Condensed Matter Theory II: Many-Body Theory (TKM II)

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Contents

Chapter 1

Introduction

Motivation

Condensed matter: solid states and liquids

→ Interactions between particles are important

→ Properties of condensed matter can be very different from those of free particles

Example (known from TKM I): an electron in a periodic potential $V(r)$.
Schrödinger equation:

$$\left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m_\mathrm{e}} + V(r)\right]\psi(r) = E\psi(r) \tag{1.1}$$

→ quasiparticle spectrum $\varepsilon(k)$ (band structure). Approximation near the band bottom:

$$\varepsilon(k) = \frac{k^2}{2m^*}\,. \tag{1.2}$$

Here m^* is the *effective mass* which can strongly differ from the free electron mass m_e.

- In GaAs, the effective mass $m^* = 0,067m_\mathrm{e}$ is smaller than the bare mass.
- In some materials (e.g., heavy-fermion compounds), the effective mass is much larger than the mass of the free electron: for example, $m^* \approx 10^3 m_\mathrm{e}$ in $\mathrm{Ce}_{1-x}\mathrm{La}_x\mathrm{Pb}_3$.
- Other properties of an electron, namely spin $s = 1/2$ and charge $q = -e$ remain the same as for the free particles.

Interactions → Novel excitations

Coulomb interaction in real materials is not necessarily weak:

$$\frac{U_\mathrm{int}}{E_\mathrm{kin}} \gtrsim 1\,, \tag{1.3}$$

In many cases a description of noninteracting particles is possible. Why?

→ Phenomenological Fermi-liquid theory (TKM I).

→ Derivation? Calculation of parameters? Beyond Fermi liquid?

→ TKM II: quantitative methods for Many-body problems

The interaction leads to modifications and limitations of single-particle picture and, therefore, to new types of excitations that do not exist in the absence of interactions.

- An important example: phonons, the quanta of sound. Other excitations: spinons, holons, polaritons, etc.
- Consider an electron which is a fermion with charge $q = -e$ and spin 1/2.
  Collective excitations in an interacting electronic gas: plasmons which are bosons with charge 0 and spin 0.
- FQHE (Fractional Quantum Hall Effect): electrons + interaction + strong magnetic field $\rightarrow$ collective state with fractional charge and fractional statistics of excitations (anyons)

Thus, properties (e.g., quantum numbers) of excitations can strongly differ from those of non-interacting particles.

Physical observables

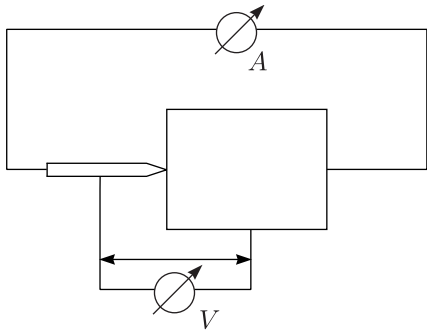
How can one describe these excitations? The naive idea is to solve the Schrödinger equation for a system consiting of N interacting particles:

$$\left[\sum_{i=1}^{N}\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}\right)+\sum_{i\neq j}^{N}U(|\mathbf{r}_i-\mathbf{r}_j|)\right]\psi_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_N)=E_\alpha\psi_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_n)\,. \tag{1.4}$$

Here, $\alpha = 0$ corresponds to the ground state, $\alpha_1, \ldots$ – excited states. However, the realistic number of interacting particles in a macroscopic system is huge: $N \approx 10^{23}$. Exact calculation is a hopeless task!

The many-particle wavefunctions $\psi_\alpha(\mathbf{r}_1, \ldots, \mathbf{r}_N; t)$ contain too much information! We do not need all this information for the analysis of physical observables. This is similar to the ideas behind statistical physics (Theo F).
What are the physical observables to be studied? These are quantities that describe

- the linear response of a system to an applied perturbation (e.g., electrical and thermal conductivity)
- the non-linear response (e.g., tunneling $I - V$ characteristics);



- thermodynamic properties (e.g., magnetic susceptibility, specific heat);
- ...

For this purposes, properties of elementary excitations will be examined:

- quantum numbers
- spectra
- life times
- ...

Very important: **Symmetry of the ground state**

- spontaneous symmetry breaking
  - → superconductivity, superfluidity
  - → (anti-)ferromagnetism
  - → CDW (Charge Density Wave)
  - → SDW (Spin Density Wave)
  - → ...

Formalism

We now need an appropriate formalism to describe all these properties: the Many-Body Green's Function Formalism. This is a field-theoretical description of condensed-matter systems.

In practice, this means that one does not use the Schrödinger equation, which is the conventional first quantization, but one uses quantum field theory (second quantization). This approach will allow us to obtain all the information that we need to calculate

- the response functions,
- thermodynamical quantities,
- spectra and decay rates of excitations,

as well as to get information about possible instabilities.

In most of the cases an exact solution of the problem is not possible and one needs certain approximations. A powerful approach – Feynman diagrammatics – is based on a systematic expansion (perturbation theory) in terms of so-called Feynman diagrams.

However, sometimes the perturbation theory is not sufficient and non-perturbative approaches must be applied, such as:

- renormalization group, which is a way to sum (most important) terms in the perturbative expansion to all orders;
- functional-integral methods;
- bosonization
- ...

Structure of the lecture course

- Introduction
- Green's functions for non-interacting particles
- Green's functions of a many-body system for $T = 0$
- Diagrammatrics for Fermi gas with weak interaction (Fermi liquids)
- Diagrammatic technique for $T \neq 0$ (Matsubara)
- Instabilities of a Fermi gas (Cooper-instability, superconductivity), diagrammatrics for superconductive systems
- Functional integral formalism
- Interacting fermions in one dimension, Luttinger liquid, Bosonization
- Introduction to the mesoscopic physics: Disorder, quantum interference, and interaction effects in quantum transport
- Interaction of electrons with magnetic impurities: Kondo effect

Chapter 2

Single-particle Green's functions

2.1 Definition of Green's functions

We start from the Hamilton operator (Hamiltonian) of a particle in potential $V(\mathbf{r})$:

$$\widehat{H} = -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V(\mathbf{r})\,. \tag{2.1}$$

The corresponding Schrödinger equation reads:

$$\mathrm{i}\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = \widehat{H}\psi(\mathbf{r},t)\,. \tag{2.2}$$

Now, we define the single-particle Green's function $G(\mathbf{r},t;\mathbf{r}',t')$ through the equation

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \widehat{H}_{\mathbf{r}}\right) G(\mathbf{r},t;\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t')\,, \tag{2.3}$$

The subscript $\mathbf{r}$ in the Hamiltonian means that the operator $\widehat{H}_{\mathbf{r}}$ acts on the variable $\mathbf{r}$ and not on $\mathbf{r}'$. In the operator language, one can write Eq. (2.3) in the following way:

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \widehat{H}\right)\widehat{G} = \widehat{\mathbb{1}}\,. \tag{2.4}$$

Here, one understands $\widehat{G}$ as an integral operator with the kernel $G(\mathbf{r},t;\mathbf{r}',t')$, i.e., $\widehat{G}f = g$ is a short-hand notation for

$$\int G(\mathbf{r},t;\mathbf{r}',t') f(\mathbf{r}',t')\,\mathrm{d}^d\mathbf{r}'\,\mathrm{d}t' = g(\mathbf{r},t)\,. \tag{2.5}$$

According to Eq. (2.4), we have

$$\widehat{G} = \left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \widehat{H}\right)^{-1}\,. \tag{2.6}$$

The potential $V(\mathbf{r})$ is t-independent; thus, the problem is translation-invariant in time. Hence, the Green function only depends on the difference of the time variables:

$$G(\boldsymbol{r}\,,t,\boldsymbol{r}\,',t') = G(\boldsymbol{r}\,,\boldsymbol{r}\,',t-t') \tag{2.7}$$

We can write G in terms of the Fourier transform from the time t to the frequency ω or, equivalently, to the energy $\varepsilon = \hbar\omega$:

$$G(\mathbf{r},\mathbf{r}',t-t') = \int \frac{\mathrm{d}\varepsilon}{2\pi}\,\exp\left(-\frac{\mathrm{i}}{\hbar}\varepsilon(t-t')\right) G(\varepsilon;\mathbf{r},\mathbf{r}')\,. \tag{2.8}$$

The Fourier transformation of Eq. (2.4) is:

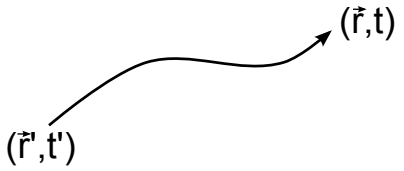
$$(\varepsilon - \widehat{H}_{\mathbf{r}})G(\varepsilon; \mathbf{r}, \mathbf{r}') \;=\; \delta(\mathbf{r} - \mathbf{r}')\,, \tag{2.9}$$

or, equivalently,

$$\widehat{G} \;=\; (\varepsilon - \widehat{H})^{-1}\,. \tag{2.10}$$

Physical interpretation

The Green's function $G(\mathbf{r}, t, \mathbf{r}', t')$ describes the probability amplitude of the process $(\mathbf{r}', t') \mapsto (\mathbf{r}, t)$, i.e. the probability amplitude for a particle that is located at point $\mathbf{r}'$ at time t' to be found at point $\mathbf{r}$ at time t. We can draw an analogy to a classical problem of diffusion. The diffusion equation (D – diffusion coefficient) has the form similar to Eq. (2.3):



$$\left(\frac{\partial}{\partial t} - D\boldsymbol{\nabla}^2\right) P(\mathbf{r}, t; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')\,. \tag{2.11}$$

However, here the Green's function $P(\mathbf{r}, t; \mathbf{r}', t')$ describes the probability (rather than the quantum-mechanical probability amplitude) of the transition $(\mathbf{r}', t') \mapsto (\mathbf{r}, t)$.

2.2 Green's functions of free particles

Equations

$$\begin{aligned} (i\hbar\partial_t - \widehat{H})\widehat{G} \;&=\; \widehat{\mathbb{1}}, \\ (\varepsilon - \widehat{H})\widehat{G} \;&=\; \widehat{\mathbb{1}} \end{aligned} \tag{2.12}$$

do not define $\widehat{G}$ uniquely. To demonstrate this, we will consider the simple Hamiltonian of a free particle:

$$\widehat{H} \mapsto \widehat{H}_0 = -\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}\,. \tag{2.13}$$

In view of the spatial translational symmetry, the coordinates enter the Green's function G_0 of a free particle through the difference $\mathbf{r} - \mathbf{r}'$. The equation for the Green's function in ε-representation is given by:

$$\left(\varepsilon + \frac{\hbar^2\boldsymbol{\nabla}_r^2}{2m}\right) G_0(\varepsilon, \mathbf{r} - \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\,. \tag{2.14}$$

We perform the Fourier transformation from the coordinate to the momentum ($r \mapsto p$),

$$G_0(\varepsilon, \mathbf{r} - \mathbf{r}') = \int \frac{\mathrm{d}^d p}{(2\pi)^d}\, G_0(\varepsilon, \mathbf{p}) \exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot(\mathbf{r} - \mathbf{r}')\right)\,. \tag{2.15}$$

Inserting this into Eq. (2.14) yields

$$\left(\varepsilon - \frac{p^2}{2m}\right) G_0(\varepsilon, \mathbf{p}) = 1 \tag{2.16}$$

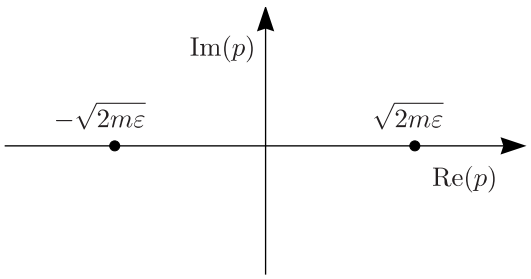
and thus

$$G_0(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon - \frac{p^2}{2m}} \,. \tag{2.17}$$

Returning to the position space (and replacing for brevity $\mathbf{r} - \mathbf{r}' \to \mathbf{r}$), we thus obtain the Green's function as an integral over momenta:

$$G_0(\varepsilon, \mathbf{r}) = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \frac{\exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)}{\varepsilon - \frac{p^2}{2m}} \,. \tag{2.18}$$

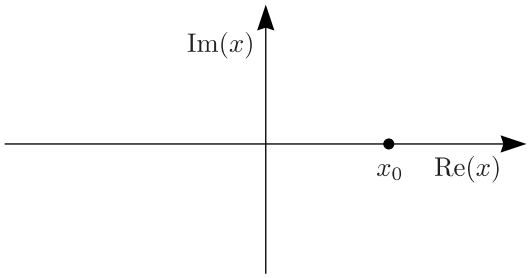
The integrand has two singularities (poles) on the real axis: $p = \pm\sqrt{2m\varepsilon}$.



2.2.1 Residues

Let $f(x)$ be a smooth function. Consider the integral

$$\int \mathrm{d}x \, \frac{f(x)}{x - x_0} \,. \tag{2.19}$$

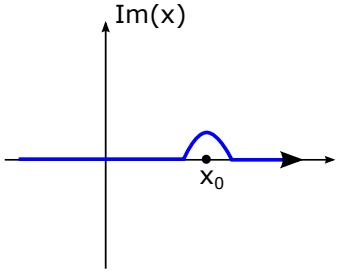


How can this integral be understood? There are different possibilities:

(i) Principal value integral denoted as $\mathcal{P}\int dx$ or, equivalently, $⨍\, dx$:

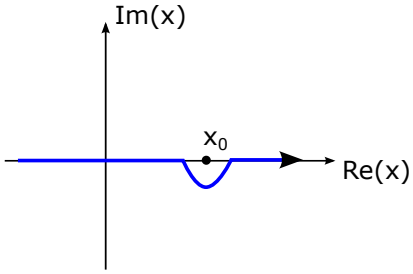
$$\mathcal{P}\int \mathrm{d}x \, \frac{f(x)}{x - x_0} \equiv ⨍ \mathrm{d}x \, \frac{f(x)}{x - x_0} = \lim_{\delta \mapsto 0} \left\{ \int_{-\infty}^{x_0 - \delta} \mathrm{d}x \, \frac{f(x)}{x - x_0} + \int_{x_0 + \delta}^{\infty} \mathrm{d}x \, \frac{f(x)}{x - x_0} \right\} . \tag{2.20}$$

(ii) Go around the point x_0 along the half-circle in the upper half-plane.



$$\int_{-\infty}^{\infty} \mathrm{d}x \, \frac{f(x)}{x - x_0} \to ⨍_{-\infty}^{\infty} \mathrm{d}x \, \frac{f(x)}{x - x_0} - \mathrm{i}\pi f(x_0) \,. \tag{2.21}$$

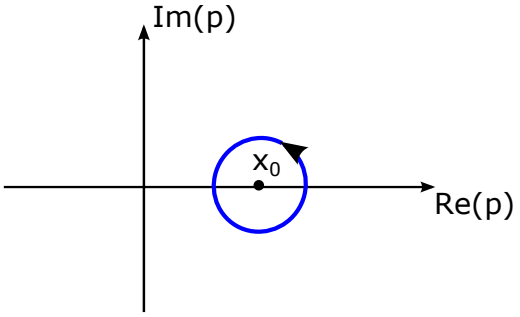
(iii) Go around the point x_0 along the half-circle in the lower half-plane.



$$\int_{-\infty}^{\infty} \mathrm{d}x\, \frac{f(x)}{x-x_0} \to \fint_{-\infty}^{\infty} \mathrm{d}x\, \frac{f(x)}{x-x_0} + \mathrm{i}\pi f(x_0)\,. \qquad (2.22)$$

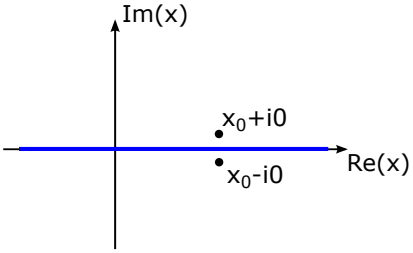
The integrals in (ii) and (iii) differ by an integral over the contour encircling x_0. By residue theorem,

$$\oint dx \frac{f(x)}{x-x_0} = 2\pi\mathrm{i}\sum \mathrm{Res} = 2\pi\mathrm{i} f(x_0).$$



The possibilities (ii) and (iii) can be obtained by shifting the pole into the complex plane and performing the integral along the real axis:

$$\begin{aligned}
\text{(ii)} \quad &= \int_{-\infty}^{\infty} dx \frac{f(x)}{x-x_0+i0} = \fint_{-\infty}^{\infty} \mathrm{d}x\, \frac{f(x)}{x-x_0} - \mathrm{i}\pi f(x_0) \\
\text{(iii)} \quad &= \int_{-\infty}^{\infty} dx \frac{f(x)}{x-x_0-i0} = \fint_{-\infty}^{\infty} \mathrm{d}x\, \frac{f(x)}{x-x_0} + \mathrm{i}\pi f(x_0).
\end{aligned} \qquad (2.23)$$



A concise way to express this is as follows:

$$\frac{1}{x-x_0 \pm \mathrm{i}0} = \mathcal{P}\frac{1}{x-x_0} \mp \mathrm{i}\pi\delta(x-x_0)\,. \qquad (2.24)$$

2.3 Retarded and advanced Green's functions

We return to the Green's function G_0. Three options (i), (ii), and (iii) yield three different Green's functions; all of them satisfy the equation (2.16) defining the Green's function.
(i) has no physical meaning,

$$\text{(i)} = \frac{\text{(ii)} + \text{(iii)}}{2}\,. \qquad (2.25)$$

(ii) corresponds to the so-called retarded Green function:

$$G_0^R(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon - \frac{p^2}{2m} + \mathrm{i}0}\,, \qquad G_0^R(\varepsilon, \mathbf{r}) = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \frac{\exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)}{\varepsilon - \frac{p^2}{2m} + \mathrm{i}0}\,. \qquad (2.26)$$

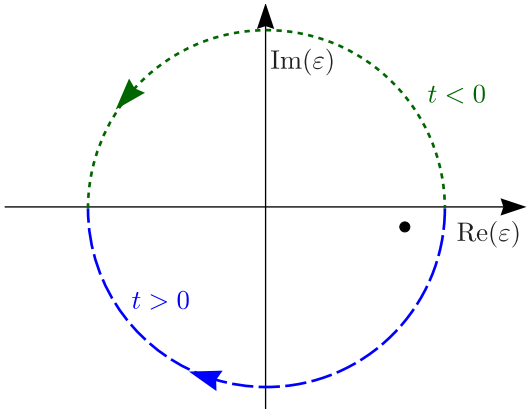
(iii) gives the advanced Green function:

$$G_0^A(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon - \frac{p^2}{2m} - \mathrm{i}0}\,, \qquad G_0^A(\varepsilon, \mathbf{r}) = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \frac{\exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)}{\varepsilon - \frac{p^2}{2m} - \mathrm{i}0}\,. \qquad (2.27)$$

Let us look at the Fourier transforms to the time representation, $\varepsilon \mapsto t$ (we set $\hbar = 1$):

$$G_0^R(t,p) = \int \frac{\mathrm{d}\varepsilon}{2\pi} \exp(-\mathrm{i}\varepsilon t) \frac{1}{\varepsilon - \frac{p^2}{2m} + \mathrm{i}0} \,. \tag{2.28}$$

For the calculation of this integral we will use the residue theorem.



For negative times, the integration contour must be closed in the upper complex half-plane and for positive times in the lower complex half-plane, so that the contour integral along this semi-circle does not contribute (because of the exponential function). The result is:

$$G_0^R(t,p) = \begin{cases} 0 & \text{for} \quad t < 0, \\ -\mathrm{i} \exp\left(-\mathrm{i}\frac{p^2}{2m} t\right) & \text{for} \quad t > 0. \end{cases} \tag{2.29}$$

Since this Green's function vanishes for negative times, it is called retarded.
For the advanced Green's function one obtains:

$$G_0^A(t,p) = \int \frac{\mathrm{d}\varepsilon}{2\pi} \exp(-\mathrm{i}\varepsilon t) \frac{1}{\varepsilon - \frac{p^2}{2m} - \mathrm{i}0} = \begin{cases} \mathrm{i} \exp\left(-\mathrm{i}\frac{p^2}{2m} t\right) & \text{for} \quad t < 0, \\ 0 & \text{for} \quad t > 0. \end{cases} \tag{2.30}$$

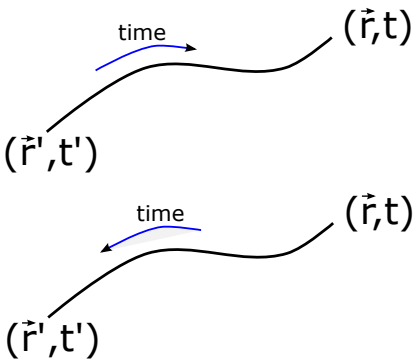
The Green's functions, Fourier-transformed with respect to the momentum $\mathbf{p}$, are:

$$\begin{aligned} G_0^R(t,r) &= \int \frac{d^d p}{(2\pi)^d} \exp\left(\mathrm{i}\mathbf{p}\cdot\mathbf{r}\right) G_0^R(t,p) = \Theta(t) \frac{1}{(2\pi)^d} \left(\frac{2\pi m}{\mathrm{i}t}\right)^{\frac{d}{2}} \exp\left(-\frac{\mathrm{i}mr^2}{2t}\right) \\ G_0^A(t,r) &= \int \frac{d^d p}{(2\pi)^d} \exp\left(\mathrm{i}\mathbf{p}\cdot\mathbf{r}\right) G_0^A(t,p) = -\Theta(-t) \frac{1}{(2\pi)^d} \left(\frac{2\pi m}{\mathrm{i}t}\right)^{\frac{d}{2}} \exp\left(-\frac{\mathrm{i}mr^2}{2t}\right), \end{aligned}$$

where $\Theta(t)$ is the Heaviside step function.

The retarded Green function describes the evolution forwards in time and the advanced Green function the evolution backwards in time:

$$\begin{aligned} G^R(\mathbf{r},t,\mathbf{r}',t') &\neq 0 \quad \text{for } t > t' \\ G^A(\mathbf{r},t,\mathbf{r}',t') &\neq 0 \quad \text{for } t < t' \end{aligned}$$



2.4 Green's Functions of particles in external potential

We now want to determine Green's functions for Hamiltonians with a potential: $\widehat{H} = \widehat{H}_0 + \widehat{V}$. Recall the equation for the Green's function:

$$(\varepsilon - \widehat{H}_0 - \widehat{V})G(\varepsilon, \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\,. \tag{2.31}$$

The Hamilton operator $\widehat{H}$ has a set of eigenfunctions ψ_α with the corresponding eigenvalues ε_α satisfying the stationary Schrödinger equation:

$$\widehat{H}\psi_\alpha = \varepsilon_\alpha \psi_\alpha\,, \tag{2.32}$$

$$\psi_\alpha^* \widehat{H} = \varepsilon_\alpha \psi_\alpha^*\,. \tag{2.33}$$

It follows from $(\varepsilon - \widehat{H})\widehat{G} = \widehat{\mathbb{1}}$ that

$$\psi_\alpha^*(\varepsilon - \widehat{H})\widehat{G} = \psi_\alpha^*\,. \tag{2.34}$$

Using Eq. (2.33), we obtain

$$(\varepsilon - \varepsilon_\alpha)\int \mathrm{d}r\, \psi_\alpha^*(\mathbf{r})G(\varepsilon; \mathbf{r}, \mathbf{r}') = \psi_\alpha^*(\mathbf{r}')\,, \tag{2.35}$$

which implies that

$$G(\varepsilon; \mathbf{r}, \mathbf{r}') = \sum_\alpha \psi_\alpha(\mathbf{r}) A_\alpha \psi_\alpha^*(\mathbf{r}')\,, \quad \text{with} \;\; (\varepsilon - \varepsilon_\alpha)A_\alpha = 1\,. \tag{2.36}$$

Therefore

$$G^R(\varepsilon; \mathbf{r}, \mathbf{r}') = \sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{\varepsilon - \varepsilon_\alpha + \mathrm{i}0}\,, \tag{2.37}$$

$$G^A(\varepsilon, \mathbf{r}, \mathbf{r}') = \sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{\varepsilon - \varepsilon_\alpha - \mathrm{i}0}\,. \tag{2.38}$$

Equivalently, this result can be derived by using the operator formalism and bra-ket notations. The Schrödinger equation and its conjugate read

$$\widehat{H}|\psi_\alpha\rangle = \varepsilon_\alpha |\psi_\alpha\rangle\,, \tag{2.39}$$

$$\langle\psi_\alpha|\widehat{H} = \varepsilon_\alpha \langle\psi_\alpha|\,. \tag{2.40}$$

One can expand $\widehat{H}$ in terms of eigenenergies:

$$\widehat{H} = \sum_{\alpha,\beta} |\psi_\alpha\rangle\langle\,\psi_\alpha \mid \widehat{H} \mid \psi_\beta\rangle\langle\psi_\beta| = \sum_\alpha \epsilon_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|, \tag{2.41}$$

which yields

$$\widehat{G}^{R,A} = \sum_\alpha \frac{|\psi_\alpha\rangle\langle\psi_\alpha|}{\varepsilon - \varepsilon_\alpha \pm \mathrm{i}0}\,. \tag{2.42}$$

It is useful to define the spectral weight

$$\mathcal{A}(\varepsilon, \mathbf{r}, \mathbf{r}') = \frac{\mathrm{i}}{2\pi}\left\{G^R(\varepsilon; \mathbf{r}, \mathbf{r}') - G^A(\varepsilon, \mathbf{r}, \mathbf{r}')\right\}. \tag{2.43}$$

Using

$$\frac{1}{x \pm \mathrm{i}0} = \mathcal{P}\frac{1}{x} \mp \mathrm{i}\pi\delta(x)\,, \tag{2.44}$$

we write the spectral weight in terms of eigenfuctions and eigenenergies:

$$\begin{aligned}
\mathcal{A}(\varepsilon, \mathbf{r}, \mathbf{r}') &= \frac{i}{2\pi}\left[\sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{\varepsilon - \varepsilon_\alpha + i0} - \sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{\varepsilon - \varepsilon_\alpha - i0}\right] \\
&\overset{(2.44)}{=} \frac{i}{2\pi}\left[\sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{\varepsilon - \varepsilon_\alpha} - i\pi\sum_\alpha \psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')\delta(\varepsilon - \varepsilon_\alpha)\right. \\
&\quad \left. - \sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{\varepsilon - \varepsilon_\alpha} - i\pi\sum_\alpha \psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')\delta(\varepsilon - \varepsilon_\alpha)\right] \\
&= \sum_\alpha \psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')\delta(\varepsilon - \varepsilon_\alpha)\,.
\end{aligned} \tag{2.45}$$

The spectral weight is non-zero at those energies for which there are eigenstates (i.e. for energies belonging to the spectrum of the Hamiltonian).
The Green's functions can be written in terms of the spectral weight:

$$G^{R,A}(\varepsilon; \mathbf{r}, \mathbf{r}') = \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}(\varepsilon_1, \mathbf{r}, \mathbf{r}')}{\varepsilon - \varepsilon_1 \pm \mathrm{i}0}\,. \tag{2.46}$$

Indeed:

$$\int_{-\infty}^{\infty} d\varepsilon_1 \frac{\mathcal{A}(\varepsilon_1, \mathbf{r}, \mathbf{r}')}{\varepsilon - \varepsilon_1 \pm i0} \overset{(2.45)}{=} \int_{-\infty}^{\infty} d\varepsilon_1 \frac{\sum_\alpha \psi_\alpha(r)\psi_\alpha^*(r')\delta(\varepsilon_1 - \varepsilon_\alpha)}{\varepsilon - \varepsilon_1 \pm i0} = \sum_\alpha \frac{\psi_\alpha(r)\psi_\alpha^*(r')}{\varepsilon - \varepsilon_\alpha \pm i0}.$$

For the states of discrete spectrum at $\varepsilon = \varepsilon_\alpha$, the spectral weight $\mathcal{A}$ has a δ-peak and Green's functions $G^{R,A}$ have poles.

2.5 Dyson equation

Let us now return to the equation for Green's functions again:

$$(\varepsilon - \widehat{H})G(\varepsilon; \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\,. \tag{2.47}$$

We multiply from the left with G_0 and use $\widehat{H} = \widehat{H}_0 + \widehat{V}$

$$\widehat{G}_0(\varepsilon - \widehat{H})\widehat{G} = \widehat{G}_0\,, \tag{2.48}$$

$$\underbrace{\widehat{G}_0(\varepsilon - \widehat{H}_0)}_{=\widehat{\mathbb{1}}}\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}\,. \tag{2.49}$$

Thus, we obtain an equation for $\widehat{G}$ in terms of $\widehat{G}_0$ and $\widehat{V}$:

$$\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}\,. \tag{2.50}$$

This equation for $\widehat{G}$ is called **Dyson equation** . When written explicitly in the coordinate representation, it is an integral equation:

$$G(\varepsilon, \mathbf{r}, \mathbf{r}') = G_0(\varepsilon, \mathbf{r}, \mathbf{r}') + \int \mathrm{d}r'' \, G_0(\varepsilon, \mathbf{r}, \mathbf{r}'')V(\mathbf{r}'')G(\varepsilon, \mathbf{r}'', \mathbf{r}')\,. \tag{2.51}$$

The equations holds both for $\widehat{G}^R$ (in which case all entering Green's functions are retarded) and for $\widehat{G}^A$ (all entering Green's functions are advanced):

$$\widehat{G}^{R/A} = \widehat{G}_0^{R/A} + \widehat{G}_0^{R/A}\widehat{V}\widehat{G}^{R/A}\,, \tag{2.52}$$

$$G^{R/A}(\varepsilon,\mathbf{r},\mathbf{r}') = G_0^{R/A}(\varepsilon,\mathbf{r},\mathbf{r}') + \int d^dr''\, G_0^{R/A}(\varepsilon,\mathbf{r},\mathbf{r}'')V(\mathbf{r}'')G^{R/A}(\varepsilon,\mathbf{r}'',\mathbf{r}'). \tag{2.53}$$

These integral equations can be solved by iterations.

- First order approximation:
$$G(\varepsilon,\mathbf{r},\mathbf{r}') = G_0(\varepsilon,\mathbf{r},\mathbf{r}')\,, \tag{2.54}$$
- Second order approximation:
$$\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}_0\,, \tag{2.55}$$
- n-th order approximation:
$$\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}_0\widehat{V}\widehat{G}_0 + \dots\,. \tag{2.56}$$

  In coordinate representation:

$$\begin{aligned} G(\varepsilon,\mathbf{r},\mathbf{r}') &= G_0(\varepsilon,\mathbf{r},\mathbf{r}') + \int d^dr'' G_0(\varepsilon,\mathbf{r},\mathbf{r}'')V(\mathbf{r}'')G_0(\varepsilon,\mathbf{r}'',\mathbf{r}') \\ &+ \int d^dr'' \int d^dr''' G_0(\varepsilon,\mathbf{r},\mathbf{r}'')V(\mathbf{r}'')G_0(\varepsilon,\mathbf{r}'',\mathbf{r}''')V(\mathbf{r}''')G_0(\varepsilon,\mathbf{r}''',\mathbf{r}') + \dots \end{aligned} \tag{2.57}$$

Equivalently, this expansion can be obtained from

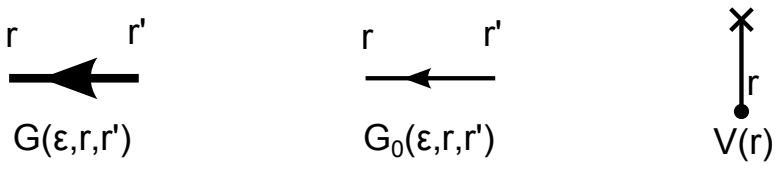
$$\widehat{G} = (\varepsilon - \widehat{H})^{-1} = (\varepsilon - \widehat{H}_0 - \widehat{V})^{-1} = (\widehat{G}_0^{-1} - \widehat{V})^{-1} \tag{2.58}$$

by expanding in $\widehat{V}$.

2.6 Diagrams

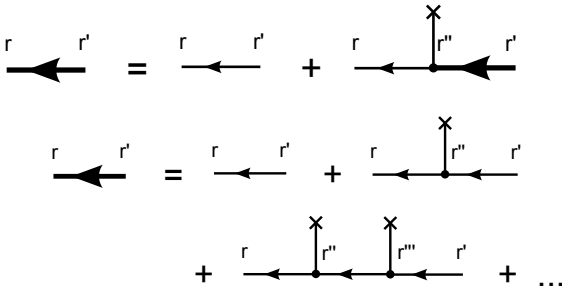
Let us define rules of the diagram technique.

- Graphical representation of the elements of Dyson equation in coordinate representation:



  The equations now take the following graphical form

$$G = G_0 + G_0VG \tag{2.59}$$



$$G = G_0 + G_0VG_0 + G_0VG_0VG_0 + \dots \tag{2.60}$$

- Integration over all intermediate coordinates is assumed in diagrams.

We remind that for G^R all Green functions in the equation are retarded and for G^A all are advanced.
By Fourier transformation we go to momentum space:

$$G^R(\varepsilon;\mathbf{r}_1,\mathbf{r}_2) = \int \frac{\mathrm{d}^d p_1}{(2\pi)^d}\,\frac{\mathrm{d}^d p_2}{(2\pi)^d}\,\exp(\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_1 - \mathrm{i}\mathbf{p}_2\cdot\mathbf{r}_2) G^R(\varepsilon;\mathbf{p}_1,\mathbf{p}_2)\,, \tag{2.61}$$

$$G_0^R(\varepsilon;\mathbf{p}_1,\mathbf{p}_2) = \underbrace{\frac{1}{\varepsilon - \frac{p_1^2}{2m} + \mathrm{i}0}}_{=G_0^R(\varepsilon;\mathbf{p}_1)} (2\pi)^d \delta(\mathbf{p}_1 - \mathbf{p}_2)\,, \tag{2.62}$$

$$V(\mathbf{r}) = \int \frac{\mathrm{d}^d q}{(2\pi)^d}\,\exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}) V(\mathbf{q})\,, \tag{2.63}$$

Thus, we obtain for the Fourier transform of equation (2.53):

$$\begin{aligned} G^R(\varepsilon;\mathbf{p}_1,\mathbf{p}_2) = G_0^R(\varepsilon;\mathbf{p}_1)(2\pi)^d\delta(\mathbf{p}_1-\mathbf{p}_2) + G_0^R(\varepsilon;\mathbf{p}_1)\int \mathrm{d}^d r_3 \int \frac{\mathrm{d}^d q}{(2\pi)^d}\,\frac{\mathrm{d}^d p_3}{(2\pi)^d}\,\exp(-\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_3) \\ \times \exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}_3) V(\mathbf{q}) \exp(\mathrm{i}\mathbf{p}_3\cdot\mathbf{r}_3) G^R(\varepsilon;\mathbf{p}_3,\mathbf{p}_2)\,. \end{aligned} \tag{2.64}$$

The integral over $\mathbf{r}_3$ yields a δ-function:

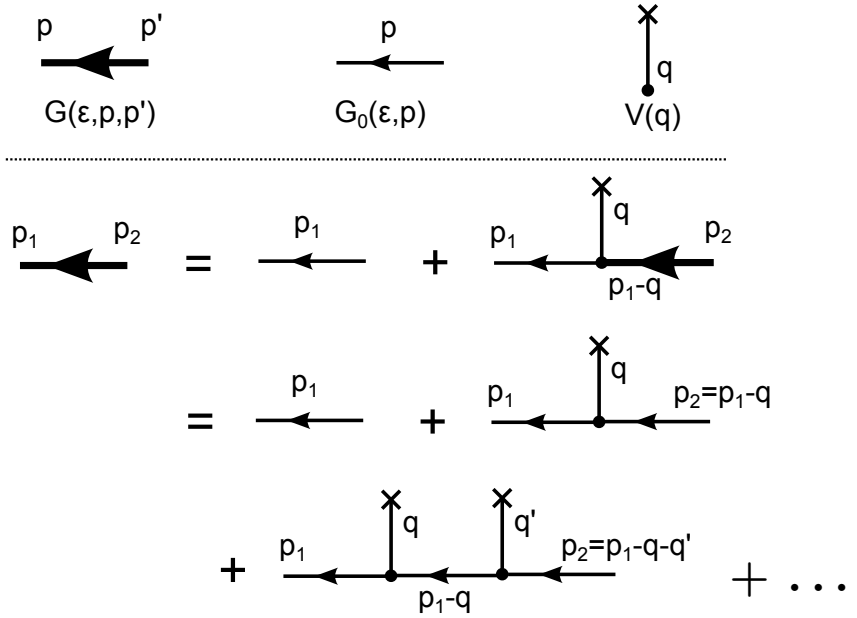
$$\int \mathrm{d}^d r_3\,\exp(-\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_3)\exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}_3)\exp(\mathrm{i}\mathbf{p}_3\cdot\mathbf{r}_3) = (2\pi)^d\delta(\mathbf{q}+\mathbf{p}_3-\mathbf{p}_1)\,. \tag{2.65}$$

This allows us to take the integral over $\mathbf{q}$, yielding

$$\begin{aligned} G^R(\varepsilon;\mathbf{p}_1,\mathbf{p}_2) &= G_0^R(\varepsilon;\mathbf{p}_1)(2\pi)^d\delta(\mathbf{p}_1-\mathbf{p}_2) + \int \frac{\mathrm{d}^d p_3}{(2\pi)^d}\, G_0^R(\varepsilon;\mathbf{p}_1) V(\mathbf{p}_1-\mathbf{p}_3) G^R(\varepsilon;\mathbf{p}_3,\mathbf{p}_2) = \\ &= G_0^R(\varepsilon;\mathbf{p}_1)(2\pi)^d\delta(\mathbf{p}_1-\mathbf{p}_2) \\ &\quad + \int \frac{\mathrm{d}^d q}{(2\pi)^d}\, G_0^R(\varepsilon;\mathbf{p}_1) V(\mathbf{q}) G_0^R(\varepsilon,\mathbf{p}_2)(2\pi)^d\delta(\mathbf{p}_1-\mathbf{q}-\mathbf{p}_2) + \dots\,. \end{aligned} \tag{2.66}$$

2.6.1 Diagrammatics in momentum space

Elements of the diagrammatic technique and equation for the Green's function in momentum representation:



- Momentum conservation at each vertex
- Factor $(2\pi)^d \delta(\mathbf{p}_1 - \mathbf{p}_2 - \sum_i \mathbf{q}_i)$
- Integrate over all internal momenta

$$\int \prod_i \frac{\mathrm{d}^d q_i}{(2\pi)^d} \cdots$$

2.7 Scattering amplitudes

Recall the scattering problem in quantum mechanics. Scattering of a plane wave $e^{i\mathbf{kr}}$ on a static, one-particle potential $V(\mathbf{r})$ is described by the wave function

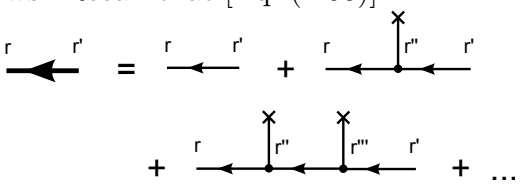
$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} + \chi_{\mathbf{k}}(\mathbf{r}), \tag{2.67}$$

where $\chi_{\mathbf{k}}(\mathbf{r})$ has the form of a spherical wave

$$\chi_{\mathbf{k}}(\mathbf{r}) = f(\mathbf{k}, k\mathbf{n}) \frac{e^{ik|\mathbf{r}|}}{|\mathbf{r}|}, \quad |\mathbf{r}| \to \infty, \quad \mathbf{n} = \frac{\mathbf{r}}{|\mathbf{r}|}, \quad k = |\mathbf{k}|. \tag{2.68}$$

The function $f(\mathbf{k}, k\mathbf{n})$ is known as the scattering amplitude.
It can be expressed in terms of the Green's function as follows. Recall that [Eq. (2.60)]

$$G^R = G_0^R + G_0^R V G_0^R + G_0^R V G_0^R V G_0^R + \dots \tag{2.69}$$



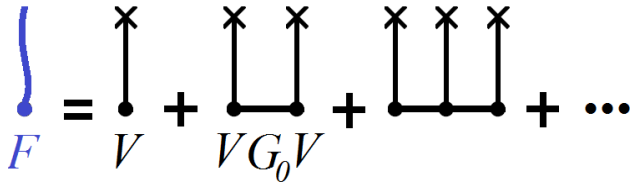
The full retarded Green's function can be written as ("amputation" of external legs G_0^R)

$$G^R = G_0^R + G_0^R F^R G_0^R, \tag{2.70}$$

where

$$F^R(\varepsilon, \mathbf{p}_1, \mathbf{p}_2) = V(\mathbf{p}_1 - \mathbf{p}_2) + \int \frac{d^3 p_3}{(2\pi)^3} V(\mathbf{p}_1 - \mathbf{p}_3) G_0^R(\varepsilon, \mathbf{p}_3) V(\mathbf{p}_3 - \mathbf{p}_2) + \dots . \tag{2.71}$$

This equation can be represented diagrammatically as



The function $F^R(\varepsilon, \mathbf{p}_1, \mathbf{p}_2)$ satisfies the equation

$$F^R(\varepsilon, \mathbf{p}_1, \mathbf{p}_2) = V(\mathbf{p}_1 - \mathbf{p}_2) + \int \frac{d^3 p_3}{(2\pi)^3} \frac{V(\mathbf{p}_1 - \mathbf{p}_3) F^R(\varepsilon, \mathbf{p}_3, \mathbf{p}_2)}{\varepsilon - p_3^2/(2m) + i0}. \tag{2.72}$$

When taken on the mass-shell,

$$\varepsilon = \frac{k_1^2}{2m} = \frac{k_2^2}{2m}, \tag{2.73}$$

it is related to the scattering amplitude from Eq. (2.68) as follows:

$$f(\mathbf{k}_1, \mathbf{k}_2) = -\frac{m}{2\pi} F^R(\varepsilon = k_1^2/(2m), \mathbf{k}_1, \mathbf{k}_2), \quad k_1^2/(2m) = k_2^2/(2m). \tag{2.74}$$

2.8 Time-dependent problems

We now consider the Hamiltonian with a time-dependent potential

$$\widehat{H} = -\frac{\boldsymbol{\nabla}^2}{2m} + V(\mathbf{r}, t)\,. \tag{2.75}$$

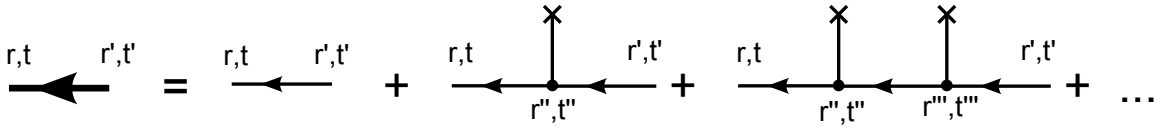
$$\left(\mathrm{i}\frac{\partial}{\partial t} - \widehat{H}(\mathbf{r}, t)\right) G(\mathbf{r}, t; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')\,, \tag{2.76}$$

$$\left(\mathrm{i}\frac{\partial}{\partial t} - \widehat{H}_0\right) G_0(\mathbf{r}, t; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')\,. \tag{2.77}$$

Because of translation invariance in time, the free Green's function G_0 only depends on time differences. The full Green's function $G(\mathbf{r}, t; \mathbf{r}', t'')$ obeys the integral equation where one has to integrate over intermediate coordinates and times:

$$G(\mathbf{r}, t; \mathbf{r}', t') = G_0(\mathbf{r} - \mathbf{r}', t - t') + \int \mathrm{d}r''\mathrm{d}t''\, G_0(\mathbf{r} - \mathbf{r}'', t - t'')V(\mathbf{r}'', t'')G(\mathbf{r}'', t''; \mathbf{r}', t')\,. \tag{2.78}$$

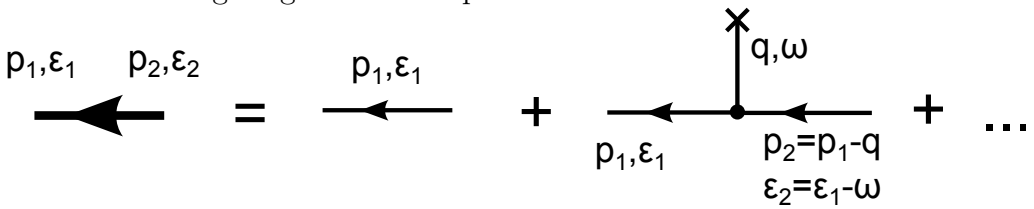
The solution can be expanded in a series in V in full analogy with the time-independent case. The graphical representation of the equation is essentially the same (but with integration over all intermediate $\mathbf{r}$ and t):



Performing Fourier transformation to the momentum-energy space,

$$G(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \int \frac{\mathrm{d}^d p_1}{(2\pi)^d}\frac{\mathrm{d}^d p_2}{(2\pi)^d}\frac{\mathrm{d}\varepsilon_1}{2\pi}\frac{\mathrm{d}\varepsilon_2}{2\pi}\, \exp(\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_1 - \mathrm{i}\mathbf{p}_2\cdot\mathbf{r}_2 - \mathrm{i}\varepsilon_1 t_1 + \mathrm{i}\varepsilon_2 t_2) G(\mathbf{p}_1, \varepsilon_1; \mathbf{p}_2, \varepsilon_2)\,, \tag{2.79}$$

we arrive at the following diagrammatic representation:



Now in each vertex there is a change in energy of the Green's function due to the external potential.

Diagrammatic rules:

- energy-momentum conservation at each vertex
- Factor $(2\pi)^d\delta(\mathbf{p}_1 - \mathbf{p}_2 - \sum_i \mathbf{q}_i)\cdot 2\pi\delta(\varepsilon_1 - \varepsilon_2 - \sum_i \omega_i)$
- integrate over internal momenta and energies: $\displaystyle\int\prod_i \frac{\mathrm{d}^d q_i}{(2\pi)^d}\frac{\mathrm{d}\omega_i}{2\pi}$

The first nontrivial term (linear in V) in the perturbation series is called Born approximation. This is a meaningful approximation if the potential is weak.

Chapter 3

Green's functions in many-body systems

Up to now we have considered a single-particle problem. Now we turn to systems of many interacting particles. We consider a Hamiltonian of a such a many-body problem:

$$\widehat{H} = \sum_{i=1}^{N} \left[-\frac{1}{2m} \boldsymbol{\nabla}_i^2 + V(\mathbf{r}_i) \right] + \frac{1}{2} \sum_{i \neq j} U(\mathbf{r}_i, \mathbf{r}_j) \equiv \widehat{H}_0 + \widehat{U} \,, \tag{3.1}$$

where $\widehat{H}_0$ is the sum of one-particles Hamiltonians and $\widehat{U}$ describes the interaction between particles.

In order to introduce the formalism of Green's functions in many-body setting, we will need the second quantization formalism.

3.1 Second quantization

We consider a basis of one-particle states

$$\psi_k(\mathbf{r}) \qquad\qquad k = 1, 2, \ldots$$

This yields a basis for N-particle wave functions:

$$\psi_{k_1}(\mathbf{r}_1) \ldots \psi_{k_N}(\mathbf{r}_N) \,. \tag{3.2}$$

We can write any many-body wave function as an expansion in this basis:

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) = \sum_{k_1, \ldots, k_N} C(k_1, \ldots, k_N; t) \psi_{k_1}(\mathbf{r}_1) \ldots \psi_{k_N}(\mathbf{r}_N) \,, \tag{3.3}$$

The coefficients $C(k_1, \ldots, k_N; t)$ should be symmetric for bosons and antisymmetric for fermions to respect the symmetries of the wave functions.

It is convenient to introduce a many-particle basis that takes into account the boson/fermion statistics. We can achieve this by using the symmetrization/antisymmetrization operator:

$$S^{(\pm)} = c^{(\pm)} \sum_P (\pm 1)^P P, \tag{3.4}$$

where the sign + corresponds to bosons and − to fermions. Here $c^{(\pm)}$ is a normalization constant and P denotes permutation, for instance:

$$P_{12} \psi_{k_1}(r_1) \psi_{k_2}(r_2) = \psi_{k_2}(r_1) \psi_{k_1}(r_1).$$

This leads to the representation of occupation numbers for many-body states and to second-quantized forms of operators, as discussed below separately for bosons and fermions.

3.1.1 Bosons

The one-particle states are labeled by the index $k = 1, 2, \ldots$. The new many-particle basis states are characterized by occupation numbers n_1, n_2, ...:

$$n_k = \text{number of particle in state } k \qquad \sum_k n_k = N.$$

One sums over all possibilities of states (3.2) such that $\{k_1, k_2, \ldots, k_N\}$ corresponds to the occupation numbers $(n_1, n_2, \ldots)$, which are $\{\underbrace{1\ldots1}_{n_1}\underbrace{2\ldots2}_{n_2}\ldots\}$ + all permutations:

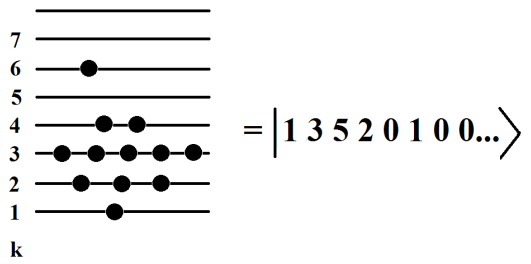
$$\Phi_{n_1,n_2,n_3,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \left(\frac{n_1!n_2!\ldots}{N!}\right)^{\frac{1}{2}} \sum_{\{k_1,k_2,\ldots,k_N\}\Leftrightarrow(n_1,n_2,n_3,\ldots)} \psi_{k_1}(\mathbf{r}_1)\psi_{k_2}(\mathbf{r}_2)\ldots\psi_{k_N}(\mathbf{r}_N)\,. \tag{3.5}$$

Then, we expand an arbitrary many-body wave-function in these many-body basis states:

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N,t) = \sum_{n_1,n_2,\ldots} \widetilde{C}(n_1,n_2,\ldots,t)\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\,. \tag{3.6}$$

We will denote $\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ by $|n_1,n_2,\ldots\rangle$.
The states are normalized:

$$\langle n_1,n_2,\ldots|n_1',n_2',\ldots\rangle = \delta_{n_1,n_1'}\delta_{n_2,n_2'}\ldots\,. \tag{3.7}$$



The projector

$$\sum_{n_1,n_2,\ldots} |n_1,n_2,\ldots\rangle\langle n_1,n_2,\ldots| = \mathbb{1}\,, \tag{3.8}$$

is the unit operator in the space of the states $|n_1,n_2,\ldots\rangle$, the so-called **Fock space**.

The next step is to introduce **creation and annihilation operators** $a_k^\dagger$ and a_k. For bosons, they obey the commutation relations:

$$[a_k, a_{k'}^\dagger] = \delta_{kk'}\,, \quad [a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0\,. \tag{3.9}$$

The operators change the occupation numbers of the corresponding states:

$$a_k|n_k\rangle = n_k^{\frac{1}{2}}|n_k-1\rangle\,, \quad a_k^\dagger|n_k\rangle = (n_k+1)^{\frac{1}{2}}|n_k+1\rangle\,, \quad a_k^\dagger a_k|n_k\rangle = n_k|n_k\rangle\,. \tag{3.10}$$

$a_k^\dagger a_k$ is the particle number operator. Any states $|n_1,n_2,\ldots\rangle$ can be written as a result of an application of creation operators on the vacuum state $|0,0,\ldots\rangle \equiv |0\rangle$:

$$|n_1,n_2,\ldots\rangle = \prod_k \frac{(a_k^\dagger)^{n_k}}{(n_k!)^{\frac{1}{2}}}|0\rangle\,. \tag{3.11}$$

We want to write the Hamiltonian in terms of the creation and annihilation operators.

Consider first the non-interacting part. Acting with it on a Fock-space basis state (3.5), one obtains

$$\sum_i \widehat{H}_0(\mathbf{r}_i)\Phi_{n_1,n_2,n_3,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$$

$$= \sum_k n_k (H_0)_{kk} \Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N) + \sum_{k\neq k'} n_k^{\frac{1}{2}} (n_{k'}+1)^{\frac{1}{2}} (H_0)_{k'k} \Phi_{n_1,n_2,\ldots,n_k-1,\ldots,n_{k'}+1,\ldots}\,, \tag{3.12}$$

where

$$\widehat{H}_0\psi_k = \sum_{k'} (H_0)_{kk'}\psi_{k'}\,, \quad \text{with } (H_0)_{k'k} = \langle k'|H_0|k\rangle = \int \mathrm{d}^d r\, \psi^*_{k'}(\mathbf{r})\widehat{H}_0(\mathbf{r})\psi_k(\mathbf{r})\,. \tag{3.13}$$

The factors n_k (in the first term) and $n_k^{\frac{1}{2}}(n_{k'}+1)^{\frac{1}{2}}$ (in the second term) in Eq. (3.12) originate from combinatorial factors and from the normalization factors in (3.5). In particular, the factor in the second term follows from

$$\left(\frac{n_1!n_2!\ldots}{N!}\right)^{\frac{1}{2}} (n_{k'}+1) = n_k^{1/2}(n_{k'}+1)^{1/2}\left(\frac{n_1!n_2!\ldots(n_k-1)!\ldots(n_{k'}+1)!}{N!}\right)^{\frac{1}{2}}\,. \tag{3.14}$$

Here $(n_{k'}+1)$ is how many times each of the terms in $\Phi_{n_1,n_2,\ldots,n_k-1,\ldots,n_{k'}+1,\ldots}$ is obtained when the left-hand-side of Eq. (3.13) is evaluated.

According to Eq. (3.13), one can write the action of the non-interacting part of the Hamiltonian in the second-quantization language as follows:

$$\sum_i \widehat{H}_0(\mathbf{r}_i)\Phi_{n_1,n_2,n_3,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \sum_{k,k'} (H_0)_{k'k} a^\dagger_{k'}a_k|n_1,n_2,\ldots\rangle. \tag{3.15}$$

Since this is true for any basis state, we have an operator identity

$$\sum_i \widehat{H}_0(\mathbf{r}_i) \Leftrightarrow \sum_{k,k'} (H_0)_{k'k} a^\dagger_{k'}a_k\,. \tag{3.16}$$

Exactly in the same way one can consider the interaction part of the Hamiltonian. The calculation proceeds analogously, and we obtain:

$$\frac{1}{2}\sum_{i\neq j} U(\mathbf{r}_i,\mathbf{r}_j) \;\Leftrightarrow\; \frac{1}{2}\sum_{k,l,m,n} U_{kl;mn} a^\dagger_k a^\dagger_l a_n a_m\,, \tag{3.17}$$

where

$$U_{kl;mn} = \int \mathrm{d}r\,\mathrm{d}r'\,\psi^*_k(\mathbf{r})\psi^*_l(\mathbf{r}')U(\mathbf{r},\mathbf{r}')\psi_m(\mathbf{r})\psi_n(\mathbf{r}')\,. \tag{3.18}$$

Thus, the full Hamiltonian has the following second-quantization representation:

$$\widehat{H} \;\Leftrightarrow\; \sum_{k,l}(H_0)_{kl}a^\dagger_k a_l + \frac{1}{2}\sum_{k,l,m,n} U_{kl;mn}a^\dagger_k a^\dagger_l a_n a_m\,. \tag{3.19}$$

3.1.2 Fermions

For fermions the occupation number is either zero or one (Pauli principle):

$$n_k = 0, 1.$$

The appropriate (antisymmetrized) many-body basis is given by

$$\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \frac{1}{(N!)^{\frac{1}{2}}} \sum_{\substack{\text{Permutations}\\ \text{of } \{k_1,\ldots,k_N\}}} (-1)^P \psi_{k_{p_1}}(\mathbf{r}_1)\ldots\psi_{k_{p_N}}(\mathbf{r}_N)$$

$$= \frac{1}{(N!)^{\frac{1}{2}}} \begin{vmatrix} \psi_{k_1}(\mathbf{r}_1) & \dots & \psi_{k_1}(\mathbf{r}_N) \\ \vdots & \ddots & \vdots \\ \psi_{k_N}(\mathbf{r}_1) & \dots & \psi_{k_N}(\mathbf{r}_N) \end{vmatrix} . \tag{3.20}$$

The above determinant is called Slater determinant.

The fermionic creation and annihilation operators satisfy the anti-commutation relations:

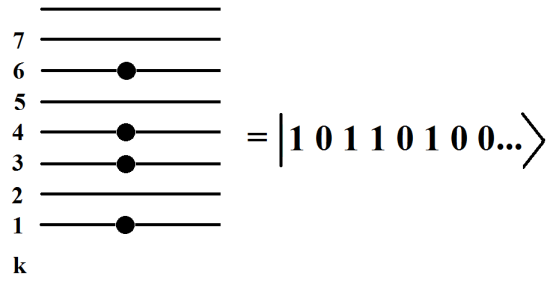
$$\{a_k, a_{k'}^\dagger\} = \delta_{kk'} , \quad \{a_k, a_{k'}\} = \{a_k^\dagger, a_{k'}^\dagger\} = 0 . \tag{3.21}$$

and obey

$$a^\dagger|0\rangle = 1\rangle , \quad a|1\rangle = |0\rangle , \quad a^\dagger|1\rangle = 0 , \quad a|0\rangle = 0 , \quad a_k^\dagger a_k = n_k . \tag{3.22}$$

In analogy with the bosonic case, many-body states (3.20) that form the basis of the Fock space are labeled by occupation numbers and are generated by action of creation operators on the vacuum state:

$$|n_1, n_2, \dots\rangle = (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \dots |0\rangle ,$$
$$\text{with } |0\rangle \equiv |0, 0, \dots\rangle . \tag{3.23}$$



The Hamiltonian expressed in terms of creation/annihilation operators has the same structure as for bosons:

$$\widehat{H} \;\Leftrightarrow\; \sum_{k,l} (H_0)_{kl} a_k^\dagger a_l + \frac{1}{2} \sum_{k,l,m,n} U_{kl;mn} a_k^\dagger a_l^\dagger a_n a_m . \tag{3.24}$$

3.2 Field operators

We perform a transformation from the basis of single-particle states ψ_k to the basis labeled by the spatial coordinate $\mathbf{r}$. The field operator is an operator in the Fock space given by

$$\widehat{\Psi}(\mathbf{r}) = \sum_k a_k \psi_k(\mathbf{r}) . \tag{3.25}$$

Here the functions $\psi_k(\mathbf{r})$ serve as coefficients. In the same way one defines

$$\widehat{\Psi}^\dagger(\mathbf{r}) = \sum_k \psi_k^*(\mathbf{r}) a_k^\dagger . \tag{3.26}$$

We calculate the commutation relations of these new operators. Let us first consider bosons:

$$[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')] = \sum_{k,k'} \psi_k(\mathbf{r}) \psi_{k'}^*(\mathbf{r}') [a_k, a_{k'}^\dagger] = \sum_k \psi_k(\mathbf{r}) \psi_k^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') , \tag{3.27}$$

$$[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}(\mathbf{r}')] = [\widehat{\Psi}^\dagger(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')] = 0 . \tag{3.28}$$

For fermions one obtains:

$$\{\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}') , \quad \{\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}(\mathbf{r}')\} = \{\widehat{\Psi}^\dagger(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')\} = 0 . \tag{3.29}$$

One can put the above formulas together in the form

$$[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')]_\mp \equiv \widehat{\Psi}(\mathbf{r}) \widehat{\Psi}^\dagger(\mathbf{r}') \mp \widehat{\Psi}^\dagger(\mathbf{r}') \widehat{\Psi}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}') , \tag{3.30}$$

where the upper sign corresponds to bosons and the lower one to fermions.

Performing the transformation in Eqs. (3.19), (3.24), we express the Hamiltonian in terms of the field operators:

$$\widehat{H} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r}) H_0(\mathbf{r}) \widehat{\Psi}(\mathbf{r}) + \frac{1}{2} \int \mathrm{d}r\, \mathrm{d}r'\, \widehat{\Psi}^\dagger(\mathbf{r}) \widehat{\Psi}^\dagger(\mathbf{r}') U(\mathbf{r},\mathbf{r}') \widehat{\Psi}(\mathbf{r}') \widehat{\Psi}(\mathbf{r})\,. \tag{3.31}$$

Up to now we have neglected the existence of spin. Including spin, $\mathbf{r} \mapsto \mathbf{r}, \sigma$, we have field operators $\widehat{\Psi}_\sigma(\mathbf{r})$, with the commutation relations

$$[\widehat{\Psi}_\sigma(\mathbf{r}), \widehat{\Psi}^\dagger_{\sigma'}(\mathbf{r}')]_\mp = \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma\sigma'}\,. \tag{3.32}$$

The representation in terms of field operators is applicable to any 1-, 2-, (...)-particle operators. For example, the operator $\varrho_{\mathbf{r}_0}$ of density of particles at a given point $\mathbf{r}_0$ is written in the first-quantized form as

$$\varrho_{\mathbf{r}_0} = \sum_{i=1}^N \delta(\mathbf{r}_i - \mathbf{r}_0) = \sum_{i=1}^N \varrho_{\mathbf{r}_0}(\mathbf{r}_i)\,, \quad \text{with } \varrho_{\mathbf{r}_0}(\mathbf{r}) = \delta(\mathbf{r}_0 - \mathbf{r})\,. \tag{3.33}$$

Thus, in the language of second quantization, the density operator is given by

$$\widehat{\varrho}_{\mathbf{r}_0} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r}) \delta(\mathbf{r}_0 - \mathbf{r}) \widehat{\Psi}(\mathbf{r}) = \widehat{\Psi}^\dagger(\mathbf{r}_0)\widehat{\Psi}(\mathbf{r}_0)\,. \tag{3.34}$$

The total particle number operator is given by the spatial integral of the density operator:

$$\widehat{N} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}(\mathbf{r})\,. \tag{3.35}$$

For many-body systems in a grand-canonical ensemble, it is convenient to consider as the Hamilton operator

$$\widehat{H}' = \widehat{H} - \mu \widehat{N}\,,$$

where μ is the chemical potential. With this shift, the non-interacting Hamiltonian becomes

$$H_0(\mathbf{r}) \mapsto H_0'(\mathbf{r}) = -\frac{1}{2m}\boldsymbol{\nabla}^2 + V(\mathbf{r}) - \mu\,, \tag{3.36}$$

i.e., the energy is counted from the chemical potential.

The grand canonical distribution then takes the form

$$\exp\left(-\frac{E_n - \mu N_n}{k_B T}\right) \equiv \exp\left(-\frac{E_n'}{k_B T}\right) \quad \xrightarrow{T\to 0} \quad \text{only ground state } E_0' \text{ survives}\,, \tag{3.37}$$

so that at $T = 0$ the system is in the ground state of $\widehat{H}'$ with the minimum energy E_0'. Let us emphasize that the ground state of the many-body system can be essentially changed by the chemical potential. For example, for a system of electrons in a metal, the ground state of $\widehat{H}$ would be a the state without any electron, while the ground state of $\widehat{H}'$—which corresponds to the $T = 0$ limit of the grand canonical distribution—is the filled Fermi sea.

Below we will frequently denote $\widehat{H}'$ again as $\widehat{H}$ in order to simplify notations.

3.3 Schrödinger vs. Heisenberg representations

The standard picture in quantum mechanics is the **Schrödinger picture**, in which the states are time dependent and obey the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}|\phi(t)\rangle_S = \widehat{H}|\phi(t)\rangle_S\,. \tag{3.38}$$

The Hamilton operator $\widehat{H}$ is t-independent, if there is no external t-dependence. The Schrödinger equation yields the unitary time evolution of the states described by the evolution operator $\mathcal{U}(t,0) = \exp(-\mathrm{i}\widehat{H}t)$:

$$|\phi(t)\rangle_S = \exp(-\mathrm{i}\widehat{H}t)|\phi(0)\rangle_S = \mathcal{U}(t,0)|\phi(0)\rangle_S\,. \tag{3.39}$$

The evolution operator is unitary: $\mathcal{U}(t,0)\,\mathcal{U}^\dagger(t,0) = \mathbb{1}$.

In the **Heisenberg picture**, the wave function is t-independent:

$$|\phi\rangle = |\phi(0)\rangle_S = \mathcal{U}^{-1}(t,0)|\phi(t)\rangle_S = \mathcal{U}^\dagger(t,0)|\phi(t)\rangle_S.$$

The t-dependence is then moved from the wave functions to operators:

$$O_H(t) = \exp(\mathrm{i}\widehat{H}t)O_S\exp(-\mathrm{i}\widehat{H}t) = \mathcal{U}^\dagger(t,0)\underbrace{O_H(0)}_{=O_S}\mathcal{U}(t,0). \tag{3.40}$$

Here $O_H(t)$ is the operator in the Heisenberg picture and O_S the operator in the Schrödinger picture. The operator $O_H(t)$ obeys the Heisenberg equation

$$\mathrm{i}\frac{\partial}{\partial t}O_H(t) = [O_H(t), \widehat{H}]\,. \tag{3.41}$$

These two pictures are equivalent when computing matrix elements:

$$\langle\phi_1(t)|O|\phi_2(t)\rangle_S = \langle\phi_1|O(t)|\phi_2\rangle_H\,. \tag{3.42}$$

The Hamilton operator is independent of the picture (no need in subscript "S" or "H"):

$$\widehat{H}_H = \exp(\mathrm{i}\widehat{H}_S t)\widehat{H}_S\exp(-\mathrm{i}\widehat{H}_S t) = \widehat{H}_S. \tag{3.43}$$

In the Heisenberg picture, the Hamiltonian is expressed in terms of the t-dependent field operators $\widehat{\Psi}(t)$ in the same way as it is expressed through $\widehat{\Psi}$ in the Schrödinger picture:

$$\begin{aligned}\widehat{H} &= \exp(\mathrm{i}\widehat{H}t)\widehat{H}\exp(-\mathrm{i}\widehat{H}t)\\ &= \exp(\mathrm{i}\widehat{H}t)\left\{\int \mathrm{d}r\;\widehat{\Psi}^\dagger(\mathbf{r})\widehat{H}_0\widehat{\Psi}(\mathbf{r}) + \frac{1}{2}\iint \mathrm{d}r\,\mathrm{d}r'\;\widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}^\dagger(\mathbf{r}')U(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}')\widehat{\Psi}(\mathbf{r})\right\}\exp(-\mathrm{i}\widehat{H}t)\\ &= \int \mathrm{d}r\;\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{H}_0(\mathbf{r})\widehat{\Psi}(\mathbf{r},t) + \frac{1}{2}\iint \mathrm{d}r\,\mathrm{d}r'\;\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{\Psi}^\dagger(\mathbf{r}',t)U(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r},t).\end{aligned} \tag{3.44}$$

For Heisenberg operators the commutator

$$[\widehat{\Psi}(\mathbf{r},t), \widehat{\Psi}^\dagger(\mathbf{r}',t')]_\mp \tag{3.45}$$

has, in general, a complicated form (it is expressed in terms of Green's functions of the many-body problem defined below). However, at equal times $t = t'$ the commutator becomes simple:

$$\begin{aligned}[\widehat{\Psi}(\mathbf{r},t), \widehat{\Psi}^\dagger(\mathbf{r}',t)]_\mp &= [\exp(\mathrm{i}\widehat{H}t)\widehat{\Psi}(\mathbf{r})\exp(-\mathrm{i}\widehat{H}t), \exp(\mathrm{i}\widehat{H}t)\widehat{\Psi}(\mathbf{r}')\exp(-\mathrm{i}\widehat{H}t)]\\ &= \exp(\mathrm{i}\widehat{H}t)[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')]\exp(-\mathrm{i}\widehat{H}t) = \delta(\mathbf{r}-\mathbf{r}')\,.\end{aligned} \tag{3.46}$$

3.3.1 Schrödinger equation for $\widehat{\Psi}(\mathbf{r},t)$

Now we use Eq. (3.41) and to derive the evolution equation (analog of Schrödinger equation) for the field operator in the Heisenberg picture:

$$\begin{aligned} \mathrm{i}\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{r},t) &= [\widehat{\Psi}(\mathbf{r},t),\widehat{H}] \\ &= \int \mathrm{d}r\,[\widehat{\Psi}(\mathbf{r},t),\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{H}_0(\mathbf{r})\Psi(\mathbf{r},t)] \\ &+ \frac{1}{2}\iint \mathrm{d}r\,\mathrm{d}r'\,U(\mathbf{r}',\mathbf{r}'')[\widehat{\Psi}(\mathbf{r},t),\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{\Psi}^\dagger(\mathbf{r}',t)U(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r},t)]. \end{aligned} \tag{3.47}$$

Using Eq. (3.46), we obtain for the required commutators (both for bosons and fermions)

$$[\widehat{\Psi}(\mathbf{r},t),\widehat{\Psi}^\dagger(\mathbf{r}',t)\widehat{H}_0(\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)] = \widehat{H}_0(\mathbf{r})\widehat{\Psi}(\mathbf{r},t)\delta(\mathbf{r}-\mathbf{r}'), \tag{3.48}$$

and

$$\begin{aligned} [\widehat{\Psi}(\mathbf{r},t),\widehat{\Psi}^\dagger(\mathbf{r}',t)\widehat{\Psi}^\dagger(\mathbf{r}'',t)U(\mathbf{r}',\mathbf{r}'')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r}'',t)] &= \delta(\mathbf{r}-\mathbf{r}'')\widehat{\Psi}^\dagger(\mathbf{r}',t)U(\mathbf{r}',\mathbf{r}'')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r}'',t) \\ +\delta(\mathbf{r}-\mathbf{r}')\widehat{\Psi}^\dagger(\mathbf{r}'',t)U(\mathbf{r}',\mathbf{r}'')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r}'',t). \end{aligned} \tag{3.49}$$

Substituting Eqs. (3.48) and (3.49) into Eq. (3.47), and using $U(\mathbf{r}',\mathbf{r}'') = U(\mathbf{r}'',\mathbf{r}')$, we arrive at

$$\mathrm{i}\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{r},t) = \left(-\frac{\boldsymbol{\nabla}^2}{2m} + V(\mathbf{r}) - \mu\right)\widehat{\Psi}(\mathbf{r},t) + \int \mathrm{d}r'\,\widehat{\Psi}^\dagger(\mathbf{r}',t)U(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r},t)\,. \tag{3.50}$$

This equation is nonlinear, so that the field operators behave in a nontrivial way.

3.4 Green's function

We define the Green's function of a many-body system as

$$G_{\sigma_1\sigma_2}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = -\mathrm{i}\langle\phi_0|\mathcal{T}\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)|\phi_0\rangle\,, \tag{3.51}$$

where $|\phi_0\rangle$ is the exact ground state, $\widehat{\Psi}_{\sigma_i}(\mathbf{r}_i,t_i)$ are Heisenberg operators, and $\mathcal{T}\widehat{\Psi}_1(t_1)\widehat{\Psi}_2(t_2)\ldots\widehat{\Psi}_n(t_n)$ is the chronological product, which is defined in the following way:

$$\begin{aligned} \mathcal{T}\widehat{\Psi}_1(t_1)\widehat{\Psi}_2(t_2)\ldots\widehat{\Psi}_n(t_n) &= \widehat{\Psi}_{i_1}(t_{i_1})\widehat{\Psi}_{i_2}(t_{i_2})\ldots\widehat{\Psi}_{i_n}(t_{i_n}) \times \begin{cases} 1 & \text{for bosons} \\ (-1)^P & \text{for fermions} \end{cases}, \\ & \text{with } t_{i_1} > t_{i_2} > \ldots > t_{i_n}\,. \end{aligned} \tag{3.52}$$

The symbol $\mathcal{T}$ denotes the time-ordering operator which orders the different times such that they increase from right to left. The factor $(-1)^P$ for fermions depends on the number P of permutations of operators required for the time ordering.

We thus have:

$$\begin{aligned} G_{\sigma_1\sigma_2}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) &= \begin{cases} -\mathrm{i}\langle\phi_0|\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)|\phi_0\rangle & \text{for} \quad t_1 > t_2 \\ \mp\mathrm{i}\langle\phi_0|\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)|\phi_0\rangle & \text{for} \quad t_2 > t_1 \end{cases} \\ &\equiv -\mathrm{i}\left\{\Theta(t_1-t_2)\langle\phi_0|\widehat{\Psi}_1\widehat{\Psi}^\dagger_2|\phi_0\rangle \pm \Theta(t_2-t_1)\langle\phi_0\widehat{\Psi}^\dagger_2\widehat{\Psi}_1|\phi_0\rangle\right\}, \end{aligned} \tag{3.53}$$

where, as before, the upper sign is for bosons and lower for fermions.

- Under the assumption that the spin symmetry is not broken, it holds that

$$G_{\sigma_1\sigma_2}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \delta_{\sigma_1\sigma_2} G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)\,. \tag{3.54}$$

  For simplicity, we will frequently discard the spin degree of freedom below.

- If there is translational invariance in the coordinate space, then it is convenient to go to the momentum space by Fourier transformation:

$$G(\mathbf{p}_1,t_1;\mathbf{p}_2,t_2) = -\mathrm{i}\langle\phi_0|\mathcal{T}\widehat{\Psi}(\mathbf{p}_1,t_1)\widehat{\Psi}^\dagger(\mathbf{p}_2,t_2)|\phi_0\rangle \xrightarrow{\text{transl. inv.}} G(\mathbf{p}_1;t_1,t_2)\cdot(2\pi)^d\delta(\mathbf{p}_1-\mathbf{p}_2)\,. \tag{3.55}$$

- If there is translational invariance with respect to time, then it is convenient to go to the energy space by Fourier transformation:

$$G(\mathbf{p}_1,\omega_1,\mathbf{p}_2,\omega_2) \xrightarrow{\text{transl. inv. in time}} G(\mathbf{p}_1,\mathbf{p}_2,\omega_1)\cdot 2\pi\,\delta(\omega_1-\omega_2)\,. \tag{3.56}$$

3.5 Non-interacting fermions

Consider the non-interacting case, $U = 0$, with the Hamiltonian given by $\widehat{H} = \widehat{H}_0$. We will analyze the connection between the Green's function $G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)$ defined in Sec. 3.4 within the many-body formalism and the single-particle Green's function of Chapter 2.

The single-particle Green's function $G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)$ as defined in Chapter 2 is as a solution of the following equation:

$$\left[\mathrm{i}\partial_{t_1} - \widehat{H}_0(\mathbf{r}_1)\right] G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \delta(\mathbf{r}_1-\mathbf{r}_2)\delta(t_1-t_2)\,, \tag{3.57}$$

with

$$\widehat{H}_0(\mathbf{r}_1) = -\frac{\boldsymbol{\nabla}^2}{2m} + V(r) - \mu\,. \tag{3.58}$$

We prove now that (3.53) obeys Eq. (3.57). For this purpose, we act with $\left[\mathrm{i}\partial_{t_1} - \widehat{H}_0(\mathbf{r}_1)\right]$ on the Green function of the many-body formalism, Eq.(3.53):

$$\begin{aligned}
&\left[i\partial_{t_1} - \widehat{H}_0(\mathbf{r}_1)\right] G_{\sigma_1\sigma_2}(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2) \overset{(3.53)}{=} -i\left[i\partial_{t_1} - \widehat{H}_0(\mathbf{r}_1)\right]\Big[\Theta(t_1-t_2)\langle\,\phi_0\mid\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)\mid\phi_0\rangle\\
&\quad \pm\Theta(t_2-t_1)\langle\,\phi_0\mid\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\mid\phi_0\rangle\Big]\\
&\quad = i(-i)\delta(t_1-t_2)\Big[\langle\,\phi_0\mid\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)\mid\phi_0\rangle \mp\langle\,\phi_0\mid\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\mid\phi_0\rangle\Big]\\
&\quad -i\Theta(t_1-t_2)\langle\,\phi_0\mid\left[i\partial_{t_1} - \widehat{H}_0(\mathbf{r}_1)\right]\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)\mid\phi_0\rangle\\
&\quad \mp i\Theta(t_2-t_1)\langle\,\phi_0\mid\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)\left[i\partial_{t_1} - \widehat{H}_0(\mathbf{r}_1)\right]\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\mid\phi_0\rangle.
\end{aligned}$$

By using

$$(\mathrm{i}\partial_t - \widehat{H}_0)\widehat{\Psi}(\mathbf{r},t) = 0 \tag{3.59}$$

(which follows from Eq. (3.50) in the absence of interaction, $U = 0$), we obtain:

$$\begin{aligned}
\left[\mathrm{i}\partial_{t_1} - \widehat{H}_0(\mathbf{r}_1)\right] G_{\sigma_1\sigma_2}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) &= \delta(t_1-t_2)\langle\phi_0|\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_1) \mp \widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_1)\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)|\phi_0\rangle\\
&= \delta(t_1-t_2)\delta(\mathbf{r}_1-\mathbf{r}_2)\delta_{\sigma_1\sigma_2}\,.
\end{aligned} \tag{3.60}$$

Thus, indeed, the Green's function of the many-body formalism satisfies, in the absence of interaction, Eq. (3.57) or, in a brief form,

$$(\mathrm{i}\partial_t - \widehat{H})\widehat{G} = \widehat{\mathbb{1}}\,. \tag{3.61}$$

In the rest of this subsection we consider the case of **fermions**.

We know from Sec. 2.2, 2.3 that Eq. (3.61) does not uniquely determine the Green function since one should specify the shift of poles in the complex plane of frequency. To determine the explicit form of the Green's function, we use the second-quantization form of the Hamilton operator,

$$\widehat{H} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}}\,, \tag{3.62}$$

with

$$\varepsilon_{\mathbf{p}} = \frac{p^2}{2m} - \mu. \tag{3.63}$$

and the field operator written in terms of the plane waves,

$$\widehat{\Psi}^\dagger(\mathbf{r}) = \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}} \frac{\exp(-\mathrm{i}\mathbf{p}\cdot\mathbf{r})}{\sqrt{V}}\,, \quad \widehat{\Psi}(\mathbf{r}) = \sum_{\mathbf{p}} a_{\mathbf{p}} \frac{\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r})}{\sqrt{V}}\,. \tag{3.64}$$

For the Green's function we need the operators in the Heisenberg picture. By using

$$[a^\dagger_{\mathbf{p}} a_{\mathbf{p}}, a^\dagger_{\mathbf{p}}] = a^\dagger_{\mathbf{p}}\,, \tag{3.65}$$

or, equivalently,

$$a^\dagger_{\mathbf{p}} a_{\mathbf{p}} \cdot a^\dagger_{\mathbf{p}} = a^\dagger_{\mathbf{p}}(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + 1)\,, \tag{3.66}$$

and, therefore,

$$\exp(\mathrm{i}\varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} t) a^\dagger_{\mathbf{p}} \exp(-\mathrm{i}\varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} t) = a^\dagger_{\mathbf{p}} \exp[\mathrm{i}\varepsilon_{\mathbf{p}}(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + 1)t] \exp(-\mathrm{i}\varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} t) = a^\dagger_{\mathbf{p}} \exp(\mathrm{i}\varepsilon_{\mathbf{p}} t)\,, \tag{3.67}$$

we obtain the Heisenberg operators

$$\widehat{\Psi}^\dagger(\mathbf{r}, t) = e^{\mathrm{i}\widehat{H}t} \widehat{\Psi}^\dagger(\mathbf{r}) e^{-\mathrm{i}\widehat{H}t} = \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}} \frac{\exp(-\mathrm{i}\mathbf{p}\cdot\mathbf{r} + \mathrm{i}\varepsilon_{\mathbf{p}} t)}{\sqrt{V}}\,, \tag{3.68}$$

$$\widehat{\Psi}(\mathbf{r}, t) = e^{\mathrm{i}\widehat{H}t} \widehat{\Psi}(\mathbf{r}) e^{-\mathrm{i}\widehat{H}t} = \sum_{\mathbf{p}} a_{\mathbf{p}} \frac{\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}} t)}{\sqrt{V}}\,. \tag{3.69}$$

The ground state has all single-particle states up to the Fermi level filled:

$$|\phi_0\rangle = \prod_{|\mathbf{p}|<p_F} a^\dagger_{\mathbf{p}} |0\rangle\,. \tag{3.70}$$

The Green's function for $t_1 > t_2$ is given by:

$$\begin{aligned} G(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) &= \frac{1}{V} \sum_{\mathbf{p}_1, \mathbf{p}_2} (-\mathrm{i}) \exp(-\mathrm{i}\varepsilon_{\mathbf{p}_1} t_1 + \mathrm{i}\varepsilon_{\mathbf{p}_2} t_2 + \mathrm{i}\mathbf{p}_1\mathbf{r}_1 - \mathrm{i}\mathbf{p}_2\mathbf{r}_2) \langle \underbrace{\phi_0 | a_{\mathbf{p}_1} a^\dagger_{\mathbf{p}_2} | \phi_0 \rangle}_{=\delta_{\mathbf{p}_1\mathbf{p}_2}\Theta(|\mathbf{p}_1|-p_F)} \\ &= -\mathrm{i}\frac{1}{V} \sum_{\mathbf{p}} \exp[-\mathrm{i}\varepsilon_{\mathbf{p}}(t_1 - t_2) + \mathrm{i}\mathbf{p}\cdot(\mathbf{r}_1 - \mathbf{r}_2)] \Theta(|\mathbf{p}| - p_F)\,, \end{aligned} \tag{3.71}$$

and for $t_1 < t_2$:

$$G(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \frac{1}{V} \sum_{\mathbf{p}_1, \mathbf{p}_2} \mathrm{i} \exp(-\mathrm{i}\varepsilon_{\mathbf{p}_1} t_1 + \mathrm{i}\varepsilon_{\mathbf{p}_2} t_2 + \mathrm{i}\mathbf{p}_1 \mathbf{r}_1 - \mathrm{i}\mathbf{p}_2 \mathbf{r}_2) \langle \underbrace{\phi_0 | a^\dagger_{\mathbf{p}_2} a_{\mathbf{p}_1} | \phi_0 \rangle}_{=\delta_{\mathbf{p}_1 \mathbf{p}_2} \Theta(p_F - |\mathbf{p}_1|)}$$

$$= \mathrm{i} \frac{1}{V} \sum_{\mathbf{p}} \exp[-\mathrm{i}\varepsilon_{\mathbf{p}}(t_1 - t_2) + \mathrm{i}\mathbf{p}(\mathbf{r}_1 - \mathbf{r}_2)] \Theta(p_F - |\mathbf{p}|) \,. \tag{3.72}$$

For the Fourier transform, one obtains:

$$G(\mathbf{p}, t) = \begin{cases} -\mathrm{i} \exp(-\mathrm{i}\varepsilon_{\mathbf{p}} t) \Theta(|\mathbf{p}| - p_F) & \text{for} \quad t > 0 \\ \mathrm{i} \exp(-\mathrm{i}\varepsilon_{\mathbf{p}} t) \Theta(p_F - |\mathbf{p}|) & \text{for} \quad t < 0 \end{cases}$$

$$= -\mathrm{i} \exp(-\mathrm{i}\varepsilon_{\mathbf{p}} t) \left[\Theta(|\mathbf{p}| - p_F) \Theta(t) - \Theta(p_F - |\mathbf{p}|) \Theta(-t) \right] . \tag{3.73}$$

We transform the Green's function to the energy space (with the terms $\mp 0t$ in the exponent introduced for convergence):

$$G(\mathbf{p}, \varepsilon) = \int \mathrm{d}t \, \exp(\mathrm{i}\varepsilon t) G(\mathbf{p}, t)$$

$$= -\mathrm{i} \left\{ \Theta(|\mathbf{p}| - p_F) \int_0^\infty \exp[\mathrm{i}(\varepsilon - \varepsilon_{\mathbf{p}})t - 0t] - \Theta(p_F - |\mathbf{p}|) \int_{-\infty}^0 \mathrm{d}t \, \exp[\mathrm{i}(\varepsilon - \varepsilon_{\mathbf{p}})t + 0t] \right\}$$

$$= -\mathrm{i} \left[\Theta(|\mathbf{p}| - p_F) \frac{1}{-\mathrm{i}(\varepsilon - \varepsilon_{\mathbf{p}}) + 0} - \Theta(p_F - |\mathbf{p}|) \frac{1}{\mathrm{i}(\varepsilon - \varepsilon_{\mathbf{p}}) + 0} \right] =$$

$$= \frac{\Theta(|\mathbf{p}| - p_F)}{\varepsilon - \varepsilon_{\mathbf{p}} + \mathrm{i}0} + \frac{\Theta(p_F - |\mathbf{p}|)}{\varepsilon - \varepsilon_{\mathbf{p}} - \mathrm{i}0}$$

$$\equiv \frac{1}{\varepsilon - \varepsilon_{\mathbf{p}} + \mathrm{i}0 \, \mathrm{sign}(|\mathbf{p}| - p_F)} \,. \tag{3.74}$$

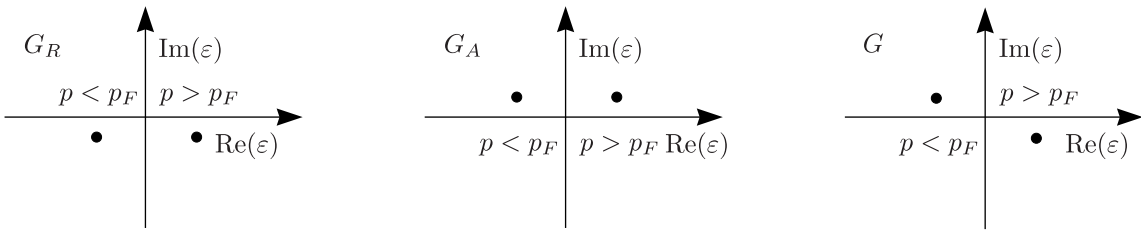
The Green's function is neither

$$G^R = \frac{1}{\varepsilon - \varepsilon_{\mathbf{p}} + \mathrm{i}0} \,, \tag{3.75}$$

nor

$$G^A = \frac{1}{\varepsilon - \varepsilon_{\mathbf{p}} - \mathrm{i}0} \,; \tag{3.76}$$

whether the pole is shifted as in G^R or as in G^A depends on the relation between $|\mathbf{p}|$ and p_F. The pole structure of the Green's functions G^R, G^A, and G in the complex plane of ε is illustrated in the figure:



According to Eq. (3.73), the particles with $p > p_F$ move forward in time, i.e., the Green function is non-zero when the particle is first created by the operator $a^\dagger_{\mathbf{p}}$ and later annihilated by $a_{\mathbf{p}}$. For $p < p_F$ the situation is opposite: the operator $a^\dagger_{\mathbf{p}}$ act at a later time than $a_{\mathbf{p}}$, i.e., the particle moves backward in time. This can be physically understood as a hole in the

filled Fermi see that moves forward in time. (Cf. positron as a hole in the filled see of Dirac electrons with negative energies, or, equivalently a Dirac electron moving backwards in time.)

The retarded and advanced Green's functions can be also defined in the many-body formalism. Specifically, in the case of fermions:

$$G^R(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = -\mathrm{i}\langle\phi_0|\{\widehat{\Psi}(\mathbf{r}_1,t_1),\widehat{\Psi}^\dagger(\mathbf{r}_2,t_2)\}|\phi_0\rangle\Theta(t_1-t_2)\,, \tag{3.77}$$

and

$$G^A(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \mathrm{i}\langle\phi_0|\{\widehat{\Psi}(\mathbf{r}_1,t_1),\widehat{\Psi}^\dagger(\mathbf{r}_2,t_2)\}|\phi_0\rangle\Theta(t_2-t_1)\,. \tag{3.78}$$

Analogous formulas holds also for bosons; one should only replace anticommutators $\{\widehat{\Psi}(\mathbf{r}_1,t_1),\widehat{\Psi}^\dagger(\mathbf{r}_2,t_2)\}$ with commutators $[\widehat{\Psi}(\mathbf{r}_1,t_1),\widehat{\Psi}^\dagger(\mathbf{r}_2,t_2)]$.

As an example of calculation of the Green function of **free bosons**, see Sec. 5.1 where the Green function of acoustic phonons is derived.

3.6 Spectral (Lehmann) representation

For definiteness, we focus on the case of **fermions** in this subsection. The derivation of the Lehmann representation as of general analytical properties of zero-temperature Green functions to the case of bosons can be straightforwardly extended to bosons. These $T=0$ results are the limiting case of finite-T formulas derived below in Sec. 4.10.1.

We start from the general definition (because of time-translational invariance we set $t_1=t$ and $t_2=0$):

$$\begin{aligned} \mathrm{i}G(\mathbf{r},\mathbf{r}',t) &= \langle\phi_0|\mathcal{T}\widehat{\Psi}(\mathbf{r},t)\widehat{\Psi}^\dagger(\mathbf{r}',0)|\phi_0\rangle & (3.79)\\ &= \Theta(t)\langle\phi_0|\widehat{\Psi}(\mathbf{r},t)\widehat{\Psi}^\dagger(\mathbf{r}',0)|\phi_0\rangle - \Theta(-t)\langle\phi_0|\widehat{\Psi}^\dagger(\mathbf{r}',0)\widehat{\Psi}(\mathbf{r},t)|\phi_0\rangle\,. & (3.80)\end{aligned}$$

Consider the grand-canonical ensemble. The Hamilton operator $\widehat{H}' = \widehat{H} - \mu\widehat{N}$ obeys the eigenvalue equation

$$\widehat{H}'|\phi_n^{(N)}\rangle = E_n'|\phi_n^{(N)}\rangle\,, \tag{3.81}$$

with the energy

$$E_n' = E_n^{(N)} - \mu N\,. \tag{3.82}$$

The eigenstates $|\phi_n^{(N)}\rangle$ are labeled by n and (N), where N stands for the number of particles. These eigenstates obey the conditions:

$$\sum_{n,N}|\phi_n^{(N)}\rangle\langle\phi_n^{(N)}| = \widehat{\mathbb{1}} \tag{3.83}$$

and

$$\langle\,\phi_n^{(N)}\mid\phi_m^{(M)}\rangle = \delta_{nm}\delta_{NM}. \tag{3.84}$$

We insert the resolution of the identity operator, Eq. (3.83), into the expression for the Green's function. Then matrix elements of the following type appear:

$$\begin{aligned}\langle\phi_m^{(N-1)}|\widehat{\Psi}(\mathbf{r},t)|\phi_n^{(N)}\rangle &= \langle\phi_m^{(N-1)}|\exp(\mathrm{i}\widehat{H}'t)\widehat{\Psi}(\mathbf{r})\exp(-\mathrm{i}\widehat{H}'t)|\phi_n^{(N)}\rangle\\ &= \exp\left[\mathrm{i}(E_m'-E_n')t\right]\langle\phi_m^{(N-1)}|\widehat{\Psi}(\mathbf{r})|\phi_n^{(N)}\rangle\\ &= \exp\left[\mathrm{i}(E_m^{(N-1)}-E_n^{(N)}+\mu)t\right]\langle\phi_m^{(N-1)}|\widehat{\Psi}(\mathbf{r})|\phi_n^{(N)}\rangle\,. \end{aligned}\tag{3.85}$$

Thus, we have pulled out the time dependence of the matrix element. The ground state is $|\phi_0^{(N)}\rangle$. The Green's function is then written as:

$$\begin{aligned}
\mathrm{i}G(\mathbf{r},\mathbf{r}',t) &\overset{(3.80)}{=} \Theta(t)\sum_m \langle\phi_0^{(N)}|\widehat{\Psi}(\mathbf{r},t)|\phi_m^{(N+1)}\rangle\langle\phi_m^{(N+1)}|\widehat{\Psi}^\dagger(\mathbf{r}',0)|\phi_0^{(N)}\rangle \\
&\quad - \Theta(-t)\sum_m \langle\phi_0^{(N)}|\widehat{\Psi}^\dagger(\mathbf{r}',0)|\phi_m^{(N-1)}\rangle\langle\phi_m^{(N-1)}|\widehat{\Psi}(\mathbf{r},t)|\phi_0^{(N)}\rangle \\
&= \Theta(t)\sum_m \exp\left[\mathrm{i}(E_0^{(N)} - E_m^{(N+1)} + \mu)t\right]\langle\phi_0^{(N)}|\widehat{\Psi}(\mathbf{r})|\phi_m^{(N+1)}\rangle\langle\phi_m^{(N+1)}|\widehat{\Psi}(\mathbf{r}')^\dagger|\phi_0^{(N)}\rangle \\
&\quad - \Theta(-t)\sum_m \exp\left[\mathrm{i}(E_m^{(N-1)} - E_0^{(N)} + \mu)t\right]\langle\phi_0^{(N)}|\widehat{\Psi}^\dagger(\mathbf{r}')|\phi_m^{(N-1)}\rangle\langle\phi_m^{(N-1)}|\widehat{\Psi}(\mathbf{r})|\phi_0^{(N)}\rangle\,.
\end{aligned} \tag{3.86}$$

We go to the energy space by Fourier transformation, which can be straightforwardly performed since all the time dependence is now in the exponential factors:

$$\begin{aligned}
G(\mathbf{r},\mathbf{r}',\varepsilon) &= \int dt\, e^{\mathrm{i}\varepsilon t}\, G(\mathbf{r},\mathbf{r}',t) \\
&= \sum_m \left\{ \frac{\langle\phi_0^{(N)}|\widehat{\Psi}(\mathbf{r})|\phi_m^{(N+1)}\rangle\langle\phi_m^{(N+1)}|\widehat{\Psi}^\dagger(\mathbf{r}')|\phi_0^{(N)}\rangle}{\varepsilon + E_0^{(N)} - E_m^{(N+1)} + \mu + \mathrm{i}0} + \frac{\langle\phi_0^{(N)}|\widehat{\Psi}^\dagger(\mathbf{r}')|\phi_m^{(N-1)}\rangle\langle\phi_m^{(N-1)}|\widehat{\Psi}(\mathbf{r})|\phi_0^{(N)}\rangle}{\varepsilon + E_m^{(N-1)} - E_0^{(N)} + \mu - \mathrm{i}0} \right\}.
\end{aligned} \tag{3.87}$$

We note that

$$\varepsilon_m^{(+)} \overset{\text{def}}{=} E_m^{(N+1)} - E_0^{(N)} \tag{3.88}$$

is the energy of a **particle-like** excitation and, therefore,

$$\varepsilon_m^{(-)} \overset{\text{def}}{=} E_0^{(N)} - E_m^{(N-1)} \tag{3.89}$$

is the energy of a **hole-like** excitation. The former corresponds to creating a particle $(N) \to (N+1)$ and the latter to removing a particle (i.e. creating a hole).

Since $|\phi_0^{(N)}\rangle$ is the ground state, we have $E_0' < E_m'$. It follows that

$$E_0{}^{(N)} - \mu N < E_m^{(N+1)} - \mu(N+1) \quad \text{and} \quad E_0^{(N)} - \mu N < E_m^{(N-1)} - \mu(N-1), \tag{3.90}$$

and, therefore

$$\varepsilon_m^{(+)} > \mu \quad \text{and} \quad \varepsilon_m^{(-)} < \mu. \tag{3.91}$$

According to Eq. (3.87), the poles of the Green's function are located at

- 1st term:

$$\varepsilon = \varepsilon_m^{(+)} - \mu > 0, \tag{3.92}$$

- 2nd term:

$$\varepsilon = \varepsilon_m^{(-)} - \mu < 0. \tag{3.93}$$

We can write the Green's function (3.87) in the **Lehmann representation** using the **spectral weight**

$$\begin{aligned}\mathcal{A}(\mathbf{r},\mathbf{r}';\varepsilon_1) &= \sum_m \Big\{ \langle\phi_0^{(N)}|\widehat{\Psi}(\mathbf{r})|\phi_m^{(N+1)}\rangle\langle\phi_m^{(N+1)}|\widehat{\Psi}^\dagger(\mathbf{r}')|\phi_0^{(N)}\rangle\delta(\varepsilon_1-\varepsilon_m^{(+)}+\mu) \\ &\qquad +\langle\phi_0^{(N)}|\widehat{\Psi}^\dagger(\mathbf{r}')|\phi_m^{(N-1)}\rangle\langle\phi_m^{(N-1)}|\widehat{\Psi}(\mathbf{r})|\phi_0^{(N)}\rangle\delta(\varepsilon_1-\varepsilon_m^{(-)}+\mu)\Big\} \\ &\equiv \mathcal{A}^{(+)}(\varepsilon_1;\mathbf{r},\mathbf{r}')+\mathcal{A}^{(-)}(\varepsilon_1;\mathbf{r},\mathbf{r}'), \end{aligned} \tag{3.94}$$

where $\mathcal{A}^{(+)} \neq 0$ only for $\varepsilon_1 > 0$ and $\mathcal{A}^{(-)} \neq 0$ only for $\varepsilon_1 < 0$. Hence, the result for the Green function can be written in a very compact form:

$$G(\mathbf{r},\mathbf{r}';\varepsilon) = \int \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}(\mathbf{r},\mathbf{r}';\varepsilon_1)}{\varepsilon-\varepsilon_1+\mathrm{i}0\mathrm{sign}(\varepsilon)} \equiv \int_0^\infty \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}^{(+)}(\varepsilon_1;\mathbf{r},\mathbf{r}')}{\varepsilon-\varepsilon_1+\mathrm{i}0} + \int_{-\infty}^0 \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}^{(-)}(\varepsilon_1;\mathbf{r},\mathbf{r}')}{\varepsilon-\varepsilon_1-\mathrm{i}0}\,. \tag{3.95}$$

The corresponding formulas for retarded and advanced Green functions defined by Eqs. (3.77) and (3.78) are given by:

$$G^R(\mathbf{r},\mathbf{r}';\varepsilon) = \int \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}(\mathbf{r},\mathbf{r}';\varepsilon_1)}{\varepsilon-\varepsilon_1+\mathrm{i}0}\,, \tag{3.96}$$

$$G^A(\mathbf{r},\mathbf{r}';\varepsilon) = \int \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}(\mathbf{r},\mathbf{r}';\varepsilon_1)}{\varepsilon-\varepsilon_1-\mathrm{i}0}\,, \tag{3.97}$$

with the same spectral weight $\mathcal{A}(\mathbf{r},\mathbf{r}';\varepsilon_1)$. (The derivation is fully analogous.) Thus, we obtain the causality relation:

$$G(\varepsilon) = \begin{cases} G^R(\varepsilon) & \text{for} \quad \varepsilon > 0, \\ G^A(\varepsilon) & \text{for} \quad \varepsilon < 0. \end{cases} \tag{3.98}$$

Obviously, location of poles in Eqs. (3.95), (3.96), and (3.97) is as follows:

- Eq.(3.95) $\rightarrow$

$$G: \quad \text{poles at} \begin{cases} \mathrm{Im}\,(\varepsilon) < 0 & \text{for} \quad \mathrm{Re}\,(\varepsilon) > 0, \\ \mathrm{Im}\,(\varepsilon) > 0 & \text{for} \quad \mathrm{Re}\,(\varepsilon) < 0. \end{cases}$$

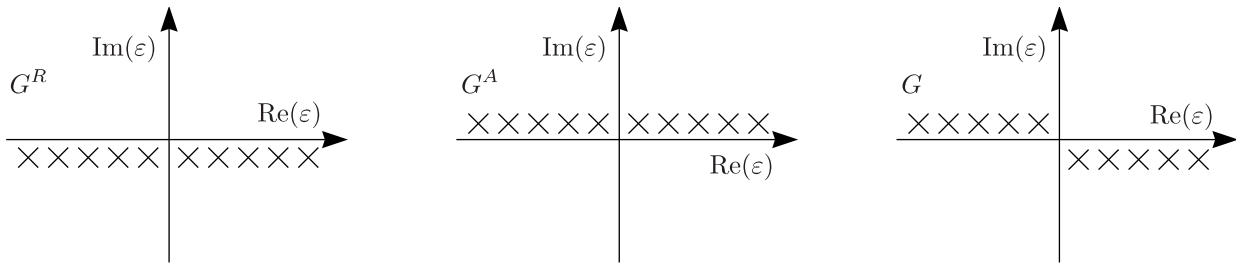
- Eq. (3.96) $\rightarrow$

$$G^R: \quad \text{poles at } \mathrm{Im}\,(\varepsilon) < 0$$

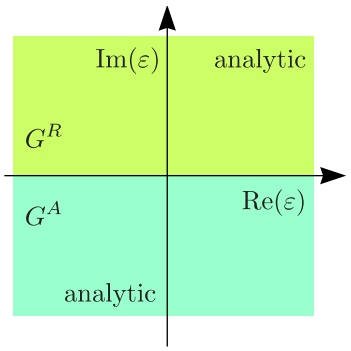
- Eq. (3.97) $\rightarrow$

$$G^A: \quad \text{poles at } \mathrm{Im}\,(\varepsilon) > 0$$

Graphical representation of poles in the integrals (3.95), (3.96), and (3.97):



Thus, G^R is analytical function in the half-plane $\mathrm{Im}\,(\varepsilon) > 0$, and G^A is analytical function in the half-plane $\mathrm{Im}\,(\varepsilon) < 0$.



