Chapter 2

Interactions in quantum many-body physics. Superfluidity and superconductivity

In this chapter, we turn to **quantum** systems of many interacting particles. We will consider systems of interacting bosons and of interacting fermions. We will see that the interaction, in combination with quantum character of the system, leads to emergence of collective states of matter characterized by spontaneous symmetry breaking and remarkable properties: superfluidity and superconductivity.

2.1 Second quantization

For dealing efficiently with problems of many interacting particles, the formalism of **second quantization** (occupation-number representation) is an extremely useful tool. We introduce it here both for systems of interacting bosons and fermions. The formalism can be then straightforwardly generalized to systems involving both fermions and bosons (as e.g. in the case of electron-phonon interaction).

Consider a Hamiltonian of a many-body problem:

$$\widehat{H} = \sum_{i=1}^{N} \underbrace{\left[-\frac{\hbar^2}{2m} \boldsymbol{\nabla}_i^2 + U(\mathbf{r}_i) \right]}_{\widehat{H}_0(\mathbf{r}_i)} + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) \equiv \widehat{H}_0 + \widehat{V} \,, \tag{2.1}$$

where $\widehat{H}_0$ is the sum of one-particles Hamiltonians and $\widehat{V}$ describes the interaction between particles. Let us further consider some orthonormal basis of one-particle states

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

This yields a basis for N-particle wave functions:

$$\psi_{k_1}(\mathbf{r}_1) \ldots \psi_{k_N}(\mathbf{r}_N) \,. \tag{2.2}$$

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

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) = \sum_{k_1, \ldots, k_N} C(k_1, \ldots, k_N; t) \psi_{k_1}(\mathbf{r}_1) \ldots \psi_{k_N}(\mathbf{r}_N) \,, \tag{2.3}$$

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

It is convenient to introduce another many-particle basis that takes into account the boson/fermion statistics, i.e. the symmetry or antisymmetry of the many-body wavefunction. We can achieve this by using the symmetrization/antisymmetrization operator:

$$S^{(\pm)} = c^{(\pm)} \sum_P (\pm 1)^P P, \tag{2.4}$$

where the sign + corresponds to bosons and − to fermions. Here $c^{(\pm)}$ is a normalization constant and P denotes permutations of the set $\{k_1, k_2, \ldots\}$, for instance:

$$P_{12}\psi_{k_1}(\mathbf{r}_1)\psi_{k_2}(\mathbf{r}_2) = \psi_{k_2}(\mathbf{r}_1)\psi_{k_1}(\mathbf{r}_2).$$

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.

2.1.1 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, ...:

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

One sums over all states (2.2) such that $\{k_1, k_2, \ldots, k_N\}$ corresponds to the occupation numbers $(n_1, n_2, \ldots)$. The corresponding sets $\{k_1, k_2, \ldots, k_N\}$ are $\{\underbrace{1\ldots1}_{n_1}\underbrace{2\ldots2}_{n_2}\ldots\}$ + all distinct permutations:

$$\Phi_{n_1,n_2,n_3,\ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \left(\frac{n_1! n_2! \ldots}{N!}\right)^{\frac{1}{2}} \sum_{\{k_1,k_2,\ldots,k_N\}\Leftrightarrow(n_1,n_2,n_3,\ldots)} \psi_{k_1}(\mathbf{r}_1)\psi_{k_2}(\mathbf{r}_2)\ldots\psi_{k_N}(\mathbf{r}_N)\,. \tag{2.5}$$

The prefactor in the r.h.s. of Eq. (2.5) ensures the normalization of the state $\Phi_{n_1,n_2,n_3,\ldots}$.

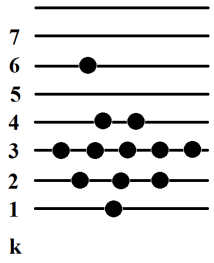
An arbitrary many-body wave-function can be expanded in these many-body basis states:

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) = \sum_{n_1,n_2,\ldots} \widetilde{C}(n_1, n_2, \ldots, t)\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N)\,. \tag{2.6}$$

We will denote $\Phi_{n_1,n_2,\ldots}$ by $|n_1, n_2, \ldots\rangle$.

These states are orthogonal and normalized:

$$\langle n_1, n_2, \ldots | n_1', n_2', \ldots\rangle = \delta_{n_1,n_1'}\delta_{n_2,n_2'}\ldots\,. \tag{2.7}$$



$= |1\,3\,5\,2\,0\,1\,0\,0\ldots\rangle$

Further, the system of these states is complete:

$$\sum_{n_1,n_2,\ldots} |n_1, n_2, \ldots\rangle\langle n_1, n_2, \ldots| = \mathbb{1}\,. \tag{2.8}$$

Thus, the states $|n_1, n_2, \ldots\rangle$ form a complete orthonormal system, i.e., an orthonormal basis in the many-body Hillbert space. This Hilbert space (including states with any total number N of particles) is known as **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:

$$[a_k, a_{k'}^\dagger] = \delta_{kk'}\,, \quad [a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0\,. \tag{2.9}$$

For any given k the algebra of operators $a_k^\dagger$, a_k is identical to the algebra of raising and lowering operators for a harmonic oscillator. We thus have

$$a_k|n_k\rangle = n_k^{\frac{1}{2}}|n_k - 1\rangle\,, \tag{2.10}$$

$$a_k^\dagger|n_k\rangle = (n_k + 1)^{\frac{1}{2}}|n_k + 1\rangle\,, \tag{2.11}$$

$$a_k^\dagger a_k|n_k\rangle = n_k|n_k\rangle\,. \tag{2.12}$$

The operator $a_k^\dagger$ increases the occupation of the state k by one (thus "creation operator"), while a_k diminishes the occupation number by one (thus "annihilation operator"). Clearly, $a_k^\dagger a_k$ is the operator of the number of particles in the state k.

