Theorie der Kondensierten Materie II SS 2017

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Blatt 8
Lösungsvorschlag

1. Drude conductivity

(a) **Use the rules of the diagrammatic technique to evaluate the Drude conductivity.**

In the lecture, we have derived an expression for the Drude conductivity in the low frequency limit $\omega \to 0$:

$$\sigma^{\alpha\beta}(q=0,\omega)=\frac{1}{\omega}\int\frac{\mathrm{d}\epsilon}{4\pi V}\left[\mathrm{th}\left(\frac{\epsilon}{2T}\right)-\mathrm{th}\left(\frac{\epsilon-\omega}{2T}\right)\right]\int \mathrm{d}^d r_3 \mathrm{d}^d r_1 j_1^\alpha G^R_{13}(\epsilon) j_3^\beta G^A_{31}(\epsilon-\omega),$$

This expression depends on the realization of the disorder. We need to average the expression w.r.t. the distribution function of the disorder potential which we assume to be the Gaussian white noise disorder. In order to obtain the Drude result, we need to take into account only the term where both Green's functions are averaged separately. After the disorder average the Green's functions are translational invariant and can thus be Fourier transformed:

$$G^R_{13}(\epsilon) \to \int \frac{\mathrm{d}^d p}{(2\pi)^d} \mathrm{e}^{i\boldsymbol{p}(\boldsymbol{r}_1-\boldsymbol{r}_3)} G^R(\epsilon,\boldsymbol{p}).$$

The current operators can now easily related to the velocity operators $v^\alpha = p^\alpha/m$. Using the definition of the current operators we find, e.g. for the operator j_3^β:

$$e^{-i\boldsymbol{p}_1\boldsymbol{r}_3} j_3^\beta e^{i\boldsymbol{p}_2\boldsymbol{r}_3} = \frac{ie}{2m}\left[-ip_1^\beta e^{-i(\boldsymbol{p}_1-\boldsymbol{p}_2)\boldsymbol{r}_3} - ip_2^\beta e^{-i(\boldsymbol{p}_1-\boldsymbol{p}_2)\boldsymbol{r}_3}\right] = \frac{e}{2m}(p_1^\beta+p_2^\beta)e^{-i(\boldsymbol{p}_1-\boldsymbol{p}_2)\boldsymbol{r}_3}.$$

Then the spatial integration yields the delta function requiring $p_1^\beta = p_2^\beta$, which leads to the simple velocity operator.

In the low frequency limit, we expand the distribution functions (since this is the term that vanishes in this limit)

$$\mathrm{th}\left(\frac{\epsilon}{2T}\right)-\mathrm{th}\left(\frac{\epsilon-\omega}{2T}\right) \approx \omega\frac{\partial}{\partial\epsilon}\mathrm{th}\left(\frac{\epsilon}{2T}\right)$$

and then neglect the ω-dependence in G^A. We now arrive at

$$\sigma_0^{\alpha\beta} = e^2\int\frac{\mathrm{d}\epsilon}{4\pi}\left[\frac{\partial}{\partial\epsilon}\mathrm{th}\left(\frac{\epsilon}{2T}\right)\right]\int\frac{\mathrm{d}^d p}{(2\pi)^d} v^\alpha v^\beta G^R(\epsilon,\boldsymbol{p})G^A(\epsilon,\boldsymbol{p})$$

The angular integration can be performed by using the isotropy of the problem:

$$\int \mathrm{d}^d p v^\alpha v^\beta = \delta_{\alpha\beta}\frac{1}{d}\int \mathrm{d}^d p \frac{p^2}{m^2}$$

Since the derivative of the hyperbolic tangent function has peak at $\epsilon = 0$ with the width $\sim T$, the integral over p is dominated by the region close to the Fermi energy. We re-write this integral with the help of the density of states and find

$$\int \mathrm{d}^d p\, v^2\, G^R G^A \approx \nu_0 v_\mathrm{F}^2 \int \mathrm{d}\xi \frac{1}{\epsilon - \xi + \frac{i}{2\tau}} \frac{1}{\epsilon - \xi - \frac{i}{2\tau}}$$

$$= 2\pi\nu_0 v_\mathrm{F}^2 \tau$$

which is independent of ϵ. The remaining integral over ϵ is now trivial. We finally find

$$\sigma_0^{\alpha\beta} = \delta^{\alpha\beta}\frac{e^2\nu_0 v_\mathrm{F}^2\tau}{d}$$

(b) **Discussion in 3D and 2D and the diffusion constant.**

The density-density correlation function of a disordered system in the long-wavelength and low energy limit has a pole structure corresponding to the diffusion equation

$$(\partial_t - D\nabla^2)\rho = 0,$$

where the diffusion coefficient reads $D = v_\mathrm{F}^2\tau/d$. We can thus easily rewrite the expression for the conductivity obtained in part (a) as

$$\sigma_0 = e^2\nu_0 D.$$

This form is called Einstein relation.