Let us now assume that we have a **translation-invariant system in coordinate space.** We perform then transformation to the momentum space:

$$G(\mathbf{r},\mathbf{r}';\varepsilon) = G(\mathbf{r}-\mathbf{r}';\varepsilon) \;\mapsto\; G(\mathbf{p};\varepsilon)\,. \tag{3.99}$$

An eigenstate $|\phi_m^{(N)}\rangle$ is then characterized by a momentum $\mathbf{p}$, so that we denote it as $|m,N,\mathbf{p}\rangle$, and the field operaror is

$$\widehat{\Psi}(\mathbf{r}) = \sum_{\mathbf{p}} \frac{1}{\sqrt{V}} \hat{a}_{\mathbf{p}} \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r})\,. \tag{3.100}$$

We obtain the Lehmann representation of the Green's function

$$G(\mathbf{p};\varepsilon) = \int \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}(\mathbf{p};\varepsilon_1)}{\varepsilon - \varepsilon_1 + \mathrm{i}0\mathrm{sign}(\varepsilon)}\,, \tag{3.101}$$

where the spectral weight

$$\mathcal{A}(\mathbf{p};\varepsilon_1) = \sum_m \Big\{ |\langle 0,N,\mathbf{p}=\mathbf{0}|\hat{a}_{\mathbf{p}}|m,N+1,\mathbf{p}\rangle|^2 \, \delta(\varepsilon_1 - \varepsilon^{(+)}(m,\mathbf{p}) + \mu) \tag{3.102}$$

$$+ \, |\langle m,N-1,-\mathbf{p}|\hat{a}_{\mathbf{p}}|0,N,\mathbf{p}=\mathbf{0}\rangle|^2 \, \delta(\varepsilon_1 - \varepsilon^{(-)}(m,-\mathbf{p}) + \mu) \Big\}\,. \tag{3.103}$$

is real. The retarded and advanced Green functions read

$$G^{R/A}(\mathbf{p};\varepsilon) \;=\; \int \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}(\mathbf{p};\varepsilon_1)}{\varepsilon - \varepsilon_1 \pm \mathrm{i}0}\,, \tag{3.104}$$

and

$$G(\mathbf{p};\varepsilon) = \begin{cases} G^R(\mathbf{p};\varepsilon) & \text{for} \quad \varepsilon > 0, \\ G^A(\mathbf{p};\varepsilon) & \text{for} \quad \varepsilon < 0. \end{cases} \tag{3.105}$$

We note that

$$[G^R(\mathbf{p};\varepsilon)]^* = G^A(\mathbf{p};\varepsilon)\,. \tag{3.106}$$

Using

$$\frac{1}{\varepsilon - \varepsilon_1 \pm \mathrm{i}0} = \mathcal{P}\frac{1}{\varepsilon - \varepsilon_1} \mp \mathrm{i}\pi\delta(\varepsilon - \varepsilon_1)\,, \tag{3.107}$$

we see that the real parts of all Green functions are equal:

$$\mathrm{Re}\, G(\mathbf{p};\varepsilon) = \mathrm{Re}\, G^R(\mathbf{p};\varepsilon) = \mathrm{Re}\, G^A(\mathbf{p};\varepsilon) = \mathcal{P}\int \mathrm{d}\varepsilon_1 \, \frac{\mathcal{A}(\varepsilon_1;\mathbf{p})}{\varepsilon - \varepsilon_1}\,. \tag{3.108}$$

At the same time, the imaginary parts differ and are expressed through the spectral weight as follows:

$$\left.\begin{array}{l} \mathrm{Im}\, G^R(\mathbf{p};\varepsilon) \\ \mathrm{Im}\, G^A(\mathbf{p};\varepsilon) \\ \mathrm{Im}\, G(\mathbf{p};\varepsilon) \end{array}\right\} = \pi\mathcal{A}(\mathbf{p};\varepsilon) \times \left\{\begin{array}{l} -1 \\ +1 \\ -\mathrm{sign}(\varepsilon) \end{array}\right. \tag{3.109}$$

Any meaningful approximation should respect these general analytic properties.

The spectral weight is normalized (**exercise**):

$$\int d\varepsilon \mathcal{A}(\mathbf{p},\varepsilon) = 1. \tag{3.110}$$

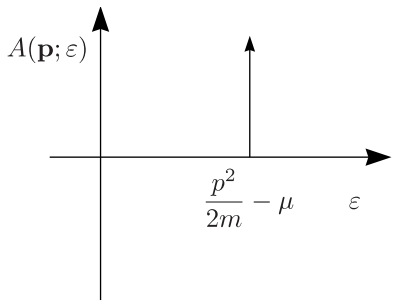
As we have shown above, pole in the Green function $G(\mathbf{p};\varepsilon)$ corresponds to excitations, which yield a nonzero spectral weight $\mathcal{A}(\mathbf{p};\varepsilon)$.

In a non-interacting system the Green function has the form

$$G(\mathbf{p};\varepsilon) = \frac{1}{\varepsilon + \mu - \frac{p^2}{2m} + \mathrm{i0sign}(\varepsilon)}\,. \tag{3.111}$$

The spectral weight is given by

$$\mathcal{A}(\mathbf{p};\varepsilon) = \delta\left(\varepsilon + \mu - \frac{p^2}{2m}\right)\,. \tag{3.112}$$

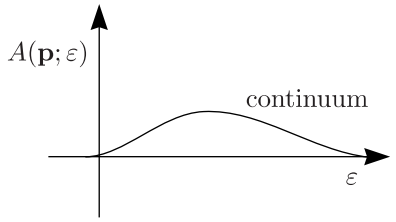


How does this change in the presence of interaction? We assume here that the system is in **Fermi-liquid** state. The Fermi-liquid theory was discussed in TKM I, where its basic properties were postulated. In Sec. 3.12 below we will derive the Fermi liquid theory in the framework of Green's function formalism.

If the excitation consists of many Fermi-liquid quasiparticles, then the momentum is

$$\mathbf{p} = \sum_i \mathbf{p}_i \tag{3.113}$$

and ε is <u>not</u> a unique function of p. The corresponding contribution to $\mathcal{A}(\mathbf{p};\varepsilon)$ will be thus spread over a broad interval of energies—a continuum. This contribution is also known as "incoherent background".



Now consider excitations with $\mathbf{p}$ be the momentum of one quasiparticle. The Landau-Fermi-Liquid theory tells us that the pole survives, and

$$G^{-1}(\mathbf{p};\varepsilon) = 0$$

is the dispersion relation of the quasiparticles. The general structure of the pole is (see Sec. 3.12 below for detailed derivation)

$$G(\mathbf{p};\varepsilon) = \frac{Z}{\varepsilon + \mu - \varepsilon(\mathbf{p})}\,, \tag{3.114}$$

where the renormalization constant Z satisfies $0 < Z < 1$. The constant Z is called "quasiparticle residue" or "quasiparticle weight".

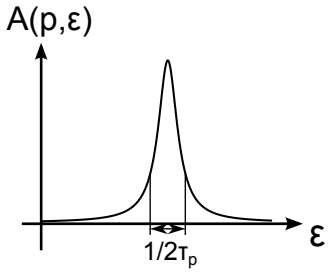
We write the energy in the form

$$\varepsilon(\mathbf{p}) = \mathrm{Re}\,\varepsilon(\mathbf{p}) \pm \mathrm{i}\,\mathrm{Im}\,\varepsilon(\mathbf{p}) \quad \text{with} \quad \mathrm{Im}\,\varepsilon(\mathbf{p}) = \frac{1}{2\tau(\mathbf{p})}\,, \tag{3.115}$$

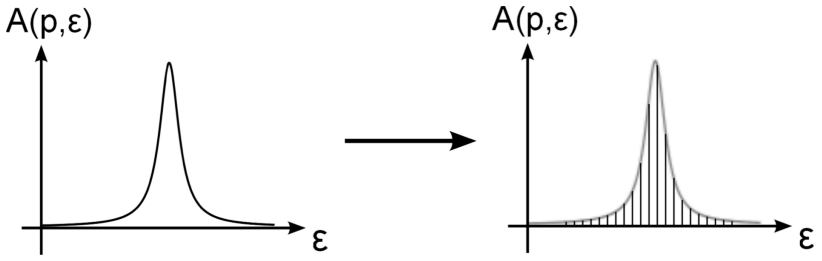
where $\tau(\mathbf{p})$ is the lifetime of the quasiparticle. [The sign of the imaginary part in the denominator of Eq. (3.114) is determined by Eq. (3.109).] It follows that

$$\pi\mathcal{A}(\mathbf{p};\varepsilon) = |\mathrm{Im}\,G(\mathbf{p};\varepsilon)| = \frac{Z\cdot\frac{1}{2\tau(\mathbf{p})}}{\left[\varepsilon+\mu-\mathrm{Re}\,\varepsilon(\mathbf{p})\right]^2+\left[\frac{1}{2\tau(\mathbf{p})}\right]^2}\,. \tag{3.116}$$

Thus, we get a quasiparticle peak in the spectral weight that has Lorentz (or, equivalently, Breit-Wigner) shape centered at $\varepsilon = \mathrm{Re}\,\varepsilon(\mathbf{p}) - \mu$ with width $1/2\tau(\mathbf{p})$.



The width, which is equal to the shift of the pole from the real axis, determines the decay rate of the quasiparticle. Note that the shift of the pole to the complex plane emerges in the thermodynamic limit. For a finite system, all poles (corresponding to energies of different many-body states) are at the real axis, see Lehmann representation above. They yield a dense set of delta functions in the spectral weight. In the thermodynamic limit, these delta functions merge into the quasiparticle peak:



Thermodynamic limit Finite system

The total spectral weight $\mathcal{A}(\mathbf{p};\varepsilon)$ is a sum of the incoherent background and the quasiparticle peak.

3.7 Interaction representation

In the Schrödinger picture states develop in time:

$$\mathrm{i}\frac{\partial}{\partial t}|\phi(t)\rangle = \widehat{H}|\phi(t)\rangle\,, \quad |\phi(t)\rangle = \exp(-\mathrm{i}\widehat{H}t)|\phi(0)\rangle\,, \tag{3.117}$$

and operators are time-independent. In the Heisenberg representation, operators develop in time

$$\mathrm{i}\frac{\partial}{\partial t}O(t) = [O(t),\widehat{H}]\,, \quad O(t) = \exp(\mathrm{i}\widehat{H}t)O(0)\exp(-\mathrm{i}\widehat{H}t)\,, \tag{3.118}$$

where $O(0) \equiv O_S$ and the states $|\phi\rangle$ are time-independent.
We introduce now one more representation that will be particularly useful for developing the perturbative expansion—the **interaction representation**. For this purpose, we split up the Hamiltonian in the free part and the interacting part: $\widehat{H} = \widehat{H}_0 + \widehat{U}$.

$$\left(\mathrm{i}\frac{\partial}{\partial t} - \widehat{H}_0\right)|\phi(t)\rangle = \widehat{U}|\phi(t)\rangle\,. \tag{3.119}$$

In general, $\widehat{U}$ can also be t-dependent, for example by adiabatic switching: $\widehat{U} \mapsto \widehat{U}\exp(-\lambda|t|)$ with $\lambda \mapsto +0$ that will be used below.
In the interaction representation (labeled by subscript "I"), the states are developed in time by the non-interacting Hamiltonian:

$$|\phi_I(t)\rangle = \exp(\mathrm{i}\widehat{H}_0 t)|\phi(t)\rangle\,. \tag{3.120}$$

Inserting this in the Schrödinger equation (3.119), we obtain:

$$\left(\mathrm{i}\frac{\partial}{\partial t} - \widehat{H}_0\right)\exp(-\mathrm{i}\widehat{H}_0 t)|\phi_I(t)\rangle \;=\; \widehat{U}\exp(-\mathrm{i}\widehat{H}_0 t)|\phi_I(t)\rangle\,, \tag{3.121}$$

which yields

$$\mathrm{i}\frac{\partial}{\partial t}|\phi_I(t)\rangle \;=\; \widehat{U}_I(t)|\phi_I(t)\rangle\,, \tag{3.122}$$

where

$$\widehat{U}_I(t) \;=\; \exp(\mathrm{i}\widehat{H}_0 t)\widehat{U}\exp(-\mathrm{i}\widehat{H}_0 t) \tag{3.123}$$

is the interaction operator in the interaction representation. In general, an operator in interaction representation is related to operator O of Schrödinger representation via

$$O_I(t) \;=\; \exp(\mathrm{i}\widehat{H}_0 t)\,O\,\exp(-\mathrm{i}\widehat{H}_0 t)\,. \tag{3.124}$$

(In general, Schrödinger operator O can be time-dependent: $O = O_{\mathrm{Schr}}(t)$.) The operators in the interaction representation have thus free dynamics determined by the operator $\exp(\mathrm{i}\widehat{H}_0 t)$, i.e., they evolve according to the free Hamiltonian $\widehat{H}_0$. The states in the interaction representation evolve as a result of the interaction, Eq. (3.122).

We solve Eq. (3.122) for $t > t_0$ with the boundary condition $|\phi_I(t)\rangle|_{t=t_0} = |\phi_I(t_0)\rangle$. Naively, one gets:

$$\begin{aligned} |\phi_I(t)\rangle \;&=\; \exp\left(-\mathrm{i}\int_{t_0}^{t}\mathrm{d}t_1\,\widehat{U}_I(t_1)\right)|\phi_I(t_0)\rangle\,. \\ &\equiv\; \sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int_{t_0}^{t}\mathrm{d}t_1\ldots\int_{t_0}^{t}\mathrm{d}t_n\,\widehat{U}_I(t_1)\ldots\widehat{U}_I(t_n)|\phi_I(t_0)\rangle \quad \textbf{(naive)} \end{aligned} \tag{3.125}$$

However, Eq. (3.125) is wrong, since $[\widehat{U}_I(t'), \widehat{U}_I(t'')] \neq 0$ in general. To find the correct solution, we solve the equation by iteration:

$$|\phi_I(t)\rangle = |\phi_I(t)\rangle_0 + |\phi_I(t)\rangle_1 + |\phi_I(t)\rangle_2 + \ldots\,, \tag{3.126}$$

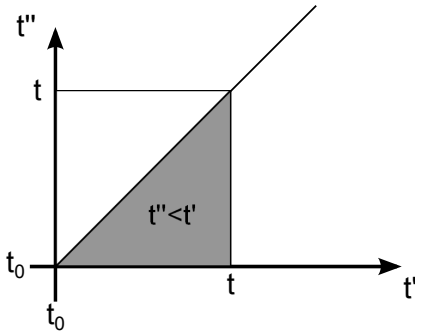
where $|\phi_I(t)\rangle_0 \sim U^0$, $|\phi_I(t)\rangle_1 \sim U^1$, and so on,

$$|\phi_I(t)\rangle_0 \stackrel{\text{def}}{=} |\phi_I(t_0)\rangle \tag{3.127}$$

$$|\phi_I(t)\rangle_1 = (-\mathrm{i}) \int_{t_0}^{t} \mathrm{d}t_1 \widehat{U}_I(t_1)|\phi_I(t_1)\rangle_0 \; = -\mathrm{i} \int_{t_0}^{t} \mathrm{d}t_1 \widehat{U}_I(t_1)|\phi_I(t_0)\rangle \,. \tag{3.128}$$

The second-order term reads:

$$\begin{aligned} |\phi_I(t)\rangle_2 &= (-\mathrm{i}) \int_{t_0}^{t} \mathrm{d}t_1 \, \widehat{U}_I(t_1)|\phi_I(t_1)\rangle_1 \\ &= (-\mathrm{i})^2 \int_{t_0}^{t} \mathrm{d}t_1 \, \widehat{U}_I(t_1) \int_{t_0}^{t_1} \mathrm{d}t_2 \, \widehat{U}_I(t_2)|\phi_I(t_0)\rangle \\ &= \frac{(-\mathrm{i})^2}{2} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t} \mathrm{d}t_2 \, \mathcal{T}\widehat{U}_I(t_1)\widehat{U}_I(t_2)|\phi_I(t_0)\rangle \,. \end{aligned} \tag{3.129}$$



The factor $1/2$ here comes from the fact that we integrate over the area $t_2 < t_1$ in the second line of Eq. (3.129) (triangle in the picture), whereas in the last line we integrate over the entire t_1, t_2-plane (square). and order operators in time. The time ordering $\mathcal{T}$ is what differs the correct second-order term (3.129) from the naive one [second-order term in Eq. (3.125)]. It is now clear that in the n-th order, we will get the term as in the n-th order of Eq.(3.125) but with time ordering. The factor $1/n!$ will emerge when we will replace an integral over $t > t_1 > t_2 > t_3 > \ldots > t_0$ by an integral without restrictions on the order of time variables (and with time ordering of operators), since there are $n!$ possible orderings of time variables.

The total result is thus given by:

$$\begin{aligned} |\phi_I(t)\rangle &= \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}t_1 \ldots \int_{t_0}^{t} \mathrm{d}t_n \, \mathcal{T}\widehat{U}_I(t_1) \ldots \widehat{U}_I(t_n)|\phi_I(t_0)\rangle \\ &\equiv \mathcal{T} \exp\left\{ -\mathrm{i} \int_{t_0}^{t} \mathrm{d}t_1 \, \widehat{U}_I(t_1) \right\} |\phi_I(t_0)\rangle \equiv \widehat{S}(t,t_0)|\phi_I(t_0)\rangle. \end{aligned} \tag{3.130}$$

Here

$$\widehat{S}(t,t_0) \stackrel{\text{def}}{=} \mathcal{T} \exp\left\{ -\mathrm{i} \int_{t_0}^{t} \mathrm{d}t_1 \, \widehat{U}_I(t_1) \right\} \tag{3.131}$$

is the evolution operator in the interaction picture:

$$|\phi_I(t)\rangle = \widehat{S}(t,t_0)|\phi_I(t_0)\rangle \,. \tag{3.132}$$

It contains all the information on how a state in the interaction representation evolves in time. Using the evolution in the Schrödinger representation,

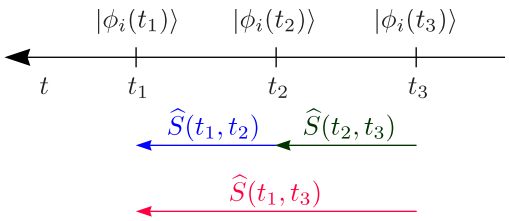
$$|\phi(t)\rangle = \exp\left[-\mathrm{i}\widehat{H}(t-t_0)\right] |\phi(t_0)\rangle \,, \tag{3.133}$$

and the relation (3.120) between the states in Schrödinger and interaction pictures, one obtains another formula for the evolution operator:

$$\widehat{S}(t,t_0) = \exp(\mathrm{i}\widehat{H}_0 t) \exp\left[-\mathrm{i}\widehat{H}(t-t_0)\right] \exp(-\mathrm{i}\widehat{H}_0 t_0) \,. \tag{3.134}$$

3.7.1 Properties of the evolution operator

- $\widehat{S}(t_1,t_2)\widehat{S}(t_2,t_3)=\widehat{S}(t_1,t_3)$



- $\widehat{S}$ is unitary: $\widehat{S}^{-1}(t,t_0)=\widehat{S}^{\dagger}(t,t_0)$.
- $\widehat{S}(t_2,t_1)=\widehat{S}^{-1}(t_1,t_2)=\widehat{S}^{\dagger}(t_1,t_2)$.

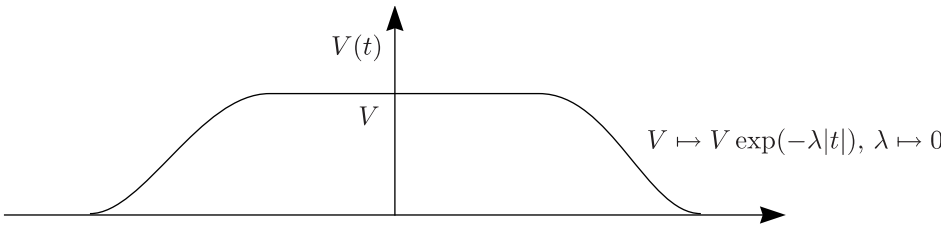
These properties follow immediately from Eq. (3.134). They can also be derived from the $\mathcal{T}$ exp formula (3.131).
Now we transform the Green's function into interaction representation. We assume first $t_1>t_2$, in which case

$$G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=-\mathrm{i}\langle\phi_0|\widehat{\Psi}(\mathbf{r}_1,t_1)\widehat{\Psi}^{\dagger}(\mathbf{r}_2,t_2)|\phi_0\rangle\,, \tag{3.135}$$

where $|\phi_0\rangle$ is the exact many-body state. Since at $t=0$ the interaction representation is the same as the Schrödinger representation, we can write for the exact many-body ground state

$$|\phi_0\rangle=|\phi_{0,I}(0)\rangle=\widehat{S}(0,-\infty)|\phi_{0,I}(-\infty)\rangle\,. \tag{3.136}$$

We assume that at large positive and negative times the interaction is adiabatically switched on/off ($\lambda\to+0$):



Thus, at $t=-\infty$ we have a non-interacting ground state:

$$|\phi_{0,I}(-\infty)\rangle=|0\rangle\,. \tag{3.137}$$

(i.e. Fermi see filled up to the chemical potential in the case of fermions). Now, let us transform the field operators (subscipts "H" , "S", and "I" denote Heisenberg, Schrödinger, and interaction representations, respectively):

$$\begin{aligned}\widehat{\Psi}_H(\mathbf{r},t)&=\exp(\mathrm{i}\widehat{H}t)\widehat{\Psi}_S(\mathbf{r})\exp(-\mathrm{i}\widehat{H}t)=\exp(\mathrm{i}\widehat{H}t)\exp(-\mathrm{i}\widehat{H}_0t)\widehat{\Psi}_I(\mathbf{r},t)\exp(\mathrm{i}\widehat{H}_0t)\exp(-\mathrm{i}\widehat{H}t)\\&=\widehat{S}^{-1}(t,0)\widehat{\Psi}_I(\mathbf{r},t)\widehat{S}(t,0)\,,\end{aligned} \tag{3.138}$$

and, analogously,

$$\widehat{\Psi}^{\dagger}_H(\mathbf{r},t)=\widehat{S}^{-1}(t,0)\widehat{\Psi}^{\dagger}_I(\mathbf{r},t)\widehat{S}(t,0)\,. \tag{3.139}$$

Then, upon transformation into the interaction representation, the Green's function takes the form:

$$\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=\langle 0|\widehat{S}^{-1}(0,-\infty)\widehat{S}^{-1}(t_1,0)\widehat{\Psi}_I(\mathbf{r}_1,t_1)\widehat{S}(t_1,0)\widehat{S}^{-1}(t_2,0)\widehat{\Psi}^{\dagger}_I(\mathbf{r}_2,t_2)\widehat{S}(t_2,0)\widehat{S}(0,-\infty)|0\rangle\,. \tag{3.140}$$

Using

$$\widehat{S}^{-1}(0,-\infty)\widehat{S}^{-1}(t_1,0) = \widehat{S}(-\infty,0)\widehat{S}(0,t_1) = \widehat{S}(-\infty,t_1) = \widehat{S}^{-1}(+\infty,-\infty)\widehat{S}(+\infty,t_1)\,, \quad (3.141)$$

$$\widehat{S}(t_1,0)\widehat{S}^{-1}(t_2,0) = \widehat{S}(t_1,t_2)\,, \quad (3.142)$$

and

$$\widehat{S}(t_2,0)\widehat{S}(0,-\infty) = \widehat{S}(t_2,-\infty)\,, \quad (3.143)$$

we rewrite Eq. (3.140) as

$$\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \langle 0|\widehat{S}^{-1}(+\infty,-\infty)\widehat{S}(+\infty,t_1)\widehat{\Psi}_I(\mathbf{r}_1,t_1)\widehat{S}(t_1,t_2)\widehat{\Psi}_I^\dagger(\mathbf{r}_2,t_2)\widehat{S}(t_2,-\infty)|0\rangle\,. \quad (3.144)$$

We define

$$\widehat{S}(+\infty,-\infty) \stackrel{\text{def}}{=} \widehat{\mathcal{S}}. \quad (3.145)$$

With adiabatic switching on and off of the interaction, the ground state develops into the ground state:

$$\widehat{S}(+\infty,-\infty)|0\rangle = \exp(\mathrm{i}\alpha)|0\rangle = \langle 0|\widehat{\mathcal{S}}|0\rangle\cdot|0\rangle\,, \quad (3.146)$$

and

$$\langle 0|S^{-1}(+\infty,-\infty) = \exp(-\mathrm{i}\alpha)\langle 0| = \langle 0|\widehat{\mathcal{S}}|0\rangle^{-1}\cdot\langle 0|\,, \quad (3.147)$$

where $e^{i\alpha}$ is a phase factor (i.e., α is real). We thus get

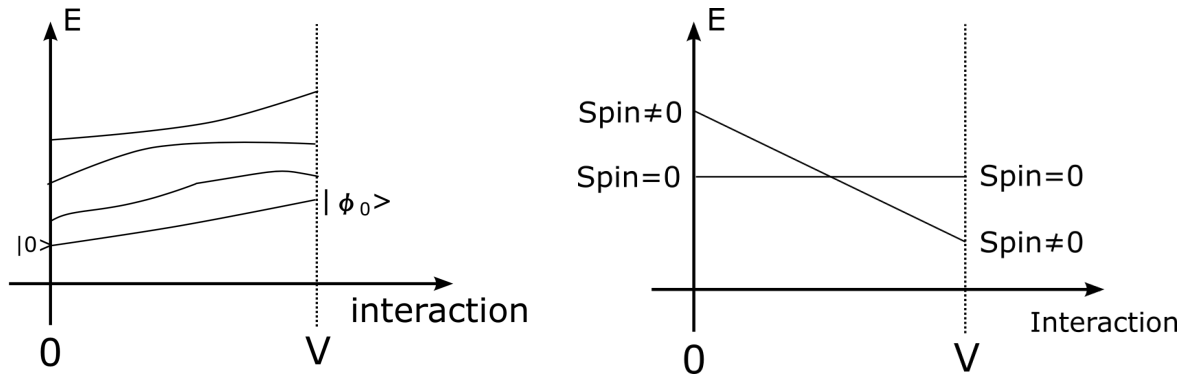
$$\begin{aligned}\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) &= \frac{\langle 0|\widehat{S}(+\infty,t_1)\widehat{\Psi}_I(\mathbf{r}_1,t_1)\widehat{S}(t_1,t_2)\widehat{\Psi}_I^\dagger(\mathbf{r}_2,t_2)\widehat{S}(t_2,-\infty)|0\rangle}{\langle 0|\widehat{\mathcal{S}}|0\rangle}\\ &= \frac{\langle 0|\mathcal{T}[\widehat{\mathcal{S}}\widehat{\Psi}_I(\mathbf{r}_1,t_1)\widehat{\Psi}_I^\dagger(\mathbf{r}_2,t_2)]|0\rangle}{\langle 0|\widehat{\mathcal{S}}|0\rangle}\\ &= \langle 0|\widehat{\mathcal{S}}|0\rangle^{-1}\langle 0|\mathcal{T}\Big[\exp\left(-\mathrm{i}\int\limits_{-\infty}^{+\infty}\mathrm{d}t_1'\widehat{U}_I(t_1')\right)\widehat{\Psi}_I(\mathbf{r}_1,t_1)\widehat{\Psi}_I^\dagger(\mathbf{r}_2,t_2)\Big]|0\rangle\,. \quad (3.148)\end{aligned}$$

Performing the expansion of $\mathcal{T}\exp$, one obtains the perturbative series for the Green's function:

$$\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \langle 0|\widehat{\mathcal{S}}|0\rangle^{-1}\sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int\limits_{-\infty}^{+\infty}\mathrm{d}t_1'\ldots\mathrm{d}t_n'\,\langle 0|\mathcal{T}[\widehat{U}_I(t_1')\ldots\widehat{U}_I(t_n')\widehat{\Psi}_I(\mathbf{r}_1,t_1)\widehat{\Psi}_I^\dagger(\mathbf{r}_2,t)]|0\rangle\,. \quad (3.149)$$

It will be a starting point for developing the Feynman diagrammatic expansion below.

Comment: We have assumed above that the interacting ground state is adiabatically connected to the no-interacting one. This assumption is not entirely trivial. Specifically, it holds in the **absence** of spontaneous symmetry breaking (left figure):



In the case of **spontaneous symmetry breaking** (such as e.g. ferromagnetism, superconductivity, etc) the assumption does not hold (energy levels cross; see the right figure for the case of ferromagnetism). We will consider a situation with spontaneous symmetry breaking later (Chapter 5 and Sec. 6.3 on superconductivity).

3.8 Diagrammatic techniques

From now on, we change the notation: $\widehat{\Psi}_I(\mathbf{r},t) \mapsto \hat{\psi}_0(\mathbf{r},t)$. The subscript "0" here is introduced since the time evolution of operators in the interaction picture is governed by the free Hamilton operator, $\widehat{H}_0$ (i.e., it is like in the Heisenberg picture but with $\widehat{H} \to \widehat{H}_0$).

We will develop the technique for calculating matrix elements entering the expansion (3.149),

$$\langle 0|\mathcal{T}[\widehat{U}_0(t_1')\dots\widehat{U}_0(t_n')\hat{\psi}_0(\mathbf{r}_1,t_1)\hat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]|0\rangle\,, \tag{3.150}$$

where $\widehat{U}_0(t)$ is the interaction operator in the interaction representation, Specifically, we will consider the case of fermions with two-particle potential interaction,

$$\widehat{U}_0(t) = \frac{1}{2}\int \mathrm{d}r\,\mathrm{d}r'\,\hat{\psi}_0^\dagger(\mathbf{r},t)\psi_0^\dagger(\mathbf{r}',t)U(\mathbf{r}-\mathbf{r}')\hat{\psi}_0(\mathbf{r}',t)\hat{\psi}_0(\mathbf{r},t)\,. \tag{3.151}$$

For other problems (e.g., electrons interacting with phonons), the diagram technique is developed in an analogous way.

3.8.1 Wick theorem

The **Wick theorem** plays a key role in evaluation of averages of the type of Eq. (3.150). We present first its formulation:

$$\langle 0|\mathcal{T}[\dots]|0\rangle = \sum \text{products of pairwise averages (contractions)} \cdot (\pm 1)^P\,, \tag{3.152}$$

where $(-1)^P$ is again the permutation factor for fermions with P counting the permutations required to bring the operators in the averages together.

As an example of application of Wick theorem, consider

$$\begin{aligned}
\langle 0|\mathcal{T}\hat{\psi}_0(1)\hat{\psi}_0^\dagger(2)\hat{\psi}_0(3)\hat{\psi}_0^\dagger(4)|0\rangle &= \langle\, 0 \mid \mathcal{T}[\hat{\psi}_0\overbrace{(1)\hat{\psi}_0^\dagger}(2)\hat{\psi}_0\overbrace{(3)\hat{\psi}_0^\dagger}(4)] \mid 0\rangle \\
&= (-1)^0\langle\, 0 \mid \mathcal{T}[\hat{\psi}_0(1)\hat{\psi}_0^\dagger(2)] \mid 0\rangle\langle\, 0 \mid \mathcal{T}[\hat{\psi}_0(3)\hat{\psi}_0^\dagger(4)] \mid 0\rangle \\
&+ (-1)^2\langle\, 0 \mid \mathcal{T}[\hat{\psi}_0(1)\hat{\psi}_0^\dagger(4)] \mid 0\rangle\langle\, 0 \mid \mathcal{T}[\hat{\psi}_0^\dagger(2)\hat{\psi}_0(3)] \mid 0\rangle \\
&= \langle 0|\mathcal{T}\hat{\psi}_0(1)\hat{\psi}_0^\dagger(2)|0\rangle\langle 0|\mathcal{T}\hat{\psi}_0(3)\hat{\psi}_0^\dagger(4)|0\rangle + \langle 0|\mathcal{T}\hat{\psi}_0(1)\hat{\psi}_0^\dagger(4)|0\rangle \underbrace{\langle 0|\mathcal{T}\hat{\psi}_0^\dagger(2)\hat{\psi}_0(3)|0\rangle}_{=-\langle 0|\mathcal{T}\hat{\psi}_0(3)\hat{\psi}_0^\dagger(2)|0\rangle} \\
&\overset{(3.51)}{=} \mathrm{i}G^{(0)}(1,2)\mathrm{i}G^{(0)}(3,4) - \mathrm{i}G^{(0)}(1,4)\mathrm{i}G^{(0)}(3,2)\,.
\end{aligned} \tag{3.153}$$

Here we use short-hand notations: $\hat{\psi}_0(1) \equiv \hat{\psi}_0(\mathbf{r}_1,t_1)$ etc. In the present case there are two possible contraction patterns (1-2, 3-4 and 1-4, 2-3), which are shown in the first line of Eq. (3.153), so that the sum (3.152) contains two terms.

We sketch now the **proof** of the Wick theorem. We introduce for momenta $|\mathbf{p}| < p_F$ the hole creation and annihilation operators $b_\mathbf{p}^\dagger$, $b_\mathbf{p}$ defined as

$$a_\mathbf{p} = b_\mathbf{p}^\dagger, \quad a_\mathbf{p}^\dagger = b_\mathbf{p}. \tag{3.154}$$

The operators $b_p/b_p^\dagger$ annihilate/create holes in the Fermi sea. We will use $a_{\mathbf{p}}/a_{\mathbf{p}}^\dagger$ for $|\mathbf{p}| > p_F$ and $b_{\mathbf{p}}/b_{\mathbf{p}}^\dagger$ for $|\mathbf{p}| < p_F$.

The field operator can be presented as

$$\hat{\psi}_0(\mathbf{r},t) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} a_{\mathbf{p}} \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}}t) = \left(\sum_{|\mathbf{p}|<p_F} + \sum_{|\mathbf{p}|>p_F}\right) a_{\mathbf{p}} \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}}t)$$
$$= \sum_{|\mathbf{p}|<p_F} b_{\mathbf{p}}^\dagger \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}}t) + \sum_{|\mathbf{p}|>p_F} a_{\mathbf{p}} \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}}t) \equiv \hat{\psi}_0^{(h)\dagger}(\mathbf{r},t) + \hat{\psi}_0^{(p)}(\mathbf{r},t)\,, \tag{3.155}$$

and analogously

$$\hat{\psi}_0^\dagger(\mathbf{r},t) = \hat{\psi}_0^{(h)}(\mathbf{r},t) + \hat{\psi}_0^{(p)\dagger}(\mathbf{r},t)\,. \tag{3.156}$$

The upper indices denote: (h) = hole and (p) = particle. We have:

$$a_{\mathbf{p}}|0\rangle = 0 \;\; (|\mathbf{p}| > p_F), \quad b_{\mathbf{p}}|0\rangle = 0 \;\; (|\mathbf{p}| < p_F) \quad \Rightarrow \quad \psi_0^{(p)}|0\rangle = 0\,, \quad \psi_0^{(h)}|0\rangle = 0, \tag{3.157}$$

and the conjugate equations

$$\langle 0|a_{\mathbf{p}}^\dagger = 0 \;\; (|\mathbf{p}| > p_F), \quad \langle 0|b_{\mathbf{p}}^\dagger = 0 \;\; (|\mathbf{p}| < p_F) \quad \Rightarrow \quad \langle 0|\psi_0^{(p)\dagger} = 0\,, \quad \langle 0|\psi_0^{(h)\dagger} = 0. \tag{3.158}$$

Normal product

We introducte the normal product (normal ordering) of operators:

$$\mathcal{N}(\mathcal{O}_1\mathcal{O}_2\ldots) \stackrel{\text{def}}{=} \{\text{all creation operators are placed to the left of all annihilation ones}\}\cdot(\pm 1)^P\,, \tag{3.159}$$

where P is the required permutation. (The factor $(-1)^P$ is there in the case of fermions; for bosons it is replaced by unity.)

For example, we have (for fermions)

$$\mathcal{N}(a_{\mathbf{p}_1} b_{\mathbf{p}_2}^\dagger a_{\mathbf{p}_3}^\dagger b_{\mathbf{p}_4} a_{\mathbf{p}_5} a_{\mathbf{p}_6}^\dagger) = -b_{\mathbf{p}_2}^\dagger a_{\mathbf{p}_3}^\dagger a_{\mathbf{p}_6}^\dagger a_{\mathbf{p}_1} b_{\mathbf{p}_4} a_{\mathbf{p}_5}\,. \tag{3.160}$$

The normal ordering is very useful since we can employ the fact that

$$\langle 0|\mathcal{N}(\mathcal{O}_1\mathcal{O}_2\ldots)|0\rangle = \pm\langle\, 0 \mid a_{\mathbf{p}'}^\dagger b_{\mathbf{k}'}^\dagger \ldots a_{\mathbf{p}} b_{\mathbf{k}} \mid 0\rangle = 0\,, \tag{3.161}$$

in view of Eqs. (3.157) and (3.158).

Contraction

The **contraction** is defined as:

$$\mathcal{O}_1\underline{\mathcal{O}_2} = \mathcal{T}(\mathcal{O}_1\mathcal{O}_2) - \mathcal{N}(\mathcal{O}_1\mathcal{O}_2), \tag{3.162}$$

where $\mathcal{O}_j$ are ψ_0 or $\psi_0^\dagger$, or their linear combination.
Properties:

- Linearity (follows from the corresponding property of $\mathcal{T}$ and $\mathcal{N}$ products):

$$(\mathcal{O}_1 + \underline{\mathcal{O}_2})\mathcal{O}_3 = \mathcal{O}_1\underline{\mathcal{O}_3} + \mathcal{O}_2\underline{\mathcal{O}_3}. \tag{3.163}$$

- (Anti-)commutativity (again follows from the corresponding property of $\mathcal{T}$ and $\mathcal{N}$ products):

$$\mathcal{O}_1\underline{\mathcal{O}_2} = \pm\mathcal{O}_2\underline{\mathcal{O}_1} \qquad \text{for bosons/fermions} \tag{3.164}$$

- Crucially, the contraction is always a c-number (not an operator). This is because the operators ψ_0, $\psi_0^\dagger$ commute (for bosons) or, respectively, anticommute (for fermions) on a c-number. To evaluate the contraction, it is thus sufficient to consider its vacuum average. This yields

$$\hat{\psi}_0(\underline{\mathbf{r}_1, t_1})\hat{\psi}_0^\dagger(\underline{\mathbf{r}_2}, t_2) = \mathrm{i}G^{(0)}(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2). \tag{3.165}$$

  (The vacuum average of the $\mathcal{T}$ product yields Green's function (times i), and the vacuum average of the $\mathcal{N}$ product is zero.) Further,

$$\hat{\psi}_0^\dagger(\underline{\mathbf{r}_1, t_1})\hat{\psi}_0^\dagger(\underline{\mathbf{r}_2}, t_2) = \hat{\psi}_0(\underline{\mathbf{r}_1, t_1})\hat{\psi}_0(\underline{\mathbf{r}_2}, t_2) = 0\,, \tag{3.166}$$

  since all creation operators (anti-)commute with each other, and all annihilation operators (anti-)commute with each other.

Wick's theorem for products of operators ($\mathcal{O}_j$ can be creation or annihilation operator, or a linear combination thereof):

$$\begin{aligned}
\mathcal{T}[\mathcal{O}_1\mathcal{O}_2\ldots\mathcal{O}_n] &= \sum \text{normal products with all possible combinations of contractions} \\
&= \mathcal{N}[\mathcal{O}_1\mathcal{O}_2\ldots\mathcal{O}_n] + \mathcal{N}[\underline{\mathcal{O}_1\mathcal{O}_2}\mathcal{O}_3\ldots\mathcal{O}_n] + \mathcal{N}[\underline{\mathcal{O}_1\mathcal{O}_2\mathcal{O}_3}\ldots\mathcal{O}_n] + \ldots \\
&+ \mathcal{N}[\underline{\mathcal{O}_1\mathcal{O}_2}\underline{\mathcal{O}_3\mathcal{O}_4}\ldots\mathcal{O}_n] + \ldots
\end{aligned} \tag{3.167}$$

In other words, a time-ordered product of creation and annihilation operators can be rewritten as the normal-ordered product of these operators plus a sum of the normal-ordered products with a single contraction among operators performed in all possible ways, plus a sum of the normal-ordered products with all possible double contractions, etc., plus all full contractions.

This formulation of the Wick theorem concerns operators (and not just their vacuum averages) and thus is more general then the one given in the beginning of this subsection.

The proof proceeds in the following way. Let us first assume that the times are ordered: $t_1 > t_2 > \ldots > t_n$. We have to bring the product $\mathcal{O}_1\mathcal{O}_2\ldots\mathcal{O}_n$ to the normal form. For this purpose, we will consecutively interchange (bring to normal order) pairs of operators. For each such exchange, we will use

$$\mathcal{T}(\mathcal{O}_1\mathcal{O}_2) = \mathcal{N}(\mathcal{O}_1\mathcal{O}_2) + \mathcal{O}_1\underline{\mathcal{O}_2}. \tag{3.168}$$

This will produce exactly the structure in the r.h.s. of Eq. (3.167). (For those pairs of operators that already stands in the normal order, the contraction is equal to zero.)

Having obtained the proof for $t_1 > t_2 > \ldots > t_n$, we can perform an arbitrary permutation of operators in the l.h.s. and in all terms in the r.h.s. This is possible since $\mathcal{T}$ product, $\mathcal{N}$, and the contraction are invariant with respect to the order of operators, up to the factor $(\pm 1)^P$. This completes the proof for an arbitrary order of times.

Using the operator version of the Wick theorem, Eq. (3.167), it is easy to prove the **Wick theorem for the vacuum expectation values**, Eq. (3.152). Indeed, let us take the vacuum expectation value of both sides of Eq. (3.167). In view of (3.161), only the terms in which all operators are contracted survive in the r.h.s. of Eq. (3.167) when the expectation value $\langle 0|\ldots|0\rangle$ is computed. Thus, we get:

$$\langle\, 0 \mid \mathcal{T}[O_1\ldots O_n] \mid 0\rangle = \underline{O_1O_2}\,\underline{O_3O_4}\ldots\underline{O_{n-1}O_n} + \text{all other terms with } \frac{n}{2} \text{ contractions},$$

(3.169)

which is the statement of the theorem.

3.9 Feynman diagrams

Now we generate an expansion of the Green's function [Eq. (3.149)]

$$\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=\langle 0|\widehat{\mathcal{S}}|0\rangle^{-1}\sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int\limits_{-\infty}^{+\infty}\mathrm{d}t_1'\ldots\mathrm{d}t_n'\,\langle 0|\mathcal{T}[\widehat{U}_0(t_1')\ldots\widehat{U}_0(t_n')\hat{\psi}_0(\mathbf{r}_1,t_1)\hat{\psi}_0^\dagger(\mathbf{r}_2,t)]|0\rangle\,. \tag{3.170}$$

in powers of interaction. The interaction operator $\widehat{U}_0(t)$ in the interaction representation reads:

$$\begin{aligned}\widehat{U}_0(t) &= e^{\mathrm{i}\widehat{H}_0t}\widehat{U}e^{-\mathrm{i}\widehat{H}_0t}=e^{\mathrm{i}\widehat{H}_0t}\frac{1}{2}\int dr\,dr'\,\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r})e^{-\mathrm{i}\widehat{H}_0t}\\ &= \frac{1}{2}\int dr\,dr'\,\psi_0^\dagger(\mathbf{r},t)\psi_0^\dagger(\mathbf{r}',t)U(\mathbf{r}-\mathbf{r}')\psi_0(\mathbf{r}',t)\psi_0(\mathbf{r},t)\end{aligned} \tag{3.171}$$

- 0th order:

$$\mathrm{i}G^{(0)}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=\langle 0|\mathcal{T}\hat{\psi}_0(\mathbf{r}_1,t_1)\hat{\psi}_0^\dagger(\mathbf{r}_2,t_2)|0\rangle\,. \tag{3.172}$$

- 1st order:

$$\mathrm{i}G^{(1)}(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2) = \langle 0|\widehat{\mathcal{S}}|0\rangle^{-1}\cdot(-\mathrm{i})\int dt\langle\,0\mid\mathcal{T}[\widehat{U}_0(t)\hat{\psi}_0(\mathbf{r}_1,t_1)\hat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]\mid 0\rangle\,. \tag{3.173}$$

Analyze the matrix element entering this contribution:

$$\begin{aligned}&\langle\,0\mid\mathcal{T}[\widehat{U}_0(t)\hat{\psi}_0(\mathbf{r}_1,t_1)\hat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]\mid 0\rangle\\ &\overset{(3.171)}{=} -\int drdr'\,U(\mathbf{r}-\mathbf{r}')\langle 0|\mathcal{T}[\hat{\psi}_0^\dagger(\mathbf{r},t+0)\hat{\psi}_0^\dagger(\mathbf{r}',t+0)\hat{\psi}_0(\mathbf{r},t)\hat{\psi}_0(\mathbf{r}',t)\hat{\psi}_0(\mathbf{r}_1,t_1)\hat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]|0\rangle\\ &\overset{(3.152)}{=} \int drdr'\,U(\mathbf{r}-\mathbf{r}')\Big[\langle\,0\mid\mathcal{T}[\hat{\psi}_0^\dagger(\mathbf{r}',t+0)\hat{\psi}_0(\mathbf{r}',t)]\mid 0\rangle\\ &\quad\times\quad\langle\,0\mid\mathcal{T}[\hat{\psi}_0^\dagger(\mathbf{r},t+0)\hat{\psi}_0(\mathbf{r}_1,t_1)]\mid 0\rangle\langle\,0\mid\mathcal{T}[\hat{\psi}_0(\mathbf{r},t)\hat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]\mid 0\rangle+5\text{ more terms}\Big]\,.\\ &= \frac{1}{2}\int\mathrm{d}r\mathrm{d}r'\,U(\mathbf{r}-\mathbf{r}')\left\{-[\mathrm{i}G^{(0)}(\mathbf{r}',\mathbf{r}',-0)][\mathrm{i}G^{(0)}(\mathbf{r}_1,\mathbf{r},t_1-t)][\mathrm{i}G^{(0)}(\mathbf{r},\mathbf{r}_2,t-t_2)]\right.\\ &\quad\left.+5\text{ more terms}\right\}\end{aligned} \tag{3.174}$$

Comments: There are four $\hat{\psi}$ / $\hat{\psi}^\dagger$ operators which come from the interaction, and two which are external, i.e., six operators in total. To tell the $\mathcal{T}$-product that it should order the field operators taken at the same time t (those originating from the interaction) in a proper way, one adds an additional $+0$ in $\hat{\psi}^\dagger$, because these stands to the left. After application of the Wick theorem, one gets $3!=6$ terms originating from different patterns of contractions. The sign in front of each term is determined by the parity of the corresponding permutation.

The first-order term in the Green's function thus has the form

$$G^{(1)}(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2)=\frac{1}{\langle 0|\widehat{\mathcal{S}}|0\rangle}$$

$$\times \frac{1}{2}\int \mathrm{d}r\mathrm{d}r'dt\, U(\mathbf{r}-\mathbf{r}')\left\{[\mathrm{i}G^{(0)}(\mathbf{r}',\mathbf{r}',-0)][\mathrm{i}G^{(0)}(\mathbf{r}_1,\mathbf{r},t_1-t)][\mathrm{i}G^{(0)}(\mathbf{r},\mathbf{r}_2,t-t_2)]\right.$$
$$\left. + 5 \text{ more terms}\right\} . \tag{3.175}$$

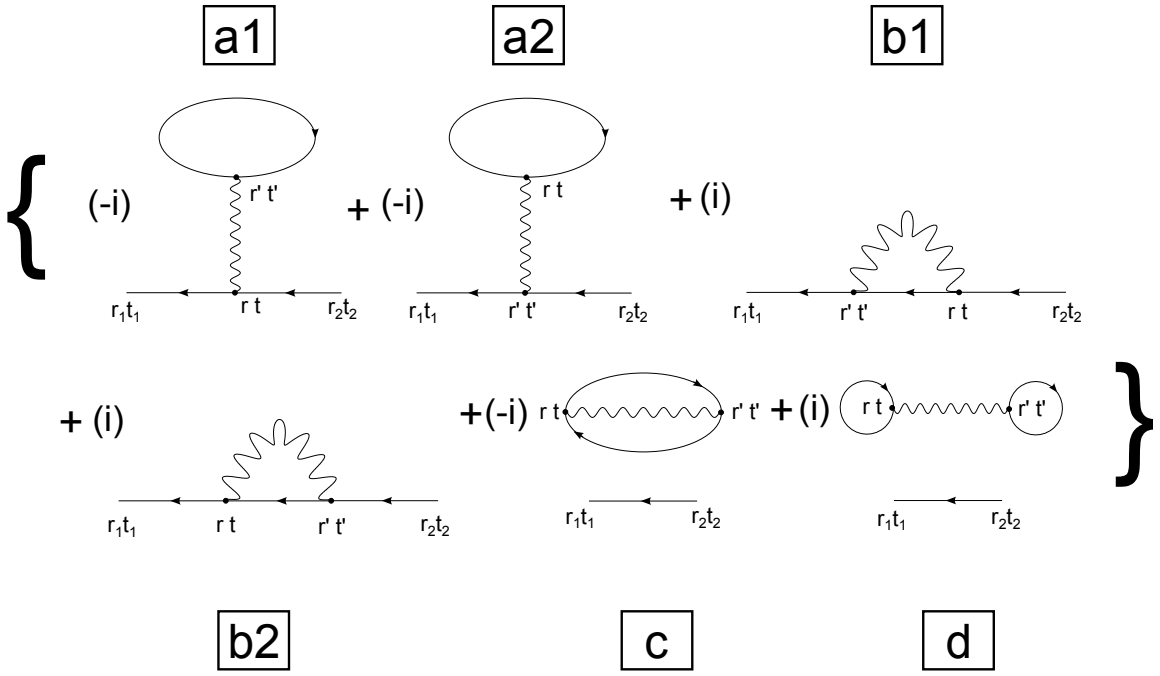
Let us now draw diagrams for expression (3.175). The basic elements of the diagrams are:

$G^{(0)}(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2)$ = 

$U(\mathbf{r}-\mathbf{r}')\delta(t-t')$ = 

With this graphical representation of the free Green's functions and interaction potential, the 1st-order correction takes the following form:

$$G^{(1)}(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2) \overset{(3.175)}{=} \frac{1}{\langle 0|\widehat{\mathcal{S}}|0\rangle}\frac{1}{2}\int drdr'dtdt' \times$$



We see that the factor in front of each diagram inside the curly brackets is equal to $i(-1)^L$, where L is the number of closed loops. As we will see below, this is a particular case of a general rule for the prefactor.

It is easy to see that $a_1 = a_2$ and $b_1 = b_2$, since we can exchange $\mathbf{r} \leftrightarrow \mathbf{r}'$ under the integral. As a result, we get for the Green's function up to the first order:

$$G = \frac{1}{\langle 0|\widehat{\mathcal{S}}|0\rangle}\left\{ \quad + \quad \text{(-i)} \quad + \text{(i)} \quad + \text{(-i/2)} \quad + \text{(i/2)} \quad + O(U^2) \right\}$$

(3.176)

Now we consider the denominator:

$$\langle 0|\widehat{\mathcal{S}}|0\rangle = \langle\, 0 \mid \mathcal{T}[e^{-i\int_{-\infty}^{\infty} dt\, \widehat{U}_0(t)}] \mid 0\rangle = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int dt\, dt' \,\ldots \langle\, 0 \mid \mathcal{T}[U_0(t)U_0(t')\ldots] \mid 0\rangle$$

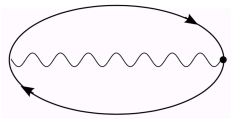
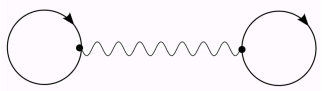
$$= \sum_{n=0}^{\infty} \frac{(-i)^n}{2^n n!} \int dt\, dt' \,\ldots \int dr\, dr'\, dr''\, dr'''\,\ldots U(\mathbf{r}-\mathbf{r}')\ldots$$

$$\times \langle\, 0 \mid \mathcal{T}[\hat{\psi}_0^\dagger(\mathbf{r}, t+0)\hat{\psi}_0^\dagger(\mathbf{r}', t+0)\hat{\psi}_0(\mathbf{r}', t)\hat{\psi}_0(\mathbf{r}, t)\ldots] \mid 0\rangle$$

Keeping the terms of zeroth and first order in interaction ($n = 0$ and 1), we get

$$\begin{aligned}
&\langle 0|\widehat{\mathcal{S}}|0\rangle \\
&= 1 - \frac{i}{2}\int dt\, dr\, dr'\, U(\mathbf{r}-\mathbf{r}')\langle\, 0 \mid \mathcal{T}[\hat{\psi}_0^\dagger(\mathbf{r}, \overbrace{t+0)\hat{\psi}_0^\dagger(\mathbf{r}', \overbrace{t+0)\hat{\psi}_0(\mathbf{r}', t)\hat{\psi}_0(\mathbf{r}}, t)}] \mid 0\rangle + \ldots \\
&= 1 - \frac{i}{2}\int dt\, dr\, dr'\, U(\mathbf{r}-\mathbf{r}') \Big\{ -\langle\, 0 \mid \mathcal{T}\left[\hat{\psi}_0^\dagger(\mathbf{r}, t+0)\hat{\psi}_0(\mathbf{r}', t)\right] \mid 0\rangle\langle\, 0 \mid \mathcal{T}\left[\hat{\psi}_0^\dagger(\mathbf{r}', t+0)\hat{\psi}_0(\mathbf{r}, t)\right] \mid 0\rangle \\
&\qquad + \langle\, 0 \mid \mathcal{T}\left[\hat{\psi}_0^\dagger(\mathbf{r}, t+0)\hat{\psi}_0(\mathbf{r}, t)\right] \mid 0\rangle\langle\, 0 \mid \mathcal{T}\left[\hat{\psi}_0^\dagger(\mathbf{r}', t+0)\hat{\psi}_0(\mathbf{r}', t)\right] \mid 0\rangle \Big\} + \ldots \\
&= 1 + \frac{i}{2}\int dt\;\, dt'\, dr\, dr'\, U(\mathbf{r}-\mathbf{r}')\delta(t-t') \left[-G^{(0)}(\mathbf{r}', \mathbf{r}, t'-t)G^{(0)}(\mathbf{r}, \mathbf{r}', t-t') \right. \\
&\qquad\qquad \left. + G^{(0)}(\mathbf{r}, \mathbf{r}, -0)G^{(0)}(\mathbf{r}', \mathbf{r}', -0)\right] + \ldots
\end{aligned} \tag{3.177}$$

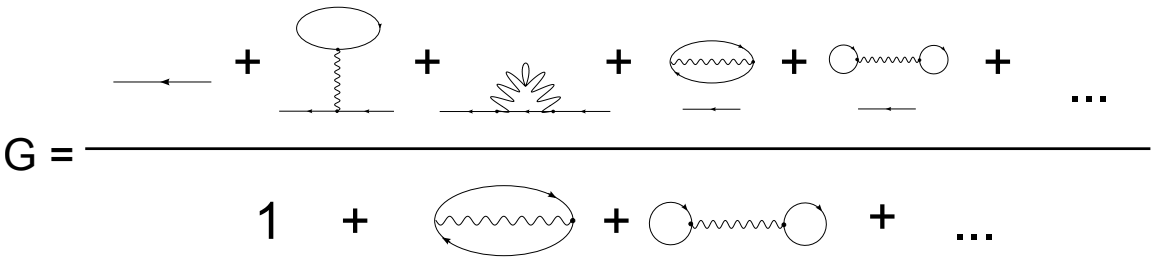
Diagrammatically, this reads:

$\langle 0|\hat{S}|0\rangle = 1 - \frac{i}{2}$  $+ \frac{i}{2}$  $+ O(U^2)\,.$ (3.178)

The diagrams for $\langle 0|\widehat{\mathcal{S}}|0\rangle$ have no external legs. They are called **"vacuum diagrams"**.

Inserting Eq. (3.178) into Eq. (3.176), we see that the vacuum diagrams (arising from the expansion of the denominator $\langle 0|\widehat{\mathcal{S}}|0\rangle$) exactly **eliminate the disconnected diagrams** for G, i.e., the last two diagrams in Eq. (3.176).

The structure of the expansion in Eq. (3.176) is schematically as follows (coefficients are not shown):



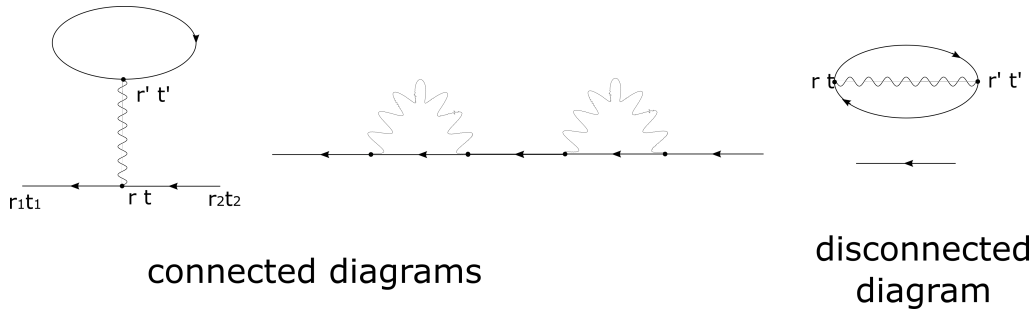
It can be shown that the role of denominator (vacuum diagrams) in this formula is in cancelation of disconnected diagrams in all orders of the perturbation theory.

3.9.1 Rules of diagrammatic technique for Green's function

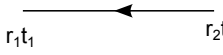
Let us consider the n-th order term in the expansion of the Green's function. The perturbative expansion outlined above leads to the following diagrammatic rules:

(1). Draw all topologically different **connected** diagrams with two external legs and $2n$ interaction vertices (n pairs of vertices; each pair is connected by an interaction line). At each vertex, there is one incoming fermionic line, one outgoing fermionic line, and one interaction line.

As illustration, here are examples of connected diagrams (one of order $n = 1$ and one of order $n = 2$) and an example of a disconnected diagram (that does not appear in the expansion, since all such diagrams are cancelled as explained above).



(2). Each straight line corresponds to the fermionic Green's function $G^{(0)}$:



$$= G^{(0)}(r_1, r_2, t_1 - t_2).$$

(3). Wavy lines are interaction lines:

$$= U(r - r')\delta(t - t').$$

(4). Integrate over t and $\mathbf{r}$ corresponding to all internal vertices.
For a spinful system, also perform summations over spin projections σ for all internal vertices. This will lead to an additional factor $2S + 1$ for each closed loop, i.e., to the overall additional factor $(2S + 1)^L$ equal to 2^L for spin 1/2. Here L is the number of closed fermionic loops.

(5). The overall factor of the diagram is $\mathrm{i}^n(-1)^L$, where L is the number of closed fermionic loops and n is the number of interaction lines (n-th order diagram). The factor $(-1)^L$ comes from the swapping of fermionic operators during the contractions.

We explain how the remaining factors combine into simply i^n. From Eqs. (3.149) and (3.151) we see that there is a factor $(-\mathrm{i})^n/n!$ from the expansion of the time-ordered exponential and additionally $1/2^n$ from the n-th power of the interaction operator:

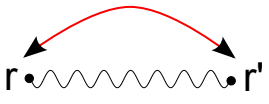
$$\begin{aligned} iG^{(n)} &= \frac{(-i)^n}{n!} \int \ldots \langle\, 0 \mid \mathcal{T}\left[U_0(1) \ldots U_0(n) \ldots\right] \mid 0 \rangle \\ &= \frac{(-i)^n}{2^n n!} \int \ldots U_0(r_1 - r_1') \ldots U_0(r_n - r_n') \langle\, 0 \mid \mathcal{T}\left[\ldots\right] \mid 0 \rangle. \end{aligned} \tag{3.179}$$

Further, a factor i^{2n+1} results from writing the contractions in terms of Green's functions, see Eq. (3.165). In addition, there is a factor $-\mathrm{i}$ originating from i in the l.h.s. of Eq. (3.179). Combining these factors, we get

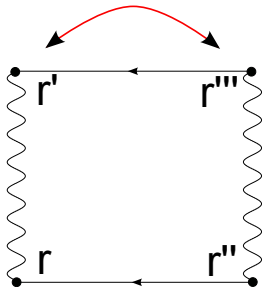
$$\frac{-i(-i)^n i^{2n+1}}{2^n \cdot n!} = \frac{i^n}{2^n \cdot n!}. \tag{3.180}$$

Now we should take into account that there will be topologically equivalent diagrams that are, however, different since they originate from different contraction patterns and thus have different positions of the integration variables $r, r', \ldots, r^{(2n)}$. Examples are pairs of topologically equivalent diagrams a1, a2 and b1, b2 in the above calculation of first-order diagrams which differed by swapping $r \leftrightarrow r'$. This produced a factor of 2 when only topologically distinct diagrams (a, b) were counted. Let us now calculate the analogous factor (i.e. the number of different but topologically identical diagrams) in n-th order. We have the integration over $r, r', \ldots, r^{(2n)}$.

By swapping two internal variables (e.g., $r \leftrightarrow r'$) belonging to the same interaction operator, i.e., connected by the interaction line $U(r - r')$, we get a factor of 2 for each pair, as we saw in the first-order calculation. Since we have n such pairs, this results in a factor 2^n.



In addition, there are permutations of interaction operators, which correspond to the permutation of interaction lines as shown on the right. Because of n lines of interaction this gives us in addition a factor $n!$.



Thus, the total number of topologically equivalent diagrams for the n-th order of expansion for the Green's function is $2^n n!$. (One can prove that all of them indeed originate from distinct contractions.) This factor $2^n n!$ exactly cancels the denominator of Eq. (3.180). The resulting factor is thus $\mathrm{i}^n(-1)^L$ as stated above.

(6). In some diagrams (e.g., in both diagrams of the first order), one has contractions of operators originating from the same interaction operator and thus belonging to the same time t: both ends of the fermionic line are attached to the same interaction line. This gives the Green function at zero time $t - t = 0$. It should be defined more carefully, however, since the Green function is discontinuous at zero time. The correct way of understanding such contractions is

$$G^{(0)}(\mathbf{r}, t; \mathbf{r}', t) = G^{(0)}(\mathbf{r}, \mathbf{r}'; 0) \;\mapsto\; G^{(0)}(\mathbf{r}, \mathbf{r}', -0). \tag{3.181}$$

This rule (shift -0) follows from the fact in the interaction operator (3.171) the operators $\psi_0^\dagger(t)$ stand to the left of $\psi_0(t)$:

$$\langle\, 0 \mid \hat{\psi}_0^\dagger(\mathbf{r}', t)\hat{\psi}_0(\mathbf{r}, t) \mid 0\rangle = -\langle\, 0 \mid \mathcal{T}[\hat{\psi}_0(\mathbf{r}, t)\hat{\psi}_0^\dagger(\mathbf{r}', t + 0) \mid 0\rangle = -iG^{(0)}(\mathbf{r}, \mathbf{r}', -0)\,. \tag{3.182}$$

For $\mathbf{r} = \mathbf{r}'$ (bubbles formed by a single fermionic lines), this gives the free density:

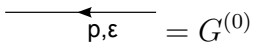
$$G^{(0)}(\mathbf{r}, \mathbf{r}, -0) = -i\langle\, 0 \mid \mathcal{T}[\hat{\psi}_0(\mathbf{r}, t)\hat{\psi}_0^\dagger(\mathbf{r}, t + 0) \mid 0\rangle = i\langle\, 0 \mid \hat{\psi}_0^\dagger(\mathbf{r}, t)\hat{\psi}_0(\mathbf{r}, t) \mid 0\rangle = in^{(0)}. \tag{3.183}$$

3.9.2 Diagrammatic rules in momentum space

Because of translation invariance in space and time, it is convenient to perform the Fourier transformation and to calculate diagrams in the energy-momentum space. The corresponding diagrammatic rules are obtained straightforwardly from the above coordinate-space rules and are formulated below.

(1). The diagrams are the same. Each line (fermionic or interaction) carries an energy ε and a momentum $\mathbf{p}$. There is momentum-energy conservation at each vertex (where two fermionic lines and one interaction line meet).

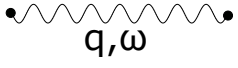
(2). Each fermionic line $(\mathbf{p}, \varepsilon)$ corresponds to a free Green's function $G^{(0)}(\mathbf{p}, \varepsilon)$:



$$= G^{(0)}(\mathbf{p}, \varepsilon),$$

$$G^{(0)}(\mathbf{p}, \varepsilon) = \frac{1}{\varepsilon - \varepsilon_{\mathbf{p}} + \mathrm{i}0\,\mathrm{sign}(\varepsilon)}\,, \quad \varepsilon_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m} - \mu\,. \tag{3.184}$$

(3). Each interaction line $(\mathbf{q}, \omega)$ yields a factor $U(\mathbf{q})$ (Fourier transform of the interaction), independent of frequency ω:



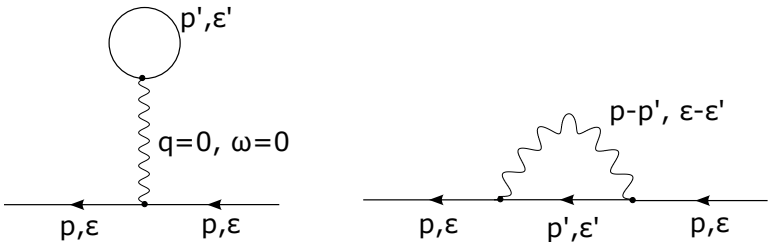
$$= U(\mathbf{q}).$$

(4). Integration over all n independent internal momenta and energies:

$$\int \prod_i \frac{\mathrm{d}^d p_i}{(2\pi)^d} \frac{\mathrm{d}\omega_i}{2\pi}\,. \tag{3.185}$$

(5). The overall factor for the diagram is $\mathrm{i}^n(-1)^L$. For a spinful system, summation over spin projections leads to an extra factor $(2S+1)^L$.

(6). Some diagrams contain elements as shown below, with both ends of a fermionic line [here $(\mathbf{p}', \varepsilon')$] attached to the same interaction line.



The interaction over the energy of this line (here ε') can then be performed directly, since nothing else depends on this energy. (We recall that the interaction line does not depend on the energy that it carries.) The result is:

$$\int \frac{\mathrm{d}\varepsilon'}{2\pi}\, G^{(0)}(\mathbf{p}', \varepsilon') \exp[-\mathrm{i}\varepsilon'(-0)] = \frac{1}{2\pi} 2\pi \mathrm{i}\Theta(p_F - p') = \mathrm{i}n_{p'}\,, \tag{3.186}$$

where -0 comes from the fact that this line corresponds to $G(\mathbf{r}, \mathbf{r}', t = -0)$ in the time-coordinate representation.

To demonstrate Eq. (3.186), we calculate the integral by closing the integration contour:

$$\int \frac{d\varepsilon'}{2\pi} G^{(0)}(\mathbf{p}', \varepsilon') \underbrace{e^{i\varepsilon' 0}}_{\text{close the contour in upper half-plane}} = \int \frac{d\varepsilon'}{2\pi} \frac{e^{i0\varepsilon'}}{\varepsilon' - \varepsilon_{p'} + i0\mathrm{sign}(\varepsilon_{p'})}$$

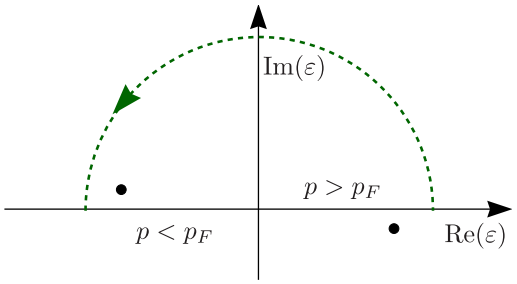
$$= \frac{1}{2\pi} 2\pi i \Theta(p_F - p') = i\Theta(p_F - p') = i n_{p'} \qquad \text{Fermi function.}$$

Here

$$\varepsilon_p = \frac{p^2}{2m} - \mu = \begin{cases} > 0, & p > p_F, \\ < 0, & p < p_F, \end{cases}$$

so that we have the pole at

$$\varepsilon' = \begin{cases} \varepsilon_p - i0, & p > p_F, \\ \varepsilon_p + i0, & p < p_F. \end{cases}$$



For the case of a bubble formed by a single fermionic line, we can directly integrate (3.186) over the corresponding momentum $\mathbf{p}'$ as well (since nothing else depends on this momentum). The integral is

$$\int \frac{\mathrm{d}^3 p'}{(2\pi)^3} \mathrm{i} n_{p'} = \mathrm{i} n \,, \tag{3.187}$$

where n is the electron density (per spin projection).

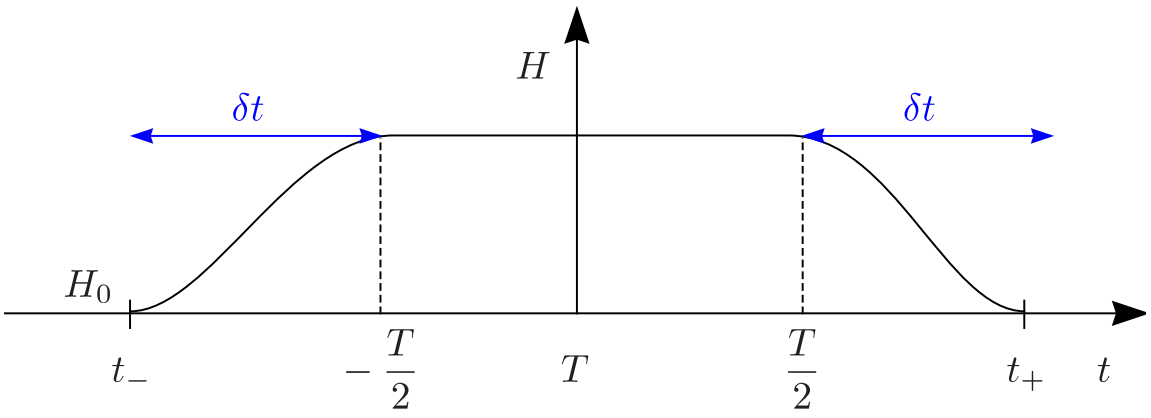
3.10 Vacuum diagrams and ground-state energy

In the calculation of the Green's function, vacuum diagrams, emerging from the perturbative expansion of $\langle 0|\widehat{\mathcal{S}}|0\rangle$, were exactly canceled. However, they are important on they own. Specifically, they carry information about the energy of the ground state, as we are going to show.

We have seen that

$$\langle 0|\widehat{\mathcal{S}}|0\rangle \equiv \langle \phi_{0,I}(-\infty)|\widehat{S}(+\infty,-\infty)|\phi_{0,I}(-\infty)\rangle = \exp(\mathrm{i}\alpha) \,, \tag{3.188}$$

where α is some phase. What is the physical meaning of α?
Let us consider the following protocol of adiabatic switching on and off of the interaction, as shown in the figure:



Here T is the time during which the interaction is on, δt is duration of the switching on and switching off processes, and $T \gg \delta t \gg$ any other time scale. The first inequality here is because we consider $T \to \infty$ limit, and the second inequality here implies adiabaticity. We rewrite $\langle 0|\widehat{\mathcal{S}}|0\rangle$ as

$$\begin{aligned} \langle\, 0 \mid \widehat{\mathcal{S}} \mid 0 \,\rangle &= \langle\, \psi_{0,I}(-\infty) \mid \hat{S}(\infty,-\infty) \mid \psi_{0,I}(-\infty) \rangle \\ &= \langle\, \psi_{0,I}(t_-) \mid \hat{S}^\dagger(-\infty,t_-)\hat{S}(\infty,t_+)\hat{S}(t_+,t_-)\hat{S}(t_-,-\infty) \mid \psi_{0,I}(-\infty) \rangle \end{aligned}$$

$$= \langle \psi_{0,I}(t_-) \mid \hat{S}^\dagger(-\infty, t_-)\hat{S}(\infty, t_+)\hat{S}(t_+, t_-) \mid \psi_{0,I}(t_-)\rangle.$$

For $t \geq t_+$ and $t \leq t_-$ there is no interaction: $\widehat{U} = 0$, and thus $\widehat{U}_I = 0$ It follows that

$$\begin{aligned} \hat{S}(\infty, t_+) &= \mathcal{T} \exp\left[\int_{t_+}^{\infty} dt' \, \widehat{U}_I(t')\right] = \mathcal{T}\exp[0] = \widehat{\mathbb{1}}, \\ \hat{S}^\dagger(-\infty, t_-) &= \hat{S}(t_-, -\infty) = \widehat{\mathbb{1}}. \end{aligned}$$

As a result, we express $\langle 0|\widehat{\mathcal{S}}|0\rangle$ through the states $\phi_{0,I}(t_\pm)$:

$$\langle 0|\widehat{\mathcal{S}}|0\rangle = \langle \phi_{0,I}(t_-)|\widehat{S}(t_+, t_-)|\phi_{0,I}(t_-)\rangle \equiv \langle \phi_{0,I}(t_-)|\phi_{0,I}(t_+)\rangle \,. \tag{3.189}$$

For $t < t_-$ or $t > t_+$ the interaction-representation state $|\phi_{0,I}(t)\rangle$ is related to the Schrödinger state $|\phi_0(t)\rangle$ via

$$|\phi_{0,I}(t)\rangle = \exp(\mathrm{i}\widehat{H}_0 t)|\phi_0(t)\rangle = \exp(\mathrm{i}E_0 t)|\phi_0(t)\rangle \,, \tag{3.190}$$

where E_0 is the ground-state energy of the non-interacting system. Thus, we have

$$\langle 0|\widehat{\mathcal{S}}|0\rangle = \exp[\mathrm{i}E_0(t_+ - t_-)]\langle \phi_0(t_-)|\phi_0(t_+)\rangle \,. \tag{3.191}$$

For the time interval $t_- + \delta t < t < t_+ - \delta t$, where the interaction is fully operative, the Schrödinger state $|\phi_0(t)\rangle$ is related to the Heisenberg state $|\phi_0\rangle$ by

$$|\phi_0(t)\rangle = \exp(-\mathrm{i}Et)|\phi_0\rangle \,, \tag{3.192}$$

where E is the ground state energy of the interacting system. Since $T \gg \delta t$, we use this relation in the whole range $t_- < t < t_+$, discard the difference between T and $T + \delta t$, and obtain the following result:

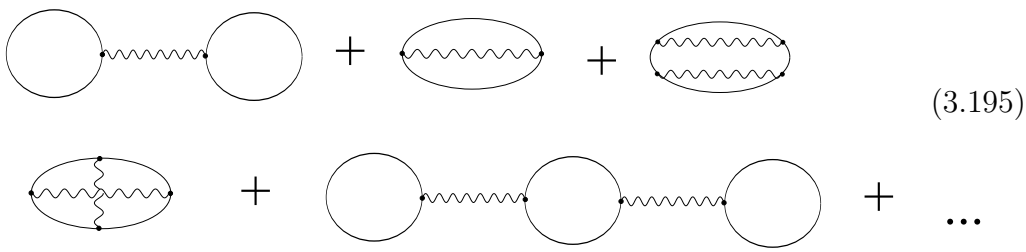
$$\langle 0|\widehat{\mathcal{S}}|0\rangle = \exp[\mathrm{i}E_0(t_+ - t_-)]\exp[-\mathrm{i}E(t_+ - t_-)] = \exp[-\mathrm{i}(E - E_0)T] \,. \tag{3.193}$$

Thus, we have established a relation between the interaction-induced change in the ground state energy $E - E_0$ and the sum of vacuum diagrams $\langle 0|\widehat{\mathcal{S}}|0\rangle$:

$$E - E_0 = \frac{\mathrm{i}}{T}\ln(\langle 0|\widehat{\mathcal{S}}|0\rangle \,. \tag{3.194}$$

3.10.1 Vacuum diagrams: Symmetry factors

We have

$\langle 0|\widehat{\mathcal{S}}|0\rangle = 1 +$  (3.195)

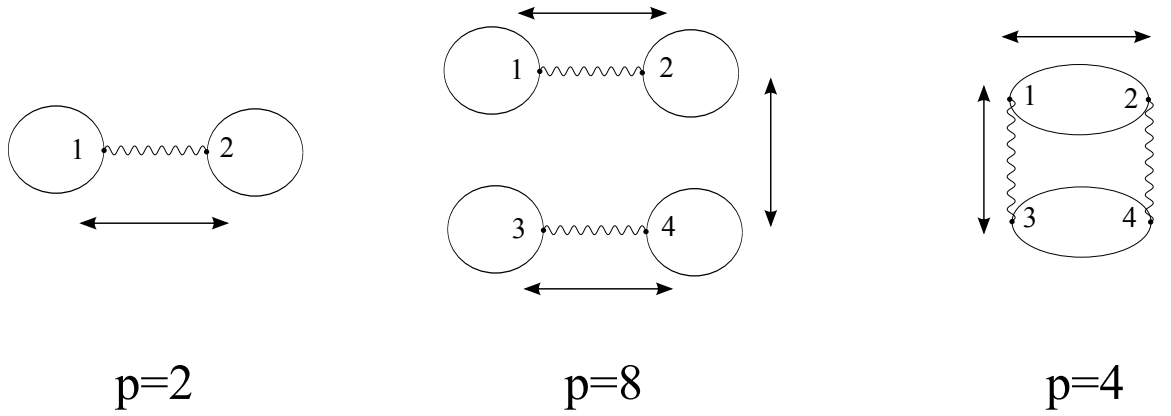
Note that the series here includes all vacuum diagrams (i.e., diagrams without external legs), including disconnected ones. The rules of the diagrammatic technique for vacuum diagrams are largely analogous to those for Green function diagrams. There is, however, one essential difference: the symmetry factors. In diagrams for the Green's function, the factor $1/(2^n n!)$ was exactly canceled by the number of distinct but topologically equivalent diagrams, which

come from interchanging the vertices (2^n) and interchanging the lines ($n!$), see item (5) in the list of rules in Sec. 3.9.1. For vacuum diagrams the situation is different.
To explain this, let us analyze the first diagram in Eq. (3.195), which is the Hartree diagram. We have already calculated this contribution in Eq. (3.177):

$$\langle 0|\widehat{\mathcal{S}}|0\rangle = 1 - \frac{i}{2}\int dt\, dr\, dr'\, U(\mathbf{r}-\mathbf{r}')\langle\, 0 \mid \mathcal{T}[\hat{\psi}_0^\dagger(\mathbf{r},\underline{t+0})\hat{\psi}_0^\dagger(\mathbf{r}',\underline{t+0})\hat{\psi}_0(\mathbf{r}',t)\hat{\psi}_0(\underline{\mathbf{r}},t)] \mid 0\rangle + \dots \tag{3.196}$$

The factor 1/2 here is exactly the factor $1/(2^n n!)$ for $n = 1$. However, now we have a single possibility of contractions that yield such diagram, so that this factor is not compensated. This is related to the fact that interchanging the vertices 1 and 2 leads to the same contractions and therefore identically the same diagram. This diagram has the symmetry factor 2, which leads to an additional factor 1/2 in front of this diagram in the expansion of $\langle 0|\widehat{\mathcal{S}}|0\rangle$, as we have already obtained in Eq. (3.178).

Examples of symmetry factors p of vacuum diagrams are shown in the figure:



For each diagram, symmetry transformation that map the diagram onto itself (i.e. preserve exactly the set of contractions, e.g., [1-2, 2-1, 3-4, 4-3] for the rightmost diagram) are indicated.

Thus, each vacuum diagram gets an additional factor $1/p$, where p represents the symmetry of the diagram, as illustrated in figure above. This factor arises in addition to the factor $\mathrm{i}^n(-1)^L$ [and the factor $(2S+1)^L$ for spinful systems], see rule (5) of the diagrammatics for Green functions.

Except for the additional factor $1/p$, the diagrammatic rules are the same as for Green function diagrams.

3.10.2 Linked cluster expansion

We have found above the relation between interaction-induced change in the ground-state energy and $\langle 0|\widehat{\mathcal{S}}|0\rangle$ given by the sum of all vacuum diagrams (here T denotes the time during which the interaction is effective):

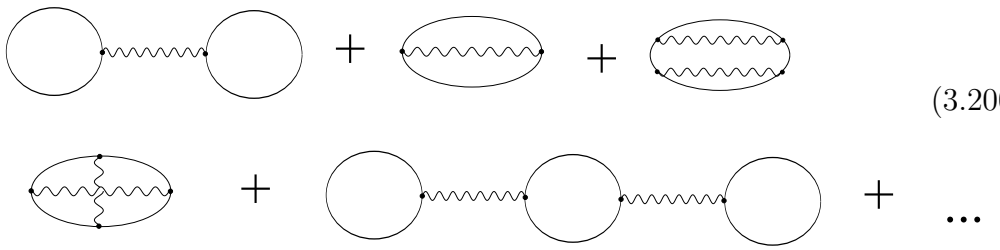
$$E - E_0 = \frac{\mathrm{i}}{T}\ln\langle 0|\widehat{\mathcal{S}}|0\rangle\Big|_{T\mapsto\infty}, \tag{3.197}$$

$$\langle 0|\widehat{\mathcal{S}}|0\rangle = \sum \text{all vacuum diagrams.} \tag{3.198}$$

The statement of the linked cluster expansion is:

$$\ln\langle 0|\widehat{\mathcal{S}}|0\rangle = \sum \text{all } \underline{\text{connected}} \text{ vacuum diagrams,} \tag{3.199}$$

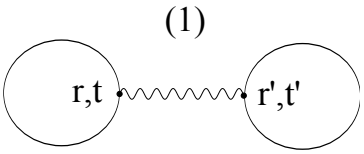
i.e,

$\ln\langle 0|\widehat{\mathcal{S}}|0\rangle =$  (3.200)

where now only <u>connected</u> vacuum diagrams are included (i.e., those that do not decouple in two or more totally disconnected pieces).

To prove this, consider an example of a connected vacuum diagram: the first (Hartree) diagram in the r.h.s. of Eq. (3.200).
Writing it explicitly in $\mathbf{r}, t$–representation, we get

$$\begin{aligned}(1) &= \frac{i}{2}\int \mathrm{d}r\,\mathrm{d}r'\,\mathrm{d}t\,\mathrm{d}t'\,G^{(0)}(\mathbf{r},\mathbf{r},-0)G^{(0)}(\mathbf{r}',\mathbf{r}',-0)\delta(t-t')U(\mathbf{r}-\mathbf{r}') \\ &\propto T\,, \end{aligned} \tag{3.201}$$

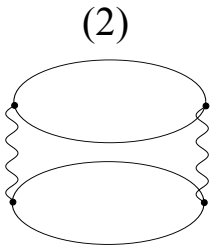


because of

$$\int \mathrm{d}t\,\mathrm{d}t'\,\delta(t-t') = T\,. \tag{3.202}$$

It is quite obvious that all connected vacuum diagrams have this behaviour; here is one more example:

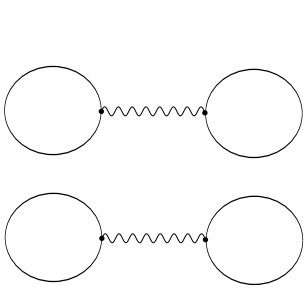
$$\begin{aligned}(2) &= \frac{-1}{4}\int dr\,dr'\,dr''\,dr'''dt\,dt'\,dt''\,dt'''\,G^{(0)}(\mathbf{r}-\mathbf{r}',t-t') \\ &\times\ G^{(0)}(\mathbf{r}'-\mathbf{r},t'-t)G^{(0)}(\mathbf{r}''-\mathbf{r}''',t''-t''')G^{(0)}(\mathbf{r}'''-\mathbf{r}'',t'''-t'') \\ &\times\ U(\mathbf{r}-\mathbf{r}'')U(\mathbf{r}'-\mathbf{r}''')\delta(t-t'')\delta(t'-t''') \\ &= \frac{-1}{4}\int dr\,dr'\,dr''\,dr'''dt\,dt'\,G^{(0)}(\mathbf{r}-\mathbf{r}',t-t')G^{(0)}(\mathbf{r}'-\mathbf{r},t'-t) \\ &\times\ G^{(0)}(\mathbf{r}''-\mathbf{r}''',t-t')G^{(0)}(\mathbf{r}'''-\mathbf{r}'',t'-t)U(\mathbf{r}-\mathbf{r}'')U(\mathbf{r}'-\mathbf{r}''') \\ &= \frac{-1}{4}\int dr\,dr'\,dr''\,dr'''dt_2\,dt_1\,G^{(0)}(\mathbf{r}-\mathbf{r}',t_2)G^{(0)}(\mathbf{r}'-\mathbf{r},-t_2) \\ &\times\ G^{(0)}(\mathbf{r}''-\mathbf{r}''',t_2)G^{(0)}(\mathbf{r}'''-\mathbf{r}'',-t_2)U(\mathbf{r}-\mathbf{r}'')U(\mathbf{r}'-\mathbf{r}''') \\ &\propto \int dt_1 = T\end{aligned}$$



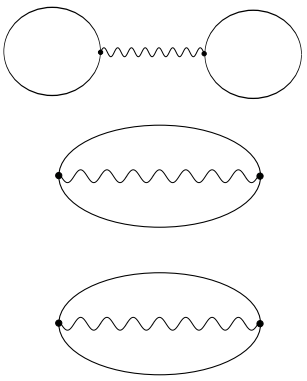
The factor T comes from the integration over the simultaneous shift of all times at vertices.

For disconnected vacuum diagrams, one finds in the same way that if the diagram consists of m disconnected parts, it scales as T^m, as illustrated in the figure:

$$\begin{aligned}\text{two disconnected parts} &\sim T^2 \\ \text{three disconnected parts} &\sim T^3 \\ \ldots &\sim \ldots\end{aligned}$$



T^2



T^3

Hence, the sum of all connected vacuum diagrams is equal to the linear-in-T term in the expansion of $\langle 0|\widehat{\mathcal{S}}|0\rangle$ in powers of T. Expanding the r.h.s. of Eq. (3.193) in powers of T yields

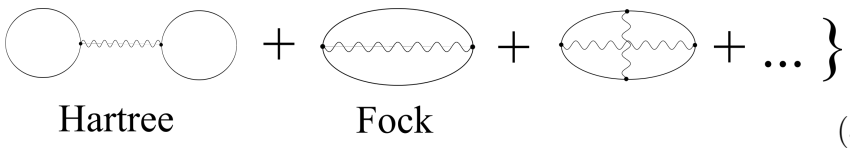
$$\langle 0|\widehat{\mathcal{S}}|0\rangle \overset{(3.193)}{=} e^{-i(E-E_0)T} = 1 - i(E-E_0)T - \frac{1}{2}(E-E_0)^2T^2 + \dots \tag{3.203}$$

Therefore, the sum of all connected vacuum diagrams is equal to $\ln\langle 0|\widehat{\mathcal{S}}|0\rangle = -i(E-E_0)T$, which proves the statement of the linked cluster expansion formulated above.

This is valid independently of presence or absence of translational invariance in space.

If the system possesses spatial translation invariance, then any connected diagram will be proportional to the volume V. (Translational invariance in space assumes that we consider a limit $V \to \infty$.) In this case, it is natural to consider the energy density

$$\frac{E-E_0}{V} = \frac{i}{T\cdot V}\cdot$$



(3.204)

Let us analyze the first two diagrams using the diagrammatic rules for fermions with spin 1/2.

Hartree Term

For the Hartree term, we obtain:

$$\frac{E_H}{V} = \mathrm{i}^2\cdot(-1)^2\cdot\frac{1}{2}\int\frac{\mathrm{d}^dp}{(2\pi)^d}\int\frac{\mathrm{d}^dp'}{(2\pi)^d}\,\mathrm{i}n_p\cdot\mathrm{i}n_{p'}\cdot U(q=0)\cdot 2^2\,. \tag{3.205}$$

The factor $(-1)^2$ comes from the two loops and the factor 2^2 from the spin. The factor $1/2$ is the symmetry factor of the diagram and n_p is the fermionic distribution function. With

$$n_p = \begin{cases} 1 & \text{for} \quad p < p_F \\ 0 & \text{for} \quad p > p_F \end{cases}\,, \tag{3.206}$$

one obtains:

$$2\int\frac{\mathrm{d}^dp}{(2\pi)^d}\,n_p = n\,, \tag{3.207}$$

where n is the total density. The end result is then:

$$\frac{E_H}{V} = \frac{1}{2}n^2U(q=0)\,. \tag{3.208}$$

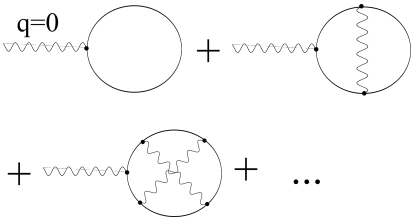
For Coulomb interaction

$$U(\mathbf{r}-\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\,, \tag{3.209}$$

the Fourier transform in three dimensions is given by

$$U(\mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2}\,. \tag{3.210}$$

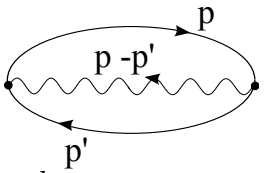
At $q = 0$ the potential has a singularity: $U(0) = \infty$, which yields an infinite Hartree term. However, for such a long-range (Coulomb) interaction one will have charge neutrality: the density of fermions (say, electrons with negative charge) will be exactly compensated by the positively-charged background. The interaction with this background will thus cancel the Hartree term. Note that the exact fermion density includes also higher-order diagrams as shown in the figure to the right.



Fock (exchange) Term

Let us now look at the exchange diagram:

$$\frac{E_{\rm ex}}{V} = -\frac{1}{2}\cdot 2\int\frac{\mathrm{d}^d p}{(2\pi)^d}\int\frac{\mathrm{d}^d p'}{(2\pi)^d}\,n_p n_{p'} U(\mathbf{p}-\mathbf{p}')\,, \tag{3.211}$$



where 1/2 is the symmetry factor and 2 comes from the spin.

For Coulomb interaction in three dimensions the result of the integration reads:

$$\frac{E_{\rm ex}}{V} = -\frac{e^2(3\pi^2 n)^{\frac{4}{3}}}{4\pi^3}\,. \tag{3.212}$$

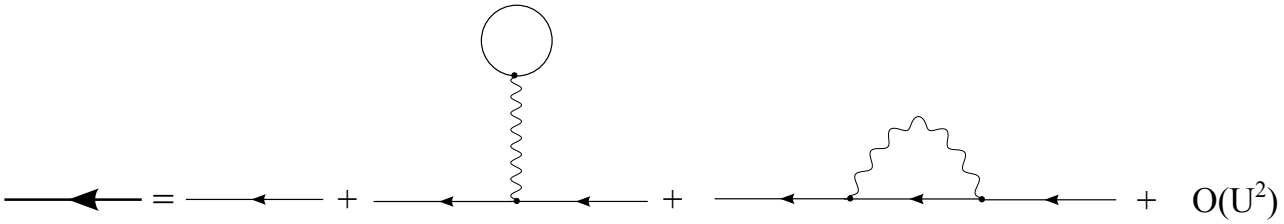
The sum of the two contributions is given by:

$$\boxed{\frac{E_H + E_{\rm ex}}{V} = \int\frac{\mathrm{d}^d p}{(2\pi)^d}\int\frac{\mathrm{d}^d p'}{(2\pi)^d}\,n_p n_{p'}\left[2U(0) - U(\mathbf{p}-\mathbf{p}')\right]\,.} \tag{3.213}$$

3.11 Self-energy. Microscopic basis for Fermi-liquid theory

3.11.1 Definition of self-energy. Green's function near the quasiparticle peak. Quasiparticle life time

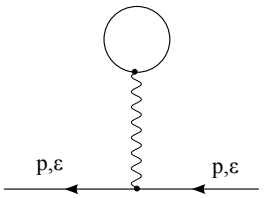
Let us go back to the expansion of the Green's functions for a system of fermions with spin 1/2.



(3.214)

Here the thick line in the l.h.s. corresponds to the full Green's function. The individual terms in the r.h.s. are (we remind that $\varepsilon_p = p^2/2m - \mu$):

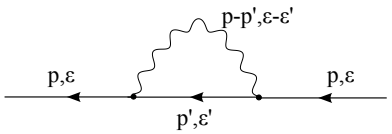
$$= G^{(0)}(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon - \varepsilon_p + i0\,\mathrm{sign}\,\varepsilon}, \tag{3.215}$$



$$= 2iU(0)\frac{1}{(\varepsilon - \varepsilon_p + i0\,\mathrm{sign}\,\varepsilon)^2}\, i\int \frac{d^d p'}{(2\pi)^d} n_{p'}(-1)$$

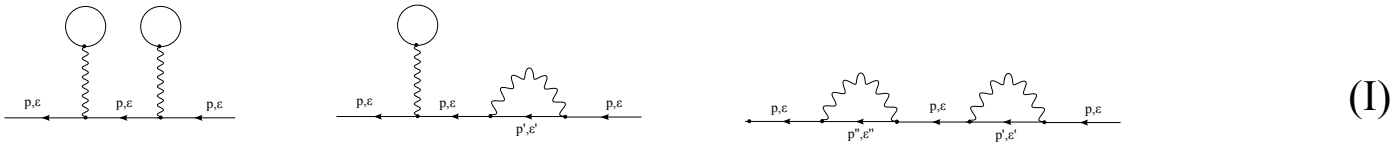
$$= \frac{nU(0)}{(\varepsilon - \varepsilon_p + i0\,\mathrm{sign}\,\varepsilon)^2}, \tag{3.216}$$

(the factor 2 due to spin; n is the total density for both spin projections)

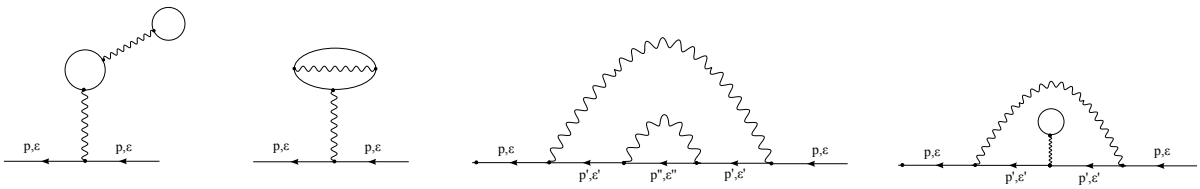


$$= -\frac{1}{(\varepsilon - \varepsilon_p + i0\,\mathrm{sign}\,\varepsilon)^2}\int \frac{d^d p'}{(2\pi)^d} U(\mathbf{p} - \mathbf{p'}) n_{p'}\,. \tag{3.217}$$

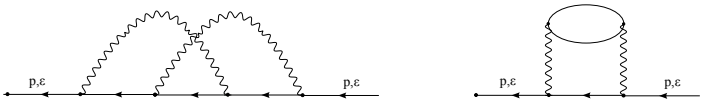
Let us go to the second order. We can classify the whole set of diagrams of the second order as follows:



(I)



(IIa)



(IIb)

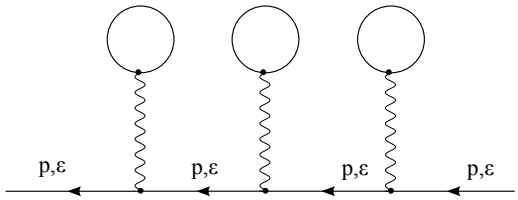
All diagrams in (I) contain the factor

$$\frac{1}{(\varepsilon - \varepsilon_p + \mathrm{i0sign}\varepsilon)^3}\,, \tag{3.218}$$

while all diagrams in (IIa) and (IIb) contain the factor

$$\frac{1}{(\varepsilon - \varepsilon_p + \mathrm{i0sign}\varepsilon)^2}\,. \tag{3.219}$$

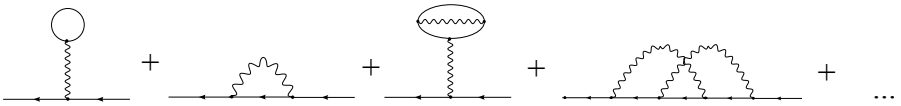
In higher-order contributions we will have terms with higher powers of the bare Green's function at the external energy and momentum, e.g.



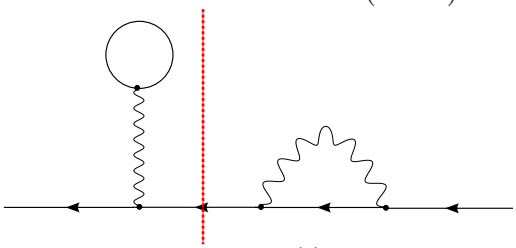
$$\propto \frac{1}{(\varepsilon - \varepsilon_p + i0\,\mathrm{sign}\,\varepsilon)^4}.$$

Therefore, the singularity becomes stronger and stronger with each order of the perturbation theory for the Green function. This implies that one has to sum an infinite series to obtain meaningful results.

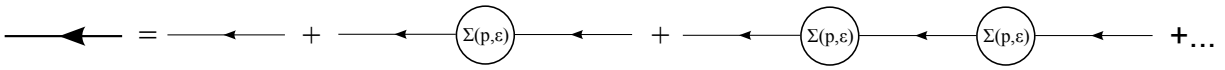
The structure of the diagrammatic series suggests that it is convenient to introduce the **self-energy** $\Sigma(\varepsilon, \mathbf{p})$ defined as a sum of all diagrams which can not be divided into two disconnected parts by cutting a single fermionic line $G^{(0)}(\varepsilon, \mathbf{p})$. (Such diagrams are called "one-particle-irreducible".) In other words, only those diagrams belong to the self-energy $\Sigma(\varepsilon, \mathbf{p})$ which have only two outer $G^{(0)}(\varepsilon, \mathbf{p})$, like (3.216),(3.217) and diagrams (IIa),(IIb) of the second order. These outer two Green's functions are not included in the self-energy Σ:

$G^{(0)}(\varepsilon, \mathbf{p})\Sigma(\varepsilon, \mathbf{p})G^{(0)}(\varepsilon, \mathbf{p}) =$  ... (3.220)

An example of a reducible diagram—which thus does not belong to the self-energy $\Sigma(\varepsilon, \mathbf{p})$—is shown to the right.

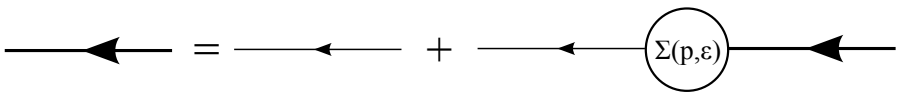


One can get the full Green function $G(\varepsilon, \mathbf{p})$ from the bare Green function $G^{(0)}(\varepsilon, \mathbf{p})$ and the self energy $\Sigma(\varepsilon, \mathbf{p})$ by summing a geometric series:



(3.221)

which can be equivalently written in the form of Dyson equation for G:



(3.222)

Algebraically, this equation reads

$$G = G^{(0)} + G^{(0)}\Sigma G\,. \tag{3.223}$$

Its solution is

$$G^{-1} = [G^{(0)}]^{-1} - \Sigma\,, \tag{3.224}$$

or, explicitly,

$$G(\varepsilon, \mathbf{p}) = \frac{1}{[G^{(0)}(\varepsilon, \mathbf{p})]^{-1} - \Sigma(\varepsilon, \mathbf{p})} = \frac{1}{\varepsilon - \varepsilon_p + \mathrm{i0sign}\varepsilon - \Sigma(\varepsilon, \mathbf{p})}\,. \tag{3.225}$$

Introducing the real and imaginary parts of the self-energy,

$$\Sigma(\varepsilon, \mathbf{p}) = \mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p}) + \mathrm{i}\,\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p})\,, \tag{3.226}$$

we thus obtain for the Green's function:

$$\begin{aligned} G(\varepsilon, \mathbf{p}) &= \frac{1}{\varepsilon - \varepsilon_p - \mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p}) - i\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p})} \\ &= \frac{\varepsilon - \varepsilon_p - \mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p})}{[\varepsilon - \varepsilon_p - \mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p})]^2 + [\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p})]^2} + i\frac{\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p})}{[\varepsilon - \varepsilon_p - \mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p})]^2 + [\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p})]^2}. \end{aligned} \tag{3.227}$$

It follows from the spectral representation

$$G(\varepsilon, \mathbf{p}) = \int d\varepsilon' \frac{\mathcal{A}(\varepsilon', \mathbf{p})}{\varepsilon - \varepsilon' + i0\,\mathrm{sign}\,\varepsilon} = \fint d\varepsilon' \frac{\mathcal{A}(\varepsilon', \mathbf{p})}{\varepsilon - \varepsilon'} - i\pi\mathcal{A}(\varepsilon, \mathbf{p})\,\mathrm{sign}\;\varepsilon$$

that

$$\mathrm{sign}\,\mathrm{Im}\,G(\varepsilon, \mathbf{p}) = -\mathrm{sign}\,\varepsilon\,, \tag{3.228}$$

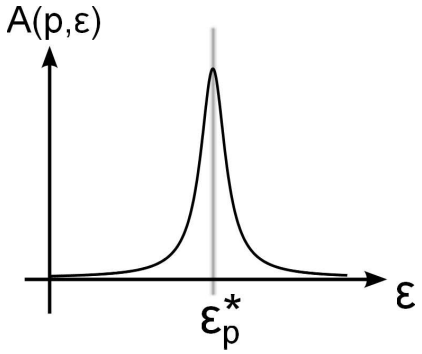
which means

$$\mathrm{sign}\,\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p}) = -\mathrm{sign}\,\varepsilon\,. \tag{3.229}$$

Thus, $\mathrm{Im}\,\Sigma$ produces by itself an imaginary shift of proper sign in the denominator of Green's function [first line of Eq. (3.227)].

The spectral weight is given by

$$\begin{aligned} \mathcal{A}(\varepsilon, \mathbf{p}) &= -\frac{1}{\pi}\mathrm{Im}\,G(\varepsilon, \mathbf{p})\,\mathrm{sign}\,\varepsilon \overset{(3.227)}{=} -\frac{1}{\pi}\,\mathrm{sign}\,\varepsilon \frac{\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p})}{[\varepsilon - \varepsilon_p - \mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p})]^2 + [\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p})]^2} \\ &\overset{(3.229)}{=} \frac{|\mathrm{Im}\,\Sigma(\varepsilon, \mathbf{p})|}{|\varepsilon - \varepsilon_p - \mathrm{Re}\,\Sigma(\mathbf{p}, \varepsilon)|^2 + |\mathrm{Im}\,\Sigma(\mathbf{p}, \varepsilon)|^2}\,. \end{aligned} \tag{3.230}$$



The spectral weight has the form of a peak centered at ε_p^*, where ε_p^* is the solution of the equation

$$\varepsilon - \varepsilon_p - \mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p}) = 0 \tag{3.231}$$

considered as an equation for ε at given p.

Hence,

$$\varepsilon_p^* = \varepsilon_p + \mathrm{Re}\,\Sigma(\varepsilon_p^*, \mathbf{p})\,. \tag{3.232}$$

We make an expansion in the vicinity of $\varepsilon = \varepsilon_p^*$:

$$\varepsilon - \varepsilon_p - \mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p}) \simeq \underbrace{\left[1 - \frac{\partial}{\partial\varepsilon}\mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p})\Big|_{\varepsilon=\varepsilon_p^*}\right]}_{Z_p^{-1}}(\varepsilon - \varepsilon_p^*) = Z_p^{-1}(\varepsilon - \varepsilon_p^*)\,, \tag{3.233}$$

with

$$Z_p = \frac{1}{1 - \frac{\partial}{\partial\varepsilon}\mathrm{Re}\,\Sigma(\varepsilon, \mathbf{p})\big|_{\varepsilon=\varepsilon_p^*}}. \tag{3.234}$$

This yields the following result for the Green's function (3.227) in the vicinity of the pole:

$$G(\varepsilon,\mathbf{p}) \simeq \frac{1}{Z_p^{-1}(\varepsilon-\varepsilon_p^*)-\mathrm{i}\,\mathrm{Im}\,\Sigma(\varepsilon,\mathbf{p})} = \frac{Z_p}{\varepsilon-\varepsilon_p^*+\mathrm{i}\,\Gamma(\varepsilon,\mathbf{p})}\,, \tag{3.235}$$

$$\Gamma(\varepsilon,\mathbf{p}) = -Z_p\,\mathrm{Im}\,\Sigma(\varepsilon,\mathbf{p}), \qquad |\Gamma| = \frac{1}{2\tau}\,. \tag{3.236}$$

Since these formulas are valid only near $\varepsilon \approx \varepsilon_p^*$, one can replace $\mathrm{Im}\,\Sigma(\varepsilon,\mathbf{p}) \mapsto \mathrm{Im}\,\Sigma(\varepsilon_p^*,\mathbf{p})$ and $\Gamma(\varepsilon,\mathbf{p}) \mapsto \Gamma(\varepsilon_p^*,\mathbf{p})$ in Eqs. (3.235), (3.236). According to Eq. (3.235), $|\Gamma(\varepsilon_p^*,\mathbf{p})|$ is the decay rate of the quasiparticles.