Any state $|n_1, n_2, \ldots\rangle$ of the Fock space can be written as a result of an application of creation operators on the vacuum state $|0, 0, \ldots\rangle \equiv |0\rangle$:

$$|n_1, n_2, \ldots\rangle = \prod_k \frac{(a_k^\dagger)^{n_k}}{(n_k!)^{\frac{1}{2}}}|0\rangle\,. \tag{2.13}$$

Now 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 (2.5), one obtains

$$\begin{aligned}\sum_i \widehat{H}_0(\mathbf{r}_i)&\Phi_{n_1,n_2,n_3,\ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \\ &= \sum_k n_k\,(H_0)_{kk}\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \\ &+ \sum_{k\neq k'} n_k^{\frac{1}{2}}(n_{k'} + 1)^{\frac{1}{2}}(H_0)_{k'k}\Phi_{n_1,n_2,\ldots,n_k-1,\ldots,n_{k'}+1,\ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N)\,,\end{aligned} \tag{2.14}$$

where $\widehat{H}_0\psi_k = \sum_{k'}(H_0)_{k'k}\psi_{k'}$, with the single-particle matrix elements

$$(H_0)_{k'k} \equiv \langle k'|H_0|k\rangle = \int \mathrm{d}^d r\, \psi_{k'}^*(\mathbf{r})\widehat{H}_0(\mathbf{r})\psi_k(\mathbf{r})\,. \tag{2.15}$$

Indeed each of the operators $\widehat{H}_0(\mathbf{r}_i)$ acts on one single-particle state in each term $\psi_{k_1}(\mathbf{r}_1)\ldots\psi_{k_N}(\mathbf{r}_N)$ in $\Phi_{n_1,n_2,n_3,\ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$. It can either leave the corresponding particle in its original state k_i or move it to another state k', which yields two terms in the r.h.s. of Eq. (2.14).

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. (2.14) originate from combinatorial factors and from the normalization factors in (2.5). Specifically, the factor n_k in the first term arises because each of the terms in $(H_0)_{kk}\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ arises under action of $\sum_i \widehat{H}_0(\mathbf{r}_i)$ on $\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ exactly n_k times. For example:

$$\begin{aligned}\Big[\widehat{H}_0(\mathbf{r}_1) + \widehat{H}_0(\mathbf{r}_2) + \widehat{H}_0(\mathbf{r}_3)\Big]&\,[\psi_{k_1}(\mathbf{r}_1)\psi_{k_1}(\mathbf{r}_2)\psi_{k_2}(\mathbf{r}_3)] \\ &= [2(H_0)_{k_1k_1} + (H_0)_{k_2k_2}]\,\psi_{k_1}(\mathbf{r}_1)\psi_{k_1}(\mathbf{r}_2)\psi_{k_2}(\mathbf{r}_3) + \text{other terms.}\end{aligned} \tag{2.16}$$

The factor in the second term follows from

$$\left(\frac{n_1!n_2!\ldots}{N!}\right)^{\frac{1}{2}}(n_{k'} + 1) = n_k^{1/2}(n_{k'} + 1)^{1/2}\left(\frac{n_1!n_2!\ldots(n_k - 1)!\ldots(n_{k'} + 1)!\ldots}{N!}\right)^{\frac{1}{2}}\,. \tag{2.17}$$

Here $(n_{k'}+1)$ is how many times each of the terms in $(H_0)_{k'k}\Phi_{n_1,n_2,\ldots,n_k-1,\ldots,n_{k'}+1,\ldots}$ is obtained when $\sum_i \widehat{H}_0(\mathbf{r}_i)$ acts on $\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$. For example:

$$\left[\widehat{H}_0(\mathbf{r}_1)+\widehat{H}_0(\mathbf{r}_2)+\widehat{H}_0(\mathbf{r}_3)\right]\left[\psi_{k_1}(\mathbf{r}_1)\psi_{k_1}(\mathbf{r}_2)\psi_{k_2}(\mathbf{r}_3)+\psi_{k_1}(\mathbf{r}_1)\psi_{k_2}(\mathbf{r}_2)\psi_{k_1}(\mathbf{r}_3)+\psi_{k_2}(\mathbf{r}_1)\psi_{k_1}(\mathbf{r}_2)\psi_{k_1}(\mathbf{r}_3)\right]$$
$$= 3\,(H_0)_{k_1k_2}\,\psi_{k_1}(\mathbf{r}_1)\psi_{k_1}(\mathbf{r}_2)\psi_{k_1}(\mathbf{r}_3)+\text{other terms}. \tag{2.18}$$

According to Eq. (2.14), one can write the action of the non-interacting part of the Hamiltonian in the second-quantization language as follows:

$$\sum_i \widehat{H}_0(\mathbf{r}_i)\Phi_{n_1,n_2,n_3,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\sum_{k,k'}(H_0)_{k'k}\,a^\dagger_{k'}a_k|n_1,n_2,\ldots\rangle. \tag{2.19}$$

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

$$\sum_i \widehat{H}_0(\mathbf{r}_i) \iff \sum_{k,k'}(H_0)_{k'k}\,a^\dagger_{k'}a_k\,. \tag{2.20}$$