There is another representation making use of the (particle-number-)density n. In three spatial dimensions we have $\nu_0 = mp_\mathrm{F}/\pi^2$ and $n = p_\mathrm{F}^3/(3\pi^2)$. Using these relations we can express the conductivity as

$$\sigma_0 = \frac{e^2 n\tau}{m}.$$

In 2D we have $\nu_0 = m/\pi$ and $n = p_\mathrm{F}^2/(2\pi)$. We can again find the same result as in 3D:

$$\sigma_0 = \frac{e^2 n\tau}{m}.$$

In 2D it is also possible to express the result as

$$\sigma_0 = \frac{e^2}{\pi}E_\mathrm{F}\tau.$$

Restoring the Planck's constant in the prefactor: $e^2/(\pi\hbar) = 2e^2/h$, where the factor e^2/h is known as the conductance quantum.

2. Non-crossing approximation

(a) Extra smallness of the diagrams with crossed impurity lines.

Let us first analyze the left diagram of Fig. 1.

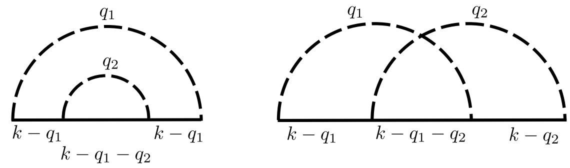

Abbildung 1: Second order contributions to the self-energy.

The structure of this diagram is

$$\int_{q_1,q_2} W(q_1)W(q_2)G^2(\underbrace{k-q_1}_{=\tilde{q}_1})G(\underbrace{k-q_1-q_2}_{=\tilde{q}_2}).$$

The main contribution of the integrand come from the region where all Green's functions are close to the Fermi surface. Here, the integrations are decoupled. We can estimate the phase space by two independent spherical shells with radius p_F. The width of the shells in a disordered system is given by the inverse mean free path $\Delta p \sim 1/l$. Thus the phase space scales as

$$\Omega_1 \sim (4\pi p_\mathrm{F}^2/l)^2.$$

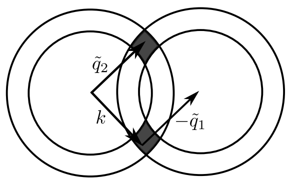

Abbildung 2: Restricted phase space for the integration over $\tilde{q}_2$.

If we now look at the right diagram of Fig. 1 (crossed impurity lines), we need to compute

$$\int_{q_1,q_2} G(\underbrace{k-q_1}_{=\tilde{q}_1})G(\underbrace{k-q_2}_{=\tilde{q}_2})G(\underbrace{k-q_1-q_2}_{\tilde{q}_1+\tilde{q}_2-k})$$

We have now an additional constraint compared to the other diagram. One integration (say over $\tilde{q}_1$) is again restricted to a spherical shell, while the integration over $\tilde{q}_2$ is restricted to the intersection of two spherical shells (see Fig. 2). The intersection can be approximated by a ring of radius $\approx p_\mathrm{F}$ and a cross section $\Delta p^2 = 1/l^2$. The phase space for this diagram scales as

$$\Omega_2 \sim (4\pi p_\mathrm{F}^2/l)(2\pi p_\mathrm{F}/l^2) \quad \Rightarrow \quad \frac{\Omega_2}{\Omega_1} \sim \frac{2}{p_\mathrm{F} l} = \frac{1}{E_\mathrm{F}\tau} \ll 1.$$

We can thus neglect the diagrams with crossed impurity lines if the mean free path is much larger than the Fermi-wavelength or equivalently if the scattering time is much larger than the inverse Fermi energy.