3.11.2 Mass and Fermi velocity renormalization

We proceed now with a calculation of the renormalization of Fermi velocity and of effective mass. The Fermi momentum p_F of the interacting system is defined by the condition

$$\varepsilon_{p_F}^* = 0\,, \tag{3.237}$$

where ε_p^* is determined by Eq. (3.232). Now we linearize the dispersion equation (3.231) with respect to ε and $p-p_F$. This yields, with $v_F = p_F/m$,

$$\left[1-\frac{\partial}{\partial\varepsilon}\mathrm{Re}\,\Sigma(\varepsilon,\mathbf{p})\Big|_{\substack{\varepsilon=0\\p=p_F}}\right]\varepsilon - v_F(p-p_F)\left[1+\frac{\partial}{\partial\varepsilon_p}\mathrm{Re}\,\Sigma(\varepsilon,\mathbf{p})\Big|_{\substack{\varepsilon=0\\p=p_F}}\right] = 0\,. \tag{3.238}$$

(Note that, according to the definition of p_F of the interacting system, Eq. (3.237), $\mathrm{Re}\Sigma(0,p_F)$ here is incorporated in p_F, see also Eq.(3.244) below.)

The solution of Eq. (3.238) for ε is by definition ε_p^*, which is thus given by

$$\varepsilon_p^* = v_F^*(p-p_F)\,, \tag{3.239}$$

where v_F^* is the renormalized Fermi velocity:

$$v_F^* = v_F\frac{1+\partial_{\varepsilon_p}\mathrm{Re}\,\Sigma(\varepsilon,\mathbf{p})\big|_{\substack{\varepsilon=0\\p=p_F}}}{1-\partial_{\varepsilon}\mathrm{Re}\,\Sigma(\varepsilon,\mathbf{p})\big|_{\substack{\varepsilon=0\\p=p_F}}}. \tag{3.240}$$

We thus obtain the effective mass:

$$m^* = \frac{p_F}{v_F^*} = m\frac{1-\dfrac{\partial}{\partial\varepsilon}\mathrm{Re}\,\Sigma(\varepsilon,\mathbf{p})\Big|_{\substack{\varepsilon=0\\p=p_F}}}{1+\dfrac{\partial}{\partial\varepsilon_p}\mathrm{Re}\,\Sigma(\varepsilon,\mathbf{p})\Big|_{\substack{\varepsilon=0\\p=p_F}}}\,. \tag{3.241}$$

In combination with Eq. (3.234), this result for the effective mass can also be written as

$$\frac{m}{m^*} = Z\left[1+\frac{\partial}{\partial\varepsilon_p}\mathrm{Re}\,\Sigma(\varepsilon,\mathbf{p})\Big|_{\substack{p=p_F\\\varepsilon=0}}\right], \qquad , \tag{3.242}$$

where $Z = Z_{p=p_F}$ is the residue at the Fermi surface,

$$Z^{-1} = 1-\frac{\partial}{\partial\varepsilon}\mathrm{Re}\,\Sigma(\varepsilon,\mathbf{p})\Big|_{\substack{\varepsilon=0\\p=p_F}}\,. \tag{3.243}$$

Let us emphasize once more that p_F in the above formulas is the Fermi momentum of the interacting system. Setting $p = p_F$ in Eq. (3.232) and using Eq. (3.237), one finds a relation

$$\frac{p_F^2}{2m} = \mu - \mathrm{Re}\,\Sigma(0, p_F)\,. \tag{3.244}$$

This should be compared with the analogous relation for a non-interacting system with the same chemical potential μ:

$$\frac{\left(p_F^{(0)}\right)^2}{2m} = \mu\,. \tag{3.245}$$

Thus, for a fixed value of the chemical potential, interaction leads to a shift of the Fermi momentum. One can show that the relation between the Fermi momentum and the density in the interacting system is the same as in the non-interacting system:

$$n = \frac{1}{3\pi^2}\,p_F^3\,, \qquad n^{(0)} = \frac{1}{3\pi^2}\left(p_F^{(0)}\right)^3\,. \tag{3.246}$$

This statement is known as Luttinger theorem (we omit its proof).

The formalism of Green functions and the diagrammatic perturbation theory thus provide a microscopic justification and a quantitative description of the Fermi-liquid theory that was introduced on phenomenological level in TKM-1. More specifically,

- The quasiparticle pole remains, which is the key property of the Fermi liquid. The theory yields the residue Z_p whose physical meaning is $Z_p = |\langle \mathrm{quasiparticle}_{\mathbf{p}}|c_{\mathbf{p}}^\dagger|\phi_0\rangle|^2 < 1$. The quasiparticle residue $Z = Z_{p_F}$ is no longer equal to unity, at variance with the free-fermion system. Since Z is the quasiparticle contribution to the integral of spectral weight (which is normalized to unity), one has $0 < Z < 1$. We will provide another proof of this below, which will also shed more light on the physical meaning of Z.

- Quasiparticles decay with a rate $|\Gamma|$. We will show below that the decay rate $|\Gamma| \ll \varepsilon$ for small ε, which means that quasiparticles are well defined.

- The quasiparticle dispersion relation is renormalized: $\varepsilon_p \mapsto \varepsilon_p^*$. This implies renormalization of the Fermi velociy, $v_F \to v_F^*$, and of the effective mass, $m \to m^*$.

3.11.3 Momentum distribution of particles in Fermi liquid

Let us analyze the distribution of particles in a Fermi liquid with respect to momenta. We have obtained above the Green's function

$$G(\mathbf{p}, \varepsilon) \simeq \frac{Z}{\varepsilon - v_F^*(p - p_F) + \mathrm{i}0\,\mathrm{sign}(\varepsilon)} + G_{\mathrm{incoh}}(\mathbf{p}, \varepsilon)\,, \tag{3.247}$$

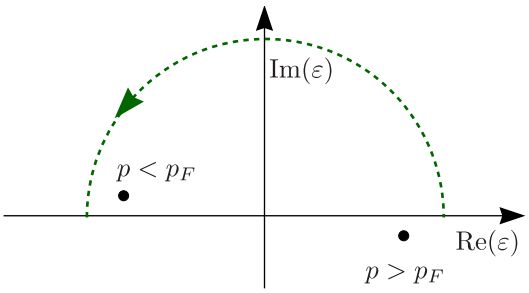
where we have replaced Γ by zero because $\Gamma \to 0$ for $\varepsilon \to 0$ and $\mathbf{p} \to \mathbf{p}_F$. (One can easily check that including Γ does not change the conclusions obtained below on the behavior of the distribution function near p_F.) The density is given by

$$\varrho(\mathbf{r}) = \langle 0|\psi^\dagger(\mathbf{r}, t)\psi(\mathbf{r}, t)|0\rangle = -\mathrm{i}G(\mathbf{r}, \mathbf{r}; t = -0) = -\mathrm{i}\int \frac{\mathrm{d}^d p}{(2\pi)^d}\,G(\mathbf{p}, t = -0)\,. \tag{3.248}$$

To calculate

$$n_p = -\mathrm{i}G(\mathbf{p}, t = -0) = -\mathrm{i}\lim_{t\to -0}\int \frac{\mathrm{d}\varepsilon}{2\pi}\,G(\mathbf{p}, \varepsilon)\exp(-\mathrm{i}\varepsilon t)\,, \tag{3.249}$$

we close the contour of energy integration in the complex plane as shown below. Further, we inspect the location of poles of the quasiparticle contribution to $G(\mathbf{p}, \varepsilon)$ given by the first term in Eq. (3.247):

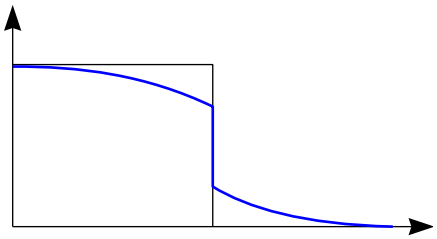


We immediately find that the contribution of this term to the integral will be Z for $p < p_F$ and zero for $p > p_F$:

$$n_p \overset{(3.247)}{=} \begin{cases} Z, & p < p_F \\ 0, & p > p_F \end{cases} + \text{background} \tag{3.250}$$

The contribution of the incoherent background is a smooth function, without any singularity at p_F. Therefore, we have a discontinuity of n_p at Fermi momentum p_F, with the magnitude of jump equal to Z:

$$n_{p_F-0} - n_{p_F+0} = Z\,. \tag{3.251}$$



This provides an additional physical meaning to Z. It is also clear from this relation that $0 < Z < 1$. For a non-interacting system we have $Z = 1$, while in a Fermi liquid $0 < Z < 1$.

3.12 Fermi liquid: Quantitative description

3.12.1 First- and second-order diagrams. Mass renormalization, Z, and quasiparticle decay rate

To the first order in interaction, we have the Hartree and Fock (exchange) self-energy diagrams:

$$\Sigma^{(1)}(\mathbf{p},\varepsilon) = \quad + \tag{3.252}$$

$$= \int \frac{\mathrm{d}^3 p'}{(2\pi)^3}\, n^{(0)}_{p'} [2U(0) - U(\mathbf{p}-\mathbf{p}')]\,, \qquad n^{(0)}_p(\mu) = \Theta\left[p^{(0)}_F(\mu) - p\right]\,.$$

The factor 2 in the Hartree term comes from spin.

Properties of $\Sigma^{(1)}(\mathbf{p},\varepsilon)$:

- It is independent of the energy ε.
- It is real: $\operatorname{Im}\Sigma^{(1)}(\mathbf{p},\varepsilon) = 0$ (since for potential interaction $U(q) \in \mathbb{R}$).

This implies that, to the first order in interaction:

- $\tau^{-1} = 2\Gamma = 0$, where τ is the lifetime and Γ the quasi-particle broadening. Hence, the quasi-particle will not decay in the first-order approximation.
- $Z = 1$ because $\Sigma^{(1)}(\mathbf{p}, \varepsilon)$ does not depend on the energy.
- Since $\Sigma^{(1)}(\mathbf{p}, \varepsilon)$ (specifically, the exchange controbution) depends on momentum $\mathbf{p}$, we obtain $m^* \neq m$, i.e., the mass gets renormalized.

Summarizing the first-order results:

$$\frac{1}{\tau^{(1)}} = 2Z^{(1)}|\text{Im } \Sigma^{(1)}(\mathbf{p}, \varepsilon_p^*)]| = 0, \tag{3.253}$$

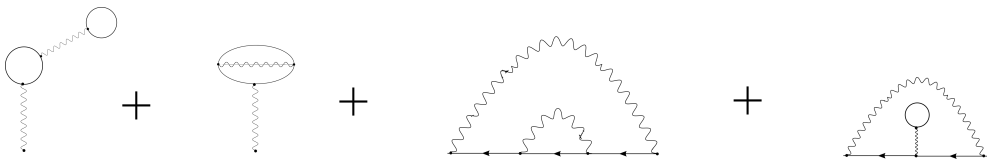
$$Z^{(1)} = \left[1 - \partial_\varepsilon \text{Re } \Sigma^{(1)}(\mathbf{p}, \varepsilon)|_{\substack{\varepsilon=0 \\ p=p_F}}\right]^{-1} = 1, \tag{3.254}$$

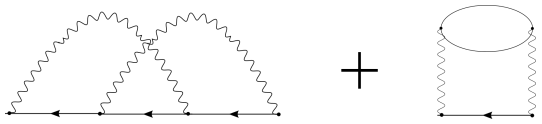
$$m^{*(1)} = \frac{m}{Z^{(1)}} \frac{1}{1 + \dfrac{\partial}{\partial \varepsilon_p} \text{Re}\, \Sigma^{(1)}(\varepsilon, \mathbf{p})\Big|_{\substack{\varepsilon=0 \\ p=p_F}}} \neq m\,. \tag{3.255}$$

To get $\tau \neq \infty$ and $Z < 1$, we thus need to proceed to the next order, i.e.., to calculate $\Sigma(\mathbf{p}, \varepsilon)$ to the 2nd order. The diagrams for $\Sigma^{(2)}$ can be subdivided into two classes:

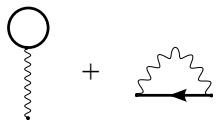
$$\Sigma^{(2)} = \Sigma^{(2a)} + \Sigma^{(2b)}\,, \tag{3.256}$$

where

$\Sigma^{(2a)} =$  (3.257)

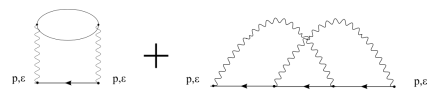
$\Sigma^{(2b)} =$  (3.258)

The diagrams $\Sigma^{(2a)}$ belong to a series of diagrams that can resummed into

 $= \Sigma^{\text{HF}}(\mathbf{p}, \varepsilon)\,.$ (3.259)

Here $\Sigma^{\text{HF}}(\mathbf{p}, \varepsilon)$ is analogous to the first-order Hartree-Fock diagrams (3.252) but with $n_p^{(0)}(\mu)$ replaced by $n_p(\mu)$. Therefore, $\Sigma^{\text{HF}}(\mathbf{p}, \varepsilon)$ has the same properties as $\Sigma^{(1)}(\mathbf{p}, \varepsilon)$: it is real and energy-independent and thus does not provide either decay rate or Z renormalization. This applies, in particular, to $\Sigma^{(2a)}$, which only provides the second-order correction to the effective mass.

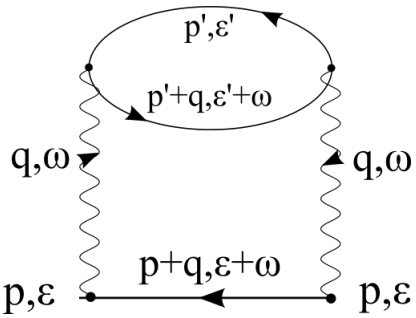
To find the decay rate and Z renormalization, one should thus analyze the diagrams $\Sigma^{(2b)}$:

$\Sigma^{(2b)} =$ 

(3.260)

Let us calculate $\Sigma^{(2b1)}$. (The second diagram,$\Sigma^{(2b2)}$, is calculated in a fully analogous way and has also similar properties.)

$$\begin{aligned}
\Sigma^{(2b1)}(\mathbf{p},\varepsilon) &= (-1)^1 i^2 2^1 \int \frac{\mathrm{d}\omega\,\mathrm{d}^3q\,\mathrm{d}\varepsilon'\,\mathrm{d}^3p'}{(2\pi)^8}\cdot G^{(0)}(\mathbf{p}+\mathbf{q},\varepsilon+\omega) \\
&\times G^{(0)}(\mathbf{p}'+\mathbf{q},\varepsilon'+\omega)G^{(0)}(\mathbf{p}',\varepsilon')\,U^2(q) \\
&= 2\int \frac{\mathrm{d}\omega\,\mathrm{d}^3q\,\mathrm{d}\varepsilon'\,\mathrm{d}^3p'}{(2\pi)^8}U^2(q) \\
&\times \frac{1}{\varepsilon+\omega-\varepsilon_{\mathbf{p}+\mathbf{q}}+i0\ \mathrm{sign}(|\mathbf{p}+\mathbf{q}|-p_F)} \\
&\times \frac{1}{\varepsilon'+\omega-\varepsilon_{\mathbf{p}'+\mathbf{q}}+i0\ \mathrm{sign}(|\mathbf{p}'+\mathbf{q}|-p_F)} \\
&\times \frac{1}{\varepsilon'-\varepsilon_{p'}+i0\ \mathrm{sign}(p'-p_F)} \qquad (3.261)
\end{aligned}$$

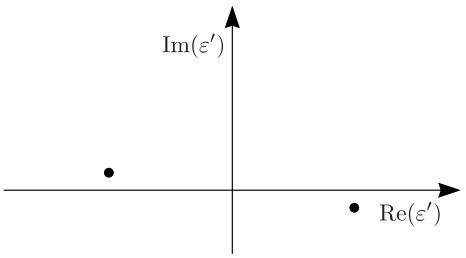


Comment: Strictly speaking, the bare Green function $G^{(0)}$ involves the bare Fermi momentum $p_F^{(0)}$ rather than p_F. However, as was discussed above [see Eq. (3.244)], the real part of the self-energy (included to all orders) will lead to renormalization $p_F^{(0)} \mapsto p_F$, where p_F is related to the exact density via Eq. (3.246). Taking this into account, we write p_F in the formula for the Green's function.

To evaluate Eq. (3.261), we first calculate the integral over ε' :

$$\begin{aligned}
&\int \frac{\mathrm{d}\varepsilon'}{2\pi}\,\frac{1}{\varepsilon'+\omega-\varepsilon_{\mathbf{p}'+\mathbf{q}}+\mathrm{i}0\,\mathrm{sign}(|\mathbf{p}'+\mathbf{q}|-p_F)}\cdot\frac{1}{\varepsilon'-\varepsilon_{p'}+\mathrm{i}0\,\mathrm{sign}(p'-p_F)} = \\
&\quad = \frac{2\pi\mathrm{i}}{2\pi}\,\frac{1}{\varepsilon_{\mathbf{p}'}-\varepsilon_{\mathbf{p}'+\mathbf{q}}+\omega+\mathrm{i}0\,\mathrm{sign}(|\mathbf{p}'+\mathbf{q}|-p_F)}\left[\Theta(|\mathbf{p}'+\mathbf{q}|-p_F)-\Theta(p'-p_F)\right]. \qquad (3.262)
\end{aligned}$$

The integral is non-zero if the poles with respect to the variable ε' are on opposite sides of the real axis:

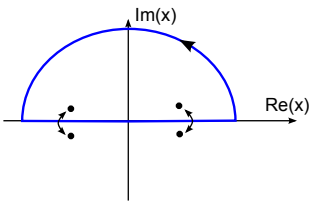


Indeed, the integral is of the form:

$$\int_{-\infty}^{\infty}\frac{dx}{2\pi}\underbrace{\frac{1}{x-z_1}\cdot\frac{1}{x-z_2}}_{x\to\infty\ \sim\ \frac{1}{x^2}},$$

and closing the contour in the complex plane leads to

$$\oint\frac{dx}{2\pi}\frac{1}{x-z_1}\cdot\frac{1}{x-z_2} = \begin{cases} i\cdot\frac{1}{z_1-z_2} & \text{for } \mathrm{Im}\,(z_1)>0, \mathrm{Im}\,(z_2)<0 \\ i\cdot\frac{1}{z_2-z_1} & \text{for } \mathrm{Im}\,(z_1)<0, \mathrm{Im}\,(z_2)>0, \\ 0 & \text{for sign } \mathrm{Im}\,(z_1)=\text{sign } \mathrm{Im}\,(z_2), \end{cases} \qquad (3.263)$$



which yields the r.h.s. of Eq. (3.262).

Now, we come to the integral over ω, which is evaluated in the same way:

$$\int \frac{d\omega}{2\pi} \frac{1}{\varepsilon+\omega-\varepsilon_{\mathbf{p}+\mathbf{q}}+i0\ \mathrm{sign}(|\mathbf{p}+\mathbf{q}|-p_F)} \cdot \frac{1}{\varepsilon_{\mathbf{p}'}-\varepsilon_{\mathbf{p}'+\mathbf{q}}+\omega+\mathrm{i}0\,\mathrm{sign}(|\mathbf{p}'+\mathbf{q}|-p_F)}$$
$$= \mathrm{i}\frac{1}{\varepsilon-\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}'}+\varepsilon_{\mathbf{p}'+\mathbf{q}}+\mathrm{i}0\,\mathrm{sign}(|\mathbf{p}+\mathbf{q}|-p_F)} \left[\Theta(|\mathbf{p}+\mathbf{q}|-p_F)-\Theta(|\mathbf{p}'+\mathbf{q}|-p_F)\right] . \tag{3.264}$$

We thus get

$$\begin{aligned}\Sigma^{(2b1)} &= -2\int \frac{d^3q\,d^3p'}{(2\pi)^6}U^2(q)\frac{1}{\varepsilon-\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}'}+\varepsilon_{\mathbf{p}'+\mathbf{q}}+i0\,\mathrm{sign}(|\mathbf{p}+\mathbf{q}|-p_F)} \\ &\times \left[\Theta(|\mathbf{p}'+\mathbf{q}|-p_F)-\Theta(p'-p_F)\right]\left[\Theta(|\mathbf{p}+\mathbf{q}|-p_F)-\Theta(|\mathbf{p}'+\mathbf{q}|-p_F)\right].\end{aligned} \tag{3.265}$$

There are two possibilities to get a non-zero product

$$\left[\Theta(|\mathbf{p}+\mathbf{q}|-p_F)-\Theta(|\mathbf{p}'+\mathbf{q}|-p_F)\right]\left[\Theta(|\mathbf{p}'+\mathbf{q}|-p_F)-\Theta(p'-p_F)\right] , \tag{3.266}$$

namely

$$|\mathbf{p}'+\mathbf{q}|>p_F\,,\quad p'<p_F\,,\quad |\mathbf{p}+\mathbf{q}|<p_F\,, \tag{3.267}$$

or

$$|\mathbf{p}'+\mathbf{q}|<p_F\,,\quad p'>p_F\,,\quad |\mathbf{p}+\mathbf{q}|>p_F\,. \tag{3.268}$$

It follows that

$$\begin{aligned}&\left[\Theta(|\mathbf{p}'+\mathbf{q}|-p_F)-\Theta(p'-p_F)\right]\left[\Theta(|\mathbf{p}+\mathbf{q}|-p_F)-\Theta(|\mathbf{p}'+\mathbf{q}|-p_F)\right] \\ =\ & -(1-n_{\mathbf{p}'+\mathbf{q}})n_{\mathbf{p}'}n_{\mathbf{p}+\mathbf{q}}-n_{\mathbf{p}'+\mathbf{q}}(1-n_{\mathbf{p}'})(1-n_{\mathbf{p}+\mathbf{q}}),\end{aligned}$$

where $n_p=\Theta(p_F-p)$ is the Fermi distribution function. Thus, we obtain:

$$\begin{aligned}\Sigma^{(2b1)}(\mathbf{p},\varepsilon) = 2\int \frac{\mathrm{d}^3q\,\mathrm{d}^3p'}{(2\pi)^6}\,U^2(q)\frac{1}{\varepsilon-\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}'}+\varepsilon_{\mathbf{p}'+\mathbf{q}}+\mathrm{i}0\,\mathrm{sign}(|\mathbf{p}+\mathbf{q}|-p_F)}\times \\ \times\left[(1-n_{\mathbf{p}'+\mathbf{q}})n_{\mathbf{p}'}n_{\mathbf{p}+\mathbf{q}}+n_{\mathbf{p}'+\mathbf{q}}(1-n_{\mathbf{p}'})(1-n_{\mathbf{p}+\mathbf{q}})\right] .\end{aligned} \tag{3.269}$$

The real part of Eq. (3.269) yields, upon substitution in Eq. (3.243) a correction of order U^2 to Z (equal to unity up to order U^1 as explained above). Note that while this correction is finite in 3D and 2D, it diverges in 1D, leading to a breakdown of the Fermi liquid in 1D, as will be discussed later in this course (see Sec. 7.1 below).

We focus now on the imaginary part of the self-energy, yielding a finite decay rate. The imaginary part originates from the shift $+\mathrm{i}0\,\mathrm{sign}(|\mathbf{p}+\mathbf{q}|-p_F)$ in the denominator in Eq. (3.269). We will use

$$\mathrm{Im}\frac{1}{x+\mathrm{i}0}=-\pi\delta(x)\,,\quad \mathrm{Im}\frac{1}{x-\mathrm{i}0}=\pi\delta(x). \tag{3.270}$$

Note that, depending on $\mathrm{sign}(|\mathbf{p}+\mathbf{q}|-p_F)$, we get opposite signs in front of the δ-function in Eq. (3.270). Further, for $|\mathbf{p}+\mathbf{q}|>p_F$ only the product $(1-n)nn$ in Eq. (3.269) contributes, while the product $n(1-n)(1-n)$ is strictly zero because it involves $1-n_{\mathbf{p}+\mathbf{q}}=0$. On the contrary, for $|\mathbf{p}+\mathbf{q}|>p_F$, only the product $n(1-n)(1-n)$ is effective. Therefore, we obtain:

$$\mathrm{Im}\,\Sigma^{(2b1)}(\mathbf{p},\varepsilon)=2\pi\int\frac{\mathrm{d}^3q\,\mathrm{d}^3p'}{(2\pi)^6}\,\delta\left(\varepsilon-\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}'}+\varepsilon_{\mathbf{p}'+\mathbf{q}}\right)U^2(q)$$

$$\times \left[\underbrace{(1-n_{\mathbf{p}'+\mathbf{q}})n_{\mathbf{p}'}n_{\mathbf{p}+\mathbf{q}}}_{(1)} - \underbrace{n_{\mathbf{p}'+\mathbf{q}}(1-n_{\mathbf{p}'})(1-n_{\mathbf{p}+\mathbf{q}})}_{(2)} \right] . \qquad (3.271)$$

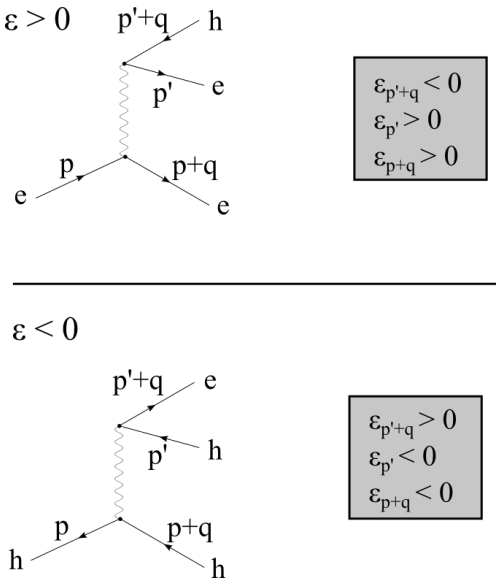
We recall that $\operatorname{sign}\varepsilon_p = \operatorname{sign}(p-p_F)$ and that $n_p = \Theta(p_F - p)$. Thus, the first term in square brackets in Eq. (3.271) is non-zero if $\varepsilon_{p'+q} > 0$, $\varepsilon_{p'} < 0$ and $\varepsilon_{p+q} < 0$, and therefore $\varepsilon = \varepsilon_{\mathbf{p}+\mathbf{q}} + \varepsilon_{\mathbf{p}'} - \varepsilon_{\mathbf{p}'+\mathbf{q}} < 0$, while the second term is non-zero when $\varepsilon_{p'+q} < 0$, $\varepsilon_{p'} > 0$ and $\varepsilon_{p+q} > 0$, which gives $\varepsilon > 0$.

Hence, the second term [labeled (2) in Eq. (3.271)] corresponds to decay of a particle above the Fermi surface. This physical process can be characterized as

$$\mathrm{e} \to \mathrm{eeh},$$

where "e" is an electron and "h" is a hole. An incoming electron uses some of its energy to excite an electron from the Fermi sea or, in other words, creates an electron-hole pair. The first term, labeled (1) in Eq. (3.271), corresponds to a process

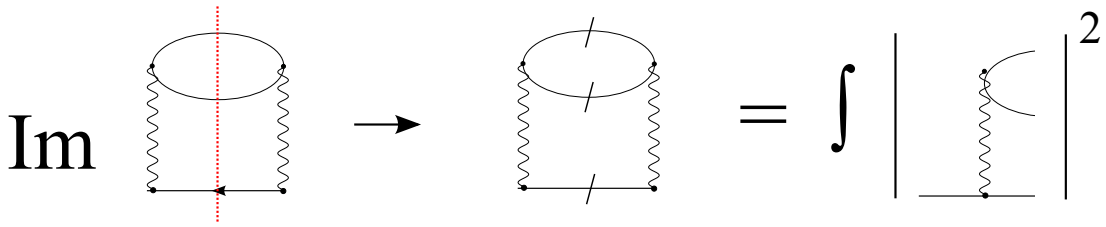
$$\mathrm{h} \to \mathrm{hhe}.$$



The imaginary part of the self-energy $\operatorname{Im}\Sigma$ thus corresponds to real decay processes $\mathrm{e} \to \mathrm{eeh}$ or $\mathrm{h} \to \mathrm{hhe}$ (in the second order). One sees a correspondence between Eq. (3.271) and Fermi's Golden Rule:

$$W = \frac{2\pi}{\hbar} \sum_f |\langle f|H_{\mathrm{int}}|i\rangle|^2 \delta(E_i - E_f).$$

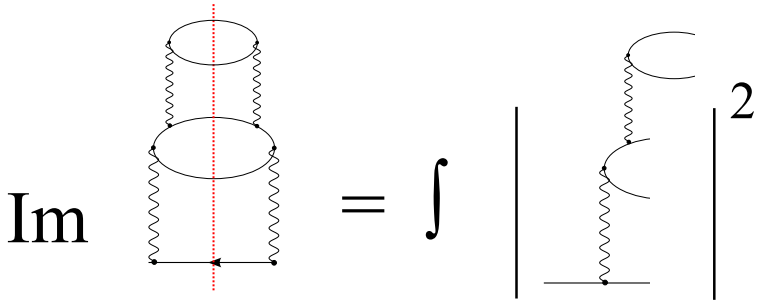
This correspondence can be schematically shown as follows:



where the crossed line denotes the imaginary part of the Green's function,

$$\operatorname{Im} G^{(0)}(\varepsilon, \mathbf{p}) = -\pi\delta(\varepsilon - \varepsilon_p)\operatorname{sign}\varepsilon_p,$$

and the integral goes over the momenta characterizing the final state. This holds also for higher-order diagrams, e.g.,



Let us return to the analysis of $\mathrm{Im}\,\Sigma^{(2b1)}(\mathbf{p},\varepsilon)$, Eq. (3.271). For $\varepsilon > 0$ and thus $\varepsilon_{p'+q} < 0$, $\varepsilon_{p'} > 0$ and $\varepsilon_{p+q} > 0$, we have

$$\varepsilon = \underbrace{\varepsilon_{p+q}}_{>0} + \underbrace{\varepsilon_{p'}}_{>0} + \underbrace{|\varepsilon_{p'+q}|}_{>0} \qquad \rightarrow \qquad \begin{array}{c} 0 \le \varepsilon_{p+q} \le \varepsilon \\ 0 \le \varepsilon_{p'} \le \varepsilon \end{array} \tag{3.272}$$

we obtain the following behavior of the quasi-particle broadening

$$\begin{aligned} \mathrm{Im}\,\Sigma^{(2b1)}(\mathbf{p},\varepsilon) &\overset{(3.271)}{=} \int \frac{d^3q\, d^3p'}{(2\pi)^3} \ldots = \int \frac{d^3(p+q)\, d^3p'}{(2\pi)^3} \ldots = \int d|p+q|\, d|p'| \ldots \\ &= \int d\varepsilon_{p+q} d\varepsilon_{p'} \ldots \propto \varepsilon^2 \qquad \text{for small } \varepsilon\,. \end{aligned} \tag{3.273}$$

Thus, to second order we find the following behaviour of $\mathrm{Im}\,\Sigma$:

$$\mathrm{Im}\,\Sigma(\mathbf{p},\varepsilon_p) \propto \varepsilon_p^2 \propto (p - p_F)^2. \tag{3.274}$$

Hence, in the vicinity of the Fermi surface

$$\mathrm{Im}\,\Sigma(\mathbf{p},\varepsilon_p) \ll \varepsilon_p \qquad \text{for } \varepsilon_p \to 0. \tag{3.275}$$

$\Rightarrow$ Quasiparticles are well defined: $\Gamma \sim \mathrm{Im}\,\Sigma(\mathbf{p},\varepsilon_p) \ll \varepsilon_p$ and $Z > 0$.

$\Rightarrow$ Fermi liquid.

Comment: More accurately, one should check that the angular integration does not bring any additional peculiarities and thus does not modify the scaling (3.274). A calculation of the integral shows that this indeed the case for 3D systems. In that case, the decay rate is dominated by generic processes of two-electron collisions, i.e., those with generic momentum transfers between electrons, $0 < q \lesssim 2k_F$. For 2D systems some modification does occur: an additional logarithmic factor appears in Eq.(3.274). This enhancement originates from "nearly 1D" processes in which two colliding electrons experience nearly forward or nearly backward scattering (momentum transfer q close to zero or to $2k_F$). In particular, for a spinful 2D system with a point-like interaction $U(\mathbf{r}-\mathbf{r}') = g\delta(\mathbf{r}-\mathbf{r}')$, the second-order diagrams (3.260) yield

$$\Gamma = -\mathrm{Im}\,\Sigma(\mathbf{p},\epsilon_p) \simeq \frac{1}{16\pi}\left(\frac{mg}{\pi}\right)^2 \frac{\epsilon_p^2}{\mu} \ln\frac{\mu}{\epsilon_p}. \tag{3.276}$$

The result (3.276) has almost the same form as in the conventional (3D) Fermi liquid, Eq. (3.274). However, the conventional Fermi-liquid ϵ_p^2 scaling of the decay rate Γ is modified in 2D by a large logarithmic factor $\ln(\mu/\epsilon_p)$. Clearly, the Fermi-liquid condition (3.275) remains valid in a 2D system: $\Gamma \ll \epsilon_p$ for small ϵ_p. At the same, the appearance of an additional logarithmic factor signals that, with lowering dimensionality, the behavior deviates from the canonical (3D) Fermi-liquid behavior. We will see in Chapter 7 below that in 1D case the Fermi-liquid behavior breaks down completely; the resulting state of matter is called "Luttinger liquid".

3.12.2 Fermi-liquid with Coulomb interaction

Up to now, we assumed that the interaction is of finite range. Here, we consider a 3D system with Coulomb interaction, $U(r) = e^2/r$. The Fourier transform of the Coulomb potential is given by

$$U(\mathbf{q}) = \frac{4\pi e^2}{q^2}. \tag{3.277}$$

We will see that the Fermi-liquid theory works in this case as well. However, the perturbative analysis should be modified: one cannot simply do the perturbation theory in the bare Coulomb interaction but rather should take screening into account, which corresponds to a partial resummation of the perturbative expansion.

We remind that, according to Eq.(3.241), the effective mass is expressed through the real part of the self-energy as follows:

$$m^* = m\,\frac{1-\left.\dfrac{\partial}{\partial\epsilon}\mathrm{Re}\,\Sigma(\epsilon,\mathbf{p})\right|_{\epsilon=0,\,p=p_F}}{1+\left.\dfrac{\partial}{\partial\epsilon_p}\mathrm{Re}\,\Sigma(\epsilon,\mathbf{p})\right|_{\epsilon=0,\,p=p_F}}, \tag{3.278}$$

To the first order in interaction, the self-energy is given by the sum of Hartree and Fock diagrams, Eq. (3.252),

$$\begin{aligned}\Sigma^{(1)}(\mathbf{p},\varepsilon) &= \quad + \\ &= \int\frac{\mathrm{d}^3k}{(2\pi)^3}\left[2U(0)-U(\mathbf{p}-\mathbf{k})\right]\underbrace{n_k}_{\Theta(p_F-k)} \\ &= \frac{1}{(2\pi)^2}\int_0^{p_F}\mathrm{d}k\,k^2\int_{-1}^{1}\mathrm{d}\cos\theta\,\left[2U(0)-U(\mathbf{p}-\mathbf{k})\right],\end{aligned} \tag{3.279}$$

where θ is the angle between vectors $\mathbf{p}$ and $\mathbf{k}$. (The self-energy does not depend on the direction of $\mathbf{p}$.) Note that, strictly speaking, the bare Hartree-Fock diagrams would involve $p_F^{(0)}$ and correspondingly $n^{(0)}$. However, dressing of the fermionic line in the Hartree-Fock diagrams leads to renormalization $p_F^{(0)}\mapsto p_F$ and $n^{(0)}\mapsto n$, see Eq. (3.259) and text below it. This is taken into account in Eq. (3.279).

The Hartree diagram is quite generally a constant that does not depend on ϵ and $\mathbf{p}$ and hence does not contribute to the effective mass. For the case of Coulomb interaction, Eq. (3.277), that we consider here, there is a peculiarity: the Hartree term diverges, as it is proportional to $U(0)=\infty$. However, this divergence is canceled by the interaction with positive background.

We thus focus on the second, Fock, term Σ_F in Eq. (3.279), with $-U(\mathbf{p}-\mathbf{k})$ in the integrand. Assuming for definiteness $p>p_F$, we find:

$$\begin{aligned}\Sigma_F(p,\epsilon) &= -\frac{4\pi e^2}{(2\pi)^2}\int_0^{p_F}\mathrm{d}k\int_{-1}^{1}\mathrm{d}\cos\theta\frac{k^2}{p^2+k^2-2pk\cos\theta} \\ &= -\frac{4\pi e^2}{(2\pi)^2}\int_0^{p_F}\mathrm{d}k\,\frac{k}{p}\,\ln\frac{p+k}{p-k} = -\frac{e^2}{\pi}\left(p_F-\frac{p^2-p_F^2}{2p}\ln\frac{p+p_F}{p-p_F}\right).\end{aligned} \tag{3.280}$$

This expression does not depend on ϵ, and hence the quasiparticle residue Z to the first order is

$$Z^{(1)} = \frac{1}{1-\left.\dfrac{\partial}{\partial\epsilon}\mathrm{Re}\,\Sigma_1(\mathbf{p},\epsilon)\right|_{\epsilon=0,\,p=p_F}} = 1, \tag{3.281}$$

and thus, the numerator in the formula (3.278) for the effective mass is unity. This is in agreement with the general Hartree-Fock result (3.254) obtained above; it holds equally for the short-range and long-range interaction.

We calculate now the expression in the denominator of Eq. (3.278),

$$\begin{aligned}\frac{\partial\Sigma_1(p,\epsilon)}{\partial\epsilon_p} &= -\frac{m}{p}\frac{4\pi e^2}{(2\pi)^2}\frac{\partial}{\partial p}\left(p_F - \frac{p^2-p_F^2}{2p}\ln\frac{p+p_F}{p-p_F}\right) \\ &= \frac{e^2 m}{\pi p}\left(\frac{p^2+p_F^2}{2p^2}\ln\frac{p+p_F}{p-p_F} - \frac{p_F}{p}\right) \underbrace{\to}_{p\to p_F} \frac{e^2 m}{\pi p_F}\ln\frac{2p_F}{p-p_F}\,. \end{aligned} \tag{3.282}$$

The result (3.282) diverges logarithmically at $p = p_F$. Thus, to first order in the Coulomb interaction,

$$m^* = 0. \tag{3.283}$$

The result (3.283) is unphysical. The divergence (3.282) originates from divergence of $U(q)$ at $q \to 0$. Since $U(q)$ becomes large at small q, considering it in the first order in this region of momenta is not justified. The proper way is to take into account the screeing, which corresponds to a resummation of a series of diagrams for the interaction line, see Sec. 3.14 below. The simplest approximation for the screening is the Thomas-Fermi screening (known from TKM 1). The resulting effective interaction reads, see Eq. (3.329) below,

$$U_{\rm eff}(\mathbf{r}-\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}e^{-\kappa|\mathbf{r}-\mathbf{r}'|}, \qquad U_{\rm eff}(\mathbf{q}) = \frac{4\pi e^2}{q^2+\kappa^2}, \tag{3.284}$$

where κ^{-1} is the screening length, $\kappa^2 = 4\pi e^2\nu$, and $\nu = mp_F/\pi^2$ is the density of states at the Fermi level. The singularity of $U(\mathbf{q})$ at $q = 0$ is now cured at the inverse screening length κ: electrons that are far apart do not experience the bare Coulomb interaction, because other electrons screen the interaction and reduce its range. Performing the calculation of the Fock self-energy Σ_F with the screened Coulomb interaction, $U \mapsto U_{\rm eff}$, we get

$$\Sigma_F(p,\epsilon) = -\frac{4\pi e^2}{(2\pi)^2}\int_0^{p_F} {\rm d}k\,\frac{k}{2p}\,\ln\frac{(p+k)^2+\kappa^2}{(p-k)^2+\kappa^2}, \tag{3.285}$$

$$\frac{\partial\Sigma_F(p,\epsilon)}{\partial\epsilon_p} = \frac{m}{p}\frac{4\pi e^2}{(2\pi)^2}\left[\frac{\kappa^2+p_F^2+p^2}{4p^2}\ln\frac{\kappa^2+(p+p_F)^2}{\kappa^2+(p-p_F)^2} - \frac{p_F}{p}\right], \tag{3.286}$$

$$\left.\frac{\partial\Sigma_F(p,\epsilon)}{\partial\epsilon_p}\right|_{p=p_F} = \frac{e^2 m}{\pi p_F}\left(\frac{\kappa^2+2p_F^2}{4p_F^2}\ln\frac{\kappa^2+4p_F^2}{\kappa^2} - 1\right). \tag{3.287}$$

It is convenient, by using $\kappa^2 = 4\pi e^2\nu$ and $\nu = mp_F/\pi^2$, to express here e^2 in terms of κ. We also note that, since the Thomas-Fermi-screened interaction (3.284) is ω-independent, we still have $Z = 1$. Thus, we get for the effective mass:

$$m^* = \frac{m}{1+\frac{\kappa^2}{4p_F^2}\left(\frac{\kappa^2+2p_F^2}{4p_F^2}\ln\frac{\kappa^2+4p_F^2}{\kappa^2}-1\right)} \underbrace{\to}_{\kappa\ll p_F} m\left(1-\frac{\kappa^2}{4p_F^2}\ln\frac{2p_F}{\kappa}\right). \tag{3.288}$$

It can be verified that the result (3.288) is controllable for $\kappa/p_F \ll 1$ ("weak Coulomb interaction"). We see that taking screening into account restores a finite value of the effective mass, i.e., the usual Fermi-liquid behavior.

Note that the value of the self-energy at $p = p_F$ and $\epsilon = 0$,

$$\Sigma_F(p_F,0) \simeq -\frac{e^2}{\pi}p_F\left(1-\frac{\pi\kappa}{2p_F}\right), \tag{3.289}$$

controls the renormalization of Fermi momentum at given chemical potential (or, alternatively, renormalization of chemical potential at fixed density) according to Eq. (3.244).

When calculating the decay rate, one should also take into account the screening of the Coulomb interaction in the second-order diagrams (3.259). (If one naively tries to calculate with the bare Coulomb interaction, one would encounter an infrared divergence originating from a singularity of $U(q)$ at $q \to 0$.) Including screening leads to the following result at $\kappa \ll p_F$ (we omit details of the calculation; renormalization of m and Z does not influence the result to the leading order):

$$\frac{1}{\tau} \simeq 2\,\mathrm{Im}\,\Sigma(\mathbf{p}, \varepsilon_p) \simeq \frac{\pi}{64}\sqrt{\frac{e^2}{v_F}}\,\frac{\varepsilon_p^2}{p_F^2/2m} \equiv \frac{\pi^{3/2}}{128}\,\frac{\kappa}{p_F}\,\frac{\varepsilon_p^2}{p_F^2/2m}\,. \tag{3.290}$$

Thus, the decay rate also shows the **Fermi-liquid behavior**, $1/\tau \propto \varepsilon_p^2$. Note that the prefactor scales with the strength of the Coulomb interaction as $(e^2)^{1/2}$, whereas naively one would expect in the second order the $(e^2)^2$ scaling. This is because one has to take screening into account, which amounts to a resummation of diagrams of all orders in the bare interaction.

3.12.3 Quasiparticle interaction function in Fermi liquid

We recall the key postulates of the Fermi-liquid theory (TKM-1):

(i) Excitations = quasi-particles with Fermi statistics,

(ii) quasi-particle energy:

$$\varepsilon(\mathbf{p}) = v_F^*(p - p_F) + \int \frac{d^3p'}{(2\pi)^3} f(\mathbf{p}, \mathbf{p}')\delta n(\mathbf{p}')\,, \qquad v_F^* = p_F/m^*\,, \tag{3.291}$$

(iii) inverse quasi-particle lifetime $1/\tau(\varepsilon) \ll$ quasi-particle energy ε,

(iv) relation between p_F and density n is not modified by interactions:

$$n = \frac{2}{(2\pi)^3}\,\frac{4}{3}\,\pi p_F^3 \qquad \text{in 3D.}$$

As we have shown above, the Green's function formalism provides a microscopic basis for justification of these postulates. In particular, (i) follows from the existence of the quasiparticle pole in the Green function, the first term in (ii) corresponds to renormalization of the mass by the real part of the self-energy, (iii) follows from the analysis of the imaginary part of the self-energy. The postulate (iv) can also be rigorously proven by using the Green's function formalism [Luttinger theorem, Eq. (3.246)] but we omitted the proof.

It remains to discuss what is the meaning of the quasiparticle interaction function $f(\mathbf{p}, \mathbf{p}')$ in (3.291) within the microscopic approach. Let us introduce a **two-particle Green's function**:

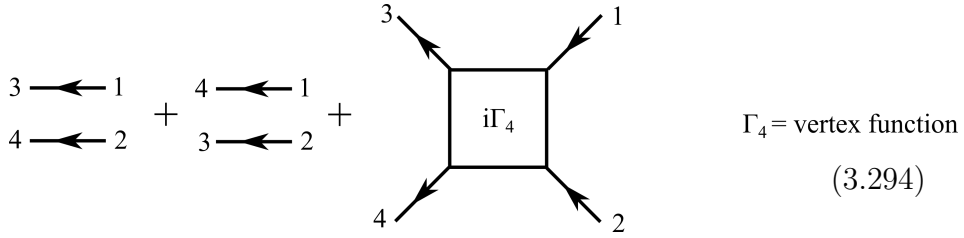
$$K(34, 12) = \langle\, \phi_0 \mid \mathcal{T}[\hat{\psi}(3)\hat{\psi}(4)\hat{\psi}^\dagger(1)\hat{\psi}^\dagger(2)] \mid \phi_0 \rangle. \tag{3.292}$$

Proceeding in the same way as for the single-particle Green's function discussed above, we can perform a transformation to the interaction representation,

$$K(34, 12) = \frac{\langle\, 0 \mid \mathcal{T}\left[\widehat{\mathcal{S}}\hat{\psi}_0(3)\hat{\psi}_0(4)\hat{\psi}_0^\dagger(1)\hat{\psi}_0^\dagger(2)\right] \mid 0\rangle}{\langle 0|\widehat{\mathcal{S}}|0\rangle}\,, \tag{3.293}$$

and, on this basis, develop the diagrammatics for the two-particle Green function. Separating the disconnected and connected parts, one finds

$K(34,12)$ =

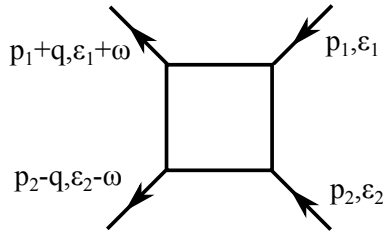


Γ_4 = vertex function

(3.294)

with all fermionic lines being thick (i.e., representing the full Green's function G) and with the vertex function (in energy-momentum representation)

$i\Gamma_4(\varepsilon_1, \mathbf{p}_1, \varepsilon_2, \mathbf{p}_2, \omega, \mathbf{q})$ =



(3.295)

Note that the external lines are not included in Γ_4 in Eq. (3.295); they only serve to indicate the vertices to which the lines can be attached as well as incoming and outgoing momenta and frequencies.

One can then show that (with $\boldsymbol{p}_1, \boldsymbol{p}_2$ on the Fermi surface):

$$f(\boldsymbol{p}_1 = \boldsymbol{n}_1 \cdot p_F,\ \boldsymbol{p}_2 = \boldsymbol{n}_2 \cdot p_F) = Z^2 \Gamma_4(\varepsilon_1 = 0, \boldsymbol{n}_1 \cdot p_F, \varepsilon_2 = 0, \boldsymbol{n}_2 \cdot p_F, \omega, q = 0)|_{\omega \to 0}. \quad (3.296)$$

Thus, the Fermi-liquid interaction function f is expressed in the microscopic approach in terms of the forward-scattering amplitude on the Fermi surface.

3.13 Linear response

Consider a system (in general, interacting) described by a Hamiltonian $\widehat{H}$. We want to investigate a reaction of the system onto a weak time-dependent perturbation of the Hamiltonian

$$\widehat{H} \mapsto \widehat{H} + \widehat{A}\, F(t)\,. \quad (3.297)$$

The ground state of the system without perturbation (in the Heisenberg picture) is $|\phi_0\rangle$. We will use the Heisenberg representation with respect to the unperturbed Hamiltonian $\widehat{H}$. (It is analogous to the interaction representation for the perturbed Hamiltonian $\widehat{H} + \widehat{A}F(t)$ if we view $\widehat{A}F(t)$ as "interaction".) In this representation, we get the following evolution equation for the state:

$$i\partial_t |\phi(t)\rangle \;=\; F(t)\widehat{A}(t)|\phi(t)\rangle \qquad \text{with } \widehat{A}(t) = e^{i\widehat{H}t}\widehat{A}_S e^{-i\widehat{H}t}, \quad (3.298)$$

where $\widehat{A}_S$ is the Schrödinger operator.

Integrating this equation over time from $-\infty$ to t and assuming that there was no perturbation at $t = -\infty$, so that the corresponding state was $|\phi(-\infty)\rangle = |\phi_0\rangle$, we get

$$\int_{-\infty}^{t} dt'\, \partial_{t'} |\phi(t')\rangle \;=\; -i \int_{-\infty}^{t} dt'\, F(t')\widehat{A}(t')|\phi(t')\rangle\,;$$

$$|\phi(t)\rangle \;=\; |\phi_0\rangle - i\int_{-\infty}^{t} dt'\, F(t')\widehat{A}(t')|\phi(t')\rangle.$$

To the first order in the perturbation F, we can replace $|\phi(t')\rangle \mapsto |\phi_0(t')\rangle$ in the r.h.s., which yields

$$|\phi(t)\rangle \approx |\phi_0\rangle - i\int_{-\infty}^{t} dt'\, F(t')\widehat{A}(t')|\phi_0\rangle \equiv |\phi_0\rangle + |\delta\phi(t)\rangle. \tag{3.299}$$

Consider a physical observable corresponding to the operator $\widehat{B}(t)$ (in Heisenberg representation). The expectation value of this observable in the absence of perturbation is

$$B_0(t) = \langle\, \phi_0 \mid \hat{B}(t) \mid \phi_0\rangle. \tag{3.300}$$

We are interested in $\delta B(t) = B(t) - B_0(t)$, where

$$B(t) = \langle\phi(t)|\widehat{B}(t)|\phi(t)\rangle \tag{3.301}$$

is the observable in the presence of the perturbation. To the linear order in F, we get

$$\begin{aligned}
\delta B(t) \;&=\; B(t) - B_0(t) = \langle\, \phi(t) \mid \hat{B}(t) \mid \phi(t)\rangle - \langle\, \phi_0 \mid \hat{B}(t) \mid \phi_0\rangle \\
&\overset{(3.299)}{\approx} \left(\langle\phi_0| + \langle\delta\phi(t)|\right) \hat{B}(t) \left(|\phi_0\rangle + |\delta\phi(t)\rangle\right) - \langle\, \phi_0 \mid \hat{B}(t) \mid \phi_0\rangle \\
&\approx \langle\, \phi_0 \mid \hat{B}(t) \mid \delta\phi(t)\rangle + \langle\, \delta\phi(t) \mid \hat{B}(t) \mid \phi_0\rangle \\
&= -\mathrm{i}\int_{-\infty}^{t} \mathrm{d}t'\, \langle\phi_0|[\widehat{B}(t), \widehat{A}(t')]|\phi_0\rangle F(t') \equiv \int_{-\infty}^{\infty} \mathrm{d}t'\, \mathscr{D}^R_{BA}(t,t')F(t')\,.
\end{aligned} \tag{3.302}$$

Here we introduced the **linear response function**

$$\mathscr{D}^R_{BA}(t,t') = -\mathrm{i}\Theta(t-t')\langle\phi_0|[\widehat{B}(t), \widehat{A}(t')]|\phi_0\rangle\,, \tag{3.303}$$

where the index R means "retarded". The formula (3.303) for the linear response function $\mathscr{D}^R_{BA}(t,t')$, which describes how the observable $B(t)$ changes under the perturbation $\widehat{A}\,F(t)$, is called **Kubo formula**.

With the diagrammatic approach developed above, we can calculate the corresponding time-ordered correlator

$$\mathscr{D}_{BA}(t,t') = -i\langle\, \phi_0 \mid \mathcal{T}\hat{B}(t)\hat{A}(t') \mid \phi_0\rangle. \tag{3.304}$$

In full analogy with the one-particle Green's function, one can show that

$$\mathscr{D}_{BA}(\omega) = \begin{cases} \mathscr{D}^R_{BA}(\omega), & \omega > 0, \\ \mathscr{D}^A_{BA}(\omega) = [\mathscr{D}^R_{BA}(\omega)]^*, & \omega < 0. \end{cases} \tag{3.305}$$

Thus, calculating $\mathscr{D}_{BA}$ we also find the response function $\mathscr{D}^R_{BA}$.

3.13.1 Density-density response function

We consider here an important special case of a linear response function: the density-density response function. To define it, we consider a scalar potential as perturbation: $F(t) \mapsto \varphi(x,t)$. The operator that couples to the potential is the density operator

$$\widehat{A}(t) \mapsto \widehat{\varrho}(x,t) = \psi^\dagger(x,t)\psi(x,t)\,, \tag{3.306}$$

and the perturbation of the Hamiltonian is given by

$$\delta\widehat{H} = \int \mathrm{d}x\, \varphi(x,t)\widehat{\varrho}(x,t)\,. \tag{3.307}$$

Further, as the observable, we also consider the density: $\widehat{B}(t) = \widehat{\varrho}(x,t)$. We have then, according to Eq. (3.302)

$$\delta\varrho(x,t) \;=\; \int_{-\infty}^{\infty} dt' \int dx'\, \mathscr{D}^R_{\varrho\varrho}(x-x',t-t')\varphi(x',t')\,, \tag{3.308}$$

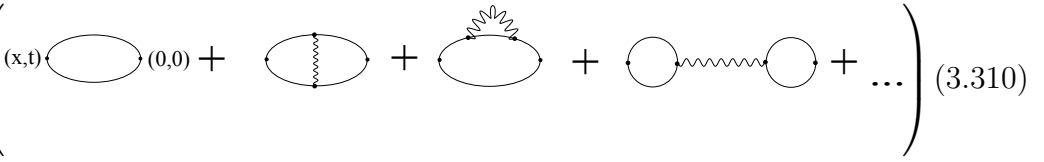
where $\mathscr{D}^R_{\varrho\varrho}(x-x',t-t')$ is the **density-density response function**:

$$\mathscr{D}^R_{\varrho\varrho}(x-x',t-t') = -\mathrm{i}\Theta(t-t')\langle\phi_0|[\widehat{\varrho}(x,t),\widehat{\varrho}(x',t')]|\phi_0\rangle = -\Pi^R(x-x',t-t')\,. \tag{3.309}$$

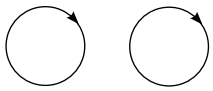
The function $\Pi^R(x-x',t-t')$ (equal to $\mathscr{D}^R_{\varrho\varrho}(x-x',t-t')$ up to a sign) is also called the **polarization operator**.

The diagrammatic approach allows us to calculate the time-ordered density-density correlation function:

$$\begin{aligned}\Pi(x,t) &= i\langle\,\phi_0 \mid \mathcal{T}\widehat{\varrho}(x,t)\widehat{\varrho}(0,0) \mid \phi_0\rangle \\ &= i\Bigg(\quad + \quad + \quad + \quad + \ldots\Bigg)\end{aligned} \tag{3.310}$$

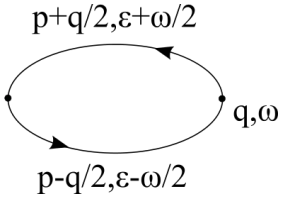


<u>*Comment:*</u> The disconnected diagram with two fermion loops shown to the right gives only a constant contribution $\langle\rho\rangle^2$ to $\Pi(x,t)$, Eq. (3.310) and is of no interest. In particular, it does not affect the calculation of Π^R below. This term does not arise at all if one slightly modifies the density operators by subtracting the average density: $\widehat{\varrho}(x,t) \mapsto \widehat{\varrho}(x,t) - \langle\rho\rangle$.



By using the diagrammatic rules we calculate $\Pi(q,\omega)$ for a non-interacting gas (the first diagram in Eq. (3.310), so-called "polarization bubble"):

$\Pi(q,\omega) = i$



$$\begin{aligned}&= (-i)(-1)\int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{\mathrm{d}\varepsilon}{2\pi}\,\frac{1}{\varepsilon+\frac{\omega}{2}-\frac{1}{2m}\left(\mathbf{p}+\frac{\mathbf{q}}{2}\right)^2+\mu+\mathrm{i}0\,\mathrm{sign}\left(\varepsilon+\frac{\omega}{2}\right)}\times \\ &\quad\times\frac{1}{\varepsilon-\frac{\omega}{2}-\frac{1}{2m}\left(\mathbf{p}-\frac{\mathbf{q}}{2}\right)^2+\mu+\mathrm{i}0\,\mathrm{sign}\left(\varepsilon-\frac{\omega}{2}\right)}\,.\end{aligned} \tag{3.311}$$

The factor $(-i)$ in front of the integral in Eq. (3.311) originates from i in the definition of the polarization operator and i^2 coming from $\langle\mathcal{T}\psi\psi^\dagger\rangle = iG$. The factor -1 comes for the fermionic loop.

We consider first the regime $|\mathbf{q}| \ll k_F$, which is usually of interest. Under this assumption, the calculations are simplified. Specifically, we have

$$\frac{1}{2m}\left(\mathbf{p}\pm\frac{\mathbf{q}}{2}\right)^2-\mu \simeq \underbrace{\frac{\mathbf{p}^2}{2m}-\mu}_{\equiv\xi} \pm\frac{\mathbf{p}\cdot\mathbf{q}}{2m} \simeq \xi \pm \frac{1}{2}v_F\mathbf{n}\cdot\mathbf{q}\,. \tag{3.312}$$

Using

$$\int \frac{d^3p}{(2\pi)^3} \ldots = \nu \int d\xi d\boldsymbol{n} \ldots \qquad \text{where} \quad \int d\boldsymbol{n} \ldots = \int \frac{d\phi\, d\cos\theta}{4\pi} \ldots ,$$

with the density of states ν at the Fermi surface and normalized angular integral, $\int d\boldsymbol{n} = 1$, we obtain:

$$\Pi(q,\omega) = \mathrm{i} \int \nu \,\mathrm{d}\xi \,\mathrm{d}\mathbf{n} \,\frac{\mathrm{d}\varepsilon}{2\pi} \,\frac{1}{\varepsilon - \xi + \frac{1}{2}\left(\omega - v_F \mathbf{n}\cdot\mathbf{q}\right) + \mathrm{i}0\,\mathrm{sign}\left(\xi + v_F \cdot \frac{\mathbf{n}\cdot\mathbf{q}}{2}\right)} \times \frac{1}{\varepsilon - \xi - \frac{1}{2}\left(\omega - v_F \mathbf{n}\cdot\mathbf{q}\right) + \mathrm{i}0\,\mathrm{sign}\left(\xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2}\right)} . \tag{3.313}$$

We will first perform the integration over the energy ε. This integral is nonzero, if

$$\mathrm{sign}\left(\xi + v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2}\right) \neq \mathrm{sign}\left(\xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2}\right) , \tag{3.314}$$

because then the two poles have opposite signs of the imaginary parts. This yields the condition restricting the values of ξ:

$$-v_F \frac{|\mathbf{n}\cdot\mathbf{q}|}{2} < \xi < v_F \frac{|\mathbf{n}\cdot\mathbf{q}|}{2} . \tag{3.315}$$

For these values we have

$$\mathrm{sign}(\xi \pm v_F \boldsymbol{n}\cdot\boldsymbol{q}/2) = \pm\,\mathrm{sign}(\boldsymbol{n}\cdot\boldsymbol{q}).$$

Performing the ε integration, we thus obtain

$$\begin{aligned}
\Pi(q,\omega) &= \mathrm{i}\nu \,\frac{2\pi\mathrm{i}}{2\pi} \int\limits_{-\frac{1}{2}v_F|\mathbf{n}\cdot\mathbf{q}|}^{\frac{1}{2}v_F|\mathbf{n}\cdot\mathbf{q}|} \mathrm{d}\xi \int \mathrm{d}\mathbf{n}\, \frac{1}{\omega - v_F\mathbf{n}\cdot\mathbf{q} + \mathrm{i}0\,\mathrm{sign}(\mathbf{n}\cdot\mathbf{q})} \mathrm{sign}(\mathbf{n}\cdot\mathbf{q}) \\
&= -\nu \int \mathrm{d}\mathbf{n}\, \frac{v_F\mathbf{n}\cdot\mathbf{q}}{\omega - v_F\mathbf{n}\cdot\mathbf{q} + \mathrm{i}0\mathrm{sign}(\omega)} \\
&= -\nu \int_{-1}^{1} \frac{d\cos\theta}{2} \int_0^{2\pi} \frac{d\phi}{2\pi}\, \frac{v_F q\cos\theta}{\omega - v_F q\cos\theta + i0\,\mathrm{sign}(\omega)} \qquad (3.316) \\
&= \frac{\nu}{2} \int_{-1}^{1} dx\, \frac{x}{x-s} \qquad (3.317)
\end{aligned}$$

with

$$s = \frac{\omega + \mathrm{i}0\,\mathrm{sign}(\omega)}{q v_F}.$$

Taking the integral

$$\int^x dy \frac{y}{y-s} = x\ln(x-s) + x\,,$$

we arrive at

$$\Pi(q,\omega) = \nu\left[1 - \frac{s}{2}\,\ln\frac{s+1}{s-1}\right] . \tag{3.318}$$

Let us analyze this result. It is important that the limits $q \to 0$ and $\omega \to 0$ for $\Pi(q,\omega)$ do not commute. Specifically, if the $\omega \to 0$ limit is taken first (which corresponds to $s \to 0$), we get

$$\lim_{q\to 0} \lim_{\omega\to 0} \Pi(q,\omega) = \nu\,. \tag{3.319}$$

This limit will determine the static (Thomas-Fermi) screening, see Sec. 3.14 below. The opposite order of limits ($q \to 0$ taken first), which corresponds to $s \to \infty$, yields

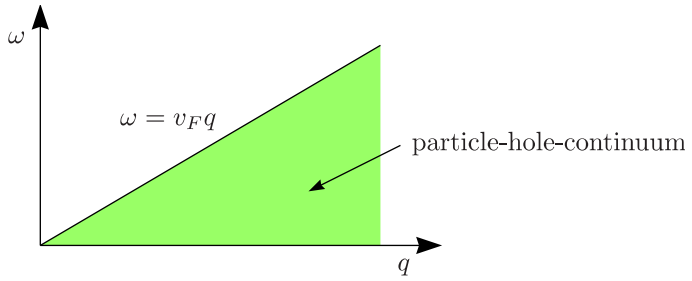
$$\lim_{\omega\to 0} \lim_{q\to 0} \Pi(q,\omega) = 0\,. \tag{3.320}$$

The physical reason for vanishing of the polarization operator in this order of limits is as follows. The polarization operator is a response of density to an external potential. If a scalar potential is uniform ($q = 0$), it does not produce any electric field and can be simply gauged out. Thus, Eq. (3.320) is a consequence of gauge invariance (or, equivalently, of charge conservation.)

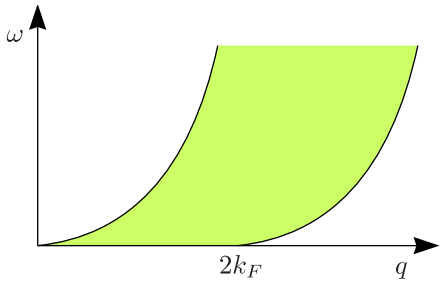
Let us analyze now under what condition the imaginary part $\mathrm{Im}\,\Pi(q,\omega)$ is nonzero. Inspecting Eq. (3.316), we see that the imaginary part is generated when the real part of the denominator is zero:

$$\omega - v_F \boldsymbol{n}\cdot\boldsymbol{q} = 0 \qquad \Rightarrow \qquad \omega = v_F \boldsymbol{n}\cdot\boldsymbol{q} < v_F \cdot q\,.$$

Thus, $\mathrm{Im}\,\Pi(q,\omega) \neq 0$ for $\omega < v_F q$. The non-zero imaginary part corresponds to the possibility of creation of real electron-hole pairs with given total values of ω and q, i.e., to dissipation. The corresponding part of the ω–q plane is called the **particle-hole continuum**.



We recall, that the above analysis was performed for $q \ll k_F$. If all momenta are considered, the particle-hole continuum is bounded by two parabolas and looks as follows:



Linearizing the parabola in the region of small q, one obtains the linear border $\omega < v_F q$ in correspondence with the limiting case $q \ll k_F$ considered above.

3.14 Coulomb interaction: Screening, random phase approximation (RPA)

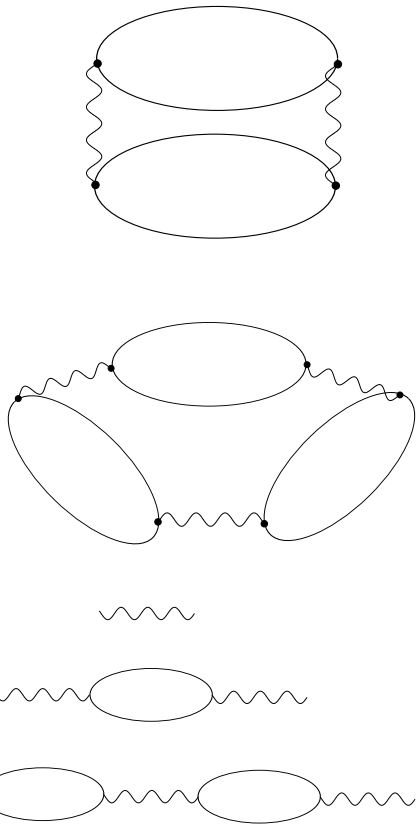
Consider a system of fermions with Coulomb interaction,

$$U(\mathbf{r}) = \frac{e^2}{|\mathbf{r}|}\,. \tag{3.321}$$

In 3D, the Fourier transform of the Columb potential reads

$$U(\mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2}\,. \tag{3.322}$$

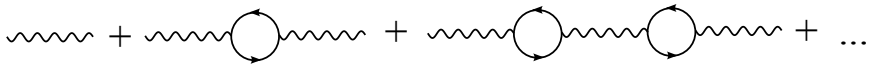
The Fourier transform of the Coulomb potential $U(\mathbf{q})$ is singular at $|\mathbf{q}| \mapsto 0$, which leads to divergencies. As an example, one can consider diagrams for the ground-state energy of the system shown to the right. See also Sec. 3.12.2.



In higher orders, one finds terms with stronger and stronger singularities that originate from a sequence of diagrams in which multiple interaction lines carry the same small momentum q, yielding factors

$$U(q)^n = \left(\frac{4\pi e^2}{q^2}\right)^n\,.$$

The corresponding diagrams for, e.g., ground state energy (or any other observable) will thus exhibit increasingly strong divergencies $\propto \int d^3q (1/q^2)^n$. In analogies with the singularities resulting from higher-order poles of the bare Green function—which motivated us to introduce the notion of self-energy, see Sec. 3.11.1— this implies a necessity to resum the series. The resummation yields an effective potential U_{eff}:

$U_{\text{eff}}(q,\omega) =$  $=$ 

$$= U(q) - U(q)\Pi(q,\omega)U(q) + U(q)\Pi(q,\omega)U(q)\Pi(q,\omega)U(q) - \dots \tag{3.323}$$

The signs in the second line of Eq. (3.323) are alternating. The $(-1)^n$ in the term with n polarization bubbles has the following origins: (a) each interaction operator comes with the factor $(-i)$ in the perurbative expansion; (b) according to the definition, the polarization bubble is equal to $-i\Pi$, see e.g. Eq. (3.311).

The series ((3.323)) leads to the Dyson equation,

$$U_{\text{eff}} = U - U\,\Pi\,U_{\text{eff}}\,, \tag{3.324}$$

and therefore

$$U_{\text{eff}}(\omega,q)\,[1 + U(q)\Pi(\omega,q)] = U(\omega,q)\,, \tag{3.325}$$

$$\boxed{U_{\text{eff}}(\omega,q) = \frac{U(q)}{1+U(q)\Pi(\omega,q)} \equiv \frac{U(q)}{\epsilon(\omega,q)}\,.} \tag{3.326}$$

The effective interaction $U_{\rm eff}$ is the **screened** Coulomb interaction. Taking screening into account cures the problem of divergencies that one encounters when naively trying to treat perturbatively the bare Coulomb interaction, see, e.g., Sec. 3.12.2 where we considered a Fermi liquid with Coulomb interaction. The last expression is Eq. (3.326) defines the effective dielectric constant

$$\epsilon(\omega, q) = 1 + U(q)\Pi(\omega, q)\,. \tag{3.327}$$

If one considers the polarization bubble in Eq. (3.323) by $(-i)$ times as the exact irreducible polarization operator Π (that cannot be divided into two parts by cutting one interaction line), Eq. (3.323) will become exact equation for the effective interaction, in analogy with the series (3.221) for the exact Green's function in terms of the self-energy. Within this analogy, equations (3.324)—(3.326) are analogs of Eqs. (3.222)—(3.225) for the fermionic Green's function. The conventional approximation is to use the leading-order diagram for the polarization operator, i.e., the polarization operator of a free system, Eq. (3.311). This approximation is known as **random phase approximation (RPA)**. If one further considers the range of relatively small wave vectors $q \ll k_F$, one can use the approximation (3.316), yielding

$$U_{\rm eff}(\omega, q) = \frac{U(q)}{1 + \nu U(q) \displaystyle\int \mathrm{d}\mathbf{n}\, \frac{v_F \mathbf{n}\cdot\mathbf{q}}{v_F \mathbf{n}\cdot\mathbf{q} - \omega - \mathrm{i}0\mathrm{sign}(\omega)}}\,. \tag{3.328}$$

It should be emphasized that we have **dynamical screening**: the effective interaction becomes frequency dependent. Physically, this can be understood as follows. If a charged particle is added to the system, other particles rearrange to form a screening cloud. This process, however, is not instantaneous, i.e, it takes some time. This retardation manifests itself in ω dependence of $U_{\rm eff}$.

3.14.1 Limiting cases of RPA

We consider now various limits of the behavior of $\Pi(\omega, q)$, and correspondingly of $\epsilon(\omega, q)$ and $U_{\rm eff}(\omega, q)$ in RPA.

(a) $\omega \to 0$ (this limit is taken first) and $q \ll 2k_F$:

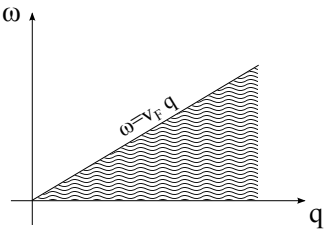
It holds that $\Pi(q) = \nu$, see Eq. (3.319). Thus,

$$U_{\rm eff}(\omega = 0, q) = \frac{U(q)}{1 + \nu U(q)} = \frac{\frac{4\pi e^2}{q^2}}{1 + \nu \frac{4\pi e^2}{q^2}} = \frac{4\pi e^2}{q^2 + \kappa^2}\,, \qquad \kappa^2 = 4\pi e^2 \nu\,. \tag{3.329}$$

The Fourier transform to real space yields

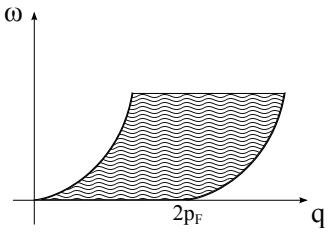
$$U_{\rm eff}(r) = \frac{e^2}{r}\exp(-\kappa r)\,. \tag{3.330}$$

This is the static (Thomas-Fermi) screening; κ is the inverse **screening length**.



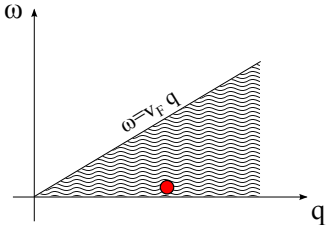
(b) $\omega = 0$ and q arbitrary:

The corresponding result is known as Lindhard function. The essential additional feature is Friedel oscillations that originate from a $2k_F$ singularity in the static polarization operator. Upon Fourier transformation to the real space, it leads to a fast oscillating part of the effective potential, which oscillates as $\cos(2k_F r)/r^3$.



(c) $\omega \neq 0$, but small ($\omega \ll q v_F$):

In this case, we get a non-zero (but small) imaginary part of the polarization operator:



$$\begin{aligned}
\text{Im } \Pi(\omega, q) &\overset{(3.316)}{=} -\nu \,\text{Im} \left(\int d\boldsymbol{n} \, \frac{v_F \boldsymbol{n} \cdot \boldsymbol{q}}{\omega - v_F \boldsymbol{n} \cdot \boldsymbol{q} + i0 \,\text{sign}(\omega)} \right) \\
&\overset{(2.24)}{=} \pi\nu \int d\boldsymbol{n} \; v_F \boldsymbol{n} \cdot \boldsymbol{q} \; \delta(\omega - v_F \boldsymbol{n} \cdot \boldsymbol{q}) \,\text{sign}(\omega) \\
&= \pi\nu \int \frac{d\phi d\cos\theta}{4\pi} v_F q \cos\theta \; \delta(\omega - v_F q \cos\theta) \,\text{sign}(\omega) \\
&= \frac{\pi}{2}\nu \int dx \; x \, \frac{\delta(\omega - x)}{v_F q} \,\text{sign}(\omega) \\
&= \nu \frac{\pi}{2} \frac{\omega \,\text{sign}(\omega)}{v_F q} = \nu \frac{\pi}{2} \frac{|\omega|}{v_F q}.
\end{aligned}$$

The polarization operator thus reads:

$$\Pi(\omega, q) \simeq \nu \left(1 + \frac{\mathrm{i}\pi}{2} \frac{|\omega|}{v_F q} \right) . \tag{3.331}$$

The emergence of the imaginary part of Π implies a non-zero imaginary part of the dielectric function $\epsilon(\omega, q)$, see Eq. (3.327). In turn, $\text{Im}\,\epsilon \neq 0$ implies presence of **dissipation**. Whenever a wave with the corresponding values of q and ω propagates in the system (see discussion of plasmons below), it will decay due to creation of particle-hole pairs—the effect known as **Landau damping**.

(d) $q \to 0$, finite ω:

$$\Pi(\omega, q) = -\nu \int \mathrm{d}\mathbf{n} \, \frac{(v_F \mathbf{n} \cdot \mathbf{q})^2}{\omega^2} = -\nu \frac{v_F^2 q^2}{3\omega^2} , \tag{3.332}$$

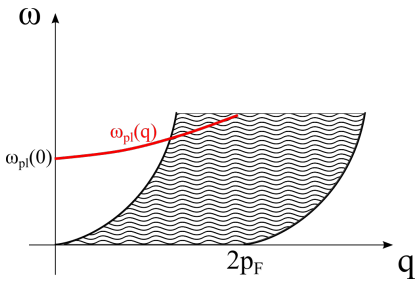
$$\epsilon(\omega, q) = 1 - \frac{4\pi e^2}{q^2} \nu \frac{v_F^2 q^2}{3\omega^2} = 1 - \left(\frac{\omega_{\text{pl}}}{\omega} \right)^2 , \tag{3.333}$$

where

$$\omega_{\text{pl}} = \left(\frac{4\pi}{3} e^2 \nu v_F^2 \right)^{\frac{1}{2}} , \tag{3.334}$$

is the **plasma frequency**.

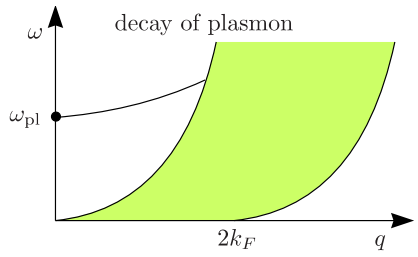
For $\omega = \omega_{\rm pl}$ we have $\varepsilon(\omega, q \to 0) = 0$, i.e., the pole of $U_{\rm eff}$. The pole in $U_{\rm eff}$ corresponds to excitations which can propagate. These excitations are collective bosonic excitations in the Fermi system with the Coulomb interaction and are called **plasmons**.



The plasmon dispersion $\omega_{\rm pl}(q)$ [with the plasma frequency (3.334) being $\omega_{\rm pl}(0)$] is determined by the equation

$$\epsilon(\omega, q) \equiv 1 + U(q)\Pi(\omega, q) = 0\,. \tag{3.335}$$

When the plasmon dispersion line enters the particle-hole continuum, the plasmons decay into particle-hole excitations as discussed above.



Chapter 4

Green's functions at $T \neq 0$. Matsubara Formalism

Above, we have developed the Green's-functions formalism at zero temperature, $T = 0$. This chapter describes the diagrammatic technique for $T \neq 0$.

For $T \neq 0$ the ground-state average is replaced by

$$\begin{aligned} \langle\, 0 \mid \ldots \mid 0 \,\rangle \qquad &\to \qquad \sum_n \frac{e^{-\beta E'_n}}{Z_G} \langle\, n \mid \ldots \mid n \,\rangle = \sum_n e^{\beta(\Omega - E'_n)} \langle\, n \mid \ldots \mid n \,\rangle \\ &= \qquad \sum_n \langle\, n \mid e^{\beta(\Omega - \widehat{H} + \mu \widehat{N})} \ldots \mid n \,\rangle, \end{aligned} \tag{4.1}$$

where n labels eigenstates of the Hamiltonian, E_n are the corresponding energies, $E'_n = E_n - \mu N_n$, and $\beta = 1/T$. Further, $Z_{\rm G}$ is the grand canonical partition function,

$$Z_{\rm G} = {\rm Tr}\, e^{-\beta(\widehat{H} - \mu \widehat{N})} = \sum_n \langle n | \exp[-\beta(\widehat{H} - \mu \widehat{N})] | n \rangle = \exp(-\beta \Omega)\,, \tag{4.2}$$

where we use the definition

$$\sum_n \langle n | \ldots | n \rangle \equiv {\rm Tr}\, \ldots\,, \tag{4.3}$$

and $\Omega(T, V, N) = (1/\beta) \ln Z_G$ is the grand canonical potential. The latter is related to free energy F and internal energy U via

$$\Omega = F - \mu N = U - ST - \mu N\,. \tag{4.4}$$

The corresponding relations in the differential form read as follows:

$$\mathrm{d}U = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}N\,, \quad \text{or} \quad \mathrm{d}\Omega = -S\,\mathrm{d}T - P\,\mathrm{d}V - N\,\mathrm{d}\mu\,. \tag{4.5}$$

Below we absorb $-\mu \widehat{N}$ in the definition of $\widehat{H}$, as we did in the $T = 0$ case.

We recall that at zero temperature we have obtained the Green function, upon transformation to the interaction representation, in the following form:

$$\begin{aligned} {\rm i}G(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) &= \langle 0 | \widehat{\mathcal{S}}^{-1} \mathcal{T} \widehat{S} \hat{\psi}_I(\mathbf{r}_1, t_1) \hat{\psi}^\dagger_I(\mathbf{r}_2, t_2) | 0 \rangle \\ &= \langle\, 0 \mid \widehat{\mathcal{S}}^{-1} \mid 0 \rangle \langle 0 | \mathcal{T} \widehat{S} \hat{\psi}_I(\mathbf{r}_1, t_1) \hat{\psi}^\dagger_I(\mathbf{r}_2, t_2) | 0 \rangle\,, \end{aligned} \tag{4.6}$$

where $|0\rangle = \langle \phi_{0,I}(-\infty)|$ is the non-interacting ground state. The transformation from the first to the second line of Eq. (4.6) was based on the property $\widehat{S}|0\rangle = \exp({\rm i}\alpha)|0\rangle$. As a result,

we have presented the Green's function as a ratio of two factors, $\langle 0|\mathcal{T}\widehat{S}\hat{\psi}_I(\mathbf{r}_1,t_1)\hat{\psi}_I^\dagger(\mathbf{r}_2,t_2)|0\rangle$ and $\langle 0|\widehat{S}|0\rangle$; each of them being an expectation vaue of a time-ordered product of interaction-representation operators (i.e., those with free dynamics) over the non-interacting ground state. Such averages are efficiently calculated via the Wick theorem, which was the basis for the perturbation theory.

At $T \neq 0$, the time-ordered Green's function can be defined as a natural generalization of the zero-temperature Green's function:

$$G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = -\mathrm{i}\,\mathrm{Tr}\left\{\exp(\beta(\Omega-\widehat{H}))\mathcal{T}\hat{\psi}_H(\mathbf{r},t)\hat{\psi}_H^\dagger(0,0)\right\}. \tag{4.7}$$

One can try to develop the perturbative expansion in the same way as for $T=0$: to perform a transformation to the interaction representation and to use a trick with switching off the interaction at $t\to\pm\infty$. In analogy with the first line of Eq. (4.6), we will then obtain

$$\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \sum_n \langle n|e^{\beta(\Omega-\widehat{H})}\widehat{S}^{-1}\mathcal{T}\,\widehat{S}\hat{\psi}_I(\mathbf{r}_1,t_1)\hat{\psi}_I^\dagger(\mathbf{r}_2,t_2)|n\rangle \tag{4.8}$$

Now we face several problems. First, Eq. (4.8) does not factorize in any simple way into a product (or ratio) of factors that are averages of time-ordered products. Second, the interaction now enters not only via $\widehat{S}$ but also via the statistical operator $e^{\beta(\Omega-\widehat{H}+\mu\widehat{N})}$, and any perturbative expansion should include this as well. Thus, an attempt to extend the $T=0$ calculation in a straightforward way fails.

A very elegant way to overcome this problem was found by Takeo Matsubara; the corresponding formalism bears his name.

4.1 Matsubara Green's function

The Matsubara Green's function is defined analogously to G but for **imaginary time**. The motivation is that the Gibbs factor $\exp(-\beta\widehat{H})$ looks like the evolution operator $U(-\mathrm{i}\beta)$,

$$e^{-\beta\widehat{H}} = e^{-i\widehat{H}t}|_{t=-i\beta}. \tag{4.9}$$

With this motivation, one considers the time t as imaginary, $t=-i\tau$, with real $\tau\in[0,\beta]$.

The Matsubara Green's function is defined as follows (recall that $\widehat{H}$ here is understood as $\widehat{H}-\mu\widehat{N}$):

$$\mathscr{G}_M(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2) = \begin{cases} -\mathrm{Tr}\,\exp[\beta(\Omega-\widehat{H})]\exp[\widehat{H}(\tau_1-\tau_2)]\hat{\psi}(\mathbf{r}_1)\exp[-\widehat{H}(\tau_1-\tau_2)]\hat{\psi}^\dagger(\mathbf{r}_2) & \text{for} \quad \tau_1>\tau_2 \\ \pm\mathrm{Tr}\,\exp[\beta(\Omega-\widehat{H})]\exp[-\widehat{H}(\tau_1-\tau_2)]\hat{\psi}^\dagger(\mathbf{r}_2)\exp[\widehat{H}(\tau_1-\tau_2)]\hat{\psi}(\mathbf{r}_1) & \text{for} \quad \tau_1<\tau_2 \end{cases}, \tag{4.10}$$

where the upper sign is for fermions and the lower sign for bosons. The operators $\hat{\psi}(\mathbf{r}_1)$ and $\hat{\psi}^\dagger(\mathbf{r}_2)$ are field operators in Schrödinger representation.

Equation (4.10) can be written in a compact form by using the following notations. First, in analogy with Heisenberg operators,

$$\hat{\psi}_H(\mathbf{r},t) = e^{i\widehat{H}t}\hat{\psi}(\mathbf{r})e^{-i\widehat{H}t}, \qquad \hat{\psi}_H^\dagger(\mathbf{r},t) = e^{i\widehat{H}t}\hat{\psi}^\dagger(\mathbf{r})e^{-i\widehat{H}t},$$

we define the "Matsubara-Heisenberg operators"

$$\psi_{\mathrm{MH}}(\mathbf{r},\tau) = \exp(\widehat{H}\tau)\hat{\psi}(\mathbf{r})\exp(-\widehat{H}\tau), \tag{4.11}$$

and

$$\overline{\psi}_{\rm MH}(\mathbf{r},\tau) = \exp(\widehat{H}\tau)\hat{\psi}^\dagger(\mathbf{r})\exp(-\widehat{H}\tau)\,. \tag{4.12}$$

Note that these operators are no longer hermitian conjugate to each other:

$$\overline{\psi}_{\rm MH}(\mathbf{r},\tau) \neq \psi^\dagger_{\rm MH}(\mathbf{r},\tau).$$

Second, we will use a compact notation for the thermodynamic average:

$$\mathrm{Tr}\,\exp[\beta(\Omega-\widehat{H})] = \langle\ldots\rangle\,, \tag{4.13}$$

Third, we define the τ-chronological product via

$$\mathcal{T}_\tau\,\psi_{\rm MH}(1)\overline{\psi}_{\rm MH}(2) = \begin{cases} \psi_{\rm MH}(1)\overline{\psi}_{\rm MH}(2) & \text{for} \quad \tau_1 > \tau_2 \\ \mp\overline{\psi}_{\rm MH}(2)\psi_{\rm MH}(1) & \text{for} \quad \tau_1 < \tau_2 \end{cases}\,, \tag{4.14}$$

with $(1) = (\mathbf{r}_1, t_1)$ and $(2) = (\mathbf{r}_2, t_2)$. With all the above conventions, the Matsubara Green's function takes the form

$$\boxed{\mathscr{G}_M(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2) = -\langle\mathcal{T}_\tau\psi_{\rm MH}(\mathbf{r}_1,\tau_1)\overline{\psi}_{\rm MH}(\mathbf{r}_2,\tau_2)\rangle\,.} \tag{4.15}$$

This formula has a remarkable similarity to the definition of the Green's function at zero T:

$$G(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2) \;\;=\;\; -i\langle\,\phi_0\mid\mathcal{T}\hat{\psi}(\mathbf{r}_1,t_1)\hat{\psi}^\dagger(\mathbf{r}_2,t_2)\mid\phi_0\rangle.$$

As we will show below, this analogy extends to the interaction representation and to the perturbative expansion.

What is the use of Matsubara Green's functions? It is immediately clear that they allow one to directly calculate thermodynamic quantities. For example, for the operator of the particle number,

$$\widehat{N} = \int \mathrm{d}^3r\,\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\,. \tag{4.16}$$

we have

$$N = \langle\widehat{N}\rangle = \int \mathrm{d}^3r\,\langle\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\rangle = \pm\int \mathrm{d}^3r\,\mathscr{G}_M(\mathbf{r},\tau;\mathbf{r},\tau+0)\,. \tag{4.17}$$

Thus, evaluation of the Matsubara Green's function directly yields $N(\mu,T)$. This can be converted into $\mu(n,T)$ where $n = N/V$ is the density. Using

$$\frac{\partial f}{\partial n} = \mu(n,T)\,, \tag{4.18}$$

one can then restore the free energy density $f = F/V$.

As we will show below, the Matsubara formalism allows one also to calculate various observables (such as response functions) at real times or frequencies by means of analytical continuation.

4.1.1 Properties of the Matsubara Green's function

(1) It is clear from the definition that

$$\mathscr{G}_M(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2) = \mathscr{G}_M(\mathbf{r}_1,\mathbf{r}_2,\tau=\tau_1-\tau_2)\,. \tag{4.19}$$

As usual, for a spatially homogeneous system, the dependence on coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ reduces to dependence on $\mathbf{r}_1-\mathbf{r}_2=\mathbf{r}$ only.

(2)
$$\delta\mathscr{G}_M \equiv \mathscr{G}_M(\mathbf{r},+0) - \mathscr{G}_M(\mathbf{r},-0) = -\langle[\psi(\mathbf{r}),\psi^\dagger(0)]_\pm\rangle = -\delta^{(3)}(\mathbf{r})\,, \tag{4.20}$$
Hence, there is a universal jump of $\mathscr{G}_M$ at $\tau = 0$, in analogy with conventional Green's functions.

(3) Equation (4.10) defines $\mathscr{G}(\mathbf{r},\tau)$ on the interval $-\beta < \tau < \beta$. (We recall that $\tau_1, \tau_2 \in [0,\beta]$.) By using the cyclic invariance of the trace, one obtains:
$$\begin{aligned}
\mathscr{G}(\mathbf{r},\tau<0) &= \pm\mathrm{Tr}[\exp(\beta\Omega)\exp(-\widehat{H}(\tau+\beta))\psi^\dagger(\mathbf{r}_2)\exp(\widehat{H}\tau)\psi(\mathbf{r}_1)] \\
&= \pm\mathrm{Tr}[\exp(\beta\Omega)\exp(\widehat{H}\tau)\psi(\mathbf{r}_1)\exp(-\widehat{H}(\tau+\beta))\psi^\dagger(\mathbf{r}_2)] \\
&= \pm\mathrm{Tr}[\exp(\beta(\Omega-\widehat{H}))\exp(\widehat{H}(\tau+\beta))\psi(\mathbf{r}_1)\exp(-\widehat{H}(\tau+\beta))\psi^\dagger(\mathbf{r}_2)] \\
&= \mp\mathscr{G}(\mathbf{r},\tau+\beta)\,, \qquad \tau+\beta>0\,.
\end{aligned} \tag{4.21}$$
Therefore, the Matsubara Green's function is β–periodic in the case of bosons and β–antiperiodic in the case of fermions. This will play a crucial role for definition of the Fourier transformation (to Matsubara frequencies) below.

4.2 The Matsubara Green's function for free particles

The free Hamiltonian is given by
$$\widehat{H}_0 = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}}\,, \tag{4.22}$$
with the dispersion relation
$$\varepsilon_{\mathbf{p}} = \frac{p^2}{2m} - \mu\,. \tag{4.23}$$
The field operators can be written in the form
$$\hat{\psi}(\mathbf{r}_1) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}_1}\exp(\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_1)\hat{a}_{\mathbf{p}_1}\,, \quad \hat{\psi}^\dagger(\mathbf{r}_2) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}_2}\exp(-\mathrm{i}\mathbf{p}_2\cdot\mathbf{r}_2)\hat{a}^\dagger_{\mathbf{p}_2}\,. \tag{4.24}$$
The Matsubara Green's function for free particles at $0<\tau<\beta$ then reads:
$$\begin{aligned}
\mathscr{G}_{M,0}(\mathbf{r}_1,\mathbf{r}_2,\tau>0) &= -\langle\psi_{\mathrm{MH}}(\mathbf{r}_1,\tau)\overline{\psi}_{\mathrm{MH}}(\mathbf{r}_2,0)\rangle \\
&= -\frac{1}{V}\sum_{\mathbf{p}_1,\mathbf{p}_2}\exp(\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_1 - \mathrm{i}\mathbf{p}_2\cdot\mathbf{r}_2) \\
&\quad\times\mathrm{Tr}[\exp(\beta(\Omega-\widehat{H}_0))\underbrace{\exp(\widehat{H}_0\tau)a_{\mathbf{p}_1}\exp(-\widehat{H}_0\tau)}_{\exp(-\varepsilon_{\mathbf{p}_1}\tau)a_{\mathbf{p}_1}}a^\dagger_{\mathbf{p}_2})] \\
&= -\frac{1}{V}\sum_{\mathbf{p}_1,\mathbf{p}_2}\exp(\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_1 - \mathrm{i}\mathbf{p}_2\cdot\mathbf{r}_2)\exp(-\varepsilon_{\mathbf{p}_1}\tau)\langle a_{\mathbf{p}_1}a^\dagger_{\mathbf{p}_2}\rangle\,.
\end{aligned} \tag{4.25}$$
The double sum over momenta reduces to a sum over one momentum since $\langle a_{\mathbf{p}_1}a^\dagger_{\mathbf{p}_2}\rangle \propto \delta_{\mathbf{p}_1\mathbf{p}_2}$. For fermions, we have
$$\langle a_{\mathbf{p}}a^\dagger_{\mathbf{p}}\rangle = 1 - \langle a^\dagger_{\mathbf{p}}a_{\mathbf{p}}\rangle = 1 - n_{\mathbf{p}}\,, \tag{4.26}$$
with the Fermi distribution
$$n_{\mathbf{p}} = \frac{1}{\exp(\beta\varepsilon_{\mathbf{p}})+1}\,, \tag{4.27}$$

and for bosons

$$\langle a_{\mathbf{p}} a_{\mathbf{p}}^{\dagger} \rangle = 1 + n_{\mathbf{p}} \,, \tag{4.28}$$

with Bose distribution

$$n_{\mathbf{p}} = \frac{1}{\exp(\beta\varepsilon_{\mathbf{p}}) - 1} \,. \tag{4.29}$$

One therefore gets

$$\begin{aligned} \mathscr{G}_{M,0}(\mathbf{r}, \tau > 0) &= -\frac{1}{V} \sum_{\mathbf{p}} \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r}) \exp(-\varepsilon_{\mathbf{p}}\tau)(1 \mp n_{\mathbf{p}}) \\ &= \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r}) \mathscr{G}_{M,0}(\mathbf{p}, \tau > 0) \,, \end{aligned} \tag{4.30}$$

with

$$\mathscr{G}_{M,0}(\mathbf{p}, \tau > 0) = -(1 \mp n_{\mathbf{p}}) \exp(-\varepsilon_{\mathbf{p}}\tau). \tag{4.31}$$

(In the second line of Eq. (4.30), we passed from summation over momenta to the integration in the standard way.) The inverse transformation reads:

$$\mathscr{G}_{M,0}(\mathbf{p}, \tau) = \int \mathrm{d}^3 r \, \exp(-\mathrm{i}\mathbf{p}\cdot\mathbf{r}) \mathscr{G}_{M,0}(\mathbf{r}, \tau) \,. \tag{4.32}$$

For $-\beta < \tau < 0$, we find

$$\begin{aligned} \mathscr{G}_{M,0}(\mathbf{p}, \tau < 0) &= \mp \mathscr{G}_{M,0}(\mathbf{p}, \tau + \beta) = \pm \exp(-\varepsilon_{\mathbf{p}}\tau) \exp(-\varepsilon_{\mathbf{p}}\beta) \left[1 \mp \frac{1}{\exp(\varepsilon_{\mathbf{p}}\beta) \pm 1} \right] \\ &= \pm \exp(-\varepsilon_{\mathbf{p}}\tau) \frac{1}{\exp(\varepsilon_{\mathbf{p}}\beta) \pm 1} \\ &= \pm \exp(-\varepsilon_{\mathbf{p}}\tau) n_{\mathbf{p}} \,. \end{aligned} \tag{4.33}$$

4.3 Interaction representation

Consider an interacting system

$$\widehat{H} = \widehat{H}_0 + \widehat{U},$$

with the term $-\mu\widehat{N}$ absorbed in $\widehat{H}_0$. We define the Matsubara-interaction representation (subscript "0" in addition to the Matsubara subscript "M") as a representation in which the operators have free Matsubara dynamics determined by H_0:

$$\psi_{M,0}(\mathbf{r}, \tau) = \exp(H_0\tau) \psi(\mathbf{r}) \exp(-H_0\tau) \,, \tag{4.34}$$

$$\overline{\psi}_{M,0}(\mathbf{r}, \tau) = \exp(H_0\tau) \psi^{\dagger}(\mathbf{r}) \exp(-H_0\tau) \,, \tag{4.35}$$

where $0 < \tau < \beta$. Relation between the Matsubara-Heisenberg and Matsubara-interaction representations:

$$\psi_{\mathrm{MH}}(\mathbf{r}, \tau) = \hat{S}^{-1}(\tau, 0) \psi_{M,0}(\mathbf{r}, \tau) \hat{S}(\tau, 0) \,, \tag{4.36}$$

where

$$\hat{S}(\tau, 0) = e^{\widehat{H}_0\tau} e^{-\widehat{H}\tau} \,. \tag{4.37}$$

is the evolution operator from 0 to τ. The general definition of the evolution operator is the same as for real times with the substitution $it \mapsto \tau$:

$$\hat{S}(\tau_1, \tau_2) = e^{\widehat{H}_0\tau_1} e^{-\widehat{H}(\tau_1 - \tau_2)} e^{-\widehat{H}_0\tau_2} \,. \tag{4.38}$$

All operators in the inetraction representation have the free dynamics determined by H_0; in particular, the interaction operator:

$$\widehat{U}_0(\tau) = \exp(\widehat{H}_0\tau)\widehat{U}\exp(-\widehat{H}_0\tau)\,. \tag{4.39}$$

Note that $\widehat{H}_0$ and $\widehat{N}$ remain independent of τ in the interaction representation, since they commute with $\widehat{H}_0$.

The equation of motion for $\hat{S}$ is given by

$$\begin{aligned}\frac{\partial\hat{S}(\tau_1,\tau_2)}{\partial\tau_1} &= e^{\widehat{H}_0\tau_1}(\widehat{H}_0-\widehat{H})e^{-\widehat{H}(\tau_1-\tau_2)}e^{-\widehat{H}_0\tau_2} = -e^{\widehat{H}_0\tau_1}\widehat{U}e^{-\widehat{H}(\tau_1-\tau_2)}e^{-\widehat{H}_0\tau_2}\\ &= -e^{\widehat{H}_0\tau_1}\widehat{U}e^{-\widehat{H}_0\tau_1}e^{\widehat{H}_0\tau_1}e^{-\widehat{H}(\tau_1-\tau_2)}e^{-\widehat{H}_0\tau_2}\\ &= -\widehat{U}_0(\tau_1)\hat{S}(\tau_1,\tau_2).\end{aligned} \tag{4.40}$$

The solution reads:

$$\boxed{\hat{S}(\tau_1,\tau_2) = \mathcal{T}_\tau \exp\left(-\int\limits_{\tau_2}^{\tau_1} \mathrm{d}\tau\,\widehat{U}_0(\tau)\right)\,.} \tag{4.41}$$

The properties of $\hat{S}$:

$$\hat{S}(\tau_1,\tau_3) = \hat{S}(\tau_1,\tau_2)\hat{S}(\tau_2,\tau_3)\,, \tag{4.42}$$

$$\hat{S}(\tau_1,\tau_2) = \hat{S}(\tau_1,0)\hat{S}^{-1}(\tau_2,0)\,. \tag{4.43}$$

Now, we can express the Matsubara Green's function in terms of the field operators in the interaction representation and the evolution operator. Consider first the case $\tau<0$ (i.e., $\tau_1>\tau_2$):

$$\begin{aligned}\mathscr{G}_M(\mathbf{r}_1,\mathbf{r}_2;\tau>0) &= -e^{\beta\Omega}\,\mathrm{Tr}[e^{-\beta H}\hat{S}^{-1}(\tau_1,0)\psi_{M,0}(\mathbf{r}_1,\tau_1)S(\tau_1,0)S^{-1}(\tau_2,0)\overline{\psi}_{M,0}(\mathbf{r}_2,\tau_2)S(\tau_2,0)]\\ &= -\exp(\beta\Omega)\mathrm{Tr}[\exp(-\beta H_0)\hat{S}(\beta,\tau_1)\psi_{M,0}(\mathbf{r}_1,\tau_1)\hat{S}(\tau_1,\tau_2)\overline{\psi}_{M,0}(\mathbf{r}_2,\tau_2)\hat{S}(\tau_2,0)]\\ &= -\exp[\beta(\Omega-\Omega_0)]\,\{\hat{S}(\beta,\tau_1)\psi_{M,0}(\mathbf{r}_1,\tau_1)\hat{S}(\tau_1,\tau_2)\overline{\psi}_{M,0}(\mathbf{r}_2,\tau_2)\hat{S}(\tau_2,0)\rangle_0\,,\end{aligned} \tag{4.44}$$

where

$$\langle\ldots\rangle_0 = \mathrm{Tr}\left(e^{\beta(\Omega_0-\widehat{H}_0)}\ldots\right)\,. \tag{4.45}$$

Proceeding in the same way for $\tau<0$ (i.e., $\tau_1<\tau_2$), we obtain

$$\mathscr{G}_M(\mathbf{r}_1,\mathbf{r}_2;\tau<0) = \pm\exp[\beta(\Omega-\Omega_0)]\,\{\hat{S}(\beta,\tau_2)\overline{\psi}_{M,0}(\mathbf{r}_2,\tau_2)\hat{S}(\tau_2,\tau_1)\psi_{M,0}(\mathbf{r}_1,\tau_1)\hat{S}(\tau_1,0)\rangle_0\,. \tag{4.46}$$

Further, for the evolution operator over the whole interval $[0,\beta]$,

$$\mathcal{S} = \hat{S}(\beta,0)\,, \tag{4.47}$$

we have

$$\begin{aligned}\langle\,\mathcal{S}\,\rangle_0 &= \mathrm{Tr}\left[e^{\beta(\Omega_0-\widehat{H}_0)}\hat{S}(\beta,0)\right] = \mathrm{Tr}\left[e^{\beta(\Omega_0-\widehat{H}_0)}e^{\widehat{H}_0\beta}e^{-\widehat{H}\beta}\right]\\ &= e^{\beta\Omega_0}\mathrm{Tr}(e^{-\beta\widehat{H}}),\end{aligned} \tag{4.48}$$

which yields

$$\boxed{\langle\mathcal{S}\rangle_0 = \exp[-\beta(\Omega-\Omega_0)]\,.} \tag{4.49}$$

Combining Eqs. (4.44) and (4.46) and using Eq. (4.49), we get the final result for the Matsubara Green's function in the interaction representation:

$$\boxed{\mathscr{G}_M(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2) = -\frac{\langle T_\tau\, \mathcal{S}\psi_{M,0}(\mathbf{r}_1,\tau_1)\overline{\psi}_{M,0}(\mathbf{r}_2,\tau_2)\rangle_0}{\langle \mathcal{S}\rangle_0}\,.} \tag{4.50}$$

Note that here was no need to use the trick with adiabatic switching on / off of the interaction in this derivation.

The denominator in Eq. (4.50) is the sum of vacuum diagrams $\langle\mathcal{S}\rangle_0$. According to Eq. (4.49), it determines the interaction-induced contribution to the grand canonical potential:

$$\Omega - \Omega_0 = -T\ln\langle\mathcal{S}\rangle_0\,. \tag{4.51}$$

According to the linked cluster expansion (see Sec. 3.10.2), $\ln\langle\mathcal{S}\rangle_0$ is the sum of all connected vacuum diagrams.