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

$$\frac{1}{2}\sum_{i\neq j}V(\mathbf{r}_i,\mathbf{r}_j) \iff \frac{1}{2}\sum_{k,l,m,n}V_{kl;mn}a^\dagger_k a^\dagger_l a_n a_m\,, \tag{2.21}$$

where

$$V_{kl;mn}=\int \mathrm{d}r\,\mathrm{d}r'\,\psi^*_k(\mathbf{r})\psi^*_l(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\psi_m(\mathbf{r})\psi_n(\mathbf{r}')\equiv\langle kl|V|mn\rangle\,. \tag{2.22}$$

Thus, the full Hamiltonian (2.1)

$$\widehat{H}=\sum_{i=1}^N\widehat{H}_0(\mathbf{r}_i)+\frac{1}{2}\sum_{i\neq j}V(\mathbf{r}_i,\mathbf{r}_j) \tag{2.23}$$

has the following **second-quantization representation**:

$$\boxed{\widehat{H} \iff \sum_{k,l}(H_0)_{kl}a^\dagger_k a_l+\frac{1}{2}\sum_{k,l,m,n}V_{kl;mn}a^\dagger_k a^\dagger_l a_n a_m\,.} \tag{2.24}$$

2.1.2 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

$$\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\frac{1}{(N!)^{\frac{1}{2}}}\sum_{\substack{\text{Permutations}\\ \text{of }\{k_1,\ldots,k_N\}}}(-1)^P\psi_{k_{p_1}}(\mathbf{r}_1)\ldots\psi_{k_{p_N}}(\mathbf{r}_N)$$
$$=\frac{1}{(N!)^{\frac{1}{2}}}\begin{vmatrix}\psi_{k_1}(\mathbf{r}_1) & \ldots & \psi_{k_1}(\mathbf{r}_N)\\ \vdots & \ddots & \vdots\\ \psi_{k_N}(\mathbf{r}_1) & \ldots & \psi_{k_N}(\mathbf{r}_N)\end{vmatrix}. \tag{2.25}$$

The above determinant is called Slater determinant.

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

$$\{a_k, a_{k'}^\dagger\} = \delta_{kk'}\,, \quad \{a_k, a_{k'}\} = \{a_k^\dagger, a_{k'}^\dagger\} = 0\,. \tag{2.26}$$

and obey

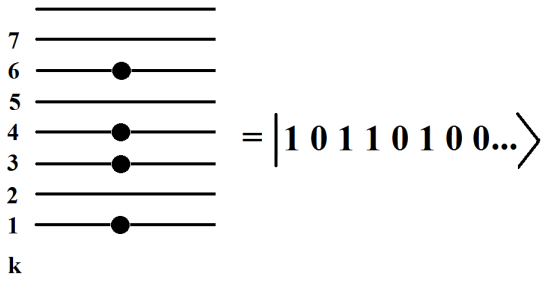
$$a_k^\dagger|0_k\rangle = |1_k\rangle\,, \qquad a_k|1_k\rangle = |0_k\rangle\,, \tag{2.27}$$

$$a_k^\dagger|1_k\rangle = 0\,, \qquad a_k|0_k\rangle = 0\,, \tag{2.28}$$

$$a_k^\dagger a_k = n_k\,. \tag{2.29}$$

In analogy with the bosonic case, many-body states (2.25) 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:

$$|n_1, n_2, \ldots\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\ldots|0\rangle\,,$$
$$\text{with } |0\rangle \equiv |0, 0, \ldots\rangle\,. \tag{2.30}$$



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

$$\widehat{H} \iff \sum_{k,l}(H_0)_{kl}a_k^\dagger a_l + \frac{1}{2}\sum_{k,l,m,n} V_{kl;mn}a_k^\dagger a_l^\dagger a_n a_m\,. \tag{2.31}$$

2.1.3 Basis transformation

When introducing second quantization, we used some basis of one-particle states labeled by k: $\psi_k(\mathbf{r})\,,\ k = 1, 2, \ldots$. There is a freedom in choosing this basis; one can transform the theory to any other basis. Consider another orthonormal basis $\chi_l(\mathbf{r})\,,\ l = 1, 2, \ldots$. The one-particle states in one basis can be expanded with respect to another basis:

$$\psi_k(\mathbf{r}) = \sum_l U_{kl}\chi_l(\mathbf{r})\,, \qquad \text{i.e.,} \qquad |\psi_k\rangle = \sum_l U_{kl}|\chi_l\rangle\,. \tag{2.32}$$

Then

$$\langle\chi_m|\psi_k\rangle = \langle\chi_m|\sum_l U_{kl}|\chi_l\rangle = \sum_l U_{kl}\delta_{ml} = U_{km}\,, \tag{2.33}$$

$$\langle\psi_k|\chi_m\rangle = U_{km}^* = U_{mk}^\dagger\,, \tag{2.34}$$

$$(UU^\dagger)_{kl} = \sum_m U_{km}U_{ml}^\dagger = \sum_m \langle\chi_m|\psi_k\rangle\langle\psi_l|\chi_m\rangle = \delta_{kl}\,, \tag{2.35}$$

where we used on the last step the completeness $\sum_m |\chi_m\rangle\langle\chi_m| = \mathbb{1}$. Equation (2.35) implies that the matrix U is unitary.