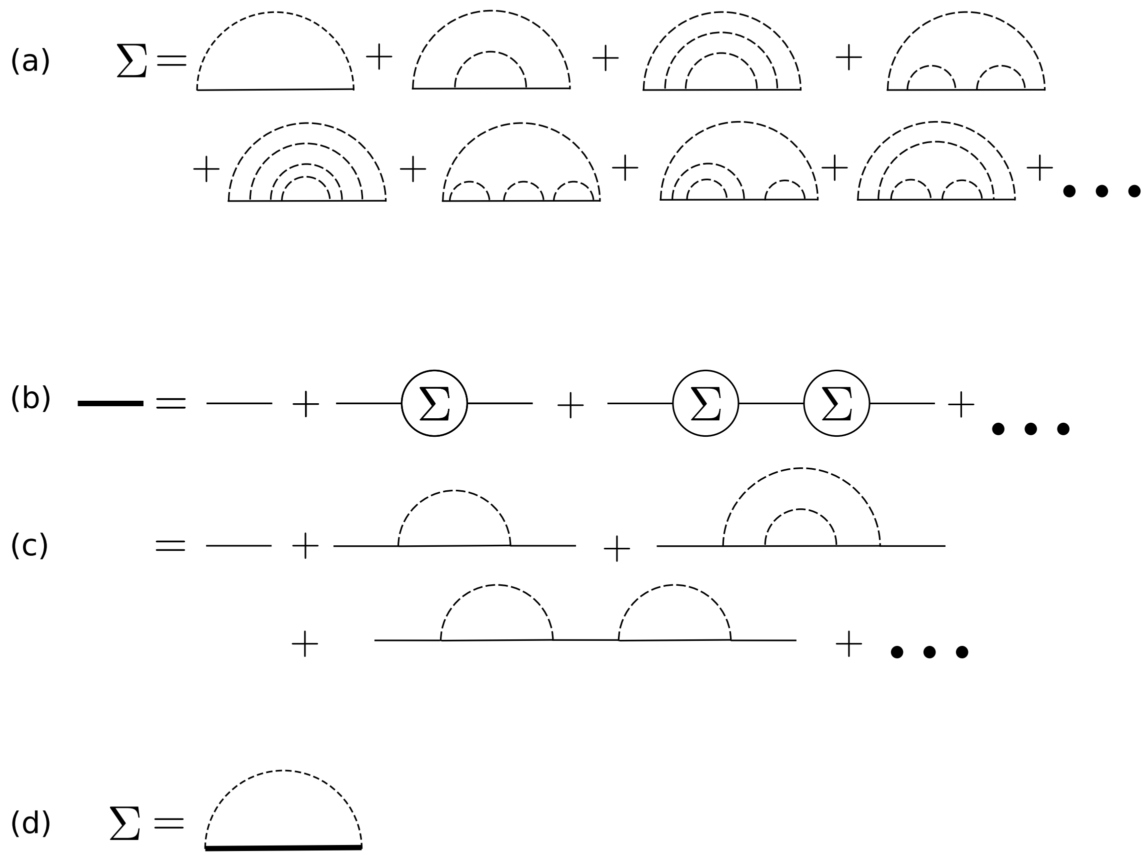

Abbildung 3: Diagrammatic summation of the rainbow diagrams (self-consistent Born approximation).

(b) **Self-consistent Born approximation**

We can sum up a whole class of diagrams of the self-energy containing no crossed impurity lines. Those diagrams are depicted in Fig. 3 (a). If we calculate the Green's function, we need to insert this self-energy between two free Green's functions, see Fig. 3 (b). A few diagrams contributing to the full Green's function are shown in Fig. 3 (c). The self-consistency equation is depicted in Fig. 3 (d). It can be easily checked that replacing the full Green's function in (d) by the diagrams in (c) reproduces the series in (a).

In order to see the self-consistency explicitly, we use the standard representation of the full Green's function by the self-energy:

$$G = \frac{1}{G_0^{-1} - \Sigma}.$$

We can thus write the self-consistency equation corresponding to the diagram in Fig. 3 (d) as

$$\Sigma^R(p,\epsilon) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{W(q)}{\epsilon - \xi_{p+q} - \Sigma^R(p+q,\epsilon)}.$$

For simplicity, we assume Gaussian white-noise disorder: $W(q) = \Gamma = const.$ Shifting the momentum q, we can make the RHS independent of p. Thus, we conclude that in this situation the self-energy is momentum independent.

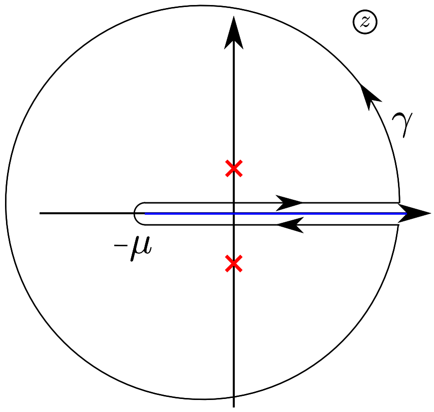

Abbildung 4: Analytic structure of f and integration contour γ.

We actually are only interested in the imaginary part of Σ since it will introduce a finite lifetime. The real part can typically be absorbed into the chemical potential. We neglect the real part in the following and additionally set $\epsilon = 0$ since we are interested only in the lifetime of the particles close to the Fermi energy. Denoting the imaginary part of Σ^R by x, we can write

$$x = \Gamma x \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{1}{(\mu - \frac{q^2}{2m})^2 + x^2}$$

This integral can be simplified (after the integration over the angles) by the substitution $\xi = q^2/(2m) - \mu$:

$$1 = \frac{\Gamma\sqrt{2m^3}}{2\pi^2} \int\limits_{-\mu}^{\infty} d\xi \frac{\sqrt{\xi + \mu}}{\xi^2 + x^2}.$$

A quick estimate of the result can be obtained by observing that in this integral the dominant contribution comes from small ξ (i.e. momenta at the Fermi surface). This yields the usual relatoin between τ and Γ, meaning that in the leading order taking into account the rainbow diagrams does not change the result. Below we describe a more precise calculation.