4.4 Wick's theorem at $T \neq 0$

Diagrammatics in Matsubara formalism is developed on the basis of formulas for the Green's function $\mathscr{G}_M$, (4.50) and for the grand canonical potential Ω, (4.51), in analogy with the $T = 0$ formalism. We expand the evolution operator

$$\widehat{\mathcal{S}} = \mathcal{T}_\tau \exp\left(-\int\limits_0^\beta \mathrm{d}\tau\, \widehat{U}_0(\tau)\right) \tag{4.52}$$

in the interaction:

$$\widehat{\mathcal{S}} = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int\limits_0^\beta \mathrm{d}\tau_1 \ldots \int\limits_0^\beta \mathrm{d}\tau_n\, \mathcal{T}_\tau \widehat{U}_0(\tau_1)\ldots\widehat{U}_0(\tau_n),, \tag{4.53}$$

with

$$\widehat{U}_0(\tau) = \frac{1}{2}\int \mathrm{d}r\mathrm{d}r'\,\overline{\psi}_{M,0}(\mathbf{r},\tau)\overline{\psi}_{M,0}(\mathbf{r}',\tau)U(\mathbf{r}-\mathbf{r}')\psi_{M,0}(\mathbf{r}',\tau)\psi_{M,0}(\mathbf{r},\tau)\,. \tag{4.54}$$

Thus, we have to evaluate thermal expectation values of the type

$$\langle \mathcal{T}_\tau \psi_{M,0}(\mathbf{r}_1,\tau_1)\ldots\overline{\psi}_{M,0}(\mathbf{r}_p,\tau_p)\rangle_0\,. \tag{4.55}$$

As in the zero-temperature technique, this is done by means of Wick theorem.

At $T = 0$, when deriving the Wick theorem for expectation values, we used the operator version of the theorem, Eq. (3.167), that expressed the chronological product as a sum of normal-ordered products. This approach is not useful at $T \neq 0$: the notion the normal ordering was defined with respect to the ground state but thermodynamic averages involve also excited states. Nevertheless, the Wick theorem for expectation values can be generalized to the case of finite temperature.

The Hamiltonian H_0 of the non-interacting system has the form

$$H_0 = \sum_\lambda \varepsilon_\lambda a_\lambda^\dagger a_\lambda\,, \tag{4.56}$$

where λ is a set of quantum numbers that label single-particle states. (Below we will assume that this is momentum $\mathbf{p}$ but this is not essential.) Eigenstates have the form (with the appropriate normalization for bosons):

$$|n_1, n_2, \ldots\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\ldots|0\rangle\,. \tag{4.57}$$

We expand the field operators in the Matsubara interaction representation in annihilation and creation operators:

$$\psi_{M,0}(\mathbf{r},\tau) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} a_{\mathbf{p}}(\tau)\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \varepsilon_{\mathbf{p}}\tau)\,, \tag{4.58}$$

and

$$\overline{\psi}_{M,0}(\mathbf{r},\tau) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} a_{\mathbf{p}}^\dagger(\tau)\exp(-\mathrm{i}\mathbf{p}\cdot\mathbf{r} + \varepsilon_{\mathbf{p}}\tau)\,. \tag{4.59}$$

Here the indices τ in $a^\dagger(\tau)$ and $a(\tau)$ do not mean any time dependence but only serve to keep the proper time ordering. The terms in the expansion of $\widehat{\mathcal{S}}$ take the form (V is volume):

$$\frac{1}{\sqrt{V}}\sum_{\mathbf{p}_1}\frac{1}{\sqrt{V}}\sum_{\mathbf{p}_2}\cdots\frac{1}{\sqrt{V}}\sum_{\mathbf{p}_1'}\frac{1}{\sqrt{V}}\sum_{\mathbf{p}_2'}\cdots\langle\mathcal{T}_\tau a_{\mathbf{p}_1}(\tau_1)a_{\mathbf{p}_2}(\tau_2)\ldots a_{\mathbf{p}_1'}^\dagger(\tau_1')a_{\mathbf{p}_2'}^\dagger(\tau_2')\rangle_0\,. \tag{4.60}$$

The average $\langle\ldots\rangle_0$ implies the sum of expectation values over the eigenstates (4.57), with the thermal weights. Obviously, it is nonzero only if every $a_{\mathbf{p}}^\dagger$ finds a partner $a_{\mathbf{p}}$. Further, the thermal distributions of populations of different single-particle states are uncorrelated. This implies decoupling of expectation values. For example,

$$\langle\,\mathcal{T}_\tau a_{\mathbf{p}}a_{\mathbf{p}'}a_{\mathbf{p}'}^\dagger a_{\mathbf{p}}^\dagger\,\rangle_0 = \langle\,\mathcal{T}_\tau a_{\mathbf{p}'}a_{\mathbf{p}'}^\dagger\,\rangle_0\langle\,T_\tau a_{\mathbf{p}}a_{\mathbf{p}}^\dagger\,\rangle_0 \qquad (\mathbf{p}\neq\mathbf{p}')\,. \tag{4.61}$$

The only special case is $\mathbf{p} = \mathbf{p}'$. These terms are, however, suppressed by a factor $1/V$,

$$\frac{1}{V^2}\sum_p\langle\,\mathcal{T}_\tau a_{\mathbf{p}}a_{\mathbf{p}}a_{\mathbf{p}}^\dagger a_{\mathbf{p}}^\dagger\,\rangle_0 = \frac{1}{V}\int\frac{d^dp}{(2\pi)^d}\langle\,\mathcal{T}_\tau a_{\mathbf{p}}a_{\mathbf{p}}a_{\mathbf{p}}^\dagger a_{\mathbf{p}}^\dagger\,\rangle_0 \sim \frac{1}{V}\xrightarrow{V\to\infty}0\,,$$

so that they are of no interest for us. In fact, one can show that the Wick theorem (formulated below) applies to them as well, i.e. it is exact also without the limit $V\to\infty$. A very elegant proof of the Wick theorem based on the functional-integral formulation of the theory will be provided below, see Sec. 6.1.4. Within the functional-integral formalism, the Wick theorem is related to exact general properties of Gaussian integrals.

To summarize, we have at $T\neq 0$ the **Wick theorem** for thermal expectation values of the type (4.55), which has essentially the same form as for $T=0$, Eq. (3.152):

$$\langle\mathcal{T}_\tau[\ldots]\rangle_0 = \sum\text{products of pairwise contractions}\cdot(\pm1)^P\,, \tag{4.62}$$

where the sum goes over all contraction patterns and $(-1)^P$ is, as usual, the permutation factor for fermions. Each pair contraction yields the thermal average of the corresponding pair product as in Eq. (4.61).

Here is an example of application of the Wick theorem:

$$\begin{aligned}
&\langle\mathcal{T}_\tau\psi_{M,0}(1)\psi_{M,0}(2)\overline{\psi}_{M,0}(1')\overline{\psi}_{M,0}(2')\rangle_0\\
&= \langle\mathcal{T}_\tau\psi_{M,0}(1)\overline{\psi}_{M,0}(2')\rangle_0\langle\mathcal{T}_\tau\psi_{M,0}(2)\overline{\psi}_{M,0}(1')\rangle_0 \mp \langle\mathcal{T}_\tau\psi_{M,0}(1)\overline{\psi}_{M,0}(1')\rangle_0\langle\mathcal{T}_\tau\psi_{M,0}(2)\overline{\psi}_{M,0}(2')\rangle_0\\
&= [-\mathscr{G}_{M,0}(1,2')][-\mathscr{G}_{M,0}(2,1')] \mp [-\mathscr{G}_{M,0}(1,1')][-\mathscr{G}_{M,0}(2,2')]\,.
\end{aligned} \tag{4.63}$$

With Wick theorem at our disposal, we can proceed with development of the perturbative expansion in powers of $\widehat{U}$ and of the corresponding diagrammatic technique, in full analogy with the $T=0$ case.

4.5 Matsubara diagrammatic technique in real space

The Matsubara diagrammatic technique is now developed in the same way as for $T = 0$, see Sec. 3.9. The rules are nearly the same, with differences in factors associated with diagrams and in the domain of time integration that follow from the comparison between the $T \neq 0$ and $T = 0$ expressions:

$$\mathscr{G}_{M,0} = -\langle \ldots \rangle_0 \qquad \text{instead of} \qquad G_0 = -\mathrm{i}\langle 0| \ldots |0\rangle,$$

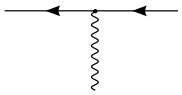
$$\widehat{\mathcal{S}} = \mathcal{T}_\tau \left\{ \exp\left(-\int \ldots \right) \right\} \qquad \text{instead of} \qquad \widehat{S} = \mathcal{T} \exp\left(-\mathrm{i} \int \ldots \right),$$

$$\int_0^\beta \mathrm{d}\tau \ldots \qquad \text{instead of} \qquad \int_{-\infty}^{+\infty} \mathrm{d}t \ldots .$$

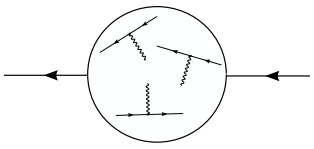
The rules are as follows:

(1) Draw all topologically different connected diagrams with $2n$ interaction vertices (i.e., n pairs of vertices; each pair is connected by an interaction line).

At each vertex, there is one incoming fermionic line, one outgoing fermionic line, and one interaction line:



Diagrams for the Green's function have two external fermionic legs (one incoming, one outgoing):



(2) $1 \longleftarrow 2 \;=\; \mathscr{G}_{M,0}(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2)$.

(3) $1 \sim\sim 2 \;=\; U(\mathbf{r_1} - \mathbf{r_2})\delta(\tau_1 - \tau_2)$.

(4) $\int \mathrm{d}r \int_0^\beta \mathrm{d}\tau$ over all internal coordinates and time arguments.

(5) Assign a factor $(-1)^n (\mp 1)^L (2S+1)^L$.

Comment on the factor $(-1)^n$*:* With each additional order of the perturbation theory one gets one additional interaction line, and with it the factor (-1) from the expansion of $\mathcal{T}_\tau \exp(-\ldots)$. At the same time, one gets two additional fermionic lines, each bringing (-1) in view of $\langle \ldots \rangle_0 = -\mathscr{G}_{M,0}$. Thus, in total, an additional factor $(-1)^3 = -1$ with each additional order, yielding $(-1)^n$ in n-th order.

(6) $\mathscr{G}_{M,0}(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2) \overset{\tau_1 = \tau_2}{=} \mathscr{G}_{M,0}(\mathbf{r}_1, \mathbf{r}_2, -0)$.

The above rules fully determine the diagrammatic expansion for the Green's function. In the case of diagrams for Ω, i.e. the vacuum diagrams, one has to take into account in addition the symmetry factors:

(7) Symmetry factors for vacuum diagrams are the same as at $T = 0$, see Sec. 3.10.1.

4.6 Matsubara frequencies

The Matsubara diagrammatics above is defined in the coordinate-"time" $(\mathbf{r}, \tau)$ space. As in the case of $T = 0$ diagrammatics, it is convenient to perform a transformation to the energy-momentum space. The transformation from coordinate to momentum space, $\mathbf{r} \to \mathbf{p}$, proceeds in the same way as for $T = 0$. As a result, each line in the diagram is characterized by a momentum, with momentum conservation in all vertices and integration over all independent internal momenta. The Matsubara Green's function of free particles in $(\mathbf{p}, \tau)$ representation has been already calculated in Sec. 4.2.

Consider now the transformation $\tau \to \omega$. The Matsubara Green's function $\mathscr{G}_M(\tau)$ was defined so far in $-\beta \le \tau < \beta$, with the property $\mathscr{G}_M(\tau < 0) = \mp\mathscr{G}_M(\tau + \beta)$. Formally, one can continue $\mathscr{G}_M(\tau)$ periodically:

$$\mathscr{G}_M(\tau) = \mp\mathscr{G}_M(\tau + \beta), \qquad \tau \in [-\infty, \infty]. \tag{4.64}$$

For a periodic function, the Fourier transformation with respect to τ involve discrete values of frequency ω_n, thus representing $\mathscr{G}_M(\tau)$ as a Fourier series (i.e., we have a sum over ω_n rather than integral):

$$\mathscr{G}_M(\tau) = \frac{1}{\beta} \sum_n \exp(-\mathrm{i}\omega_n \tau) \mathscr{G}_M(\omega_n)\,. \tag{4.65}$$

The coefficients $\mathscr{G}_M(\omega_n)$ can be obtained by

$$\mathscr{G}_M(\omega_n) = \int_0^\beta \mathrm{d}\tau\, \exp(\mathrm{i}\omega_n \tau) \mathscr{G}_M(\tau)\,. \tag{4.66}$$

The frequencies ω_n over which the summation in Eq. (4.65) is performed are (we recall that $\beta^{-1} = T$, where T is the temperature):

$$\omega_n = \begin{cases} 2n\pi T & \text{for bosons} \\ (2n+1)\pi T & \text{for fermions} \end{cases} \qquad n - \text{integer}. \tag{4.67}$$

This follows from the conditions of periodicity (bosons) or antiperiodicity (fermions). Indeed, we have for bosons

$$\begin{aligned} \mathscr{G}_M(\tau = \beta) &\overset{(4.65)}{=} \frac{1}{\beta} \sum_n e^{-i\omega_n \beta} \mathscr{G}_M(\omega_n) \overset{!}{=} \frac{1}{\beta} \sum_n \mathscr{G}_M(\omega_n) = \mathscr{G}_M(\tau = 0) \\ &\to \qquad \omega_n \beta = 2\pi n \qquad \to \qquad \omega_n = 2\pi n T, \end{aligned}$$

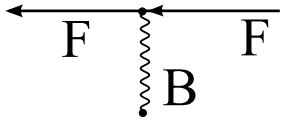
while for fermions

$$\begin{aligned} \mathscr{G}_M(\tau = \beta) &\overset{(4.65)}{=} \frac{1}{\beta} \sum_n e^{-i\omega_n \beta} \mathscr{G}_M(\omega_n) \overset{!}{=} -\frac{1}{\beta} \sum_n \mathscr{G}_M(\omega_n) = -\mathscr{G}_M(\tau = 0) \\ &\to \qquad \omega_n \beta = (2n+1)\pi n \qquad \to \qquad \omega_n = (2n+1)\pi T. \end{aligned}$$

For fermions one often writes ε_n instead of ω_n to distinguish the fermionic Matsubara energies from the bosonic frequencies (the latter are sometimes denoted by ν_n).

Very generally, every vertex involves several fermionic and bosonic lines. One then obtains after integration over the time τ associated with this vertex:

$$\int_0^\beta \mathrm{d}\tau\, \exp\left(\mathrm{i}\tau \left\{ \sum \varepsilon_n + \sum \nu_m \right\}\right) = \beta\, \delta_{\sum \varepsilon_n + \sum \nu_m,\, 0} \tag{4.68}$$



This ensures the energy conservation similarly to the momentum conservation for the transformation $\mathbf{r} \to \mathbf{p}$.

4.7 $\mathscr{G}_M(\mathbf{p}, \omega_n)$ for free particles

The Fourier transform of

$$\mathscr{G}_{M,0}(\mathbf{p}, \tau) = -[1 \mp n(\mathbf{p})] \exp(-\varepsilon_{\mathbf{p}} \tau) \,, \quad 0 < \tau < \beta \,. \tag{4.69}$$

is given by

$$\begin{aligned} \mathscr{G}_{M,0}(\mathbf{p}, \omega_n) &= -[1 \mp n(\mathbf{p})] \int_0^\beta \mathrm{d}\tau \, \exp(\mathrm{i}\omega_n \tau) \exp(-\varepsilon_{\mathbf{p}} \tau) \\ &= -[1 \mp n(\mathbf{p})] \frac{1}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{p}}} \left[\exp(\mathrm{i}\omega_n \beta) \exp(-\varepsilon_{\mathbf{p}} \beta) - 1\right] \\ &= \frac{1}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{p}}} \,. \end{aligned} \tag{4.70}$$

Here, we have used $e^{i\omega_n \beta} = \mp 1$ and

$$1 \mp n(\mathbf{p}) = 1 \mp \frac{1}{\exp(\beta \varepsilon_{\mathbf{p}}) \pm 1} = \frac{1}{1 \pm \exp(-\varepsilon_{\mathbf{p}} \beta)} \,. \tag{4.71}$$

Note that Eq. (4.70) has the same form for fermions and bosons. The difference is in the allowed values of ω_n.

It is instructive to compare the (real-time) free Green's function for $T = 0$ and the Matsubara (imaginary-time) free Green's function for $T \neq 0$; the correspondence is quite clear:

$$G^{(0)}(p, \omega) = \frac{1}{\omega - \varepsilon_p + i0 \, \mathrm{sign}(\omega)} \,, \qquad \mathscr{G}_{M,0}(p, \omega_n) = \frac{1}{i\omega_n - \varepsilon_p}.$$

For **phonons**, one can perform an analogous calculation to find the Matsubara phonon propagator:

$$D(\mathbf{k}, \nu_n) = -\frac{\omega_{\mathbf{k}}^2}{\nu_n^2 + \omega_{\mathbf{k}}^2} \,, \quad \omega_{\mathbf{k}} = s|\mathbf{k}| \,. \tag{4.72}$$

It should be compared to the $T = 0$, real-time phonon propagator calculated below, see Eq. (5.8). Again, the correspondence is clear.

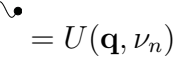
4.8 Diagrammatics in momentum-frequency domain

(1) We associate with every line an energy and a momentum $(\mathbf{q}, \omega_n)$
with $\omega_n = \varepsilon_n = (2n+1)\pi T$ for fermions and $\omega_n = \nu_n = 2n\pi T$ for bosons.

(2) Energy and momentum are conserved at every vertex.

(3) 

$= \dfrac{1}{\mathrm{i}\varepsilon_n - \varepsilon_{\mathbf{p}}} \equiv \mathscr{G}_{M,0}(\varepsilon_n, \mathbf{p})$.

(4) 

$= U(\mathbf{q}, \nu_n) \underbrace{=}_{\text{if no retardation}} U(\mathbf{q})$.

(5) Integrate over momenta and sum over frequencies for all internal loops:

$$\prod_i \left(\int \frac{\mathrm{d}^3 p_i}{(2\pi)^3} \frac{1}{\beta} \sum_{n_i} \right) \dots$$

(6) Assign a factor $(-1)^n (\mp 1)^L (2S+1)^L$, where n is the order of perturbation theory (number of interaction lines), and L the number of closed fermionic loops.

(7) For a fermionic line both ends of which are attached to the same interaction line (like in Hartree and Fock diagrams), i.e. correspond to the same Matsubara time, include a factor $e^{\mathrm{i}\varepsilon_n 0}$.

(8) For vacuum diagrams (when Ω is calculated), take into account symmetry factors.

Comment: Let us consider the correspondence between the $T = 0$ diagrammatics and the Matsubara diagrammatics for $T \neq 0$:

$$\begin{aligned} \varepsilon,\, \omega \qquad &\longrightarrow \quad \mathrm{i}\varepsilon_n,\, \mathrm{i}\nu_n \text{ with } \varepsilon_n = (2n+1)\pi T,\, \nu_n = 2n\pi T \\ \int \frac{\mathrm{d}\varepsilon}{2\pi}, \int \frac{\mathrm{d}\omega}{2\pi} \quad &\longrightarrow \quad \frac{\mathrm{i}}{\beta} \sum_{\varepsilon_n}, \; \frac{\mathrm{i}}{\beta} \sum_{\nu_n} \end{aligned}$$

Limit $T \to 0$ from Matsubara:

$$\Delta\omega_n = \omega_{n+1} - \omega_n = 2\pi T \quad \text{both for bosons and fermions,}$$

so that in the $T \to 0$ limit sums become integrals:

$$T \sum_{\omega_n} \mapsto \int \frac{\mathrm{d}\omega}{2\pi}\,, \tag{4.73}$$

as in the $T = 0$ technique. It should be stressed, however, that the corresponding frequencies are imaginary from the point of view of usual $T = 0$ technique. In particular, $\mathscr{G}_M(\omega)$ obtained in zero-T limit of the Matsubara diagrammatics is not the same as $G(\omega)$, as one still has to perform the analytic continuation from imaginary to real frequencies (see below). Upon this continuation, the $T \to 0$ limiting formulas of the Matsubara formalism transform into formulas of the conventional $T = 0$ diagrammatics.

4.9 Calculating sums over Matsubara frequencies

When evaluating Matsubara diagrams, one encounters sums over Matsubara frequencies. We present now the technique (based on contour integration in the plane of complex frequency) that allows one to evaluate such sums. The resulting expressions will be convenient for analytical continuation to real external frequencies, which is needed to obtain physical observables (such as response functions), as will be discussed later.

Let us start from a simple example and consider

$$n_{\mathbf{p}} = \langle c^\dagger_{\mathbf{p}} c_{\mathbf{p}} \rangle = \mathscr{G}(\mathbf{p}, -0) = \frac{1}{\beta} \sum_n \frac{1}{\mathrm{i}\varepsilon_n - \varepsilon_{\mathbf{p}}} \exp(\mathrm{i}\varepsilon_n 0)\,. \tag{4.74}$$

We know, of course, that the result should be given by the Fermi function but want to see how it is obtained by the Matsubara technique. To evaluate this sum, consider the Fermi function as a function of a complex variable z:

$$f(z) = \frac{1}{\exp(z\beta) + 1}\,. \tag{4.75}$$

This function has simple poles with residues $-\frac{1}{\beta}$ at $z = \mathrm{i}\varepsilon_n \equiv \mathrm{i}\,2\pi(n+1)T$ for all integer n. To check this, we caculate $f(z)$ for $z = \mathrm{i}\varepsilon_n + \delta$ with $\delta \to 0$:

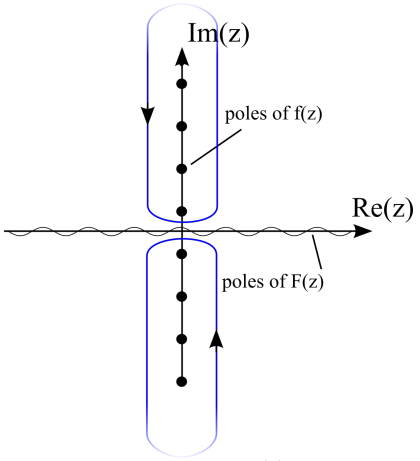
$$f(\mathrm{i}\varepsilon_n + \delta) = \frac{1}{\exp(\mathrm{i}\varepsilon_n\beta)\exp(\delta\beta) + 1} = \frac{1}{-\exp(\delta\beta) + 1} \approx \frac{1}{-\delta\beta} = \frac{-\frac{1}{\beta}}{\delta}\,. \tag{4.76}$$

Thus, $f(z)$ indeed has first-order poles on the imaginary axis, at $z = \mathrm{i}\varepsilon_n$, where ε_n are fermionic Matsubara frequencies, with the residues $-\frac{1}{\beta}$. It is easy to check that $f(z)$ does not have any other singularities in the complex plane.

It follows that, for a general function $\mathcal{F}(z)$ (satisfying assumptions formulated below),

$$\frac{1}{\beta}\sum_n \mathcal{F}(\mathrm{i}\varepsilon_n) = -\oint_{\mathcal{C}} \frac{\mathrm{d}z}{2\pi\mathrm{i}}\,\mathcal{F}(z)f(z)\,. \tag{4.77}$$

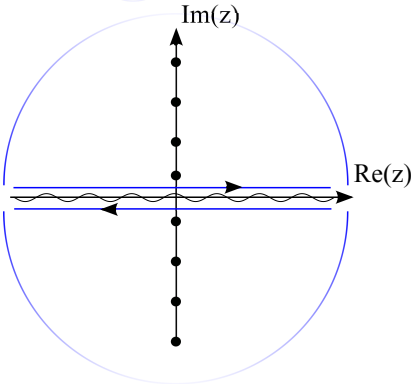
with the integration contour $\mathcal{C}$ shown in the figure to the right. (The contour consists of two parts, one above the real axis, and one below the real axis.) The assumption here is that the functions $\mathcal{F}(z)$ has its singularities (poles and/or branch cuts) only on the real axis of z.



We now transform the contour:

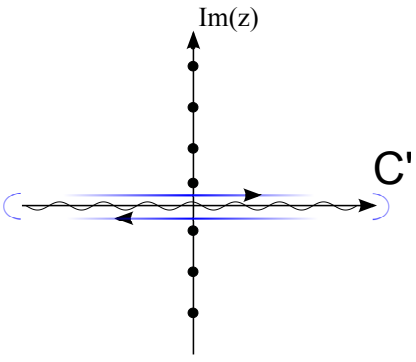
$$-\oint_{\mathcal{C}} \frac{dz}{2\pi i}\mathcal{F}(z)f(z) = -\oint_{\mathcal{C}'} \frac{dz}{2\pi i}\mathcal{F}(z)f(z)\,,$$

so that it now consists of two sections going near the real axis as well as two arcs of infinite radius. The integral over the arcs can be neglected if we assume (in addition to the above assumprion that singularities of $\mathcal{F}(z)$ are on the real axis only) that $\mathcal{F}(z)f(z)|z| \to 0$ for $|z| \to \infty$.



As a result we obtain the integral over a contour $\mathcal{C}'$ going along the real axis and encircling singularities of $\mathcal{F}(z)$ there:

$$\frac{1}{\beta}\sum_n \mathcal{F}(\mathrm{i}\varepsilon_n) = -\oint_{\mathcal{C}'} \frac{\mathrm{d}z}{2\pi\mathrm{i}}\,\mathcal{F}(z)f(z)\,. \tag{4.78}$$



Thus, we only have to calculate the integral along the real axis, which will be determined by singularities (in simple cases, poles) of $\mathcal{F}(z)$. This scheme can be extended to more complicated situations, as we will demonstrate in the following subsections.

Let us now apply the obtained result (4.78) to the example (4.74). In this case, we have

$$\mathcal{F}(z) = \frac{1}{z - \varepsilon_{\mathbf{p}}} \exp(z \cdot 0)\,. \tag{4.79}$$

First, we check that the assumptions about $\mathcal{F}(z)$ are fulfilled. First, the function $\mathcal{F}(z)$ has the only pole at $z = \varepsilon_{\mathbf{p}}$, i.e., on the real axis, as required. Second,

$$\begin{array}{ll} \text{for } \mathrm{Re}\, z > 0: & f(z) \sim e^{-\beta z} \to 0\,, \\ \text{for } \mathrm{Re}\, z < 0: & e^{z0} \to 0\,, \end{array}$$

so that

$$f(z)\mathcal{F}(z) = \frac{1}{z - \varepsilon_{\mathbf{p}}} \exp(z \cdot 0) \frac{1}{\exp(z\beta) + 1}$$

drops indeed faster than $1/|z|$. Thus, all conditions are fulfilled, so that the application of Eq. (4.78) is justified. It yields

$$n_{\mathbf{p}} = -\oint_{C'} \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{\exp(z \cdot 0)}{z - \varepsilon_{\mathbf{p}}} f(z) = f(\varepsilon_{\mathbf{p}})\,, \tag{4.80}$$

which is the correct result: $n_{\mathbf{p}}$ is equal to the Fermi function.

It is now straightforward to carry out an analogous calculation for bosons, Instead of the Fermi function function $f(z)$, we should then take the Bose function

$$g(z) = \frac{1}{\exp(\beta z) - 1}\,. \tag{4.81}$$

It is easy to check that $g(z)$ has simple poles at $z = \mathrm{i}\nu_n \equiv \mathrm{i}\, 2\pi n T$, where ν_n are bosonic Matsubara frequencies, with residues $1/\beta$. The resulting Matsubara sum, in the form valid for both fermions and bosons (upper and lower sign, as usual) reads:

$$\frac{1}{\beta} \sum_n \frac{\exp(\mathrm{i}\omega_n \cdot 0)}{\mathrm{i}\omega_n - x} = \pm \frac{1}{\exp(\beta x) \pm 1}\,. \tag{4.82}$$

For bosons, the overall minus sign in Eq. (4.82) is compensated by the minus sign in $n_{\mathbf{p}} = -\mathscr{G}_{M,0}(\mathbf{p}, -0)$, so that $n_{\mathbf{p}}$ is given by the Bose function, as it should be.

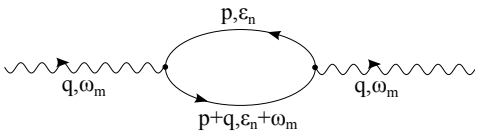
4.9.1 Polarization operator

We consider the polarization operator Π_M of free fermions at finite temperature in the Matsubara formalism. The polarization operator is defined as (-1) times the Matsubara density-density response function $\mathscr{D}^M_{\rho\rho}$, which is (see Sec. 4.106 for general definition of Matsubara response functions and their relation to physical, i.e., real time, response functions):

$$\mathscr{D}^M_{\rho\rho}(\mathbf{r}, \tau) = -\langle \mathcal{T}_\tau \widehat{\rho}(\mathbf{r}, \tau) \widehat{\rho}(0, 0) \rangle\,. \tag{4.83}$$

Thus, the polarization operator is given by Eq. (4.83) but with the opposite sign (i.e., with plus sign in front). For free fermions, this yields the following bubble diagram:

$\Pi_M(\mathbf{q}, \omega_m)$ =



(4.84)

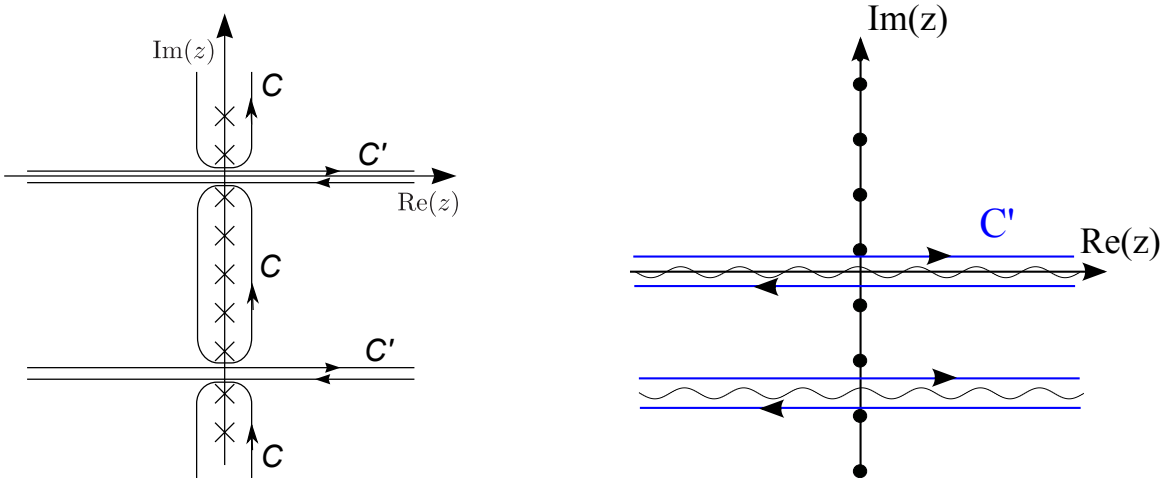
According to the rules of Matsubara diagrammatics, we get (with factor 2 for spin and -1 for fermion loop):

$$\Pi_M(\mathbf{q},\omega_m) = (-1)\cdot 2\int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{1}{\beta}\sum_{\varepsilon_n}\mathscr{G}_{M,0}(\mathbf{p}+\mathbf{q},\varepsilon_n+\omega_m)\mathscr{G}_{M,0}(\mathbf{p},\varepsilon_n). \tag{4.85}$$

The incoming frequency ω_m is bosonic. The summation over the internal fermionic energy ε_n is performed using the contour integration:

$$\begin{aligned}\frac{1}{\beta}\sum_{\varepsilon_n}\mathscr{G}_{M,0}(\mathbf{p}+\mathbf{q},\varepsilon_n+\omega_m)\mathscr{G}_{M,0}(\mathbf{p},\varepsilon_n) &= \frac{1}{\beta}\sum_{\varepsilon_n}\frac{1}{\mathrm{i}(\varepsilon_n+\omega_m)-\varepsilon_{\mathbf{p}+\mathbf{q}}}\cdot\frac{1}{\mathrm{i}\varepsilon_n-\varepsilon_{\mathbf{p}}}\\ &= -\oint_{\mathcal{C}}\frac{\mathrm{d}z}{2\pi\mathrm{i}}\underbrace{\frac{1}{z+\mathrm{i}\omega_m-\varepsilon_{\mathbf{p}+\mathbf{q}}}\,\frac{1}{z-\varepsilon_{\mathbf{p}}}}_{\mathcal{F}(z)}f(z)\,.\end{aligned} \tag{4.86}$$

The function $\mathcal{F}(z)$ has now singularities not only on the real axis $\mathrm{Im}\,z=0$ but also on a line parallel to the real axis, $\mathrm{Im}\,z=-\mathrm{i}\omega_m$. These two lines divide the imaginary axis, where poles of $f(z)$ are located, into three parts. In view of this, the integration contour $\mathcal{C}$ now consists of three parts, as shown in the figure. We deform again the contour, $\mathcal{C}\mapsto\mathcal{C}'$, such that the new contour $\mathcal{C}'$ encircles the lines $\mathrm{Im}\,z=0$ and $\mathrm{Im}\,z=-\mathrm{i}\omega_m$ where the singularities of $\mathcal{F}(z)$ are located:



The transformation is justified since the function $\mathcal{F}(z)$ decays fast at large $|z|$:

$$\mathcal{F}(z)\xrightarrow{z\to\infty}\frac{1}{z^2}.$$

We are thus left with the integral as in Eq. (4.86) but along the contour $\mathcal{C}'$. This integral is determined by singularities of $\mathcal{F}(z)$. This functions has two poles: at $z=\varepsilon_{\mathbf{p}}$ and $z=\varepsilon_{\mathbf{p}+\mathbf{q}}-i\omega_m$. Evaluating the corresponding residues, we obtain

$$-\oint_{\mathcal{C}'}\frac{\mathrm{d}z}{2\pi\mathrm{i}}\,\frac{1}{z+\mathrm{i}\omega_m-\varepsilon_{\mathbf{p}+\mathbf{q}}}\,\frac{1}{z-\varepsilon_{\mathbf{p}}}f(z) = \frac{f(\varepsilon_{\mathbf{p}+\mathbf{q}}-\mathrm{i}\omega_m)}{\varepsilon_{\mathbf{p}+\mathbf{q}}-\mathrm{i}\omega_m-\varepsilon_{\mathbf{p}}}+\frac{f(\varepsilon_{\mathbf{p}})}{\varepsilon_{\mathbf{p}}+\mathrm{i}\omega_m-\varepsilon_{\mathbf{p}+\mathbf{q}}}. \tag{4.87}$$

Using the periodicity of the Fermi function,

$$f(x+\mathrm{i}\omega_m) = \frac{1}{\exp(\beta x)\exp(\mathrm{i}\beta\omega_m)+1} = f(x)\,, \tag{4.88}$$

we finally arrive at

$$\Pi_M(\mathbf{q},\omega_m) = 2\int\frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{f(\varepsilon_{\mathbf{p}+\mathbf{q}})-f(\varepsilon_{\mathbf{p}})}{\mathrm{i}\omega_m-(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}})}\,. \tag{4.89}$$

4.10 From imaginary to real times (frequencies)

We have defined and analyzed the Matsubara Green's function in imaginary time $t = -i\tau$:

$$\mathscr{G}_M(\mathbf{r},\tau) = -\mathrm{Tr}\left\{\exp[\beta(\Omega-\widehat{H})]\mathcal{T}_\tau \psi_{MH}(\mathbf{r},\tau)\overline{\psi}_{MH}(0,0)\right\} \tag{4.90}$$

The great advantage of the Matsubara Green's function (as well as more complicated Matsubara correlation functions, such as response functions) was the possibility to perform a perturbative diagrammatic analysis. However, in order to use the results, we should be able to establish a connection between Matsubara-formalism quantities and physical observables. For thermodynamic observables, such a connection is straightforward: Eq. (4.51) directly relates the grand thermodynamic potential to the sum of connected vacuum Matsubara diagrams. But what about dynamical observables? They depend on real times or energies (frequencies), whereas the Matsubara Green functions and response functions depend on imaginary times or frequencies. It is thus crucially important to establish a connection between the Matsubara and real-time correlators. This connection is established via the Lehmann representation. Derivation of the Lehmann representation at $T \neq 0$ is fully analogous to its $T = 0$ derivation, see Sec. 3.6. We perform this analysis first for the Green function (Sec. 4.10.1); generalization to the linear-response functions (Sec. 4.10.2) is straightforward.

4.10.1 Real-time Green's functions at $T \neq 0$

Consider the real-time Green's function at finite T, Eq. (4.7):

$$G(\mathbf{r},t) = -\mathrm{iTr}\left\{\exp(\beta(\Omega-\widehat{H}))\mathcal{T}_t \psi(\mathbf{r},t)\psi^\dagger(0,0)\right\}, \tag{4.91}$$

where $\psi(\mathbf{r},t)$ are operators in conventional (real-time) Heisenberg representation. As we know already from the $T = 0$ analysis, the Green function $G(\mathbf{r},t)$, upon transformation to $G(\mathbf{p},\omega)$ does not have simple analytic properties when considered as a function of complex ω. (It has singularities both in upper and lower half-plane.) We will see that at $T > 0$ the analytical properties of $G(\mathbf{p},\omega)$ are even more complicated. We introduce two Green functions that have simple analytical properties: the retarded (G^R) and advanced (G^A) Green's functions. The definition is a natural generalization of the $T = 0$ definition, Eqs. (3.77) and (3.78):

$$G^R(\mathbf{r},t) = \begin{cases} -\mathrm{iTr}\left(\exp(\beta(\Omega-\widehat{H}))[\psi(\mathbf{r},t),\psi^\dagger(0,0)]_\pm\right) & \text{for} \quad t>0, \\ 0 & \text{for} \quad t<0, \end{cases} \tag{4.92}$$

$$G^A(\mathbf{r},t) = \begin{cases} 0 & \text{for} \quad t>0, \\ \mathrm{iTr}\left(\exp(\beta(\Omega-\widehat{H}))[\psi(\mathbf{r},t),\psi^\dagger(0,0)]_\pm\right) & \text{for} \quad t<0. \end{cases} \tag{4.93}$$

Lehmann-representation for the retarded Green's function:

$$\begin{aligned} G^R(\mathbf{r},t) &= -i\Theta(t)\langle\,[\psi(\mathbf{r},t),\psi^\dagger(0,0)]_\pm\,\rangle \\ &= -i\Theta(t)e^{\beta\Omega}\sum_n \langle\, n \mid e^{-\beta H}\{\psi(\mathbf{r},t)\psi^\dagger(0,0) \pm \psi^\dagger(0,0)\psi(\mathbf{r},t)\} \mid n\rangle \\ &= -i\Theta(t)e^{\beta\Omega}\sum_n e^{-\beta E_n}\langle\, n \mid e^{iHt}\psi(\mathbf{r})e^{-iHt}\psi^\dagger(0) \pm \psi^\dagger(0)e^{iHt}\psi(\mathbf{r})e^{-iHt} \mid n\rangle \\ &= -i\Theta(t)e^{\beta\Omega}\sum_{n,m} e^{-\beta E_n}\left[e^{i(E_n-E_m)t}\langle\, n \mid \psi(\mathbf{r}) \mid m\rangle\langle\, m \mid \psi^\dagger(0) \mid n\rangle\right. \end{aligned}$$

$$\pm\, e^{i(E_m-E_n)t}\langle\, n \mid \psi^\dagger(0) \mid m\rangle\langle\, m \mid \psi(\mathbf{r}) \mid n\rangle\big]\,.$$

With

$$\langle\, n \mid \psi(\mathbf{r}) \mid m\rangle = e^{-i(\mathbf{p}_n-\mathbf{p}_m)\mathbf{r}}\langle\, n \mid \psi(0) \mid m\rangle \tag{4.94}$$

we get

$$\begin{aligned} G^R(\mathbf{r},t) &= -i\Theta(t)e^{\beta\Omega}\sum_{n,m} e^{-\beta E_n}\left[e^{i(E_n-E_m)t}e^{-i(\mathbf{p}_n-\mathbf{p}_m)\mathbf{r}}\langle\, n \mid \psi(0) \mid m\rangle\langle\, m \mid \psi^\dagger(0) \mid n\rangle\right. \\ &\quad \left.\pm\, e^{i(E_m-E_n)t}e^{-i(\mathbf{p}_m-\mathbf{p}_n)\mathbf{r}}\langle\, n \mid \psi^\dagger(0) \mid m\rangle\langle\, m \mid \psi(0) \mid n\rangle\right]. \end{aligned}$$

Exchanging the summation variables $m \leftrightarrow n$ in the second term and then combining both terms, we obtain

$$G^R(\mathbf{r},t) = -i\Theta(t)e^{\beta\Omega}\sum_{n,m}(e^{-\beta E_n} \pm e^{-\beta E_m})e^{i(E_n-E_m)t}e^{-i(\mathbf{p}_n-\mathbf{p}_m)\mathbf{r}}\,|\langle\, n \mid \psi(0) \mid m\rangle|^2\,.$$

Fourier transformation to the momentum space yields

$$\begin{aligned} G^R(\mathbf{p},t) &= \int d^3r\, G^R(\mathbf{r},t)e^{-i\mathbf{pr}} \\ &= -i\Theta(t)e^{\beta\Omega}\sum_{n,m}(e^{-\beta E_n} \pm e^{-\beta E_m})e^{i(E_n-E_m)t}(2\pi)^3\delta(\mathbf{p}+\mathbf{p}_n-\mathbf{p}_m)\,|\langle\, n \mid \psi(0) \mid m\rangle|^2\,. \end{aligned}$$

Now we perform also the Fourier transformation from t to ω:

$$\begin{aligned} G^R(\mathbf{p},\omega) &= \int dt\, G^R(\mathbf{p},t)e^{i\omega t} \\ &= -ie^{\beta\Omega}\sum_{n,m}(e^{-\beta E_n} \pm e^{-\beta E_m})(2\pi)^3\delta(\mathbf{p}+\mathbf{p}_n-\mathbf{p}_m)\,|\langle\, n \mid \psi(0) \mid m\rangle|^2\int_0^\infty dt\, e^{[i(\omega+E_n-E_m)-0]t} \\ &= e^{\beta\Omega}\sum_{n,m}(e^{-\beta E_n} \pm e^{-\beta E_m})(2\pi)^3\delta(\mathbf{p}+\mathbf{p}_n-\mathbf{p}_m)\,|\langle\, n \mid \psi(0) \mid m\rangle|^2\,\frac{1}{\omega+E_n-E_m+i0}. \end{aligned}$$

The result can be written as the spectral representation

$$G^R(\mathbf{p},\omega) = \int_{-\infty}^{+\infty} \mathrm{d}\omega'\,\frac{\mathcal{A}(\mathbf{p},\omega')}{\omega-\omega'+\mathrm{i}0}\,, \tag{4.95}$$

with the (real) spectral function

$$\begin{aligned} \mathcal{A}(\mathbf{p},\omega) = \sum_{n,m} &\exp(\beta\Omega)\,[\exp(-\beta E_n) \pm \exp(-\beta E_m)]\,|\langle n|\psi(0)|m\rangle|^2 \\ &\times (2\pi)^3\delta(\mathbf{p}-\mathbf{p}_m+\mathbf{p}_n)\delta(\omega-E_m+E_n)\,. \end{aligned} \tag{4.96}$$

A fully analogous derivation for the advanced Green's function G^A yields

$$G^A(\mathbf{p},\omega) = \int_{-\infty}^{+\infty} \mathrm{d}\omega'\,\frac{\mathcal{A}(\mathbf{p},\omega')}{\omega-\omega'-\mathrm{i}0} = [G^R(\mathbf{p},\omega)]^*\,, \tag{4.97}$$

with the same spectral function (4.96). In full consistency with their retarded (respectively, advanced) character, G^R is analytic in the upper half-plane and G^A in the lower half-plane of complex ω. Performing an analogous derivation for the Green function G, Eq. (4.91), we get

$$G(\omega,\mathbf{p}) = \mathrm{Re}\, G^R(\mathbf{p},\omega) + \left\{ \begin{array}{c} \mathrm{i}\tanh\frac{\omega}{2T} \\ \mathrm{i}\coth\frac{\omega}{2T} \end{array} \right\} \mathrm{Im}\, G^R(\mathbf{p},\omega)\,. \tag{4.98}$$

Now we perform an analogous derivation for $\mathscr{G}_M$:

$$\begin{aligned}
\mathscr{G}_M(\mathbf{r},\tau>0) &= -\langle\, \psi_{MH}(\mathbf{r},\tau)\bar{\psi}_{MH}(0,0)\,\rangle \\
&= -e^{\beta\Omega}\sum_n e^{-\beta E_n}\langle\, n \mid \psi_{MH}(\mathbf{r},\tau)\bar{\psi}_{MH}(0,0)\mid n\rangle \\
&= -e^{\beta\Omega}\sum_n e^{-\beta E_n}\langle\, n \mid e^{\tau H}\psi(\mathbf{r})e^{-\tau H}\psi^\dagger(0)\mid n\rangle \\
&= -e^{\beta\Omega}\sum_n e^{-\beta E_n}e^{(E_n-E_m)\tau}\langle\, n \mid \psi(\mathbf{r})\mid m\rangle\langle\, m\mid \psi^\dagger(0)\mid n\rangle \\
&\overset{(4.94)}{=} -e^{\beta\Omega}\sum_n e^{-\beta E_n}e^{(E_n-E_m)\tau}e^{-i(\mathbf{p}_n-\mathbf{p}_m)\mathbf{r}}\,|\langle\, n\mid\psi(0)\mid m\rangle|^2
\end{aligned}$$

Fourier transformation $\mathbf{r}\to\mathbf{p}$:

$$\mathscr{G}_M(\mathbf{p},\tau>0) = -e^{\beta\Omega}\sum_n e^{-\beta E_n}e^{(E_n-E_m)\tau}(2\pi)^3\delta(\mathbf{p}+\mathbf{p}_n-\mathbf{p}_m)\,|\langle\, n\mid\psi(0)\mid m\rangle|^2\,.$$

Fourier transformation $\tau\to\omega_n$:

$$\begin{aligned}
\mathscr{G}_M(\mathbf{p},\omega_n) &= -e^{\beta\Omega}\sum_n e^{-\beta E_n}(2\pi)^3\delta(\mathbf{p}+\mathbf{p}_n-\mathbf{p}_m)\,|\langle\, n\mid\psi(0)\mid m\rangle|^2\int_0^\beta d\tau\, e^{(E_n-E_m)\tau}e^{i\omega_n\tau} \\
&= -e^{\beta\Omega}\sum_n e^{-\beta E_n}(2\pi)^3\delta(\mathbf{p}+\mathbf{p}_n-\mathbf{p}_m)\,|\langle\, n\mid\psi(0)\mid m\rangle|^2\,\frac{1}{E_n-E_m+i\omega_n} \\
&\times \left(e^{(E_n-E_m)\beta}\underbrace{e^{i\omega_n\beta}}_{=\mp 1}-1\right) \\
&= e^{\beta\Omega}\sum_n(e^{-\beta E_n}\pm e^{-\beta E_m})(2\pi)^3\delta(\mathbf{p}+\mathbf{p}_n-\mathbf{p}_m)\,|\langle\, n\mid\psi(0)\mid m\rangle|^2\,\frac{1}{i\omega_n+E_n-E_m}.
\end{aligned} \tag{4.99}$$

This can be written as

$$\mathscr{G}_M(\mathbf{p},\omega_n) = \int_{-\infty}^{+\infty}\mathrm{d}\omega'\,\frac{\mathcal{A}(\mathbf{p},\omega')}{\mathrm{i}\omega_n-\omega'}\,. \tag{4.100}$$

with the same spectral function (4.96).

Comparing Eq. (4.100) with Eq. (4.95) and using the analyticity of G^R in the upper half-plane ($\mathrm{Im}\,\omega>0$), we get

$$\mathscr{G}_M(\omega_n) = G^R(\mathrm{i}\omega_n) \qquad \text{for all}\ \ \omega_n>0\,. \tag{4.101}$$

We do not indicate here the momentum argument $\mathbf{p}$, since it is the same on both sides of the equality. Via the same token, comparing Eq. (4.100) with Eq. (4.97) and using the analyticity of G^A in the lower half-plane ($\mathrm{Im}\,\omega<0$), we find

$$\mathscr{G}_M(\omega_n) = G^A(\mathrm{i}\omega_n) \qquad \text{for all}\ \ \omega_n<0\,. \tag{4.102}$$

Note that, according to Eq.(4.100), $\mathscr{G}_M(\mathbf{p}, -\omega_n) = \mathscr{G}_M^*(\mathbf{p}, \omega_n)$.

Equation (4.101) is the sought relation between the Matsubara Green's function $\mathscr{G}_M$ and the real-time Green's function G^R. It allows one to restore G^R (which has information about physical properties of the system at real times or frequencies) from the Matsubara (imaginary-time) Green's function $\mathscr{G}_M$ by means of **analytical continuation**. Specifically, imagine that we have calculated (by diagrammatic means) $\mathscr{G}_M(\omega_n)$. We should then find a function $\mathcal{F}(z)$ such that, first, it is analytical in the upper half-plane, $\mathrm{Im}\,\omega > 0$ and, second

$$\mathcal{F}(\mathrm{i}\omega_n) = \mathscr{G}_M(\omega_n) \quad \text{for all} \;\; \omega_n > 0. \tag{4.103}$$

Then this function yields the sought G^R:

$$G^R(\omega) = \mathcal{F}(\omega)\,, \quad \text{analytic for} \quad \mathrm{Im}\,\omega > 0\,. \tag{4.104}$$

Once G^R have been determined, one can immediately find also G by using Eq. (4.98).

Consider a simple **example: free particles**. The Matsubara Green's functions then reads [Eq. (4.70)]:

$$\mathscr{G}_M(\mathbf{p}, \epsilon_n) = \frac{1}{i\epsilon_n - \epsilon_p}$$

Performing an analytical continuation, we easily find

$$G^R(\mathbf{p}, \epsilon) = \frac{1}{\epsilon - \epsilon_p + i0}. \tag{4.105}$$

4.10.2 Linear response at $T \neq 0$

In Sec. (4.10.1) we explained in detail how the real-time Green's function G^R is obtained from the Matsubara (imaginary-time) Green's function $\mathscr{G}_M$. This is achieved by analytic continuation from imaginary to real frequencies. This idea is straightforwardly generalized to response functions. The Matsubara response function is defined as follows:

$$\mathscr{D}_{BA}^M(\tau) = -\langle \mathcal{T}_\tau \widehat{B}(\tau)\widehat{A}(0)\rangle\,, \quad \langle \ldots \rangle = \mathrm{Tr}[\exp(\beta(\Omega - \widehat{H}))]\,. \tag{4.106}$$

For instance, if $\widehat{B}$ is the density operator $\widehat{\rho}(\mathbf{r})$ and $\widehat{A}$ the density operator $\widehat{\rho}(\mathbf{r}')$, we have the density-density Matsubara response function (4.83).

The physical (real-time) response function is defined at $T \neq 0$ according to the linear-response theory, Eq. (3.303):

$$\mathscr{D}_{BA}^R(t) = -i\Theta(t)\langle\, [\widehat{B}(t), \widehat{A}(0)]\,\rangle. \tag{4.107}$$

The Matsubara function (4.106) can be calculated diagrammatically. At the same time, for physical applications, we need the real-time response function ((4.107)). The question is thus how to find $\mathscr{D}_{BA}^R$ from the known (diagrammatically calculated) $\mathscr{D}_{BA}^M$. The relation between $\mathscr{D}_{BA}^R$ and $\mathscr{D}_{BA}^M$ is established by Lehmann representation in exactly the same way, as the relation between G^R and $\mathscr{G}_M$ obtained in Sec. (4.10.1). The resulting relation has exactly the same form:

$$\mathscr{D}_{BA}^R(i\omega_n) = \mathscr{D}_{BA}^M(\omega_n)\,. \tag{4.108}$$

Thus, in order to determine $\mathscr{D}_{BA}^R$, one should first calculate (diagrammatically) the Matsubara response function $\mathscr{D}_{BA}^M(\omega_n)$ and then to find a function $\mathcal{F}(z)$, analytic in the upper half-plane $\mathrm{Im}\,\omega > 0$, such that

$$\mathcal{F}(i\omega_n) = \mathscr{D}_{BA}^M(\omega_n) \quad \text{for all} \;\; \omega_n > 0\,. \tag{4.109}$$

Then the function $\mathcal{F}(z)$ yields the sought physical response function (analytic in the half-plane $\mathrm{Im}\,\omega > 0$),

$$\mathscr{D}^R_{BA}(\omega) = \mathcal{F}(\omega)\,. \tag{4.110}$$

Example: Polarization operator. The Matsubara polarization operator was calculated above, see Eq. (4.89):

$$\Pi_M(\mathbf{q},\omega_n) = 2\int \frac{\mathrm{d}^3 p}{(2\pi)^3}\,\frac{f(\varepsilon_{\mathbf{p}+\mathbf{q}}) - f(\varepsilon_{\mathbf{p}})}{\mathrm{i}\omega_n - (\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}})}\,. \tag{4.111}$$

The analytic continuation is straightforward, yielding

$$\Pi^R(\mathbf{q},\omega) = 2\int \frac{\mathrm{d}^3 p}{(2\pi)^3}\,\frac{f(\varepsilon_{\mathbf{p}+\mathbf{q}}) - f(\varepsilon_{\mathbf{p}})}{\omega - \varepsilon_{\mathbf{p}+\mathbf{q}} + \varepsilon_{\mathbf{p}} + \mathrm{i}0}\,. \tag{4.112}$$

4.11 Example: Coulomb drag in Matsubara formalism

This section serves as another illustration of the technique of finite-temperature calculation of response functions. As explained above, this requires, first, a diagrammatic calculation of the Matsubara response function and, second, an analytic continuation from imaginary to real frequencies. Here the technique is illustrated by a somewhat sophisticated example of Coulomb drag in bilayer 2D systems. The calculation requires evaluation of Matsubara sums and analytical continuation for both fermions (electrons) and bosons (dynamically screened, retarded Coulomb interaction). The presentation is based on the paper I. V. Gornyi, A. D. Mirlin, F. von Oppen, Phys. Rev. B 70, 245302 (2004). In Sec. 4.11.1 we will define the physical observable of interest (drag conductivity), identify the corresponding diagrams, calculate them in the Matsubara formalism, and present the results of analytic continuation to real frequencies. A detailed exposition of the analytic continuation is presented in Sec. 4.11.2.

Comments:

(i) Note that we do not discuss here the analysis of resulting expressions (integrals of products involving retarded and advanced Green's functions) in different regimes of parameters. Our goal here is to demonstrate how these general expressions are derived by means of Matsubara formalism and analytical continuation.

(ii) Notations used in this section for Matsubara Green functions is slightly different from those used above. We do not write here the subscript (or superscript) "M" but instead include the imaginary unit in the Matsubara-frequency argument. In particular, we denote the Matsubara drag conductivity $\sigma^D(i\Omega_k)$ rather than $\sigma^D_M(\Omega_k)$, the Matsubara Green function $\mathscr{G}(i\epsilon_k)$ rather than $\mathscr{G}_M(\epsilon_k)$, and so on. Such notations, frequently used in scientific literature, indicate that Matsubara quantities correspond to physical quantities calculated at imaginary frequencies $\mathrm{i}\omega_n$ (where ω_n are Matsubara frequencies).

4.11.1 Definition of the problem, diagrams, and results

The Coulomb-drag signal in a double-layer system is the voltage V developing in the open-circuit passive layer when a current I is applied in the active layer. The drag resistance (also known as transresistance) is then defined by $R_D = V/I$. In a simple picture of Coulomb drag, the carriers of the active layer transfer momentum to the carriers of the passive layer by interlayer electron-electron scattering. A voltage V develops in the passive layer, which balances this momentum transfer.

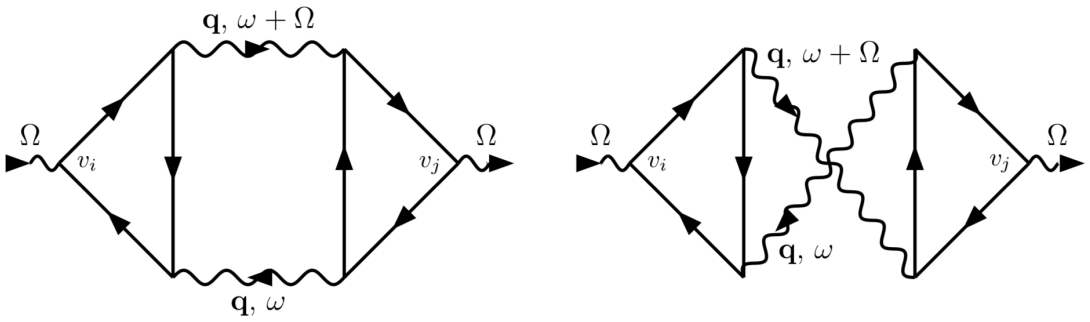


Figure 4.1: The diagrams contributing to the drag conductivity to leading order in the dynamically screened interlayer interaction $U(\mathbf{q},\omega)$ (wavy lines). The full lines represent the electron Green's function. The external vertices labelled by the velocity operator v_i are vector (current) vertices while the internal vertices are scalar (density) vertices.

To calculate the drag resistance, we use the Kubo approach which expresses the drag conductivity $\sigma^D_{ij}(\mathbf{Q},\Omega)$ in terms of a current-current correlation function,

$$\sigma^D_{ij}(\mathbf{Q},\Omega) = \frac{1}{\Omega S}\int_0^\infty dt\, e^{i\Omega t}\left\langle [j_i^{(1)\dagger}(\mathbf{Q},t), j_j^{(2)}(\mathbf{Q},0)]\right\rangle . \tag{4.113}$$

where i,j label the components of the drag conductivity tensor, $\mathbf{Q},\Omega$ denote the wave vector and frequency of the applied field, S is the area of the sample, and $j_i^{(l)}$ denotes the ith component of the current operator in the lth layer. The *dc* drag conductivity follows by taking the limit

$$\sigma^D_{ij} = \sigma^D_{ij}(\mathbf{Q}=0,\Omega\to 0). \tag{4.114}$$

When computing the retarded correlation function appearing in Eq. (4.113) within the Matsubara technique, the leading diagrams in the limit of weak (screened) interlayer interaction $U(\mathbf{q},\omega)$ are shown in Fig. 4.1. Analytically, these diagrams are given by the expression

$$\sigma^D_{ij}(i\Omega_k) = \frac{e^2T}{2\Omega_k S}\sum_{\mathbf{q},\omega_n}\Gamma_i^{(1)}(\mathbf{q},i\omega_n+i\Omega_k,i\omega_n)\Gamma_j^{(2)}(\mathbf{q},i\omega_n,i\omega_n+i\Omega_k)U(\mathbf{q},i\omega_n+i\Omega_k)U(\mathbf{q},i\omega_n). \tag{4.115}$$

Here, ω_n and Ω_k denote bosonic Matsubara frequencies and the vector $\mathbf{\Gamma}^{(l)}(\mathbf{q},i\omega_n,i\omega_m)$ is the triangle vertex of layer l as defined by the diagrams in Fig. 4.2. Neglecting *intra*layer interactions, it takes the analytical form

$$\begin{aligned}\mathbf{\Gamma}(\mathbf{q},i\omega_n,i\omega_m) &= T\sum_{\epsilon_k}\mathrm{tr}\left\{\mathscr{G}(i\epsilon_k)e^{i\mathbf{qr}}\mathscr{G}(i\epsilon_k+i\omega_m)\mathbf{v}\mathscr{G}(i\epsilon_k+i\omega_n)e^{-i\mathbf{qr}}\right. &(4.116)\\ &+ \left.\mathscr{G}(i\epsilon_k)e^{-i\mathbf{qr}}\mathscr{G}(i\epsilon_k-i\omega_n)\mathbf{v}\mathscr{G}(i\epsilon_k-i\omega_m)e^{i\mathbf{qr}}\right\}, &(4.117)\end{aligned}$$

where $\mathscr{G}$ denotes the Matsubara Green's function, ϵ_k is a fermionic Matsubara frequency, and $\mathbf{v}$ represents the velocity operator. Summing over the Matsubara frequency ω_n, performing the analytical continuation to a real frequency Ω, and finally taking the limit $\Omega\to 0$ yields for the *dc* drag conductivity

$$\sigma^D_{ij} = \frac{e^2}{16\pi TS}\sum_{\mathbf{q}}\int_{-\infty}^{\infty}\frac{d\omega}{\sinh^2(\omega/2T)}\Gamma_i^{(1)}(\mathbf{q},\omega+i0,\omega-i0)\Gamma_j^{(2)}(\mathbf{q},\omega-i0,\omega+i0)|U(\mathbf{q},\omega)|^2. \tag{4.118}$$

In the sequel, we will use a short-hand notation, $\mathbf{\Gamma}(\mathbf{q},\omega)\equiv\mathbf{\Gamma}(\mathbf{q},\omega+i0,\omega-i0)$.

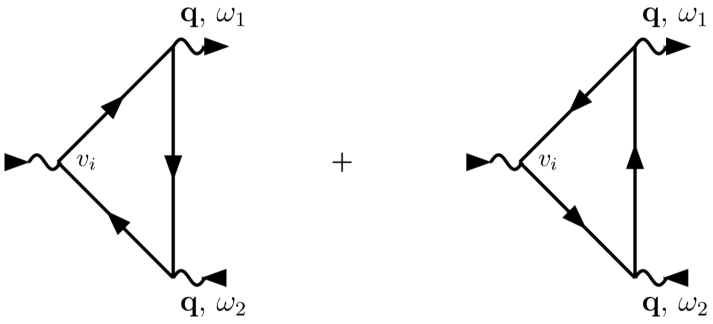


Figure 4.2: Diagrams defining the triangle vertex $\mathbf{\Gamma}(\mathbf{q},\omega_1,\omega_2)$.

The triangle vertex $\mathbf{\Gamma}(\mathbf{q},\omega)$ is obtained by analytic continuation of (4.116). The result has the form $\mathbf{\Gamma}=\mathbf{\Gamma}^{(a)}+\mathbf{\Gamma}^{(b)}$ with the two contributions

$$\begin{aligned}\mathbf{\Gamma}^{(a)}(\mathbf{q},\omega)&=\int\frac{d\epsilon}{4\pi i}\tanh\frac{\epsilon+\omega-\mu}{2T}\\&\times\mathrm{tr}\left\{\mathbf{v}G^R(\epsilon+\omega)e^{i\mathbf{qr}}G^R(\epsilon)e^{-i\mathbf{qr}}G^R(\epsilon+\omega)-\mathbf{v}G^A(\epsilon+\omega)e^{i\mathbf{qr}}G^A(\epsilon)e^{-i\mathbf{qr}}G^A(\epsilon+\omega)\right\}\\&+(\omega,\mathbf{q}\to-\omega,-\mathbf{q}),\end{aligned}\tag{4.119}$$

$$\begin{aligned}\mathbf{\Gamma}^{(b)}(\mathbf{q},\omega)&=\int\frac{d\epsilon}{4\pi i}\left(\tanh\frac{\epsilon+\omega-\mu}{2T}-\tanh\frac{\epsilon-\mu}{2T}\right)\\&\times\mathrm{tr}\left\{\mathbf{v}G^A(\epsilon+\omega)e^{i\mathbf{qr}}[G^A(\epsilon)-G^R(\epsilon)]e^{-i\mathbf{qr}}G^R(\epsilon+\omega)\right\}+(\omega,\mathbf{q}\to-\omega,-\mathbf{q}).\end{aligned}\tag{4.120}$$

Here, $G^R(\epsilon)$ and $G^A(\epsilon)$ denote the retarded and advanced Green's's functions, respectively, and μ is the chemical potential.

For small ω, the expressions for $\mathbf{\Gamma}(\mathbf{q},\omega)$ simplify to

$$\mathbf{\Gamma}^{(a)}(\mathbf{q},\omega)=\frac{\omega}{2\pi i}\mathrm{tr}\left\{\mathbf{v}G^R(\epsilon)e^{i\mathbf{qr}}G^R(\epsilon)e^{-i\mathbf{qr}}G^R(\epsilon)-(G^R\to G^A)\right\}\tag{4.121}$$

$$\mathbf{\Gamma}^{(b)}(\mathbf{q},\omega)=\frac{\omega}{i\pi}\mathrm{tr}\left\{\mathbf{v}G^A(\epsilon)e^{i\mathbf{qr}}[G^A(\epsilon)-G^R(\epsilon)]e^{-i\mathbf{qr}}G^R(\epsilon)\right\}.\tag{4.122}$$

It is also useful to note that $\mathbf{\Gamma}^{(a)}(\mathbf{q},\omega)$ can be expressed as

$$\mathbf{\Gamma}^{(a)}(\mathbf{q},\omega)=\frac{\omega}{\pi}\nabla_{\mathbf{q}}\mathrm{Im}\,\mathrm{tr}\left\{e^{i\mathbf{qr}}G^R(\epsilon)e^{-i\mathbf{qr}}G^R(\epsilon)\right\},\tag{4.123}$$

which shows that $\mathbf{\Gamma}^{(a)}(\mathbf{q},\omega)$ gives only a longitudinal contribution (parallel to $\mathbf{q}$) to $\mathbf{\Gamma}(\mathbf{q},\omega)$.

4.11.2 Analytical continuation

Here, we perform the analytical continuation of the Matsubara expressions for the drag conductivity and the triangle vertex $\mathbf{\Gamma}$. To calculate the Matsubara sum over $\omega_n=2\pi nT$ in Eq. (4.115), the standard contour integration in the complex ω plane is done,

$$T\sum_{\omega_n}F(i\omega_n)=\frac{1}{4\pi i}\int_{C_b}d\omega\;F(\omega)\;\coth\frac{\omega}{2T}.\tag{4.124}$$

The integrand has branch cuts at Im $\omega=0$ and Im $\omega=-\Omega_k$, where Ω_k represents the external frequency. The integration contour C_b thus contains three parts, see Fig. 4.3

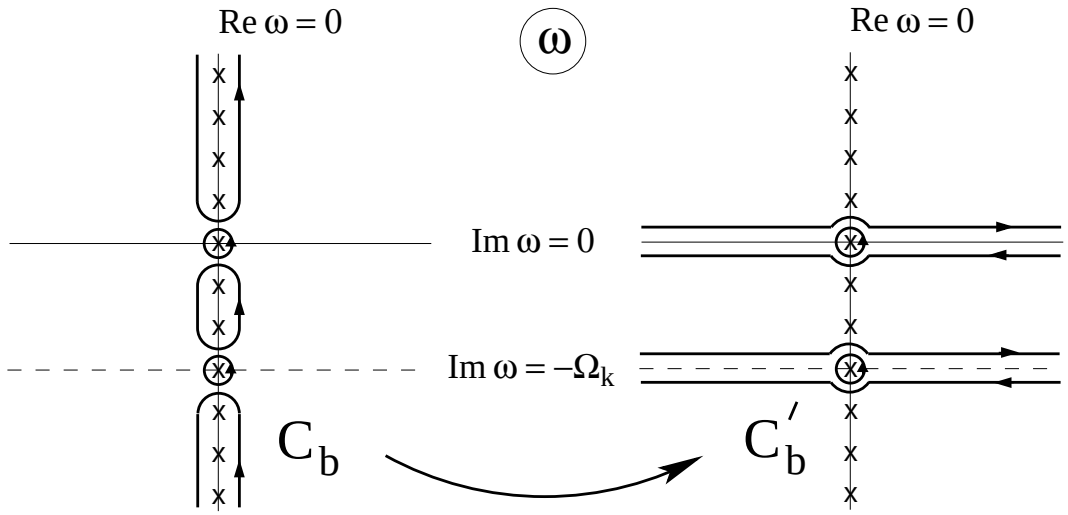


Figure 4.3: Contours for the ω-integration.

Deforming the contour as shown in Fig. 4.3, we get four terms corresponding to four lines (above and below of both the branch cuts) forming the new contour,

$$\begin{aligned}
\sigma_{ij}^{D}(i\Omega_k) &= -\frac{e^2}{8\Omega_k S}\sum_{\mathbf{q}}\int_{-\infty}^{\infty} d\omega\, \coth\frac{\omega}{2T} \\
&\times \Big[\Gamma_i^{(1)}(\mathbf{q},\omega+i\Omega_k,\omega+i0)\Gamma_j^{(2)}(\mathbf{q},\omega+i0,\omega+i\Omega_k)U(\mathbf{q},\omega+i\Omega_k)U(\mathbf{q},\omega+i0) \\
&- \Gamma_i^{(1)}(\mathbf{q},\omega+i\Omega_k,\omega-i0)\Gamma_j^{(2)}(\mathbf{q},\omega-i0,\omega+i\Omega_k)U(\mathbf{q},\omega+i\Omega_k)U(\mathbf{q},\omega-i0) \\
&+ \Gamma_i^{(1)}(\mathbf{q},\omega+i0,\omega-i\Omega_k)\Gamma_j^{(2)}(\mathbf{q},\omega-i\Omega_k,\omega+i0)U(\mathbf{q},\omega+i0)U(\mathbf{q},\omega-i\Omega_k) \\
&- \Gamma_i^{(1)}(\mathbf{q},\omega-i0,\omega-i\Omega_k)\Gamma_j^{(2)}(\mathbf{q},\omega-i\Omega_k,\omega-i0)U(\mathbf{q},\omega-i0)U(\mathbf{q},\omega-i\Omega_k)\Big].
\end{aligned} \tag{4.125}$$

In the third and fourth terms we have used $\coth(z+i\Omega_k/2T)=\coth z$. The contributions of points $\omega=0$ and $\omega=-i\Omega_k$ cancel the integral over the small circles around these points, so that the integrals above should be understood in the principal value sense.

We now perform the analytical continuation $i\Omega_k\to\Omega+i0$ and take the limit $\Omega\to 0$. The first and the last terms coming from outer sides of branch cuts vanish in the limit $\Omega\to 0$. This yields

$$\begin{aligned}
\sigma_{ij}^{D} &= -\frac{e^2}{8\pi S}\sum_{\mathbf{q}}\int_{-\infty}^{\infty} d\omega\, \coth\frac{\omega}{2T}\,\frac{\partial}{\partial\omega} \\
&\times \Big[\Gamma_i^{(1)}(\mathbf{q},\omega+i0,\omega-i0)\Gamma_j^{(2)}(\mathbf{q},\omega-i0,\omega+i0)U(\mathbf{q},\omega+i0)U(\mathbf{q},\omega-i0)\Big].
\end{aligned} \tag{4.126}$$

Using

$$\frac{\partial}{\partial\omega}\coth\frac{\omega}{2T} = -\frac{1}{2T\sinh^2(\omega/2T)}, \tag{4.127}$$

we arrive at Eq. (4.118).

The next step is the analytical continuation of the triangle vertex. The summation over the fermionic Matsubara energies $\epsilon_k=(2k+1)\pi T$ in Eq. (4.116) is performed using the integral

$$T\sum_{\epsilon_k} F(i\epsilon_k) = \frac{1}{4\pi i}\int_{C_f} d\epsilon F(\epsilon)\,\tanh\frac{\epsilon}{2T}, \tag{4.128}$$

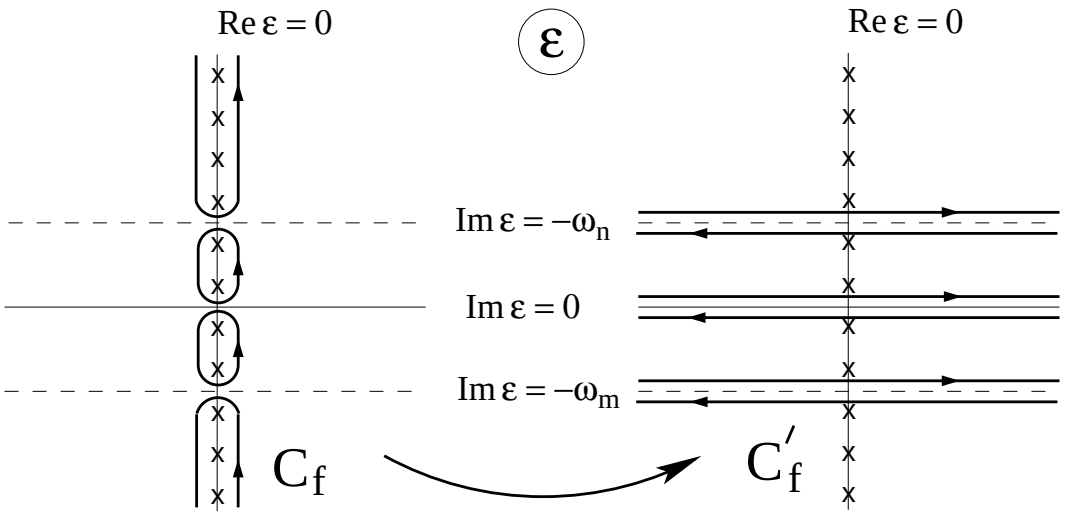


Figure 4.4: Contours for the ϵ-integration.

along the contour C_f shown in Fig. 4.4. Since the triangle vertex depends on two frequencies $i\omega_m$ and $i\omega_n$, the integrand now has three branch cuts in the complex plane of ϵ, namely at $\mathrm{Im}\,\epsilon = 0$, $\mathrm{Im}\,\epsilon = -\omega_m$, and $\mathrm{Im}\,\epsilon = -\omega_n$. Similarly to C_b, the contour C_f can be deformed into a set of six lines going on both sides of each of the branch cuts (see Fig. 4.4), yielding

$$\begin{aligned}\mathbf{\Gamma}(\mathbf{q}, i\omega_m, i\omega_n) &= \int_{-\infty}^{\infty} \frac{d\epsilon}{4\pi i} \tanh\frac{\epsilon}{2T} \mathrm{tr}\left\{\mathbf{v}\,[G^R(\epsilon) - G^A(\epsilon)] e^{i\mathbf{qr}} \mathscr{G}(\epsilon - i\omega_n) e^{-i\mathbf{qr}} \mathscr{G}(\epsilon + i\omega_m - i\omega_n)\right. \\ &- \mathbf{v}\,\mathscr{G}(\epsilon + i\omega_n) e^{i\mathbf{qr}} [G^R(\epsilon) - G^A(\epsilon)] e^{-i\mathbf{qr}} \mathscr{G}(\epsilon + i\omega_m) \\ &+ \left.\mathbf{v}\,\mathscr{G}(\epsilon - i\omega_m + i\omega_n) e^{i\mathbf{qr}} \mathscr{G}(\epsilon - i\omega_m) e^{-i\mathbf{qr}} [G^R(\epsilon) - G^A(\epsilon)]\right\} \\ &+ (\omega_n \to -\omega_m, \mathbf{q} \to -\mathbf{q}). \end{aligned} \tag{4.129}$$

In this formula $G^{R,A}(\epsilon) = \mathscr{G}(\epsilon \pm i0)$ and we have used

$$\tanh\left(z - \frac{i\omega_m}{2T}\right) = \tanh z.$$

The equation (4.129) is valid irrespective of the relation between ω_m, ω_n, and 0. Performing the analytical continuation to real frequencies $i\omega_m \to \omega_1 + i0$ and $i\omega_n \to \omega_2 - i0$ (and shifting the integration variables $\epsilon \to \epsilon + \omega_2$ and $\epsilon \to \epsilon + \omega_1$ in the first and third terms, respectively) we obtain

$$\begin{aligned}\mathbf{\Gamma}(\mathbf{q}, \omega_1 + i0, \omega_2 - i0) &= \int_{-\infty}^{\infty} \frac{d\epsilon}{4\pi i} \\ &\times \mathrm{tr}\left\{\tanh\frac{\epsilon + \omega_2}{2T}\ \mathbf{v}\,[G^R(\epsilon + \omega_2) - G^A(\epsilon + \omega_2)] e^{i\mathbf{qr}} G^R(\epsilon) e^{-i\mathbf{qr}} G^R(\epsilon + \omega_1)\right. \\ &- \tanh\frac{\epsilon}{2T}\ \mathbf{v}\, G^A(\epsilon + \omega_2) e^{i\mathbf{qr}} [G^R(\epsilon) - G^A(\epsilon)] e^{-i\mathbf{qr}} G^R(\epsilon + \omega_1) \\ &+ \left.\tanh\frac{\epsilon + \omega_1}{2T}\ \mathbf{v}\, G^A(\epsilon + \omega_2) e^{i\mathbf{qr}} G^A(\epsilon) e^{-i\mathbf{qr}} [G^R(\epsilon + \omega_1) - G^A(\epsilon + \omega_1)]\right\} \\ &+ (\omega, \mathbf{q} \to -\omega, -\mathbf{q}). \end{aligned} \tag{4.130}$$

Setting $\omega_1 = \omega_2$ and collecting the contributions containing only retarded (from the first term) and only advanced (from the third term) Green's functions, we arrive [up to a redefinition of zero of fermionic energies, which are counted from the chemical potential in Eq. (4.130)] at Eq. (4.119) for $\mathbf{\Gamma}^{(a)}$. The remaining terms constitute the expression (4.120) for $\mathbf{\Gamma}^{(b)}$.

Chapter 5

Superconductivity

We consider interacting system of Fermions (electrons). If the interaction is repulsive and not too strong, the system is in the Fermi-liquid phase. This was considered in previous chapters. (Note that a strong repulsive interaction can lead to instabilities such as ferromagnetic Stoner instability.)

The situation turns out to be dramatically different if the interaction is attractive. In this case, an arbitrarily weak interaction leads to instability: the system becomes superconducting. The Coulomb interaction between electrons is repulsive. What can lead to attraction? The most conventional mechanism is the interaction mediated by phonons.

5.1 Phonon Green's function

Consider free acoustic phonons with the Hamilton operator

$$\widehat{H} = \sum_{\mathbf{k}} \omega_k \left(\hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \frac{1}{2} \right), \tag{5.1}$$

where $\omega_k = s|\mathbf{k}|$ and s is the sound velocity. Introduce the bosonic field operator (which describes, up to a proportionality coefficient, the local fluctuation of ion density, see TKM I)

$$\widehat{\Phi}(\mathbf{r}) = i \sum_{\mathbf{k}} \sqrt{\frac{\omega_k}{2V}} \left(\hat{b}_{\mathbf{k}} e^{i\,\mathbf{k}\cdot\mathbf{r}} - \hat{b}^\dagger_{\mathbf{k}} e^{-i\,\mathbf{k}\cdot\mathbf{r}} \right). \tag{5.2}$$

The Heisenberg operator at time t is then

$$\widehat{\Phi}(\mathbf{r},t) = i \sum_{\mathbf{k}} \sqrt{\frac{\omega_k}{2V}} \left(\hat{b}_{\mathbf{k}} e^{i\,\mathbf{k}\cdot\mathbf{r} - i\omega_k t} - \hat{b}^\dagger_{\mathbf{k}} e^{-i\,\mathbf{k}\cdot\mathbf{r} + i\omega_k t} \right). \tag{5.3}$$

The field $\widehat{\Phi}$ is real in the sense $\widehat{\Phi}(\mathbf{r},t) = \widehat{\Phi}^\dagger(\mathbf{r},t)$, which is a manifestation of the fact that phonons do not carry charge. This should be contrasted to charged matter fields which are complex (two distinct operators $\hat{\psi}$ and $\hat{\psi}^\dagger$; invariance of the corresponding theory with respect to global phase transformations $\hat{\psi} \to e^{i\phi}\hat{\psi}$ corresponds to charge conservation).

The (zero-temperature) phonon Green's function is defined as

$$D(\mathbf{r},t;\mathbf{r}',t') = -i\langle 0|\mathcal{T}\widehat{\Phi}(\mathbf{r},t)\widehat{\Phi}(\mathbf{r}',t')|0\rangle, \tag{5.4}$$

where $|0\rangle$ denotes the ground state (no phonons). As usual, translational invariance in space and time implies that

$$D(\mathbf{r},t;\mathbf{r}',t) = D(\mathbf{r}-\mathbf{r}',t-t'). \tag{5.5}$$

We set $\mathbf{r}-\mathbf{r}' \to \mathbf{r}$ and $t-t' \to t$.

For $t>0$ we have

$$\begin{aligned} D(\mathbf{r},t) &= -i\sum_{\mathbf{k}}\left(\sqrt{\frac{\omega_{\mathbf{k}}}{2V}}\right)^2 \langle 0|b_{\mathbf{k}}e^{i\mathbf{kr}-i\omega_{\mathbf{k}}t}b_{\mathbf{k}}^{\dagger}|0\rangle \\ &= -i\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}}{2V}e^{i\mathbf{kr}-i\omega_{\mathbf{k}}t}. \end{aligned} \tag{5.6}$$

Similarly, for $t<0$:

$$\begin{aligned} D(\mathbf{r},t) &= -i\sum_{\mathbf{k}}\left(\sqrt{\frac{\omega_{\mathbf{k}}}{2V}}\right)^2 \langle 0|b_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}e^{-i\mathbf{kr}+i\omega_{\mathbf{k}}t}|0\rangle \\ &= -i\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}}{2V}e^{-i\mathbf{kr}+i\omega_{\mathbf{k}}t} = -i\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}}{2V}e^{i\mathbf{kr}+i\omega_{\mathbf{k}}t} \end{aligned} \tag{5.7}$$

On the last step we made a change of the variable $\mathbf{k}\to-\mathbf{k}$ and used $\omega_{\mathbf{k}}=\omega_{-\mathbf{k}}$.

Fourier transformation from $\mathbf{r},t$ to $\mathbf{q},\omega$ finally yields the phonon Green's function in momentum-frequency representation

$$\begin{aligned} D(\mathbf{k},\omega) &= -i\frac{\omega_{\mathbf{k}}}{2}\left[\int_0^{\infty}dt\, e^{i\omega t-i\omega_{\mathbf{k}}t-0t}+\int_{-\infty}^{0}dt\, e^{i\omega t+i\omega_{\mathbf{k}}t+0t}\right] \\ &= -i\frac{\omega_{\mathbf{k}}}{2}\left[\frac{1}{-i(\omega-\omega_{\mathbf{k}}+i0)}+\frac{1}{i(\omega+\omega_{\mathbf{k}}-i0)}\right] \\ &= \frac{\omega_{\mathbf{k}}}{2}\left[\frac{1}{\omega-\omega_{\mathbf{k}}+i0}-\frac{1}{\omega+\omega_{\mathbf{k}}-i0}\right] \\ &= \frac{\omega_{\mathbf{k}}^2}{\omega^2-\omega_{\mathbf{k}}^2+i0}. \end{aligned} \tag{5.8}$$

5.2 Electron-phonon interaction. Phonon-mediated electron-electron interaction

Hamiltonian of the electron-phonon interaction (Fröhlich Hamiltonian)

$$\widehat{H}_{\rm int} = g\int \mathrm{d}^3r\, \hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r})\widehat{\Phi}(\mathbf{r})\,, \tag{5.9}$$

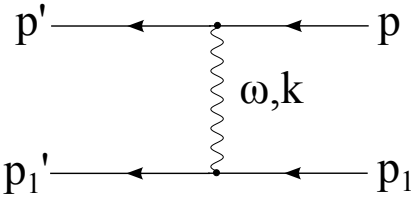
where g is a (material-dependent) constant. Equation (5.9) is written under several simplifying assumptions:

(i) only acoustic phonons are retained (otherwise there would be a sum over all branches);

(ii) it is assumed that phonons are either exactly longitudinal or exactly transverse, as in an isotropic medium; then, only longitudinal phonons contribute;

(iii) Thomas-Fermi approximation for screened Coulomb interaction: $4\pi e^2/(q^2+k_{\rm TF}^2) \longrightarrow 4\pi e^2/k_{\rm TF}^2$, so that the interaction is effectively local.

The electron-phonon interaction induces an effective electron-electron interaction through an intermediate phonon. It is represented by the following element of a Feynman diagram:



Here the wavy line represents the Green's function (or, equivalenty, propagator) of the phonons calculated above

$$D(\mathbf{r},t) = -i\langle 0|\mathcal{T}\widehat{\Phi}(\mathbf{r},t)\widehat{\Phi}(\mathbf{r}',t')|0\rangle\,, \quad D(k,\omega) = \frac{\omega_k^2}{\omega^2-\omega_k^2+\mathrm{i}0}\,, \quad \omega_k = c|\mathbf{k}|\,. \tag{5.10}$$

In the Matsubara (finite-temperature) formalism we have correspondingly

$$D_M(k,\nu_m) = -\frac{\omega_k^2}{\nu_m^2+\omega_k^2}\,. \tag{5.11}$$

Taking into account that every electron-phonon vertex yields a factor g, we obtain the effective electron-electron interaction mediated by phonons

$$U_{\text{eff}}(k,\omega) = g^2 D(k,\omega) = g^2\frac{\omega_k^2}{\omega^2-\omega_k^2+\mathrm{i}0}\,. \tag{5.12}$$

One says that the effective interaction emerges when phonons are integrated out. (This terminology becomes particularly transparent in the functional-integral formalism of the quantum field theory.)

Characteristic values of phonon momenta:

$$k = |\mathbf{p}-\mathbf{p}'| \sim p_F \quad\Longrightarrow\quad \omega_k \sim \omega_D \;\text{ Debye frequency }\; (\sim 100-1000\,\text{K for metals}) \tag{5.13}$$

On the other hand, characteristic energy transfers ω are set by temperature T and by the superconducting gap Δ (which will be determined below) and satisfy

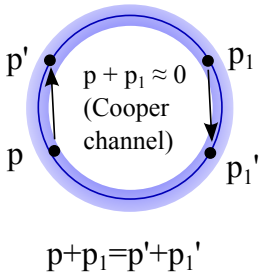
$$\omega \ll \omega_D. \tag{5.14}$$

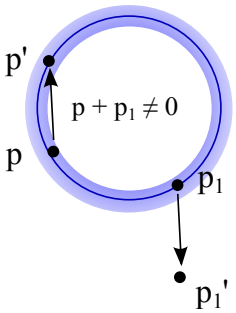
According to Eqs. (5.13) and (5.14), relevant values of ω are much smaller than those of ω_k. Thus, Eq. (5.12) reduces to

$$U_{\text{eff}}(k,\omega) \simeq -g^2 < 0\,, \qquad \text{for} \quad \omega_k \sim \omega_D, \quad \omega \ll \omega_D \tag{5.15}$$

Therefore, phonons induce an effective attraction between electrons.

The attraction is efficient only for electrons that have opposite momenta: $\mathbf{p} \simeq -\mathbf{p_1}$. Indeed, only under this condition two electrons near the Fermi surface can exchange a large momentum $\mathbf{k}$ (of order p_F) such that the resulting electrons with momenta $\mathbf{p}' = \mathbf{p}+\mathbf{k}$ and $\mathbf{p}_1' = \mathbf{p_1}-\mathbf{k}$ remain close to the Fermi surface.





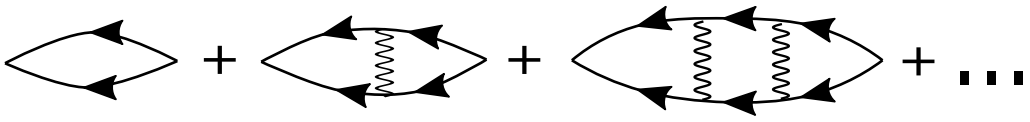
The condition $\mathbf{p}+\mathbf{p_1} \simeq 0$ determines the so-called Cooper channel.

5.3 Cooper instability of a Fermi liquid with attractive interactions

We explore the superconducting instability of a system of fermions with weak attractive interaction. The physics of the instability is formation (one uses the word "condensation") of Cooper pairs. To reveal this instability we consider the response function in the Cooper channel:

$$C(\mathbf{r},t) = -\mathrm{i}\langle\mathcal{T}\psi_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)\psi_\downarrow^\dagger(0,0)\psi_\uparrow^\dagger(0,0)\rangle\,. \tag{5.16}$$

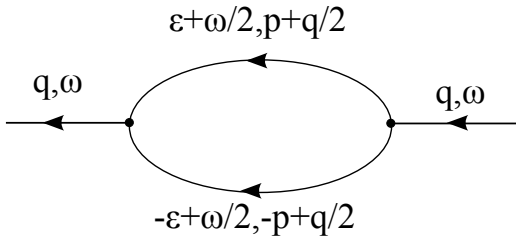
The dominant diagrammatic series for this correlation function is the sum of ladder diagrams:



Indeed, in this series, the condition of Cooper channel (the sum of momenta of interacting electrons is zero, $\mathbf{p} + \mathbf{p_1} \simeq 0$) is fulfilled for each interaction line.

We begin by calculating the first diagram: the bubble without interaction $C^{(0)}(\mathbf{r}, t)$. As usual, we transform to the frequency-momentum representation:

$C^{(0)}(q,\omega)\ =$



We are interested in the behavior of the correlation function at small q and ω. The calculation is similar to that of the density response function in Sec. 3.13.1. Note, however, the crucial difference: arrows on Green functions in the bubble are parallel here (Cooper channel, the sum q of electron momenta is small), while there were anti-parallel there (correspondingly, the difference q of electron momenta was small).

According to the rules of the diagrammatic technique, we have

$$C^{(0)}(q,\omega) = -\mathrm{i}(-1)\int \frac{\mathrm{d}\varepsilon}{2\pi}\int \frac{\mathrm{d}^d p}{(2\pi)^d}\, G\left(\varepsilon + \frac{\omega}{2}, p + \frac{q}{2}\right) G\left(-\varepsilon + \frac{\omega}{2}, -p + \frac{q}{2}\right), \tag{5.17}$$

where $G(\omega, q)$ are free-electron Green's functions. We introduce

$$\xi = \frac{p^2}{2m} - \mu\,, \qquad \int \frac{\mathrm{d}^d p}{(2\pi)^d} \;\longrightarrow\; \nu \int \mathrm{d}\xi \int \mathrm{d}\mathbf{n}\,, \tag{5.18}$$

where ν is the density of states at the Fermi energy, and $\mathbf{n}$ is the unit vector in the direction of $\mathbf{p}$. Expanding the denominators of Green's functions up to the linear order in small momentum $\mathbf{q}$, see Eq. (3.312), we get

$$C^{(0)}(q,\omega) = \mathrm{i}\nu \int \mathrm{d}\xi \int \mathrm{d}\mathbf{n} \int \frac{\mathrm{d}\varepsilon}{2\pi} \frac{1}{\varepsilon + \frac{\omega}{2} - \xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} + \mathrm{i}0\,\mathrm{sign}\left(\frac{\xi + v_F \mathbf{n}\cdot\mathbf{q}}{2}\right)} \times$$
$$\times \frac{1}{-\varepsilon + \frac{\omega}{2} - \xi + \frac{v_F \mathbf{n}\cdot\mathbf{q}}{2} + \mathrm{i}0\,\mathrm{sign}\left(\xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2}\right)}\,. \tag{5.19}$$

We perform first the integration over ϵ. The integral is different from zero if the poles are on the opposite sides of the real axis. There are two such cases: either

$$\xi + v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} > 0\,, \quad \xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} > 0 \qquad \text{(case I)} \tag{5.20}$$

or

$$\xi + v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} < 0\,, \quad \xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} < 0 \qquad \text{(case II)}. \tag{5.21}$$

Evaluating the ε integrals by means of the residue theorem and combining both contributions, we get

$$C^{(0)}(q,\omega) = \nu \left[\int\limits_{\text{(I)}} \mathrm{d}\xi \int \mathrm{d}\mathbf{n}\, \frac{-1}{2\xi - \omega - \mathrm{i}0} + \int\limits_{\text{(II)}} \mathrm{d}\xi \int \mathrm{d}\mathbf{n}\, \frac{1}{2\xi - \omega + \mathrm{i}0} \right]. \tag{5.22}$$

The dominant contribution comes from the region $|\xi| > |\omega|$, $|v_F \mathbf{n}\cdot\mathbf{q}|$. In this range of ξ, one of the conditions (5.20) and (5.21) is fulfilled (the first one for positive ξ, the second one for negative ξ). Further, we neglect ω in the denominators in Eq. (5.22). The ξ intergrals in Eq. (5.22) then take the form of logarithmic integrals

$$\int\limits_{\max(|\omega|,|v_F\mathbf{n}\cdot\mathbf{q}|)}^{\varepsilon^*} \frac{\mathrm{d}\xi}{|\xi|}\,. \tag{5.23}$$

Since we will use the non-interacting bubble $C^{(0)}(q,\omega)$ as an element of geometric series for $C(q,\omega)$ of the interacting theory, the upper ("ultraviolet") cutoff ε^* is determined by the range of validity of the model with constant interaction. For the phonon-mediated attraction, which is our main focus here, we thus have Debye frequency as a cutoff $\varepsilon^* = \omega_D$. On the other hand, if we would perform an analogous calculation for the Cooper-channel repulsion due to Coulomb interaction, we would have Fermi energy as a cutoff $\varepsilon^* = \varepsilon_F$.

On the lower (infrared) side, the logarithmic divergence (5.23) is cut off either by frequency ω or by momentum $|v_F\mathbf{n}\cdot\mathbf{q}|$. Since there is also $\mathbf{n}$ integration in Eq. (5.22), the dominant contribution will come from typical $\mathbf{n}$ for which $|\mathbf{n}\cdot\mathbf{q}| \sim q$. Thus, we get

$$C^{(0)}(q,\omega) \simeq -\nu \ln \frac{\varepsilon^*}{\max(|\omega|, v_F q)}\,. \tag{5.24}$$

The fact that the Cooper-channel response $C^{(0)}(q,\omega)$ of a non-interacting Fermi gas is divergent in the limit $q,\omega \to 0$ implies an instability of the system with respect to an arbitrarily weak attractive interaction as we are going to discuss.

We return to the full series of ladder diagrams for $C(q,\omega)$ [see figure below Eq. (5.16)]. Every wavy (interaction) line is a constant

$$\lambda = -g^2\,,$$

see Eq. (5.15). In the real space this means a local interaction

$$U(\mathbf{r},\mathbf{r}';t,t') = \lambda\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')\,, \tag{5.25}$$

i.e. the interaction line is essentially contracted to a single point. (In other words, integrations within bubbles separated by an impurity line are decoupled.) The diagram of n-th order in interaction is thus $\lambda^n[C^{(0)}(q,\omega)]^{n+1}$. Summing up the geometric series, we get

$$C(q,\omega) = \frac{C^{(0)}(q,\omega)}{1-\lambda C^{(0)}(q,\omega)}\,. \tag{5.26}$$

Substituting here Eq. (5.24) and setting for simplicity $q = 0$, we get

$$C(q,\omega) = -\frac{\nu \ln\left(\frac{\varepsilon^*}{\omega}\right)}{1+\lambda\nu \ln\left(\frac{\varepsilon^*}{\omega}\right)}\,. \tag{5.27}$$

Let us analyse the final result (5.27). For repulsive interaction, $\lambda > 0$, there is no singularities. At the same time, for attractive interaction, $\lambda < 0$, we encounter a singularity at

$$\omega \sim \varepsilon^* \exp\left(-\frac{1}{|\lambda|\nu}\right)\,. \tag{5.28}$$

A slightly more accurate calculation of the integrals in Eq. (5.22) yields at $q = 0$ and $\omega > 0$

$$C^{(0)}(\omega) = \nu \left[-\int_0^{\varepsilon^*} \frac{d\xi}{2\xi - \omega - i0} + \int_{-\varepsilon^*}^{0} \frac{d\xi}{2\xi - \omega + i0} \right] \tag{5.29}$$

$$= -\nu \left[\frac{1}{2} \ln \frac{2\varepsilon^*}{-\omega - i0} + \frac{1}{2} \ln \frac{2\varepsilon^*}{\omega - i0} \right] = -\nu \left[\ln \frac{2\varepsilon^*}{\omega} + \frac{i\pi}{2} \right]. \tag{5.30}$$

The response function $C(\omega)$, Eq. (5.26), has a pole at a real value $C^{(0)}(\omega) = 1/\lambda < 0$. Continuing (5.30) into the complex plane, we find the position of the pole:

$$\omega = 2i\,\varepsilon^* \exp\left(-\frac{1}{|\lambda|\nu} \right). \tag{5.31}$$

The pole of the response function in the upper half-plane $\mathrm{Im}\,\omega > 0$ of complex ω implies an **instability**: the response function is retarded and should be regular in the half-plane $\mathrm{Im}\,\omega > 0$. Thus, our assumption (on which the calculation was based) that the ground state is of normal Fermi-liquid type is inconsistent: this state is unstable with respect to (arbitrarily weak) attractive interaction.

The instability indicates **spontaneous symmetry breaking** characterized by emergence of the anomalous correlation function $\langle \mathcal{T}\psi_\uparrow\psi_\downarrow \rangle$ and $\langle \mathcal{T}\psi_\uparrow^\dagger\psi_\downarrow^\dagger \rangle$:

$$\langle \mathcal{T}\psi_\uparrow\psi_\downarrow \rangle\,,\ \langle \mathcal{T}\psi_\uparrow^\dagger\psi_\downarrow^\dagger \rangle\ \neq 0 \tag{5.32}$$

In the limit of large r, t, the Cooper correlator (5.16) decouples into a product of anomalous averages:

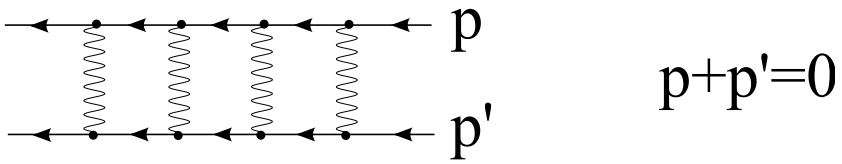
$$\langle \mathcal{T}\psi_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)\psi_\uparrow^\dagger(0,0)\psi_\downarrow^\dagger(0,0) \rangle \longrightarrow \langle \mathcal{T}\psi_\uparrow\psi_\downarrow \rangle \langle \mathcal{T}\psi_\uparrow^\dagger\psi_\downarrow^\dagger \rangle. \tag{5.33}$$

This is a spontaneous breaking of the $U(1)$ symmetrie. Indeed, consider the $U(1)$ transformation (with a constant ϕ)

$$\psi \ \to\ e^{i\phi}\psi\,, \qquad \psi^\dagger \to e^{-i\phi}\psi\,,$$

The Hamiltonian, which contains terms of the type $\psi^\dagger\psi$ and $\psi^\dagger\psi^\dagger\psi\psi$, is invariant with respect to this transformation. At the same, the ground state is not invariant, as is manifested in Eq. (5.32). There is a clear analogy with ferromagnetism, where divergence of the magnetic susceptibility in the paramagnetic state signals spontaneous breaking of symmetry [$O(3)$ in the case of isotropic system] characterized by anomalous (ferromagnetic) average (average magnetization).

With a slight modification, the same calculation as above for the Cooper response function can be performed for the scattering amplitude in the Cooper channel. It is given by a sum of ladder diagrams with external ends satisfying $\mathbf{p} + \mathbf{p}' = 0$:



The first term (one interaction line) is simply the bare vertex λ, and the denominator of the geometric series is the same as above, so that we get

$$\Gamma(\omega) = \frac{\lambda}{1 + \lambda\nu \ln\left(\frac{\varepsilon^*}{\omega}\right)}\,. \tag{5.34}$$

Singularity of the scattering amplitude signals formation of bound states (Cooper pairs). The scale ω, Eq. (5.28), at which the singularity occurs determines, up to numerical coefficients of order unity, the value of the **superconducting gap** Δ (at zero temperature) as well as the **critical temperature** T_c of the superconducting transition. It is important to emphasize a **non-analytic** dependence of this scale on the interaction strength λ. Indeed, the result (5.28) is non-perturbative with respect to a weak interaction λ: an attempt to expand in power series in λ would yield zero in all orders.

The ω dependence of the amplitude Γ shows that the effective Cooper-channel interaction changes as a function of the energy scale ω. (Alternatively, one can consider a change with momentum scale q.) Equation (5.34) can be equivalently presented in the form of a differential equation

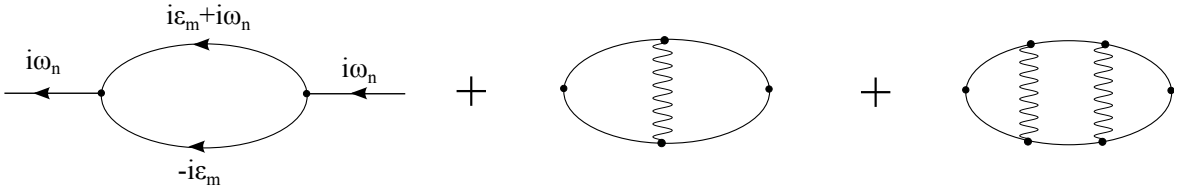
$$\begin{aligned} -\frac{d\Gamma^{-1}}{d\ln\omega} &= \nu \\ \text{or, equivalently} \qquad -\frac{d\Gamma}{d\ln\omega} &= -\nu\Gamma^2\,, \end{aligned} \tag{5.35}$$

with the condition

$$\Gamma(\epsilon^*) = \lambda. \tag{5.36}$$

Equation (5.35) can be viewed as **renormalization flow** of the Cooper-channel interaction constant. It is initially defined at the ultraviolet scale ϵ^*, see Eq. (5.36) and then gets renormalized when one proceeds to lower energy scales. Such renormalization plays an extremely important role in many physical phenomena. The general formalism is known under the name **renormalization group (RG)**.

Let us generalize the analysis to calculate explicitly T_c. We use the Matsubara formalism and calculate the Cooper susceptibility at finite temperature T and zero wave vector $\mathbf{q}$. We have the same sum of ladder diagrams but now with imaginary Matsubara frequencies:



Here the external frequency is bosonic,

$$\omega_n = 2n\pi T\,, \tag{5.37}$$

while internal energies (to be summed over) are femionic,

$$\varepsilon_m = (2m+1)\pi T\,. \tag{5.38}$$

Summing the geometric series, one finds

$$\chi_c(\mathrm{i}\omega_n) = \frac{\chi_c^{(0)}(\mathrm{i}\omega_n)}{1+\lambda\chi_c^{(0)}(\mathrm{i}\omega_n)}\,, \tag{5.39}$$

where

$$\chi_c^{(0)}(\mathrm{i}\omega_n) = T\sum_m \nu\int \mathrm{d}\xi\,\frac{1}{(\mathrm{i}\varepsilon_m+\mathrm{i}\omega_n-\xi)(-\mathrm{i}\varepsilon_m-\xi)}\,. \tag{5.40}$$

To determine T_c, we focus on the static susceptibility, $\omega_n = 0$. We perform the summation over Matsubara frequencies:

$$T\sum_m \frac{1}{(\mathrm{i}\varepsilon_m - \xi)(-\mathrm{i}\varepsilon_m - \xi)} = \frac{1}{2\xi}\tanh\left(\frac{\xi}{2T}\right). \tag{5.41}$$

Thus

$$\chi_c^{(0)}(\mathrm{i}\omega_n = 0) = T\sum_m \nu \int \mathrm{d}\xi\, \frac{1}{\varepsilon_m^2 + \xi^2} = \nu \int_{-\omega_D}^{\omega_D} \mathrm{d}\xi\, \frac{1}{2\xi}\tanh\left(\frac{\xi}{2T}\right) = \nu \ln\left(\frac{2e^\gamma}{\pi}\,\frac{\omega_D}{T}\right), \tag{5.42}$$

where $\gamma \approx 0.577$ is the Euler-Mascheroni constant. We have used a sharp upper cutoff (BCS model) and put the Debye frequency ω_D as a cutoff having in mind the attractive interaction mediated by phonons. Substituting Eq. (5.42) into Eq. (5.39), we find that the susceptibility diverges at the critical temperature (here $\lambda = -g^2 < 0$)

$$T_C = \frac{2e^\gamma}{\pi}\omega_D \exp\left(-\frac{1}{|\lambda|\nu}\right). \tag{5.43}$$

Below this temperature, the system becomes unstable and the superconducting order develops.