Now, if $a_k^\dagger$ are creation operators for the states $\psi_k(\mathbf{r})$, and $b_l^\dagger$ are creation operators for the states $\chi_l(\mathbf{r})$, they should be related by the same matrix U:

$$a_k^\dagger = \sum_l U_{kl}b_l^\dagger \equiv \sum_l \langle\chi_l|\psi_k\rangle b_l^\dagger \quad \text{and thus} \quad a_k = \sum_l U_{kl}^* b_l = \sum_l U_{lk}^\dagger b_l \equiv \sum_l \langle\psi_k|\chi_l\rangle b_l\,. \tag{2.36}$$

The reverse transformation reads (we use unitarity of U, which implies $U^{-1} = U^\dagger$):

$$b_l^\dagger = \sum_k U_{lk}^\dagger a_k^\dagger \equiv \sum_k \langle\psi_k|\chi_l\rangle a_k^\dagger \qquad \text{and} \qquad b_l = \sum_k U_{kl}a_k \equiv \sum_k \langle\chi_l|\psi_k\rangle a_k\,. \tag{2.37}$$

Check that the canonical commutation relations preserve their form under a basis transformation. Consider for example bosons, so that $[a_k, a_{k'}^\dagger] = \delta_{kk'}$. In the transformed basis we have then:

$$[b_l, b_{l'}^\dagger] = \sum_{k,k'} U_{kl} U_{l'k'}^\dagger [a_k, a_{k'}^\dagger] = \sum_{k,k'} U_{kl} U_{l'k'}^\dagger \delta_{kk'} = \sum_k U_{kl} U_{l'k}^\dagger = \delta_{ll'} \,, \tag{2.38}$$

so that the form of commutation relations is indeed preserved as expected.

The form of the second-quantized Hamiltonian (2.24) is also preserved with respect to basis transformation. (The matrix elements there should be of course calculated in the same basis to which the creation and annihilation operators correspond).

Consider a non-interacting system,

$$\hat{H} = \sum_{kk'} (H_0)_{kk'} a_k^\dagger a_{k'} \,. \tag{2.39}$$

Under basis transformation, this Hamiltonian becomes

$$\hat{H} = \sum_{ll'} (\tilde{H}_0)_{ll'} b_l^\dagger b_{l'} \,, \tag{2.40}$$

where

$$(\tilde{H}_0)_{ll'} = \sum_{kk'} U_{kl} (H_0)_{kk'} U_{l'k'}^\dagger \,, \qquad \text{i.e.,} \qquad \tilde{H}_0 = U^T H_0 (U^T)^\dagger \,. \tag{2.41}$$

Since H_0 is a Hermitian matrix, one can choose a unitary matrix U^T that diagonalizes it:

$$\tilde{H}_0 = \mathrm{diag}(\epsilon_1, \epsilon_2, \ldots) \,, \qquad \text{i.e.,} \qquad (\tilde{H}_0)_{ll'} = \epsilon_l \delta_{ll'} \,, \tag{2.42}$$

so that

$$\hat{H} = \sum_l \epsilon_l b_l^\dagger b_l \,. \tag{2.43}$$

Eigenstates of $\hat{H}$ are then Fock-space basis states $\Phi_{n_1,n_2,\ldots}$ in the basis corresponding to operators $b_l^\dagger$, b_l, and eigenenergies are $E_{n_1,n_2,\ldots} = \sum_l n_l \epsilon_l$.

2.1.4 Field operators

Let us 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

$$\widehat{\Psi}(\mathbf{r}) = \sum_k a_k \psi_k(\mathbf{r}) \,. \tag{2.44}$$

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

$$\widehat{\Psi}^\dagger(\mathbf{r}) = \sum_k \psi_k^*(\mathbf{r}) a_k^\dagger \,. \tag{2.45}$$

These formulas are a special case of the transformation (2.37). We calculate the commutation relations of these new operators. Let us first consider bosons:

$$[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')] = \sum_{k,k'} \psi_k(\mathbf{r}) \psi_{k'}^*(\mathbf{r}') \underbrace{[a_k, a_{k'}^\dagger]}_{\delta_{kk'}} = \sum_k \psi_k(\mathbf{r}) \psi_k^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \,, \tag{2.46}$$

$$[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}(\mathbf{r}')] = [\widehat{\Psi}^\dagger(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')] = 0 \,. \tag{2.47}$$

For fermions one obtains in the same way:

$$\{\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')\} = \delta(\mathbf{r}-\mathbf{r}')\,, \quad \{\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}(\mathbf{r}')\} = \{\widehat{\Psi}^\dagger(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')\} = 0\,. \tag{2.48}$$

One can put the above formulas together in the form

$$[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')]_\mp \equiv \widehat{\Psi}(\mathbf{r})\widehat{\Psi}^\dagger(\mathbf{r}') \mp \widehat{\Psi}^\dagger(\mathbf{r}')\widehat{\Psi}(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}')\,, \tag{2.49}$$

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

Performing the transformation in Eqs. (2.24), (2.31), we express the Hamiltonian in terms of the field operators:

$$\boxed{\widehat{H} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r}) H_0(\mathbf{r}) \widehat{\Psi}(\mathbf{r}) + \frac{1}{2}\int \mathrm{d}r\, \mathrm{d}r'\, \widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}^\dagger(\mathbf{r}') V(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}')\widehat{\Psi}(\mathbf{r})\,.} \tag{2.50}$$

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

$$[\widehat{\Psi}_\sigma(\mathbf{r}), \widehat{\Psi}^\dagger_{\sigma'}(\mathbf{r}')]_\mp = \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma\sigma'}\,. \tag{2.51}$$

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

$$\varrho_{\mathbf{r}_0} = \sum_{i=1}^N \delta(\mathbf{r}_i - \mathbf{r}_0) = \sum_{i=1}^N \varrho_{\mathbf{r}_0}(\mathbf{r}_i)\,, \quad \text{with } \varrho_{\mathbf{r}_0}(\mathbf{r}) = \delta(\mathbf{r}_0 - \mathbf{r})\,. \tag{2.52}$$

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

$$\widehat{\varrho}_{\mathbf{r}_0} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r})\delta(\mathbf{r}_0-\mathbf{r})\widehat{\Psi}(\mathbf{r}) = \widehat{\Psi}^\dagger(\mathbf{r}_0)\widehat{\Psi}(\mathbf{r}_0)\,. \tag{2.53}$$

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

$$\widehat{N} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}(\mathbf{r})\,. \tag{2.54}$$

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

$$H_0(\mathbf{r}) \mapsto H_0'(\mathbf{r}) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U(\mathbf{r}) - \mu\,, \tag{2.55}$$

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

The grand canonical distribution then takes the form

$$\exp\left(-\frac{E_n - \mu N_n}{k_B T}\right) \equiv \exp\left(-\frac{E_n'}{k_B T}\right) \quad \xrightarrow{T\to 0} \quad \text{only ground state } E_0' \text{ survives}\,, \tag{2.56}$$

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.