Now we show how the above integral can be performed using the methods of the complex analysis. First of all we define the function

$$f(z) = \frac{\sqrt{z + \mu}}{z^2 + x^2}$$

in the complex plane, where we choose the following branch of the square root:

$$\sqrt{z + \mu} = \sqrt{|z + \mu|}\, \mathrm{e}^{i\theta/2},$$

Here $\theta \in [0, 2\pi)$ is the (unique) argument of the complex number $z + \mu$. With this definition of the square root, the function f has a discontinuity along the real axis for $z \geq -\mu$ (branch cut). There are furthermore two first order poles at $z = \pm ix$. The analytic structure of f as well as the integration contour in the complex plane are depicted in Fig. 4.

We perform now the integration along the contour γ. We can use the Residue theorem to evaluate the integral. On the other hand we can parametrize the path and perform the integration explicitly. The large circle as well as the small circle (around the branch point) give no contribution. Above the branch cut we have $\theta = 0$ and below $\theta = 2\pi$. Hence, we can write

$$\int_\gamma \mathrm{d}z f(z) = 2\pi i \left(\frac{\sqrt{ix+\mu}}{2ix} - \frac{\sqrt{-ix+\mu}}{2ix} \right) = \int_{-\mu}^{\infty} \mathrm{d}t \frac{\sqrt{t+\mu}}{t^2+x^2} + \int_{\infty}^{-\mu} \mathrm{d}t \frac{-\sqrt{t+\mu}}{t^2+x^2}$$

The order of integration limits can be interchanged in the second integral such that we can solve the equation for the unknown integral:

$$I := \int_{-\mu}^{\infty} \mathrm{d}t \frac{\sqrt{t+\mu}}{t^2+x^2} = \frac{\pi}{2x} \left(\sqrt{ix+\mu} - \sqrt{-ix+\mu} \right).$$

We can now simplify the square roots under the conditions $\mu > 0$ and $x < 0$ (retarded self-energy has negative imaginary part).

$$\begin{aligned} I &= \frac{\pi \sqrt[4]{x^2+\mu^2}}{2x} \left(\mathrm{e}^{\frac{i}{2}(2\pi - \arctan(-x/\mu))} - \mathrm{e}^{\frac{i}{2}\arctan(-x/\mu)} \right) \\ &= -\frac{\pi \sqrt[4]{x^2+\mu^2}}{x} \cos\left[\frac{1}{2} \arctan(-x/\mu) \right]. \end{aligned}$$

Using simple trigonometric relations we can establish the following equations for $\alpha \in (0, \pi/2)$:

$$\cos\frac{\alpha}{2} = \frac{\sin\alpha}{\sqrt{2}\sqrt{1-\cos\alpha}}, \qquad \sin\alpha = \frac{\tan\alpha}{\sqrt{1+\tan^2\alpha}}, \qquad \cos\alpha = \frac{1}{\sqrt{1+\tan^2\alpha}},$$

and thus

$$\cos\frac{\alpha}{2} = \frac{\tan\alpha}{\sqrt{2}\sqrt[4]{1+\tan^2\alpha}\sqrt{\sqrt{1+\tan^2\alpha}-1}}.$$

We can finally express the integral as

$$I = \frac{\pi}{\sqrt{2}} \frac{1}{\sqrt{\sqrt{x^2+\mu^2}-\mu}}$$

We can now solve the self-consistency equation and find

$$x = -\frac{\Gamma m^{3/2}\sqrt{\mu}}{\sqrt{2}\pi} \sqrt{1 + \frac{\Gamma^2 m^3}{8\pi^2\mu}}$$

From the imaginary part of the self energy we can read off the scattering time as $x = -1/(2\tau)$. With the help of the DOS at the Fermi level we can write

$$\tau = \frac{1}{2\pi\nu_0\Gamma} \left(1 + \frac{\Gamma^2 m^3}{8\pi^2\mu} \right)^{-1/2}.$$

In the lecture we only considered the first Born approximation which yields the prefactor of the square root. In the self-consistent calculation we now get a slightly different result originating from the higher order diagrams. The parameter that controls the smallness of the higher order contributions can be estimated by plugging the first order result $\Gamma = (2\pi\nu_0\tau)^{-1}$ into the ratio inside the square root:

$$\left.\frac{\Gamma^2 m^3}{8\pi^2\mu}\right|_{\Gamma=(2\pi\nu_0\tau)^{-1}} = \frac{1}{16}\frac{1}{(E_\mathrm{F}\tau)^2}.$$