5.4 BCS theory: Brief reminder

For completeness, we include a reminder of the BCS theory as was presented in TKM I.

We consider the Hamiltonian

$$\widehat{H} = \sum_{p,\alpha} \xi_p a^\dagger_{p,\alpha} a_{p,\alpha} + \frac{1}{2}\sum_{\substack{p+p'=q+q' \\ \alpha,\beta}} V_{p,p',q,q} a^\dagger_{p,\alpha} a^\dagger_{p',\beta} a_{q',\beta} a_{q,\alpha}\,, \tag{5.44}$$

with

$$V_{p,p',q,q'} = \frac{1}{V}\begin{cases} \lambda & \text{for} \quad |\xi_{\max}| < \omega_D\,, \\ 0 & \text{otherwise}\,, \end{cases} \tag{5.45}$$

where α, β are spin indices, V is the volume, $\lambda < 0$ the interaction constant, and

$$|\xi_{\max}| = \max(|\xi_p|, |\xi_{p'}|, |\xi_q|, |\xi_{q'}|)\,, \quad \xi_p = v_F(p - p_F)\,. \tag{5.46}$$

Only such electrons interact with each other that belong to a narrow shell (of width ω_D) around the Fermi energy. Further, one keeps only pairs with

$$p' = -p\,, \qquad q' = -q$$

(Cooper-channel interaction): only particles with opposite momenta interact with each other. We are left with the BCS Hamiltonian

$$\widehat{H}_{\mathrm{BCS}} = \sum_{p,\alpha} \xi_p a^\dagger_{p,\alpha} a_{p,\alpha} + \frac{\lambda}{V}\sum_{\substack{p,q \\ |\xi_p|,|\xi_q|<\omega_D}} a^\dagger_{p,\uparrow} a^\dagger_{-p,\downarrow} a_{q,\downarrow} a_{-q,\uparrow}\,, \tag{5.47}$$

Note that spins within the Cooper pair (i.e. of two particles with opposite momenta) are opposite since $\sum_p a^\dagger_{p,\uparrow} a^\dagger_{-p,\downarrow}$ is identically zero in view of Fermi statistics.

Mean-field solution: introduce **anomalous expectation values**

$$\Delta^* = \frac{|\lambda|}{V} \sum_p \langle a^\dagger_{p,\uparrow} a^\dagger_{-p,\downarrow} \rangle \,, \tag{5.48}$$

$$\Delta = \frac{|\lambda|}{V} \sum_p \langle a_{p,\downarrow}, a_{-p,\uparrow} \rangle \,. \tag{5.49}$$

Cooper pairs have total momentum zero and total spin zero. The BCS theory describes the simplest possible type of the superconducting order—***s*-wave spin-singlet pairing**. However, this is not the only possible superconducting order. Many high-temperature superconductors exhibit d-wave spin-singlet pairing. Also, there are some materials that show p-wave spin-triplet pairing.

The mean-field Hamiltonian reads

$$\widehat{H}_{\mathrm{MF}} = \sum_p \xi_p (a^\dagger_{p,\uparrow} a_{p,\uparrow} + a^\dagger_{p,\downarrow} a_{p,\downarrow}) + \sum_p \left(\Delta a^\dagger_{p,\downarrow} a^\dagger_{-p,\uparrow} + \Delta^* a_{p,\uparrow} a_{-p,\downarrow} \right) . \tag{5.50}$$

To diagonalize this Hamiltonian, we introduce (Bogoliubov transformation)

$$c_{p,\uparrow} = u_p a_{p,\uparrow} + v_p a^\dagger_{-p,\downarrow} \,, \quad c_{p,\downarrow} = u_p a_{p,\downarrow} - v_p a^\dagger_{-p,\uparrow} \,. \tag{5.51}$$

The coefficients u_p, v_p of this transformation should be determined from the condition that terms of the type cc and $c^\dagger c^\dagger$ cancel:

$$\widehat{H} = E_0 + \sum_{p,\alpha} \varepsilon_p c^\dagger_{p,\alpha} c_{p,\alpha} \,. \tag{5.52}$$

It is sufficient to consider $\Delta \in \mathbb{R}$. Then u_p and v_p can be also chosen real, $u_p = u_{-p} = u_p^*$ and $v_p = v_{-p} = v_p^*$. The result is

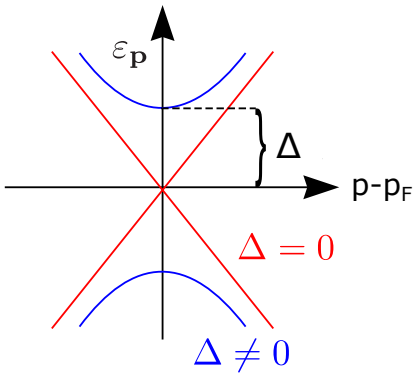
$$u_p^2 = \frac{1}{2} \left(1 + \frac{\xi_p}{\varepsilon_p} \right) , \quad v_p^2 = \frac{1}{2} \left(1 - \frac{\xi_p}{\varepsilon_p} \right) , \tag{5.53}$$

with

$$\varepsilon_p = (\xi_p^2 + \Delta^2)^{\frac{1}{2}} \,. \tag{5.54}$$

Hence, one obtains a change in the dispersion relation: an **energy gap** emerges.

This figure shows ε_p and its mirror reflection, $-\varepsilon_p$. The gap between the ground state and the lowest excited state, which is obtained by breaking the Cooper pair and creating a pair of excitations at the Fermi surface, is 2Δ.



Substituting the inverted Bogloliubov transformation

$$a_{p,\uparrow} = u_p c_{p,\uparrow} - v_{p'} c^\dagger_{-p,\downarrow} \,, \quad a_{p,\downarrow} = u_p c_{p,\downarrow} + v_p c^\dagger_{-p,\uparrow} \,, \tag{5.55}$$

in the definition of Δ, one obtains the self-consistency equation

$$\Delta = \frac{|\lambda|}{2V} \sum_p u_p v_p \qquad \Longrightarrow \qquad \Delta = \frac{|\lambda|}{V} \sum_p \frac{\Delta}{(\xi_p^2 + \Delta^2)^{\frac{1}{2}}} \,, \tag{5.56}$$

and thus, after cancelling Δ on both sides of the equation,

$$1 = \frac{|\lambda|}{2V} \sum_p \frac{1}{(\xi_p^2 + \Delta^2)^{\frac{1}{2}}} \,. \tag{5.57}$$

We replace the summation by an integral and evaluate the integral:

$$\begin{aligned} 1 &= \frac{|\lambda|}{2}\nu \int_{-\omega_D}^{\omega_D} \mathrm{d}\xi \, \frac{1}{(\xi^2 + \Delta^2)^{\frac{1}{2}}} = |\lambda|\nu \int_0^{\omega_D/\Delta} \frac{dx}{\sqrt{1+x^2}} \\ &= |\lambda|\nu \ln(\sqrt{1+x^2} + x)\Big|_0^{\omega_D/\Delta} \simeq |\lambda|\nu \ln \frac{2\omega_D}{\Delta} \,, \end{aligned} \tag{5.58}$$

where we used $\omega_D/\delta \gg 1$. Thus, we finally get the value of the gap:

$$\boxed{\Delta = 2\omega_D \exp\left(-\frac{1}{|\lambda|\nu}\right) .} \tag{5.59}$$

Comparing (5.59) with (5.43), one finds the universal ratio of the zero-temperature gap to critical temperature within the BCS theory:

$$\frac{2\Delta(T=0)}{T_c} = \frac{2\pi}{\gamma} \approx 3.53. \tag{5.60}$$

The BCS ground state $|\Phi_{\mathrm{BCS}}\rangle$ satisfies $c_{p\sigma}|\Phi_{\mathrm{BCS}}\rangle = 0$ for all p, σ. This yields

$$|\Phi_{\mathrm{BCS}}\rangle = \prod_p \left(u_p + v_p a^\dagger_{p,\uparrow} a^\dagger_{-p,\downarrow}\right)|0\rangle \,. \tag{5.61}$$

Note there are in fact many equivalent ground state that are obtained from this one by a transformation $a^\dagger \to a^\dagger e^{i\phi}$:

$$|\Phi^{(\phi)}_{\mathrm{BCS}}\rangle = \prod_p \left(u_p + v_p e^{2i\phi} a^\dagger_{p,\uparrow} a^\dagger_{-p,\downarrow}\right)|0\rangle \,. \tag{5.62}$$

The existence of a manifold of degenerate ground state is a manifestation of spontaneous symmetry breaking. Note that these states are not characterized by a given particle number N. (These are states with a given phase ϕ). One can obtain a state with a fixed number of particles N by taking the appropriate linear combination

$$|\Phi^{(N)}_{\mathrm{BCS}}\rangle = \int \frac{d\phi}{2\pi} e^{-iN\phi} |\Phi^{(\phi)}_{\mathrm{BCS}}\rangle \,. \tag{5.63}$$

5.5 Green functions in a superconductor

The Green function formalism is a very powerful approach for calculating various physical observables. Thus, it is important to develop it also for superconducting systems. At the same time, in view of the spontaneous symmetry breaking in a superconducting state, the Green function formalism requires modification in this situation. The appropriate formalism was developed by Nambu and Gorkov.

Below we consider the simplest model: uniform system, no external fields, constant interaction (as in the BCS model) and will rederive in this way the BCS solution. The Green

function formalism has proven to be very useful in a variety of more complicated problems: superconducting systems subjected to external electromagnetic fields, spatially inhomogeneous setups, disordered superconductors, etc.

We consider the $T = 0$ technique; in the finite-temperature (Matsubara) formalism one proceeds in an analogous way. First, we define the normal Green function,

$$G_{\alpha\beta}(1,2) = -\mathrm{i}\langle \mathcal{T}\psi_\alpha(1)\psi^\dagger_\beta(2)\rangle\,, \qquad \text{1} \leftarrow \text{2} \tag{5.64}$$

where we use compact notations for arguments, $1 = (\mathbf{r_1}, t_1)$ and α, β are spin indices. In addition, one defines **anomalous Green functions**

$$F_{\alpha\beta}(1,2) = -\mathrm{i}\langle \mathcal{T}\psi_\alpha(1)\psi_\beta(2)\rangle\,, \qquad \text{1} \leftrightarrow \text{2} \tag{5.65}$$

and

$$\overline{F}_{\alpha\beta}(1,2) = -\mathrm{i}\langle \mathcal{T}\psi^\dagger_\alpha(1)\psi^\dagger_\beta(2)\rangle\,. \qquad \text{1} \rightarrow \leftarrow \text{2} \tag{5.66}$$

The anomalous Green functions are zero in normal state since they break the U(1) invariance $\psi \to e^{i\phi}\psi$. They become non-zero in superconducting state in view of the spontaneous symmetry breaking.

The averaging in these formulas goes over the superconducting ground state, which in the BCS theory has the form (5.61). If one wants to think instead in terms of a ground state $|N\rangle$ with given number of particles, then the correlator F should be understood as $-\mathrm{i}\langle N|\mathcal{T}\psi_\alpha(1)\psi_\beta(2)|N{+}2\rangle$. The state $|N{+}2\rangle$ contains one additional Cooper pair in comparison with $|N\rangle$.

5.5.1 Equations for Green functions

We start with the Hamiltonian

$$\widehat{H} = \int \mathrm{d}^3 r \left\{ \hat\psi^\dagger_\alpha \left(-\frac{\boldsymbol{\nabla}^2}{2m} - \mu \right) \hat\psi_\alpha + \frac{\lambda}{2} \hat\psi^\dagger_\alpha \hat\psi^\dagger_\gamma \hat\psi_\gamma \hat\psi_\alpha \right\}. \tag{5.67}$$

The ultraviolet cutoff ω_D is implicitly assumed and will be taken into account at the appropriate stage.

We want to derive (and then solve) equations for Green functions defined above. To this end, we first derive the equations of motion for $\hat\psi$ and $\hat\psi^\dagger$. Using

$$\mathrm{i}\frac{\partial}{\partial t}\hat\psi_\alpha = [\hat\psi_\alpha, \widehat{H}]\,, \qquad \mathrm{i}\frac{\partial}{\partial t}\hat\psi^\dagger_\alpha = [\hat\psi^\dagger_\alpha, \widehat{H}]\,, \tag{5.68}$$

we get

$$\mathrm{i}\frac{\partial}{\partial t}\hat\psi_\alpha(x) = -\left(\frac{\boldsymbol{\nabla}^2}{2m} + \mu \right) \hat\psi_\alpha(x) + \lambda \hat\psi^\dagger_\gamma(x)\hat\psi_\gamma(x)\hat\psi_\alpha(x)\,, \tag{5.69}$$

and

$$\mathrm{i}\frac{\partial}{\partial t}\hat\psi^\dagger_\alpha(x) = \left(\frac{\boldsymbol{\nabla}^2}{2m} + \mu \right) \hat\psi^\dagger_\alpha(x) - \lambda \hat\psi^\dagger_\alpha(x)\hat\psi^\dagger_\gamma(x)\hat\psi_\gamma(x)\,, \tag{5.70}$$

where $x = (\mathbf{r}, t)$. Multiplying Eq. (5.69) with $-\mathrm{i}\psi^\dagger_\beta(x')$ and performing the average $\langle \mathcal{T}\ldots\rangle$, we obtain an equation of motion for the Green function G:

$$\left(\mathrm{i}\frac{\partial}{\partial t} + \frac{\boldsymbol{\nabla}^2}{2m} + \mu \right) G_{\alpha\beta}(x,x') + \mathrm{i}\lambda \langle \mathcal{T}\hat\psi^\dagger_\gamma(x)\hat\psi_\gamma(x)\hat\psi_\alpha(x)\hat\psi^\dagger_\beta(x')\rangle = \delta_{\alpha\beta}\delta(x-x')\,. \tag{5.71}$$

The delta function on the r.h.s. originates from the time derivative acting on a discontinuity in $G_{\alpha\beta}(x,x')$ resulting from time ordering.

Equation (5.71) is exact but cannot be solved without making an approximation. We proceed in spirit of mean-field approximation and decouple the correlation function involving four ψ-operators in terms of products of pairwise Green functions:

$$\langle \mathcal{T}\hat{\psi}^\dagger_\gamma(x)\hat{\psi}_\gamma(x)\hat{\psi}_\alpha(x)\hat{\psi}^\dagger_\beta(x')\rangle \approx \langle \mathcal{T}\psi_\gamma(x)\psi_\alpha(x)\rangle\langle \mathcal{T}\psi^\dagger_\gamma(x)\psi^\dagger_\beta(x')\rangle\,, \tag{5.72}$$

We have discarded the other two terms in Eq. (5.72), namely $\langle \mathcal{T}\psi^\dagger_\gamma(x)\psi_\gamma(x)\rangle\langle \mathcal{T}\psi_\alpha(x)\psi^\dagger_\beta(x')\rangle$ and $-\langle \mathcal{T}\psi_\gamma(x)^\dagger\psi_\alpha(x)\rangle\langle \mathcal{T}\psi_\gamma(x)\psi^\dagger_\beta(x')\rangle$. They only lead to an additive correction to the chemical potential and are not essential for our analysis. The r.h.s. of Eq. (5.72) is nothing but

$$\mathrm{i}^2 F_{\gamma\alpha}(x,x)\overline{F}_{\gamma\beta}(x,x')\,. \tag{5.73}$$

The spin structure is $G_{\alpha\beta}\propto\delta_{\alpha\beta}$ and

$$F_{\alpha\beta},\,\overline{F}_{\alpha\beta}\propto g_{\alpha\beta}=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\,, \tag{5.74}$$

the latter formula being a manifestation of the singlet pairing. Hence, one can write $G_{\alpha\beta}=G\,\delta_{\alpha\beta}$, $F_{\alpha\beta}=F\,g_{\alpha\beta}$, and $\overline{F}_{\alpha\beta}=\overline{F}\,g_{\alpha\beta}$. Further, we note that

$$\sum_\gamma g_{\gamma\alpha}g_{\gamma\beta}=\delta_{\alpha\beta}\,. \tag{5.75}$$

We thus reduce Eq. (5.71) to the form

$$\boxed{\left(\mathrm{i}\frac{\partial}{\partial t}+\frac{\boldsymbol{\nabla}^2}{2m}+\mu\right)G(x-x')-\mathrm{i}\lambda F(0)\overline{F}(x-x')=\delta(x-x')\,.} \tag{5.76}$$

We have used here the translational invariance, $G(x,x')=G(x-x')$ etc.

In the same way, we obtain from Eq. (5.70) the following equation for $\overline{F}$:

$$\left(\mathrm{i}\frac{\partial}{\partial t}-\frac{\boldsymbol{\nabla}^2}{2m}-\mu\right)\overline{F}(x-x')=-\mathrm{i}\lambda\langle \mathcal{T}\hat{\psi}^\dagger_\alpha(x)\hat{\psi}^\dagger_\gamma(x)\hat{\psi}_\gamma(x)\hat{\psi}^\dagger_\beta(x')\rangle=0\,. \tag{5.77}$$

Note that the r.h.s. here is zero: the function $\overline{F}$ has no discontinuity at $t=t'$ since $\psi^\dagger(x)$ and $\psi^\dagger(x')$ anticommute at $t=t'$. Performing again a mean-field-like decoupling

$$\langle \mathcal{T}\hat{\psi}^\dagger_\alpha(x)\hat{\psi}^\dagger_\gamma(x)\hat{\psi}_\gamma(x)\hat{\psi}^\dagger_\beta(x')\rangle \approx \langle \mathcal{T}\hat{\psi}^\dagger_\alpha(x)\hat{\psi}^\dagger_\gamma(x)\rangle\langle \mathcal{T}\hat{\psi}_\gamma(x)\hat{\psi}^\dagger_\beta(x')\rangle\,, \tag{5.78}$$

we obtain

$$\boxed{\left(\mathrm{i}\frac{\partial}{\partial t}-\frac{\boldsymbol{\nabla}^2}{2m}-\mu\right)\overline{F}(x-x')+\mathrm{i}\lambda\overline{F}(0)G(x-x')=0\,.} \tag{5.79}$$

Equations (5.76) and (5.79) form a system of two equations for the functions G and $\overline{F}$. In these equations, $F(0)$ and $\overline{F}(0)$ are complex-conjugate constants:

$$F(0)=-\mathrm{i}\langle\psi_\uparrow(x)\psi_\downarrow(x)\rangle\,,\qquad \overline{F}(0)=-\mathrm{i}\langle\psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x)\rangle=F^*(0)\,. \tag{5.80}$$

Fourier transformation of these equations yields

$$(\varepsilon-\xi_p)G(\varepsilon,p)-\mathrm{i}\lambda F(0)\overline{F}(\varepsilon,p)=1\,, \tag{5.81}$$

and

$$(\varepsilon + \xi_p)\overline{F}(\varepsilon, p) + \mathrm{i}\lambda F^*(0) G(\varepsilon, p) = 0\,. \tag{5.82}$$

The solution for $G(\varepsilon, p)$ reads

$$G(\varepsilon, p) = \frac{\varepsilon + \xi_p}{\varepsilon^2 - \xi_p^2 - \Delta^2}\,, \tag{5.83}$$

where

$$\Delta^2 = \lambda^2 |F(0)|^2\,. \tag{5.84}$$

We decompose this result into a sum of two fractions, each with a single pole:

$$G(\varepsilon, p) = \frac{u_p^2}{\varepsilon - \varepsilon_p} + \frac{v_p^2}{\varepsilon + \varepsilon_p}\,, \tag{5.85}$$

where

$$u_p^2 = \frac{1}{2}\left(1 + \frac{\xi_p}{\varepsilon_p}\right)\,, \quad v_p^2 = \frac{1}{2}\left(1 - \frac{\xi_p}{\varepsilon_p}\right)\,, \tag{5.86}$$

and

$$\varepsilon_p = (\xi_p^2 + \Delta^2)^{\frac{1}{2}}\,. \tag{5.87}$$

We know from general analytic properties of the Green function G (considered as a function of ε) that its singularities at $\varepsilon > 0$ should be in the lower half plane (i.e. we should shift $\varepsilon \to \varepsilon + \mathrm{i}0$), while for $\varepsilon < 0$ the singularities should be in the upper half plane (i.e. we should shift $\varepsilon \to \varepsilon - \mathrm{i}0$). Restoring the proper analytic structure of singularities, we thus get

$$\boxed{G(\varepsilon, p) = \frac{u_p^2}{\varepsilon - \varepsilon_p + \mathrm{i}0} + \frac{v_p^2}{\varepsilon + \varepsilon_p - \mathrm{i}0} = \frac{\varepsilon + \xi_p}{(\varepsilon - \varepsilon_p + \mathrm{i}0)(\varepsilon + \varepsilon_p - \mathrm{i}0)}\,.} \tag{5.88}$$

The Green function is a sum of contributions of Bogoliubov quasiparticles and quasiholes with weights u_p^2 and v_p^2, respectively.

Having determined $G(\varepsilon, p)$, we find from Eq. (5.82) the anomalous Green function $\overline{F}(\varepsilon, p)$:

$$\overline{F}(\varepsilon, p) = -\mathrm{i}\lambda \frac{F^*(0)}{(\varepsilon - \varepsilon_p + \mathrm{i}0)(\varepsilon + \varepsilon_p - \mathrm{i}0)}\,. \tag{5.89}$$

Substituting this in the identity

$$F^*(0) = \int \frac{\mathrm{d}\varepsilon}{2\pi} \frac{\mathrm{d}^3 p}{(2\pi)^3}\, \overline{F}(\varepsilon, p)\,, \tag{5.90}$$

one obtains the self-consistency equation

$$1 = \mathrm{i}|\lambda| \int \frac{\mathrm{d}\varepsilon\, \mathrm{d}^3 p}{(2\pi)^4} \frac{1}{(\varepsilon - \varepsilon_p + \mathrm{i}0)(\varepsilon + \varepsilon_p - \mathrm{i}0)}\,. \tag{5.91}$$

Performing the ε integration, we get

$$1 = |\lambda| \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2\epsilon_p} = |\lambda| \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2\sqrt{\xi_p^2 + \Delta^2}} = |\lambda|\, \nu \int_{-\omega_D}^{\omega_D} \frac{d\xi_p}{2\sqrt{\xi_p^2 + \Delta^2}}\,. \tag{5.92}$$

In the last form of Eq. (5.92) we have restored the ultraviolet cutoff (ω_D). Equation (5.92) is identical to (5.92) and leads to the result (5.59) for the zero-temperature gap Δ (which we repeat here for completeness):

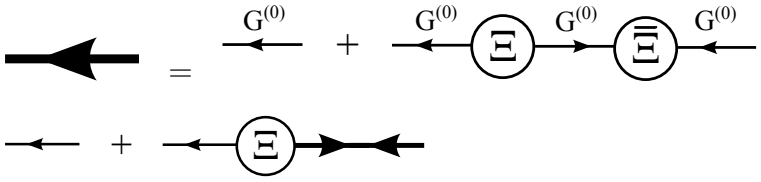
$$\boxed{\Delta = 2\omega_D \exp\left(-\frac{1}{|\lambda|\nu}\right)\,.} \tag{5.93}$$

5.5.2 Diagrammatic representation

We present here a diagrammatic version of the derivation of equations fro Green functions in a superconductor presented in Sec. 5.5.1. This will allow us to see the connection with (and differences from) the corresponding derivation for normal systems.

In analogy with Eqs. (3.222), (3.223) we have a Dyson series for the Green function:

$G_{\alpha\beta}$ =



$$= G^{(0)}_{\alpha\beta} + G^{(0)}_{\alpha\gamma}\,\Xi_{\gamma\delta}\,\overline{F}_{\delta\beta}\,. \tag{5.94}$$

Here Ξ and $\bar{\Xi}$ are the anomalous self-energies. (The normal self-energy is discarded as it is not essential for this analysis.) Including the energy and momentum arguments, we have

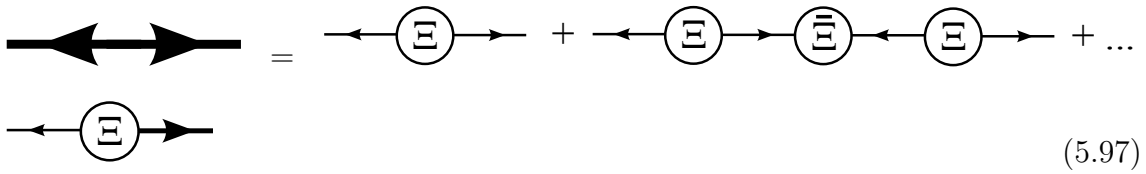
$$G_{\alpha\beta}(\varepsilon,p) = G^{(0)}_{\alpha\beta}(\varepsilon,p) + G^{(0)}_{\alpha\gamma}(\varepsilon,p)\,\Xi_{\gamma\delta}(\varepsilon,p)\overline{F}_{\delta\beta}(\varepsilon,p)\,. \tag{5.95}$$

As discussed above, the spin structure is $G_{\alpha\beta} = G\delta_{\alpha\beta}$ and $F_{\alpha\beta} = Fg_{\alpha\beta}$, $\overline{F}_{\alpha\beta} = \overline{F}g_{\alpha\beta}$, see Eq. (5.74), so that Eq. (5.95) reduces to

$$G(\varepsilon,p) = G^{(0)}(\varepsilon,p) - G^{(0)}(\varepsilon,p)\,\Xi(\varepsilon,p)\overline{F}(\varepsilon,p) \tag{5.96}$$

Similarly, we have an equation of Dyson type for the anomalous Green function:

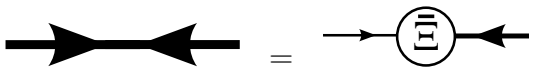
$F_{\alpha\beta}$ =



(5.97)

and, analogously,

$\overline{F}_{\alpha\beta}$ =



(5.98)

In the algebraic form, they read

$$F_{\alpha\beta}(\varepsilon,p) = G^{(0)}_{\alpha\gamma}(\varepsilon,p)\Xi_{\gamma\delta}(\varepsilon,p)G_{\delta\beta}(-\varepsilon,-p)\,, \tag{5.99}$$

$$\overline{F}_{\alpha\beta}(\varepsilon,p) = G^{(0)}_{\alpha\gamma}(-\varepsilon,-p)\overline{\Xi}_{\gamma\delta}(\varepsilon,p)G_{\delta\beta}(\varepsilon,p)\,, \tag{5.100}$$

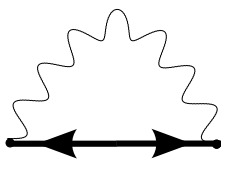
or, after taking care about the spin structure,

$$F(\varepsilon,p) = G^{(0)}(\varepsilon,p)\Xi(\varepsilon,p)G(-\varepsilon,-p)\,, \tag{5.101}$$

$$\overline{F}(\varepsilon,p) = G^{(0)}(-\varepsilon,-p)\overline{\Xi}(\varepsilon,p)G(\varepsilon,p)\,. \tag{5.102}$$

Equations (5.96) and (5.102) represent a system of two equations for two functions $G(\varepsilon,p)$ and $\overline{F}(\varepsilon,p)$. To solve them, we need to close the system and thus to make an approximation for the self-energies Ξ, $\overline{\Xi}$. This is done by using an analog of self-consistent Hartree-Fock approximation (3.259). The corresponding diagram for the anomalous self-energy Ξ looks as follows:

Ξ =



(5.103)

and similarly for $\overline{\Xi}$. For the point-like interaction of strength λ the self-energy is a constant in momentum-energy representation and is equal to

$$\Xi = i\lambda \int \frac{d^3p\, d\varepsilon}{(2\pi)^4}\, F(\epsilon,p) \equiv i\lambda F(0)\,, \qquad \overline{\Xi} = i\lambda \int \frac{d^3p\, d\varepsilon}{(2\pi)^4}\, \overline{F}(\epsilon,p) \equiv i\lambda F^*(0)\,. \tag{5.104}$$

Using

$$[G^{(0)}(\varepsilon,p)]^{-1} = \varepsilon - \xi_p\,, \qquad \xi_p = \frac{p^2}{2m} - \mu\,,$$

we thus rewrite Eqs. (5.96) and (5.102) in the form

$$(\varepsilon - \xi_p)G(\epsilon,p) - i\lambda F(0)\overline{F}(\varepsilon,p) = 1\,, \tag{5.105}$$

$$(\varepsilon + \xi_p)\overline{F}(\varepsilon,p) + i\lambda F^*(0)G(\varepsilon,p) = 0\,. \tag{5.106}$$

This system is identical to equations (5.81) and (5.82). The rest of the solution in Sec. 5.5.1 thus follows.

5.5.3 Nambu-Gorkov Matrix Formalism

Green functions in a superconductor (as defined above) in the matrix form:

$$\begin{aligned} G_{\uparrow\uparrow}(1,2) &= -i\langle\, \mathcal{T}\psi_\uparrow(1)\psi^\dagger_\uparrow(2)\,\rangle = G(1,2) \\ G_{\downarrow\downarrow}(1,2) &= -i\langle\, \mathcal{T}\psi_\downarrow(1)\psi^\dagger_\downarrow(2)\,\rangle = G(1,2) \\ F_{\uparrow\downarrow}(1,2) &= -i\langle\, \mathcal{T}\psi_\uparrow(1)\psi_\downarrow(2)\,\rangle = F(1,2) \\ \bar{F}_{\downarrow\uparrow}(1,2) &= -i\langle\, \mathcal{T}\psi^\dagger_\downarrow(1)\psi^\dagger_\uparrow(2)\,\rangle = -\overline{F}(1,2) \end{aligned} \tag{5.107}$$

We introduce the **Nambu spinor**:

$$\boldsymbol{\psi} = \begin{pmatrix} \psi_\uparrow \\ \psi^\dagger_\downarrow \end{pmatrix}\,, \qquad \boldsymbol{\psi}^\dagger = \begin{pmatrix} \psi^\dagger_\uparrow & \psi_\downarrow \end{pmatrix}\,. \tag{5.108}$$

The **matrix Green function** is then defined according to

$$\begin{aligned} \hat{G}(1,2) &= -i\langle\, \mathcal{T}\boldsymbol{\psi}\,(1) \otimes \boldsymbol{\psi}^\dagger(2)\,\rangle \\ &= \begin{pmatrix} -i\langle\, \mathcal{T}\psi_\uparrow(1)\psi^\dagger_\uparrow(2)\,\rangle & -i\langle\, \mathcal{T}\psi_\uparrow(1)\psi_\downarrow(2)\,\rangle \\ -i\langle\, \mathcal{T}\psi^\dagger_\downarrow(1)\psi^\dagger_\uparrow(2)\,\rangle & -i\langle\, \mathcal{T}\psi^\dagger_\downarrow(1)\psi_\downarrow(2)\,\rangle \end{pmatrix} \\ &= \begin{pmatrix} G(1,2) & F(1,2) \\ -\overline{F}(1,2) & -G(2,1) \end{pmatrix}\,. \end{aligned} \tag{5.109}$$

In the absence of interaction we have

$$\begin{aligned} (i\partial_{t_1} - \hat{H}_0)G(1,2) &= \delta(r_1 - r_2)\delta(t_1 - t_2)\,, \\ i\partial_{t_1}F(1,2) &= i\partial_{t_1}\overline{F}(1,2) = 0\,, \end{aligned}$$

which can be cast in the matrix form

$$(i\partial_{t_1} - \hat{H}_0\tau_z)\hat{G}(1,2) = \delta(r - r')\delta(t - t')\mathbb{1}\,, \tag{5.110}$$

where τ_z is the third Pauli matrix in the Nambu space. Transforming to the energy-momentum representation, we get

$$(\varepsilon - \xi_p\tau_z + i0\,\mathrm{sign}\,\varepsilon)\,\hat{G}(\epsilon,p) = \mathbb{1}\,, \tag{5.111}$$

where we have included the infinitesimal shift $\varepsilon \to \varepsilon + i0\,\mathrm{sign}\,\varepsilon$ to indicate the analytical properties of $\hat{G}$. In the presence of interaction, we have equations (5.81) and (5.82), which correspond to the following **matrix equation for the Green function**:

$$\begin{pmatrix} \epsilon - \xi_p & -\Delta \\ -\Delta^* & \epsilon + \xi_p \end{pmatrix} \hat{G}(\epsilon, p) = \mathbb{1}\,, \tag{5.112}$$

or, equivalently,

$$(\epsilon - \xi_p \tau_z - \Delta\tau_+ - \Delta^*\tau_-)\,\hat{G}(\epsilon, p) = \mathbb{1}\,, \tag{5.113}$$

where

$$\tau_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \tau_+ = \frac{1}{2}(\tau_x + i\tau_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \tau_- = \frac{1}{2}(\tau_x - i\tau_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Matrix Hamiltonians corresponding to Eq. (5.112) and its various generalizations are frequently called **Bogoliubov-de Gennes Hamiltonians**.

Chapter 6

Functional integral formalism

Goal of this Chapter: to develop a powerful approach to many-body condensed-matter quantum field theory based on integrals over field configuration (**"functional integrals"**). It is an approach alternative to (but also equivalent to) the operator approach presented above. In particular, it reproduces the Wick theorem, perturbative diagrammatic expansion, etc. However, the functional-integral approach has many very important advantages—which is why it is so broadly used in scientific research in modern condensed matter physics. These advantages become especially important in situations when one has to go beyond the simple perturbation theory—including, in particular, the situations when (i) an infinite resummation of diagrams is needed that corresponds to the action of the renormalization group, or (ii) a spontaneous symmetry breaking occurs, or (iii) physically relevant degrees of freedom corresponding to low-energy excitations are qualitatively different from microscopic degrees of freedom in the original formulation of the problem.

Another fundamentally important aspect of the functional-integral formalism is that it emphasizes deep connections between the classical and quantum physics and the role of the action functional in the quantum physics.

The functional-integral formalism presented below is a many-body generalization of Feynman's path-integral approach to quantum mechanics.

6.1 Bosons

We consider first the case of bosons and later generalize the formalism to the case of fermions.

6.1.1 Coherent states

The corresponding second-quantization formalism was presented in Sec. 3.1.1. The bosonic creation and annihilation operators, $a_k^\dagger$ and a_k, satisfy canonical commutation relations. The basis of the Fock space (Hilbert space of the many-body problem), is obtained by the action of creation operators on the vacuum state, see Eq. (3.11), which we repeat here for convenience:

$$|n_1, n_2, \ldots\rangle = \prod_k \frac{(a_k^\dagger)^{n_k}}{\sqrt{n_k!}} |0\rangle \,. \tag{6.1}$$

Any state in the Fock space is a linear superposition of the basis states (6.1):

$$|\phi\rangle = \sum_{n_1, n_2, \ldots} C_{n_1, n_2, \ldots} |n_1, n_2, \ldots\rangle. \tag{6.2}$$

We look for Fock-space states $|\phi\rangle$ that are eigenstates of all annihilation operators a_k. Such states are called **bosonic coherent states**. A coherent state is thus determined by the set of eigenvalue conditions,

$$a_k|\phi\rangle = \phi_k|\phi\rangle \qquad \text{for all } k\,, \tag{6.3}$$

where $\{\phi_k\}$ is a set of complex numbers, $\phi_k \in \mathbb{C}$. Equation (6.3) imlplies the following relation between the coefficients $C_{n_1,n_2,\ldots}$

$$\sqrt{n_k}\, C_{n_1,n_2,\ldots,n_k,\ldots} = \phi_k C_{n_1,n_2,\ldots,n_k-1,\ldots}\,. \tag{6.4}$$

This formula expresses $C_{n_1,n_2,\ldots,n_k,\ldots}$ through $C_{n_1,n_2,\ldots,n_k-1,\ldots}$. Using it consecutively, we can express all coefficients through $C_{0,0,\ldots}$. Setting $C_{0,0,\ldots} = 1$ (which is an arbitrary choice; the coherent states $|\phi\rangle$ that we obtain will not be normalized to unity), we thus get

$$C_{n_1,n_2,\ldots} = \prod_k \frac{\phi_k^{n_k}}{\sqrt{n_k!}}\,. \tag{6.5}$$

Substituting this in Eq. (6.2) and using (6.1), we obtain

$$\boxed{|\phi\rangle = \sum_{n_1,n_2,\ldots} \prod_k \frac{(\phi_k a_k^\dagger)^{n_k}}{n_k!}|0\rangle = \exp\left[\sum_k \phi_k a_k^\dagger\right]|0\rangle\,.} \tag{6.6}$$

Taking the hermitean conjugate of Eqs. (6.3), we find that "bra-states" $\langle\phi|$ corresponding to the coherent states $|\phi\rangle$ are left eigenstates of the creation operators $a_k^\dagger$:

$$\langle\phi| = \langle 0|\exp\left[\sum_k \phi_k^* a_k\right]\,; \tag{6.7}$$

$$\langle\phi|a_k^\dagger = \langle\phi|\phi_k^*\,. \tag{6.8}$$

Inspecting how the operator $a_k^\dagger$ acts on the coherent state $|\phi\rangle$, we find

$$a_k^\dagger|\phi\rangle = a_k^\dagger \exp\left[\sum_k \phi_k a_k^\dagger\right]|0\rangle = \frac{\partial}{\partial\phi_k}|\phi\rangle\,, \tag{6.9}$$

and the adjoint relation

$$\langle\phi|a_k = \frac{\partial}{\partial\phi_k^*}\langle\phi|\,. \tag{6.10}$$

It is instructive to check that Eqs. (6.3) and (6.9) representing the action of the operators a_k and $a_k^\dagger$ on coherent states are consistent with the commutation relations $[a_j, a_k^\dagger] = \delta_{jk}$. Indeed,

$$\begin{aligned}[a_j, a_k^\dagger]|\phi\rangle &= a_j a_k^\dagger|\phi\rangle - a_k^\dagger a_j|\phi\rangle = a_j\frac{\partial}{\partial\phi_k}|\phi\rangle - a_k^\dagger\phi_j|\phi\rangle = \frac{\partial}{\partial\phi_k}a_j|\phi\rangle - \phi_j a_k^\dagger|\phi\rangle \\ &= \left(\frac{\partial}{\partial\phi_k}\phi_j - \phi_j\frac{\partial}{\partial\phi_k}\right)|\phi\rangle = \delta_{jk}|\phi\rangle\,.\end{aligned} \tag{6.11}$$

We further calculate the overlap of two coherent states $|\phi\rangle$ and $|\psi\rangle$:

$$\langle\psi|\phi\rangle = \sum_{m_1,m_2,\ldots}\sum_{n_1,n_2,\ldots}\prod_j \frac{(\psi_j^*)^{m_j}}{\sqrt{m_j!}}\prod_k \frac{\phi_k^{n_k}}{\sqrt{n_k!}}\,\langle m_1, m_2, \ldots|n_1, n_2, \ldots\rangle \tag{6.12}$$

$$= \sum_{n_1,n_2,\ldots} \prod_k \frac{(\psi_k^* \phi_k)^{n_k}}{n_k!} = \exp\left[\sum_k \psi_k^* \phi_k\right] . \tag{6.13}$$

In the second line of Eq. (6.13) we used the orthonormality of basis states of the Fock space,

$$\langle m_1, m_2, \ldots | n_1, n_2, \ldots \rangle = \delta_{m_1,n_1} \delta_{m_2,n_2} \ldots . \tag{6.14}$$

As a particular case of Eq. (6.13), we find the normalization of a coherent state $|\phi\rangle$:

$$\langle \phi | \phi \rangle = \exp\left[\sum_k \phi_k^* \phi_k\right] . \tag{6.15}$$

The crucial property of coherent states is that they form a **complete set of states** in the Fock space: any vector in the Fock space can be expanded as a linear combination of coherent states with some coefficients. (In fact, the set of coherent states is even overcomplete.) The completeness is expressed by the following identity

$$\boxed{\int \prod_j \frac{d\,\mathrm{Re}\,\phi_j \, d\,\mathrm{Im}\,\phi_j}{\pi} \, e^{-\sum_k \phi_k^* \phi_k} |\phi\rangle\langle\phi| = \mathbb{1} \, .} \tag{6.16}$$

To prove Eq. (6.16), it is useful to consider first the case of only one single-particle state, $k = 1$, with the corresponding occupation number n_1. The l.h.s. of Eq. (6.16) then reduces to

$$\int \frac{d\,\mathrm{Re}\,\phi_1 \, d\,\mathrm{Im}\,\phi_1}{\pi} \, e^{-\phi_1^* \phi_1} |\phi_1\rangle\langle\phi_1| = \int \frac{\rho \, d\rho \, d\theta}{\pi} \, e^{-\rho^2} \sum_{m_1} \frac{(\rho e^{i\theta})^{m_1}}{\sqrt{m_1!}} \sum_{n_1} \frac{(\rho e^{-i\theta})^{n_1}}{\sqrt{n_1!}} |m_1\rangle\langle n_1| \, , \tag{6.17}$$

where we introduced polar coordinates $\phi = \rho e^{i\theta}$. Performing the θ integration and after this the ρ integration,

$$\int d\theta \, e^{i\theta(m-n)} = 2\pi \delta_{m,n} \, . \tag{6.18}$$

$$\int 2\rho \, d\rho \, e^{-\rho^2} \rho^{2n} = n! \, , \tag{6.19}$$

we get

$$\int \frac{d\,\mathrm{Re}\,\phi_1 \, d\,\mathrm{Im}\,\phi_1}{\pi} \, e^{-\phi_1^* \phi_1} |\phi_1\rangle\langle\phi_1| = \sum_{n_1} |n_1\rangle\langle n_1| \, . \tag{6.20}$$

It is now straightforward to extend this caluclation to the general case of many single-particle states, $k = 1, 2, \ldots$,

$$\int \prod_j \frac{d\,\mathrm{Re}\,\phi_j \, d\,\mathrm{Im}\,\phi_j}{\pi} \, e^{-\sum_k \phi_k^* \phi_k} |\phi\rangle\langle\phi| = \sum_{n_1,n_2\ldots} |n_1, n_2, \ldots\rangle\langle n_1, n_2, \ldots| = \mathbb{1} \, , \tag{6.21}$$

which proves Eq. (6.16). On the last step, we used the completeness of the basis $|n_1, n_2, \ldots\rangle$ in the Fock space.

Using the completeness relation (6.16), we can write the trace of any operator $\hat{A}$ as

$$\mathrm{Tr}\, \hat{A} = \int \mathcal{D}(\phi^*, \phi) e^{-\sum_k \phi_k^* \phi_k} \langle \phi | \hat{A} | \phi \rangle \, , \tag{6.22}$$

where we have introduced a short-hand notation for the integration measure,

$$\mathcal{D}(\phi^*,\phi) \equiv \prod_j \frac{d\,\mathrm{Re}\,\phi_j\, d\,\mathrm{Im}\,\phi_j}{\pi}\,. \tag{6.23}$$

A very important property of coherent states is a simple form of matrix elements of **normal-ordered operators** between coherent states. Consider a generic operator $\hat{A}$. Bring it to the normal-ordered form, with all creation operators $a_j^\dagger$ staying to the left of all annihilation operators a_k. After this, replace every operator $a_j^\dagger$ by a complex variable ϕ_j^* and every operator a_j by a complex variable ψ_j. In this way, one gets a function $A(\{\phi_k^*,\psi_k\})$ of complex variables $\{\phi_k^*,\psi_k\}$, which is in one-to-one correspondence with the normal-ordered form of the operator $\hat{A}$. As an example, consider the conventional Hamiltonian operator of a system with two-body interaction,

$$\hat{H} = \sum_{k,l} h_{kl} a_k^\dagger a_l + \frac{1}{2}\sum_{k,l,m,n} U_{kl;mn} a_k^\dagger a_l^\dagger a_m a_n\,. \tag{6.24}$$

The form (6.24) of the Hamiltonian operator is clearly normal-ordered, so that the corresponding function $H(\{\phi_k^*,\psi_k\})$ reads

$$H(\{\phi_k^*,\psi_k\}) = \sum_{k,l} h_{kl}\phi_k^*\psi_l + \frac{1}{2}\sum_{k,l,m,n} U_{kl;mn}\phi_k^*\phi_l^*\psi_m\psi_n\,. \tag{6.25}$$

If an operator is given in a form that is not normal ordered, one can always bring it to the normal-ordered form by using commutation relations between $a_k^\dagger$ and a_j.

Assume now that we have an operator $\hat{A}(\{a_k^\dagger,a_k\})$ in a normal-ordered form characterized by the function $A(\{\phi_k^*,\psi_k\})$. Then the matrix element of $\hat{A}$ between two coherent states $\langle\phi|$ and $|\psi\rangle$ can be straightforwardly found:

$$\langle\phi|\hat{A}(\{a_k^\dagger,a_k\})|\psi\rangle = A(\{\phi_k^*,\psi_k\})e^{\sum_k \phi_k^*\psi_k}\,. \tag{6.26}$$

To obtain Eq. (6.26), we have used Eq. (6.3) for the right-action of a_k and Eq. (6.8) for the left-action of $a_k^\dagger$.

6.1.2 Quantum partition function as a coherent-state functional integral

The goal of this and the next subsections is to work out a presentation of Green's functions and of the partition function in terms of coherent-state functional integrals. This can be done in the real-time formalism (appropriate at zero temperature) or within the Matsubara (imaginary-time) formalism appropriate for temperature $T \neq 0$. The presentation below is in the imaginary time. The zero-temperature, real-time formulation can be obtained by setting $\beta \to \infty$ and performing the so-called Wick rotation from imaginary to real times: $\tau \to it$ with real t.

We begin by developing a functional-integral representation of the partition function

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}\,. \tag{6.27}$$

Using Eq. (6.22), we get

$$Z = \int \mathcal{D}(\phi^*,\phi)\, e^{-\sum_k \phi_k^*\phi_k}\langle\phi|e^{-\beta(\hat{H}-\mu\hat{N})}|\phi\rangle\,. \tag{6.28}$$

We divide the "time" interval β into a large number M of small intervals $\beta/M = \Delta\tau$ and write

$$e^{-\beta(\hat{H}-\mu\hat{N})} = \left[e^{-\Delta\tau(\hat{H}-\mu\hat{N})}\right]^M \equiv \underbrace{e^{-\Delta\tau(\hat{H}-\mu\hat{N})}e^{-\Delta\tau(\hat{H}-\mu\hat{N})}\ldots e^{-\Delta\tau(\hat{H}-\mu\hat{N})}}_{M \text{ factors}} . \tag{6.29}$$

In the end of the calculation we will take the continuum limit $M \to \infty$. Since $\Delta\tau$ is small, we expand each of the exponential factors in Eq. (6.29),

$$e^{-\Delta\tau(\hat{H}-\mu\hat{N})} = 1 - \Delta\tau(\hat{H}-\mu\hat{N}) + O((\Delta\tau)^2) . \tag{6.30}$$

The terms $O((\Delta\tau)^2)$ will vanish in the continuum limit.

As a next step, we insert the resolution of unity in terms of coherent states, Eq. (6.16), between every two consecutive exponential factors in Eq. (6.29). We write the Hamiltonian in the normal-ordered form $\hat{H}(\{a_k^\dagger, a_k\})$ characterized by the function $H(\{\phi_k^*, \psi_k\})$. The normal-ordered form of $\hat{N}$ is $\hat{N} = \sum_k a_k^\dagger a_k$, so that $N(\{\phi_k^*, \psi_k\}) = \sum_k \phi_k^*\psi_k$. After the insertion of resolutions of identity, each of the factors $1-\Delta\tau(\hat{H}-\mu\hat{N})$ will be surrounded by two coherent states corresponding to the consecutive time steps, thus forming the matrix element

$$\begin{aligned}\langle\phi_n|1-\Delta\tau(\hat{H}-\mu\hat{N})|\phi_{n-1}\rangle &= \exp\left[\sum_k \phi_{k,n}^*\phi_{k,n-1}\right]\left\{1-\Delta\tau\left[H(\phi_n^*,\phi_{n-1}) - \mu\sum_k \phi_{k,n}^*\phi_{k,n-1}\right]\right\} \\ &\simeq \exp\left\{\sum_k \phi_{k,n}^*\phi_{k,n-1} - \Delta\tau\left[H(\phi_n^*,\phi_{n-1}) - \mu\sum_k \phi_{k,n}^*\phi_{k,n-1}\right]\right\} .\end{aligned} \tag{6.31}$$

Here $\phi_n = \{\phi_{n,k}\}$ is the coherent state from the resolution of identity on time step $n = 1, 2, \ldots, M-1$. Further, $\phi_0 = \phi_M$ is the coherent state (corresponding to the time $\tau = 0$, or, equivalently, $\tau = \beta$) from the trace in Eq. (6.28). The index n is thus the time index, while the index k labels single-particle states. In the second line of Eq. (6.31), we have again neglected corrections of the order $(\Delta\tau)^2$, which is justified by the continuum limit $M \to \infty$. Substituting Eqs. (6.29), (6.30), and (6.31) into Eq. (6.28), we obtain

$$Z = \lim_{M\to\infty}\int\prod_{n=1}^{M}\mathcal{D}(\phi_n^*,\phi_n)\exp\sum_{k,n}\left[\phi_{k,n}^*(\phi_{k,n-1}-\phi_{k,n}) + \Delta\tau\,\mu\phi_{k,n}^*\phi_{k,n-1} - \Delta\tau\,H(\phi_n^*,\phi_{n-1})\right] . \tag{6.32}$$

Taking the limit $M \to \infty$ (i.e., $\Delta\tau \to 0$), we rewrite Eq. (6.32) in the continuum notations $(n\cdot\Delta\tau \to \tau)$,

$$Z = \int_{\phi(0)=\phi(\beta)}\mathcal{D}(\phi^*,\phi)\exp\{-S[\phi^*,\phi]\} , \tag{6.33}$$

where the integration goes over fields $\phi(\tau) = \{\phi_k(\tau)\}$ and the functional S is given by

$$S[\phi^*,\phi] = \int_0^\beta d\tau\left[\sum_k \phi_k^*(\tau)(\partial_\tau - \mu)\phi_k(\tau) + H(\phi^*(\tau),\phi(\tau))\right] . \tag{6.34}$$

The functional S has the meaning of the (imaginary-time) action. Indeed, Eq. (6.34) is fully analogous to the formula for the action familiar from the classical mechanics, $S = \int dt\,(\sum_k p_k\dot{q}_k - h)$, where $\{q_k, p_k\}$ are canonically conjugate coordinates and momenta and h is the Hamiltonian. We used during the derivation the canonically conjugated operators

$a_k^\dagger, a_k$, which is why the corresponding fields $\{\phi_k^*, \phi_k\}$ (analogous to $\{q_k, p_k\}$) enter the expression for the action.

In particular, for the Hamiltonian (6.24) (with a conventional, two-body interaction), the action functional S has the form

$$S[\phi^*, \phi] = \int_0^\beta d\tau \left[\sum_{k,l} \phi_k^*(\tau)[(\partial_\tau - \mu)\delta_{kl} + h_{kl}]\phi_l(\tau) + \frac{1}{2} \sum_{k,l,m,n} U_{kl;mn}\phi_k^*(\tau)\phi_l^*(\tau)\phi_m(\tau)\phi_n(\tau) \right]. \tag{6.35}$$

Equations (6.33) and (6.34) provide a representation of the partition function in terms of a **functional integral**: the integration in (6.33) goes over fields $\phi(\tau) = \{\phi_k(\tau)\}$, which are functions of time τ and of the index k labelling single-particle states (usually the spatial coordinate $\mathbf{r}$). Let us emphasize that the fields $\phi(\tau)$ over which the integral in Eq. (6.33) is carried out are periodic in imaginary time, $\phi(0) = \phi(\beta)$. This is the property of the **bosonic** functional integral. If we perform the Fourier transformation from time to frequency, $\tau \to \omega_n$, we will get the familiar bosonic Matsubara frequencies,

$$\omega_n = 2\pi n T\,, \qquad n \in \mathbb{Z}\,. \tag{6.36}$$

6.1.3 Green's functions in terms of functional integrals

Now we are ready to express Green's functions as functional integrals. Consider the two-point Matsubara Green's function, Eq. (4.15),

$$\begin{aligned} \mathscr{G}_M(k_1, \tau_1; k_2, \tau_2) &= -\langle \mathcal{T}_\tau\, a_{k_1,\mathrm{MH}}(\tau_1)\overline{a}_{k_2,\mathrm{MH}}(\tau_2)\rangle \\ &= -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\mathcal{T}_\tau\, a_{k_1,\mathrm{MH}}(\tau_1)\overline{a}_{k_2,\mathrm{MH}}(\tau_2)\right], \end{aligned} \tag{6.37}$$

where

$$a_{k,\mathrm{MH}}(\tau) = e^{(\hat{H}-\mu\hat{N})\tau}\, a_k\, e^{-(\hat{H}-\mu\hat{N})\tau} \tag{6.38}$$

$$\overline{a}_{k,\mathrm{MH}}(\tau) = e^{(\hat{H}-\mu\hat{N})\tau}\, a_k^\dagger\, e^{-(\hat{H}-\mu\hat{N})\tau} \tag{6.39}$$

are the Matsubara-Heisenberg operators. As in the preceding calculation of the partition function, we keep the index k for labelling single-particle states. In the common representation of field operators, this will be the spatial coordinate $\mathbf{r}$.

Consider the case $\tau_1 > \tau_2$. Substituting (6.38) and (6.39) into Eq. (6.37), we get

$$\mathscr{G}_M(k_1, \tau_1; k_2, \tau_2) = -\frac{1}{Z}\mathrm{Tr}\left[e^{-(\beta-\tau_1)(\hat{H}-\mu\hat{N})}\, a_{k_1}\, e^{-(\tau_1-\tau_2)(\hat{H}-\mu\hat{N})}\, a_{k_2}^\dagger\, e^{-\tau_2(\hat{H}-\mu\hat{N})}\right], \tag{6.40}$$

where a_k, $a_k^\dagger$ are Schrödinger (time-indepedent) operators. It is instructive to rewrite this as

$$\begin{aligned} \mathscr{G}_M(k_1, \tau_1; k_2, \tau_2) &= -\frac{1}{Z}\mathrm{Tr}\left[\exp\left(-\int_{\tau_1}^\beta d\tau(\hat{H}-\mu\hat{N})\right) a_{k_1}^{(\tau_1)} \exp\left(-\int_{\tau_2}^{\tau_1} d\tau(\hat{H}-\mu\hat{N})\right)\right. \\ &\times \left. a_{k_2}^{\dagger(\tau_2)} \exp\left(-\int_0^{\tau_2} d\tau(\hat{H}-\mu\hat{N})\right)\right]. \end{aligned} \tag{6.41}$$

The upper labels (τ_1) and (τ_2) of the creation and annihilation operators here are introduced only for convenience – these are the time-independent Schrödinger operators. The role of the labels is just to indicate at what position these operators stay in the time-ordered structure

that is transparent in Eq. (6.41): the evolution operator from time 0 till τ_2, then operator $a^\dagger_{k_2}$, then evolution from τ_2 till τ_1, then a_{k_1}, and finally evolution from τ_1 till β.

We perform now the same procedure as in course of the derivation of the functional-integral representation of the partition function in Sec. 6.1.2, which has allowed us to bring Eq. (6.27) into the form (6.33), (6.34). The only difference is that we have now in addition operators $a^{(\tau_1)}_{k_1}$ and $a^{\dagger(\tau_2)}_{k_2}$ acting at the corresponding time steps. When acting on coherent states, they will produce factors $\phi_{k_1}(\tau_1)$ and $\phi^*_{k_2}(\tau_2)$, respectively. We thus obtain

$$\mathscr{G}_M(k_1,\tau_1;k_2,\tau_2) = -\frac{1}{Z}\int_{\phi(0)=\phi(\beta)} \mathcal{D}(\phi^*,\phi)\,\phi_{k_1}(\tau_1)\phi^*_{k_2}(\tau_2)\exp\{-S[\phi^*,\phi]\}\,, \tag{6.42}$$

with the action given by Eq. (6.34).

Consider now the case of the opposite time order, $\tau_2 > \tau_1$. Repeating the same steps, we come to exactly the same result, Eq. (6.42). It is a remarkable property of the functional integral that it generates automatically time-ordered averages of the operator formalism. Thus, Eq. (6.42) together with the action (6.34) is a **functional-integral representation of the (Matsubara) Green function**.

This analysis can be straightforwardly generalized to many-point Green functions. For example,

$$\begin{aligned}&\langle \mathcal{T}_\tau\, a_{k_1,\mathrm{MH}}(\tau_1)a_{k_2,\mathrm{MH}}(\tau_2)\overline{a}_{k_3,\mathrm{MH}}(\tau_3)\overline{a}_{k_4,\mathrm{MH}}(\tau_4)\rangle \\ &\qquad = \frac{1}{Z}\int_{\phi(0)=\phi(\beta)} \mathcal{D}(\phi^*,\phi)\,\phi_{k_1}(\tau_1)\phi_{k_2}(\tau_2)\phi^*_{k_3}(\tau_3)\phi^*_{k_4}(\tau_4)\exp\{-S[\phi^*,\phi]\}\,.\end{aligned} \tag{6.43}$$

6.1.4 Perturbation theory: Gaussian integrals and Wick theorem

We show now how the perturbative expansion of the Green's function is obtained within the functional-integral formalism. For this purpose, we will need properties of Gaussian integrals (in a generalized sense) – namely, multidimensional intergrals of a multidimensional Gaussian (exponential of a quadratic form) multiplied by a polynomial. As we will see below, the Wick theorem is in exact correspondence with properties of such integrals. We thus begin this section by presenting key formulas for Gaussian integrals. In all of them the integration goes over N-component vector $\mathbf{x}$, either real or complex.

We consider first the case of **real integration variables**. Here $\mathbf{x} = (x_1,\ldots,x_N) \in \mathbb{R}^N$ and the integration measure is $d(\mathbf{x}) = \prod_{i=1}^N dx_i$. Further, A is an $N\times N$ symmetric positive-definite matrix, and $\mathbf{J}$ is an N-component vector. Then

$$\int d(\mathbf{x})\, e^{-\frac{1}{2}\mathbf{x}^T A\mathbf{x} + \boldsymbol{J}^T\mathbf{x}} = \frac{(2\pi)^{N/2}}{(\det A)^{1/2}}\, e^{\frac{1}{2}\boldsymbol{J}^T A^{-1}\boldsymbol{J}}\,. \tag{6.44}$$

Brief sketch of the proof:

- Consider first $\mathbf{J} = 0$ and a diagonal matrix A. The integral is then a product of N conventional one-dimensional Gaussian integrals and the result follows.
- Still $\mathbf{J} = 0$ but now with an arbitrary real symmetric positive-definite matrix A. Such matrix can be diagonalized by an orthogonal transformation. Peforming a rotation of the intergartion variables by the corresponding orthogonal matrix, one can reduce the integral to the preceding case.
- Now consider $\mathbf{J} \neq 0$. Performing a shift of the variable $\mathbf{x} - A^{-1}\mathbf{J} = \mathbf{x}'$, one transforms the integral (6.44) to the preceding case, and the result follows.

- Finally, by virtue of analytic continuation, the result (6.44) can be extended also onto complex symmetric matrices A whose real part is positive definite (which guarantees the convergence)

The formula (6.44) is very useful as a generating function for integrals of polynomials with the Gaussian weight $\exp(-\frac{1}{2}\mathbf{x}^T A\mathbf{x})$. Indeed, differentiating the left-hand side over J_k produces a factor x_k under the integral. Thus, taking the second derivative $\partial^2/\partial J_k \partial J_l$ and then setting $\mathbf{J} = 0$, we get

$$\int d(\mathbf{x})\, x_k x_l\, e^{-\frac{1}{2}\mathbf{x}^T A\mathbf{x}} = \frac{(2\pi)^{N/2}}{(\det A)^{1/2}}\, (A^{-1})_{kl}\,. \tag{6.45}$$

Defining averages with the Gaussian weight,

$$\langle \ldots \rangle = \frac{\int d(\mathbf{x})\, (\ldots)\, e^{-\frac{1}{2}\mathbf{x}^T A\mathbf{x}}}{\int d(\mathbf{x})\; e^{-\frac{1}{2}\mathbf{x}^T A\mathbf{x}}}\,, \tag{6.46}$$

we therefore have

$$\langle x_k x_l \rangle = (A^{-1})_{kl}\,. \tag{6.47}$$

In the same way, we can calculate averages of products of a larger number of components of $\mathbf{x}$. For example,

$$\begin{aligned} \langle x_j x_k x_l x_m \rangle &= (A^{-1})_{jk}(A^{-1})_{lm} + (A^{-1})_{jl}(A^{-1})_{km} + (A^{-1})_{jm}(A^{-1})_{kl} \\ &\equiv \langle x_j x_k \rangle \langle x_l x_m \rangle + \langle x_j x_l \rangle \langle x_k x_m \rangle + \langle x_j x_m \rangle \langle x_k x_l \rangle\,. \end{aligned} \tag{6.48}$$

We see that the result is the sum of the terms with all possible pairings. It is not difficult to show (exercise) that this remains true also in a general case of an average of order $2n$:

$$\langle x_{j_1} x_{j_2} \ldots x_{j_{2n}} \rangle = \sum_{\substack{\text{all inequivalent pairings} \\ \text{of } \{j_1, \ldots j_{2n}\}}} \langle x_{j_{p_1}} x_{j_{p_2}} \rangle \langle x_{j_{p_3}} x_{j_{p_4}} \rangle \ldots \langle x_{j_{p_{2n-1}}} x_{j_{p_{2n}}} \rangle\,. \tag{6.49}$$

Equivalently, one can sum in Eq. (6.49) over all permutations $\{p_1, \ldots, p_{2n}\}$ of $\{1, \ldots, 2n\}$ and then divide by $2^n n!$ (a number of times each pairing combination will be encountered).

We recognize in Eq. (6.49) the statement of the **Wick theorem** (for real fields) that was obtained in the preceding chapters within the operator formalism. From the point of view of the functional-integral formalism, the Wick theorem is nothing but the property of Gaussian integrals.

Let us discuss generalization to the case of **complex integration variables**. Now $\mathbf{x} = (x_1, \ldots, x_N) \in \mathbb{C}^N$ and the integration measure is $d(\mathbf{x}^\dagger, \mathbf{x}) = \prod_{i=1}^N (d\mathrm{Re}\, x_i\, d\mathrm{Im}\, x_i)$. Further, A is an $N \times N$ complex positive-definite matrix, and $\mathbf{J_1}$, $\mathbf{J_2}$ are vectors from $\mathbb{C}^N$. The complex analog of Eq. (6.44) reads

$$\int d(\mathbf{x}^\dagger, \mathbf{x})\, e^{-\mathbf{x}^\dagger A\mathbf{x} + \mathbf{J_1}^\dagger \mathbf{x} + \mathbf{x}^\dagger \mathbf{J_2}} = \frac{\pi^N}{\det A}\, e^{\mathbf{J_1}^\dagger A^{-1} \mathbf{J_2}}\,. \tag{6.50}$$

The proof proceeds in a close analogy with that for the real case. In the simplest situation, the matrix A is Hermitian; however, the proof can be also extended onto non-Hermitian matrices with a positive-definite Hermitian part $\frac{1}{2}(A + A^\dagger)$.

In full analogy with its real counterpart, Eq. (6.50) serves a generator of correlation functions of components of $\mathbf{x}^\dagger$ and $\mathbf{x}$ with the Gaussian weight,

$$\langle \ldots \rangle = \frac{\int d(\mathbf{x}^\dagger, \mathbf{x})\, (\ldots)\, e^{-\mathbf{x}^\dagger A\mathbf{x}}}{\int d(\mathbf{x}^\dagger, \mathbf{x})\; e^{-\mathbf{x}^\dagger A\mathbf{x}}}\,, \tag{6.51}$$

For this purpose, one differentiates (6.50) with respect to components of sources $\mathbf{J_1}^\dagger$ and $\mathbf{J_2}$ and then sets $\mathbf{J_1} = \mathbf{J_2} = 0$. This yields

$$\langle x_k^* x_l \rangle = (A^{-1})_{lk} \,, \tag{6.52}$$

and

$$\begin{aligned} \langle x_j^* x_k^* x_l x_m \rangle &= (A^{-1})_{lj}(A^{-1})_{mk} + (A^{-1})_{lk}(A^{-1})_{mj} \\ &= \langle x_j^* x_l \rangle \langle x_k^* x_m \rangle + \langle x_k^* x_l \rangle \langle x_j^* x_m \rangle \,. \end{aligned} \tag{6.53}$$

The general formula (**Wick theorem** for complex fields) reads

$$\langle x_{j_1}^* x_{j_2}^* \dots x_{j_n}^* x_{k_1} x_{k_2} \dots x_{k_n} \rangle = \sum_{\text{permutations } P} \langle x_{j_1}^* x_{k_{p_1}} \rangle \langle x_{j_2}^* x_{k_{p_2}} \rangle \dots \langle x_{j_n}^* x_{k_{p_n}} \rangle \,, \tag{6.54}$$

where the sum goes over permutations $P = \{p_1, \dots, p_n\}$ of $\{1, \dots, n\}$.

Development of the perturbative expansion for the partition function and the Green functions is now quite straightforward. Consider first the partition function Z of a system with two-body interaction given by the functional integral (6.33) with the action (6.35). Expanding in powers of the interaction U, we will obtain in each order of the perturbation theory Gaussian integrals that can be evaluated using the formulas presented above in this section. This will generate exactly the same diagrammatic expansion for the free energy (vacuum diagrams) that we obtained earlier within the operator formalism. Similarly, consider the Green function (6.42). Again, expanding in the interaction, we will generate a perturbative series. In each order, we will have to compute Gaussian integrals. This will reproduce the perturbative diagrammatic expansion for the Green function that has been obtained in the framework of the operator formalism.

In this connection, it is useful to write down a **functional version of the Gaussian integrals** discussed above. Consider, for example, the real case. Integration of an N-component vector $\mathbf{x} = (x_1, \dots, x_N) \in \mathbb{R}^N$ becomes in the continuum limit an integration over functions $x(\tau)$. Similarly, the vector $\mathbf{J}$ becomes a function $J(\tau)$, and the matrix A becomes a kernel $A(\tau, \tau')$ of an integral operator (acting on functions of τ). The Gaussian-integral formula (6.44) takes the form

$$\begin{aligned} &\int Dx(\tau) \exp\left[-\frac{1}{2} \int d\tau d\tau' x(\tau) A(\tau, \tau') x(\tau') + \int d\tau J(\tau) x(\tau) \right] \\ &\qquad = \left(\det \frac{A}{2\pi} \right)^{-1/2} \exp\left[\frac{1}{2} \int d\tau d\tau' J(\tau) A^{-1}(\tau, \tau') J(\tau') \right] . \end{aligned} \tag{6.55}$$

Here $A^{-1}(\tau, \tau')$ is the kernel of the inverse operator A^{-1} which is defined by

$$\int d\tau' A(\tau, \tau') A^{-1}(\tau', \tau'') = \delta(\tau - \tau'') \,. \tag{6.56}$$

Equation (6.47) for the correlation function takes the form

$$\langle x(\tau) x(\tau') \rangle) = A^{-1}(\tau, \tau') \,. \tag{6.57}$$

Equation (6.49) retains its form, with each two-point correlation function given now by Eq. (6.57). In the context of the perturbative expansion for the partition function and Green functions, $A^{-1}(x, x')$ will be the Green function of non-interacting system.

6.2 Fermions

The goal of this section is to generalize the above functional-integral formalism to the case of fermions. However, one encounters an apparent difficulty related to the fact that fermionic operators satisfy **anticommutation** relations, instead of commutation relations for bosons. Indeed, to proceed in analogy with bosons, we would like to introduce coherent states $|\eta\rangle$ that satisfy, for all fermionic annihilation operators a_k, the eigenvalue condition

$$a_k|\eta\rangle = \eta_k|\eta\rangle\,. \tag{6.58}$$

Since the fermionic operators satisfy the anticommutation relations,

$$[a_j, a_k]_+ = 0\,, \qquad \text{where} [A, B]_+ = AB + BA\,, \tag{6.59}$$

we obtain, by acting with $[a_j, a_k]_+$ on $|\eta\rangle$,

$$\eta_j\eta_k + \eta_k\eta_j = 0\,. \tag{6.60}$$

Therefore, eigenvalues η_k should also anticommute. Thus, they cannot be conventional numbers but should be rather "anticommuting numbers". The required mathematical construction is known under the name of **Grassmann algebra**, and η_k are termed **"Grassmann variables"**.

6.2.1 Grassmann algebra

A Grassmann algebra is defined by a set of generators (which we will term **"Grassmann variables"**) η_i with $i = 1, \ldots, N$. These generators anticommute:

$$\eta_j\eta_k + \eta_k\eta_j = 0\,. \tag{6.61}$$

An immediate consequence of this is that

$$\eta_j^2 = 0\,. \tag{6.62}$$

In the algebra, one can add and multiply elements and also multiply them by complex numbers. As a consequence, any element of the Grassmann algebra is a linear combination, with complex coefficients of the basis elements formed by all possible products of generators $1, \{\eta_k\}, \{\eta_k\eta_j\}, \ldots, \eta_1\eta_2\ldots\eta_N$:

$$\xi = c_0 + \sum_{n=1}^{N} \sum_{j_1<j_2<\ldots<j_n} c_{j_1,\ldots,j_n}\eta_{j_1}\eta_{j_2}\ldots\eta_{j_n}\,, \qquad \text{with} \;\; c_0, c_{j_1,\ldots,j_n} \in \mathbb{C}\,, \tag{6.63}$$

where the summation goes over all ordered subsets $j_1 < j_2 < \ldots < j_n$ of $(1, 2, \ldots, N)$. It is easy to see that the number of basis elements is 2^N, i.e. the Grassmann algebra with N generators has dimension 2^N.

One can extend notions of calculus to the case of Grassmann variables. An analytic **function** $f(\eta_1, \ldots, \eta_N)$ is defined by a series expansion

$$f(\eta_1, \ldots, \eta_N) = c_0 + \sum_{n=1}^{N} \sum_{j_1<j_2<\ldots<j_n} c_{j_1,\ldots,j_n}\eta_{j_1}\eta_{j_2}\ldots\eta_{j_n}\,, \qquad \text{with} \;\; c_0, c_{j_1,\ldots,j_n} \in \mathbb{C}\,. \tag{6.64}$$

Note that the series is finite. As simple examples, for $N = 1$ we have

$$f(\eta) = c_0 + c_1\eta\,, \tag{6.65}$$

for $N = 2$ we have

$$f(\eta_1, \eta_2) = c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2\,, \tag{6.66}$$

and so on.

Differentiation with respect to a Grassmann variable is defined by the rule

$$\frac{\partial}{\partial\eta_j}\eta_k = \delta_{jk}\,. \tag{6.67}$$

This is sufficient to define the action of the derivative on any function (6.64). Note, however, that before the derivative $\frac{\partial}{\partial\eta_j}$ can act on η_j that enters a product of several Grassmann variables, one should use anticommutation relations to place η_j directly after $\frac{\partial}{\partial\eta_j}$. Example:

$$\frac{\partial}{\partial\eta_2}(c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2) = c_2 - c_{1,2}\eta_1 \tag{6.68}$$

$$\frac{\partial}{\partial\eta_1}(c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2) = c_1 + c_{1,2}\eta_2 \tag{6.69}$$

$$\frac{\partial}{\partial\eta_1}\frac{\partial}{\partial\eta_2}(c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2) = -c_{1,2} \tag{6.70}$$

$$\frac{\partial}{\partial\eta_2}\frac{\partial}{\partial\eta_1}(c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2) = c_{1,2}\,. \tag{6.71}$$

Note that the operators $\frac{\partial}{\partial\eta_k}$ and $\frac{\partial}{\partial\eta_j}$ anticommute.

Integration over the Grassmann variables, is defined by the rules

$$\int d\eta_j = 0\,, \qquad \int d\eta_j\,\eta_j = 1\,. \tag{6.72}$$

This is a formal algebraic definition; one should not think about an integral in the usual sense (as a limit of the Riemann sum) in this context. For example, the question of integration domain makes no sense for the Grassmann integration. A consecutive application of these rules allows one to evaluate an integral, also over several Grassmann variables, of any function of these variables. Remarkably, the Grassmann integration is essentially equivalent to the Grassmann differentiation. For example,

$$\int d\eta_2(c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2) = c_2 - c_{1,2}\eta_1 \tag{6.73}$$

$$\int d\eta_1(c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2) = c_1 + c_{1,2}\eta_2 \tag{6.74}$$

$$\int d\eta_1 d\eta_2(c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2) = -c_{1,2} \tag{6.75}$$

$$\int d\eta_2 d\eta_1(c_0 + c_1\eta_1 + c_2\eta_2 + c_{1,2}\eta_1\eta_2) = c_{1,2}\,. \tag{6.76}$$

Note that an integral of derivative (over the same Grassmann variable) is zero:

$$\int d\eta_1\,\frac{\partial}{\partial\eta_1} f(\eta_1, \ldots) = 0\,. \tag{6.77}$$

This is in analogy with the conventional calculus: $\int_{-\infty}^{\infty} dx\,\partial_x g(x, \ldots) = 0$ for any function g vanishing at $x \to \pm\infty$.

6.2.2 Grassmann Gaussian Integrals

We start from the simplest Grassmann Gaussian integral, which requires two Grassmann variables that we will denote η and η^*. Note that η and η^* should be considered as two independent Grassmann variables.

$$\int d\eta^* d\eta \, e^{-\eta^* a \eta} = a \,, \tag{6.78}$$

where a is an arbitrary complex number. This result is immediately obtained by expanding the exponential, $e^{-\eta^* a \eta} = 1 - \eta^* a \eta$, and using the integration rules. Now we generalize (6.78) to a multidimensional case. Consider two N-component vectors of Grassmann variables $\eta^* = \{\eta_j^*\}$ and $\eta = \{\eta_j\}$, with $j = 1, 2, \ldots, N$. Then for any complex matrix A,

$$\int d(\eta^*, \eta) e^{-\eta^{*T} A \eta} = \det A \,, \tag{6.79}$$

where $d(\eta^*, \eta) = \prod_{j=1}^N d\eta_j^* d\eta_j$. To prove (6.79), one can expand the exponential in the power series. According to the rules of the Grassmann integration, only the term of the highest, N-th, order in this expansion will contribute to the integral. This will give a homogeneous polynomial of N-th order with respect to matrix elements of A. It is not difficult to show that this polynomial is $\det A$.

Now we include in the exponential, in addition to the quadratic form, terms that are linear with respect to η and η^*:

$$\int d(\eta^*, \eta) e^{-\eta^{*T} A \eta + \xi^{*T} \eta + \eta^{*T} \xi} = \det A \, e^{\xi^{*T} A^{-1} \xi} \,, \tag{6.80}$$

where ξ and ξ^* are N-component vectors of Grassmann variables. The formula (6.80) is a direct analog of Eq. (6.50) for Gaussian integral over conventional complex variables. A remarkable similarity of the two formulas is evident. The only essential difference is that $(\det A)^{-1}$ in the conventional case becomes $(\det A)$ in the Grassmann case. Like in the case of ordinary Gaussian integral, one can prove Eq. (6.80) by performing a shift of variables that reduces it to the integral (6.79). Indeed, a shift of the variable is a legitimate operation also for Grassmann integrals, by virtue of the identity

$$\int d\eta f(\eta) = \int d\eta f(\eta + \zeta) \,. \tag{6.81}$$

We can obtain integrals of products of Grassmann variables with the Gaussian weight by expanding (or, equivalently, differentiating) Eq. (6.80) with respect to components of the sources ξ and ξ^*. For example, we get in this way

$$\int d(\eta^*, \eta) \, \eta_j \eta_k^* \, e^{-\eta^{*T} A \eta} = \det A \, (A^{-1})_{jk} \,, \tag{6.82}$$

Defining

$$\langle \ldots \rangle = \frac{\int d(\eta^*, \eta) \, (\ldots) \, e^{-\eta^{*T} A \eta}}{\int d(\eta^*, \eta) \; e^{-\eta^{*T} A \eta}} \,, \tag{6.83}$$

we obtain

$$\langle \eta_j \eta_k^* \rangle = (A^{-1})_{jk}. \tag{6.84}$$

In the same way, one gets higher-order correlation functions

$$\langle \eta_{j_1} \eta_{j_2} \ldots \eta_{j_n} \eta_{k_n}^* \ldots \eta_{k_2}^* \eta_{k_1}^* \rangle \;\; = \sum_{\text{permutations } P} \mathrm{sgn}(P) \, (A^{-1})_{j_1 k_{p_1}} (A^{-1})_{j_2 k_{p_2}} \ldots (A^{-1})_{j_n k_{p_n}}$$

$$= \sum_{\text{permutations } P} \text{sgn}(P) \, \langle \eta_{j_1} \eta^*_{k_{p_1}} \rangle \langle \eta_{j_2} \eta^*_{k_{p_2}} \rangle \ldots \langle \eta_{j_n} \eta^*_{k_{p_n}} \rangle \,, \quad (6.85)$$

where the sum goes over permutations $P = \{p_1, \ldots, p_n\}$ of $\{1, \ldots, n\}$, and $\text{sgn}(P)$ is the sign of the permutation.

Equations (6.84) and (6.85) are direct counterparts of the corresponding formulas for ordinary ("bosonic") Gaussian integrals, Eqs. (6.52) and (6.54). Equation (6.85) is at the heart of the Wick theorem for fermionic systems. The essential difference with respect to the conventional ("bosonic") version is the emergence of the factor $\text{sgn}(P)$.

6.2.3 Fermion coherent states

Consider a fermionic many-body system, with creation and annihilation operators $a_k^\dagger, a_k$, satisfying the anticommutation relations. We introduce Grassmann generators ("anticommuting variables") η_j. In order to proceed, we allow for a multiplication of states from the fermionic Fock space with elements of the Grassmann algebra. We further require that the Grassmann generators η_j anticommute with operators $a_k^\dagger, a_k$:

$$[\eta_j, a_k]_+ = 0 \,, \qquad [\eta_j, a_k^\dagger]_+ = 0 \,. \quad (6.86)$$

The fermionic coherent states are now defined by a formula analogous to that in the bosonic case:

$$|\eta\rangle = \exp\left[-\sum_k \eta_k a_k^\dagger \right] |0\rangle \,. \quad (6.87)$$

Expanding the exponential, we can write Eq. (6.87) in the form

$$|\eta\rangle = \prod_k (1 - \eta_k a_k^\dagger) |0\rangle \,. \quad (6.88)$$

It is now straightforward to check that the state $|\eta\rangle$ satisfies the eigenvalue conditions

$$a_k |\eta\rangle = \eta_k |\eta\rangle \,, \quad (6.89)$$

in full analogy with the bosonic case. The adjoint of the coherent state ("bra" state) reads

$$\langle \eta| = \langle 0| \exp\left[-a_k \sum_k \eta_k^* \right] = \langle 0| \exp\left[\sum_k \eta_k^* a_k \right] \,. \quad (6.90)$$

As has been already emphasized before, one should view η_k and η_k^* as independent Grassmann variables. As in the bosonic case, adjoint coherent states are left eigenstates of creation operators:

$$\langle \eta | a_k^\dagger = \langle \eta | \eta_k^* \,. \quad (6.91)$$

Analogy with the bosonic case extends to further properties of the coherent states. We summarize them below (the proof is left as an exercise):

- Right action of $a_k^\dagger$ and left action of a_k:

$$a_k^\dagger |\eta\rangle = -\frac{\partial}{\partial \eta_k} |\eta\rangle \,, \qquad \langle \eta | a_k = \frac{\partial}{\partial \eta_k^*} \langle \eta| \,. \quad (6.92)$$

- Overlap (here η_k and ψ_k^* are two sets of Grassmann variables):

$$\langle \psi | \eta \rangle = \exp\left[\sum_k \psi_k^* \eta_k \right] \,. \quad (6.93)$$

- Completeness:

$$\boxed{\int \mathcal{D}(\eta^*,\eta)\exp\left[-\sum_k \eta_k^*\eta_k\right]|\eta\rangle\langle\eta| = \mathbb{1}} \qquad \text{with} \quad \mathcal{D}(\eta^*,\eta) = \prod_j d\eta_j^* d\eta_j \,. \tag{6.94}$$

- Trace of an operator in terms of coherent-state matrix elements. Consider an arbitrary operator $\hat{A}$ acting in the Fock space. Using Eq. (6.94), we can express its trace as

$$\mathrm{Tr}\,\hat{A} = \int \mathcal{D}(\eta^*,\eta)\, e^{-\sum_k \eta_k^*\eta_k}\langle -\eta|\hat{A}|\eta\rangle \,. \tag{6.95}$$

Note an important difference with respect to the bosonic case: minus sign in the bra-state $\langle -\eta|$. It emerges because of anticommutation relations between Grassmann variables, which implies that $\mathrm{Tr}\,\hat{A}|\eta\rangle\langle\eta| = \langle -\eta|\hat{A}|\eta\rangle$.

- Matrix elements of normal-ordered operators between coherent states. Assume that we have an operator $\hat{A}(\{a_k^\dagger, a_k\})$ in a normal-ordered form. We associate with it a function $A(\{\psi_k^*, \eta_k\})$ of Grassmann variables by a substitution $a_k^\dagger \to \psi_k^*$ and $a_k \to \eta_k$. Then the matrix element of $\hat{A}$ between two coherent states $\langle\psi|$ and $|\eta\rangle$ has a simple form:

$$\langle\psi|\hat{A}(\{a_k^\dagger, a_k\})|\eta\rangle = A(\{\psi_k^*, \eta_k\})\, e^{\sum_k \psi_k^*\eta_k} \,. \tag{6.96}$$

6.2.4 Fermionic partition function and Green's functions as functional integrals

We have now all prerequisites to derive the coherent-state functional-integral representation of the partition function and the Green's functions in the fermionic case. Since all key formulas of the coherent-state formalism for fermions—see Eqs. (6.94), (6.22), and (6.96)—have nearly the same form as for bosons, the derivation proceeds in the same way as in Sec. 6.1.2, 6.1.3.

The partition function

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} \tag{6.97}$$

can be presented, by using Eq. (6.95), in terms of an integral over fermionic coherent states (as before, k is the index labelling single-particle states):

$$Z = \int \mathcal{D}(\psi^*,\psi)\, e^{-\sum_k \psi_k^*\psi_k}\langle -\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle \,. \tag{6.98}$$

Dividing the "time" interval β in a large number M of small intervals and inserting the resolution of unity in terms of fermionic coherent states, Eq. (6.94), between each two consecutive intervals [i.e., at times $\tau = (n/M)\beta$ with $n = 1, 2, \ldots, M-1$], we get

$$Z = \int_{\substack{\psi(\beta)=-\psi(0)\\ \psi^*(\beta)=-\psi^*(0)}} \mathcal{D}(\psi^*,\psi)\exp\{-S[\psi^*,\psi]\} \,, \tag{6.99}$$

where the integration goes over Grassmann fields $\psi(\tau) = \{\psi_k(\tau)\}$ and the action functional S has the same form as for bosons:

$$S[\psi^*,\psi] = \int_0^\beta d\tau \left[\sum_k \psi_k^*(\tau)(\partial_\tau - \mu)\psi_k(\tau) + H(\psi^*(\tau),\psi(\tau))\right] . \tag{6.100}$$

An essential difference in comparison with the bosonic case is the **antiperiodic boundary conditions**. They originate from the form of the matrix element in the r.h.s. of Eq. (6.98) as follows. In the original discrete-time form, we define

$$\psi_0 = \psi \,, \qquad \psi_0^* = \psi^* \tag{6.101}$$

and

$$\psi_M = -\psi\,, \qquad \psi^*_M = -\psi^*\,, \tag{6.102}$$

where ψ, ψ^* are from Eq. (6.98). Then the matrix element in the r.h.s. of Eq. (6.98) becomes $\langle\psi_M|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi_0\rangle$, with antiperiodic conditions

$$\psi_M = -\psi_0\,, \qquad \psi^*_M = -\psi^*_0\,, \tag{6.103}$$

and the exponential factor becomes $e^{-\sum_k \psi^*_{k,0}\psi_{k,0}} \equiv e^{-\sum_k \psi^*_{k,M}\psi_{k,M}}$. Passing to the continuum limit, we get Eq. (6.99).

Extending the calculation to the Matsubara Green function of the many-body fermionic system,

$$\begin{aligned}\mathscr{G}_M(k_1,\tau_1;k_2,\tau_2) &= -\langle\mathcal{T}_\tau\, a_{k_1,\mathrm{MH}}(\tau_1)\overline{a}_{k_2,\mathrm{MH}}(\tau_2)\rangle \\ &= -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\mathcal{T}_\tau\, a_{k_1,\mathrm{MH}}(\tau_1)\overline{a}_{k_2,\mathrm{MH}}(\tau_2)\right]\,,\end{aligned} \tag{6.104}$$

where

$$a_{k,\mathrm{MH}}(\tau) = e^{(\hat{H}-\mu\hat{N})\tau}\, a_k\, e^{-(\hat{H}-\mu\hat{N})\tau}\,, \tag{6.105}$$

$$\overline{a}_{k,\mathrm{MH}}(\tau) = e^{(\hat{H}-\mu\hat{N})\tau}\, a^\dagger_k\, e^{-(\hat{H}-\mu\hat{N})\tau}\,, \tag{6.106}$$

one finds

$$\mathscr{G}_M(k_1,\tau_1;k_2,\tau_2) = -\frac{1}{Z}\int_{\substack{\psi(\beta)=-\psi(0)\\ \psi^*(\beta)=-\psi^*(0)}} \mathcal{D}(\psi^*,\psi)\,\psi_{k_1}(\tau_1)\psi^*_{k_2}(\tau_2)\exp\{-S[\psi^*,\psi]\}\,, \tag{6.107}$$

with the action given by Eq. (6.100). The result can be straightforwardly extended to higher-order correlation functions, e.g.,

$$\begin{aligned}&\langle\mathcal{T}_\tau\, a_{k_1,\mathrm{MH}}(\tau_1)a_{k_2,\mathrm{MH}}(\tau_2)\overline{a}_{k_3,\mathrm{MH}}(\tau_3)\overline{a}_{k_4,\mathrm{MH}}(\tau_4)\rangle \\ &= \frac{1}{Z}\int_{\substack{\psi(\beta)=-\psi(0)\\ \psi^*(\beta)=-\psi^*(0)}} \mathcal{D}(\psi^*,\psi)\,\psi_{k_1}(\tau_1)\psi_{k_2}(\tau_2)\psi^*_{k_3}(\tau_3)\psi^*_{k_4}(\tau_4)\exp\{-S[\psi^*,\psi]\}\,.\end{aligned} \tag{6.108}$$

We have thus obtained representations of the partition function and of Green's functions of a many-body fermionic system in terms of coherent state path integrals. They are very much similar to those for bosons. One of essential differences is the antiperiodic boundary conditions in τ for fermions. Upon Fourier transformation, $\tau \to \omega_n$, they imply that the corresponding frequencies are

$$\omega_n = (2n+1)\pi T\,, \qquad n \in \mathbb{Z}\,, \tag{6.109}$$

which are familiar fermionic Matsubara frequencies. In the same way as for bosons, the perturbative expansion is obtained by expanding e^{-S} in a power series with respect to the interaction-induced part of the action and then evaluating the resulting Gaussian integrals over Grassmann variables.

6.3 Superconductivity via functional integral

In this Section, we demonstrate the power of the functional-integral formalism by applying it to the problem of superconductivity. We show how the mean field solution arises as a saddle point of the functional integral and how the effective low-energy long-wave-length theory (Ginzburg-Landau theory) is derived from the microscopic theory.

6.3.1 Formulation in terms of the functional integral

We begin with the Hamiltonian of a Fermi system with weak attraction, Eq. (5.67),

$$\widehat{H} = \int \mathrm{d}^3 r \left\{ \hat{\psi}^\dagger_\sigma(\mathbf{r}) \left(-\frac{\boldsymbol{\nabla}^2}{2m} - \mu \right) \hat{\psi}_\sigma(\mathbf{r}) - g \hat{\psi}^\dagger_\uparrow(\mathbf{r}) \hat{\psi}^\dagger_\downarrow(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) \right\} . \tag{6.110}$$

Here $g > 0$ is the strength of attraction ($g = -\lambda$ in previous notations). Clearly, the operator (6.110) has a normal-ordered form. Using results of Sec. 6.2.4, we write the partition function of the theory in terms of a functional integral,

$$Z = \int_{\substack{\psi(\beta) = -\psi(0) \\ \psi^*(\beta) = -\psi^*(0)}} \mathcal{D}(\psi^*, \psi) \exp\{-S[\psi^*, \psi]\} , \tag{6.111}$$

where the action S is given by

$$S[\psi, \psi^*] \;=\; \int_0^\beta d\tau \int \mathrm{d}^3 r \left[\psi^*_\sigma(\mathbf{r}, \tau) \left(\partial_\tau - \frac{\boldsymbol{\nabla}^2}{2m} - \mu \right) \psi_\sigma(\mathbf{r}, \tau) - g \psi^*_\uparrow(\mathbf{r}, \tau) \psi^*_\downarrow(\mathbf{r}, \tau) \psi_\downarrow(\mathbf{r}, \tau) \psi_\uparrow(\mathbf{r}, \tau) \right] . \tag{6.112}$$

It should be emphasized that, whereas $\hat{\psi}, \hat{\psi}^\dagger$ in Eq. (6.110) are operators, ψ, ψ^* in Eq. (6.112) are Grassmann variables. The boundary conditions in τ are antiperiodic for ψ, ψ^*, as always for Grassmann fields representing fermions. We will not write explicitly the boundary conditions in formulas below. All integrations $\int d\tau$ below are understood as $\int_0^\beta d\tau$.

Next we perform the **Hubbard-Stratonovich transformation** in the Cooper channel. The idea of this transformation is to decouple the quartic term in Eq. (6.112) by means of introducing a new field that will eventually serve the role of the order parameter in the symmetry-broken phase. Such transformations are very useful in various interacting fermionic problems, as they allow one to reformulate the theory on terms of appropriate degrees of freedom, to explore the symmetry breaking, and to derive an effective low-energy, long-distance theory of the problem. In the present case, the appropriate Hubbard-Stratonovich transformation reads:

$$\exp\left[g \int d\tau d^3 r \, \psi^*_\uparrow(\mathbf{r}, \tau) \psi^*_\downarrow(\mathbf{r}, \tau) \psi_\downarrow(\mathbf{r}, \tau) \psi_\uparrow(\mathbf{r}, \tau) \right] =$$

$$\mathcal{N} \int \mathcal{D}(\Delta^*, \Delta) \exp\left\{ \int d\tau \mathrm{d}^3 r \left[-\frac{1}{g} \Delta^*(\mathbf{r}, \tau) \Delta(\mathbf{r}, \tau) + \Delta^*(\mathbf{r}, \tau) \psi_\downarrow(\mathbf{r}, \tau) \psi_\uparrow(\mathbf{r}, \tau) + \psi^*_\uparrow(\mathbf{r}, \tau) \psi^*_\downarrow(\mathbf{r}, \tau) \Delta(\mathbf{r}, \tau) \right] \right\} . \tag{6.113}$$

For brevity, it is convenient to omit the $(\mathbf{r}, \tau)$ arguments in such formulas; Eq. (6.113) then takes the form

$$\exp\left[g \int d\tau d^3 r \, \psi^*_\uparrow \psi^*_\downarrow \psi_\downarrow \psi_\uparrow \right] = \mathcal{N} \int \mathcal{D}(\Delta^*, \Delta) \exp\left\{ \int d\tau \mathrm{d}^3 r \left[-\frac{1}{g} \Delta^* \Delta + \Delta^* \psi_\downarrow \psi_\uparrow + \psi^*_\uparrow \psi^*_\downarrow \Delta \right] \right\} . \tag{6.114}$$

The integration in Eq. (6.114) goes over a bosonic (i.e., commuting) complex field $\Delta(\mathbf{r}, \tau)$. Equation (6.114) follows from general formulas for Gaussian integrals. Indeed, the r.h.s. of Eq. (6.114) is the continuum version of the Gaussian integral (6.50). The normalization factor $\mathcal{N}$ is a constant originating from the factor $[\det(A/\pi)]^{-1}$ in (6.50); it is a constant (does not

depend on any of the fields), and we discard it below. (One can also say that this constant is absorbed in the integration measure $\mathcal{D}(\Delta^*, \Delta)$.)

It is worth pointing out that one can perform the Hubbard-Stratonovich decoupling of the quartic term in the l.h.s. of Eq. (6.114) also in different ways. We carry out here a decoupling in the Cooper channel, since we develop a theory of superconductivity and the chosen decoupling field Δ corresponds to the expected order parameter.

Substituting the Hubbard-Stratonovich decoupling formula (6.114), into Eq. (6.111) with the action (6.112), we obtain the partition function Z as an integral over Grassmann fields ψ, ψ^* and a complex bosonic field Δ, Δ^*:

$$Z = \int \mathcal{D}(\psi^*, \psi) \int \mathcal{D}(\Delta^*, \Delta) \exp\left\{-S[\psi, \psi^*, \Delta, \Delta^*]\right\} , \tag{6.115}$$

$$S[\psi, \psi^*, \Delta, \Delta^*] = \int d\tau d^d r \left[\psi^*_\sigma \left(\partial_\tau - \frac{\boldsymbol{\nabla}^2}{2m} - \mu\right) \psi_\sigma + \frac{1}{g}\Delta^*\Delta - \Delta^*\psi_\downarrow\psi_\uparrow - \psi^*_\uparrow\psi^*_\downarrow\Delta\right] . \tag{6.116}$$

At this point, it is convenient to switch to matrix notation introduced in Sec. 5.5.3 by defining the Nambu spinor

$$\Psi = \begin{pmatrix} \psi_\uparrow \\ \psi^*_\downarrow \end{pmatrix} , \qquad \bar{\Psi} = \begin{pmatrix} \psi^*_\uparrow & \psi_\downarrow \end{pmatrix} . \tag{6.117}$$

Then the partition function takes the form

$$Z = \int \mathcal{D}(\bar{\Psi}, \Psi) \int \mathcal{D}(\Delta^*, \Delta) \exp\left\{-S[\Psi, \bar{\Psi}, \Delta, \Delta^*]\right\} , \tag{6.118}$$

$$S[\Psi, \bar{\Psi}, \Delta, \Delta^*] = \int d\tau d^d r \left[\frac{1}{g}\Delta^*\Delta + \bar{\Psi}(\partial_\tau + h_\Delta)\Psi\right] , \tag{6.119}$$

$$h_\Delta = \begin{pmatrix} -\frac{\boldsymbol{\nabla}^2}{2m} - \mu & -\Delta \\ -\Delta^* & \frac{\boldsymbol{\nabla}^2}{2m} + \mu \end{pmatrix} . \tag{6.120}$$

The structure of the matrix h_Δ is that of the Bogoliubov-de Gennes Hamiltonian, and the inverse matrix $(-\partial_\tau - h_\Delta)^{-1}$ has a structure of the Gorkov-Nambu matrix Green function. We emphasize, however, that the pairing Δ here is a fluctuating field: it is a function of the imaginary time τ and the coordinate $\mathbf{r}$. In the functional integral (6.118), we integrate over all configurations $\Delta(\tau, \mathbf{r})$ (with periodic boundary conditions in τ, since this field is bosonic).

Since the action (6.119) is quadratic with respect to the fermionic (Grassmann) fields $\Psi, \bar{\Psi}$, the integration over them is of Gaussian form and can be now performed exactly, yielding

$$Z = \int \mathcal{D}(\Delta^*, \Delta) \exp\left[-\frac{1}{g}\int d\tau d^d r\, \Delta^*\Delta\right] \det(-\partial_\tau - h_\Delta) . \tag{6.121}$$

Using the identity

$$\ln \det A = \mathrm{tr} \ln A , \tag{6.122}$$

we rewrite Eq. (6.121) in the form

$$Z = \int \mathcal{D}(\Delta^*, \Delta) \exp\left\{-S[\Delta, \Delta*]\right\} , \tag{6.123}$$

with the action

$$S[\Delta, \Delta^*] = \frac{1}{g}\int d\tau d^d r\, \Delta^*\Delta - \mathrm{tr} \ln(-\partial_\tau - h_\Delta) . \tag{6.124}$$

We have therefore reformulated the original theory of interacting fermions, which was defined by the Hamiltonian (6.110), or, equivalently, by the functional integral over Grassmann fields (6.111), as a theory of complex bosonic field Δ, Δ^* defined by the functional integral with the action (6.112). Up to this point, all transformations were exact. To proceed further, we will have to make approximations.

6.3.2 Stationary point of the functional integral: Mean-field approximation

We can expect that the dominant contribution to the functional integral (6.123) will be given by a vicinity of the minima of the action (6.124). To find them, we vary Eq. (6.124) with respect to $\Delta(\mathbf{r}, \tau)$.

Mathematical Intermezzo. Let $z = x + iy \in \mathbb{C}$ be a complex variable (with real part x and imaginary part y) and $z^* = x - iy$ its complex conjugate. Then one can define derivatives with respect to z and z^*:

$$\partial_z = \frac{1}{2}(\partial_x - i\partial_y)\,, \qquad \partial_{z^*} = \frac{1}{2}(\partial_x + i\partial_y)\,. \tag{6.125}$$

One has

$$\partial_z z = 1\,, \qquad \partial_z z^* = 0\,, \qquad \partial_{z^*} z = 0\,, \qquad \partial_{z^*} z^* = 1\,. \tag{6.126}$$

One can therefore operates with ∂_z and ∂_{z^*} when acting on analytic functions $f(z, z*)$ essentially by viewing z and z^* as independent variables. In particular, in our case, we have as a result of variation of the first term in Eq. (6.124),

$$\frac{\delta}{\delta\Delta(\mathbf{r},\tau)}\,\frac{1}{g}\int d\tau d^d r\,\Delta^*\Delta = \frac{1}{g}\Delta^*(\mathbf{r},\tau)\,. \tag{6.127}$$

Mathematical Intermezzo. Imagine that we have a function $f(\hat{A})$ of a matrix $\hat{A}$. Further, let matrix $\hat{A}$ be dependent on some parameter z. Then

$$\partial_z \mathrm{tr}\, f(\hat{A}) = \mathrm{tr}\,[f'(\hat{A})\partial_z \hat{A}]\,, \tag{6.128}$$

where $f'(x)$ is the derivative of $f(x)$. Thus, under the trace, functions of matrices can be differentiated over a parameter as conventional functions.
Proof: Consider first $f(x) = x^n$. Then

$$\partial_z \mathrm{tr}\,\hat{A}^n = \sum_{k=0}^{n} \mathrm{tr}\,[\hat{A}^k(\partial_z\hat{A})\hat{A}^{n-k-1}] = n\,\mathrm{tr}\,[\hat{A}^{n-1}\partial_z\hat{A}]\,, \tag{6.129}$$

where we used $\mathrm{tr}\,\hat{B}\hat{C} = \mathrm{tr}\,\hat{C}\hat{B}$. This proves Eq. (6.128) for the case $f(x) = x^n$. Generalization to any analytic function $f(x)$ is obtained by expanding it in Taylor series. Thus, variation of the second term in Eq. (6.124) yields

$$\frac{\delta}{\delta\Delta(\mathbf{r},\tau)}\,\mathrm{tr}\ln(-\partial_\tau - h_\Delta) = \mathrm{tr}\left[(-\partial_\tau - h_\Delta)^{-1}\frac{\delta}{\delta\Delta(\mathbf{r},\tau)}(-\partial_\tau - h_\Delta)\right] = G_{\Delta;21}(\mathbf{r},\tau;\mathbf{r},\tau)\,, \tag{6.130}$$

where G_Δ is the matrix Green function,

$$G_\Delta = (-\partial_\tau - h_\Delta)^{-1}, \tag{6.131}$$

satisfying, with explicitly shown coordinate dependence,

$$(-\partial_\tau - h_\Delta) G_\Delta(\mathbf{r},\tau;\mathbf{r}',\tau') = \delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau')\mathbb{1}\,. \tag{6.132}$$

The subscript "21" in Eq. (6.130) denote the corresponding matrix element of the 2×2 Green function in the Nambu space.

Combining everything, we thus obtain the stationary-point equation

$$\frac{1}{g}\Delta^*(\mathbf{r},\tau) = G_{\Delta;21}(\mathbf{r},\tau;\mathbf{r},\tau)\,. \tag{6.133}$$

The stationary solution is expected to be homogeneous in space and time, $\Delta(\mathbf{r},\tau)=\Delta_0$. The Green function G_Δ in such a homogeneous configuration can be straightforwardly found by the Fourier transformation:

$$G_\Delta(\omega_n,p) = \begin{pmatrix} i\omega_n - \xi_p & \Delta_0 \\ \Delta_0^* & i\omega_n + \xi_p \end{pmatrix}^{-1}, \qquad \xi_p = \frac{p^2}{2m} - \mu\,, \tag{6.134}$$

so that the 21 matrix element of G_Δ is

$$G_{\Delta;21}(\omega_n,p) = \frac{\Delta_0^*}{\omega_n^2 + \xi_p^2 + |\Delta_0|^2}\,. \tag{6.135}$$

The stationary point equation thus reduces to

$$\frac{1}{g}\Delta_0^* = \frac{T}{V}\sum_{\mathbf{p},n} \frac{\Delta_0^*}{\omega_n^2 + \xi_p^2 + |\Delta_0|^2}\,. \tag{6.136}$$

Here it is important to recall that $\operatorname{tr}\ln(-\partial_\tau - h_\Delta)$ in the action (6.124) had its origin in integration over Grassmann fields ψ^*,ψ with antiperiodic boundary conditions. For the same reason, the Green function G_Δ satisfies antiperiodic boundary conditions in time τ. Correspondingly, the Matsubara energies ω_n are of fermionic type, $\omega_n = (2n+1)\pi T$. We perform summation over Matsubara frequencies [cf. Eq. (5.41)]:

$$T\sum_n \frac{1}{\omega_n^2 + \xi_p^2 + |\Delta_0|^2} = \frac{1}{2\sqrt{\xi_p^2 + |\Delta_0|^2}} \tanh\left(\frac{\sqrt{\xi_p^2 + |\Delta_0|^2}}{2T}\right)\,. \tag{6.137}$$

Replacing, as usual, $V^{-1}\sum_{\mathbf{p}} \to \nu\int d\xi_p$, where ν is the density of states at the Fermi level, we thus cast Eq. (6.136) into the form

$$1 = g\nu \int_{-\omega_D}^{\omega_D} d\xi_p \, \frac{\tanh\left(\sqrt{\xi_p^2 + |\Delta_0|^2}/2T\right)}{2\sqrt{\xi_p^2 + |\Delta_0|^2}}\,. \tag{6.138}$$

Here, we have restored the ultraviolet cutoff ω_D determined by the interval of ξ_p for which the attraction holds.