In the many-body quantum physics, one frequently calls $\widehat{H}'$ the Hamiltonian and denotes is again as $\widehat{H}$ in order to simplify notations.

2.2 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

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\phi(t)\rangle_S = \widehat{H}|\phi(t)\rangle_S\,. \tag{2.57}$$

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 $\mathcal{U}(t,0) = \exp(-\mathrm{i}\widehat{H}t/\hbar)$:

$$|\phi(t)\rangle_S = \exp(-\mathrm{i}\widehat{H}t/\hbar)|\phi(0)\rangle_S = \mathcal{U}(t,0)|\phi(0)\rangle_S\,. \tag{2.58}$$

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:

$$O_H(t) = \exp(\mathrm{i}\widehat{H}t/\hbar)O_S\exp(-\mathrm{i}\widehat{H}t/\hbar) = \mathcal{U}^\dagger(t,0)\underbrace{O_H(0)}_{=O_S}\mathcal{U}(t,0). \tag{2.59}$$

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

$$\mathrm{i}\hbar\frac{\partial}{\partial t}O_H(t) = [O_H(t), \widehat{H}]\,. \tag{2.60}$$

These two pictures are equivalent when computing matrix elements:

$$\langle\phi_1(t)|O|\phi_2(t)\rangle_S = \langle\phi_1|O(t)|\phi_2\rangle_H\,. \tag{2.61}$$

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

$$\widehat{H}_H = \exp(\mathrm{i}\widehat{H}_S t/\hbar)\widehat{H}_S\exp(-\mathrm{i}\widehat{H}_S t/\hbar) = \widehat{H}_S. \tag{2.62}$$

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:

$$\begin{aligned}\widehat{H} &= \exp(\mathrm{i}\widehat{H}t/\hbar)\widehat{H}\exp(-\mathrm{i}\widehat{H}t/\hbar)\\ &= \exp(\mathrm{i}\widehat{H}t/\hbar)\left\{\int \mathrm{d}r\;\widehat{\Psi}^\dagger(\mathbf{r})\widehat{H}_0\widehat{\Psi}(\mathbf{r}) + \frac{1}{2}\iint \mathrm{d}r\,\mathrm{d}r'\;\widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}')\widehat{\Psi}(\mathbf{r})\right\}\exp(-\mathrm{i}\widehat{H}t/\hbar)\\ &= \int \mathrm{d}r\;\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{H}_0(\mathbf{r})\widehat{\Psi}(\mathbf{r},t) + \frac{1}{2}\iint \mathrm{d}r\,\mathrm{d}r'\;\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{\Psi}^\dagger(\mathbf{r}',t)V(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r},t).\end{aligned} \tag{2.63}$$

For Heisenberg operators the commutator

$$[\widehat{\Psi}(\mathbf{r},t), \widehat{\Psi}^\dagger(\mathbf{r}',t')]_\mp \tag{2.64}$$

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:

$$\begin{aligned}[\widehat{\Psi}(\mathbf{r},t), \widehat{\Psi}^\dagger(\mathbf{r}',t)]_\mp &= [\exp(\mathrm{i}\widehat{H}t/\hbar)\widehat{\Psi}(\mathbf{r})\exp(-\mathrm{i}\widehat{H}t/\hbar), \exp(\mathrm{i}\widehat{H}t/\hbar)\widehat{\Psi}(\mathbf{r}')\exp(-\mathrm{i}\widehat{H}t/\hbar)]\\ &= \exp(\mathrm{i}\widehat{H}t/\hbar)[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')]\exp(-\mathrm{i}\widehat{H}t/\hbar) = \delta(\mathbf{r}-\mathbf{r}')\,.\end{aligned} \tag{2.65}$$

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

Now we use Eq. (2.60) and to derive the evolution equation (analog of Schrödinger equation) for the field operator in the Heisenberg picture:

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{r},t) &= [\widehat{\Psi}(\mathbf{r},t),\widehat{H}] \\ &= \int \mathrm{d}r\,[\widehat{\Psi}(\mathbf{r},t),\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{H}_0(\mathbf{r})\Psi(\mathbf{r},t)] \\ &+ \frac{1}{2}\iint \mathrm{d}r\,\mathrm{d}r'\,[\widehat{\Psi}(\mathbf{r},t),\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{\Psi}^\dagger(\mathbf{r}',t)V(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r},t)]. \end{aligned} \tag{2.66}$$

Using Eq. (2.65), we obtain for the required commutators (both for bosons and fermions)

$$[\widehat{\Psi}(\mathbf{r},t),\widehat{\Psi}^\dagger(\mathbf{r}',t)\widehat{H}_0(\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)] = \widehat{H}_0(\mathbf{r})\widehat{\Psi}(\mathbf{r},t)\delta(\mathbf{r}-\mathbf{r}'), \tag{2.67}$$

and

$$\begin{aligned} [\widehat{\Psi}(\mathbf{r},t),\widehat{\Psi}^\dagger(\mathbf{r}',t)\widehat{\Psi}^\dagger(\mathbf{r}'',t)V(\mathbf{r}',\mathbf{r}'')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r}'',t)] &= \delta(\mathbf{r}-\mathbf{r}'')\widehat{\Psi}^\dagger(\mathbf{r}',t)V(\mathbf{r}',\mathbf{r}'')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r}'',t) \\ +\delta(\mathbf{r}-\mathbf{r}')\widehat{\Psi}^\dagger(\mathbf{r}'',t)V(\mathbf{r}',\mathbf{r}'')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r}'',t). \end{aligned} \tag{2.68}$$

Substituting Eqs. (2.67) and (2.68) into Eq. (2.66), and using $V(\mathbf{r}',\mathbf{r}'') = V(\mathbf{r}'',\mathbf{r}')$, we arrive at

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{r},t) = \left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + U(\mathbf{r}) - \mu\right)\widehat{\Psi}(\mathbf{r},t) + \int \mathrm{d}r'\,\widehat{\Psi}^\dagger(\mathbf{r}',t)V(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r},t)\,. \tag{2.69}$$

This equation is nonlinear, so that the field operators behave in a nontrivial way. The term $-\mu$ in brackets in Eq. (2.69) is present if the evolution of the Heisenberg operator $\widehat{\Psi}(\mathbf{r},t)$ is defined via the Hamiltonian $\widehat{H}' = \widehat{H} - \mu\widehat{N}$, and is absent if the original Hamiltonian $\widehat{H}$ is used, see Eq. (2.55).

2.3 Correlations in a free Fermi gas

Before turning to interacting systems, let us discuss some applications of the second-quantization formalism to a non-interacting system. Specifically, we consider a free (i.e., non-interacting) Fermi gas. Even though the system is non-interacting, it is characterized by correlations that are caused by Fermi statistics.

We consider a gas of N free electrons (fermions with spin 1/2). Single-particle eigenstates that diagonalize the free Hamiltonian are plane waves. The ground state is given by

$$|\Phi_0\rangle = \prod_{\boldsymbol{k},\sigma:\ |\boldsymbol{k}|<k_F} c^\dagger_{\boldsymbol{k},\sigma}|0\rangle\,, \tag{2.70}$$

where $\boldsymbol{k}$ is the wave vector (related to the momentum $\boldsymbol{p}$ via $\boldsymbol{p} = \hbar\boldsymbol{k}$) and $c^\dagger_{\boldsymbol{k},\sigma}$ is a creation operator for an electron with wave vector $\boldsymbol{k}$ and spin projection σ. The value of k_F is determined by the number of particles N. Namely

$$N = \left(\sum_{\boldsymbol{k},\sigma:\ |\boldsymbol{k}|<k_F} 1\right) = 2\left(\sum_{\boldsymbol{k}:\ |\boldsymbol{k}|<k_F} 1\right) = \frac{2V}{(2\pi)^3}\int_{|\boldsymbol{k}|<k_F} d^3k = V\cdot\frac{k_F^3}{3\pi^2} \tag{2.71}$$

Thus $n = k_F^3/3\pi^2$ and, equivalently, $k_F = (3\pi^2 n)^{1/3}$, where $n \equiv N/V$ is the density of electrons. The field operators are

$$\Psi_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\,\mathbf{r}} c_{\boldsymbol{k}\,\sigma}\,. \tag{2.72}$$

Check the average density:

$$\begin{aligned}
\langle\Phi_0|\hat{\rho}(\mathbf{r})|\Phi_0\rangle &= \sum_\sigma \langle\Phi_0|\hat{\Psi}^\dagger_\sigma(\mathbf{r})\hat{\Psi}_\sigma(\mathbf{r})|\Phi_0\rangle \\
&= \sum_\sigma \sum_{\boldsymbol{k}\,,\boldsymbol{k}\,'} \frac{e^{-i\boldsymbol{k}\,'\mathbf{r}}}{\sqrt{V}} \cdot \frac{e^{i\boldsymbol{k}\,\mathbf{r}}}{\sqrt{V}} \langle\Phi_0|\hat{c}^\dagger_{\boldsymbol{k}\,,\sigma}\hat{c}_{\boldsymbol{k}\,',\sigma}|\Phi_0\rangle \\
&= \sum_\sigma \sum_{\boldsymbol{k}\,,\boldsymbol{k}\,'} \frac{e^{-i\boldsymbol{k}\,'\mathbf{r}}}{\sqrt{V}} \cdot \frac{e^{i\boldsymbol{k}\,\mathbf{r}}}{\sqrt{V}} \,\delta_{\boldsymbol{k}\,,\boldsymbol{k}\,'}\,\Theta(k_F - |\boldsymbol{k}\,|) = n\,.
\end{aligned} \tag{2.73}$$

We used here

$$\langle\Phi_0|\hat{c}^\dagger_{\boldsymbol{k}\,,\sigma}\hat{c}_{\boldsymbol{k}\,',\sigma'}|\Phi_0\rangle = \delta_{\boldsymbol{k}\,\boldsymbol{k}\,'}\delta_{\sigma\sigma'}\Theta(k_F - |\boldsymbol{k}\,|) \qquad (T=0). \tag{2.74}$$

2.3.1 One-particle correlation function

The **one-particle correlation function** (equivalently, one-particle density matrix) is defined via

$$G_\sigma(\mathbf{r}-\mathbf{r}') = \langle\Phi_0|\hat{\Psi}^\dagger_\sigma(\mathbf{r})\hat{\Psi}_\sigma(\mathbf{r}')|\Phi_0\rangle\,. \tag{2.75}$$