Equation (6.138) is the BCS gap equation determining the dependence of the gap $|\Delta_0|$ on temperature T. At zero temperature, $\tanh(\varepsilon_p/T) \to \operatorname{sgn}(\varepsilon)$, and Eq. (6.138) reduces to Eq. (5.58). With increasing temperature, the gap $|\Delta_0|$ decreases, turning to zero at $T=T_c$. The critical temperature is thus determined by the equation

$$1 = g\nu \int\limits_{-\omega_D}^{\omega_D} \mathrm{d}\xi \, \frac{1}{2\xi} \tanh\left(\frac{\xi}{2T}\right)\,, \tag{6.139}$$

which is exactly the equation derived in Sec. 5.3 for the temperature at which the Cooper instability of a normal system develops. The result for T_c is given by Eq. (5.43), which we repeat here:

$$T_c = \frac{2e^\gamma}{\pi}\omega_D \exp\left(-\frac{1}{|\lambda|\nu}\right), \tag{6.140}$$

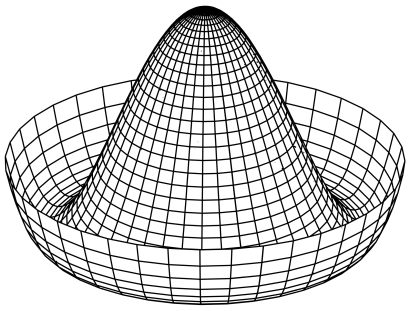
where $\gamma \approx 0.577$ is the Euler-Mascheroni constant.

What we have obtained is the **mean-field solution** of the original theory (6.110). We thus see that the saddle-point approximation to the functional integral is equivalent to the mean-field approximation. The exact functional-integral formulation of the theory, Eqs. (6.123) and (6.124), allows one to make important further progress by including fluctuations of $\Delta(\mathbf{r}, \tau)$, as will be discussed below.

It is important to emphasize that Eq. (6.136) fixes the absolute value of Δ_0 but not its phase. Indeed, if Δ_0 is a solution of this equation, then $\Delta_0 e^{i\phi_0}$ is also a solution for any $\phi \in \mathbb{R}$. Thus, the action $S[\Delta, \Delta^*]$, Eq, (6.124) has a continuous set of minima, $\Delta = \Delta_0 e^{i\phi_0}$. This is a consequence of the fact that the action is invariant with respect to the global gauge transformations,

$$S[\Delta, \Delta^*] = S[\Delta e^{i\phi_0}, \Delta^* e^{-i\phi_0}]\,. \tag{6.141}$$

Presence of many degenerate minima (each of them not invariant with respect to the transformation $\Delta \to e^{i\phi_0}\Delta$) of the action that is invariant withe respect to this transformation is a manifestation of the **spontaneous symmetry breaking** that occurs when the minimum of the action it at $\Delta_0 \neq 0$, i.e. in the superconducting phase $T < T_c$.



This figure illustrates qualitatively the action S (vertical axis) as a function of complex Δ_0 in the symmetry-broken phase $T < T_c$. The horizontal plane is $(\mathrm{Re}\,\Delta_0, \mathrm{Im}\,\Delta_0)$.

6.3.3 Ginzburg-Landau theory

Consider the system in the superconducting phase close to the critical temperature: $T < T_c$ and $T_c - T \ll T_c$. Then the order parameter Δ is small compared to T. Using this fact, one can expand the action $S[\Delta, \Delta^*]$, Eq, (6.124), in Δ (and its spatial and temporal derivatives). The first term of the action is a simple quadratic function, so the only non-trivial part of this procedure is the expansion of the second term, $-\mathrm{tr}\ln(-\partial_\tau - h_\Delta)$.

Mathematical Intermezzo. For matrices (or operators) $\hat{A}$, $\hat{B}$ one has

$$\mathrm{tr}\,\ln(\hat{A}\hat{B}) = \mathrm{tr}\,\ln\hat{A} + \mathrm{tr}\,\ln\hat{B}\,, \tag{6.142}$$

$$\mathrm{tr}\,\ln(1+\hat{A}) = \sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}\mathrm{tr}\,\hat{A}^n\,. \tag{6.143}$$

Equation (6.142) follows from $\det(\hat{A}\hat{B}) = \det\hat{A}\,\det\hat{B}$. Equation (6.143) is immediately obtained by expanding the $\ln(1+\hat{A})$ in a power series.

Using these formulas, we get

$$\mathrm{tr}\ln(-\partial_\tau - \hat{h}_\Delta) = \mathrm{tr}\ln(-\partial_\tau - \hat{h}_0 + \hat{\Delta}) \;=\; \mathrm{tr}\ln\left\{(-\partial_\tau - \hat{h}_0)\left[1 + (-\partial_\tau - \hat{h}_0)^{-1}\hat{\Delta}\right]\right\}$$

$$= \quad \mathrm{tr}\ln \hat{G}_0^{-1} - \sum_{k=1}^{\infty} \frac{1}{2k} \mathrm{tr}[(\hat{G}_0\,\hat{\Delta})^{2k}]\,, \tag{6.144}$$

where hats emphasize that we deal with matrices in the Nambu space, we have defined

$$\hat{\Delta} = \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix}, \qquad \hat{h}_0 = \hat{h}_\Delta\big|_{\Delta=0}\,, \qquad \hat{G}_0 = \hat{G}_\Delta\big|_{\Delta=0}\,, \tag{6.145}$$

and $\hat{G}_\Delta = (-\partial_\tau - h_\Delta)^{-1}$ is the matrix Green function that was defined in Eq. (6.131). While expanding the logarithm in the last expression in Eq. (6.144), we have taken into account that only terms of even order in Δ contribute in view of the symmetry of the action.

Equation (6.144) yields the desired expansion of $\mathrm{tr}\ln(-\partial_\tau - \hat{h}_\Delta)$ in powers of Δ. The term of zeroth order in Δ [the first term in Eq. (6.144)] is just a constant and we discard it. Let us consider the term of second order in Δ. It has the form

$$\begin{aligned} -\frac{1}{2}\mathrm{tr}[(\hat{G}_0\,\hat{\Delta})^2] \;&=\; \int d\tau_1 d^3r_1 d\tau_2 d^3r_2\, G_{0,11}(\tau_2,\mathbf{r_2};\tau_1,\mathbf{r_1})\Delta(\tau_1,\mathbf{r_1})G_{0,22}(\tau_1,\mathbf{r_1};\tau_2,\mathbf{r_2})\Delta^*(\tau_2,\mathbf{r_2}) \\ &=\; -\frac{T}{V}\sum_{\epsilon_n,\omega_m,\mathbf{p},\mathbf{q}} G_{0,11}(\epsilon_n,\mathbf{p})\Delta(\omega_m,\mathbf{q})G_{0,22}(\epsilon_n-\omega_m,\mathbf{p}-\mathbf{q})\Delta^*(-\omega_m,-\mathbf{q})\,, \end{aligned} \tag{6.146}$$

where the summation goes over fermionic Matsubara frequencies ϵ_n and bosonic Matsubara frequencies ω_m. The normal-state matrix Green function $\hat{G}_0$ has the structure

$$\hat{G}_0(\epsilon_n,\mathbf{p}) = \begin{pmatrix} G_0(\epsilon_n,\mathbf{p}) & 0 \\ 0 & -G_0(-\epsilon_n,-\mathbf{p}) \end{pmatrix} = \begin{pmatrix} \frac{1}{i\epsilon_n - \xi_{\mathbf{p}}} & 0 \\ 0 & \frac{1}{i\epsilon_n + \xi_{-\mathbf{p}}} \end{pmatrix}, \tag{6.147}$$

where $\hat{G}_0(\epsilon_n,\mathbf{p})$ is the conventional free-fermion Green function. The 22 element of (6.147) is the hole Green function. Substituting (6.147) into (6.146) and using $\Delta^*(-\omega_m,-\mathbf{q}) = [\Delta(\omega_m,\mathbf{q})]^*$, we get

$$\begin{aligned} -\frac{1}{2}\mathrm{tr}[(\hat{G}_0\,\hat{\Delta})^2] \;&=\; \frac{T}{V}\sum_{\epsilon_n,\omega_m,\mathbf{p},\mathbf{q}} G_0(\epsilon_n,\mathbf{p})G_0(-\epsilon_n+\omega_m,-\mathbf{p}+\mathbf{q})|\Delta(\omega_m,\mathbf{q})|^2 \\ &=\; \sum_{\omega_m,\mathbf{q}} \chi_c^{(0)}(\omega_m,\mathbf{q})|\Delta(\omega_m,\mathbf{q})|^2\,, \end{aligned} \tag{6.148}$$

where

$$\begin{aligned} \chi_c^{(0)}(\omega_m,\mathbf{q}) \;&=\; \frac{T}{V}\sum_{\epsilon_n,\mathbf{p}} G_0(\epsilon_n,\mathbf{p})G_0(-\epsilon_n+\omega_m,-\mathbf{p}+\mathbf{q}) \\ &=\; \frac{T}{V}\sum_{\epsilon_n,\mathbf{p}} \frac{1}{(i\epsilon_n - \xi_{\mathbf{p}})(-i\epsilon_n + i\omega_m - \xi_{-\mathbf{p}+\mathbf{q}})} \end{aligned} \tag{6.149}$$

is the Cooper-channel susceptibility of the normal state that was introduced in Sec. 5.3, see the formula (5.40) for $\chi_c^{(0)}(\omega_m)$ at $\mathbf{q}=0$. Combining Eq. (6.148) with the first term in Eq. (6.124), we obtain the quadratic part of the action $S[\Delta,\Delta^*]$:

$$S^{(2)}[\Delta,\Delta^*] = \sum_{\omega_m,\mathbf{q}} \left[\frac{1}{g} - \chi_c^{(0)}(\omega_m,\mathbf{q})\right] |\Delta(\omega_m,\mathbf{q})|^2\,. \tag{6.150}$$

Expanding $[g^{-1} - \chi_c^{(0)}(\omega_m, \mathbf{q})]$ in Eq. (6.150) with respect to ω_m and $\mathbf{q}$, one obtains an expansion in temporal and spatial derivatives. To get the quadratic-in-Δ term without derivatives, we should evaluate $[g^{-1} - \chi_c^{(0)}(0,0)]$ According to Eq. (5.42),

$$\chi_c^{(0)}(0,0) = T\sum_n \nu \int \mathrm{d}\xi \, \frac{1}{\epsilon_n^2 + \xi^2} = \nu \int\limits_{-\omega_D}^{\omega_D} \mathrm{d}\xi \, \frac{1}{2\xi} \tanh\left(\frac{\xi}{2T}\right) = \nu \ln\left(\frac{2e^\gamma}{\pi}\,\frac{\omega_D}{T}\right) , \qquad (6.151)$$

where $\gamma \approx 0.577$ is the Euler-Mascheroni constant. Using also the formula for the critical temperature, Eq. (5.43),

$$T_c = \frac{2e^\gamma}{\pi}\omega_D \exp\left(-\frac{1}{g\nu}\right) , \qquad (6.152)$$

we obtain

$$\frac{1}{g} - \chi_c^{(0)}(0,0) = \nu \ln\frac{T}{T_c} \simeq \nu\frac{T - T_c}{T_c} . \qquad (6.153)$$

On the last step, we have expanded in a small parameter $(T - T_c)/T_c$. Thus, we find

$$S^{(2)}[\Delta, \Delta^*] = \int d\tau d^3r \left[a(T)|\Delta|^2 + \ldots\right] , \qquad (6.154)$$

where

$$a(T) = \nu\,\frac{T - T_c}{T_c} . \qquad (6.155)$$

The coefficient $a(T)$ changes sign at $T = T_c$, becoming negative at $T < T_c$, which signifies instability of the normal state.

To ensure convergence of the integral at $T \leq T_c$, one has to include the next-order term $S^{(4)}$. Let us evaluate it. In the calculation of this term, derivatives can be neglected, as the corresponding contribution will be small compared to the gradient contribution to $S^{(2)}$ considered below. We then have, according to Eqs. (6.144) and (6.147),

$$S^{(4)}[\Delta, \Delta^*] = \frac{1}{4}\mathrm{tr}[(\hat{G}_0\,\hat{\Delta})^4] \simeq \frac{T}{2V}\sum_{\epsilon_n, \mathbf{p}} G_0^2(\epsilon_n, \mathbf{p}) G_0^2(-\epsilon_n, -\mathbf{p}) \int d\tau d^3r \, |\Delta|^4 , \qquad (6.156)$$

The sum and integral are easily calculated

$$\frac{T}{V}\sum_{\epsilon_n, \mathbf{p}} G_0^2(\epsilon_n, \mathbf{p}) G_0^2(-\epsilon_n, -\mathbf{p}) = \frac{T}{V}\sum_{\epsilon_n, \mathbf{p}} \frac{1}{(\epsilon_n^2 + \xi_p^2)^2} = \nu T \sum_{\epsilon_n} \int_{-\omega_D}^{\omega_D} d\xi \frac{1}{(\epsilon_n^2 + \xi^2)^2}$$

$$= \nu T \frac{\pi}{2}\sum_{\epsilon_n} \frac{1}{|\epsilon_n|^3} = \frac{\nu}{(\pi T)^2}\sum_{n=0}^{\infty} \frac{1}{(2n+1)^3} = \frac{7}{8}\zeta(3)\frac{\nu}{(\pi T)^2} . \qquad (6.157)$$

Thus, we obtain the quartic term in the action

$$S[\Delta, \Delta^*] = \int d\tau d^3r \left[a(T)|\Delta|^2 + b|\Delta|^4 + \ldots\right] , \qquad (6.158)$$

where

$$b = \frac{7}{16}\zeta(3)\frac{\nu}{(\pi T)^2} . \qquad (6.159)$$

The coefficient b is positive and ensures convergence.

Let us return to the quadratic part of the action $S^{(2)}[\Delta, \Delta^*]$, Eq. (6.150). Expanding $[g^{-1} - \chi_c^{(0)}(\omega_m, \mathbf{q})]$ in $\mathbf{q}$, we will find terms with spatial gradients in the action. From symmetry

considerations, it is clear that the term linear in $\mathbf{q}$ vanishes, so that one has to expand to the second order in $\mathbf{q}$. As we have already discussed earlier in context of similar calculations of the polarization operator, it is sufficient, in the leading order, to keep the linear-in-q term in $\chi_{-\mathbf{p}+\mathbf{q}}$ in the denominator of Eq. (6.149):

$$\xi_{-\mathbf{p}+\mathbf{q}} \simeq \xi_{-\mathbf{p}} - \frac{\mathbf{pq}}{m} \,. \tag{6.160}$$

Expanding after this up to the second order in $\mathbf{q}$, it is not dfficult to estimate the resulting sum over the Matsubara frequencies and momenta $\mathbf{p}$. Two factors $\mathbf{p}/m$ under sum yield $\sim v_F^2$, and two additional factors $(i\epsilon_n - \xi_{-\mathbf{p}})$ in the denominator yield $\sim 1/T^2$. We thus have

$$\chi_c^{(0)}(0,\mathbf{q}) \simeq \chi_c^{(0)}(0,0) - K\mathbf{q}^2 \,, \tag{6.161}$$

where

$$K = c_K \, \nu \left(\frac{v_F}{T}\right)^2 \,, \tag{6.162}$$

and c_K is a numerical coefficient. Accurate calculation of this coefficient yields

$$c_K = \frac{7\zeta(3)}{48\pi^2} \,. \tag{6.163}$$

Including this term, we get the **Ginzburg-Landau action** in the conventional form

$$S[\Delta,\Delta^*] = \int d\tau d^3r \left[a(T)|\Delta|^2 + b|\Delta|^4 + K|\partial_{\mathbf{r}}\Delta|^2 + \ldots\right] \,, \tag{6.164}$$

We have thus derived the Ginzburg-Landau action from the microscopic Hamiltonian by means of the functional integral technique. One can now apply the standard machinery (as was discussed in the Theory F: Statistical Physics course) to analyze properties of the system near the phase transition.

6.3.4 Outlook

Let us also list some further extensions, without going into details:

- Extension of the expansion, to include also terms with temporal derivatives: Time-dependent Ginzburg-Landau formalism
- Extension to spatially non-uniform problems
- Stationary-point approximation to the Ginzburg-Landau action, yielding equations for the time and spatial variation of the order parameter
- Charged particles: Including coupling to the electromagnetric field (by means of minimal coupling that follows from gauge invariance); Anderson-Higgs mechanism of generation of mass of the photon.
- Other types of interaction in the microscopic Hamiltonian
- ...

Finally, it should be emphasized that the program presented above for s-wave superconductivity (functional integral formalism, Hubbard-Stratonovich transformation, derivation of effective action, spontaneous symmetry breaking, expansion around mean-field solution, ...) is very general. It applies, with suitable modifications, to a great variety of problems, including superconductivity with anisotropic types of pairing (d-wave, p-wave, ...), magnetism, disordered systems, etc.

Chapter 7

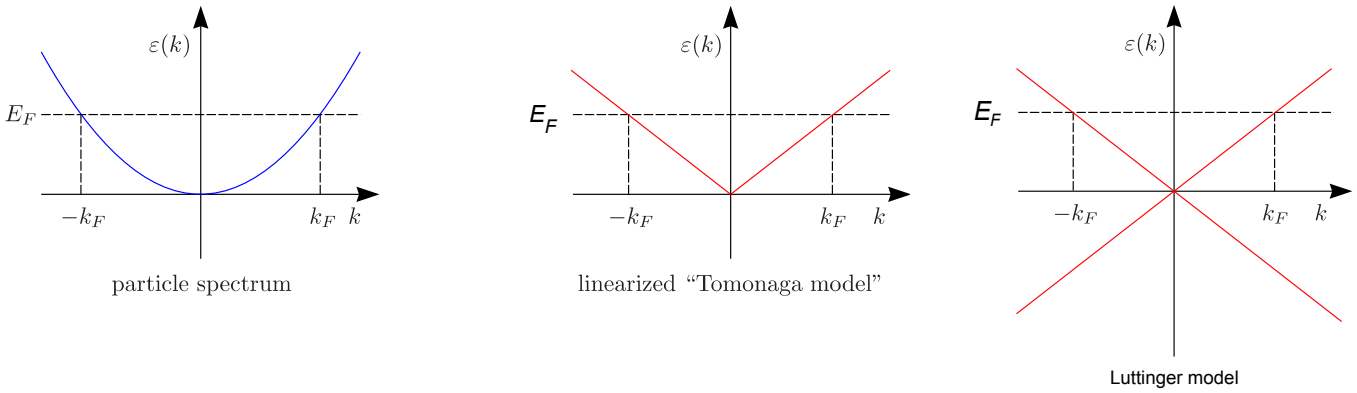
Interacting Fermions in 1D: Bosonization and Luttinger Liquids

In $d > 1$ spatial dimensions, a fermionic system with a not too strong repulsive interaction forms a Fermi liquid. An attractive interaction in $d > 1$ dimensions leads to spontaneous symmetry breaking and superconducting order. As we discuss in this chapter, in one dimension (1D) any interaction, either repulsive or attractive, destroys the Fermi liquid – due to a very different mechanism. The resulting state is known as **Luttinger liquid**. In fact, Luttinger liquids are ubiquitous in the physics of interacting 1D systems: in particular, they also emerge in the cases of interacting 1D bosons and spin chains.

7.1 Breakdown of Fermi liquid state in 1D

Consider first free fermions in 1D. The special feature of one dimension is that the Fermi surface consists of only two points: $k = k_F,\ -k_F$. We will be interested in the low-energy excitations, as only they are relevant for sufficiently low temperatures, $T \ll E_F$. Thus, only momenta k in the vicinity of $\pm k_F$ will be important. In view of this, we can **linearize** the dispersion relation in the vicinity of each of the Fermi points:

$$\varepsilon_k = \frac{k^2}{2m} - \mu \quad \longrightarrow \quad \begin{cases} (k - k_F)v_F\,, & k \approx k_F \\ (-k - k_F)v_F & k \approx -k_F \end{cases} \tag{7.1}$$



We thus have two branches of particles: **right-movers** that have a constant velocity v_F and **left-movers** with a constant velocity $-v_F$. We include all states with energies down to $-\infty$ in both branches. While not affecting the physics at sufficiently low temperatures

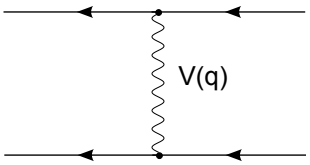
$T \ll E_F$, this will make the interacting model analytically solvable. The resulting model is called **Luttinger model**.

The kinetic term in the Hamiltonian now has the following form:

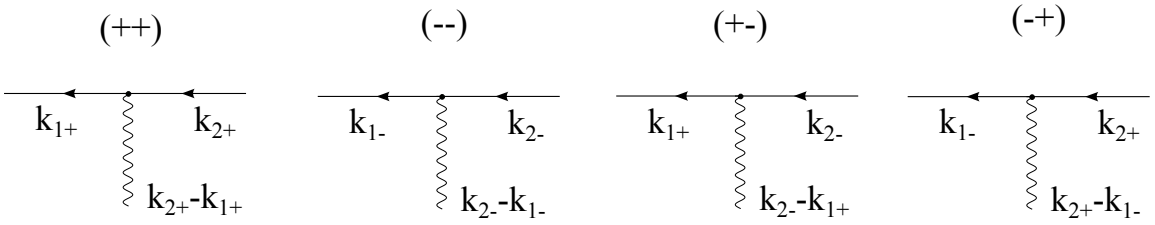
$$H_0 = v_F \sum_k \left[(k - k_F) a^\dagger_{+,k} a_{+,k} + (-k - k_F) a^\dagger_{-,k} a_{-,k} \right] , \tag{7.2}$$

where "+" stands for the right-movers and "-" for the left-movers. At this stage, we discard the spin degree of freedom. (One can think about spin-polarized fermions.) We will first develop the theory of spinless Luttinger liquid, and include spin at a later stage.

Let us turn now to the interaction. Assume a momentum-dependent interaction $V(q)$:



We can classify vertices connecting the interaction line with tho fermion lines according to the branches to which the fermion belongs before and after the scattering event:



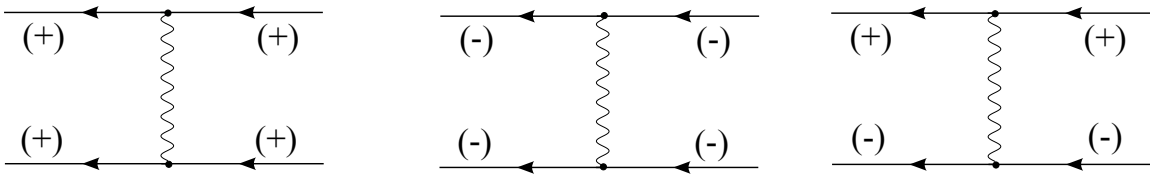
For $(++)$ and $(--)$ vertices, the transferred momentum is small, $q = k_1 - k_2 \ll k_F$. In view of this, we approximate the corresponding interaction $V(k_1 - k_2)$ by $V(0)$:

$$V(k_1 - k_2) \approx V(0) \equiv g \qquad \text{for} \;\; (++)\,, \;\; (--)\,. \tag{7.3}$$

On the other hand, For $(+-)$ and $(-+)$ vertices, the transferred momentum is $|q| = |k_1 - k_2| \approx 2k_F$. If we assume that the interaction range is sufficiently large, then $V(2k_F)$ is small, and we can neglect it:

$$V(k_1 - k_2) \approx V(2k_F) \;\mapsto\; 0 \qquad \text{for} \;\; (+-)\,, \;\; (-+)\,. \tag{7.4}$$

(We will return to the effect of $2k_F$ processes below.) We are then left with the following interaction diagrams that all correspond to forward scattering: every fermion remains on the same branch where it was before the collision:



The corresponding interaction part of the Hamiltonian reads:

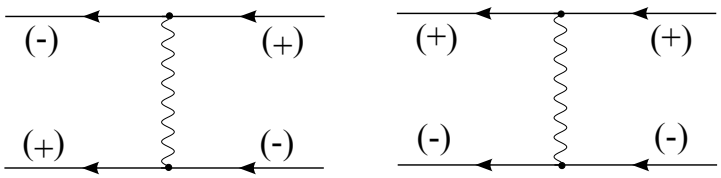
$$H_{\rm int} = \frac{g}{2L} \sum_q \sum_{\alpha=\pm} \left[\varrho_\alpha(q) \varrho_{-\alpha}(-q) + \varrho_\alpha(q) \varrho_\alpha(-q) \right] , \tag{7.5}$$

where $\varrho_\alpha(q)$ are the density operators

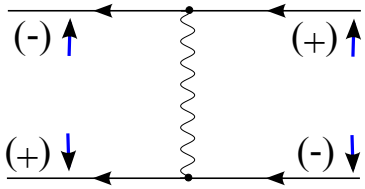
$$\varrho_\alpha(q) = \sum_k a^\dagger_{\alpha,k+q} a_{\alpha,k} \,. \tag{7.6}$$

One can also consider a model with different coupling constants for the two terms in Eq. (7.5). Traditional notations are g_2 for the coupling in the first term (scattering of right-movers on left-movers) and g_4 for the coupling in the second term (scattering between particles within the same chiral branch). However, this does not bring any new physics. We will thus set $g_2 = g_4 = g$.

Let us now briefly return to the processes with $\approx 2k_F$ momentum transfer (backscattering) that have been neglected above. It is clear that, in view of the momentum conservation, the corresponding scattering process may only be of the form shown on the left figure below:



However, in a spinless situation, it is the same process as shown in the right figure – which corresponds to the forward scattering. Including the backscattering process thus would not produce any new term in the Hamiltonian (7.5); it would only correct the coupling, $V(0) \to V(0) - V(2k_F)$, which does not play any essential role. On the other hand, in the presence of spin, the situation is different: there is a back-scattering ($2k_F$) process which is distinct from forward-scattering processes:



The corresponding coupling is traditionally denoted g_1. In the spinful case, in the presence of such g_1 term, the model is not exactly solvable anymore. One first solves the model at $g_1 = 0$ and then analyzes the effect of g_1 by using renormalization-group framework (to be discussed in the end of this chapter).

We return to the spinless case. The Hamiltonian of the **Luttinger model (without spin)**

$$H = H_0 + H_{\rm int} \tag{7.7}$$

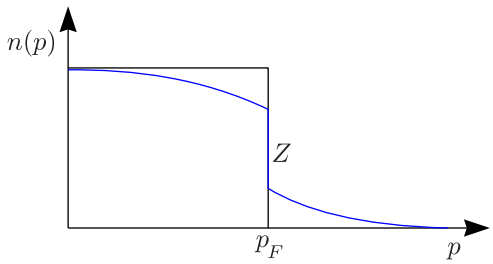
is given by the sum of Eqs. (7.2) and (7.5). To demonstrate the breakdown of the Fermi-liquid theory, let us try to calculate the corresponding residue Z by perturbation theory with respect to $H_{\rm int}$. We remind that in the Fermi-liquid state, the Green function has the form (see Sec. 3.11)

$$G(\varepsilon, p) \simeq \frac{Z}{\varepsilon - \epsilon_p + i\Gamma(\varepsilon, p)} \,, \tag{7.8}$$

where $\epsilon_p = v_F^*(p - p_F)$ and $\operatorname{sign}\Gamma(\varepsilon, p) = \operatorname{sign}\varepsilon$. The quasiparticle residue Z is given by

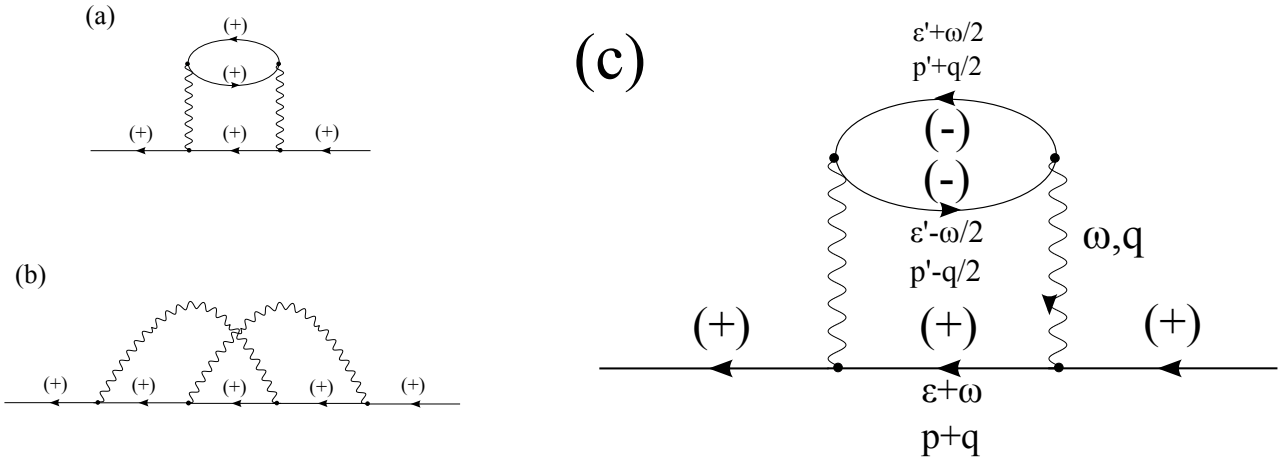
$$Z = \left. \frac{1}{1 - \frac{\partial}{\partial\varepsilon}{\rm Re}\Sigma(\varepsilon, p)} \right|_{\substack{p=p_F \\ \varepsilon=\varepsilon_F}} . \tag{7.9}$$

It determines the discontinuity of the occupation number at the Fermi momentum:



In the Fermi liquid $0 < Z < 1$. The singularity at the Fermi energy determines all key properties of the Fermi liquid. In other words, the Fermi liquid behavior is crucially based on $Z > 0$, which means that there are are well defined fermionic quasiparticles analogous to the particles in a non-interacting system.

To calculate perturbatively Z, we should first calculate the self-energy Σ. Let us calculate $\Sigma_+(\varepsilon, p)$ of right-moving quasiparticles at zero temperature. (Clearly, the self-energy for left movers has the same behavior.) The first-oder diagrams do not depend on ε and thus do not affect Z, see Eq. (3.254). We thus analyze second-order diagrams, as we did in Sec. 3.12.1 for higher-dimensional systems. We have the following three diagrams:



The diagrams (a) and (b) cancel exactly: $(a) + (b) = 0$, and we focus on the diagram (c). [*Remark:* in the presence of spin, $(a) = -2(b)$.]

The diagram (c) yields:

$$\Sigma_+(\varepsilon, p) = \mathrm{i}^2 g^2 \int \frac{\mathrm{d}q\, \mathrm{d}\omega}{(2\pi)^2}\, \mathrm{i}\Pi_-(\omega, q) G_+^{(0)}(\varepsilon + \omega, p + q)\,, \tag{7.10}$$

with

$$G_\pm^{(0)}(\varepsilon, p) = \frac{1}{\varepsilon - v_F(\pm p - p_F) + \mathrm{i}0\,\mathrm{sign}(\varepsilon)}\,, \tag{7.11}$$

and

$$\Pi_-(\omega, q) = \mathrm{i} \int \frac{\mathrm{d}\varepsilon'\, \mathrm{d}p'}{(2\pi)^2} G_-^{(0)}\left(\varepsilon' + \frac{\omega}{2}, p' + \frac{q}{2}\right) G_-^{(0)}\left(\varepsilon' - \frac{\omega}{2}, p' - \frac{q}{2}\right)\,. \tag{7.12}$$

It is convenient to count momenta of right- and left-movers from the corresponding Fermi momenta. In other words, we define

$$\tilde{p} = \begin{cases} p - p_F & \text{for right-movers} \\ p + p_F & \text{for left-movers} \end{cases} \tag{7.13}$$

and then omit tilde. Since we only consider forward-scattering processes, this is fully justified. Intetgration over ε' in Eq. (7.12) yields, see Eq. (3.262):

$$\Pi_-(\omega,q) = -\int \frac{\mathrm{d}p'}{2\pi}\, \frac{\Theta\left(p'+\frac{q}{2}\right)-\Theta\left(p'-\frac{q}{2}\right)}{-v_F\left(p'+\frac{q}{2}\right)+v_F\left(p'-\frac{q}{2}\right)-\omega+i0\,\mathrm{sign}\left(p'+\frac{q}{2}\right)}\,. \tag{7.14}$$

Integration over p' is trivial and yields

$$\Pi_-(\omega,q) = \frac{1}{2\pi}\,\frac{q}{v_F q+\omega+\mathrm{i}0\,\mathrm{sign}(\omega)}\,. \tag{7.15}$$

Substituting (7.15) into the integral for Σ_+, Eq. (7.10), we get

$$\begin{aligned}
\Sigma_+(\epsilon,p) &= -ig^2\int \frac{dqd\omega}{(2\pi)^2}\, {G_+}^{(0)}(\epsilon+\omega,p+q)\frac{1}{2\pi}\,\frac{q}{v_F q+\omega+i0\,\mathrm{sign}(\omega)} \\
&= -ig^2\int \frac{dqd\omega}{(2\pi)^3}\,\frac{1}{\epsilon+\omega-v_F(p+q)+i0\,\mathrm{sign}(\epsilon+\omega)}\cdot\frac{q}{v_F q+\omega+i0\,\mathrm{sign}(\omega)} \\
&= -ig^2\int \frac{dqd\omega}{(2\pi)^3}\,\frac{1}{\epsilon+\omega-v_F(p+q)+i0\,\mathrm{sign}(p+q)}\cdot\frac{q}{v_F q+\omega+i0\,\mathrm{sign}(-q)} \\
&= \frac{g^2}{(2\pi)^2}\int dq\,\frac{q[\Theta(p+q)-\Theta(-q)]}{\epsilon-v_F(2q+p)+i0\,\mathrm{sign}\,\epsilon}
\end{aligned} \tag{7.16}$$

Since we need now the real part of $\Sigma_+(\epsilon,p)$, the shift $+i0\,\mathrm{sign}\,\epsilon$ will be of no importance. In the term proportional to $\Theta(-q)$ the integration goes effectively over $q<0$. We make the change of variable $q\to -q$ in this term. In the term proportional to $\Theta(p+q)$ the integration goes effectively over $q>-p$. We make the change of variable $q+p\to q$ in this term. After this, the integration in both terms goes over $q>0$, yielding

$$\mathrm{Re}\,\Sigma_+(\epsilon,p) = \frac{g^2}{(2\pi)^2}\int_0^\infty dq\left[\frac{q}{\epsilon+v_F(2q-p)}+\frac{q-p}{\epsilon-v_F(2q-p)}\right] \tag{7.17}$$

Using

$$\begin{aligned}
\frac{q}{\epsilon+v_F(2q-p)} &= \frac{1}{2v_F}\left(1+\frac{v_Fp-\epsilon}{\epsilon+v_F(2q-p)}\right), \\
\frac{q-p}{\epsilon-v_F(2q-p)} &= \frac{1}{2v_F}\left(-1+\frac{\epsilon-v_Fp}{\epsilon-v_F(2q-p)}\right),
\end{aligned}$$

we get

$$\mathrm{Re}\,\Sigma_+(\varepsilon,p) = \frac{g^2}{(2\pi)^2}\,\frac{1}{2v_F}(v_Fp-\varepsilon)\int\limits_0^\infty \mathrm{d}q\,\left[\frac{1}{2v_Fq+\varepsilon-v_Fp}+\frac{1}{2v_Fq-\varepsilon-v_Fp}\right]. \tag{7.18}$$

We see that the integral is logarithmically divergent at large q. We have thus to introduce an ultraviolet (UV) cutoff $q_{\max}$. The physical reason for the necessity of the cutoff is the linearization of the spectrum that we have performed. This implies that physically $q_{\max}\sim p_F$. We thus have

$$\mathrm{Re}\,\Sigma_+(\epsilon,p) = -\frac{g^2}{(4\pi v_F)^2}(\epsilon-v_Fp)\left[\ln\left|\frac{2v_Fq_{\max}}{\epsilon-v_Fp}\right|+\ln\left|\frac{2v_Fq_{\max}}{\epsilon+v_Fp}\right|\right], \tag{7.19}$$

where we have taken into account that $\epsilon,\ v_F p \ll v_F q_{\max}$. Combining both terms together and defining the UV cutoff energy scale $\Lambda = v_F q_{\max}$ (on physical reasons explained above $\Lambda \sim E_F$), we finally obtain

$$\boxed{\mathrm{Re}\,\Sigma_+(\varepsilon,p) = -\frac{g^2}{(4\pi v_F)^2}(\varepsilon - v_F p)\ln\left|\frac{4\Lambda^2}{\varepsilon^2 - v_F^2 p^2}\right|\,.} \tag{7.20}$$

Substituting this result in Eq. (7.9) for the residue Z, we get

$$Z = \left.\frac{1}{1-\frac{\partial}{\partial\varepsilon}\mathrm{Re}\,\Sigma(\varepsilon,p)}\right|_{\varepsilon=\varepsilon_p} \simeq \left[1 + \frac{g^2}{(4\pi v_F)^2}\ln\left(\frac{\Lambda^2}{0}\right)\right]^{-1} = 0\,. \qquad (!) \tag{7.21}$$

This implies that the actual ground state of the system is not of Fermi-liquid type. Due to infrared singularities, fermionic quasiparticles are not well defined (at least not in the usual Fermi-liquid sense). As we will see below, the divergent logarithms can be resummed and in fact give rise to power laws with non-trivial, interaction-dependent exponents. A beautiful and powerful way to do this, and more generally, to calculate various observables in the problem, is to switch from fermionic to **bosonic** formulation of the theory.

7.2 From fermions to bosons

We want to present the theory in terms of bosonic density operators

$$\varrho_\alpha(q) = \sum_k a^\dagger_{\alpha,k+q} a_{\alpha,k}\,. \tag{7.22}$$

Clearly, each such operator creates particle-hole excitations when acting on the fermionic ground state (Fermi sea).

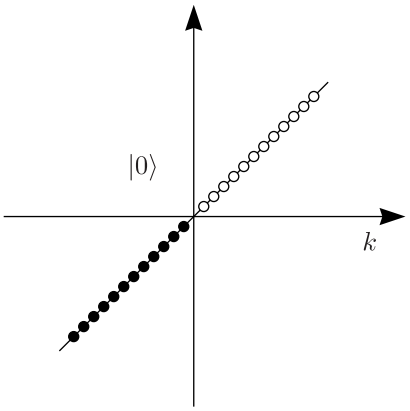
The interaction part of the Hamiltonian $H_{\rm int}$ has a simple (quadratic) form in terms of ρ_α. But what about the free part H_0? Let us show that there is an exact correspondence between the free fermionic and bosonic theories in 1D.

Since right- and left-movers decouple in the absence of interaction, we consider now only one branch: right-movers. Let us first illustrate the equivalence by considering low-lying states in two theories. We assume a system of size L, so that all energies are discrete.

- Fermions: Single particle states have the following momenta and energies:

$$k_j = \frac{2\pi}{L} j\,, \qquad \epsilon_j = v_F k_j\,, \tag{7.23}$$

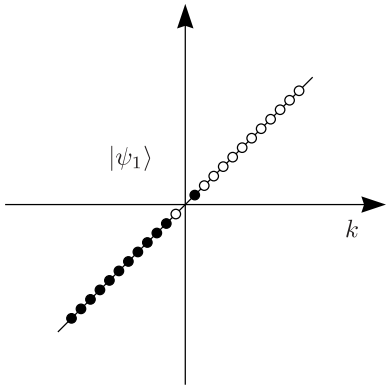
with k_j extending from $-\infty$ to $+\infty$. The ground state of the fermionic system $|0\rangle_f$ is the filled Fermi sea:



• Bosons: Single-particle excitations have momenta $k_j = \frac{2\pi}{L} j > 0$ and energies $\omega_j = v_F k_j > 0$. Ground state $|0\rangle_b$: no excitations at all.

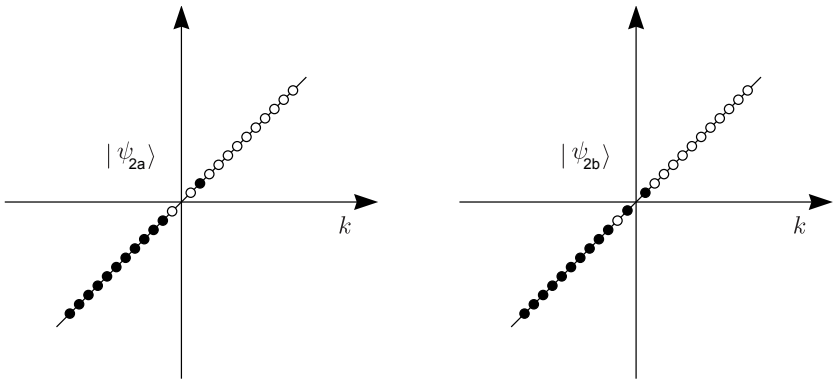
We assign the energy zero to ground states in both models and compared excited states in them. Obviously, all excitations energies in both models are quantized in units of $k_1 = 2\pi/L$. Let us consider excited states with excitations energies E up to $3v_F k_1$:

(i) $E = v_F k_1$.
On the fermionic side, there is clearly just one state:



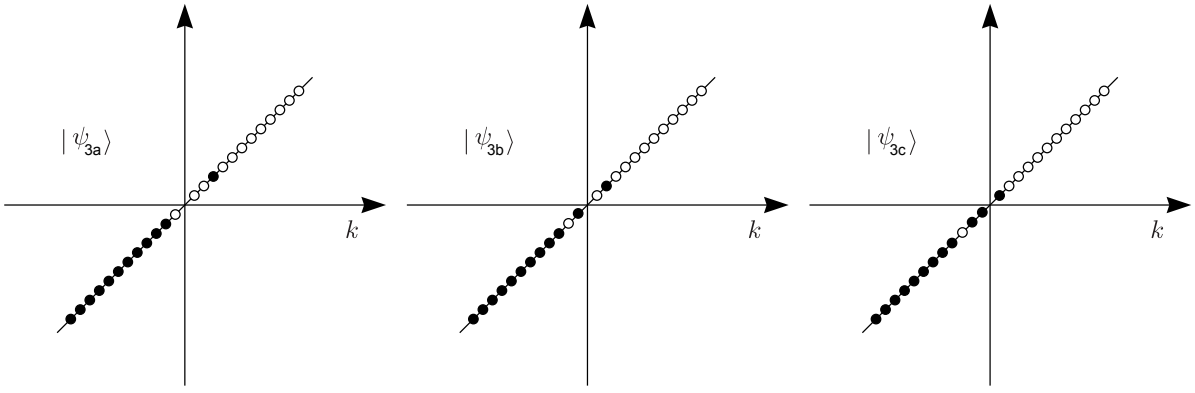
In the bosonic theory, there is also one state:
$|1k_1\rangle$ (one excited boson with momentum k_1).

(ii) $E = 2v_F k_1$.
In the fermionic theory, there are two such (linearly independent) states:



In the bosonic theory, there are also two such states:
$|2k_1\rangle$ (two excited bosons with momentum k_1)
$|1k_2\rangle$ (one excited boson with momentum k_2).

(ii) $E = 3v_F k_1$.
In the fermionic theory, there are three such states:



In the bosonic theory, there are also two such states:
$|3k_1\rangle$ (three excited bosons with momentum k_1)
$|1k_1\,,\,1k_2\rangle$ (one boson with momentum k_1 and one boson with momentum k_2)
$|1k_3\rangle$ (one excited boson with momentum k_3).

One can prove that this agreement holds for all excitation energies. We thus have a correspondence between Hilbert spaces of the fermionic and bosonic theories, and we expect that the free-fermion Hamiltonian can be rewritten in terms of free bosons. Let us show that this is indeed the case. The free-fermion part of the Hamiltonian is

$$H_0 = v_F \sum_k \left[k a^\dagger_{+,k} a_{+,k} + (-k) a^\dagger_{-,k} a_{-,k} \right] = v_F \sum_{\alpha,k} \alpha k \, a^\dagger_{\alpha,k} a_{\alpha,k} \,, \tag{7.24}$$

We want to express H_0 through the density operators

$$\varrho_\alpha(q) = \sum_k a^\dagger_{\alpha,k+q} a_{\alpha,k} \,. \tag{7.25}$$

For this purpose, we calculate, using fermionic anticommutation relations

$$\{a^\dagger_{\alpha,k}, a^\dagger_{\alpha,k}\} = \delta_{\alpha\alpha'}\delta_{kk'} \,, \tag{7.26}$$

the commutator of density operators

$$\begin{aligned}
[\varrho_\alpha(q), \varrho_{\alpha'}(-q')] &= \left[\sum_p a^\dagger_{\alpha,p+q} a_{\alpha,p} \,, \sum_{p'} a^\dagger_{\alpha',p'-q'} a_{\alpha',p'} \right] \\
&= \sum_{p,p'} (a^\dagger_{\alpha,p+q} a_{\alpha,p} a^\dagger_{\alpha',p'-q'} a_{\alpha',p'} - a^\dagger_{\alpha',p'-q'} a_{\alpha',p'} a^\dagger_{\alpha,p+q} a_{\alpha,p}) \\
&= \sum_{p,p'} (a^\dagger_{\alpha,p+q} (\delta_{p,p'-q'}\delta_{\alpha\alpha'} - a^\dagger_{\alpha',p'-q'} a_{\alpha,p}) a_{\alpha',p'} - a^\dagger_{\alpha',p'-q'} (\delta_{p',p+q}\delta_{\alpha\alpha'} - a^\dagger_{\alpha,p+q} a_{\alpha',p'}) a_{\alpha,p} \\
&= \delta_{\alpha\alpha'} \sum_p \left(a^\dagger_{\alpha,p+q} a_{\alpha,p+q'} - a^\dagger_{\alpha,p+q-q'} a_{\alpha,p} \right)
\end{aligned} \tag{7.27}$$

Consider first the case $q = q'$. (We will show later that for $q \neq q'$ the commutator is zero.) We have

$$[\varrho_\alpha(q), \varrho_\alpha(-q)] = \sum_p \left(a^\dagger_{\alpha,p+q} a_{\alpha,p+q} - a^\dagger_{\alpha,p} a_{\alpha,p} \right) = \sum_p (\hat{n}_{\alpha,p+q} - \hat{n}_{\alpha,p}) \,, \tag{7.28}$$

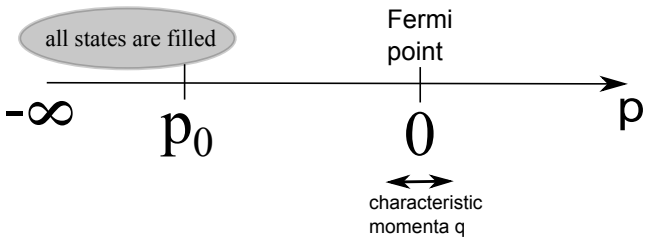
where

$$\hat{n}_{\alpha,p} = a^\dagger_{\alpha,p} a_{\alpha,p} \tag{7.29}$$

are fermionic occupation number operators. Naively, one could conclude, by splitting the resulting expression in (7.28) in two sums and shifting the summation variable in one of them, that the result is zero:

$$\sum_p (\hat{n}_{\alpha,p+q} - \hat{n}_{\alpha,p}) \stackrel{?}{=} \sum_p \hat{n}_{\alpha,p+q} - \sum_p \hat{n}_{\alpha,p} = \sum_p \hat{n}_{\alpha,p} - \sum_p \hat{n}_{\alpha,p} = 0 \,. \tag{7.30}$$

However, this conclusion is incorrect, since both sums (7.30) are UV-divergent, so that one subtracts one infinity from the other. We thus proceed in a more careful way. Let us consider right-movers for definiteness. We are only interested in states that are obtained from the ground state (Fermi sea with all $p < 0$ filled) by exciting fermionic particles with momenta in some range around zero (certainly $p \ll p_F$). We can thus safely assume that there is a momentum $p_0 < 0$ (deeply in the Fermi sea) such that we do not touch fermions with momenta $p < p_0$; in all relevant processes states below p_0 keep occupation unity.



We have

$$\begin{aligned}
[\varrho_+(q),\varrho_+(-q)] &= \sum_p (\hat{n}_{+,p+q}-\hat{n}_{+,p}) \\
&= \sum_{p>p_0}[\hat{n}_{+,p+q}-\hat{n}_{+,p}] + \sum_{p<p_0}\underbrace{[\overbrace{\hat{n}_{+,p+q}}^{=1}-\overbrace{\hat{n}_{+,p}}^{=1}]}_{=0} \\
&= \sum_{p>p_0}[\hat{n}_{+,p+q}-\hat{n}_{+,p}] = \sum_{p>p_0+q}\hat{n}_{+,p}-\sum_{p>p_0}\hat{n}_{+,p} = -\sum_{p=p_0}^{p_0+q}\underbrace{\hat{n}_{+,p}}_{=1} \\
&= -\frac{qL}{2\pi} \qquad (7.31)
\end{aligned}$$

For left-movers ($\alpha=-$) the calculation is carried out in the same way; the result for both chiral branches reads:

$$[\varrho_\alpha(q),\varrho_\alpha(-q)] = -\frac{\alpha qL}{2\pi}\,. \qquad (7.32)$$

For $q\neq q'$ the calculation is performed in an analogous way but now we get the sum

$$\sum_{p=p_0}^{p_0+q} a^\dagger_{\alpha,p}a_{\alpha,p+q'-q}\,,$$

which yields zero since all states below and near p_0 are occupied.

Hence, we get the following result for the commutator of density operators:

$$\boxed{[\varrho_\alpha(q),\varrho_{\alpha'}(-q')] = \delta_{\alpha\alpha'}\delta_{qq'}\frac{(-\alpha)qL}{2\pi}\,.} \qquad (7.33)$$

To cast these relations in the form of canonical Bose commutations relations, we observe that

$$\begin{aligned}
\varrho_+(q)|0\rangle &= 0 \qquad \text{for } q<0\,, \\
\varrho_-(q)|0\rangle &= 0 \qquad \text{for } q>0\,, \qquad (7.34)
\end{aligned}$$

and

$$\varrho^\dagger_\alpha(q) = \left(\sum_k a^\dagger_{\alpha,k+q}a_{\alpha,k}\right)^\dagger = \sum_k a^\dagger_{\alpha,k}a_{\alpha,k+q} = \sum_k a^\dagger_{\alpha,k-q}a_{\alpha,k} = \varrho_\alpha(-q) \qquad (7.35)$$

We thus define the bosonic creation and annihilation operators $b^\dagger, b$ as follows:

$$\text{right-movers:} \quad \left.\begin{aligned}\varrho_+(q) &= b^\dagger_{+,q}\left(\tfrac{qL}{2\pi}\right)^{\frac{1}{2}} \\ \varrho_+(-q) &= b_{+,q}\left(\tfrac{qL}{2\pi}\right)^{\frac{1}{2}}\end{aligned}\right\} \quad q>0 \qquad (7.36)$$

and

$$\text{left-movers:} \quad \left.\begin{array}{l} \varrho_-(-q) = b^\dagger_{-,-q} \left(\frac{qL}{2\pi}\right)^{\frac{1}{2}} \\ \varrho_-(q) = b_{-,-q} \left(\frac{qL}{2\pi}\right)^{\frac{1}{2}} \end{array}\right\} \qquad q > 0\,. \tag{7.37}$$

According to Eq. (7.33) the operators, $b^\dagger, b$ satisfy canonical bosonic commutation relations

$$\boxed{[b^\dagger_{\alpha,q}, b_{\alpha',q'}] = -\delta_{\alpha\alpha'}\delta_{qq'}}\,. \tag{7.38}$$

According to (7.34), (7.35), all annihilation operators b yield zero, when acting on vacuum (ground state).

It still remains to express H_0 through the density operators ϱ. For this purpose, we inspect commutation relations of H_0 with the density operators. We have

$$\begin{aligned} [H_0, \varrho_\alpha(q)] &= \left[v_F \sum_{\alpha',k'} k'\alpha' a^\dagger_{\alpha',k'} a_{\alpha',k'}, \sum_k a^\dagger_{\alpha,k+q} a_{\alpha,k} \right] \\ &= v_F \sum_{k,k',\alpha'} k'\alpha' \left(a^\dagger_{\alpha',k'} a_{\alpha',k'} a^\dagger_{\alpha,k+q} a_{\alpha,k} - a^\dagger_{\alpha,k+q} a_{\alpha,k} a^\dagger_{\alpha',k'} a_{\alpha',k'} \right) \\ &= v_F \alpha \sum_k \left[(k+q) a^\dagger_{k+q,\alpha} a_{k,\alpha} - k a^\dagger_{k+q,\alpha} a_{k,\alpha} \right] = v_F \alpha q\, \varrho_\alpha(q)\,. \end{aligned} \tag{7.39}$$

Commutation relations with all the creation and annihilation operators uniquely define an operator. We thus should find an expression for H_0 in terms of density operators that satisfies the commutation relations (7.39). It is easy to see that the required expression has the form

$$\boxed{H_0 = \frac{\pi v_F}{L} \sum_{\alpha,q} \varrho_\alpha(q)\varrho_\alpha(-q)\,.} \tag{7.40}$$

Indeed, according to the commutation relations (7.33),

$$[H_0, \varrho_\alpha(q)] = \left[\frac{\pi v_F}{L} \sum_{\alpha',q'} \varrho_{\alpha'}(q')\varrho_{\alpha'}(-q'), \varrho_\alpha(q) \right] = v_F \alpha q \varrho_\alpha(q)\,, \tag{7.41}$$

reproducing Eq. (7.39) as required.

Therefore, both the free part of the Hamiltonian, H_0, and the interaction part $H_{\rm int}$ are expressed in a form quadratic with respect to the density operators, and thus quadratic with respect to the canonical bosonic operators $b, b^\dagger$. We come to a very important conclusion: the interacting fermionic theory from which we started can be exactly reformulated as a theory of **free bosons**. Below we explore consequences of this remarkable mapping.

7.3 Spinless Luttinger liquid: Bosonic excitations

We have derived the Hamiltonian of the spinless **Luttinger liquid** in the bosonized form, which is given by a sum of Eqs. (7.40) and (7.5):

$$\begin{aligned} H &= H_0 + H_{\rm int} = \frac{\pi v_F}{L} \sum_{\alpha,q} \varrho_\alpha(q)\varrho_\alpha(-q) + \frac{g}{2L} \sum_{\alpha,q} [\varrho_\alpha(q)\varrho_{-\alpha}(-q) + \varrho_\alpha(q)\varrho_\alpha(-q)] \\ &= \frac{1}{2L} \sum_{q,\alpha} [(2\pi v_F + g)\varrho_\alpha(q)\varrho_\alpha(-q) + g\varrho_\alpha(q)\varrho_{-\alpha}(-q)] \end{aligned}$$

$$= \frac{1}{2L}\sum_q \{(2\pi v_F+g)[\varrho_+(q)\varrho_+(-q)+\varrho_-(q)\varrho_-(-q)]+g[\varrho_+(q)\varrho_-(-q)+\varrho_-(q)\varrho_+(-q)]\}$$

$$= \frac{1}{L}\sum_{q>0} \{(2\pi v_F+g)[\varrho_+(q)\varrho_+(-q)+\varrho_-(q)\varrho_-(-q)]+g[\varrho_+(q)\varrho_-(-q)+\varrho_-(q)\varrho_+(-q)]\} + \text{const.} \quad (7.42)$$

We discard the constant and rewrite this in terms of the canonical bosonic operators b, $b^\dagger$ introduced in Eqs. (7.36) and (7.37):

$$H = \frac{1}{L}\sum_{q>0}\frac{qL}{2\pi}\left[(2\pi v_F+g)[b^\dagger_{+,q}b_{+,q}+b_{-,-q}b^\dagger_{-,-q}]+g(b^\dagger_{+,q}b^\dagger_{-,-q}+b_{+,q}b_{-,-q})\right]. \quad (7.43)$$

The result can be presented in the matrix form:

$$H = \sum_{q>0}\frac{q}{2\pi}\begin{pmatrix} b^\dagger_{+,q} & b_{-,-q}\end{pmatrix}\begin{pmatrix} 2\pi v_F+g & g \\ g & 2\pi v_F+g\end{pmatrix}\begin{pmatrix} b_{+,q} \\ b^\dagger_{-,-q}\end{pmatrix}. \quad (7.44)$$

There is a clear analogy with the mean-field Hamiltonian in the problem of superconductivity, Eq. (5.50). An important difference is, however, that here we deal with a Hamiltonian of bosons, whereas it was fermionic in the case of superconductivity. We thus perform a **bosonic Bogoliubov transformation** to diagonalize the Hamiltonian:

$$\begin{aligned} \tilde{b}_{+,q} &= \cosh\theta_q\, b_{+,q} + \sinh\theta_q\, b^\dagger_{-,-q}\ ; \\ \tilde{b}^\dagger_{-,-q} &= \sinh\theta_q\, b_{+,q} + \cosh\theta_q\, b^\dagger_{-,-q}\ , \end{aligned} \quad (7.45)$$

or, in the matrix notations,

$$\begin{pmatrix} \tilde{b}_{+,q} \\ \tilde{b}^\dagger_{-,-q}\end{pmatrix} = \begin{pmatrix} \cosh\theta_q & \sinh\theta_q \\ \sinh\theta_q & \cosh\theta_q\end{pmatrix}\begin{pmatrix} b_{+,q} \\ b^\dagger_{-,-q}\end{pmatrix}. \quad (7.46)$$

Note that, while in the case of fermionic Bogoliubov transformation, the corresponding 2×2 matrix was unitary, here it is pseudounitary, i.e. satisfies the relation $M^\dagger\tau_3 M = \tau_3$, where $\tau_3 = \mathrm{diag}(1,-1)$ is the third Pauli matrix. The difference originates from the requirement that the transformation should preserve the commutation relations in the bosonic case, in contrast to anticommutation relations in the fermionic case. The inverse transformation reads:

$$\begin{pmatrix} b_{+,q} \\ b^\dagger_{-,-q}\end{pmatrix} = \begin{pmatrix} \cosh\theta_q & -\sinh\theta_q \\ -\sinh\theta_q & \cosh\theta_q\end{pmatrix}\begin{pmatrix} \tilde{b}_{+,q} \\ \tilde{b}^\dagger_{-,-q}\end{pmatrix}. \quad (7.47)$$

Substituting this in (7.44), we get

$$H = \sum_{q>0}\frac{gq}{2\pi}\begin{pmatrix} \tilde{b}^\dagger_{+,q} & \tilde{b}_{-,-q}\end{pmatrix}\begin{pmatrix} \cosh\theta_q & -\sinh\theta_q \\ -\sinh\theta_q & \cosh\theta_q\end{pmatrix}\begin{pmatrix} 1+{}^{2\pi v_F}/_{g} & 1 \\ 1 & 1+{}^{2\pi v_F}/_{g}\end{pmatrix}\begin{pmatrix} \cosh\theta_q & -\sinh\theta_q \\ -\sinh\theta_q & \cosh\theta_q\end{pmatrix}\begin{pmatrix} \tilde{b}_{+,q} \\ \tilde{b}^\dagger_{-,-q}\end{pmatrix}$$

$$= \sum_{q>0}\frac{gq}{2\pi}\begin{pmatrix} \tilde{b}^\dagger_{+,q} & \tilde{b}_{-,-q}\end{pmatrix}\begin{pmatrix} \cosh(2\theta_q)[1+{}^{2\pi v_F}/_{g}]-\sinh(2\theta_q) & \sinh(2\theta_q)[1+{}^{2\pi v_F}/_{g}]-\cosh(2\theta_q) \\ \sinh(2\theta_q)[1+{}^{2\pi v_F}/_{g}]-\cosh(2\theta_q) & \cosh(2\theta_q)[1+{}^{2\pi v_F}/_{g}]-\sinh(2\theta_q)\end{pmatrix}\begin{pmatrix} \tilde{b}_{+,q} \\ \tilde{b}^\dagger_{-,-q}\end{pmatrix}. \quad (7.48)$$

Requiring that the matrix in (7.48) is diagonal, one gets the condition

$$\sinh(2\theta_q)[1+{}^{2\pi v_F}/_{g}]-\cosh(2\theta_q) = 0\,, \quad (7.49)$$

or, equivalently,

$$\coth(2\theta_q) = 1 + \frac{2\pi v_F}{g}\,. \tag{7.50}$$

This implies

$$\sinh(2\theta_q) = \mathrm{sign}(g)\,\frac{1}{\sqrt{[1+{}^{2\pi v_F}/_{g}]^2 - 1}}\,. \tag{7.51}$$

Diagonal elements of the matrix in Eq. (7.48) are then equal to

$$\begin{aligned}
\cosh(2\theta_q)[1+{}^{2\pi v_F}/_{g}] - \sinh(2\theta_q) &= \sinh(2\theta_q)\,\{\coth(2\theta_q)[1+{}^{2\pi v_F}/_{g}] - 1\} \\
&= \frac{\mathrm{sign}(g)}{\sqrt{[1+{}^{2\pi v_F}/_{g}]^2 - 1}}\left([1+{}^{2\pi v_F}/_{g}]^2 - 1\right) \\
&= \mathrm{sign}(g)\,\sqrt{[1+{}^{2\pi v_F}/_{g}]^2 - 1}\,.
\end{aligned} \tag{7.52}$$

Therefore, the Hamiltonian (7.48) takes the form

$$\begin{aligned}
H &= \sum_{q>0} \frac{|g|q}{2\pi}\sqrt{[1+{}^{2\pi v_F}/_{g}]^2 - 1}\,\left(\tilde{b}^\dagger_{+,q}\tilde{b}_{+,q} + \tilde{b}^\dagger_{-,-q}\tilde{b}_{-,-q}\right) \\
&= \sum_{q>0} q\sqrt{\left(v_F + \frac{g}{2\pi}\right)^2 - \left(\frac{g}{2\pi}\right)^2}\,\left(\tilde{b}^\dagger_{+,q}\tilde{b}_{+,q} + \tilde{b}^\dagger_{-,-q}\tilde{b}_{-,-q}\right)\,.
\end{aligned} \tag{7.53}$$

We have therefore achieved an exact transformation of an interacting fermionic system to a system of free bosons with the spectrum

$$\omega = u\,|q|\ , \tag{7.54}$$

where

$$u = \sqrt{\left(v_F + \frac{g}{2\pi}\right)^2 - \left(\frac{g}{2\pi}\right)^2} = \sqrt{v_F^2 + \frac{v_F g}{\pi}}\,. \tag{7.55}$$

These excitations of an interacting 1D fermionic system are collective density excitations—**plasmons**. The dispersion relation (7.54) is analogous to that of acoustic phonons. Clearly, u is the velocity of excitations. In the non-interacting case, $g = 0$, we have $u = v_F$. The interaction makes the plasmon velocity u larger or smaller than v_F, depending on whether it is repulsive ($g > 0$) or attractive ($g < 0$).

Comment: We recall that in the above derivation we have replaced the interaction $V(q)$ at small wave vector q with a constant $V(0) = g$. One can also keep the momentum dependence, thus obtaining the theory (7.42) with $g \mapsto g(q)$. It is diagonalized in the same way by Bogoliubov transformation (but with θ_q depending on q). This results in the spectrum of plasmons

$$\omega = u_q\,|q|\ , \qquad u_q = \sqrt{v_F^2 + \frac{v_F g(q)}{\pi}}\,, \tag{7.56}$$

which includes corrections to the linear dispersion. For most purposes, the leading approximation of linear dispersion, Eq. (7.54), is sufficient, and we will stick to it below. However, in some cases, one has to go beyond it and take into account the q-dependence of the plasmon velocity, Eq. (7.56).

7.3.1 From momentum- to coordinate-space representation

Let us rewrite the Luttinger-liquid Hamiltonian in the coordinate representation. We define the real-space density operators

$$\varrho_\alpha(x) = \frac{1}{L}\sum_{q\neq 0} e^{-iqx}\varrho_\alpha(q) + \varrho_\alpha^{(0)}\,. \tag{7.57}$$

The constant term $\varrho_\alpha^{(0)}$ is the background density (i.e. it represents information about the total number of particles); we discard it below. (We will include it later when necessary.) The Hamiltonian (7.42) takes the form

$$H = \frac{1}{2}\int dx\left\{2\pi v_F\left[\varrho_+^2(x)+\varrho_-^2(x)\right] + g\left[\varrho_+(x)+\varrho_-(x)\right]^2\right\}\,. \tag{7.58}$$

The commutation relations (7.33) yield, upon Fourier transformation,

$$[\varrho_\alpha(x),\varrho_{\alpha'}(x')] = \delta_{\alpha\alpha'}\frac{\alpha}{2\pi i}\frac{\partial}{\partial x}\delta(x-x')\,. \tag{7.59}$$

We define the fields $\phi(x)$ and $\theta(x)$ via

$$\partial_x\phi(x) = -\pi[\varrho_+(x)+\varrho_-(x)]\,, \tag{7.60}$$

$$\partial_x\theta(x) = \pi[\varrho_+(x)-\varrho_-(x)]\,. \tag{7.61}$$

Note that $\partial_x\phi(x)$ is equal (up to a factor $-\pi$) to the total density, while $\partial_x\theta(x)$ is equal (up to a factor π/v_F) to the total current. Using (7.59), we find the commutator of ϕ and $\partial_x\theta$ fields:

$$[\phi(x),\partial_{x'}\theta(x')] = i\pi\delta(x-x')\,. \tag{7.62}$$

Therefore, the fields $\phi(x)$ and

$$\Pi(x) = \frac{1}{\pi}\partial_x\theta(x) \tag{7.63}$$

are canonically conjugate: if $\phi(x)$ is considered as a coordinate, then $\Pi(x)$ is the corresponding canonical momentum:

$$[\phi(x),\Pi(x')] = i\delta(x-x')\,. \tag{7.64}$$

Let is now express the Hamiltonian in terms of these new fields ϕ and Π. According to Eqs. (7.60), (7.61), (7.63), the chiral density operators ρ_+ and ρ_- are expressed in terms of ϕ and Π as follows:

$$\rho_+(x) = \frac{1}{2}\left[\Pi(x) - \frac{1}{\pi}\partial_x\phi(x)\right]\,, \qquad \rho_-(x) = -\frac{1}{2}\left[\Pi(x) + \frac{1}{\pi}\partial_x\phi(x)\right]\,. \tag{7.65}$$

Thus,

$$\rho_+ + \rho_- = -\frac{1}{\pi}\partial_x\phi\,, \qquad \rho_+^2+\rho_-^2 = \frac{1}{2}\left[\Pi^2 + \frac{1}{\pi^2}(\partial_x\phi)^2\right]\,. \tag{7.66}$$

Substituting this in Eq. (7.58), we get

$$\begin{aligned} H &= \frac{1}{2}\int dx\left\{\pi v_F\left[\Pi^2+\frac{1}{\pi^2}(\partial_x\phi)^2\right] + \frac{g}{\pi^2}(\partial_x\phi)^2\right\} \\ &= \frac{1}{2\pi}\int dx\left[v_F(\pi\Pi)^2 + \left(v_F+\frac{g}{\pi}\right)(\partial_x\phi)^2\right] \end{aligned}$$

$$= \frac{1}{2\pi}\int dx\left[uK(\pi\Pi)^2+\frac{u}{K}(\partial_x\phi)^2\right], \tag{7.67}$$

where

$$u=\left(v_F^2+\frac{v_F g}{\pi}\right)^{1/2}=\frac{v_F}{K} \tag{7.68}$$

is the velocity defined in Eq. (7.55) and the dimensionless constant K is given by

$$K=\left(\frac{v_F}{v_F+\frac{g}{\pi}}\right)^{1/2}=\left(1+\frac{g}{\pi v_F}\right)^{-1/2}. \tag{7.69}$$

The Hamiltonian (7.67) has the same form as that of an elastic string. Diagonalizing it (in analogy with calculation of a spectrum of acoustic phonons in TKM 1), one reproduces, of course, the above result $\omega = uq$.

The constant K is the only dimensionless coupling that controls the physics of the spinless Luttinger liquid. In the absence of interaction one has $K = 1$, for repulsive interaction $K < 1$, and for attractive interaction $K > 1$. We will see below that $K \neq 1$ will be responsible for all non-trivial properties of the system.

As was mentioned above, one can consider a more general version of the Hamiltonian (7.5), with two different couplings: g_2 and g_4:

$$H_{\rm int}=\frac{1}{2L}\sum_q\sum_{\alpha=\pm}\left[g_2\,\varrho_\alpha(q)\varrho_{-\alpha}(-q)+g_4\,\varrho_\alpha(q)\varrho_\alpha(-q)\right], \tag{7.70}$$

In this case, the same analysis leads to exactly the same form of the Hamiltonian, Eq.(7.67), with the parameters

$$u = \left[\left(v_F+\frac{g_4}{2\pi}\right)^2-\left(\frac{g_2}{2\pi}\right)^2\right]^{1/2}, \tag{7.71}$$

$$K = \left[\frac{v_F+(g_4-g_2)/2\pi}{v_F+(g_4+g_2)/2\pi}\right]^{1/2}. \tag{7.72}$$

It is worth noting that the constant g_4 enters everywhere in combination $v_F + g_4/2\pi$. In the absence of g_2 interaction we would have a free-fermion theory ($K = 1$) but with modified velocity. It is the g_2 interaction between + and − chiral branches that is responsible for a non-trivial value $K \neq 1$.

7.4 Luttinger liquid with spin: Spin-charge separation

We consider now a system with spin (1/2). In full analogy with Eq. (7.22), we introduce density operators $\varrho_{\alpha s}(q)$ for each of the spin components, as labeled by the additional subscript $s =\uparrow,\downarrow$. Within each of the spin components, these operators satisfy the same commutation relations as in the spinless case, Eq. (7.33); density operators with different spin indices commute.

The Hamiltonian is given by a direct generalization of Eq. (7.58):

$$H=\frac{1}{2}\int dx\left[2\pi v_F\left(\varrho_{+\uparrow}^2+\varrho_{+\downarrow}^2+\varrho_{-\uparrow}^2+\varrho_{-\downarrow}^2\right)+g\left(\varrho_{+\uparrow}+\varrho_{+\downarrow}+\varrho_{-\uparrow}+\varrho_{-\downarrow}\right)^2\right]. \tag{7.73}$$

Here we assume a single interaction constant g. More generally, one can allow for different constants depending on whether the particles are on same or different chiral branches, and

whether they have same or opposite spins. We will discuss below what will be the effect of this.

It is worth recalling that in the spinful case there are in principle $2k_F$ processes of g_1 type that are not included in Eq. (7.73) since they are usually weak, see discussion in Sec. 7.1.

In order to diagonalize the Hamiltonian, we introduce, for each of the chiral branches, $\alpha = \pm$, the charge and spin densities:

$$\varrho_\alpha = \frac{1}{\sqrt{2}}(\varrho_{\alpha\uparrow} + \varrho_{\alpha\downarrow}) , \tag{7.74}$$

$$\sigma_\alpha = \frac{1}{\sqrt{2}}(\varrho_{\alpha\uparrow} - \varrho_{\alpha\downarrow}) . \tag{7.75}$$

This is a unitary transformation; the commutation relations remain the same. In terms of these operators, the Hamiltonian reads

$$\begin{aligned} H &= \frac{1}{2}\int dx \left[2\pi v_F \left(\varrho_+^2 + \sigma_+^2 + \varrho_-^2 + \sigma_-^2\right) + 2g\left(\varrho_+ + \varrho_-\right)^2\right] \\ &= H_\rho + H_\sigma , \end{aligned} \tag{7.76}$$

where

$$H_\rho = \frac{1}{2}\int dx \left[2\pi v_F \left(\varrho_+^2 + \varrho_-^2\right) + 2g\left(\varrho_+ + \varrho_-\right)^2\right] , \tag{7.77}$$

$$H_\sigma = \frac{1}{2}\int dx \; 2\pi v_F \left(\sigma_+^2 + \sigma_-^2\right) . \tag{7.78}$$

We see that the spin and charge degrees of freedom decouple. We consider both sectors separately:

- Charge excitations, Hamiltonian H_ρ. This Hamiltonian has exactly the same form as that for spinless problem, Eq. (7.58) but with $g \mapsto 2g$. We thus have the following spectrum of charge density excitations:

$$\omega = u_\rho |q| , \qquad u_\rho = \sqrt{\left(v_F + \frac{g}{\pi}\right)^2 - \left(\frac{g}{\pi}\right)^2} , \tag{7.79}$$

  and the constant K in the charge sector

$$K_\rho = \left(1 + \frac{2g}{\pi v_F}\right)^{-1/2} . \tag{7.80}$$

- Spin excitations, Hamiltonian H_σ. This Hamiltonian is identical to that of spinless problem without interaction. Therefore, we find in the spin sector

$$\omega = u_\sigma |q| , \qquad u_\sigma = v_F , \tag{7.81}$$

$$K_\sigma = 1 . \tag{7.82}$$

Remarkably, due to interaction, the charge and spin excitations fully decouple and have different dynamics—the phenomenon known as **spin-charge separation**. If we create some local perturbation (hump) of electron density (which carry both charge and spin) around a point $x = 0$ and then let it evolve starting from time $t = 0$, it will split in charge and spin

perturbations propagating with different velocities. Specifically, at time t we will have peaks of charge density around $\pm v_\rho t$ and of spin density around $\pm v_\sigma t$.

More generally, we can consider a model with several interaction parameters:

$$H_{\rm int} = H_2 + H_4\,, \tag{7.83}$$

$$H_2 = \frac{1}{2}\int dx \sum_\alpha \sum_{s=\uparrow,\downarrow} \left[g_{2\parallel}\ \varrho_{\alpha,s}\varrho_{-\alpha,s} + g_{2\perp}\ \varrho_{\alpha,s}\varrho_{-\alpha,-s}\right], \tag{7.84}$$

$$H_4 = \frac{1}{2}\int dx \sum_\alpha \sum_{s=\uparrow,\downarrow} \left[g_{4\parallel}\ \varrho_{\alpha,s}\varrho_{\alpha,s} + g_{4\perp}\ \varrho_{\alpha,s}\varrho_{\alpha,-s}\right]. \tag{7.85}$$

Here, in analogy with the spinless case, see Eq. (7.5), H_4 describes interaction of fermions on the same chiral branch, while H_2 the scattering of fermions from different branches. In addition, the subscript $\parallel$ corresponds to interaction of fermions with the same spin, and $\perp$ to that of fermions with opposite spins. Repeating the analysis, one finds again the spin-charge separation, with each sector described by the theory of the same form as that for spinless problem. The corresponding parameters are:

$$u_\rho = \left[\left(v_F + \frac{g_{4\parallel}+g_{4\perp}}{2\pi}\right)^2 - \left(\frac{g_{2\parallel}-g_{2\perp}}{2\pi}\right)^2\right]^{1/2}, \tag{7.86}$$

$$K_\rho = \left[\frac{v_F + (g_{4\parallel}+g_{4\perp}-g_{2\parallel}-g_{2\perp})/2\pi}{v_F + (g_{4\parallel}+g_{4\perp}+g_{2\parallel}+g_{2\perp})/2\pi}\right]^{1/2}, \tag{7.87}$$

$$u_\sigma = \left[\left(v_F + \frac{g_{4\parallel}-g_{4\perp}}{2\pi}\right)^2 - \left(\frac{g_{2\parallel}+g_{2\perp}}{2\pi}\right)^2\right]^{1/2}, \tag{7.88}$$

$$K_\sigma = \left[\frac{v_F + (g_{4\parallel}-g_{4\perp}-g_{2\parallel}+g_{2\perp})/2\pi}{v_F + (g_{4\parallel}-g_{4\perp}+g_{2\parallel}-g_{2\perp})/2\pi}\right]^{1/2}. \tag{7.89}$$

It is seen that in the general case also the Luttinger-liquid constant in the spin sector, K_σ, is different from unity.

In full analogy with the spinless case, Eqs. (7.60) and (7.61), one can make a transformation to the fields ϕ_ρ, θ_ρ in the charge sector and to the fields ϕ_σ, θ_σ in the spin sector. Then in each of the sectors the Hamiltonian will take the form (7.67), with the corresponding parameters given by Eqs. (7.86) – (7.89).

7.5 Concept of Luttinger liquid

The concept of Luttinger liquid was introduced by Haldane. It plays the role analogous to the concept of Fermi liquid for higher-dimensional systems. Let us comment on this point.

The Fermi liquid state is characterized by the renormalized Fermi velocity v_F^* and the quasiparticle interaction function $f(\mathbf{p},\mathbf{p}')$. For weak interactions, we were able to calculate them perturbatively, see Sec. 3.12. However, the concept of Fermi liquid is more general and holds also for strong interactions. In that case, the Fermi liquid parameters v_F^* and $f(\mathbf{p},\mathbf{p}')$ cannot be calculated analytically and should be considered as phenomenological parameters. They can be measured experimentally, at least in principle.

The situation with the Luttinger liquid state in 1D interacting systems is analogous. Above, we have derived the bosonic theory characterized by two parameters u and K for spinless particles and by four parameters u_ρ, K_ρ, u_σ, K_σ for spinful particles starting from a model

with linear spectrum (Luttinger model). In this situation, the parameters of the theory were calculated analytically, for any strength of the interaction g. However, in a realistic situation, the spectrum of fermions is not linear (e.g., it is $\varepsilon_k = k^2/2m - \mu$ in the absence of lattice). In that case, the calculation of parameters u and K is still controllable if the interaction is weak $g/v_F \ll 1$. However, if the interaction is strong $g/v_F \gtrsim 1$ and the fermionic spectrum is curved, the calculation of parameters is not controllable any more. Nevertheless, the system is still in the Luttinger liquid state (precisely in the same way as a strongly-interacting 3D system may be in Fermi-liquid state). However, the Luttinger-liquid parameters u and K (or u_ρ , K_ρ , u_σ , K_σ in the spinful case) should be now considered as phenomenological parameters.

7.6 Fermionic operators in the bosonized form

Let us summarize where we stand now. We have reformulated the Hamitlonian of the theory in the bosonized form — in terms of density operators. This has allowed us to identify the collective bosonic excitations and to calculate their spectrum. This is sufficient if one wants to calculate, e.g., the density response of a Luttinger liquid. However, for many observables it is not sufficient, since one needs to calculate the single-fermion Green's function. This is needed if one studies, e.g., the tunneling density of states or the effect of impurities in a Luttinger liquid. To calculate the fermion Green's function, we have to be able to express the fermionic operator in the bosonized language. We are now going to derive this formula, which is one of central formulas of the bosonization theory.

We use the logic analogous to the one used above for the derivation of the bosonized form of H_0. Let us calculate the commutator of the fermionic creation operator (on the chiral branch α) with the corresponding density operator:

$$[\varrho_\alpha(x), \psi_\alpha^\dagger(x')] = [\psi_\alpha^\dagger(x)\psi_\alpha(x), \psi_\alpha^\dagger(x')] = \psi_\alpha^\dagger(x)\{\psi_\alpha(x), \psi_\alpha^\dagger(x')\} = \delta(x-x')\psi_\alpha^\dagger(x)\,, \qquad (7.90)$$

where we used the anticommutation relations for the fermionic operators. We now want to identify the bosonic expression for $\psi_\alpha^\dagger$ using Eq. (7.90) which tells us that its commutator with ρ_α yields again $\psi_\alpha^\dagger$.

For this purpose, let us first look at the analogous problem for the case of a system with just one degree of freedom: the coordinate $\hat{q}$ (and the conjugate momentum $p = -i\frac{\partial}{\partial q}$). Imagine that we want to find an operator $\hat{\mathcal{O}}$ satisfying

$$[\hat{q}, \hat{\mathcal{O}}] = \hat{\mathcal{O}}\,. \qquad (7.91)$$

Rewriting this formula, we get

$$\hat{q}\hat{\mathcal{O}} = \hat{\mathcal{O}}(\hat{q}+1) \qquad \Longrightarrow \qquad \hat{\mathcal{O}}^{-1}\hat{q}\hat{\mathcal{O}} = \hat{q}+1\,. \qquad (7.92)$$

The solution is well known:

$$\hat{\mathcal{O}} = \exp\left(-\frac{\partial}{\partial q}\right) = \exp(-i\hat{p}) \qquad (\times \text{ const})\,, \qquad (7.93)$$

which is a manifestation of the fact that the momentum is the generator of translations.

Therefore, the solution of Eq. (7.90) is exponential of the operator canonically conjugate to $\psi_\alpha^\dagger$ (times i). To identify such operator, we recall the commutation relations between the density operators, Eq. (7.59),

$$[\varrho_\alpha(x), \varrho_{\alpha'}(x')] = \delta_{\alpha\alpha'}\frac{\alpha}{2\pi i}\frac{\partial}{\partial x}\delta(x-x')\,. \qquad (7.94)$$

Let us define the fields $\phi_\alpha(x)$ via

$$\phi_\alpha(x) = 2\pi\alpha \int_{-\infty}^{x} \varrho_\alpha(x')\, dx' \,. \tag{7.95}$$

Then we have

$$[\varrho_\alpha(x), \phi_\alpha(x')] = i\delta(x - x') \,, \tag{7.96}$$

which are the required canonical commutation relations. Thus,

$$\psi_\alpha^\dagger(x) = A\, U_\alpha^\dagger \, \exp\left[-i\alpha k_F x - i\phi_\alpha(x)\right] \,, \tag{7.97}$$

where A is a constant prefactor to be specified below. The factor $e^{i\alpha k_F x}$ corresponds to the constant background density $\varrho_\alpha^{(0)} = k_F/2\pi$ of right- and left-movers. We recall that the density $\varrho_\alpha(x)$ in Eq. (7.95) is the fluctuating density on top of this background, see Eq. (7.57) and the comment below it. We have further included ladder operators $U_\alpha^\dagger$ that raise or lower the overall fermion number (so-called Klein factors), which are needed to make this identity exact (but will be of no importance in the rest of this chapter); we will give a definition of these operators below. Using Eqs. (7.60) and (7.61), we can express the exponent in Eq. (7.97) through the fields $\phi(x)$ and $\theta(x)$:

$$\boxed{\psi_\alpha^\dagger(x) = A\, U_\alpha^\dagger \, \exp\left\{-i\alpha k_F x - i[\theta(x) - \alpha\phi(x)]\right\}.} \tag{7.98}$$

The hermitian conjugate of this identity yields the bosonized representation of ψ_α:

$$\boxed{\psi_\alpha(x) = A\, U_\alpha \, \exp\left\{i\alpha k_F x + i[\theta(x) - \alpha\phi(x)]\right\}.} \tag{7.99}$$

Now we briefly comment on the Klein factors $U_\alpha^\dagger$. The operator $\psi_\alpha^\dagger$ in the l.h.s. of Eq. (7.98) clearly increases the total number of fermions N_α in the α chiral branch by one. On the other hand, the bosonic operators $\theta(x)$ and $\phi(x)$ (and thus any function of them) do not change the total number of fermions. Therefore, to make Eq. (7.98) a true operator identity, one has to include ladder operators that modify appropriately the total number of fermions:

$$\begin{aligned} U_+^\dagger \, |N_+,\, N_-\rangle &= |N_+ + 1,\, N_-\rangle \,, \\ U_-^\dagger \, |N_+,\, N_-\rangle &= |N_+,\, N_- + 1\rangle \,, \\ U_\alpha U_\alpha^\dagger = U_\alpha^\dagger U_\alpha &= 1 \,. \end{aligned} \tag{7.100}$$

The operators U_α, $U_\alpha^\dagger$ commute with all bosonic operators ϕ, θ. In order to guarantee the anticommutation relations between fermionic operators on different chiral branches, one also requires anticommutation of the corresponding Klein factors:

$$\{U_\alpha, U_{\alpha'}\} = \{U_\alpha^\dagger, U_{\alpha'}^\dagger\} = \{U_\alpha^\dagger, U_{\alpha'}\} = 0 \qquad \text{for} \quad \alpha \neq \alpha' \,. \tag{7.101}$$

It can be checked by using the commutation relations for bosonic fields θ and ϕ that the fermionic operators defined by Eq. (7.98) satisfy the required anticommutation relations

$$\{\psi_\alpha(x), \psi_\alpha(x')\} = \{\psi_\alpha^\dagger(x), \psi_\alpha^\dagger(x')\} = 0 \,. \tag{7.102}$$

Further, by calculating the anticommutator $\{\psi_\alpha^\dagger(x), \psi_\alpha(x')\}$, one fixes the value of the constant A in Eq. (7.98):

$$A = \frac{1}{\sqrt{2\pi\lambda}} \,, \tag{7.103}$$

where λ is the ultraviolet (short-distance) cutoff length. The necessity to introduce the ultraviolet cutoff in the theory was already discussed above ($\lambda \sim u/\Lambda$, where Λ is the energy-space UV cutoff). On a formal level, λ is introduced in the Fourier-expansion formulas:

$$\left.\begin{matrix}\phi(x)\\ \theta(x)\end{matrix}\right\} = \frac{i\pi}{L}\sum_{q\neq 0}\frac{1}{q}\, e^{-iqx}\left[\mp\varrho_+(q) - \varrho_-(q)\right] e^{-|q|\lambda/2}\,. \tag{7.104}$$

Physically, λ can be determined, e.g., by the lattice constant or by a non-zero interaction range. The fact that $A \sim \lambda^{-1/2}$ is clear from dimensional reasons: the fermionic operator $\psi(x)$ in 1D should have the dimension $(\text{length})^{-1/2}$. We will also confirm this value of A below by checking that Eq. (7.98) with (7.103) reproduces correctly the Green function of free fermions.

7.7 Fermionic Green's function

In this section we calculate, by using the bosonization formalism, the fermionic Green's function. This will allow us to determine several key physical properties of the Luttinger liquid.

In the context of Luttinger-liquid theory, it turns out to be more convenient to explore Green's functions not in the energy-momentum (p,ω) space but rather in real space (x,t). We thus start from writing down the free-fermion Green's function of the Luttinger model in the (x,t) space. This will later serve as a very useful benchmark for the bosonization theory, which should reproduce the free-fermion theory when one sets the interaction $g = 0$, i.e. $u = v_F$ and $K = 1$.

7.7.1 Green functions of free fermions in 1D with linear spectrum

It is convenient to define

$$G^{>}_{\alpha}(t,x) = -i\langle\psi_\alpha(x,t)\psi^\dagger_\alpha(0,0)\rangle\,, \tag{7.105}$$

$$G^{<}_{\alpha}(t,x) = i\langle\psi^\dagger_\alpha(0,0)\psi_\alpha(x,t)\rangle\,. \tag{7.106}$$

The conventional (causal) Green function is in these notations

$$G_\alpha(t,x) \equiv -i\langle\mathcal{T}\psi_\alpha(x,t)\psi^\dagger_\alpha(0,0)\rangle = \Theta(t)G^{>}_{\alpha}(t,x) + \Theta(-t)G^{<}_{\alpha}(t,x)\,. \tag{7.107}$$

Let us focus below on right movers for definiteness. We have [see Eq. (3.73)] for the functions $G^{>}_{+}$ and $G^{<}_{+}$ at $T = 0$ in the (p,t) space:

$$G^{>}_{+}(t,p) = -ie^{-iv(p-p_F)t}\,\Theta(p-p_F)\,, \tag{7.108}$$

$$G^{<}_{+}(t,p) = ie^{-iv(p-p_F)t}\,\Theta(-p+p_F)\,, \tag{7.109}$$

where $v \equiv v_F$, and we used the linearized spectrum of the Luttinger model, $\epsilon_p = v(p-p_F)$. Performing the Fourier transformation $p \longrightarrow x$, we get

$$G^{>}_{+}(t,x) = \int\frac{dp}{2\pi}e^{ipx}G^{>}_{+}(t,p) = e^{ip_Fx}\,\frac{1}{2\pi}\,\frac{1}{x-vt+i0}\,, \tag{7.110}$$

where $+i0$ is required by the convergence of the p integral. When considered as a function of complex time t, the function $G^{>}_{+}(t,x)$ is analytic (has no singularities) in the lower half-plane, $\mathrm{Im}\,t < 0$. Similarly,

$$G^{<}_{+}(t,x) = e^{ip_Fx}\,\frac{1}{2\pi}\,\frac{1}{x-vt-i0}\,. \tag{7.111}$$

Combining these two formulas, we get, according to Eq. (7.107),

$$G_+(t,x) = e^{ip_F x}\,\frac{1}{2\pi}\,\frac{1}{x - vt + i0\,\mathrm{sign}\,t}\,. \tag{7.112}$$

The corresponding formulas for left-movers are obtained by replacing $p \mapsto -p$ in the (p,t) representation and $x \mapsto -x$ in the (x,t) representation.

Calculating the density $n_\alpha = -iG^<_\alpha(0,0)$, we see that it is infinite according to Eq. (7.111). This is not surprising since these formulas have been written for a system with linear spectrum and without cutoff. In the presence of the ultraviolet cutoff represented by the short-scale cutoff length λ, these formulas get modified according to $i0 \mapsto i\lambda$; in particular, Eq. (7.112) becomes

$$G_+(t,x) = e^{ip_F x}\,\frac{1}{2\pi}\,\frac{1}{x - vt + i\lambda\,\mathrm{sign}\,t}\,. \tag{7.113}$$

The density is then $n_\alpha = 1/2\pi\lambda$, i.e. λ^{-1} plays the role of k_F.

7.7.2 Bosonic functional integral formulation of Luttinger-liquid theory

We reformulate the Luttinger liquid theory using the functional-integral formalism developed in Chapter 6. We can start directly from Eq. (7.67) for the Hamiltonian expressed in terms of the field $\phi(x)$ and its canonically conjugate momentum $\Pi(x) = (1/\pi)\partial_x\theta(x)$. The partition function Z is then

$$Z = \int \mathcal{D}\phi\,\mathcal{D}\theta\,\exp[-S]\,, \tag{7.114}$$

where the (Matsubara) action reads

$$S[\theta,\phi] = \int d\tau dx\left\{-\frac{i}{\pi}\partial_x\theta\,\partial_\tau\phi + \frac{1}{2\pi}\left[uK(\partial_x\theta)^2 + \frac{u}{K}(\partial_x\phi)^2\right]\right\}. \tag{7.115}$$

The action is quadratic with respect to the fields ϕ, θ, which reflects the fact that we deal with a free bosonic theory. The Green functions are obtained as functional integrals with the weight e^{-S} determined by this action:

$$\begin{aligned}\langle \mathcal{T}_\tau \mathcal{O}_1(\tau_1)\mathcal{O}_2(\tau_2)\rangle &= \frac{1}{Z}\int \mathcal{D}\phi\,\mathcal{D}\theta\;\mathcal{O}_1(\phi(\tau_1),\theta(\tau_1))\;\mathcal{O}_2(\phi(\tau_2),\theta(\tau_2))\exp[-S]\\ &\equiv \langle \mathcal{O}_1(\phi(\tau_1),\theta(\tau_1))\;\mathcal{O}_2(\phi(\tau_2),\theta(\tau_2))\rangle\,.\end{aligned} \tag{7.116}$$

Note that in the l.h.s. of (7.116) the symbol $\langle\ldots\rangle$ means the quantum-mechanical average at equilibrium (over the ground state at $T=0$), while in the last expression $\langle\ldots\rangle$ means averaging in the sense of functional integral with the weight e^{-S}.

If $\mathcal{O}_1$, $\mathcal{O}_2$ depend only on the ϕ field and do not depend on θ, one can integrate e^{-S} over θ and to get the action $S[\phi]$ depending only on ϕ fields:

$$\int \mathcal{D}\theta\;\exp\{-S[\theta,\phi]\} = \exp\{-S[\phi]\}\;\times \mathrm{const}\,, \tag{7.117}$$

with

$$S[\phi] = \frac{1}{2\pi uK}\int d\tau dx\left[(\partial_\tau\phi)^2 + u^2(\partial_x\phi)^2\right]. \tag{7.118}$$

Similarly,

$$\int \mathcal{D}\phi\;\exp\{-S[\theta,\phi]\} = \exp\{-S[\theta]\}\;\times \mathrm{const}\,, \tag{7.119}$$

with

$$S[\theta] = \frac{K}{2\pi u}\int d\tau dx\left[(\partial_\tau\theta)^2 + u^2(\partial_x\theta)^2\right] . \tag{7.120}$$

Note that equations (7.118) and (7.120) demonstrate an emergent invariance of the theory (at $T = 0$) with respect to rotations in $(x, u\tau)$ plane. It corresponds to the "Lorentz invariance" in (x, ut) plane, where t is the real time, with u playing a role of the "light velocity"

The action $S[\theta, \phi]$ in the (q, ω) space:

$$\begin{aligned} S &= \frac{1}{2\pi}\int \frac{dq\, d\omega}{(2\pi)^2}\ \begin{pmatrix}\phi & \theta\end{pmatrix}_{-q,-\omega}\begin{pmatrix}(u/K)q^2 & iq\omega\\ iq\omega & uKq^2\end{pmatrix}\begin{pmatrix}\phi\\ \theta\end{pmatrix}_{q,\omega} \\ &= \frac{1}{2}\int \frac{dq\, d\omega}{(2\pi)^2}\ \begin{pmatrix}\phi & \theta\end{pmatrix}_{-q,-\omega} M_{q,\omega}\begin{pmatrix}\phi\\ \theta\end{pmatrix}_{q,\omega}, \qquad M_{q,\omega} = \frac{1}{\pi}\begin{pmatrix}(u/K)q^2 & iq\omega\\ iq\omega & uKq^2\end{pmatrix}. \end{aligned} \tag{7.121}$$

This is written in the limit $T \to 0$, when the Matsubara summation can be replaced by integration. For finite T, one should consider ω in Eq. (7.121) as bosonic Matsubara frequency ω_n and replace $\int(d\omega/2\pi)$ by $T\sum_{\omega_n}$. The correlation functions will be determined by the inverse of the matrix $M_{q,\omega}$, which reads

$$M^{-1}_{q,\omega} = \frac{\pi}{u^2q^2 + \omega^2}\begin{pmatrix}uK & -i\omega/q\\ -i\omega/q & u/K\end{pmatrix}. \tag{7.122}$$

7.7.3 Evaluation of fermionic Green's function via bosonic functional integral

Using the bosonized representation of the fermionic operator, Eq. (7.98), the (Matsubara) fermionic Green function is given by

$$\begin{aligned} \mathscr{G}_+(x,\tau) &= -\langle \mathcal{T}_\tau \psi_+(x,\tau)\psi^\dagger_+(0,0)\rangle \\ &= -\frac{1}{2\pi\lambda}e^{ik_Fx}\left\langle \mathcal{T}_\tau \exp\left\{i[\theta(x,\tau) - \phi(x,\tau)]\right\}\exp\left\{-i[\theta(0,0) - \phi(0,0)]\right\}\right\rangle . \end{aligned} \tag{7.123}$$

(We focus on the Green function of right-movers for definiteness.) This can be rewritten, according to Eq. (7.116), in terms of a functional integral:

$$\mathscr{G}_+(x,\tau) = -\frac{1}{2\pi\lambda}e^{ik_Fx}\left\langle \exp\left\{i[\theta(x,\tau) - \phi(x,\tau)]\right\}\exp\left\{-i[\theta(0,0) - \phi(0,0)]\right\}\right\rangle , \tag{7.124}$$

where $\langle \ldots \rangle$ means functional averaging with the weight e^{-S} and the action $S[\theta, \phi]$ given by Eq. (7.115).

The crucial point that allows us to evaluate this integral exactly is that it is of Gaussian type: the action is quadratic with respect to the fields and the expression under $\langle \ldots \rangle$ is exponential of a functional that is linear in the fields. We recall Eq. (6.44) for the Gaussian integral (in real version),

$$\int d(\mathbf{x})\, e^{-\frac{1}{2}\mathbf{x}^T A\mathbf{x} + \boldsymbol{J}^T\mathbf{x}} = \frac{(2\pi)^{N/2}}{(\det A)^{1/2}}\, e^{\frac{1}{2}\boldsymbol{J}^T A^{-1}\boldsymbol{J}} , \tag{7.125}$$

which can be rewritten as

$$\langle e^{\boldsymbol{J}^T\mathbf{x}}\rangle = e^{\frac{1}{2}\boldsymbol{J}^T A^{-1}\boldsymbol{J}} \,. \tag{7.126}$$

On the other hand,

$$\langle x_k x_l\rangle = (A^{-1})_{kl} \,. \tag{7.127}$$

Therefore,

$$\boxed{\left\langle \exp\left\{\boldsymbol{J}^T\mathbf{x}\right\}\right\rangle = \exp\left\{\frac{1}{2}\left\langle(\boldsymbol{J}^T\mathbf{x})^2\right\rangle\right\} \,.} \tag{7.128}$$

In application to the average for the Green's function, Eq. (7.124), this yields

$$\mathscr{G}_+(x,\tau) = -\frac{1}{2\pi\lambda}e^{ik_F x}\exp\left\{-\frac{1}{2}\left\langle[\theta(x,\tau)-\phi(x,\tau)-\theta(0,0)+\phi(0,0)]^2\right\rangle\right\}. \tag{7.129}$$

Using the fact that $\langle\phi^2(x,\tau)\rangle = \langle\phi^2(0,0)\rangle$ (and similarly for $\langle\theta^2\rangle$ and $\langle\phi\theta\rangle$) in view of the translational invariance of the theory, we rewrite this formula as follows:

$$\mathscr{G}_+(x,\tau) = -\frac{1}{2\pi\lambda}e^{ik_F x}\exp\left[\mathcal{B}_{\phi\phi}(x,\tau)+\mathcal{B}_{\theta\theta}(x,\tau)-2\mathcal{B}_{\phi\theta}(x,\tau)\right] \,, \tag{7.130}$$

where

$$\mathcal{B}_{\phi\phi}(x,\tau) = \langle\phi(x,\tau)\phi(0,0)-\phi^2(0,0)\rangle \,, \tag{7.131}$$

$$\mathcal{B}_{\theta\theta}(x,\tau) = \langle\theta(x,\tau)\theta(0,0)-\theta^2(0,0)\rangle \,, \tag{7.132}$$

$$\mathcal{B}_{\phi\theta}(x,\tau) = \langle\phi(x,\tau)\theta(0,0)-\phi(0,0)\theta(0,0)\rangle \,. \tag{7.133}$$

Let us emphasize a remarkable character of Eq. (7.130): **the fermionic Green's function of the Luttinger model is given (up to a certain prefactor) by an exponential of the Green's function of free bosons!**

It remains to calculate the bosonic correlation functions. In the (q,ω) representation they are immediately given by the matrix M^{-1}, Eq. (7.122), according to the properties of Gaussian integrals, Eq. (7.127). We only have to perform the Fourier transformation. Let us do it for $\mathcal{B}_{\phi\phi}(x,\tau)$, focussing on the limit $T=0$ (when the Matsubara summation becomes an integral). We have

$$\mathcal{B}_{\phi\phi}(x,\tau) = \int\frac{dq\,d\omega}{(2\pi)^2}\,\frac{\pi uK}{u^2q^2+\omega^2}\left(e^{iqx-i\omega\tau}-1\right)e^{-\lambda|q|} \,, \tag{7.134}$$

where we have taken into account the UV cutoff length λ by including a factor that cuts momenta above $1/\lambda$ according to Eq. (7.104). It is instructive to rewrite this formula by introducing the two-component "relativistic" momentum $\mathbf{P} = (P_0, P_1) = (\omega, uq)$:

$$\mathcal{B}_{\phi\phi}(x,\tau) = K\int\frac{dP_0\,dP_1}{4\pi}\,\frac{1}{\mathbf{P}^2}\left(e^{-iP_0\tau+iP_1x/u}-1\right)e^{-(\lambda/u)|P_1|} \,. \tag{7.135}$$

We see that in a broad range of P the integral is logarithmic: it is of the type

$$-K\int\frac{dP_0\,dP_1}{4\pi}\,\frac{1}{\mathbf{P}^2} = -\frac{K}{4}\int\frac{d(P^2)}{P^2} \,. \tag{7.136}$$

The logarithmic behavior is bounded on the ultraviolet (large P) side by $P^2\sim(\lambda/u)^{-2}$ due to the regularization and at the infrared (small P) side by $P^2\sim(\tau^2+x^2/u^2)^{-1}$. Therefore, we have

$$\mathcal{B}_{\phi\phi}(x,\tau) \simeq -\frac{K}{4}\ln\frac{x^2+u^2\tau^2}{\lambda^2} \,. \tag{7.137}$$

Equation (7.137) demonstrates once more importance of introducing the UV cutoff λ. This is the leading behavior when the logarithm is large; an exact calculation yields

$$\mathcal{B}_{\phi\phi}(x,\tau) = -\frac{K}{4}\ln\frac{x^2+(u|\tau|+\lambda)^2}{\lambda^2}\,. \tag{7.138}$$

The result (7.138) is a manifestation of the fact that the correlation function of a free massless boson field is logarithmic (in coordinate space) in $1+1=2$ dimensions. The coefficient in front of the logarithm depends on the coupling constant K. Since the fermionic Green function is an exponential of the bosonic one, we can already foresee that remarkable consequence: **the Green's function of fermions will show a power-law dependence, with an exponent depending on the interaction strength.**

To complete the calculation, we still need the correlation functions $\mathcal{B}_{\theta\theta}(x,\tau)$ and $\mathcal{B}_{\phi\theta}(x,\tau)$. As is clear from Eq. (7.122) (or, equivalently from a comparison of Eqs. (7.118) and (7.120)), the first of them differs from $\mathcal{B}_{\phi\phi}(x,\tau)$ only by a replacement $K \mapsto K^{-1}$:

$$\mathcal{B}_{\theta\theta}(x,\tau) = -\frac{1}{4K}\ln\frac{x^2+(u|\tau|+\lambda)^2}{\lambda^2}\,. \tag{7.139}$$

The correlation function $\mathcal{B}_{\phi\theta}(x,\tau)$ is given by

$$\mathcal{B}_{\phi\theta}(x,\tau) = \int \frac{dq\,d\omega}{(2\pi)^2}\,\frac{-i\omega/q}{u^2q^2+\omega^2}\left(e^{iqx-i\omega\tau}-1\right)e^{-\lambda|q|}\,, \tag{7.140}$$

This integral does not produce a big logarithm cut off by λ: such a contribution vanishes since the factor $-i\omega/q$ is odd with respect to ω and q. For this reason, the contribution of the correlation function $\mathcal{B}_{\phi\theta}(x,\tau)$ will be of no importance for the scaling of such observables like the tunneling density of states (calculated below). Still, it is needed to get the exact formula for the Green function. We omit technical details of the evaluation of the integral in Eq. (7.140) and present the result:

$$\mathcal{B}_{\phi\theta}(x,\tau) = -\frac{i}{2}\mathrm{Arg}(-ix+u\tau+\lambda\,\mathrm{sign}\,\tau) = -\frac{1}{4}\ln\frac{ix+u\tau+\lambda\,\mathrm{sign}\,\tau}{-ix+u\tau+\lambda\,\mathrm{sign}\,\tau}\,. \tag{7.141}$$

Substituting Eqs. (7.138), (7.139), and (7.141) in Eq. (7.130), we obtain

$$\begin{aligned}\mathscr{G}_+(x,\tau) &= -\frac{1}{2\pi\lambda}e^{ik_Fx}\left[\frac{\lambda^2}{x^2+(u|\tau|+\lambda)^2}\right]^{(K+K^{-1})/4}\left(\frac{ix+u\tau+\lambda\,\mathrm{sign}\,\tau}{-ix+u\tau+\lambda\,\mathrm{sign}\,\tau}\right)^{1/2}\\ &= -\frac{i}{2\pi}e^{ik_Fx}\frac{\lambda^\gamma}{(x+iu\tau+i\lambda\,\mathrm{sign}\,\tau)^{1+\gamma/2}(x-iu\tau-i\lambda\,\mathrm{sign}\,\tau)^{\gamma/2}}\,,\end{aligned} \tag{7.142}$$

where we have defined

$$\boxed{\gamma = \frac{K+K^{-1}-2}{2}\,.} \tag{7.143}$$

Performing an analytical continuation $\tau \to it$, we obtain from this Matsubara Green function the real-time Green function (we take into account an additional factor i in the definition of the latter):

$$\boxed{G_+(x,t) = \frac{1}{2\pi}e^{ik_Fx}\frac{\lambda^\gamma}{(x-ut+i\lambda\,\mathrm{sign}\,t)^{1+\gamma/2}(x+ut-i\lambda\,\mathrm{sign}\,t)^{\gamma/2}}\,.} \tag{7.144}$$

The shift of the singularities to the complex plane is determined by analytical properties of the Green function as a function of complex variable t, see Sec. 7.7.1.