Using (2.74), we get

$$\begin{aligned}
G_\sigma(\mathbf{r}-\mathbf{r}') &= \frac{1}{V}\sum_{\boldsymbol{k}\,,\boldsymbol{k}\,'} e^{-i\boldsymbol{k}\,\mathbf{r}+i\boldsymbol{k}\,'\mathbf{r}'} \langle\Phi_0|\hat{c}^\dagger_{\boldsymbol{k}\,,\sigma}\hat{c}_{\boldsymbol{k}\,',\sigma}|\Phi_0\rangle \\
&= \int_{|\boldsymbol{k}\,|<k_F} \frac{d^3k}{(2\pi)^3} e^{-i\boldsymbol{k}\,(\mathbf{r}-\mathbf{r}')} = \frac{3n}{2}\cdot\frac{(\sin x - x\cos x)}{x^3}\,, \qquad x \equiv k_F|\mathbf{r}-\mathbf{r}'|.
\end{aligned} \tag{2.76}$$

The diagonal ($\mathbf{r}=\mathbf{r}'$) elements of the density matrix are $G_\sigma(0) = n/2$ (the factor 1/2 because n was defined as a total density for two spin projections). The off-diagonal ($\mathbf{r}\neq\mathbf{r}'$) elements decay towards zero with increasing $x = k_F|\mathbf{r}-\mathbf{r}'|$. Sharp Fermi edge leads to quantum-mechanical interference effects on the scale of the Fermi wave length.

2.3.2 Two-particle correlation function

Now we define a **pair correlation function**, which is the probability density to find a particle at $\mathbf{r}$ with spin σ and another particle at $\mathbf{r}'$ with spin σ':

$$\begin{aligned}
G^{(2)}_{\sigma,\sigma'}(\mathbf{r}-\mathbf{r}') &= \langle\Phi_0|\hat{\Psi}^\dagger_\sigma(\mathbf{r})\hat{\Psi}^\dagger_{\sigma'}(\mathbf{r}')\hat{\Psi}_{\sigma'}(\mathbf{r}')\hat{\Psi}_\sigma(\mathbf{r})|\Phi_0\rangle \\
&= \left[\langle\Phi_0|\hat{\rho}_\sigma(\mathbf{r})\hat{\rho}_{\sigma'}(\mathbf{r}')|\Phi_0\rangle - \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma,\sigma'}\cdot n\right]\,,
\end{aligned} \tag{2.77}$$

where $\rho_\sigma(\mathbf{r}) = \hat{\Psi}^\dagger_\sigma(\mathbf{r})\hat{\Psi}_\sigma(\mathbf{r})$ is the density operator.
We have

$$G^{(2)}_{\sigma,\sigma'}(\mathbf{r}-\mathbf{r}') = \frac{1}{V^2}\sum_{\boldsymbol{k}\,,\boldsymbol{k}\,',\boldsymbol{q}\,,\boldsymbol{q}\,'} e^{-i(\boldsymbol{k}\,-\boldsymbol{k}\,')\mathbf{r}}\cdot e^{-i(\boldsymbol{q}\,-\boldsymbol{q}\,')\mathbf{r}'} \langle\Phi_0|\hat{c}^\dagger_{\boldsymbol{k}\,,\sigma}\hat{c}^\dagger_{\boldsymbol{q}\,,\sigma'}\hat{c}_{\boldsymbol{q}\,',\sigma'}\hat{c}_{\boldsymbol{k}\,',\sigma}|\Phi_0\rangle\,. \tag{2.78}$$

After action of the product $\hat{c}^\dagger_{\boldsymbol{k}\,,\sigma}\hat{c}^\dagger_{\boldsymbol{q}\,,\sigma'}\hat{c}_{\boldsymbol{q}\,',\sigma'}\hat{c}_{\boldsymbol{k}\,',\sigma}$ on $|\Phi_0\rangle$, we should again get $|\Phi_0\rangle$ (otherwise the matrix element is zero).

If $\sigma \neq \sigma'$, this is only possible for $\boldsymbol{q} = \boldsymbol{q}\,'$ and $\boldsymbol{k} = \boldsymbol{k}\,'$. Thus,

$$G^{(2)}_{\sigma,\sigma'}(\mathbf{r}-\mathbf{r}') = \left(\frac{1}{V}\right)^2 \sum_{\boldsymbol{k},\boldsymbol{q}} \langle \Phi_0 | \hat{n}_{\boldsymbol{k},\sigma} \hat{n}_{\boldsymbol{q},\sigma'} | \Phi_0 \rangle = \left(\frac{n}{2}\right)^2 , \qquad \sigma \neq \sigma' , \tag{2.79}$$

where $n_{\boldsymbol{k},\sigma} = c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}$. Thus, there is no correlations for $\sigma \neq \sigma'$: the correlation function is equal to its disconnected part $\langle \Phi_0 | \hat{\rho}_\sigma(\mathbf{r}) | \Phi_0 \rangle \langle \Phi_0 | \hat{\rho}_{\sigma'}(\mathbf{r}') | \Phi_0 \rangle = (n/2)^2$.

If, however, $\sigma = \sigma'$, then there are two possibilities to get a non-zero matrix element entering Eq. (2.78):

(i) $\boldsymbol{q} = \boldsymbol{q}\,'$ and $\boldsymbol{k} = \boldsymbol{k}\,'$, or (ii) $\boldsymbol{q} = \boldsymbol{k}\,'$ and $\boldsymbol{k} = \boldsymbol{q}\,'$.