Equation (7.144) is the final result for the fermionic Green function (at zero T). Let us analyze it. First, consider the non-interacting case, $g = 0$. In this case, $u = v$ and $K = 1$. Equation (7.143) yields then $\gamma = 0$. Therefore, we see that Eq. (7.144) reproduces correctly the Green's function of free fermions, Eq. (7.113). Now return to the interacting case, when $K \neq 1$. Then, according to Eq. (7.143), the index $\gamma > 0$. Therefore, instead of a single pole at $x = vt$, the Green's function exhibits power-law singularities at $x = \pm ut$ with exponents depending on the interaction strength.

7.7.4 Distribution of particles over momenta

We use the result for the Green function to calculate the distribution of particles in the Fermi liquid over momenta.

$$n_+(p) = -i \int dx\, e^{-ipx} G_+(x, t = -0) = -\frac{i}{2\pi} \int dx\, e^{-i(p-p_F)x} \frac{\lambda^\gamma}{(x - i\lambda)^{1+\gamma/2}(x + i\lambda)^{\gamma/2}}. \quad (7.145)$$

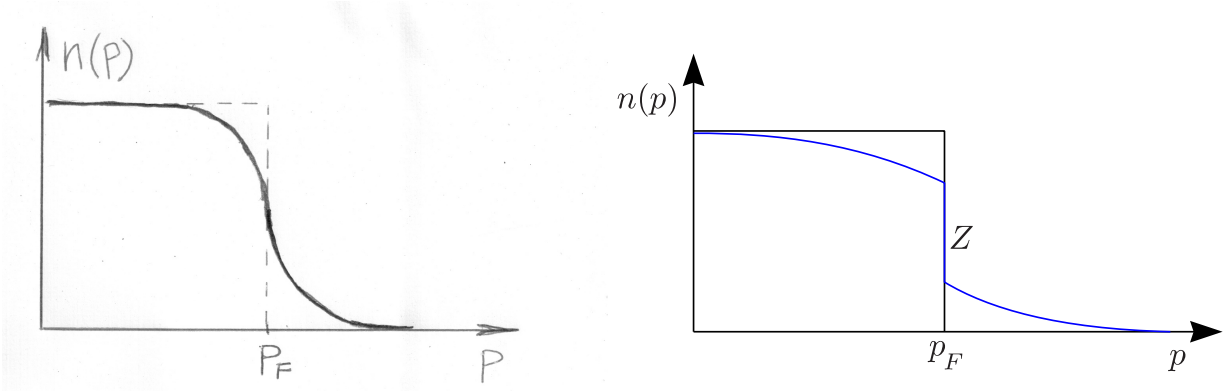
We subtract $n_+(p_F)$. After this, the ultraviolet regularization is not needed, since the integral converges anyway at small x:

$$n_+(p) - n_+(p_F) = -\frac{i}{2\pi} \int dx \left(e^{-i(p-p_F)x} - 1\right) \frac{\lambda^\gamma}{x^{1+\gamma}}\,. \quad (7.146)$$

The integral can be estimated (up to a numerical prefactor) by dimensional analysis, yielding

$$n_+(p) - n_+(p_F) \sim -\,\mathrm{sign}(p - p_F)\lambda^\gamma |p - p_F|^\gamma\,. \quad (7.147)$$

Thus, $n(p)$ is continuous at $p = p_F$ (shown schematically in the left figure below), in contrast to the Fermi liquid, where it has a jump of height Z (right figure). This is in full consistency with our earlier perturbative analysis that suggested that $Z = 0$ in the interacting 1D system. Now we see that $n(p)$ in the Luttinger liquid is continuous but shows a power-law singularity at $p = p_F$, with the index γ given by Eq. (7.143).



7.7.5 Tunneling density of states

A closely related quantity is the tunneling density of states.

$$\nu_+(\epsilon) = -\frac{1}{\pi}\mathrm{Im}\, G^R_+(0, \epsilon) = -\frac{1}{\pi}\mathrm{Im} \int dt\, e^{i\epsilon t}\, G^R_+(x = 0, t)\,, \quad (7.148)$$

where G^R is the retarded Green's function. The retarded function can be calculated in the same way as we calculated the causal Green's function, Eq. (7.144), and shows the same scaling. After the Fourier transformation, the scaling behavior $G^R(0, t) \sim \lambda^\gamma (ut)^{-1-\gamma}$ translates into

$$\nu(\epsilon) \sim \frac{1}{u}\left(\frac{\lambda}{u}\right)^\gamma |\epsilon|^\gamma\,. \quad (7.149)$$

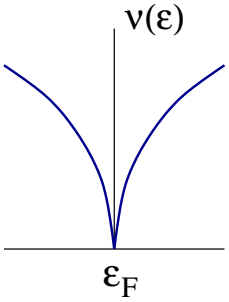
The density of states in the absence of interaction is $\nu_+^{(0)} = 1/2\pi v$. Further, u/λ is the high-energy cutoff Λ (typically of the order of Fermi energy). Thus, we can rewrite Eq. (7.149) as

$$\nu(\epsilon) \sim \nu^{(0)} \left(\frac{|\epsilon|}{\Lambda} \right)^{\gamma} . \tag{7.150}$$

As the name suggests, the tunneling density of states can be observed in experiments on tunneling from a metallic electrode to a Luttinger liquid. Then it determines the dependence of the differential conductance on the bias voltage V:

$$\frac{\partial I}{\partial V} \propto |V|^{\gamma} . \tag{7.151}$$

(Here I is the tunneling current.) The differential conductance is suppressed according to a power law at low voltages. This effect is called **"zero-bias anomaly"**.



All the calculations of the Green's function (and thus of physical observables that it determines) can be extended to the case of a non-zero temperature. Then one should replace intetgration over frequency in Eq. (7.134) for $\mathcal{B}_{\phi\phi}(x,\tau)$ and in analogous formulas for $\mathcal{B}_{\theta\theta}(x,\tau)$ and $\mathcal{B}_{\phi\theta}(x,\tau)$ by a sumattion over Matsubara frequencies. The calculations still can be performed analytically. On a qualitative level, the main result is that T serves as an infrared cutoff: the behavior at distances $\tau, x/u \ll T^{-1}$ remains essentially unchanged, while at larger distances the Green's function becomes exponentially suppressed. In the energy space, this results in the smearing of singularity in $\nu(\epsilon)$ at small energies:

$$\nu(\epsilon, T) \sim \nu^{(0)} \left(\frac{\max(|\epsilon|, T)}{\Lambda} \right)^{\gamma} . \tag{7.152}$$

7.7.6 Generalization to Luttinger liquid with spin

For spinful model, the charge and spin densities were defined in Eq. (7.75). Using them, one introduces the fields ϕ_ρ, θ_ρ in the charge sector and ϕ_σ, θ_σ in the spin sector. Equivalently, one can express them in terms of fields ϕ_s and θ_s for each of the spin components:

$$\phi_\rho = \frac{1}{\sqrt{2}}(\phi_\uparrow + \phi_\downarrow) , \tag{7.153}$$

$$\phi_\sigma = \frac{1}{\sqrt{2}}(\phi_\uparrow - \phi_\downarrow) , \tag{7.154}$$

$$\theta_\rho = \frac{1}{\sqrt{2}}(\theta_\uparrow + \theta_\downarrow) , \tag{7.155}$$

$$\theta_\sigma = \frac{1}{\sqrt{2}}(\theta_\uparrow - \theta_\downarrow) . \tag{7.156}$$

Within the bosonic theory, the spin and charge sectors are decoupled. The Hamiltonian is $H = H_\rho + H_\sigma$, with each of them having the same form as the Hamiltonian for the spinless

model. In the functional integral formalism, the action is correspondingly a sum of S_ρ and S_σ, where each of them has the same form as the action for the spinless model. The charge sector is characterized by the parameters u_ρ and K_ρ, the spin sector by u_σ and K_σ. In the model with one interaction constant g one has $u_\sigma = v$ and $K_\sigma = 1$.

The ρ operators commute with σ operators. Commutation relations within each sector, i.e. for the pair (ϕ_ρ, θ_ρ) as well for the pair $(\phi_\sigma, \theta_\sigma)$ are the same as for (ϕ, θ) of the spinless theory. The expression for the fermionic operator $\psi_{\alpha,s}$ (where $\alpha = \pm$ is the chiral branch index and $s = \uparrow, \downarrow$ the spin index) in terms of these fields is immediately obtained by using Eq. (7.99) for each of the spin components and then performing the transformation (7.156):

$$\boxed{\psi_{\alpha,s}(x) = \frac{1}{\sqrt{2\pi\lambda}} U_{\alpha,s} \exp\left\{ i\alpha k_F x + \frac{i}{\sqrt{2}}[\theta_\rho(x) - \alpha\phi_\rho(x) + s\theta_\sigma(x) - s\alpha\phi_\sigma(x)] \right\}.} \qquad (7.157)$$

Since exponential factors with ρ and σ fields enter Eq. (7.157) multiplicatively and the action S is $S = S_\rho + S_\sigma$, the averaging with e^{-S} decouples in calculation of averages in the charge and spin sectors, which are of exactly the same form as for the spinless model. The formula (7.144) for the Green's function of the spinless model thus becomes in the case of a model with spin

$$G_{+,s}(x,t) = \frac{1}{2\pi} e^{ik_F x} \frac{\lambda^{\gamma_\rho}}{(x - u_\rho t + i\lambda \operatorname{sign} t)^{(1+\gamma_\rho)/2} (x + u_\rho t - i\lambda \operatorname{sign} t)^{\gamma_\rho/2}} \times \frac{\lambda^{\gamma_\sigma}}{(x - u_\sigma t + i\lambda \operatorname{sign} t)^{(1+\gamma_\sigma)/2} (x + u_\sigma t - i\lambda \operatorname{sign} t)^{\gamma_\sigma/2}}, \qquad (7.158)$$

where

$$\gamma_\rho = \frac{K_\rho + K_\rho^{-1} - 2}{4}, \qquad \gamma_\sigma = \frac{K_\sigma + K_\sigma^{-1} - 2}{4}. \qquad (7.159)$$

For the case of $K_\sigma = 1$ we have $\gamma_\sigma = 0$. The additional factor of $1/2$ in Eq. (7.159) in comparison with Eq. (7.143) originates from the factor $1/\sqrt{2}$ in the exponent of Eq. (7.157).

The behavior of the distribution of fermions over momenta $n(p)$ near p_F and of the tunneling density of states $\nu(\epsilon)$ (and correspondingly of the tunneling conductance $\partial I/\partial V$) has the same form as in the spinless case,

$$n_+(p) - n_+(p_F) \sim -\operatorname{sign}(p - p_F) \lambda^\gamma |p - p_F|^\gamma . \qquad (7.160)$$

$$\nu(\epsilon) \sim \nu^{(0)} \left(\frac{|\epsilon|}{\Lambda} \right)^\gamma , \qquad \frac{\partial I}{\partial V} \propto |V|^\gamma , \qquad (7.161)$$

now with the index γ given by

$$\gamma = \gamma_\rho + \gamma_\sigma . \qquad (7.162)$$

7.8 Impurities in a Luttinger liquid

Up to now we considered a clean system. In realistic systems, impurities frequently play an important role. If an impurity induces back-scattering of fermions, it will clearly affect transport properties of a wire (increase its resistance). It turns out that the effect of impurities in Luttinger liquid is highly peculiar: the strength of an impurity becomes strongly renormalized as a function of a wire length or of the temperature. The impurity may become much stronger or weaker depending on the value of the Luttinger-liquid parameter K (i.e. of interaction strength). This is the subject of the present section.

7.8.1 Weak impurity

We consider a spinless Luttinger liquid with the action (7.115). Let us consider a perturbation of this theory by an impurity described by a potential $\mathcal{U}(x)$ localized near a point x_0. For the impurity to produce a substantial back-scattering effect, its characteristic size should be comparable to k_F^{-1}. In the fermionic language, this means adding to the Hamiltonian of the problem a term

$$H_{\rm imp} = \int dx\, \mathcal{U}(x)\psi^\dagger(x)\psi(x)\,, \tag{7.163}$$

where $\psi(x) = \psi_+(x) + \psi_-(x)$ is the total fermionic operator, including right-moving and left-moving contributions. Let us define smooth parts of $\psi_+(x)$ and $\psi_-(x)$ via

$$\psi_+(x) = \psi_{+,\rm sm}(x)\, e^{ik_F x}\,, \qquad \psi_-(x) = \psi_{-,\rm sm}(x)\, e^{-ik_F x}\,. \tag{7.164}$$

The term "smooth" means that the characteristic momenta are much smaller than k_F. Since the impurity is localized on a short scale around the point x_0, we can approximate in Eq. (7.163) the slow factors as $\psi_{+,\rm sm}(x) \simeq \psi_{+,\rm sm}(x_0)$ and $\psi_{-,\rm sm}(x) \simeq \psi_{-,\rm sm}(x_0)$. Thus, Eq. (7.163) takes the form

$$\begin{aligned} H_{\rm imp} \;&\simeq\; \mathcal{U}_{\rm f}\left[\psi^\dagger_{+,\rm sm}(x_0)\psi_{+,\rm sm}(x_0) + \psi^\dagger_{-,\rm sm}(x_0)\psi_{-,\rm sm}(x_0)\right] \\ &+\; \mathcal{U}_{\rm b}\,\psi^\dagger_{+,\rm sm}(x_0)\psi_{-,\rm sm}(x_0) + \mathcal{U}^*_{\rm b}\psi^\dagger_{-,\rm sm}(x_0)\psi_{+,\rm sm}(x_0)\,, \end{aligned} \tag{7.165}$$

where $\mathcal{U}_{\rm f}$ and $\mathcal{U}_{\rm b}$ are $k = 0$ and $k = 2k_F$ Fourier components of $U(x)$, respectively:

$$\mathcal{U}_{\rm f} = \mathcal{U}(k=0) \equiv \int dx\, \mathcal{U}(x)\,, \qquad \mathcal{U}_{\rm b} = \mathcal{U}(k=2k_F) \equiv \int dx\, \mathcal{U}(x) e^{-2ik_F x}\,. \tag{7.166}$$

The subscripts "f" and "b" mean forward and backward scattering, respectively.

The forward-scattering term, which corresponds simply to a spatial variation of the velocity, is of no importance for our consideration. In particular, it does not affect the conductance of a wire. We discard it below and focus on the back-scattering term. The corresponding coefficient $\mathcal{U}_{\rm b}$ is the back-scattering amplitude for fermions. It reduces the conductance of a wire. In particular, for the non-interacting problem, the effect of a single impurity on the conductance g reads (to the leading order in $\mathcal{U}_{\rm b}$)

$$g = \frac{e^2}{h}\left(1 - v_F^{-2}|\mathcal{U}_{\rm b}|^2\right)\,. \tag{7.167}$$

Inserting the bosonized form of the fermionic operators, Eq. (7.99), in the back-scattering part of Eq. (7.165), we get

$$H_{\rm imp} = \frac{1}{2\pi\lambda}\left(U_+^\dagger U_-\, \mathcal{U}_{\rm b}\, e^{2i\phi(x_0)} + U_-^\dagger U_+\, \mathcal{U}^*_{\rm b}\, e^{-2i\phi(x_0)}\right)\,. \tag{7.168}$$

The Klein factors U_+ and U_- will not play any role in the analysis below, so that we omit them:

$$H_{\rm imp} = \frac{1}{2\pi\lambda}\left(\mathcal{U}_{\rm b}\, e^{2i\phi(x_0)} + \mathcal{U}^*_{\rm b}\, e^{-2i\phi(x_0)}\right)\,. \tag{7.169}$$

The formula (7.169) can be straightforwardly generalized to the case of an arbitrary random potential:

$$H_{\rm dis} = \frac{1}{2\pi\lambda}\int dx\, \left(\mathcal{U}_{\rm b}(x)\, e^{2i\phi(x)} + \mathcal{U}^*_{\rm b}(x)\, e^{-2i\phi(x)}\right)\,. \tag{7.170}$$

The impurity-induced contribution (7.169) should be added to the Luttinger-liquid Hamiltonian H. Since $H_{\rm imp}$ is not quadratic in bosonic fields, the resulting theory is not exactly solvable any more. We thus should use an approximate approach. A powerful method that will be very useful in the present context (and in a great variety of other physical problems) is the **renormalization group (RG)**. To formulate it, the functional-integral formalism is most suitable. The action of our problem (with a single impurity) reads

$$S[\phi] = S_0[\phi] + S_{\rm imp}[\phi] = \frac{1}{2\pi u K}\int d\tau dx \left[(\partial_\tau \phi)^2 + u^2(\partial_x \phi)^2\right] + \frac{1}{\pi\lambda}\mathcal{U}\int d\tau \cos(2\phi(x_0,\tau))\,, \tag{7.171}$$

where S_0 is the clean Luttinger-liquid action and $S_{\rm imp} = \int d\tau H_{\rm imp}$ is the impurity contribution. Since the impurity term depends only on ϕ field, we have used the Luttinger-liquid action in the form (7.118), with the θ field integrated out. Also, we have taken $\mathcal{U}_{\rm b}$ to be real, as its phase does not play any role, and omitted the subscript "b". Now, assuming a weak impurity, we can expand the weight e^{-S} with which functional-integral evaluation of any observable is performed:

$$e^{-S[\phi]} = e^{-S_0[\phi]-S_{\rm imp}[\phi]} \approx e^{-S_0[\phi]}\left(1 - S_{\rm imp}[\phi]\right)\,. \tag{7.172}$$

Now assume that the physical observable that we want to calculate corresponds to a certain macroscopic scale L. For example, we are interested in a conductance of a wire of length L (with an impurity somewhere in the middle of the wire). Thus, we are interested in properties of the system (response functions) at a (small) momentum $\sim L^{-1}$. In view of this, we can integrate out all momenta from the ultraviolet cutoff λ^{-1} down to L^{-1}. The renormalization group is a procedure of consecutively integrating out the momenta. This procedure includes the following steps:

Step 1. Integrating out fast fields.

We define a new ultraviolet cutoff: $\lambda \mapsto b\lambda$, with $b > 1$.
According to this, we split the fields in "fast" and"slow":

$$\phi = \phi^> + \phi^<\,, \tag{7.173}$$

where fast fields $\phi^>$ have the two-component momenta $P = (\omega/u, q)$ in the interval $(b\lambda)^{-1} < |P| < \lambda^{-1}$, while slow fields $\phi^<$ have momenta $|P| < (b\lambda)^{-1}$.
The quadratic ("free") part of the action $S_0[\phi]$ is simply

$$S_0[\phi] = S_0[\phi^>] + S_0[\phi^<]\,. \tag{7.174}$$

Now we integrate out fast fields, to obtain the new, effective action for slow fields

$$\begin{aligned}\int \mathcal{D}\phi^> e^{-S[\phi^>,\phi^<]} &= \int \mathcal{D}\phi^> e^{-S_0[\phi^>]-S_0[\phi^<]-S_{\rm imp}[\phi^>,\phi^<]} = e^{-S_0[\phi^<]}\left\langle e^{-S_{\rm imp}[\phi^>,\phi^<]}\right\rangle_{\phi^>} \\ &\simeq e^{-S_0[\phi^<]}\left(1 - \langle S_{\rm imp}[\phi^>,\phi^<]\rangle_{\phi^>}\right)\,,\end{aligned} \tag{7.175}$$

where $\langle\ldots\rangle_{\phi^>}$ means the averaging (functional integration) over $\phi^>$ with the weight $e^{-S_0[\phi^>]}$. We thus have to calculate

$$\begin{aligned}\langle S_{\rm imp}[\phi^>,\phi^<]\rangle_{\phi^>} &= \frac{\mathcal{U}}{\pi\lambda}\int d\tau\ \langle\cos(2\phi(x_0,\tau))\rangle_{\phi^>} = \frac{\mathcal{U}}{\pi\lambda}\int d\tau\,{\rm Re}\,\left\langle e^{2i\phi(x_0,\tau)}\right\rangle_{\phi^>} \\ &= \frac{\mathcal{U}}{\pi\lambda}\int d\tau\,{\rm Re}\,e^{2i\phi^<(x_0,\tau)}\left\langle e^{2i\phi^>(x_0,\tau)}\right\rangle_{\phi^>}\,.\end{aligned} \tag{7.176}$$

The average is a Gaussian integral and thus is easily performed:

$$\left\langle e^{2i\phi^>(x_0,\tau)}\right\rangle_{\phi^>} = \exp\left\{-\frac{1}{2}\,4\,\langle\phi^>(x_0,\tau)\phi^>(x_0,\tau)\rangle_{\phi^>}\right\}\,, \tag{7.177}$$

with

$$\langle \phi^{>}(x_0,\tau)\phi^{>}(x_0,\tau)\rangle_{\phi^{>}} = \int_{(b\lambda)^{-1}<P<\lambda^{-1}} \frac{dq\,d\omega}{(2\pi)^2}\frac{\pi u K}{u^2q^2+\omega^2} = \frac{K}{2}\int_{(b\lambda)^{-1}}^{\lambda^{-1}}\frac{dP}{P} = \frac{K}{2}\ln b\,, \quad (7.178)$$

so that

$$\left\langle e^{2i\phi^{>}(x_0,\tau)}\right\rangle_{\phi^{>}} = b^{-K}\,. \quad (7.179)$$

Thus,

$$\langle S_{\rm imp}[\phi^{>},\phi^{<}]\rangle_{\phi^{>}} = \frac{b^{-K}\mathcal{U}}{\pi\lambda}\int d\tau\,\cos(2\phi^{<}(x_0,\tau))\,. \quad (7.180)$$

This completes the Step 1 of the RG. We still should perform

Step 2. Rescaling.

The resulting theory has, however, the ultraviolet cutoff $b\lambda$, different from the cutoff λ of the original theory. In order to compare them, we should restore the cutoff. This is done by rescaling of coordinates:

$$x/b = x'\,, \qquad \tau/b = \tau'\,. \quad (7.181)$$

In the new coordinates x', τ', the cutoff is again λ. The new fields are

$$\phi'(x',\tau') = \phi^{<}(x,\tau)\,. \quad (7.182)$$

One should also verify that the free action S_0 retains the same form (with the same constant K) as it was originally. In general, this requires a rescaling of fields but in the present case it is not needed (S_0 contains two integrations over x and τ and two derivatives, so that the corresponding powers of b cancel.)

After the rescaling, the impurity action (7.180) takes the form

$$S'_{\rm imp}[\phi'] = \frac{1}{\pi\lambda}\,b^{1-K}\mathcal{U}\int d\tau'\cos(2\phi(x'_0,\tau'))\,. \quad (7.183)$$

It has exactly the same form as the original impurity action, see the second term in Eq. (7.171), with the **renormalized impurity strength**

$$\mathcal{U} \;\mapsto\; \mathcal{U}(b) = b^{1-K}\,\mathcal{U}\,. \quad (7.184)$$

Considering the renormalization factor b as continuously varying, we thus obtain the **RG equation**:

$$\boxed{\frac{d\,\mathcal{U}(b)}{d\ln b} = (1-K)\,\mathcal{U}(b)\,.} \quad (7.185)$$

According to Eq. (7.185), the strength of an impurity gets renormalized in a Luttinger liquid:

- For $K<1$, i.e., for repulsive interaction, the impurity becomes stronger;
- For $K>1$, i.e., for attractive interaction, the impurity becomes weaker.

For $K=1$, i.e., in the absence of interaction, the impurity is not renormalized. This should be so, since the renormalization is due to interaction between fermions.

The underlying physics of renormalization is as follows: the impurity perturbs the density of fermions around it. In an interacting system, fermions are scattered not only by a "dressed impurity" composed by the impurity itself and the cloud of fermionic density that it creates.

When does the renormalization stop? If the temperature is $T = 0$ (as we assumed in the above calculation), then the renormalization is stopped by the length L of the wire. Originally, we have the ultraviolet (UV) cutoff λ and the infrared (IR) cutoff L. Once the fast fields have been integrated out, the UV cutoff becomes $b\lambda$; the IR cutoff is still L. Then we rescale coordinates, such that the UV cutoff returns to its original value λ but the IR cutoff then becomes L/b. Obviously, this will stop at

$$b = L/\lambda\,. \tag{7.186}$$

Thus, the renormalized strength of the impurity will be

$$\mathcal{U}_{\rm ren} = \mathcal{U}(b = L/\lambda) = \left(\frac{L}{\lambda}\right)^{1-K} \mathcal{U}\,. \tag{7.187}$$

In particular, this renormalized value of the impurity strength will enter Eq. (7.167) for the conductance of the wire.

If the temperature is non-zero, then it can also provide an IR cutoff. Indeed, then the integration over τ in the original integral goes over an interval of length $\beta = 1/T$. In units of length, this corresponds to the infrared cutoff length

$$l_T = \frac{u}{T} \tag{7.188}$$

(thermal length). If $L > l_T$, then the RG flow will stopped at $b = l_T/\lambda$, yielding the renormalized impurity strength

$$\mathcal{U}_{\rm ren} = \mathcal{U}(b = l_T/\lambda) = \left(\frac{u}{T\lambda}\right)^{1-K} \mathcal{U}\,. \tag{7.189}$$

The renormalized impurity strength thus depends in this situation on temperature in a power-law way.

All these formulas are valid as long as the impurity remains weak: $\mathcal{U}(b)/u \ll 1$. The opposite limit of a strong barrier will be considered below. But before doing this, we will briefly discuss properties of a Luttinger-liquid system with many weak impurities—a disordered system.

7.8.2 Many impurities: Disordered system

Consider a Luttinger liquid with density $n_{\rm imp}$ of weak scatterers. Each scatterer is characterized by the (bare) back-scattering amplitude $\mathcal{U}$. In the absence of interaction, we would have the Drude conductivity

$$\sigma = e^2 \nu v_F^2 \tau_0\,, \tag{7.190}$$

with the (transport) scattering time τ_0,

$$(\nu\tau_0)^{-1} \sim n_{\rm imp}\mathcal{U}^2\,. \tag{7.191}$$

(The symbol $\sim$ means that we do not keep numerical coefficients.) Renormalization of the impurity strength $\mathcal{U} \mapsto \mathcal{U}(b) = b^{1-K}\mathcal{U}$ therefore implies the renormalization of the scattering time,

$$\tau_0 \mapsto \tau(b) = b^{2(K-1)}\tau_0\,, \tag{7.192}$$

and thus of the conductivity.

Consider first the case when the IR cutoff if provided by temperature (i.e. $u/T < L$). Then the renormalized time is

$$\tau = \tau_0 \left(\frac{T}{\Lambda}\right)^{2(1-K)} , \tag{7.193}$$

where $\Lambda = u/\lambda$ is the UV cutoff in units of energy. This yields the renormalized Drude conductivity

$$\sigma_D(T) = \sigma_0 \left(\frac{T}{\Lambda}\right)^{2(1-K)} . \tag{7.194}$$

We thus obtain a power-law dependence of conductivity on temperature, with an exponent determined by the Luttinger-liquid constant K (and thus by the interaction between fermions). Equation (7.194) for the conductivity holds for not too low temperatures. At lower temperatures it breaks down due to quantum interference between scattering on many impurities, which has not been taken into account and leads to Anderson localization. The Anderson localization will be a subject of the next Chapter of this course. Here we discuss it only briefly in the context of L-dependence of the conductivity; details will be in the next Chapter.

Consider the case of zero temperature. The IR cutoff is then provided by the system size L. Then, in full analogy with Eq. (7.194), we get the Drude conductivity (i.e. the conductivity discarding Anderson localization physics)

$$\sigma_D(L) = \sigma_0 \left(\frac{\lambda}{L}\right)^{2(1-K)} . \tag{7.195}$$

It is useful to introduce the conductance (inverse resistance) of a wire of length L

$$g_D(L) = \frac{\sigma_D(L)}{L} \sim \frac{e^2}{h} l_0 \lambda^{2-2K} L^{2K-3} \propto L^{2K-3} , \tag{7.196}$$

where $l_0 = v_F \tau_0$ is the bare mean free path. Consider the behavior for different values of K:

- $K = 1$, corresponding to non-interacting fermions. Then Eq. (7.196) yields $g_D(L) \propto 1/L$, which is the conventional (classical) behavior. With increasing L, the Drude conductance $g_D(L)$ decreases. When it becomes of order unity in units of e^2/h, the Anderson localization effects become crucially important, leading to exponential decay of the true conductance,

  $$g(L) \sim e^{-L/\xi}, \tag{7.197}$$

  with the localization length ξ. For the non-interacting case ($K = 1$) we have $\xi \sim l_0$.

- $K < 3/2$, including the cases of repulsive interaction as well as weak or moderately strong attraction. Qualitatively the same behavior: conductance decreases with increasing L. When it becomes of order of unity in units of e^2/h, the Anderson localization sets in, leading to the exponential suppression (7.197). The localization length ξ scales now as

  $$\xi \sim \left(l_0 \, \lambda^{2-2K}\right)^{1/(3-2K)} . \tag{7.198}$$

  The system is thus an insulator.

- $K > 3/2$, which means a strong attraction. Now we have a very unusual behavior: the conductance $g_D(L)$ increases with increasing L. As a result, the Anderson localization does not play any role. In the $L \to \infty$ limit, the conductance (and thus also the conductivity) diverge, i.e., the resistivity vanishes: the system behaves as a perfect metal, or, in a sense, as a superconductor. Indeed, the physics is similar to the superconductivity: attractive interaction between fermions leads to vanishing of resistivity. However, the analogy is not complete: in higher dimensions, the superconductivity results from a spontaneous symmetry breaking, which is not allowed in 1D.

Summarizing, we find at $K = 3/2$ a **metal-insulator transition**. In view of superconducting features of the metallic phase, it is also referred to as **1D "superconductor"-insulator transition**.

Comment: In this analysis, we have assumed a very weak bare disorder. It turns out that disorder also leads to renormalization of K: one should consider a two-parameter RG flow of K and disorder. As a result, for not so weak bare disorder, the transition is slightly shifted from $K = 3/2$.

7.8.3 Edge tunneling

We return to the problem of a single impurity. A strong barrier located at the point $x = 0$ in a Luttinger liquid can be described as a weak (tunneling) link between two halves of the system: $x < 0$ and $x > 0$. To address it, we first solve a problem of tunneling into the edge of a Luttinger liquid.

Consider a wire occupying the region $x > 0$ with an edge at $x = 0$. We want to generalize the calculation of the tunneling density of states, Sec. 7.7.5, to the case of tunneling at the edge. In principle, one can generalize the above calculation of the Green function in a problem without an edge to the present case. The Green function now will be $G(x, x'; t)$: it will depend on two coordinates in view of the lack of translational invariance. We present a simplified calculation which is sufficient to find $G(x, x'; t)$ at $x = x' = 0$.

We recall that $\phi(x, \tau) = -\pi \int_{-\infty}^{0} dx\, \rho(x, \tau)$ counts the total number of fermions to the left of the point x. Since we now have a boundary at $x = 0$, we have $\phi(x = 0, \tau) = \text{const}$. The value of this const will not be important (it just provides a constant phase to the ψ operator) and we discard it below. We thus get for the fermionic operator, according to Eq. (7.99),

$$\psi(x = 0, \tau) \sim \frac{1}{2\pi\lambda} \exp\{i\theta(x = 0, \tau)\}\,. \tag{7.199}$$

The Matsubara Green function at the edge thus becomes [in analogy with the bulk formula (7.124)]

$$\begin{aligned} \mathscr{G}(0, 0; \tau) &= -\frac{1}{2\pi\lambda} \langle \exp\{i[\theta(0, \tau) - \theta(0, 0)]\}\rangle \\ &= -\frac{1}{2\pi\lambda} \exp\left[\mathcal{B}_{\theta\theta}(0, 0; \tau)\right]\,, \end{aligned} \tag{7.200}$$

with

$$\mathcal{B}_{\theta\theta}(x, x'; \tau) = \langle \theta(x, \tau)\theta(x', 0) - \theta^2(0, 0)\rangle\,. \tag{7.201}$$

In the absence of the boundary, the correlation function $\mathcal{B}_{\theta\theta}(x, \tau)$ was found above, Eq. (7.139). If we put $x = 0$ in that formula, it yields

$$\mathcal{B}^{\text{bulk}}_{\theta\theta}(0, \tau) = -\frac{1}{2K} \ln \frac{u|\tau| + \lambda}{\lambda}\,. \tag{7.202}$$

However, there is still one important modification. The action of the θ field now is defined only on half-plane $x > 0$:

$$S[\theta] = \frac{K}{2\pi u} \int d\tau \int_0^\infty dx\, \left[(\partial_\tau\theta)^2 + u^2(\partial_x\theta)^2\right]\,, \tag{7.203}$$

which affects the correlation function. A simple and physically transparent way to evaluate this effect is to notice that the correlation function $\mathcal{B}_{\theta\theta}(x, x'; \tau)$ is the solution of the Laplace equation

$$-\frac{K}{2\pi u}(\partial_\tau^2 + u^2\partial_x^2)\mathcal{B}_{\theta\theta}(x, x'; \tau) = \delta(x - x')\delta(\tau - \tau') \tag{7.204}$$

on a half-plane $x > 0$ with the boundary conditions $\partial_x \mathcal{B}_{\theta\theta}(x, x'; \tau)|_{x=0} = 0$ and $\partial_{x'} \mathcal{B}_{\theta\theta}(x, x'; \tau)|_{x'=0} = 0$. This is a standard problem of the electrostatics, and the solution is given by the method of images:

$$\mathcal{B}_{\theta\theta}(x, x'; \tau) = \mathcal{B}_{\theta\theta}^{\text{bulk}}(x - x', \tau) + \mathcal{B}_{\theta\theta}^{\text{bulk}}(x + x', \tau)\,, \tag{7.205}$$

and thus

$$\mathcal{B}_{\theta\theta}(0, 0; \tau) = 2\mathcal{B}_{\theta\theta}^{\text{bulk}}(0, \tau) = -\frac{1}{K} \ln \frac{u|\tau| + \lambda}{\lambda}\,. \tag{7.206}$$

Substituting this in Eq. (7.200), we get

$$\mathcal{G}(0, 0; \tau) = -\frac{1}{2\pi\lambda} \exp\left[-\frac{1}{K} \ln \frac{u|\tau|}{\lambda}\right] \propto |\tau|^{-1/K}\,. \tag{7.207}$$

This yields, after Fourier transformation in the energy space the scaling of the tunneling density of states [see Sec. 7.7.5 for the corresponding calculation in the bulk]:

$$\nu(\epsilon) \sim \nu^{(0)} \left(\frac{|\epsilon|}{\Lambda}\right)^{\gamma_e}\,, \tag{7.208}$$

with the edge exponent

$$\boxed{\gamma_e = K^{-1} - 1\,.} \tag{7.209}$$

Thus, like in the bulk, there is a power-law scaling of the tunneling density of states at the edge, with an exponent determined by the Luttinger-liquid constant K (i.e., by the interaction strength). However, the edge exponent γ_e is different from the bulk exponent $\gamma = (K + K^{-1} - 2)/2$, Eq. (7.143).

7.8.4 Strong barrier

Now we are ready to study a strong impurity, i.e., a strong barrier between two halves of the wire, $x < 0$ and $x > 0$. It can be described as a weak link between the two halves, with the total Hamiltonian having a form

$$H = H_1 + H_2 + H_{\text{t}}\,, \tag{7.210}$$

where H_1 and H_2 describe Luttinger liquids on the semi-axes $x < 0$ and $x > 0$, respectively, and the tunneling part of the Hamiltonian is

$$H_{\text{t}} = t_0 \left[\psi_1^\dagger(0)\psi_2(0) + \psi_2^\dagger(0)\psi_1(0)\right]. \tag{7.211}$$

(The arguments refer to $x = 0$.) In the bosonized language, the tunneling term becomes

$$H_{\text{t}} = \frac{1}{2\pi\lambda} t_0 \left[e^{i\theta_1(0)} e^{-i\theta_2(0)} + e^{-i\theta_1(0)} e^{i\theta_2(0)}\right]. \tag{7.212}$$

We now switch to the functional-integral formulation and then perform the RG for the week tunneling in the same way as for the case of a weak impurity in Sec. 7.8.1. We split the fields θ_j (with $j = 1, 2$) into fast $\theta_j^>$ and slow $\theta_j^<$ components, integrate out fast fields, and then rescale the coordinates to restore the UV cutoff. This yields the renormalization of the tunneling amplitude:

$$t_0 \;\mapsto\; t(b) = t_0 \cdot \left\langle e^{i\theta_1^>(0,0)} \right\rangle_{\theta_1^>} \left\langle e^{-i\theta_2^>(0,0)} \right\rangle_{\theta_2^>} \cdot b\,. \tag{7.213}$$

Each of the averages here is

$$\left\langle e^{i\theta_1^>(0,0)}\right\rangle_{\theta_1^>} = \left\langle e^{-i\theta_2^>(0,0)}\right\rangle_{\theta_2^>} = \exp\left\{-\frac{1}{2}\langle\theta_j^>(0,0)\theta_j^>(0,0)\rangle_{\theta_j^>}\right\} \tag{7.214}$$

where the averaging is over functions on the half-plane (i.e, $x > 0$) with the action (7.203). The result immediately follows from Eq. (7.206):

$$\langle\theta_j^>(0,0)\theta_j^>(0,0)\rangle_{\theta_j^>} = \frac{1}{K}\ln b\,, \tag{7.215}$$

so that

$$t(b) = t_0\, b^{1-K^{-1}}\,. \tag{7.216}$$

This yields the RG equation

$$\boxed{\frac{d\,t(b)}{d\ln b} = (1-K^{-1})\,t(b)\,.} \tag{7.217}$$

These formulas hold as long as tunneling is weak, i.e. $t/u \ll 1$. The conductance of the wire in this regime is small:

$$g = \frac{e^2}{h}(|t|/u)^2\,, \tag{7.218}$$

with the renormalized amplitude t.

The infrared cutoff is set by the system size L or temperature T, i.e. $b = \min(L/\lambda, l_T/\lambda)$ in the same way as in Sec. 7.8.1.

Two RG equations—Eq. (7.185) for weak impurity and Eq. (7.217) for weak link fully describe the RG flow of the impurity strength. We see that they show the same direction of flow:

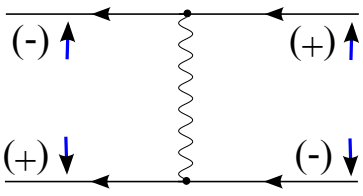
- For $K < 1$ a weak impurity becomes strong according to Eq. (7.185) and then the resulting weak link becomes still weaker according to Eq. (7.217). In the limit $T \to 0$ and $L \to \infty$, the renormalized tunneling t vanishes: **"single impurity cuts the chain!"**
- For $K > 1$ the RG flow is exactly opposite. Even if we have initially a strong barrier (i.e. weak tunneling), the tunneling becomes stronger according to Eq. (7.217), transforming into a weak impurity, which then further weakens, vanishing in the limit $T \to 0$ and $L \to \infty$.

7.9 Additional comments

7.9.1 Interaction-induced backscattering in spinful Luttinger liquid: g_1 term

We can now briefly return to the term in the Hamiltonian of the spinful Luttinger liquid that we have neglected:

$$H_{1\perp} = g_{1\perp}\int dx \sum_s \psi^\dagger_{-,s}\psi^\dagger_{+,-s}\psi_{-,-s}\psi_{+,s}\,. \tag{7.219}$$



This term involves interaction-induced backscattering and is not quadratic with respect to density fields of the bosonized theory. Using the bosonization identity for the fermionic operator in the spinful theory, Eq. (7.157), we obtain

$$H_{1\perp} = \frac{2g_{1\perp}}{(2\pi\lambda)^2} \int dx \cos\left[2\sqrt{2}\,\phi_\sigma(x)\right] . \tag{7.220}$$

The total action of the spin sector is $S = S_0 + S_{1\perp}$, where

$$S_0[\phi_\sigma] = \frac{1}{2\pi u_\sigma K_\sigma} \int d\tau dx \left[(\partial_\tau \phi_\sigma)^2 + u^2 (\partial_x \phi_\sigma)^2\right] . \tag{7.221}$$

and $S_{1\perp}[\phi_\sigma] = \int d\tau H_{1\perp}[\phi_\sigma]$. We use here the quadratic action S_0 depending on ϕ_σ field only (i.e. with θ_σ integrated out), since $S_{1\perp}$ depends on ϕ_σ only.

Considering the coupling $g_{1\perp}$ as small, one can derive the RG equation for it in the same way as this was done for the impurity-induced backscattering amplitude $\mathcal{U}$ in Sec. 7.8.1. The resulting equation reads

$$\frac{dg_{1\perp}}{d\ln b} = (2 - 2K_\sigma) g_{1\perp} . \tag{7.222}$$

Thus, depending on the value of K_σ (whether it is larger or smaller than unity), the coupling $g_{1\perp}$ either decreases or increases under RG. If $g_{1\perp}$ decreases under RG (one says then that it is an irrelevant coupling), it does not play much role: at long distances and low temperatures it will be very small and can be neglected. On the other hand, if $g_{1\perp}$ increases under RG (one says then that it is an RG-relevant coupling), the situation is totally different. At certain scale of L (or, equivalently, at sufficiently low temperature T), this coupling will become large. An analysis shows that this scale determines a gap that the spin sector acquires: the "phonons" of the spin sector become massive and cannot propagate beyond this scale. At longer scales (and lower temperatures) only charge-sector excitations remain. Thus, in such a situation, the spin-charge separation becomes really dramatic: the charge can propagate but the spin cannot! (Such a state is frequently called "Luther-Emery liquid".)

Comment: A fully accurate RG analysis requires two equations for mutual renormalization of $g_{1\perp}$ and K_σ.

7.9.2 Outlook: Further generalizations

- Spin chains
- Interacting 1D bosons
- Fractional quantum Hall edges

Chapter 8

Quantum transport in disordered systems

The subject of this Chapter is transport properties of disordered quantum systems. Physically, disorder means some concentration of impurities of a certain strength. Typical observables are the conductivity (or the conductance) of a system. We will focus on the charge conductivity but this can also be the heat conductivity. On a the quasiclassical level, the conductivity was studied in the framework of the Boltzmann kinetic equation in the Statistical Physics (Theory F) and TKM I courses. We formulate now a systematic, fully quantum approach to transport based on the linear response theory. This will allow us to explore effects in transport that are related to **quantum interference** and are missed by the Boltzmann equation. The most dramatic manifestation of these effects is **Anderson localization**.

8.1 Kubo formula for conductivity

In Sec. 3.13, we have developed the general formalism of linear response. Let is briefly repeat the main results here. One considers a perturbation of the Hamiltonian resulting from the action of a weak external field $F(t)$ ("generalized force") coupled to an operator $\widehat{A}$ ("generalized coordinate") of the system:

$$\hat{H} = \hat{H}_0 + \hat{A}\, F(t)\,. \tag{8.1}$$

One is interested in the change $\delta B(t)$ of the value of an observable $\hat{B}$ resulting from the action of the perturbation, to the linear order in perturbation. Here

$$B(t) = \langle \hat{B} \rangle_t\,, \tag{8.2}$$

where the averaging goes over the density-matrix at time t. Without perturbation the system is characterized by the equilibrium density matrix with temperature T. In Sec. 3.13 the formulas were written for $T = 0$ but they are straightforwardly extended to any equilibrium state, see Sec. 4.10.2. The result reads

$$\delta B(t) = \int \mathrm{d}t'\, \mathscr{D}^R_{BA}(t,t') F(t')\,, \tag{8.3}$$

where

$$\mathscr{D}^R_{BA}(t,t') = -\mathrm{i}\Theta(t-t')\langle [\widehat{B}(t), \widehat{A}(t')] \rangle_0 \tag{8.4}$$

and $\langle \dots \rangle_0 = \mathrm{tr} \dots \rho_0$ is the averaging over the unperturbed equilibrium state with density matrix ρ_0. (At zero temperature, this is averaging over the ground state of the unperturbed

system.) The function $\mathscr{D}^R_{BA}(t,t')$ is the **linear-response function**; the superscript "R" indicates its retarded character. Upon Fourier transformation, it becomes $\mathscr{D}^R_{BA}(\omega)$. In view of the retarded character of response, the function $\mathscr{D}^R_{BA}(\omega)$ is analytic function of the complex variable ω in the upper half-plane, $\operatorname{Im}\omega > 0$.

The formula (8.4) is the **Kubo formula**.

To obtain $\mathscr{D}^R_{BA}(\omega)$ in the diagrammatic framework, one uses the Matsubara formalism, which allows to obtain the Matsubara response function (see Sec. 4.10.2)

$$\mathscr{D}^M_{BA}(\tau) = -\langle \mathcal{T}_\tau \widehat{B}(\tau)\widehat{A}(0)\rangle_0 \,. \tag{8.5}$$

Its Fourier transform is $\mathscr{D}^M_{BA}(\omega_n)$ where ω_n are bosonic Matsubara frequencies. The real-time response function $\mathscr{D}^R_{BA}(\omega)$ is obtained by analytical continuation from the imaginary axis where it satisfies the condition

$$\mathscr{D}^R_{BA}(i\omega_n) = \mathscr{D}^M_{BA}(\omega_n)\,, \qquad \omega_n > 0, \tag{8.6}$$

to the real axis $\omega \in \mathbb{R} + i0$.

To apply the linear-response formalism to the (electric) conductivity, we need the expression for the perturbation of the Hamiltonian under applied electric field. It is convenient to use the gauge with zero scalar potential, $\varphi = 0$; the electric field is then

$$\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}\,, \tag{8.7}$$

where $\mathbf{A}$ is the vector potential.

The Hamiltonian in the absence of perturbation is

$$H_0 = \int d^3r\, \psi^\dagger(\mathbf{r}) \left[\frac{(-i\boldsymbol{\nabla})^2}{2m} + U(\mathbf{r})\right]\psi(\mathbf{r}) + H_{\text{int}}\,, \tag{8.8}$$

where $U(\mathbf{r})$ is a potential (which we will need to include the disorder) and H_{int} is the interaction part. Coupling to the vector potential $\mathbf{A}(\mathbf{r},t)$ is obtained by the substitution

$$\mathbf{p} \;\mapsto\; \mathbf{p} - \frac{e}{c}\mathbf{A} \equiv \mathbf{p}^{(\text{kin})}\,, \tag{8.9}$$

where $\mathbf{p} = -i\boldsymbol{\nabla}$ is the canonical momentum and $\mathbf{p}^{(\text{kin})}$ is the kinematic momentum. Thus, the perturbed Hamiltonian reads

$$H_0 + V(t) = \int d^3r\, \psi^\dagger(\mathbf{r}) \left[\frac{(-i\boldsymbol{\nabla} - \frac{e}{c}\mathbf{A}(\mathbf{r},t))^2}{2m} + U(\mathbf{r})\right]\psi(\mathbf{r}) + H_{\text{int}}\,, \tag{8.10}$$

Comparing with Eq. (8.8), we can read out the perturbation

$$V(t) = -\frac{1}{c}\int d^3r\, \mathbf{j}(\mathbf{r})\mathbf{A}(\mathbf{r}) + O(A^2)\,, \tag{8.11}$$

where

$$\mathbf{j}(\mathbf{r}) = \frac{e}{2m}(-i)\left[\psi^\dagger\boldsymbol{\nabla}\psi - (\boldsymbol{\nabla}\psi^\dagger)\,\psi\right]. \tag{8.12}$$

Since we are interested in linear response, we discard the term $O(A^2)$ in Eq. (8.11). The operator $j(r)$ is the current operator. In the absence of the potential $U(r)$ (i.e. in a translationally invariant system) it satisfies the conservation law

$$\operatorname{div}\mathbf{j} + \frac{\partial \rho}{\partial t} = 0\,, \tag{8.13}$$

where $\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$ is the density operator.

To calculate the conductivity, we need to find the response of a current to the applied electric field. According to the general Kubo formula (8.3), (8.4),

$$\delta\langle j_\mu(\mathbf{r})\rangle_t = \frac{i}{c}\int_{-\infty}^{t} dt' \int d^3r' \, \langle [j_\mu(\mathbf{r},t), j_\nu(\mathbf{r}',t')]\rangle_0 \, A_\nu(\mathbf{r}',t') \,. \tag{8.14}$$

However, according to Eq. (8.9), the physically measurable current in the presence of the electromagnetic field A_μ is not j_μ but rather

$$J_\mu(\mathbf{r},t) = j_\mu(\mathbf{r}) - \frac{e^2}{mc}\psi^\dagger(\mathbf{r})\psi(\mathbf{r})A_\mu(\mathbf{r},t) \,. \tag{8.15}$$

We thus need $\delta\langle J_\mu(\mathbf{r})\rangle_t$, which reads

$$\delta\langle J_\mu(\mathbf{r},t)\rangle = \int_{-\infty}^{t} dt' \int d^3r' \, Q_{\mu\nu}(\mathbf{r},t;\mathbf{r}',t')\frac{1}{c}A_\nu(\mathbf{r}',t') \,, \tag{8.16}$$

where

$$\begin{aligned} Q_{\mu\nu}(\mathbf{r},t;\mathbf{r}',t') &= i\Theta(t-t')\langle [j_\mu(\mathbf{r},t), j_\nu(\mathbf{r}',t')]\rangle_0 - \frac{e^2}{m}\langle\rho(\mathbf{r})\rangle_0 \, \delta(t-t')\delta(\mathbf{r}-\mathbf{r}')\delta_{\mu\nu} \\ &\equiv -\mathscr{D}^R_{jj;\mu\nu}(\mathbf{r},\mathbf{r}';t-t') - \frac{e^2}{m}\langle\rho(\mathbf{r})\rangle_0 \, \delta(t-t')\delta(\mathbf{r}-\mathbf{r}')\delta_{\mu\nu} \,, \end{aligned} \tag{8.17}$$

where $\mathscr{D}^R_{jj;\mu\nu}$ is the retarded current-current response function.

Consider a response on frequency ω:

$$\begin{aligned} &\mathbf{A}(\mathbf{r},t) = \mathbf{A}(\mathbf{r},\omega)e^{-i\omega t} \,; \qquad \mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r},\omega)e^{-i\omega t} \,, \\ &\mathbf{E}(\mathbf{r},\omega) = \frac{i\omega}{c}\mathbf{A}(\mathbf{r},\omega) \,. \end{aligned} \tag{8.18}$$

Equations (8.16), (8.17) become

$$\delta\langle J_\mu(\mathbf{r},\omega)\rangle = \int d^3r' \, \sigma_{\mu\nu}(\mathbf{r},\mathbf{r}';\omega)E_\nu(\mathbf{r}',\omega) \tag{8.19}$$

with

$$\boxed{\begin{aligned} \sigma_{\mu\nu}(\mathbf{r},\mathbf{r}';\omega) &= \frac{Q_{\mu\nu}(\omega)}{i\omega} \\ &= \frac{1}{i\omega}\left\{ i\int_0^\infty dt \, e^{i\omega t}\langle [j_\mu(\mathbf{r},t), j_\nu(\mathbf{r}',0)]\rangle_0 - \frac{e^2}{m}\langle\rho(\mathbf{r})\rangle_0 \, \delta(\mathbf{r}-\mathbf{r}')\delta_{\mu\nu}\right\} . \end{aligned}} \tag{8.20}$$

This is **Kubo formula for the conductivity**.

In the presence of disorder potential $U(\mathbf{r})$, the conductivity $\sigma_{\mu\nu}(\mathbf{r},\mathbf{r}';\omega)$ is not translationally invariant for a given realization of disorder. However, the translation invariance is restored upon averaging over disorder (i.e. averaging over an ensemble of systems corresponding to a given disorder strength):

$$\langle\sigma_{\mu\nu}(\mathbf{r},\mathbf{r}';\omega)\rangle_{\text{disorder}} \quad\longrightarrow\quad \sigma_{\mu\nu}(\mathbf{r}-\mathbf{r}';\omega) \,. \tag{8.21}$$

After this, one can perform also Fourier transformation $\mathbf{r} \to \mathbf{q}$:

$$\sigma_{\mu\nu}(\mathbf{q};\omega) = \int d(\mathbf{r}-\mathbf{r}') e^{-i\mathbf{q}(\mathbf{r}-\mathbf{r}')} \sigma_{\mu\nu}(\mathbf{r}-\mathbf{r}';\omega)\,. \tag{8.22}$$

Consider a response to a spatially homogeneous electric field, i.e., at $\mathbf{q}=0$. We have then

$$\sigma_{\mu\nu}(\omega) = \frac{1}{i\omega}\left[K_{\mu\nu}(\omega) - \frac{e^2}{m} n\delta_{\mu\nu}\right], \tag{8.23}$$

where

$$K_{\mu\nu}(\omega) = i\int_0^\infty dt\, d^3r\, e^{i\omega t} \langle [j_\mu(\mathbf{r},t), j_\nu(\mathbf{r}',0)]\rangle_0 \tag{8.24}$$

and $n = \langle\langle \rho(\mathbf{r})\rangle_0\rangle_{\text{disorder}}$ is the particle density. We note that the field $\mathbf{A}_\mu$ with $q=0$ and $\omega=0$ is a pure gauge, since the corresponding electric and magnetic fields are zero. Therefore, the current (which is a gauge-invariant observable) cannot be affected by such perturbation: $\delta\langle J_\mu\rangle = 0$. On the other hand,

$$\delta\langle J_\mu(\omega)\rangle = \left[K_{\mu\nu}(\omega) - \frac{e^2}{m} n\delta_{\mu\nu}\right]\frac{1}{c}\mathbf{A}_\nu(\omega)\,. \tag{8.25}$$

Thus

$$K_{\mu\nu}(0) = \frac{e^2}{m} n\delta_{\mu\nu}\,, \tag{8.26}$$

and the $q=0$ Kubo formula (8.23) can also be presented in the form

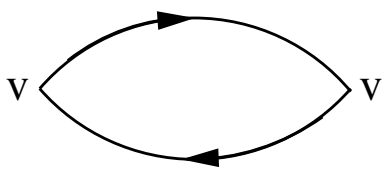
$$\sigma_{\mu\nu}(\omega) = \frac{1}{i\omega}\left[K_{\mu\nu}(\omega) - K_{\mu\nu}(0)\right]\,. \tag{8.27}$$

8.2 Kubo formula for non-interacting fermions

To determine the conductivity, we just need to evaluate the current-current response function, see Eq. (8.20). It can be obtained by analytical continuation of the corresponding Matsubara correlation function, see Eqs. (8.5) and (8.6):

$$\mathscr{D}^M_{jj;\mu\nu}(\mathbf{r},\mathbf{r}';\tau) = -\langle \mathcal{T}_\tau j_\mu(\mathbf{r},\tau) j_\nu(\mathbf{r}',0)\rangle_0\,. \tag{8.28}$$

For a system of non-interacting fermions there will be a single diagram for the correlation function (8.28), in full analogy with the density-density response function calculated in Sec. 4.9.1:



The corresponding expression is

$$\mathscr{D}^M_{jj;\mu\nu}(\mathbf{r},\mathbf{r}';\omega_m) = e^2\frac{1}{\beta}\sum_{\varepsilon_n} \hat{v}_\mu \mathscr{G}_{M,0}(\mathbf{r},\mathbf{r}';\varepsilon_n+\omega_m)\,\hat{v}_\nu\,\mathscr{G}_{M,0}(\mathbf{r}',\mathbf{r},\varepsilon_n). \tag{8.29}$$

Here $\hat{v}_\mu$ are velocity operators (with the word "operator" used in a single-particle sense),

$$F\mathbf{v}G = \frac{-i}{2m}\left[F\boldsymbol{\nabla}G - (\boldsymbol{\nabla}F)\,G\right]\,, \tag{8.30}$$

see Eq. (8.12) for the current. The velocity $\hat{v}_\mu$ in Eq. (8.29) contains derivatives with respect to $\mathbf{r}$, and $\hat{v}_\nu$ contains derivatives with respect to $\mathbf{r}'$. One should think about the factors in Eq. (8.29) forming a loop, as on the diagram, so that each velocity has one derivative acting to the right (with plus sign) and one acting to the left (with minus sign).

Analytical continuation from the Matsubara to real frequencies is performed in the same way as in Sec. 4.11.2 and is left as an exercise. The result reads

$$\begin{aligned}\mathscr{D}^R_{jj;\mu\nu}(\mathbf{r},\mathbf{r}';\omega) &= -ie^2\int\frac{dE}{2\pi}\left\{f(E+\omega)\,\hat{v}_\mu\,\left[G^R_{E+\omega}(\mathbf{r},\mathbf{r}')-G^A_{E+\omega}(\mathbf{r},\mathbf{r}')\right]\,\hat{v}_\nu\,G^A_E(\mathbf{r}',\mathbf{r})\right.\\ &+ \left. f(E)\,\hat{v}_\mu\,G^R_{E+\omega}(\mathbf{r},\mathbf{r}')\,\hat{v}_\nu\,\left[G^R_E(\mathbf{r}',\mathbf{r})-G^A_E(\mathbf{r}',\mathbf{r})\right]\right\}. \qquad (8.31)\end{aligned}$$

Substituting this in Eqs. (8.17) and (8.20), we obtain the conductivity $\sigma_{\mu\nu}(\mathbf{r},\mathbf{r}';\omega)$. Considering a response to the spatially homogeneous electric field ($q=0$). The (frequency-dependent) conductivity is then given by Eq. (8.27). There, $K_{\mu\nu}$, is defined by Eq. (8.24), i.e. it is (with a minus sign) the current-current response (8.31) integrated over $\mathbf{r}$. Thus, we get

$$\begin{aligned}\sigma_{\mu\nu}(\omega) &= \frac{1}{i\omega}\left[K_{\mu\nu}(\omega)-K_{\mu\nu}(0)\right]\\ &= -\frac{1}{\omega}\,e^2\int\frac{dE}{2\pi V}\left\{\left[f(E+\omega)\,\mathrm{tr}\,\hat{v}_\mu\,\left(G^R_{E+\omega}-G^A_{E+\omega}\right)\,\hat{v}_\nu\,G^A_E\right.\right.\\ &+ \left.\left. f(E)\,\mathrm{tr}\,\hat{v}_\mu\,G^R_{E+\omega}\,\hat{v}_\nu\,\left(G^R_E-G^A_E\right)\right]-[\text{the same with }\omega=0]\right\}, \qquad (8.32)\end{aligned}$$

where V is the volume.

Let us now focus on the longitudinal conductivity σ_{xx}. Equation (8.32) yields:

$$\begin{aligned}\sigma_{xx}(\omega) &= -\frac{1}{\omega}\,e^2\int\frac{dE}{2\pi V}\left\{f(E+\omega)\,\mathrm{tr}\left[\,\hat{v}_x\,(G^R_{E+\omega}-G^A_{E+\omega})\,\hat{v}_x\,G^A_E\right]\right.\\ &+ f(E)\,\mathrm{tr}\,\left[\hat{v}_x\,G^R_{E+\omega}\,\hat{v}_x\,(G^R_E-G^A_E)\right]\\ &+ \left. f(E)\,\mathrm{tr}\,\left[\hat{v}_x\,G^A_E\,\hat{v}_x\,G^A_E-\hat{v}_x\,G^R_E\,\hat{v}_x\,G^R_E\right]\right\}. \qquad (8.33)\end{aligned}$$

We consider the real part of the conductivity which is dominant at low frequencies (if the system is not an insulator). For this purpose we use the identities

$$\mathrm{Re}\;\mathrm{tr}\,M=\frac{1}{2}\mathrm{tr}\,(M+M^\dagger)\,,\qquad (G^R_E)^\dagger=G^A_E\,,\qquad \hat{v}_x^\dagger=\hat{v}_x\,. \qquad (8.34)$$

The result is

$$\boxed{\mathrm{Re}\,\sigma_{xx}(\omega)=-\frac{e^2}{4\pi V}\int dE\,\frac{f(E)-f(E+\omega)}{\omega}\,\mathrm{tr}\,\hat{v}_x\,(G^R_{E+\omega}-G^A_{E+\omega})\,\hat{v}_x\,(G^R_E-G^A_E)\,.} \qquad (8.35)$$

In the regime of interest, $\omega, T \ll E_F$, the energy integration goes over a vicinity of the Fermi energy, so that we can approximate

$$\int dE\,\frac{f(E)-f(E+\omega)}{\omega}(\ldots) \;\simeq\; (\ldots)_{E=E_F}\,. \qquad (8.36)$$

Thus,

$$\mathrm{Re}\,\sigma_{xx}(\omega)\simeq-\frac{e^2}{4\pi V}\mathrm{tr}\,\hat{v}_x\,(G^R_{E+\omega}-G^A_{E+\omega})\,\hat{v}_x\,(G^R_E-G^A_E)\big|_{E=E_F}\,. \qquad (8.37)$$

The corresponding formula for the complex $\sigma_{xx}(\omega)$ is immediately obtained from the real part by using analyticity of $\sigma_{xx}(\omega)$ in the half-plane $\mathrm{Im}\,\omega>0$:

$$\sigma_{xx}(\omega)\simeq-\frac{e^2}{2\pi V}\mathrm{tr}\,\hat{v}_x\,G^R_{E+\omega}\,\hat{v}_x\,(G^R_E-G^A_E)\big|_{E=E_F}\,. \qquad (8.38)$$

8.3 Disorder diagrammatics

Above, we expressed the conductivity of a system of non-interacting fermions in terms of the Green functions G_E^R, G_E^A. These Green functions are defined as

$$G_E^R = (E + i0 - \hat{H})^{-1}\,, \qquad G_E^A = (E - i0 - \hat{H})^{-1}\,,$$
$$\hat{H} = \hat{H}_0 + U(\mathbf{r}) = -\frac{\boldsymbol{\nabla}^2}{2m} + U(\mathbf{r})\,, \tag{8.39}$$

where $U(\mathbf{r})$ is the random potential. Clearly, Green functions depend on the realization of random potential. One should average the conductivity as given by Eq. (8.35) or (8.37) over the realizations of disorder. We develop now a diagrammatic technique that allows one to perform this.

Comment: In fact, fluctuations of the conductance from one realizations to another are also interesting. These are so-called **mesocopic conductance fluctuations**. However, it is natural to start from the average. One can show that if the system is a relatively good conductor (conductance $\gg e^2/h$), the fluctuations are small compared to the average.

We should first formulate a model of disorder. To simplify the analysis, let us assume that we have a high concentration of weak impurities:

$$U(\mathbf{r}) = \sum_i V_0(\mathbf{r} - \mathbf{r_i})\,, \tag{8.40}$$

where positions $\mathbf{r_i}$ of impurities are randomly distributed with a density $n_{\rm imp}$, and V_0 is a potential of an individual impurity. Consider a limit

$$n_{\rm imp} \to \infty\,, \qquad V_0 \to 0\,, \qquad n_{\rm imp} V_0^2 = {\rm const}\,. \tag{8.41}$$

It is easy to check that in this limit the statistics of the random potential $U(\mathbf{r})$ becomes Gaussian, i.e., it is characterized by a distribution of the type

$$\mathcal{P}\{U(\mathbf{r})\} = \frac{1}{Z} \exp\left\{-\frac{1}{2}\int d^3r_1 d^3r_2 U(\mathbf{r_1}) K(\mathbf{r_1} - \mathbf{r_2}) U(\mathbf{r_2})\right\}. \tag{8.42}$$

This means that the correlations of the potential $U(\mathbf{r})$ decouple into sums of products of pairwise correlations according to the Wick theorem, e.g.

$$\begin{aligned}\langle U(\mathbf{r_1})U(\mathbf{r_2})U(\mathbf{r_3})U(\mathbf{r_4})\rangle &= \langle U(\mathbf{r_1})U(\mathbf{r_2})\rangle \langle U(\mathbf{r_3})U(\mathbf{r_4})\rangle + \langle U(\mathbf{r_1})U(\mathbf{r_3})\rangle \langle U(\mathbf{r_2})U(\mathbf{r_4})\rangle \\ &+ \langle U(\mathbf{r_1})U(\mathbf{r_4})\rangle \langle U(\mathbf{r_2})U(\mathbf{r_3})\rangle\,. \end{aligned} \tag{8.43}$$

The pair correlator is

$$\langle U(\mathbf{r_1})U(\mathbf{r_2})\rangle = W(\mathbf{r_1} - \mathbf{r_2})\,, \tag{8.44}$$

where

$$\int d^3r K(\mathbf{r_1} - \mathbf{r}) W(\mathbf{r_1} - \mathbf{r_2}) = \delta(\mathbf{r_1} - \mathbf{r_2})\,. \tag{8.45}$$

The assumption of Gaussian statistics of disorder simplifies the analysis. At the same time, it does not affect the physics in any essential way.

Note that we assume here that $\langle U(\mathbf{r}\rangle = 0$. If it is not the case, one can simply include this constant as a shift of the energy.

In most of the calculations, we will make a further simplifying assumption:

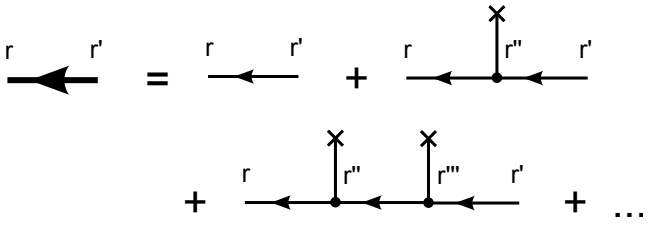
$$W(\mathbf{r_1} - \mathbf{r_2}) = \Gamma\delta(\mathbf{r_1} - \mathbf{r_2})\,. \tag{8.46}$$

This model is called "white-noise disorder". It is obtained from the above model of high concentration of weak impurity if one assumes that each impurity is characterized by a potential $V_0(\mathbf{r}-\mathbf{r_i}) = v_0\delta(\mathbf{r}-\mathbf{r_i})$, with $n_{\rm imp}\to\infty$, $v_0\to 0$, and $n_{\rm imp}v_0^2 = \Gamma$.

We use now the perturbative expansion of the Green functions in the potential U, see Sec. 2.6.

$$G^R = G_0^R + G_0^R U G_0^R + G_0^R U G_0^R U G_0^R + \dots \tag{8.47}$$

Here G_0^R is the Green function of free fermions: $G_0^R(\epsilon) = (\epsilon + i0 - \hat{H}_0)^{-1}$ with $H_0 = -\boldsymbol{\nabla}^2/2m$. The energy is the same for all Green functions in Eq. (8.47) and not indicated. A fully analogous expansion holds for G^A.



To calculate the conductivity, we need to average a product of two Green's functions. Let us start, however, from calculating the average of a single Green's function. Averaging (8.47), we obtain diagrams consisting of the following elements:

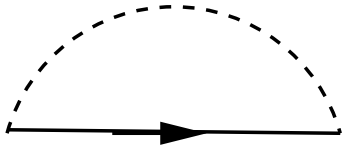
Free Green function $\quad G_0^{R,A}(\epsilon,p) = (\epsilon - p^2/2m \pm i0)^{-1}$ 

Disorder line $\quad \langle U(\mathbf{r})U(\mathbf{r}')\rangle = W(\mathbf{r}-\mathbf{r}')$

The diagrammatics has some similarity with that for an interacting system [Sec. 3.9]. However, there are essential differences:

- No diagrams with internal closed loops. For example, out of numerous diagrams that we had in the second order with respect to interaction, see figure below Eq. (3.217), only three diagrams will have their counterparts in the present case (with wavy line representing the interaction replaced by the dashed line representing the disorder).
- Disorder line does not carry any energy (contrary to the interaction line).

In full similarity with the diagrammatics for problems with interaction, we introduce the self-energy $\Sigma(\epsilon,p)$. To the lowest order in disorder correlator, we have just one diagram for the self-energy:



The corresponding analytical expression:

$$\Sigma^R(\epsilon,p) = \int (d\mathbf{p_1}) G_0^R(\mathbf{p_1}) W(\mathbf{p}-\mathbf{p_1}) = \int (d\mathbf{p_1}) \frac{1}{\epsilon + i0 - p_1^2/2m} W(\mathbf{p}-\mathbf{p_1})\,, \tag{8.48}$$

where we used a short notation for the integration measure, $(dp) = d^dp/(2\pi)^d$.

The real part of the self-energy will produce only a small correction to the energy ($\ll E_F$), so we neglect it.

Comment: If one uses the white-noise disorder model, then the integral for the real part will formally diverge on the ultraviolet limit. However, if one makes a UV cutoff, e.g., at momenta $\sim p_F$, one gets a finite and small result (for weak disorder; the exact condition will be specified below), as we have just stated.

We thus focus on the imaginary part of the self-energy.

$$\mathrm{Im}\,\Sigma^R(\epsilon,p)=\int(d\mathbf{p_1})(-\pi)\delta(\epsilon-p_1^2/2m)W(\mathbf{p}-\mathbf{p_1})\,, \tag{8.49}$$

Consider the white-noise disorder model (8.46). In the momentum space, the disorder correlation function is then simply constant:

$$W(\mathbf{q})=\Gamma\,. \tag{8.50}$$

Thus,

$$\mathrm{Im}\,\Sigma^R(\epsilon,p)=\int(d\mathbf{p_1})(-\pi)\,\delta(\epsilon-p_1^2/2m)\,\Gamma=-\pi\nu(\epsilon)\Gamma\equiv-\frac{1}{2\tau}\,. \tag{8.51}$$

Here $\nu(\epsilon)$ is the density of states at energy ϵ. Since relevant energies ϵ are close to Fermi energy, we can as usual approximate $\nu(\epsilon)$ by the density of states at the Fermi energy $\nu(E_F)$ and thus consider is as a constant (to be denoted simply as ν).

The imaginary part of the self-energy defines the **mean free time** τ. This is the mean free time with respect to the impurity scattering. It is worth emphasizing that this scattering is *elastic* (energy-conserving). This distinguishes it from inelastic scattering due to interactions (electron-electron, electron-phonon, etc.)

Thus, we find the disorder-averaged Green's functions $G^{R,A}(\epsilon,p)$: 

$$\boxed{G^{R,A}(\epsilon,p)=\frac{1}{\epsilon-\frac{p^2}{2m}-\Sigma_{R,A}}\simeq\frac{1}{\epsilon-\frac{p^2}{2m}\pm\frac{i}{2\tau}}} \tag{8.52}$$

The calculation (based on the lowest-order diagram for self-energy) is valid if the disorder is weak. The corresponding condition is $\epsilon\tau\gg1$, or, equivalently,

$$E_F\tau\gg1\,. \tag{8.53}$$

To understand the role of the imaginary part of the self-energy, it is useful to inspect its effect on the behavior of the Green function in real space. We perform the Fourier transformation:

$$G^{R,A}(\epsilon,r)=\int(dp)e^{i\mathbf{pr}}\frac{1}{\epsilon-\frac{p^2}{2m}\pm\frac{i}{2\tau}} \tag{8.54}$$

We can set $\epsilon=E_F$. The pole is shifted from to $p=p_F$ to $p\simeq p_F\pm i/2l$, where $l=v_F\tau$ is the **mean free path**. This implies that

$$G^{R,A}(\epsilon,r)\simeq G_0^{R,A}(\epsilon,r)e^{-r/2l}\,, \tag{8.55}$$

as can be indeed verified by an accurate calculation. The physical meaning of this exponential suppression of the Green function at $r\gg l$: decay of a plane-wave state (i.e. a state with a given momentum p) due to the (elastic) impurity scattering. Note that exact single-particle states do not decay, since we consider a non-interacting problem. In this respect, there is a qualitative difference with (inelastic) decay due to interaction considered earlier in this course.

8.4 Feynman path integral

Before proceeding with application of the the diagrammatic to the calculation of conductivity, we make a digression and introduce the Feynman path integral formalism for quantum-mechanical Green function (propagator). This formalism is in fact a precursor of the functional-integral formalism which was introduced in Chapter 6. While we will not use the Feynman path integral approach for actual calculation, it will be very useful for physical interpretation of diagrammatic calculations.

We consider quantum mechanics of a particle with the Hamiltonian

$$\hat{H}(t) = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{x}, t)\,, \qquad \hat{\mathbf{p}} = -i\boldsymbol{\nabla}\,. \tag{8.56}$$

The corresponding retarded Green's function $G^R(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i)$ was defined in Chapter 2. It satisfies the equation

$$(i\partial_{t_f} - H_{\mathbf{x}_f, t_f}) G^R(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \delta(t_f - t_i)\delta(\mathbf{x}_i - \mathbf{x}_f). \tag{8.57}$$

The retarded solution of this equation reads

$$iG^R(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \theta(t_f - t_i)\big\langle \mathbf{x}_f | \hat{U}(t_f, t_i) | \mathbf{x}_i \big\rangle = \theta(t_f - t_i)\big\langle \mathbf{x}_f | \mathcal{T} e^{-i\int_{t_i}^{t_f} dt' \hat{H}(t')} | \mathbf{x}_i \big\rangle, \tag{8.58}$$

where $\hat{U}(t_f, t_i)$ is the evolution operator. To present the propagator $G^R(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i)$ as a path integral, we split the time interval from t_i till t_f in a large number of smalls steps $[t_{n-1}, t_n]$, each of length Δt:

$$\hat{U}(t_f, t_i) = \hat{U}(t_f, t_{M-1})\hat{U}(t_{M-1}, t_{M-2}) \ldots \hat{U}(t_2, t_1)\hat{U}(t_1, t_i)\,. \tag{8.59}$$

The evolution operator on each of the steps can be approximated as

$$\hat{U}(t_n, t_{n-1}) = \mathcal{T} e^{-i\int_{t_{n-1}}^{t_n} dt' \hat{H}(t')} \simeq 1 - i\Delta t\, \hat{H}(t_n)\,. \tag{8.60}$$

Now we insert between each two consecutive evolution operators $\hat{U}(t_{n+1}, t_n)$ and $\hat{U}(t_n, t_{n-1})$ with $n = 1, 2 \ldots, M-1$ the following decomposition of unity:

$$\mathbb{1} = \int d^d x_n \int \frac{d^d p_n}{(2\pi)^d} \, |\mathbf{x}_n\rangle\langle \mathbf{x}_n | \boldsymbol{p}_n \rangle\langle \boldsymbol{p}_n |\,, \tag{8.61}$$

with $\big\langle \mathbf{x} | \boldsymbol{p} \big\rangle = e^{i\boldsymbol{p}\mathbf{x}}$. Note that $x_0 \equiv x_i$ and $x_M \equiv x_f$. After the last step, i.e. at time t_M, we insert

$$\mathbb{1} = \int \frac{d^d p_M}{(2\pi)^d} \, |\boldsymbol{p}_M\rangle\langle \boldsymbol{p}_M |\,. \tag{8.62}$$

As a result, the evolution operator (8.60) of each step produces the matrix element

$$\begin{aligned} \big\langle \boldsymbol{p}_n | 1 - i\Delta t\, \hat{H}(t_n) | \mathbf{x}_{n-1} \big\rangle &= [1 - i\Delta t\, \mathcal{H}(t_n, \boldsymbol{p}_n, \mathbf{x}_{n-1})]\, e^{-i\mathbf{x}_{n-1}\boldsymbol{p}_n} \\ &\simeq \exp\left[-i\Delta t\, \mathcal{H}(t_n, \boldsymbol{p}_n, \mathbf{x}_{n-1})\right] e^{-i\mathbf{x}_{n-1}\boldsymbol{p}_n}\,, \end{aligned} \tag{8.63}$$

where $\mathcal{H}(t, \boldsymbol{p}, \mathbf{x})$ is the Hamilton function corresponding to the Hamiltonian operator $\hat{H}(t)$. For the Hamiltonian (8.56) we have obviously

$$\mathcal{H}(t, \boldsymbol{p}, \mathbf{x}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}, t)\,. \tag{8.64}$$

Combining everything, we obtain

$$iG^R(\mathbf{x}_f,t_f;\mathbf{x}_i,t_i)=\theta(t_f{-}t_i)\int\prod_{n=1}^{M-1}d^dx_n\prod_{n=1}^{M}\frac{d^dp_n}{(2\pi)^d}\exp\left\{\sum_{n=1}^{M}\left[i\boldsymbol{p}_n\left(\mathbf{x}_n-\mathbf{x}_{n-1}\right)-i\Delta t\,\mathcal{H}\left(t_n,\boldsymbol{p}_n,\mathbf{x}_{n-1}\right)\right]\right\}. \tag{8.65}$$

In the continuum limit ($M\to\infty$ and $\Delta t\to 0$), this becomes

$$\boxed{iG^R(\mathbf{x}_f,t_f;\mathbf{x}_i,t_i)=\theta(t_f-t_i)\int_{x(t_i)=x_i}^{x(t_f)=x_f}\mathcal{D}\mathbf{x}(t)\int\mathcal{D}\boldsymbol{p}\,(t)\,\exp\left\{i\int_{t_i}^{t_f}dt\left[\boldsymbol{p}\,(t)\dot{\mathbf{x}}(t)-\mathcal{H}(t,\boldsymbol{p}\,(t),\mathbf{x}(t))\right]\right\}.} \tag{8.66}$$

The integral is performed over paths in the phase space $\mathbf{x}(t),\mathbf{p}(t)$ with boundary conditions $\mathbf{x}(t_i)=\mathbf{x}_i$ and $\mathbf{x}(t_f)=\mathbf{x}_f$. This version of the path integral can be derived for any Hamiltonian built out of operators $\mathbf{x}$ and $\boldsymbol{p}$. For such a general Hamiltonian, one should first transform it to the normal-ordered form in the sense that in any term involving both $\mathbf{x}$ and $\boldsymbol{p}$, all $\boldsymbol{p}$ factors should stay to the left of all $\mathbf{x}$ factors. This normal form defines the function $\mathcal{H}(t,\boldsymbol{p},\mathbf{x})$.

Now we focus on Hamiltonians of the type (8.56). In this case, the integration $\int\mathcal{D}\boldsymbol{p}\,(t)$ in Eq. (8.66) is Gaussian and can be performed exactly, see Eq. (6.55). The result reads

$$\boxed{iG^R(\mathbf{x}_f,t_f;\mathbf{x}_i,t_i)=\theta(t_f-t_i)\int_{x(t_i)=x_i}^{x(t_f)=x_f}\mathcal{D}\mathbf{x}(t)\,\exp\left\{i\int_{t_i}^{t_f}dt\,L(\mathbf{x},\dot{\mathbf{x}},t)\right\}.} \tag{8.67}$$

where $L(\mathbf{x},\dot{\mathbf{x}},t)$ is the classical Lagrangian,

$$L(\mathbf{x},\dot{\mathbf{x}},t)=\frac{m\dot{\mathbf{x}}^2}{2}-V(\mathbf{x},t)\,. \tag{8.68}$$

The functional that has emerged in the exponent of Eq. (8.67) is the classical action S evaluated on the trajectory $\mathbf{x}(t)$:

$$S[\mathbf{x}(t)]=\int_{t_i}^{t_f}dt\,L(\mathbf{x},\dot{\mathbf{x}},t)\,. \tag{8.69}$$

Thus, Eq. (8.67) can be written in a very compact form:

$$\boxed{iG^R(\mathbf{x}_f,t_f;\mathbf{x}_i,t_i)=\theta(t_f-t_i)\int_{x(t_i)=x_i}^{x(t_f)=x_f}\mathcal{D}\mathbf{x}(t)\,e^{iS[\mathbf{x}(t)]}\,.} \tag{8.70}$$

This is the Feynman path-integral formula. It presents the quantum-mechanical Green's function, i.e., the amplitude of evolution from point $\mathbf{x}_i$ at time t_i to point $\mathbf{x}_f$ at time t_f, as an integral over all paths from $(\mathbf{x}_i,t_i)$ to $(\mathbf{x}_f,t_f)$, with every path being weighted with the factor $e^{iS[\mathbf{x}(t)]}$ where $S[\mathbf{x}(t)]$ is the classical action evaluated on this path.

An analogous formula holds for the advanced Green's function (for convenience, we interchange $i\leftrightarrow f$ in indices of the arguments of G^A in order to keep $t_f>t_i$):

$$iG^A(\mathbf{x}_i,t_i;\mathbf{x}_f,t_f)=-\theta(t_f-t_i)\big\langle\mathbf{x}_i|\hat{U}(t_i,t_f)|\mathbf{x}_f\big\rangle=i[G^R(\mathbf{x}_f,t_f;\mathbf{x}_i,t_i)]^*\,, \tag{8.71}$$

so that

$$iG^A(\mathbf{x}_i,t_i;\mathbf{x}_f,t_f)=-\theta(t_f-t_i)\int_{x(t_i)=x_i}^{x(t_f)=x_f}\mathcal{D}\mathbf{x}(t)\,e^{-iS[\mathbf{x}(t)]}\,. \tag{8.72}$$

8.4.1 Stationary phase approximation

When characteristic value of the action S in the exponent are large, the path integral can be evaluated in the stationary-phase approximation. (We recall that we use units $\hbar = 1$, i.e. the action is measured in units of $\hbar$.) This situation corresponds to the quasiclassical regime. A stationary point is defined by the condition

$$\frac{\delta S[\mathbf{x}(t)]}{\delta \mathbf{x}(t)} = 0\,. \tag{8.73}$$

We know from the classical mechanics that this condition is equivalent to the Lagrange equations of motion. Therefore, a stationary point of the path integral is a classical trajectory $\mathbf{x}_{\rm cl}(t)$. We get in the stationary-phase approximation

$$iG^R(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) \simeq \theta(t_f - t_i) e^{iS[\mathbf{x}_{\rm cl}(t)]} A[\mathbf{x}_{\rm cl}(t)]\,, \tag{8.74}$$

where $A[\mathbf{x}_{\rm cl}(t)]$ results from Gaussian integration around the stationary point:

$$A[\mathbf{x}_{\rm cl}(t)] = \det\left(\frac{1}{2\pi i}\,\frac{\partial^2 S}{\partial x_\mu(t_1)\partial x_\nu(t_2)}\Big|_{\mathbf{x}(t)=\mathbf{x}_{\rm cl}(t)}\right)^{-1/2}. \tag{8.75}$$

By varying the action around the classical trajectory, one can show that

$$A[\mathbf{x}_{\rm cl}(t)] = \det\left[\frac{i}{2\pi}\,\left(m\delta_{\mu\nu}\frac{d^2}{dt^2} + \partial_{x_\mu}\partial_{x_\nu} V(\mathbf{x}_{\rm cl}(t), t)\right)\right]^{-1/2}. \tag{8.76}$$

If there are multiple classical trajectories $\mathbf{x}_{\rm cl}^{(j)}(t)$ (which will be the case for disordered systems), one should sum their contributions to the propagator:

$$iG^R(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) \simeq \theta(t_f - t_i) \sum_j e^{iS[\mathbf{x}_{\rm cl}^{(j)}(t)]} A[\mathbf{x}_{\rm cl}^{(j)}(t)]\,, \tag{8.77}$$

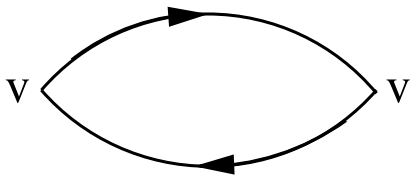
8.5 Diagrammatic calculation of conductivity

We have derived the general formula, Eq. (8.38):

$$\sigma_{xx}(\omega) \simeq \frac{e^2}{2\pi V}\left\langle \mathrm{tr}\,\hat{v}_x\, G^R_{\epsilon+\omega}\,\hat{v}_x\,(G^A_\epsilon - G^R_\epsilon)\right\rangle_{\rm disorder}\Big|_{\epsilon=E_F}, \tag{8.78}$$

where we now explicitly indicated disorder averaging.

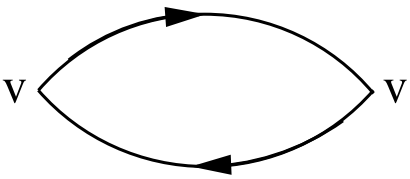
This corresponds to the sum of diagrams obtained from the bare one (shown to the right) by inserting impurity lines in all possible ways.



8.5.1 Drude conductivity

Consider first diagrams with impurity lines inserted in each of the fermionic lines but not connecting them. Then $G^R \mapsto \langle G^R\rangle$ and $G^A \mapsto \langle G^A\rangle$. For brevity, we simply write $\langle\ldots\rangle$ for $\langle\ldots\rangle_{\rm disorder}$.

This can be again represented by a simple bubble diagram but now each line means averaged Green's function $\langle G^R\rangle$ or $\langle G^A\rangle$.



$$\sigma_{xx}(\omega) = \frac{e^2}{2\pi}\int (dp)\,\frac{1}{m^2}\,p_x^2\,\langle G^R_{\epsilon+\omega}\rangle(p)\left[\langle G^A_\epsilon\rangle(p)-\langle G^R_\epsilon\rangle(p)\right]$$

$$= \frac{e^2}{2\pi m^2}\int (dp)\,\frac{p^2}{d}\,\frac{1}{\epsilon+\omega-\frac{p^2}{2m}+\frac{i}{2\tau}}\left(\frac{1}{\epsilon-\frac{p^2}{2m}-\frac{i}{2\tau}}-\frac{1}{\epsilon-\frac{p^2}{2m}+\frac{i}{2\tau}}\right), \quad (8.79)$$

where d is the spatial dimensionality. We denote $p^2/2m-\epsilon=\xi_p$. The energy ϵ is to be taken $\epsilon=E_F$. The integral is determined by the vicinity of the Fermi surface: $\xi_p\sim 1/\tau \ll E_F$. Therefore, we can approximate

$$p^2\simeq p_F^2\,,\qquad \nu(\epsilon)\simeq\nu(E_F)\equiv\nu\,,\qquad \int_{-E_F}^{\infty} d\xi_p\ldots\simeq\int_{-\infty}^{\infty}d\xi_p\ldots\,. \quad (8.80)$$

This yields

$$\sigma_{xx}(\omega)=\frac{e^2}{2\pi}\,\nu\,\frac{v_F^2}{d}\int d\xi_p\,\frac{1}{\omega-\xi_p+\frac{i}{2\tau}}\left(\frac{1}{-\xi_p-\frac{i}{2\tau}}-\frac{1}{-\xi_p+\frac{i}{2\tau}}\right). \quad (8.81)$$

The integral is straightforwardly calculated by means of Cauchy's residue theorem. The second term, i.e. the G^RG^R term, yields zero contribution (both residues are on the upper side of the real axis of ξ_p). From the first (G^RG^A) term we get

$$\sigma_{xx}(\omega)=e^2\,\frac{\nu v_F^2}{d}\,\frac{\tau}{1-i\omega\tau}\,. \quad (8.82)$$

This is exactly the Drude formula for conductivity as obtained by the classical calculation based on the Boltzmann kinetic equation (Statistical Physics and TKM I courses).

Comment: While the result comes from the G^RG^A term, we kept also the G^RG^R term in the original formula (8.79), as the integral would be UV-divergent otherwise. After approximations (8.80), the G^RG^R term becomes zero, and the G^RG^A integral UV-convergent and fully determined by the vicinity of the Fermi surface. Below in analogous calculations we will do the same approximations, so that we keep only terms of the G^RG^A type from the very beginning.

This calculation was performed for the white-noise disorder (8.50). Let us return for a moment to the general case of the disorder correlation function $W(q)$ and inspect the self-energy (8.49),

$$\frac{1}{2\tau}=-\mathrm{Im}\,\Sigma^R(\epsilon,\mathbf{p})=\int(d\mathbf{p_1})(-\pi)\delta(\epsilon-\mathbf{p_1}^2/2m)W(\mathbf{p}-\mathbf{p_1})\,. \quad (8.83)$$

Setting $\epsilon=E_F$ and $|\mathbf{p}|=p_F$, we get

$$\frac{1}{\tau}=\nu\int d\Omega\,w_p(\theta)\,,\qquad w_p(\theta)=2\pi W(\mathbf{p}-\mathbf{p_1})=2\pi W(2p_F\sin(\theta/2))\,, \quad (8.84)$$

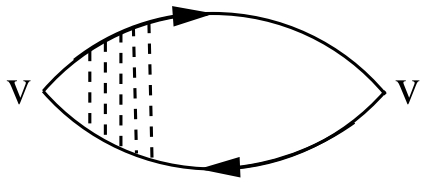
where $\int d\Omega\ldots$ is the angular integral (normalized to unity) over the direction of $\mathbf{p_1}$, and θ is the angle between $\mathbf{p_1}$ and $\mathbf{p}$. On the other hand, within the quasiclassical approximation

we obtained, in the case of general impurity scattering, the Drude formula (8.82) but with $\tau \mapsto \tau_{\rm tr}$, where $\tau_{\rm tr}$ is the transport relaxation time,

$$\frac{1}{\tau_{\rm tr}} = \nu \int d\Omega \, w_p(\theta)(1-\cos\theta) \, . \tag{8.85}$$

For the white noise disorder $W(\mathbf{q}) = \Gamma$ we have $w_p(\theta) = 2\pi\Gamma$, i.e. isotropic scattering, so that the formulas (8.84) and (8.85) yield identical results. However, for a general $w_p(\theta)$, when the scattering is anisotropic (i.e., the rate $w_p(\theta)$ is dependent on scattering angle θ), they are different: Eq. (8.84) is the total relaxation rate, while Eq. (8.85) is the transport scattering rate.

To obtain correctly the Drude conductivity (8.82) with $\tau \mapsto \tau_{\rm tr}$, one has to sum up the ladder diagrams:



Let us calculate the first of them (with one leg of the ladder, i.e., one impurity line connecting two fermionic lines):

$$\begin{aligned}
\sigma_{xx}^{(1)}(\omega) &= \frac{e^2}{2\pi} \int (dp)(dp') \, \frac{1}{m^2} \, p_x p'_x \, \langle G^R_{\epsilon+\omega}\rangle(p) \langle G^A_{\epsilon}\rangle(p) \langle G^R_{\epsilon+\omega}\rangle(p') \langle G^A_{\epsilon}\rangle(p') W(\mathbf{p}-\mathbf{p}') \\
&= \frac{e^2}{2\pi} \, \nu \, \frac{v_F^2}{d} \int d\xi_p d\xi_{p'} \, \frac{1}{(\omega - \xi_p + \frac{i}{2\tau})(-\xi_p - \frac{i}{2\tau})} \, \frac{1}{(\omega - \xi_p + \frac{i}{2\tau})(-\xi_p - \frac{i}{2\tau})} \int d\Omega \, w_p(\theta) \cos\theta \, . \\
&= e^2 \, \frac{\nu v_F^2}{d} \, \left(\frac{\tau}{1 - i\omega\tau} \right)^2 \left(\frac{1}{\tau} - \frac{1}{\tau_{\rm tr}} \right) ,
\end{aligned} \tag{8.86}$$

where we used that $\nu \int d\Omega \, w_p(\theta) \cos\theta = \tau^{-1} - \tau_{\rm tr}^{-1}$ according to Eqs. (8.84) and (8.85). It is not difficult to check that ladder diagrams yield a geometric series; the term with n legs reads

$$\sigma_{xx}^{(n)}(\omega) = e^2 \, \frac{\nu v_F^2}{d} \, \left(\frac{\tau}{1 - i\omega\tau} \right)^{n+1} \left(\frac{1}{\tau} - \frac{1}{\tau_{\rm tr}} \right)^n \tag{8.87}$$

Summing the series, one finds

$$\begin{aligned}
\sigma_{xx}(\omega) &= \sum_{n=0}^{\infty} \sigma_{xx}^{(n)}(\omega) = \frac{e^2}{2\pi} \, \nu \, \frac{v_F^2}{d} \, \frac{\tau}{1 - i\omega\tau} \sum_{n=0}^{\infty} \left(\frac{1 - \tau/\tau_{\rm tr}}{1 - i\omega\tau} \right)^n = \frac{e^2}{2\pi} \, \nu \, \frac{v_F^2}{d} \, \frac{\tau}{1 - i\omega\tau} \, \frac{1}{1 - \frac{1-\tau/\tau_{\rm tr}}{1 - i\omega\tau}} \\
&= \frac{e^2}{2\pi} \, \nu \, \frac{v_F^2}{d} \, \frac{\tau_{\rm tr}}{1 - i\omega\tau_{\rm tr}} \, .
\end{aligned} \tag{8.88}$$

We thus see that indeed the resummation of the ladder diagrams yields correctly the Drude conductivity with the transport relaxation time.

8.5.2 Interpretation of ladder diagrams in terms of path integral

We now provide a physical interpretation of the ladder diagrams in terms of the Feynman path integral, Sec. 8.4. According to Eq. (8.77),

$$G^R(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) \simeq \sum_j A_j \, e^{iS_j} \, , \qquad t_f > t_i \, , \tag{8.89}$$

where the index j labels classical trajectrories, S_j is the corresponding action and A_j the pre-exponential factor (whose specific form will not be important for the qualitative considerations). We have incorporated the factor i in A_j. In the same way,

$$G^A(\mathbf{x}_i, t_i; \mathbf{x}_f, t_f) = \left[G^R(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i)\right]^* \simeq \sum_j A_j^* \, e^{-iS_j} \,, \qquad t_f > t_i \,, \tag{8.90}$$

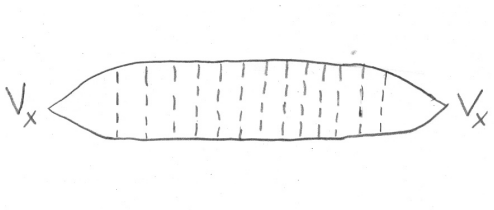
In the calculation of conductivity, or other related observables (e.g., density-density response function etc), we will have to average a product $G^R G^A$ (in fact, with some operators staying in vertices, but this is not essential for the present discussion). This yields

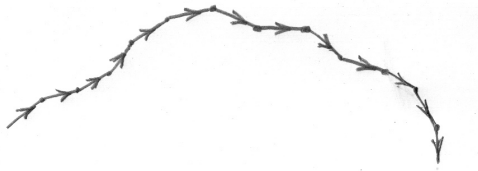
$$\langle G^R G^A \rangle = \left\langle \sum_{jk} A_j A_k^* \, e^{i(S_j - S_k)} \right\rangle . \tag{8.91}$$

The actions S_j are large, so that we have quickly varying phase factors $e^{i(S_j - S_k)}$ for $j \neq k$. In view of this, the leading contribution is given by the diagonal terms, $j = k$, i.e. by the same trajectory contributing to G^R and G^A:

$$\langle G^R G^A \rangle \simeq \left\langle \sum_j |A_j|^2 \right\rangle . \tag{8.92}$$

This is the classical approximation. The ladder diagrams (as e.g. we found for the conductivity in the case of anisotropic scattering) can be understood in this way:





quantum

classical

$$\sigma_{xx}(\omega) = \frac{e^2}{2\pi V} \left\langle \mathrm{tr}\, \hat{v}_x \, G^R_{\epsilon+\omega} \, \hat{v}_x \, G^A_{\epsilon} \right\rangle \qquad \sigma_{xx}(\omega) = e^2 \nu \int_0^\infty dt \, \langle v_x(0) v_x(t) \rangle e^{i\omega t}$$

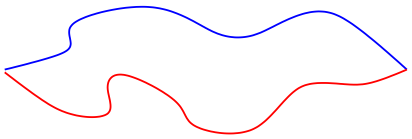
Two fermionic Green functions lines correspond physically to two trajectories, each describing a quantum-mechanical amplitude. In the classical approximation, this is the same trajectory, which thus becomes the trajectory for propagation of the probability density, in full correspondence with the Boltzmann kinetic equation formalism.

8.5.3 Quantum interference effects: Qualitative discussion

Quantum interference effects are given by terms in (8.91) that are missed by the classical approximation (8.92), i.e., by non-diagonal terms

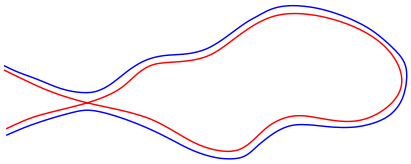
$$\langle G^R G^A \rangle_{\text{quantum interference}} = \left\langle \sum_{j \neq k} A_j A_k^* \, e^{i(S_j - S_k)} \right\rangle . \tag{8.93}$$

As discussed above, most of these terms average to zero due to phase factors.



There are, however, important exceptions. In particular, time-reversed paths (i.e., the same trajectory traversed in two opposite directions) have the same action. This assumes that the time-reversal symmetry is not broken, which requires absence of magnetic fields.

Two paths, that have the same initial and final points, follow the same classical trajectory but traverse the loop in the opposite directions.



The interference of time-reversed paths leads to **weak-localization correction to conductivity** which will be calculated below by diagrammatic means. Furthermore, as will be also discussed below, in some situations such quantum corrections proliferate and lead to **strong Anderson localization**, which totally blocks the transport.

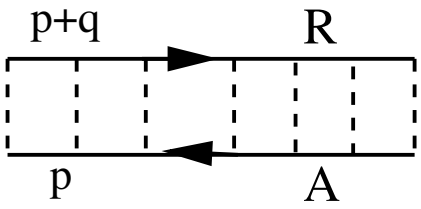
Comment: As is clear from the above discussion, localization phenomena originate from wave interference. Therefore, they are characteristic not only for quantum mechanics of a particle in random potential but also to classical waves in disordered media. In particular, the effect of interference of time-reversed paths is also known in optics where it leads to the phenomenon of enhanced back-scattering from a disordered medium. Anderson localization of classical waves has been studied in a variety of settings.

8.5.4 Diffuson and cooperon

We calculate the sums of ladder diagrams. For simplicity, we assume the white-noise disorder.

First, consider the **diffuson**, which a sum of ladder contributions to

$$\mathcal{D}(\mathbf{q},\omega) = (2\pi\nu\tau)^{-2} \int d^d(r-r') \langle G^R_{\epsilon+\omega}(\mathbf{r},\mathbf{r}') G^A_{\epsilon}(\mathbf{r}',\mathbf{r}) \rangle e^{-i\mathbf{q}(\mathbf{r}-\mathbf{r}')} \,. \tag{8.94}$$



We should sum the geometric series

$$\mathcal{D}(\mathbf{q},\omega) = \frac{1}{2\pi\nu\tau} \sum_{n=0}^{\infty} \left[\frac{1}{2\pi\nu\tau} \int (dp) G^R_{\epsilon+\omega}(\mathbf{p}+\mathbf{q}) G^A_{\epsilon}(\mathbf{p}) \right]^n \tag{8.95}$$

Calculate the integral in Eq. (8.95):

$$\int (dp) G^R_{\epsilon+\omega}(\mathbf{p}+\mathbf{q}) G^A_{\epsilon}(\mathbf{p}) \simeq \nu \int d\xi_p \, d\Omega \, \frac{1}{(\omega - \xi_p - v_F q \cos\theta + \frac{i}{2\tau})(-\xi_p - \frac{i}{2\tau})} \,, \tag{8.96}$$

where θ is the angle between $\mathbf{p}$ and $\mathbf{q}$. We perform an expansion in frequency and momentum, which is valid under the following conditions:

$$ql, \ \omega\tau \ll 1 \,. \tag{8.97}$$

We keep leading contributions coming from non-zero $\mathbf{q}$ and ω, which means expansion up to the first order in ω and the second order in $\mathbf{q}$:

$$\int (dp) G^R_{\epsilon+\omega}(\mathbf{p}+\mathbf{q}) G^A_{\epsilon}(\mathbf{p}) \ \simeq \ \nu \int d\xi_p \, d\Omega \left[\frac{1}{(-\xi_p + \frac{i}{2\tau})(-\xi_p - \frac{i}{2\tau})} \right.$$

$$+ \quad \frac{1}{(-\xi_p+\frac{i}{2\tau})^3(-\xi_p-\frac{i}{2\tau})}\, v_F^2 q^2\cos^2\theta - \frac{1}{(-\xi_p+\frac{i}{2\tau})^2(-\xi_p-\frac{i}{2\tau})}\,\omega\Bigg]\,. \tag{8.98}$$

The integrals over ξ_p belong to the following family of integrals that are easily evaluated via the Cauchy's residue theorem:

$$\int d\xi\, \frac{1}{(\xi+\frac{i}{2\tau})(\xi-\frac{i}{2\tau})^n} = -2\pi i\,(i\tau)^n\,. \tag{8.99}$$

Sometimes one needs integrals of a more general class that can also be straightforwardly evaluated:

$$\int d\xi\, \frac{1}{(\xi+\frac{i}{2\tau})^m(\xi-\frac{i}{2\tau})^n} = 2\pi i^{n-m}\,\frac{(m+n-2)!}{(m-1)!(n-1)!}\,\tau^{m+n-1} \tag{8.100}$$

The integrals over ξ_p in (8.98) are of the type (8.99) with $n = 1$, 2, and 3. Substituting their values as given by Eq. (8.99) into (8.98), we get

$$\int (dp) G^R_{\epsilon+\omega}(\mathbf{p}+\mathbf{q}) G^A_\epsilon(\mathbf{p}) \simeq 2\pi\nu\tau[1-\tau(Dq^2-i\omega)]\,, \tag{8.101}$$

where

$$D = \frac{v_F^2\tau}{d} \tag{8.102}$$

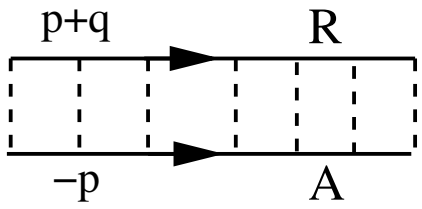
is the diffusion coefficient. Substituting this in Eq. (8.95), we get the final result for the diffuson:

$$\boxed{\mathcal{D}(\mathbf{q},\omega) = \frac{1}{2\pi\nu\tau^2}\,\frac{1}{Dq^2-i\omega}\,.} \tag{8.103}$$

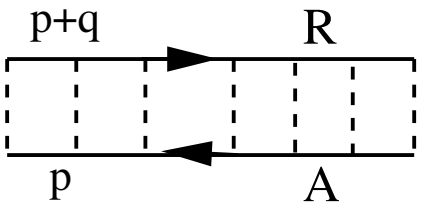
The $1/(Dq^2-i\omega)$ from of the propagator is known as "diffusion pole", since $\mathcal{D}(q,\omega)$ is the classical diffusion propagator. Indeed, its Fourier transform satisfies the diffusion equation

$$\left(\frac{\partial}{\partial t} - D\nabla_r^2\right)\mathcal{D}(r-r',t-t') = \frac{1}{2\pi\nu\tau^2}\,\delta(r-r')\delta(t-t')\,. \tag{8.104}$$

To calculate the weak-localization correction, which results from interference of time-reversed paths, we will need another type of ladder diagrams: the **cooperon** $\mathcal{C}(q,\omega)$:



Cooperon $\mathcal{C}(q,\omega)$



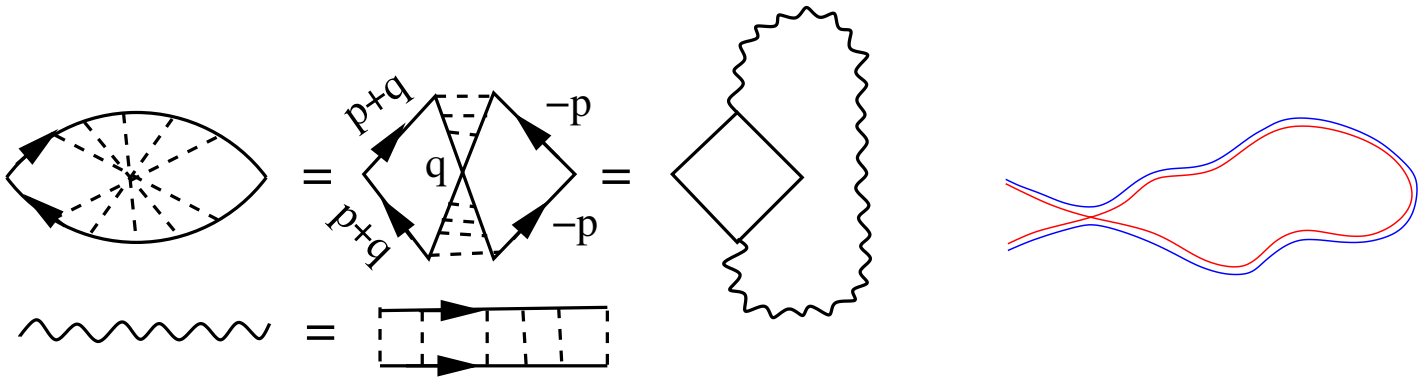
Diffuson $\mathcal{D}(q,\omega)$

If the time-reversal symmetry is preserved (no magnetic field), we have $G^A_\epsilon(\mathbf{p}) = (\epsilon - p^2/2m - i/2\tau)^{-1} = G^A_\epsilon(-\mathbf{p})$. Therefore, expressions for diagrams in the cooperon ladder are identical to those in the diffuson ladder, i.e.,

$$\mathcal{C}(q,\omega) = \mathcal{D}(q,\omega) = \frac{1}{2\pi\nu\tau^2}\,\frac{1}{Dq^2-i\omega}\,. \tag{8.105}$$

8.5.5 Weak-localization correction to conductivity

The weak-localization correction to conductivity is given by the sum of maximally crossed diagrams. The diagrams can be redrawn to make clear that they involve a cooperon loop. In the third representation below, the cooperon ladder is replaced by a wavy line. Physically, the cooperon loop corresponds to interference of time-reversed paths.



The corresponding expression reads:

$$\Delta\sigma_{\rm WL} = \frac{e^2}{2\pi}\int (dp)(dq)\frac{p_x+q_x}{m}\,\frac{-p_x}{m}\,G^R_{\epsilon+\omega}(\mathbf{p}+\mathbf{q})G^A_{\epsilon}(\mathbf{p}+\mathbf{q})G^R_{\epsilon+\omega}(-\mathbf{p})G^A_{\epsilon}(-\mathbf{p})\frac{1}{2\pi\nu\tau^2}\,\frac{1}{Dq^2-i\omega}\,. \tag{8.106}$$

The cooperon momentum q and the frequency ω are small, see Eq. (8.97). We neglect q and ω everywhere except for cooperon propagator. The p and q integrals then fully decouple. The p integral yields

$$\int (dp)\frac{p_x}{m}\,\frac{-p_x}{m}\,G^R_{\epsilon}(\mathbf{p})G^A_{\epsilon}(\mathbf{p})G^R_{\epsilon}(-\mathbf{p})G^A_{\epsilon}(-\mathbf{p}) = -\nu\frac{v_F^2}{d}\int d\xi_p\,\frac{1}{(\xi_p+\frac{i}{2\tau})^2(\xi_p-\frac{i}{2\tau})^2} = -\nu\frac{v_F^2}{d}4\pi\tau^3\,. \tag{8.107}$$

Thus, we get

$$\Delta\sigma_{\rm WL} = -\frac{e^2}{2\pi}\frac{v_F^2}{d}4\pi\nu\tau^3\frac{1}{2\pi\nu\tau^2}\int\frac{(dq)}{Dq^2-i\omega} = -e^2\,\frac{D}{\pi}\int\frac{(dq)}{Dq^2-i\omega}\,. \tag{8.108}$$

It also instructive to write down this result in the following form:

$$\Delta\sigma_{\rm WL} = -\sigma_0\frac{1}{\pi\nu}\int\frac{(dq)}{Dq^2-i\omega}\,, \tag{8.109}$$

where $\sigma_0 = e^2\nu v_F^2\tau/d$ is the zero-frequency Drude conductivity. It is worth emphasizing that the correction is negative: the weak-localization effect reduces the conductivity.

Let us analyze the result (8.108). The behavior of the integral over the cooperon momentum q depends crucially on the spatial dimensionality.

3D system. The integral over q is formally UV divergent. It should be cut off at $q\sim l^{-1}$, in view of the condition (8.97). The result reads

$$\Delta\sigma_{\rm WL} = -\frac{e^2}{(2\pi)^2}\left(\frac{\sim 1}{l}-\frac{1}{L_\omega}\right)\,, \qquad {\rm 3D}\,, \tag{8.110}$$

where

$$L_\omega = \left(\frac{D}{-i\omega}\right)^{1/2} \tag{8.111}$$

has a dimension of length. The dominant part of the correction (8.110) is controlled by the UV cutoff, $q \sim l^{-1}$; it is small compared to the Drude conductivity as

$$\Delta\sigma_{\rm WL}/\sigma_0 \sim (k_F l)^{-2} \ll 1\,. \tag{8.112}$$

We have kept in Eq. (8.110) also the subleading contribution, which depends on ω.

2D system. The integral over q is now logarithmic, with l^{-1} serving as UV cutoff and $\sim L_\omega^{-1}$ as IR cutoff. This yields

$$\Delta\sigma_{\rm WL} = -\frac{e^2}{2\pi^2}\ln\frac{L_\omega}{l}\ , \qquad {\rm 2D}\,. \tag{8.113}$$

Quasi-1D system. Now the q integral is fully determined by the infrared cutoff $\sim L_\omega^{-1}$.

$$\Delta\sigma_{\rm WL} = -\frac{e^2}{2\pi}L_\omega\ , \qquad \text{quasi-1D} \tag{8.114}$$

What we consider here is not strictly 1D system but rather quasi-1D geometry. i.e., a wire with transverse dimensions much smaller than the length L. The 1D conductivity is defined as the conductance of the wire multiplied by its length.

Crucially, the WL correction diverges in the limit $L_\omega \to \infty$ (i.e., $\omega \to 0$) for spatial dimensionality $d \leq 2$. Since the correction is negative, and the conductivity cannot become negative, the formulas will stop working in this limit. However, they imply some dramatic change of the behavior at sufficiently small ω. As we discuss below, the IR divergence of the weak-localization correction signals strong Anderson localization.

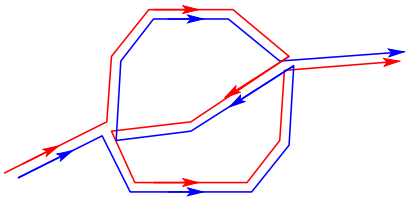
In this analysis, we considered conductivity of a non-interacting system of infinite size at finite frequency ω. Correspondingly, the IR cutoff length was set by frequency, Eq. (8.111). In a more general situation, the IR cutoff L_ω in the above formulas for $\Delta\sigma_{\rm WL}$ will be replaced by

$$L_\omega \ \longrightarrow\ \min\{L_\omega, L, L_\phi\}, \tag{8.115}$$

where L is the system size and L_ϕ is the dephasing length due to interaction-induced inelastic processes (electron-electron, electron-phonon, ... scattering).

What we have calculated is the leading, i.e. one-loop, weak-localization correction. Here "one-loop" refers to the cooperon loop. There are also higher-order (two-loop, three-loop, etc.) corrections, where counting of loops refers to diffusons and cooperons. When the one-loop correction is relatively small (see the analysis below), higher-loop corrections are still smaller.

Two paths corresponding to a two-loop diagram (with three diffusons). Drawing the corresponding diagram for the conductivity is left as an exercise.



8.6 Anderson localization

Consider the case $\omega = 0$ (i.e. $L_\omega = \infty$), with the infrared cutoff set by the system size L.

We recall that we consider a non-interacting system, which means that there is no dephasing, $L_\phi = \infty$. One can also consider an interacting Fermi-liquid system at $T = 0$; then one also has $L_\phi = \infty$ since inelastic processes governing the dephasing are absent at $T = 0$.

For convenience, assume that the systems has equal dimensions in all directions (i.e. it is $L \times L$ for 2D or $L \times L \times L$ in 3D). It is convenient to speak about the conductance $G = \sigma L^{d-2}$ ($G = 1/R$ where R is the resistance).

8.6.1 Quasi-1D system

Classically:

$$G_0(L) = \frac{\sigma_0}{L}\,. \tag{8.116}$$

Including the weak-localization correction (8.114) with $L_\omega \mapsto \sim L$, we obtain

$$G(L) = G_0(L) - C_1 \frac{e^2}{2\pi\hbar}\,. \tag{8.117}$$

Here $C_1 \sim 1$ is a numerical coefficient. To determine it, one should evaluate an analog of Eq. (8.108) with $\omega = 0$ and in a finite 1D system (i.e., with integration over q becoming a summation). The result is $C_1 = 1/3$ (for a spinless system).

For clarity, we have restored $\hbar$ in Eq. (8.117) (which we set to unity in most of the formulas). The combination $e^2/h \approx (25\,\mathrm{k\Omega})^{-1}$ is the quantum unit of the conductance. It is convenient to define the dimensionless conductance

$$g = \frac{G}{e^2/h}\,. \tag{8.118}$$

In these notations, Eq. (8.117) takes the from

$$g(L) = g_0(L) - C_1\,, \qquad g_0(L) = \frac{(h/e^2)\,\sigma_0}{L}\,. \tag{8.119}$$

We see that the weak-localization regime can extend only up to lengths $L \sim (h/e^2)\,\sigma_0$. For larger lengths, the formula (8.119) would yield a negative conductance, which can not be correct. What happens in reality is that at the length $L \sim (h/e^2)\,\sigma_0$ the system enters the strong-localization regime. In larger systems, wave functions are exponentially localized:

$$|\psi^2(x)| \sim \exp\{-|x - x_0|/\xi\}\,, \tag{8.120}$$

where

$$\xi \sim (h/e^2)\,\sigma_0 \tag{8.121}$$

is the localization length. As a result, the conductance decays exponentially with increasing L:

$$g(L) \propto \exp(-L/\xi)\,, \qquad L \gg \xi\,. \tag{8.122}$$

The localization length ξ, Eq. (8.121), can be also presented as

$$\xi \sim \nu D \sim \nu_{3\mathrm{D}} S\, v_F l \sim m p_F\, S\, v_F l \sim N l\,, \tag{8.123}$$

where S is the transverse cross-section and

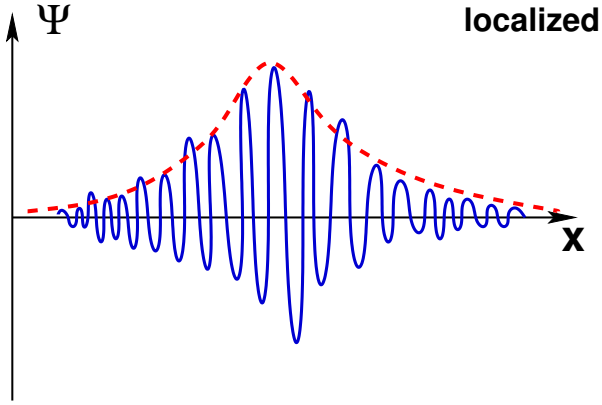
$$N \sim p_F^2 S \tag{8.124}$$

is the number of transverse channels. For a strictly 1D system, $N = 1$ and $\xi \sim l$, so that there is no room for a diffusive behavior: the ballistic regime (essentially no disorder) at $L \ll \xi$ crosses over directly into the localized regime at $L \gg \xi$.

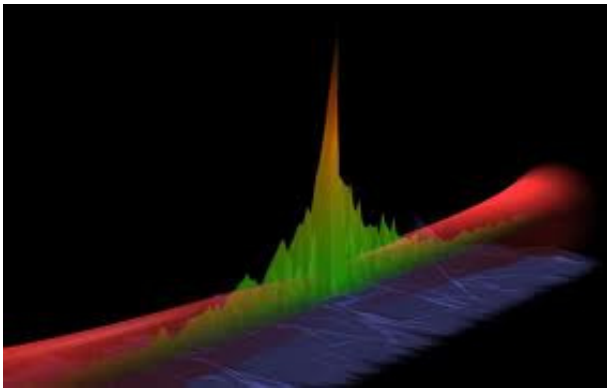
Let us summarize:

- In (quasi-)1D systems all states are localized for an arbitrarily weak disorder.
- The localization length ξ is of the order of the length of a sample with the resistance $R \sim h/e^2 \approx 25\,\mathrm{k\Omega}$.

- For $L > \xi$ (i.e., $R > 25\,\mathrm{k}\Omega$), the resistance increases exponentially with the length L.



Schematic view of localized 1D wave function



Localized 1D atomic Bose-Einstein condensate; Billy et al (Aspect group), Nature 2008

8.6.2 2D system

In 2D, the conductance $G(L)$ is equal to the conductivity $\sigma(L)$. According to Eq. (8.113), we have

$$G(L) = \sigma_0 - \frac{e^2}{2\pi^2\hbar} \ln \frac{L}{l}\,, \tag{8.125}$$

or, equivalently, for the dimensionless conductance

$$g(L) = g_0 - \frac{1}{\pi} \ln \frac{L}{l}\,, \tag{8.126}$$

where

$$g_0 = \frac{\sigma_0}{e^2/2\pi} = \frac{e^2 \nu v_F^2 \tau/2}{e^2/2\pi} = \frac{k_F l}{2} \gg 1. \tag{8.127}$$

The condition $k_F l \gg 1$ is the condition of weak disorder: the mean free path is much larger than the wave length.

The conductance decreases logarithmically with L in 2D, see Eq. (8.126). The localization length ξ is the value of L at which Eq. (8.126) would predict $g = 0$. This yields:

$$\xi \sim l \exp(\pi g_0)\,. \tag{8.128}$$

At $L \gg \xi$ the system is in the strong-localization regime. Thus, like in the (quasi-)1D geometry, all states are localized also in 2D systems. However, the localization length increases exponentially with g_0.

These results for the localization length ξ in 1D and 2D geometries have been obtained above from the extrapolation of the one-loop weak-localization correction. They can be proven by using a mapping of the localization problem to an effective field theory—replica (or supersymmetric) sigma-model. While we cannot present the sigma-model theory in this course in detail, we will give a brief outline below.

8.6.3 3D system

For weak disorder, $k_F l \gg 1$, the weak-localization correction is small: $\Delta\sigma_{\mathrm{WL}}/\sigma_0 \sim (k_F l)^{-2} \ll 1$, see Eq. (8.112). Thus, the states remain delocalized. The length dependence of dimensionless conductance $g(L)$ is

$$g(L) = \tilde{\sigma}_0 L + C_3\,, \tag{8.129}$$

where $\tilde{\sigma}_0 = \sigma_0 - \Delta\sigma_{\rm WL}(L \to \infty)$ and $C_3 \sim 1$.

On the other hand, for strong disorder ($k_F l \lesssim 1$) states become localized also in 3D (and in fact in any dimensionality). This was proven in the famous paper "Absence of diffusion in certain random lattices" by P. W. Anderson in 1958 (Nobel Prize 1977).

Idea of the proof: Consider a tight-binding model on, say, cubic lattice, with hopping V and random potential on every site with magnitude W:

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{\langle ij \rangle} t(c_i^\dagger c_j + c_j^\dagger c_i) \tag{8.130}$$

Here ϵ_i are random energies, with distribution width W: $\quad -W/2 \le \epsilon_i \le W/2$.

Consider the strong-disorder regime: $W \gg t$. To the leading order ($t/W \to 0$), every eigenstate is localized on a single site. Consider an eigenstate that is localized on a given site j_0. Develop a perturbation theory in t/W around this limit. To the first order, there will be admixture of states from sites directly adjacent to j_0, with the amplitude $\sim t/W$. To the second order, second-nearest-neighbors, i.e. sites on distance 2 from j_0 will get admixed, with the amplitude $\sim (t/W)^2$, and so on. This implies that the wave function amplitude on a site a distance r from j_0 is $\sim (t/W)^r \equiv \exp\{-r \ln(W/t)\}$, which is the exponential localization. Anderson proved that this is indeed a controllable perturbative expansion. (This is by far not trivial, as we deal with a disordered system, and rare realizations may violate the condition of applicability of perturbation theory.)

8.6.4 Scaling theory of localization. Anderson transition.

The scaling theory of localization is a heuristic theory proposed by Abrahams, Anderson, Licciardello, and Ramakrishnan (AALR) in 1979. It has been later justified through the mapping to an effective sigma-model field theory, see a discussion below.

The central idea of the scaling theory is that the conductance $g(L)$ is the only important characteristics of the system. In particular, change of the conductance with L is determined only by $g(L)$. This allows one to formulate the one-parameter scaling theory:

$$\frac{d \ln g(L)}{d \ln L} = \beta(g(L))\,, \tag{8.131}$$

where $\beta(g)$ is so-called β-function. Equation (8.131) has a form of the RG flow of a coupling constant in a field theory characterized by a single coupling. The outstanding guess of AALR was that there exists such a theory for the localization problem and that the conductance plays the role of the corresponding coupling.

Let us check that Eq. (8.131) is compatible with the behavior at large and small $g(L)$ and calculate the leading behavior of the β-function in these regimes.

- Large g: Weak-localization regime

(i) Classical behavior:

$$g(L) = \sigma_0 L^{d-2} \qquad \longrightarrow \qquad \beta(g) = d - 2\,. \tag{8.132}$$

(ii) Include weak-localization correction:

Quasi-1D system. According to Eq. (8.119), we have

$$g(L) = \frac{(h/e^2)\,\sigma_0}{L}\left(1 - C_1 \frac{L}{(h/e^2)\,\sigma_0}\right)\,, \tag{8.133}$$

so that

$$\frac{d\ln g(L)}{d\ln L} = -1 + \frac{d}{d\ln L}\ln\left(1 - C_1\frac{L}{(h/e^2)\,\sigma_0}\right) \simeq -1 - C_1\frac{L}{(h/e^2)\,\sigma_0} \simeq -1 - \frac{C_1}{g(L)}\,. \quad (8.134)$$

This has indeed the form of the one-parameter scaling equation (8.131): the r.h.s. of Eq. (8.134) depends only on $g(L)$. The corresponding β-function reads

$$\beta(g) \simeq -1 - \frac{C_1}{g}\,. \quad (8.135)$$

In this calculation, we kept the weak-localization correction to the leading order only, so that Eq. (8.135) should be understood as two leading orders of the expansion in $1/g$.

2D system. According to Eqs. (8.126) and (8.127), we have

$$g(L) = g_0\left(1 - \frac{1}{\pi g_0}\ln\frac{L}{l}\right)\,, \quad (8.136)$$

so that

$$\frac{d\ln g(L)}{d\ln L} = -\frac{1}{\pi g_0} \simeq -\frac{1}{\pi g(L)}\,. \quad (8.137)$$

This has again the form of Eq. (8.131) with

$$\beta(g) \simeq -\frac{1}{\pi g}\,. \quad (8.138)$$

3D system. According to Eq. (8.129), we have

$$g(L) = \tilde{\sigma}_0 L\left(1 + \frac{C_3}{\tilde{\sigma}_0 L}\right)\,, \quad (8.139)$$

so that

$$\frac{d\ln g(L)}{d\ln L} \simeq 1 - \frac{C_3}{\tilde{\sigma}_0 L} \simeq 1 - \frac{C_3}{g(L)}\,. \quad (8.140)$$

This has the form of Eq. (8.131) with

$$\beta(g) \simeq 1 - \frac{C_3}{g}\,. \quad (8.141)$$

Summarizing, for spatial dimensionality d, the one-loop β-function is

$$\beta(g) \simeq d - 2 - \frac{C_d}{g}\,, \qquad C_2 = \frac{1}{\pi}\,. \quad (8.142)$$

- Small g: Strong localization regime.

In this regime, the conductance decays exponentially with L:

$$g(L) \sim e^{-L/\xi}\,, \quad (8.143)$$

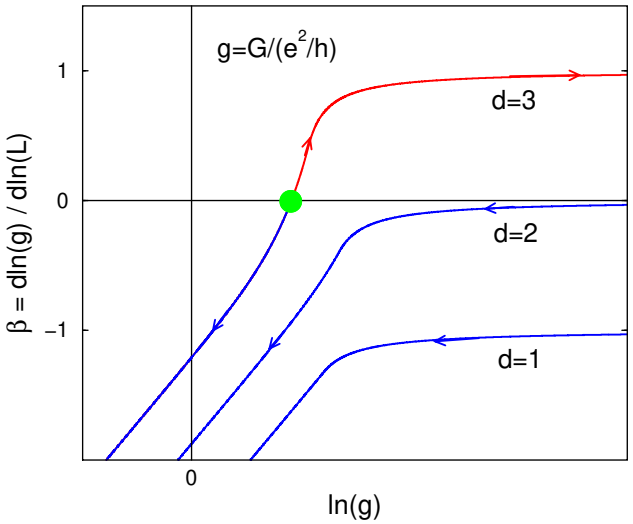
so that

$$\frac{d\ln g(L)}{d\ln L} \simeq -\frac{d}{d\ln L}\,\frac{L}{\xi} = -\frac{L}{\xi} = \ln g(L)\,. \tag{8.144}$$

This is also in full agreement with the one parameter scaling, Eq. (8.131), with

$$\beta(g) \simeq \ln g(L)\,. \tag{8.145}$$

Combining the large-g (strong localization) and small-g results, one gets the behavior of $\beta(g)$ as shown in the figure:



Beta-function $\beta(g)$ plotted vs $\ln g$.

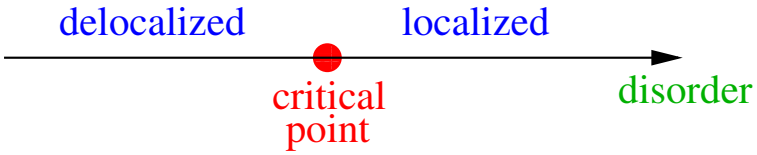
The arrows indicate the flow of $g(L)$ with increasing L.

In 1D and 2D (or, more generally, for $d \leq 2$ if one allows also fractal dimensions), the system flows from weak-localization to strong-localization with increasing L. In the thermodynamic limit the system is always an insulator: $g \to 0$ at $L \to \infty$.

On the other hand, in 3D (or, more generally, for $d > 2$) the system undergoes a phase transition: **Anderson localization transition**, also known as Anderson metal-insulator transition or, simply, Anderson transition. The transition point g_* is determined by the condition

$$\beta(g_*) = 0\,. \tag{8.146}$$

For $g > g_*$ the system flows (with increasing L) towards the metallic fixed point, $g = \infty$, while for $g < g_*$ the flow is towards the localization fixed point $g = 0$. The initial (small-system-size) value $g(l)$ can be changed by varying some parameter of the system, e.g., the strength of disorder or the energy. Therefore, under such variation the system (in the thermodynamic limit $L \to \infty$) undergoes the Anderson localization transition:



Let us analyze the critical behavior near the transition. For this purpose, we expand the β-function in the vicinity of the critical point g_*:

$$\beta(g) \simeq \beta'(g_*)\,(g - g_*)\,. \tag{8.147}$$

According to the definition of the β-function,

$$\frac{dg}{g\,\beta(g)} = d\ln L\,. \tag{8.148}$$

We consider the system which is close to the transition, i.e., $g(l) \simeq g_*$. Define the localization (correlation) length ξ as such length for which $g(\xi) = ag_*$ with $a - 1 \sim 1$. For example, we can take $a = 1/2$ on the localized side and $a = 2$ on the delocalized side. This is the length on which the system crosses over from the critical regime ($g \simeq g_*$) to the localized ($g \ll g_*$) or delocalized ($g \gg g_*$) regime. Integrating Eq. (8.148), we obtain

$$\int_{g(l)}^{ag_*} \frac{dg}{g_*\beta'(g_*)\,(g - g_*)} \simeq \ln\frac{\xi}{l}\,, \tag{8.149}$$

which yields

$$\ln\frac{\xi}{l} \simeq \frac{1}{g_*\beta'(g_*)} \ln\frac{1}{|g(l) - g_*|}\,. \tag{8.150}$$

The short-scale conductance $g(l)$ is a smooth function of a control parameter (disorder, strength, energy, ...) that is used to cross the transition. For definiteness, let's assume that this parameter is energy E. The Anderson-transition critical point E_c is then called the mobility edge. We have

$$g(l) - g_* \propto E - E_c\,. \tag{8.151}$$

Substituting this in Eq. (8.150) and exponentiating, we find the scaling of the localization (resp., correlation) length ξ:

$$\xi \propto |E - E_c|^{-\nu}\,, \tag{8.152}$$

where ν is the critical index given by

$$\nu = \frac{1}{g_*\beta'(g_*)}\,. \tag{8.153}$$

Another important exponent is the index s that governs the scaling of the conductivity on the delocalized side of the transition. It is directly related to ν. Indeed, for $L \gg \xi$ the conductance shows, to the leading approximation, the conventional (classical) scaling:

$$g(L) \sim g(\xi) \left(\frac{L}{\xi}\right)^{d-2} \sim g_* \left(\frac{L}{\xi}\right)^{d-2}\,. \tag{8.154}$$

Thus, the conductivity is

$$\sigma = \lim_{L\to\infty} \frac{\sigma(L)}{L^{d-2}} \sim \frac{g_*}{\xi^{d-2}} \propto (E - E_c)^s\,, \tag{8.155}$$

where

$$s = \nu(d - 2)\,. \tag{8.156}$$

Analytical calculation of the critical exponents in 3D is not possible, since the critical point is $g_* \sim 1$ and no small parameter is available. One can, however, consider the transition in spatial dimensionality $d = 2 + \epsilon$ with $\epsilon \ll 1$. Then, according to Eq. (8.142), the β-function is

$$\beta(g) \simeq \epsilon - \frac{1}{\pi g}\,, \tag{8.157}$$

yielding the critical point

$$g_* = \frac{1}{\pi\epsilon} \gg 1\,. \tag{8.158}$$

Substituting Eqs. (8.157) and (8.158) into (8.153) and (8.156), we get

$$\nu = \frac{1}{g_*\beta'(g_*)} = \pi g_* = \frac{1}{\epsilon}\,, \qquad s = 1\,. \tag{8.159}$$

Substituting here formally $\epsilon = 1$ to describe a 3D system, one would get $\nu = s = 1$. While this is a meaningful rough approximation, it is not an exact value of the exponent. The correct value, as obtained by numerical simulations, is $\nu = s \approx 1.57$. The difference is fully expected, since the exponents (8.159) are obtained in the leading order in $\epsilon \ll 1$. By calculating higher-loop contributions to the β-function (up to now has been done up to the four-loop order), one can obtain higher orders of the ϵ expansion for critical exponents.

We have demonstrated above that the scaling equation (8.131) is in agreement with the one-loop diagrammatic results for the weak-localization correction. One can check that this agreement remains when higher loops are taken into account. In fact, already on the two-loop level, Eq. (8.131) makes a very non-trivial prediction that can be verified diagrammatically. Specifically, to the two-loop order we expect for a 2D system

$$\beta(g) = -\frac{1}{\pi g} + \frac{C_2^{(2)}}{g^2} + O(g^{-3}) \,, \tag{8.160}$$

where $C_2^{(2)}$ is a numerical coefficient. Substituting this in Eq. (8.148) and integrating it from l (with $g(l) = g_0$) till L, one finds

$$g(L) = g_0 - \frac{1}{\pi} \ln \frac{L}{l} + \frac{C_2^{(2)}}{g_0} \ln \frac{L}{l} + \dots \,, \tag{8.161}$$

where $(\dots)$ means terms of still higher orders in $1/g_0$. A remarkably property of the two-loop contribution is the absence of the term $\sim (1/g_0) \ln^2(L/l)$. Indeed, the relative smallness of the one-loop term as compared to the classical term g_0 is $\Delta g^{(1)}_{\rm WL}/g_0 \sim (1/g_0) \ln(L/l)$, which is the factor resulting from the cooperon loop $\int (dq)/\nu D q^2$. One could thus expect for the two-loop contribution $\Delta g^{(2)}_{\rm WL}/g_0 \sim (1/g_0^2) \ln^2(L/l)$. However, such term is absent in Eq. (8.161), which is thus a non-trivial prediction. It is confirmed by diagrammatic calculation: while individual two-loop diagrams do produce such contributions, their cancel when all diagrams are summed up.

As it has been introduced above, the (8.131) is a heuristic theory. We have explained that it is in agreement with weak-localization diagrammatics in one-loop and two-loop order. One can also derive it in a fully systematic way. The path goes through the derivation of the **low-energy effective field theory** of disordered fermions. The strategy is largely analogous to the one that was used in course of derivation of the Ginzburg-Landau theory for superconductivity in Sec. 6.3. In particular, it includes Hubbard-Stratonovich transformation introducing an appropriate bosonic field, integrating out fermions, spontaneous symmetry breaking, and gradient and frequency expansion of the bosonic action (that has a form of a functional determinant). The resulting effective theory has a form of the so-called non-linear σ-model. The coupling constant of this theory is exactly the conductance $g(L)$, and the propagators of the σ-model field correspond to ladder diagrams of the original theory—diffusons and cooperons. Performing the RG analysis, one obtains the RG flow equation for $g(L)$, which has the form (8.131).

This effective theory (σ-model) is useful in many other respects. In particular, for quasi-1D geometry one can solve it exactly and thus obtain exact results for the conductance $g(L/\xi)$ in the whole range of L/ξ and for various other observables.

8.7 Mesoscopic conductance fluctuations

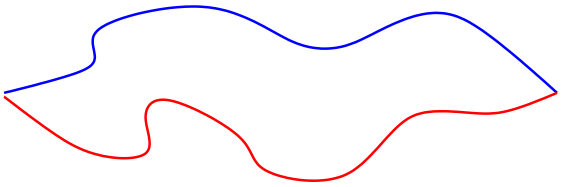
Consider now fluctuations of the conductance from one realizations to another. Such fluctuations in a disordered system are called mesoscopic. We focus on the "metallic" regime,

when the system conductance is large $g \gg 1$. We will see that the fluctuations are relatively small—in comparison with the average value. On the other hand, we will see that they are anomalously large—in comparison with classical expectation—due to quantum interference effects.

We begin with a qualitative discussion in spirit of Sec. 8.5.3. Let us recall that, from the point of view of the path-integral representation for two Green's functions, the quantum interference contribution to the conductance is given by non-diagonal contributions

$$G_{\text{quantum interference}} \sim \sum_{j \neq k} A_j A_k^* \, e^{i(S_j - S_k)} \,. \tag{8.162}$$

In the calculation of the average conductance $\langle G \rangle$, such terms did not contribute, apart from special cases of time-reversed paths and their higher-loop analogs.

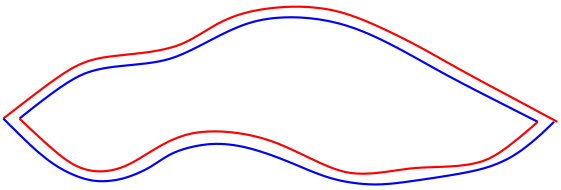


However, such terms do contribute when we calculate the variance of the conductance:

$$\begin{aligned} \langle (\delta G)^2 \rangle \sim \left\langle \left(\sum_{j \neq k} A_j A_k^* \, e^{i(S_j - S_k)} \right)^2 \right\rangle &= \left\langle \sum_{j \neq k} A_j A_k^* \, e^{i(S_j - S_k)} \sum_{j' \neq k'} A_{j'}^* A_{k'} \, e^{-i(S_{j'} - S_{k'})} \right\rangle \\ &\sim \sum_{j \neq k} \langle |A_j|^2 \rangle \langle |A_k|^2 \rangle \,, \end{aligned} \tag{8.163}$$

where we kept terms with $j = j'$ and $k = k'$ for which the phase factors cancel.

This corresponds to "pairing" of paths coming from different conductance loops:

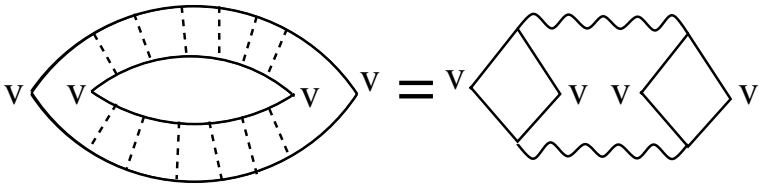


The corresponding diagrams are shown below. The conductivity in a given realization of disorder is, according to Eq. (8.38),

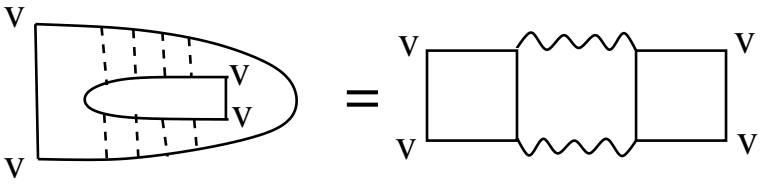
$$\sigma_{xx}(\omega) \simeq \frac{e^2}{2\pi V} \mathrm{tr} \, \hat{v}_x \, G_\epsilon^R \, \hat{v}_x \, G_\epsilon^A \,. \tag{8.164}$$

To calculate the variance, $\langle (\delta\sigma)^2 \rangle = \langle \sigma^2 \rangle - \langle \sigma \rangle^2$, we should draw two such conductivity bubbles and connect them by impurity lines. We already know that the dominant contribution will be given by diagrams with $G^R G^A$ ladders. It is easy to see that one can insert two ladders – connecting G^R of the first bubble with G^A of the second and vice versa. The ladders can be either diffusons or cooperons, depending on the relative directions of arrows in the bubble. Each diffuson diagram has its cooperon counterpart; they give equal contributions. In the second representation of each diagram in the figure, the diffuson / cooperon is represented by a wavy line.

(a)



(b)



Let us calculate the diagram (a). Choose arrow directions such that we have duffusons. (The diagram with cooperons will give exactly the same contribution.) Each of the two boxes formed by four Green's functions has the same form as was already encountered when we were calculating the weak-localization correction, see Eq. (8.107):

$$\int (dp) \frac{p_x^2}{m^2} G_\epsilon^R(\mathbf{p}) G_\epsilon^A(\mathbf{p}) G_\epsilon^R(\mathbf{p}) G_\epsilon^A(\mathbf{p}) = \nu \frac{v_F^2}{d} \int d\xi_p \frac{1}{(\xi_p + \frac{i}{2\tau})^2 (\xi_p - \frac{i}{2\tau})^2} = \nu \frac{v_F^2}{d} 4\pi\tau^3 . \quad (8.165)$$

We thus have for this diagram

$$\langle (\delta\sigma)^2 \rangle_a = V \left(\frac{e^2}{2\pi V} \right)^2 (4\pi\nu\tau^2 D)^2 \frac{1}{V} \sum_{\mathbf{q}} \left(\frac{1}{2\pi\nu\tau^2 D \mathbf{q}^2} \right)^2 = 4 \left(\frac{e^2}{2\pi V} \right)^2 \sum_{\mathbf{q}} \left(\frac{1}{\mathbf{q}^2} \right)^2 , \quad (8.166)$$

where $V = L^d$ is the system volume. We wrote $(1/V)\sum_{\mathbf{q}}$ instead of $\int (dq)$ since the sum over momenta will be determined by the smallest $q \sim L^{-1}$. (If one writes it as $\int (dq)$ at cuts off at $q \sim L^{-1}$, one obtains a correct estimate but cannot determine the numerical coefficient.) The dimensionless conductance g is related to the conductivity σ via

$$g = \frac{G}{e^2/h} \overset{\hbar=1}{=} \frac{G}{e^2/2\pi} = \frac{\sigma L^{d-2}}{e^2/2\pi} , \quad (8.167)$$

so that Eq. (8.166) yields

$$\langle (\delta g)^2 \rangle_a = \frac{4}{L^4} \sum_{\mathbf{q}} \left(\frac{1}{\mathbf{q}^2} \right)^2 = \frac{4}{\pi^4} \sum_{\mathbf{m}} \left(\frac{1}{\mathbf{m}^2} \right)^2 , \quad (8.168)$$

where we used the quantization conditions

$$q_i = \frac{\pi m_i}{L} . \quad (8.169)$$

We already see that (8.168) yields just a number of order unity. To calculate the number, one should specify the boundary conditions on the diffuson that determine allowed values of m_i in Eq. (8.169). We consider the current through a sample in x direction, so that it is connected to metallic reservoirs (leads) in x direction and to vacuum (or, more generally, insulator) in y and z directions. The corresponding boundary conditions on the diffuson $\mathcal{D}(\mathbf{r}, \mathbf{r}')$ are

$$\mathcal{D}(\mathbf{r}, \mathbf{r}') = 0 \quad \text{on boundaries with leads;} \quad (8.170)$$

$$\mathbf{n}\boldsymbol{\nabla}\mathcal{D}(\mathbf{r}, \mathbf{r}') = 0 \quad \text{on boundaries with insulator (no current),} \quad (8.171)$$

where $\mathbf{n}$ is the vector normal to the surface. This determines the values of m_i:

$$\langle (\delta g)^2 \rangle_a = \frac{4}{\pi^4} \sum_{\mathbf{m}} \left(\frac{1}{\mathbf{m}^2} \right)^2 , \qquad m_x = 1, 2, 3, \dots , \qquad m_{y,z} = 0, 1, 2, \dots \quad (8.172)$$

The diagram (b) is calculated in the same way. More precisely, there are two such diagrams with diffusons. Their contribution is found to be $\langle(\delta g)^2\rangle_b = (1/2)\langle(\delta g)^2\rangle_a$. Taking into account cooperon diagrams yields an additional overall factor of two, so that the overall result reads

$$\langle(\delta g)^2\rangle = \frac{12}{\pi^4}\sum_{\mathbf{m}}\left(\frac{1}{\mathbf{m}^2}\right)^2, \qquad m_x = 1,2,3,\dots, \qquad m_{y,z} = 0,1,2,\dots \tag{8.173}$$

As an example, consider quasi-1D geometry. Then $m_y = m_z = 0$, and Eq. (8.173) reduces to

$$\langle(\delta g)^2\rangle = \frac{12}{\pi^4}\sum_{m_x=1,2,3,\dots}\frac{1}{m_x^4} = \frac{12}{\pi^4}\,\frac{\pi^4}{90} = \frac{2}{15}\,. \tag{8.174}$$

These are the results for a spinless system. For a spinful system, the conductivity is multiplied by two, so that $\langle(\delta g)^2\rangle$ acquires an additional factor of 4. In particular, $\langle(\delta g)^2\rangle = 8/15$ in quasi-1D geometry.

Remarkably, $\langle(\delta g)^2\rangle$ is a number of order unity, independent of system size (or any microscopic parameters). It depends only on the geometry of the system. For this reason, these fluctuations are called **universal conductance fluctuations (UCF)**.

Let us demonstrate that UCF are anomalously strong. Classically, one would expect

$$\frac{\langle(\delta g)^2\rangle_{\text{classical}}}{g^2} \propto \frac{1}{V} = L^{-d} \quad \Longrightarrow \quad \langle(\delta g)^2\rangle_{\text{classical}} \propto L^{d-4}\,. \tag{8.175}$$

Thus, on the classical level, fluctuations should vanish, $\langle(\delta g)^2\rangle_{\text{classical}} \to 0$ at $L \to \infty$ for $d < 4$. The UCF are thus indeed anomalously strong, which is a result of quantum coherence throughout the whole system.

Comments:

• The universality of conductance fluctuations requires $L \ll L_T, L_\phi$, where $L_T \sim (D/T)^{1/2}$ is the thermal length and L_ϕ is the dephasing length due to interaction-induced inelastic scattering. At zero temperature, both L_T and L_ϕ are infinite, so that this condition is automatically fulfilled. With increasing temperature (and at fixed L), the condition gets violated, leading to suppression of fluctuations. At high temperatures, such that $L \gg L_\phi$, the scaling of $\langle(\delta g)^2\rangle$ with L becomes classical, Eq. (8.175).

• Experimentally, UCF are best observed by weakly varying the magnetic field B. Traces $g(B)$ demonstrating these fluctuations are termed "magnetofingerprints".

• UCF are very sensitive to global symmetries of the system. Breaking the time reversal symmetry reduces UCF by factor of 2 (diagrams with cooperons are "killed"); breaking the spin-rotational symmetry in a spinful system reduces them by factor of 4.

8.8 Interaction effects in quantum transport in disordered systems

In this Section, we study effects of electron-electron interaction on properties of a disordered system.

8.8.1 Generalities

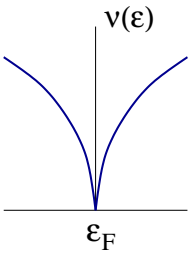
Quite generally, interaction effects can be divided into two classes:

I. Renormalization

- Fermi liquid: real part of the self-energy $\mathrm{Re}\,\Sigma(\epsilon, \mathbf{p})$, which results in
  ▷ renormalization of velocity, $v \mapsto v_*$ (or, equivalently, of the effective mass, $m \mapsto m_*$);
  ▷ renormalization of quasiparticle pole residue Z (instead of 1 in the absence of interaction)

- Luttinger liquid:
  ▷ tunneling density of states, Eq. (7.152):

$$\nu(\epsilon, T) \sim \nu^{(0)} \left(\frac{\max(|\epsilon|, T)}{\Lambda} \right)^{\gamma} ; \tag{8.176}$$



  ▷ renormalization of impurity strength, Eqs. (7.185) and (7.217)

- Kondo effect: renormalization of scattering of conduction electrons off a magnetic impurity (next Chapter)

- Fermi-edge singularity in X-ray absorption spectra

- ...

The renormalization is governed by **virtual processes**, i.e., by those with energy transfer $\gtrsim T$. Thus, it becomes stronger when T is lowered, may lead to singularities at $T \to 0$.

II. Inelastic processes. Dephasing.

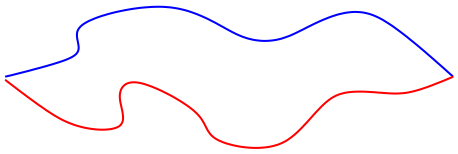
Real inelastic-scattering processes, energy transfer $\lesssim T$. Become weaker when T is lowered, vanish in the limit $T \to 0$.

- Fermi liquid: imaginary part of the mass-shell self-energy $\mathrm{Im}\,\Sigma(\mathbf{p}, \epsilon_p^*)$, which determines the quasiparticle decay rate

$$\Gamma = \frac{1}{2\tau_p} = Z\,\mathrm{Im}\,\Sigma(\mathbf{p}, \epsilon_p^*) \propto T^2\,, \tag{8.177}$$

  see Eq. (3.274). The T^2 scaling in Eq. (8.177) corresponds to the decay rate of thermal excitations, $\epsilon_p^* \sim T$; in general, one has $\left\{\max(\epsilon_p^*, T)\right\}^2$.

- Quite generally, inelastic processes determine the **dephasing time** τ_ϕ that serves as an infrared (i.e. long-time) cutoff for quantum interference phenomena. Consider interference resulting from addition of two amplitudes corresponding, in the path integral framework, to particle propagation along two different paths; see general discussion of interference phenomena in the beginning of Sec. 8.7.



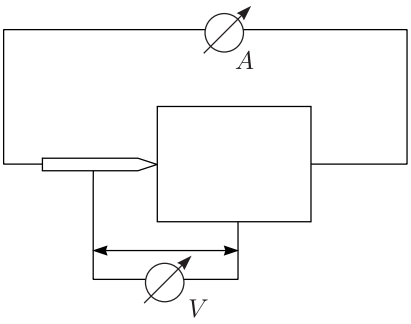
  Imagine that the particle, while propagating along one of the path experiences an inelastic scattering and thus emits an electron-hole pair (or a phonon, a photon, etc – depending on the interaction involved). Then the final states for these two amplitudes are different, and they cannot be added, so that the interference breaks down. Therefore, interference takes place only if the time of propagation along the interfering paths is

$$t \lesssim \tau_\phi, \tag{8.178}$$

where the dephasing (or, equivalently, **decoherence**) time τ_ϕ is essentially the shortest out of inelastic scattering times. For electrons in metals, the relevant inelastic times are usually the electron-electron scattering time τ_{ee} (dominant for low temperatures) and the electron-phonon scattering time τ_{e-ph} (dominant for higher temperatures).

This general discussion applies to a variety of quantum interference phenomena: weak localization, mesoscopic conductance fluctuations, Aharonov-Bohm effect in rings, double-slit experiment, etc.

8.8.2 Tunneling density of states in a disordered system: Renormalization by interaction



We consider first the effect of electron-electron interaction on the tunneling density of states (DOS) $\nu(\epsilon)$ that can be studied experimentally by measuring the differential tunneling conductance $g(V) = \partial I/\partial V$. We have discussed it before in the context of the Luttinger liquid, see Sec. 7.7.5.

The tunneling DOS is given by

$$\nu(\epsilon) = -\frac{1}{\pi}\mathrm{Im}\,\left\langle G^R(\mathbf{r},\mathbf{r};\epsilon)\right\rangle = -\frac{1}{\pi}\mathrm{Im}\int (dp)\langle G^R\rangle(\mathbf{p};\epsilon)\,, \tag{8.179}$$

where $\langle\ldots\rangle$ denotes the disorder averaging. The Green's function in a given disorder realization is

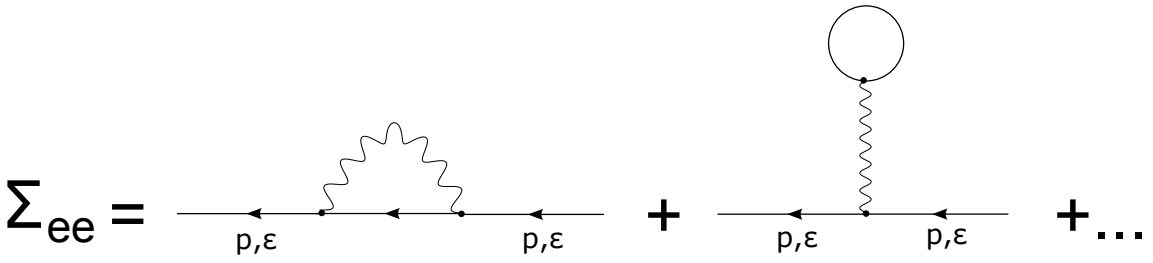
$$G^R = \left[\left(G^R_{(0)}\right)^{-1} - \Sigma^R_{ee}\right]^{-1} = G^R_{(0)} + G^R_{(0)}\Sigma^R_{ee}G^R_{(0)} + \ldots\,, \tag{8.180}$$

where $G^R_{(0)}$ is the non-interacting Green's function and Σ^R_{ee} is the self-energy induced by electron-electron interaction. It is important that both $G^R_{(0)}$ and Σ_{ee} correspond here to the same realization of disorder; the disorder averaging has not been done yet!

We will evaluate the interaction-induced correction to tunneling DOS perturbatively in the interaction U. Thus, we focus on the term of the first order in Σ_{ee} in Eq. (8.180); its contribution to Eq. (8.179) reads

$$\Delta\nu(\epsilon) = -\frac{1}{\pi}\mathrm{Im}\int (dp)\langle G^R_{(0)}\Sigma^R_{ee}G^R_{(0)}\rangle(\mathbf{p};\epsilon)\,. \tag{8.181}$$

The leading-order diagrams for the self-energy are (in a given disorder realization):



exchange (Fock) Hartree

For simplicity, we perform the calculation in $T = 0$ technique; generalization to finite T

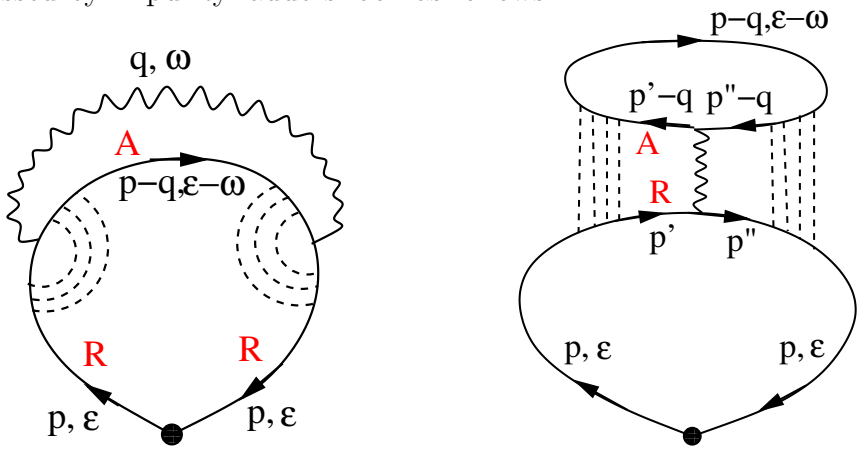
(Matsubara formalism) is rather straightforward. We recall that at $T = 0$ the Green function satisfies, see Eq. (3.98),

$$G(\epsilon) = \begin{cases} G^R(\epsilon) & \text{for} \quad \epsilon > 0, \\ G^A(\epsilon) & \text{for} \quad \epsilon < 0. \end{cases} \tag{8.182}$$

Thus, for $\epsilon > 0$, Eq. (8.181) is equivalently written as

$$\Delta\nu(\epsilon) = -\frac{1}{\pi}\mathrm{Im} \int (dp) \langle G_{(0)} \Sigma_{ee} G_{(0)} \rangle (\mathbf{p}; \epsilon) \, . \tag{8.183}$$

As for other physical observables that we have calculated above, main contributions come from diagrams with impurity ladders (in the present case, diffusons), which represent effects governed by phase coherence over large spatial scales. Since the external lines are retarded (R), the ladders can be inserted when the internal fermionic line is advanced (A), i.e. when the energy on this line satisfies $\epsilon - \omega < 0$. The exchange and Hartree diagrams for $\Delta\nu(\epsilon)$ dressed by impurity ladders look as follows:



Let us calculate the exchange diagram (the left one):

$$\begin{aligned} \Delta\nu^{\mathrm{ex}}(\epsilon) &= -\frac{1}{\pi}\,\mathrm{Im} \int (dp) \int (dq) \int_\epsilon^\infty d\omega \, (2\pi\nu\tau)^2 \left[\frac{1}{2\pi\nu\tau^2 (Dq^2 - i\omega)} \right]^2 \\ &\times \frac{1}{(\epsilon - \xi_p + \frac{i}{2\tau})^2} \, \frac{1}{\epsilon - \omega - \xi_{\mathbf{p}-\mathbf{q}} - \frac{i}{2\tau}} \, iU(\mathbf{q}, \omega) \, . \end{aligned} \tag{8.184}$$

The factor i originates from i^n, where n is the order of the perturbation theory in U (here $n = 1$). As in previous calculations (weak localization, mesoscopic conductance fluctuations), we can neglect ω and q in the denominator of the fermionic Green's function. The integration over $\mathbf{p}$ and $\mathbf{q}$ then decouple; the $\mathbf{p}$ integration yields, according to Eq. (8.99),

$$\int (dp) \frac{1}{(\epsilon - \xi_p + \frac{i}{2\tau})^2} \, \frac{1}{\epsilon - \omega - \xi_{\mathbf{p}-\mathbf{q}} - \frac{i}{2\tau}} \simeq \nu \int d\xi_p \frac{1}{(\epsilon - \xi_p + \frac{i}{2\tau})^2} \, \frac{1}{\epsilon - \xi_p - \frac{i}{2\tau}} = -2\pi i \nu \tau^2 \, . \tag{8.185}$$

We thus get for the exchange correction to DOS

$$\frac{\Delta\nu^{\mathrm{ex}}(\epsilon)}{\nu} = -\frac{1}{\pi}\mathrm{Im} \int (dq) \int_\epsilon^\infty d\omega \, U(q, \omega) \frac{1}{(Dq^2 - i\omega)^2} \, . \tag{8.186}$$

Here we kept for generality the ω dependence of the (effective) interaction $U(q, \omega)$. It is important for the case of long-range (Coulomb) interaction, when one should take into account

the dynamical screening of the interaction by the disordered fermionic system. For a short-range interaction we have $U(q)$ instead of $U(q,\omega)$. Furthermore, we can replace $U(q) \mapsto U(0)$, since the integral is governed by small q. Evaluating the ω integral, we obtain

$$\frac{\Delta\nu^{\rm ex}(\epsilon)}{\nu} = -\frac{1}{\pi}U(0)\,{\rm Im}\int (dq)\frac{i}{Dq^2 - i\epsilon} = -\frac{1}{\pi}U(0)\int (dq)\frac{Dq^2}{(Dq^2)^2+\epsilon^2}\,. \tag{8.187}$$

The expression for the interaction correction (8.187) is remarkably similar to the (real part of) weak localization correction (8.109) to the conductivity. The behavior in different spatial dimensionalities is correspondingly fully analogous to that found for the weak-localization correction in Sec. 8.5.5:

$$\frac{\Delta\nu^{\rm ex}(\epsilon)}{\nu} = -\frac{1}{\pi}U(0)\times\begin{cases} \dfrac{-1}{4\pi\sqrt{2}}\,\dfrac{\epsilon^{1/2}}{D^{3/2}} + {\rm const}\,, & {\rm 3D}\,,\\ \dfrac{1}{4\pi D}\ln\dfrac{1}{\epsilon\tau}\,, & {\rm 2D}\,,\\ \dfrac{1}{2\sqrt{2}}\,\dfrac{1}{(\epsilon D)^{1/2}}\,. & {\rm 1D}\,. \end{cases} \tag{8.188}$$

The expression for Hartree contribution [the right diagram below Eq. (8.183)] has almost the same structure as that for the exchange contribution, with the following modifications: (i) interaction line $U(q,\omega) \mapsto \overline{U(\mathbf{p}-\mathbf{p}',0)}$, where the bar means averaging over momenta $\mathbf{p}$ and $\mathbf{p}'$ on the Fermi surface, (ii) minus sign due to the internal fermionic loop, (iii) in the case of a spinful system: factor 2, due to summation over spin polarization in the internal loop. Thus, we obtain, by including the Hartree term in Eq. (8.186),

$$\frac{\Delta\nu(\epsilon)}{\nu} = -\frac{1}{\pi}\,{\rm Im}\int (dq)\int_\epsilon^\infty d\omega\left[U(q,\omega) - 2\overline{U(\mathbf{p}-\mathbf{p}',0)}\right]\frac{1}{(Dq^2 - i\omega)^2}\,. \tag{8.189}$$

For a short-range interaction $U(q)$, this takes the form [extension of Eq. 8.187]

$$\frac{\Delta\nu(\epsilon)}{\nu} = -\frac{1}{\pi}\left[U(0) - 2\overline{U(\mathbf{p}-\mathbf{p}',0)}\right]\int (dq)\frac{Dq^2}{(Dq^2)^2+\epsilon^2}\,. \tag{8.190}$$

Equations (8.189) and (8.189) are written for a spinful system; in the case of a spinless (spin-polarized) system, the factor 2 in the Hartree term should be omitted.

If the range of interaction is substantially larger than the Fermi wave length, the exchange term dominates. In the case of repulsive interaction, this implies that the correction is negative: the tunneling DOS is suppressed due to interaction. Let us estimate the magnitude of the effect. Assume a dimensionless interaction strength of order unity, $\nu U(0) \sim 1$. Consider the 1D geometry: a wire of length L. We have, according to Eq. (8.188),

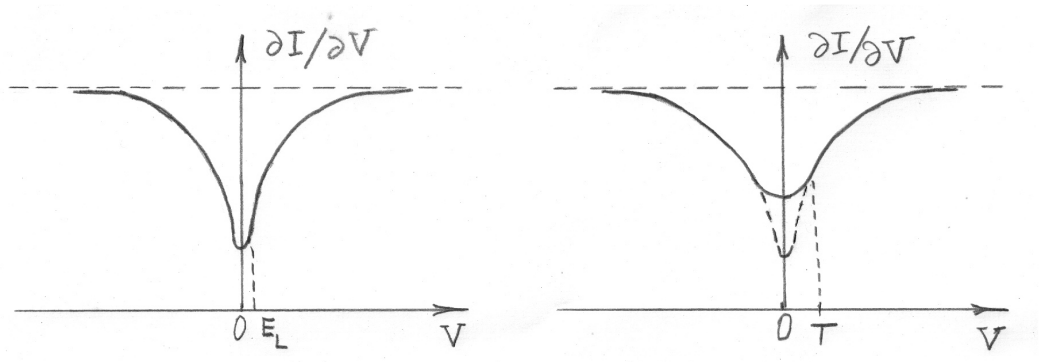
$$\frac{\Delta\nu(\epsilon)}{\nu} \sim -\frac{1}{\nu(\epsilon D)^{1/2}}\,. \tag{8.191}$$

The smallest energy ϵ for which the calculation holds is $\epsilon \sim D/L^2 \equiv E_L$ (known as Thouless energy), since we replaced the sum over $\mathbf{q}$ by an integral when obtaining Eq. (8.188). For smaller energies $\epsilon \ll E_L$, the sum over momenta is cut off by L^{-1}, and one gets $\Delta\nu(\epsilon) \simeq \Delta\nu(E_L)$. Thus, the magnitude of the effect is

$$\frac{\Delta\nu(E_L)}{\nu} \sim -\frac{1}{\nu(D/L)} \sim -\frac{L}{\xi}\,, \tag{8.192}$$

where ξ is the localization length (8.123). Thus, the correction remains relatively small, $|\Delta\nu|/\nu \ll 1$ as long as the system is short ("metallic"), $L \ll \xi$. On the other hand, at the crossover to the strong localization, $L \sim \xi$, the correction becomes large, $|\Delta\nu|/\nu \sim 1$. For strongly localized ("insulating") samples, $L \gg \xi$, the tunneling DOS gets in general strongly suppressed for small energies ϵ. (One speaks in this context about a "soft gap".) The perturbative calculation is clearly not sufficient to evaluate the specific form of this suppression.

As was discussed in Sec. 7.7.5 in the context of Luttinger liquid, the interaction suppression of the tunneling DOS is observed in the form of **zero-bias anomaly** in tunneling conductance $\partial I/\partial V$:



$T = 0$ $\qquad\qquad$ $T > E_L$

Extensions (without derivation) and comments:

(i) The above calculations were done at zero temperature. For a finite temperature, one should use the Matsubara technique, with an analytical continuation. The result is as expected on physical grounds. For $T \ll \epsilon$, the zero-temperature results hold. For $T > \epsilon$, the energy ϵ in the above formulas is replaced by temperature T (see right panel of the figure).

(ii) The analysis can be extended to the case of long-range (Coulomb) interaction. In that case, one should take into account the dynamical screening of the interaction by the disordered fermionic system. The screening is weakened by the slow (diffusive) motion of fermions. Consequently, while the results are in general similar to those for short-range interaction, there is an additional enhancement of the ZBA. For example, in 2D one finds, instead of the logarithmic singularity (8.188) at $\epsilon \to 0$, a stronger, logarithm-squared singularity:

$$\frac{\Delta\nu(\epsilon)}{\nu} = -\frac{1}{8\pi^2\nu D}\left[\ln^2\frac{D\kappa^2}{\epsilon} - \ln^2 D\kappa^2\tau\right], \tag{8.193}$$

where $\kappa = 4\pi e^2\nu$ is the 2D Thomas-Fermi screening wave vector. Furthermore, in this case, one can proceed beyond the leading order of the perturbative expansion and find the suppression of tunneling DOS at still smaller energies, where the renormalized tunneling DOS is much smaller than the bare one:

$$\frac{\nu(\epsilon)}{\nu_0} = \exp\left\{-\frac{1}{8\pi^2\nu D}\left[\ln^2\frac{D\kappa^2}{\epsilon} - \ln^2 D\kappa^2\tau\right]\right\}. \tag{8.194}$$

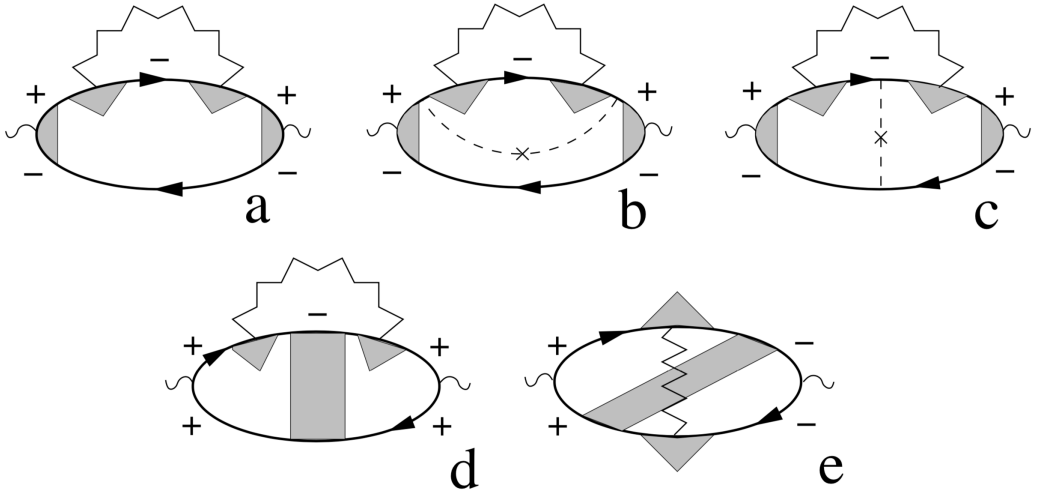
Note that the DOS vanishes even faster than a power law.

(iii) As is clear from Eq. (8.187), and is seen explicitly in the results (8.188), the interaction-induced renormalization correction in a disordered system is infrared-divergent (i.e. diverges in the limit $\epsilon \to 0$) for dimensionality $d \leq 2$. The 2D case serves as a borderline (logarithmic behavior of the perturbative correction). It is instructive to compare this with the behavior in

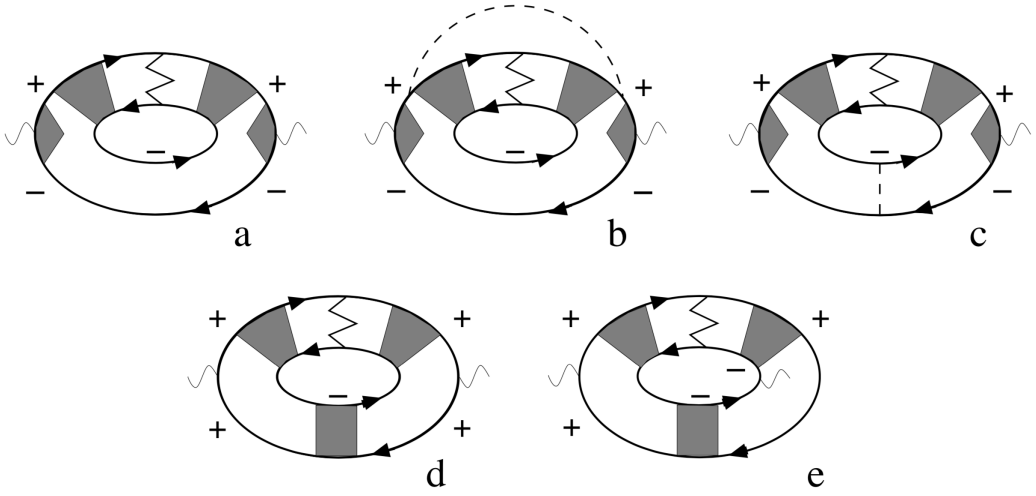
a clean system. There, perturbative renormalization corrections are infrared-divergent in $d \leq 1$ (implying a breakdown of the Fermi liquid), with logarithmic behavior in 1D, see Sec. 7.1. (It is this logarithmic perturbative divergence that yields, after proper resummation, the Luttinger-liquid behavior.) Therefore, disorder enhances the effect of interaction, by shifting the "critical dimension" (beyond which infrared divergencies occur) from $d = 1$ to $d = 2$. The physical reason for this is quite transparent: diffusing fermions spend more time in the vicinity of each other and thus interact more efficiently.

8.8.3 Interaction correction to conductivity

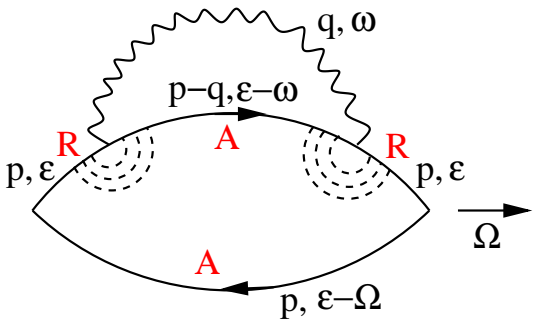
Similarly to the correction to tunneling DOS, there are interaction-induced corrections to the conductivity of exchange and Hartree types. We use diagrammatics for the conductivity of an interacting system based on the Kubo formula (8.23), (8.24). Here are the exchange diagrams ("+" and "−" mean "retarded" and "advanced", respectively; shaded blocks are diffuson ladders):



Each of the exchange diagrams has its Hartree counterpart:



To get the full set of leading-order diagrams (one-loop with respect to diffusons), one should also include diagrams obtained by flipping and/or replacement $+ \leftrightarrow -$. Let us calculate a typical diagram at $T = 0$ (diagram (a) of the exchange type), with the infrared cutoff set by the frequency Ω at which the conductivity is evaluated.



Here the external frequency $\Omega > 0$, satisfies $\Omega \ll 1/\tau$. Diffuson ladders can be inserted between retarded (R) and advanced (A) Green's function, which implies the following conditions:

$$\epsilon > 0\,, \qquad \epsilon - \Omega < 0\,, \qquad \epsilon - \omega < 0\,. \tag{8.195}$$

They determine the limits of integration over ϵ and ω:

$$\Delta\sigma^{\text{ex}-\text{a}}(\Omega) = \frac{1}{\Omega}\frac{e^2}{2\pi}\int (dp)(dq)\int_0^\Omega \frac{d\epsilon}{2\pi}\int_\epsilon^\infty \frac{d\omega}{2\pi} v_x^2 [G^R_\epsilon(p)]^2 G^A_{\epsilon-\Omega}(p) G^A_{\epsilon-\omega}(\mathbf{p}-\mathbf{q})\frac{iU(q,\omega)}{(Dq^2 - i\omega)^2\tau^2}\,. \tag{8.196}$$

Comments: (i) The formula is written for the spinless case; in the case of a spinful system to be multiplied by 2. (ii) There is a flipped diagram (a′), with the interaction line inserted in the lower fermionic line. It yields the same contribution as the diagram (a).

As in previous calculations within the disorder diagrammatic technique, we can neglect q and ω in arguments of fermionic Green functions. The p integral then gives [see general formula (8.100)]

$$\int (dp) v_x^2 [G^R(p)]^2 [G^A(p)]^2 = 4\pi\tau^2 \nu D\,, \tag{8.197}$$

so that Eq. (8.196) reduces to

$$\Delta\sigma^{\text{ex}-\text{a}}(\Omega) = \frac{\sigma_0}{2\pi^2\Omega}\int_0^\Omega d\epsilon \int (dq)\int_\epsilon^\infty d\omega\, \frac{iU(q,\omega)}{(Dq^2 - i\omega)^2} \tag{8.198}$$

As in the calculation of the correction to tunneling DOS, for a short-range interaction we can replace $U(q,\omega) \to U(0)$, which yields

$$\Delta\sigma^{\text{ex}-\text{a}}(\Omega) = -\frac{\sigma_0}{2\pi^2}\,U(0)\,\frac{1}{\Omega}\int_0^\Omega d\epsilon \int (dq)\frac{1}{Dq^2 - i\epsilon}\,. \tag{8.199}$$

Comparing to the results for the DOS correction, Eqs. (8.186) and (8.187), we see that

$$\frac{\Delta\sigma^{\text{ex}-\text{a}}(\Omega)}{\sigma_0} = \frac{1}{2\pi\Omega}\int_0^\Omega d\epsilon\,\frac{\Delta\nu^{\text{ex}}(\epsilon)}{\nu}\,. \tag{8.200}$$

Therefore, we find that for a short-range interaction $\Delta\sigma^{\text{ex}-\text{a}}(\Omega)/\sigma_0 \sim \Delta\nu^{\text{ex}}(\Omega)/\nu$, up to a numerical coefficient. An accurate calculation, including all diagrams, confirms this conclusion (it only modifies the numerical coefficient):

$$\frac{\Delta\sigma(\Omega)}{\sigma_0} \sim \frac{\Delta\nu(\Omega)}{\nu}\,. \tag{8.201}$$

In full analogy with the behavior of the weak-localization correction, Sec. 8.5.5, and of the tunneling DOS, Eq. (8.188), in various spatial dimensionalities, we have

$$\Delta\sigma(\Omega) \;\sim\; -\sigma_0 U(0)\int_{l_\Omega^{-1}}^{l^{-1}} \frac{(dq)}{Dq^2} \;\sim\; -e^2\nu U(0)\times \begin{cases} \left(\dfrac{D}{\Omega}\right)^{1/2}, & d=1\,, \\ \ln\dfrac{1}{\Omega\tau}\,, & d=2\,, \\ -\left(\dfrac{\Omega}{D}\right)^{1/2} + \text{const}, & d=3\,. \end{cases} \tag{8.202}$$

For finite temperature, the calculation can be performed in a fully analogous way by using the Matsubara formalism. The above (zero-T) results hold as long as $\Omega \gg T$. In the opposite case, $T \gg \Omega$ (which is usually the case in experiment), Ω is replaced by T.

8.8.4 Dephasing

As was discussed above (Sec. 8.8.1), the dephasing time τ_ϕ resulting from inelastic scattering properties sets the infrared cutoff for quantum interference phenomena. For sufficiently low temperatures, $1/\tau_\phi$ is dominated by electron-electron scattering. In a clean Fermi liquid, we would have

$$1/\tau_\phi(T) \sim 1/\tau_{ee}(\epsilon \sim T) \sim \frac{T^2}{E_F}\,. \tag{8.203}$$

(For simplicity, we assume that the dimensionless interaction strength is of order unity. This is not important for the discussion here.) As was pointed out above (see a comment in the end of Sec. 7.7.5), the interaction is enhanced by disorder. Thus, one can expect a much larger interaction-induced dephasing rate $1/\tau_\phi(T)$ in comparison with the clean Fermi-liquid formula (8.203). This is indeed the case. Skipping the derivation (exercise), we only present the result here:

$$\frac{1}{\tau_\phi(T)} \sim \begin{cases} \left(\dfrac{T}{\nu D^{1/2}}\right)^{2/3}, & \text{quasi-1D}\,, \\ \dfrac{T}{\nu D}\ln(\nu D)\,, & \text{2D}\,, \\ \dfrac{T^{3/2}}{\nu D^{3/2}}\,, & \text{3D}\,. \end{cases} \tag{8.204}$$

8.9 Outlook

Before closing the Chapter on quantum transport in disordered systems, let us list further important extensions, which have been a subject of active recent and current research:

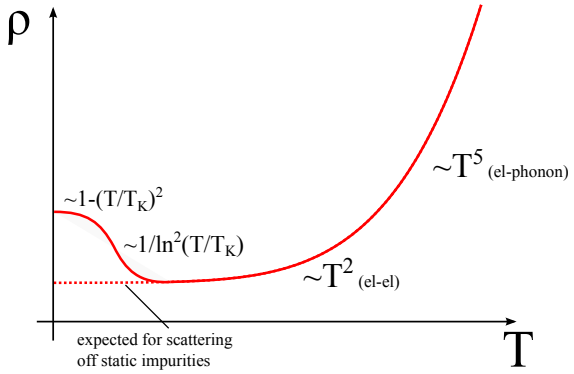
- Symmetry classification of disordered systems; field theories and localization phenomena in systems of various symmetry classes.
- Multifractality of critical wave functions as a hallmark of Anderson localization transitions.
- Classification of disordered topological insulators and superconductors; localization phenomena in topological matter (graphene, 3D Weyl / Dirac materials, surfaces of topological insulators and superconductors).

- Field theories of disordered interacting systems, renormalization group for disorder + interactions, metal-insulator and superconductor-insulator quantum phase transitions.
- "Many-body localization" (MBL): Breakdown of dephasing and ergodicity breaking at non-zero temperatures in disordered interacting systems, transitions between ergodic and MBL phases.

Chapter 9

Magnetic impurities and Kondo effect

Experimentally observed minimum in temperature dependence of resistance of some metals and alloys was a puzzle for approximately three decades (since the early 30s) . It was understood in the 60s due to works of Anderson and Kondo that the low-T increase with lowering temperature results from renormalization of electron scattering off magnetic impurities (local moments).



9.1 Anderson impurity model

The starting point of the theoretical analysis is the Anderson's model of a local magnetic moment. It describes a partly filled d or f orbital of an atom of transition metal, rare earth, or actinide element, coupled to a conduction band:

$$H = \sum_{\mathbf{k},\sigma} \epsilon_k c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_\sigma \epsilon_d n_{d,\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{\mathbf{k},\sigma} \left(V_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} d_\sigma + V^*_{\mathbf{k}} d^\dagger_\sigma c_{\mathbf{k},\sigma} \right) . \tag{9.1}$$

where $c^\dagger_{\mathbf{k},\sigma}$ is the creation operator of a conduction electron with momentum $\mathbf{k}$ and spin $\sigma =\uparrow,\downarrow$, while $d^\dagger_\sigma$ creates an electron with spin σ on the localized orbital. Further, $n_{d,\sigma} = d^\dagger_\sigma d_\sigma$. The first term in Eq. (9.1) is the kinetic energy of band electrons, the second term is the energy of the localized orbital, the third term is the Hubbard-like interaction that is operative when the orbital is doubly occupied (by electrons with opposite spin), and the last term describes hybridization between the band electrons and the orbital. The interaction $U > 0$ originates from Coulomb repulsion:

$$U = \int d\mathbf{r}\, d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} |\psi(\mathbf{r})|^2 |\psi(\mathbf{r}')|^2 , \tag{9.2}$$

where $\psi(\mathbf{r})$ is the wave function of the state on the localized orbital. The momentum dependence of the hybridization $V_{\mathbf{k}}$ is not essential; one can consider a model with $V_{\mathbf{k}} = V$ independent on $\mathbf{k}$.

In the absence of the hybridization with the continuum, the atomic orbital has four states:
▷ empty state with energy $E_0 = 0$,
▷ two degenerate states with single occupation, with energy $E_{1,\sigma} = \epsilon_d$,
▷ doubly occupied state with energy $E_2 = 2\epsilon_d + U$.

The corresponding eigenvalues of $\tilde{H}_d = H_d - \mu\, n_d$, where μ is the chemical potential (equal to the Fermi energy of the conduction band) are $\tilde{E}_0 = 0$ for zero occupation, $\tilde{E}_{1,\sigma} = \epsilon_d - \mu$ for single occupation and $\tilde{E}_2 = 2\epsilon_d + U - 2\mu$ for double occupation. Therefore, under the conditions

$$\epsilon_d - \mu < 0\,, \qquad \epsilon_d + U - \mu > 0, \tag{9.3}$$

the ground state of the orbital will be the doubly degenerate single-occupancy state with spin $S = \frac{1}{2}$, i.e., the local moment. We assume that these conditions are fulfilled. Furthermore, we will assume that the temperature is sufficiently low, $|\epsilon_d - \mu| \gg T$ and $\epsilon_d + U - \mu \gg T$, so that thermal occupations of the empty and doubly occupied states are negligible.

When the hybridization with the conduction band is included, electrons will be scattered by the local moment. Our goal will be to calculate the corresponding scattering rate. It is convenient to derive first an effective Hamiltonian by eliminating empty and doubly-occupied states of the orbital, thus mapping the Anderson impurity model to the Kondo model.

9.2 From Anderson model to Kondo model

We want to derive an effective Hamiltonian that keeps only two low-lying states (those with spin 1/2) on the orbital, projecting out the remaining two states (empty and doubly occupied). We want to include, however, transitions between the two local-moment states. They are possible in the second order of the perturbation theory and go either through the virtual doubly occupied state or through the virtual zero-occupancy state:

$$|\mathbf{k}_\downarrow;\uparrow\rangle \;\longrightarrow\; |0;\uparrow\downarrow\rangle \;\longrightarrow\; |\mathbf{k}'_\uparrow;\downarrow\rangle\,, \tag{9.4}$$

$$|\mathbf{k}_\downarrow;\uparrow\rangle \;\longrightarrow\; |\mathbf{k}_\downarrow\mathbf{k}'_\uparrow;0\rangle \;\longrightarrow\; |\mathbf{k}'_\uparrow;\downarrow\rangle\,. \tag{9.5}$$

Here we used the notation of the type $|\alpha;\beta\rangle$, where α means the state of relevant conduction electron(s) and β the state on the orbital. The total amplitude of these two processes is, according to the formulas of the second-order perturbation theory,

$$V_{\mathbf{k}'} V^*_{\mathbf{k}} \left(\frac{1}{\epsilon_{\mathbf{k}} - \epsilon_d} + \frac{1}{U + \epsilon_d - \epsilon_{\mathbf{k}}} \right) \equiv \frac{1}{2} J_{\mathbf{k}',\mathbf{k}}\,, \tag{9.6}$$

where we have set $\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}'}$ (both these energies can be replaced by the Fermi energy μ here). These processes induce the following term in the Hamiltonian:

$$\sum_{\mathbf{k},\mathbf{k}'} \frac{1}{2} J_{\mathbf{k}',\mathbf{k}} \left(c^\dagger_{\mathbf{k}',\uparrow} c_{\mathbf{k},\downarrow} S^- + c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\uparrow} S^+ \right)\,, \tag{9.7}$$

where S^α are the spin-1/2 operators corresponding to the local moment ($S^\pm = S^x \pm i S^y$). In view of the total spin symmetry, we can write the generated term in the spin-invariant form:

$$\sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k}',\mathbf{k}} \left(c^\dagger_{\mathbf{k}',\sigma'} s^\alpha_{\sigma'\sigma} c_{\mathbf{k},\sigma} \right) S^\alpha\,, \tag{9.8}$$

where s^α are spin-1/2 matrices (i.e. $\frac{1}{2}$ times the Pauli matrices). There is an implicit summation over the repeated index $\alpha = 1, 2, 3$.

The $s^z S^z$ terms that were not written in Eq. (9.7) correspond to second-order processes without spin flip:

$$|\mathbf{k}_\downarrow;\uparrow\rangle \;\longrightarrow\; |0;\uparrow\downarrow\rangle \;\longrightarrow\; |\mathbf{k}'_\downarrow;\uparrow\rangle\,, \tag{9.9}$$

$$|\mathbf{k}_\downarrow;\uparrow\rangle \;\longrightarrow\; |\mathbf{k}_\downarrow \mathbf{k}'_\uparrow;0\rangle \;\longrightarrow\; |\mathbf{k}'_\downarrow;\uparrow\rangle\,. \tag{9.10}$$

We thus obtain the Kondo model

$$H = \sum_{\mathbf{k},\sigma} \epsilon_k c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k}',\mathbf{k}} \left(c^\dagger_{\mathbf{k}',\sigma'} s^\alpha_{\sigma'\sigma} c_{\mathbf{k},\sigma}\right) S^\alpha\,. \tag{9.11}$$

For simplicity, we can discard the momentum dependence of $J_{\mathbf{k}',\mathbf{k}}$ and replace it by a constant J. Then, the model takes the form

$$\boxed{H = \sum_{\mathbf{k},\sigma} \epsilon_k c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + J \psi^\dagger_{\sigma'}(0) s^\alpha_{\sigma'\sigma} \psi_\sigma(0) S^\alpha\,,} \tag{9.12}$$

where $\psi^\dagger_\sigma(0) = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma}$ is the operator of creation of a band electron at the spatial point $\mathbf{r} = 0$ of the local moment. The generated interaction between the local moment S^α and the spin s^α of the conducting electrons is antiferromagnetic: $J > 0$.

The derivation of the Kondo model from the Anderson impurity model was first performed by Schrieffer and Wolff by means of a unitary transformation of the Hamiltonian (known as **Schrieffer-Wolff transformation**). In fact, an additional term is generated that does not depend on spin and correspond to a conventional potential scattering. It is not essential, so that we discard it.

9.3 Renormalization of scattering amplitude

The central quantity to be analyzed within the Kondo model is the scattering amplitude

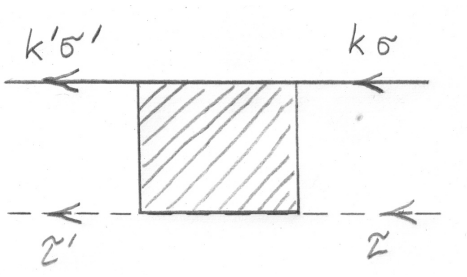
$$|\mathbf{k}\sigma,\, \tau\rangle \;\longrightarrow\; |\mathbf{k}'\sigma',\, \tau'\rangle\,, \tag{9.13}$$

where $\mathbf{k}\sigma$ denotes the state of the conducting electron and τ of the local moment. The scattering amplitude, also known as the T-matrix, is given by the mass-shell Green function without external legs, see Sec. 2.7:

$$G^R = G^R_0 + G^R_0 T^R G^R_0, \tag{9.14}$$

While we used the notation F for the T-matrix in Sec. 2.7, here we use the more conventional notation T. The amplitude of the process (9.13) is thus denoted as $T_{\mathbf{k}'\sigma',\,\tau';\,\mathbf{k}\sigma,\,\tau}$:

$T_{\mathbf{k}'\sigma',\,\tau';\,\mathbf{k}\sigma,\,\tau}$ =



(9.15)

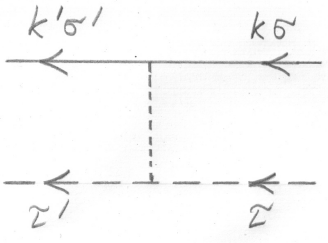
To develop a perturbative expansion for the scattering amplitude, we write the Kondo-model Hamiltonian (9.12) as $H = H_0 + H_{\rm imp}$, where H_0 is the Hamiltonian of free conduction electrons [first term in Eq. (9.12)] and $H_{\rm imp}$ describes the interaction with the magnetic impurity [second term in Eq. (9.12)]. The T-matrix is [see Eq. (2.71)]

$$T^R(\epsilon) = T(\epsilon + i0) \;=\; H_{\rm imp} + H_{\rm imp}(\epsilon + i0 - H_0)^{-1} H_{\rm imp}$$

$$+ \quad H_{\rm imp}(\epsilon + i0 - H_0)^{-1} H_{\rm imp}(\epsilon + i0 - H_0)^{-1} H_{\rm imp} + \dots \,. \qquad (9.16)$$

To the lowest order of the perturbation theory [first term on the r.h.s of Eq. (9.16)] we have

$$T^{(1)}_{\mathbf{k}'\sigma',\tau';\,\mathbf{k}\sigma,\tau} = J s^{\alpha}_{\sigma'\sigma} S^{\alpha}_{\tau'\tau} \,. \qquad (9.17)$$



(Here and below we use the convention of summation over repeated indices.) Now we inspect the second order:

$$\begin{aligned} T^{(2)}_{\mathbf{k}'\sigma',\tau';\,\mathbf{k}\sigma,\tau} &= \langle \mathbf{k}'\sigma',\, \tau' | H_{\rm imp}(\epsilon + i0 - H_0)^{-1} H_{\rm imp} | \mathbf{k}\sigma,\, \tau \rangle \\ &= J^2 \langle \mathbf{k}'\sigma',\, \tau' | \sum_{\mathbf{k_1},\mathbf{k}'_1} (c^{\dagger}_{\mathbf{k}'_1,\sigma'_1} s^{\alpha}_{\sigma'_1\sigma_1} c_{\mathbf{k}_1,\sigma_1})\, S^{\alpha} (\epsilon + i0 - H_0)^{-1} \sum_{\mathbf{k_2},\mathbf{k}'_2} (c^{\dagger}_{\mathbf{k}'_2,\sigma'_2} s^{\beta}_{\sigma'_2\sigma_2} c_{\mathbf{k}_2,\sigma_2})\, S^{\beta} | \mathbf{k}\sigma,\, \tau \rangle. \end{aligned} \qquad (9.18)$$

We need it on mass-shell, so that $\epsilon = \epsilon_{\mathbf{k}} = \epsilon'_{\mathbf{k}}$. There are two contributions:
(i) The right $H_{\rm imp}$ (which corresponds to an earlier time, as it acts first) annihilates the electron $\mathbf{k}\sigma$ of the initial state and creates $\mathbf{k}'_2\sigma'_2$ above the Fermi sea, the left (i.e. the second) $H_{\rm imp}$ annihilates $\mathbf{k}'_2\sigma'_2$ and creates $\mathbf{k}'\sigma'$ of the final state. This means

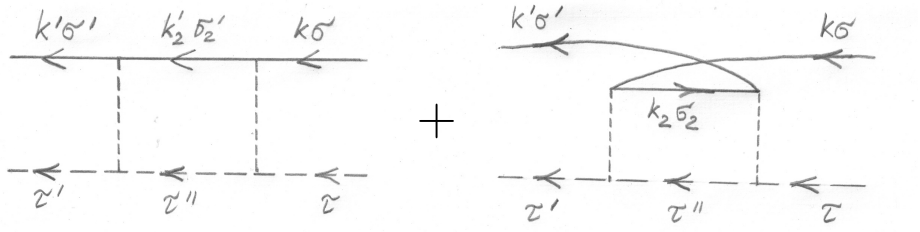
$$\mathbf{k}_2, \sigma_2 = \mathbf{k}, \sigma \,, \qquad \mathbf{k}_1, \sigma_1 = \mathbf{k}'_2, \sigma'_2, \qquad \mathbf{k}', \sigma' = \mathbf{k}'_1, \sigma'_1 \,. \qquad (9.19)$$

(ii) The first (right) $H_{\rm imp}$ annihilates an electron $\mathbf{k}_2\sigma_2$ from the Fermi sea (i.e. creates the corresponding hole) and creates an electron $\mathbf{k}'\sigma'$, the second (left) $H_{\rm imp}$ annihilates $\mathbf{k}\sigma$ and restores $\mathbf{k}_2\sigma_2$ (or, equivalently, annihilates the hole). This means

$$\mathbf{k}_1, \sigma_1 = \mathbf{k}, \sigma \,, \qquad \mathbf{k}'_1, \sigma'_1 = \mathbf{k}_2, \sigma_2, \qquad \mathbf{k}', \sigma' = \mathbf{k}'_2, \sigma'_2 \,. \qquad (9.20)$$

The diagrammatic representation of these two processes is as follows:

$$T^{(2)}_{\mathbf{k}'\sigma',\tau';\,\mathbf{k}\sigma,\tau} = \qquad (9.21)$$



Note that this diagram technique is somewhat different from the conventional Feynman diagrammatics since there is no Wick theorem for the local moment: spin operators do not satisfy the algebra of bosonic or fermionic creation and annihilation operators. On these diagrams, the time direction is explicit: from right to left. This diagrammatics can be equivalently obtained by using the expansion for the evolution operator in the interaction representation, Eq. (3.130), with $H_{\rm imp}$ being the interaction. Then the first-order term (3.128) yields (9.17), and the second-order term (3.129) yields exactly the contribution (9.18) that we are analyzing. See e.g. the book by Bruus and Flensberg for a detailed derivation of Matsubara diagrammatic rules.

The first diagram yields ($\epsilon = \epsilon_{\mathbf{k}} = \epsilon'_{\mathbf{k}}$)

$$\begin{aligned} T^{(2a)}_{\mathbf{k}'\sigma',\tau';\,\mathbf{k}\sigma,\tau} &= J^2 \sum_{\mathbf{k}'_2\sigma'_2\tau''} S^{\alpha}_{\tau'\tau''} S^{\beta}_{\tau''\tau} s^{\alpha}_{\sigma'\sigma'_2} s^{\beta}_{\sigma'_2\sigma} \, \frac{1}{\epsilon - \epsilon_{k'_2} + i0} \, [1 - f(\epsilon_{k'_2})] \\ &= J^2 (S^{\alpha} S^{\beta})_{\tau'\tau} (s^{\alpha} s^{\beta})_{\sigma'\sigma} \sum_{\mathbf{k}'_2} \frac{1}{\epsilon_k - \epsilon_{k'_2} + i0} \, [1 - f(\epsilon_{k'_2})] \, , \end{aligned} \tag{9.22}$$

where $f(\epsilon)$ is the Fermi distribution. The factor $1 - f(\epsilon_{k'_2})$ reflects the order of the operators corresponding to the internal fermionic line:

$$\langle c_{\mathbf{k}_1,\sigma_1} c^{\dagger}_{\mathbf{k}'_2,\sigma'_2} \rangle = [1 - f(\epsilon_{k'_2})] \delta_{\mathbf{k}_1,\mathbf{k}'_2} \delta_{\sigma_1,\sigma'_2} \, . \tag{9.23}$$

This is in agreement with the above physical picture of this process: the first (earlier in time) interaction operator creates the virtual state $\mathbf{k}'_2, \sigma'_2$, and the second annihilates it. At zero temperature this factor reduces to the summation going over momenta $k'_2 > k_F$.

In the same way, the second diagram yields

$$\begin{aligned} T^{(2b)}_{\mathbf{k}'\sigma',\tau';\,\mathbf{k}\sigma,\tau} &= -J^2 \sum_{\mathbf{k}_2\sigma_2\tau''} S^{\alpha}_{\tau'\tau''} S^{\beta}_{\tau''\tau} s^{\alpha}_{\sigma_2\sigma} s^{\beta}_{\sigma'\sigma_2} \, \frac{1}{\epsilon - (\epsilon_k + \epsilon_{k'} - \epsilon_{k_2}) + i0} \, f(\epsilon_{k_2}) \\ &= -J^2 (S^{\alpha} S^{\beta})_{\tau'\tau} (s^{\beta} s^{\alpha})_{\sigma'\sigma} \sum_{\mathbf{k}'_2} \frac{1}{-\epsilon_k + \epsilon_{k_2} + i0} \, f(\epsilon_{k_2}) \\ &= J^2 (S^{\alpha} S^{\beta})_{\tau'\tau} (s^{\beta} s^{\alpha})_{\sigma'\sigma} \sum_{\mathbf{k}'_2} \frac{1}{\epsilon_k - \epsilon_{k_2} - i0} \, f(\epsilon_{k_2}) \, . \end{aligned} \tag{9.24}$$

The overall minus sign in the first line of Eq. (9.24) originates from an odd permutation of fermionic operators needed for these contractions, see factor $(-1)^P$ in Eq. (3.152). The Fermi factor $f(\epsilon_{k_2})$ reflects the fact that here the virtual state with momentum $\mathbf{k}_2$ is a hole.

The renormalization effects that we are interested in are related to virtual processes (real part of $T^{(2)}$). We thus discard below $\pm i0$ in the denominators.

The conduction-electron spin operators s^{α} are $s^{\alpha} = \frac{1}{2}\sigma^{\alpha}$, where σ^{α} are Pauli matrices. We use the following identity for Pauli matrices:

$$(\sigma^{\alpha}\sigma^{\beta})_{p'p} = \delta_{\alpha\beta}\delta_{p'p} + i\epsilon_{\alpha\beta\gamma}\sigma^{\gamma}_{p'p} \, . \tag{9.25}$$

Thus, the (real part of) sum of (9.22) and (9.24) yields

$$\begin{aligned} T^{(2)}_{\mathbf{k}'\sigma',\tau';\,\mathbf{k}\sigma,\tau} &= J^2 (s^{\alpha} s^{\beta})_{\sigma'\sigma} \sum_{\mathbf{k}_2} \left\{ (S^{\alpha} S^{\beta})_{\tau'\tau} [1 - f(\epsilon_{k_2})] + (S^{\beta} S^{\alpha})_{\tau'\tau} f(\epsilon_{k_2}) \right\} \frac{1}{\epsilon_k - \epsilon_{k_2}} \\ &= \frac{J^2}{4} \sum_{\mathbf{k}_2} \frac{1}{\epsilon_k - \epsilon_{k_2}} \left\{ \delta_{\sigma'\sigma}\delta_{\tau'\tau} S(S+1) - 2 s^{\gamma}_{\sigma'\sigma} S^{\gamma}_{\tau'\tau} [1 - 2 f(\epsilon_{k_2})] \right\} \, . \end{aligned} \tag{9.26}$$

In the second line we used the identity (9.25), as well as

$$\epsilon_{\alpha\beta\gamma} S^{\alpha} S^{\beta} = \frac{1}{2} \epsilon_{\alpha\beta\gamma} [S^{\alpha}, S^{\beta}] = \frac{1}{2} \epsilon_{\alpha\beta\gamma} \epsilon_{\alpha\beta\delta} \, i S^{\delta} = i S^{\gamma} \, . \tag{9.27}$$

Note that Eq. (9.27) is general: it is not restricted to spin-1/2 of the local moment. While we considered $S = 1/2$ when deriving the Kondo model, it can be in fact formulated for any spin S, and the perturbative analysis also applies to any S.

The first term in the result (second line of) Eq. (9.26) is not particularly interesting: it does not contain a logarithmic singularity. (Such a term would arise also in the second order for conventional potential scattering.) We thus drop it. On the other hand, the second term does yield an infrared logarithm due to the additional factor $[1-2f(\epsilon_{k_2})]$ which changes sign together with $\epsilon_k - \epsilon_{k_2}$. Combining it with the first-order term (9.17), we obtain

$$\begin{aligned}\left[T^{(1)}+T^{(2)}\right]_{\mathbf{k}'\sigma',\tau';\,\mathbf{k}\sigma,\tau} &= Js^{\alpha}_{\sigma'\sigma}S^{\alpha}_{\tau'\tau}\left\{1-\frac{J}{2}\sum_{\mathbf{k}_2}\frac{1}{\epsilon_k-\epsilon_{k_2}}[1-2f(\epsilon_{k_2})]\right\} \\ &= Js^{\alpha}_{\sigma'\sigma}S^{\alpha}_{\tau'\tau}\left\{1-\frac{J}{2}\sum_{\mathbf{k}_2}\frac{\tanh(\epsilon_{k_2}/2T)}{\epsilon_k-\epsilon_{k_2}}\right\}. \qquad (9.28)\end{aligned}$$

At the Fermi level, $\epsilon_k = 0$, the sum over momenta of the virtual state in Eq. (9.28) yields

$$\sum_{\mathbf{k}_2}\frac{\tanh(\epsilon_{k_2}/2T)}{-\epsilon_{k_2}} \simeq -\nu\int d\epsilon_2\,\frac{\tanh(\epsilon_2/2T)}{\epsilon_2} \simeq -2\nu\ln\frac{\Lambda}{T}\,, \qquad (9.29)$$

where Λ is the ultraviolet cutoff (band width). On the infrared side, the logarithm is cut off by temperature. Substitution of (9.29) into (9.28) gives

$$T^{(1)}+T^{(2)} = Js^{\alpha}S^{\alpha}\left(1+\nu J\ln\frac{\Lambda}{T}\right). \qquad (9.30)$$

Equation (9.30) shows that the effective coupling increases logarithmically when temperature is lowered. This is the result originally obtained by Kondo, who used it to explain the resistivity minimum (see figure in the beginning of this chapter): increase of coupling means stronger scattering and therefore increase of resistivity (as discussed in more detail below).

This perturbative calculation is valid under the condition $T^{(2)} < T^{(1)}$. One can extend it by means of renormalization group (RG), which was done by Anderson. We briefly sketch the RG analysis. The general ideology of RG was discussed in Sec. 7.8.1 in the context of Luttinger-liquid theory. In spirit of this idea, we start from the theory with the UV cutoff Λ and then consecutively integrate out fast degrees of freedom and monitor how the effective coupling J changes. Integrating out the degrees of freedom from the shell $\Lambda' \equiv \Lambda/b < \epsilon_k < \Lambda$, we get, in analogy with Eq. (9.30), the following modification of the coupling constant:

$$J \;\mapsto\; J' = J + \nu J^2\ln\frac{\Lambda}{\Lambda'} \equiv J + \nu J^2\ln b\,. \qquad (9.31)$$

This can be written in a differential form:

$$\frac{dJ}{d\ln b} = \nu J^2\,, \qquad (9.32)$$

where J is the running coupling associated with the scale Λ/b. This equation can be immediately integrated:

$$\frac{dJ}{\nu J^2} = d\ln b \qquad \Longrightarrow \qquad (\nu J)^{-1} = (\nu J_0)^{-1} - \ln b \qquad \Longrightarrow \qquad J = \frac{J_0}{1-\nu J_0\ln b}\,, \qquad (9.33)$$

where J_0 is the bare coupling (i.e. the one at the initial cutoff Λ), and J is the effective coupling resulting from lowering the cutoff down to Λ/b. The renormalization will be stopped by the temperature T. Setting $b = \Lambda/T$, we get for the renormalized dimensionless coupling νJ:

$$\nu J = \frac{\nu J_0}{1-\nu J_0\ln(\Lambda/T)} = \frac{1}{\ln(T/T_K)}\,, \qquad (9.34)$$

where T_K is the Kondo temperature,

$$T_K = \Lambda \exp\left(-\frac{1}{\nu J_0}\right) . \tag{9.35}$$

The obtained scattering amplitude allows one to find the cross-section of electron scattering off impurity:

$$\sigma_{\mathbf{k}'\mathbf{k}} = \frac{1}{2(2S+1)} \sum_{\sigma'\sigma\tau'\tau} |T_{\mathbf{k}'\sigma',\,\tau';\,\mathbf{k}\sigma,\,\tau}|^2 . \tag{9.36}$$

(This includes averaging over initial spin states and summation over final spin states.) In the lowest order, we get, according to Eq. (9.17), and by using the identity (9.25),

$$\sigma_{\mathbf{k}\mathbf{k}'} = \frac{1}{4} J_0^2 \, S(S+1) \tag{9.37}$$

$$= \frac{3}{16} J_0^2 \qquad \text{for } S = \frac{1}{2} . \tag{9.38}$$

This yields the transport relaxation rate

$$\frac{1}{\tau^{(0)}} = \frac{\pi}{2} \, n_{\text{imp}} \, \nu J_0^2 S(S+1), \tag{9.39}$$

which determines the contribution of magnetic impurities to the resistivity:

$$\rho_{\text{imp}}^{(0)} = \frac{3}{e^2 \nu v_F^2 \tau^{(0)}} = \frac{3\pi}{2} \, \frac{1}{e^2 v_F^2} \, n_{\text{imp}} \, J_0^2 S(S+1) . \tag{9.40}$$

Here n_{imp} is the impurity concentration. According to Eq. (9.34), the renormalization due to higher-order processes amounts to a replacement in these formulas

$$J_0^2 \;\longrightarrow\; \frac{1}{\nu^2 \ln^2(T/T_K)} , \tag{9.41}$$

which determines the law of increase of resistivity.

The RG analysis assumes that the renormalized dimensionless coupling νJ is small, so that it is valid for $T > T_K$ (weak-coupling regime). When the temperature is lowered down to $T \sim T_K$, the theory enters the strong-coupling regime. The physics at $T < T_K$ requires a different analysis. We only briefly state the result for the case of the impurity spin $S = 1/2$. The local moment forms a singlet with conducting electrons, which serves as a potential scatterer. Therefore, the increase of resistivity with lowering T stops at T_K, i.e., the resistivity saturates (see the schematic figure in the beginning of this Chapter).

9.3.1 Outlook

A great variety of important extensions:

- Anisotropic coupling
- Multichannel Kondo models
- Strong coupling regimes; Wilson's numerical RG
- Kondo lattices: dense arrays of local moments
- Kondo effect in quantum dots
- ...