This yields

$$\langle \Phi_0 | \hat{c}^\dagger_{\boldsymbol{k},\sigma} \hat{c}^\dagger_{\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{q}\,',\sigma} \hat{c}_{\boldsymbol{k}\,',\sigma} | \Phi_0 \rangle = n_{\boldsymbol{k},\sigma} n_{\boldsymbol{q},\sigma} (\delta_{\boldsymbol{k},\boldsymbol{k}'} \delta_{\boldsymbol{q},\boldsymbol{q}'} - \delta_{\boldsymbol{k},\boldsymbol{q}'} \delta_{\boldsymbol{q},\boldsymbol{k}'}). \tag{2.80}$$

This is an example of a general Wick theorem, which plays a very important role in many-body quantum theory (to be studied in TKM-2 course). Substituting Eq. (2.80) into Eq. (2.78), we obtain

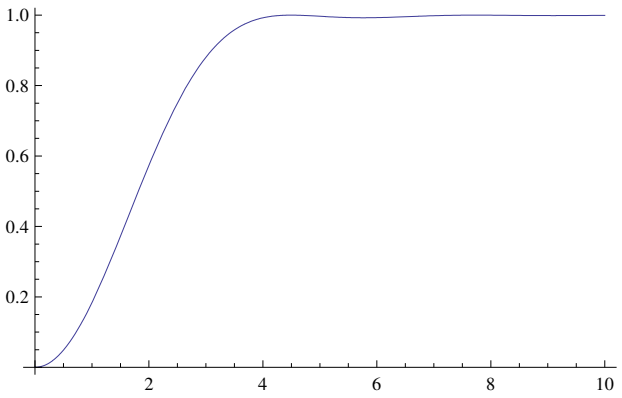
$$\begin{aligned} G^{(2)}_{\sigma,\sigma}(\mathbf{r}-\mathbf{r}') &= \left(\frac{1}{V}\right)^2 \sum_{|\boldsymbol{k}|<k_F,\ |\boldsymbol{q}|<k_F} \left(1 - e^{-i(\boldsymbol{k}-\boldsymbol{q})(\mathbf{r}-\mathbf{r}')}\right) \\ &= \left(\frac{n}{2}\right)^2 - [G_\sigma(\mathbf{r}-\mathbf{r}')]^2 = \left(\frac{n}{2}\right)^2 \left[1 - \left(\frac{3(\sin x - x\cos x)}{x^3}\right)^2\right], \end{aligned} \tag{2.81}$$

where again $x = k_F|\mathbf{r}-\mathbf{r}'|$. The constant term $(n/2)^2$ in Eq. (2.81) corresponds to a disconnected part of the correlation function, $\langle \Phi_0 | \hat{\rho}_\sigma(\mathbf{r}) | \Phi_0 \rangle \langle \Phi_0 | \hat{\rho}_{\sigma'}(\mathbf{r}') | \Phi_0 \rangle$; the second term is the connected correlation function.

Figure: $g_{\sigma\sigma}(r) \equiv \left(\frac{2}{n}\right)^2 G^{(2)}_{\sigma,\sigma}(r)$

as a function of $x = k_F r$.

A "hole" due to the Pauli principle at $x \sim 1$ (i.e. $r \sim k_F^{-1}$) is manifest. Electron seem to "repel" each other, although there is no real interaction. The effect is entirely due to Fermi statistics.



One can check that

$$\frac{n}{2} \int d^3 r (g_{\sigma,\sigma}(r) - 1) = -1 , \tag{2.82}$$

i.e., the "hole" corresponds to exactly one "missing" electron.

2.4 Weakly interacting Bose gas

2.4.1 Hamiltonian, Bose-Einstein condensation, and Bogoliubov approximation

We consider a system of bosons with a weak repulsive interaction $V(\mathbf{r}-\mathbf{r}')$. The Hamiltonian is given by Eq. (2.50). The single-particle Hamiltonian H_0 is that of free particles in a box

of volume V. The interaction is assumed to be short-ranged, and we approximate it by a delta-function interaction, $V(\mathbf{r}-\mathbf{r}') = U_0\delta(\mathbf{r}-\mathbf{r}')$ with $U_0 > 0$ (repulsion). The Hamiltonian thus reads

$$\widehat{H} = \int \mathrm{d}r \left[-\widehat{\Psi}^\dagger(\mathbf{r})\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\widehat{\Psi}(\mathbf{r}) + \frac{U_0}{2}\,\widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}(\mathbf{r})\widehat{\Psi}(\mathbf{r})\right], \tag{2.83}$$

or, equivalently, in terms of momentum-space creation and annihilation operators, with commutation relations $[a_{\mathbf{p}}, a^\dagger_{\mathbf{p}'}] = \delta_{\mathbf{p}\mathbf{p}'}$,

$$\widehat{H} = \sum_{\mathbf{p}} \epsilon_p^{(0)} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + \frac{U_0}{2V} \sum_{\mathbf{p}_1+\mathbf{p}_2=\mathbf{p}_3+\mathbf{p}_4} a^\dagger_{\mathbf{p}_1} a^\dagger_{\mathbf{p}_2} a_{\mathbf{p}_3} a_{\mathbf{p}_4}\,, \tag{2.84}$$

where $\epsilon_p^{(0)} = p^2/2m$.

We consider the limit of low temperature. Let N be the total number of particles. In a non-interacting Bose gas, almost all particles are then in condensate, i.e., in the state with momentum $\mathbf{p} = 0$. We assume a weak interaction, so that this is the case also in the presence of interaction. We denote the number of particles in the $\mathbf{p} = 0$ state by N_0, i.e. $\langle a_0^\dagger a_0\rangle = N_0$. Since N_0 is macroscopically large, we make an approximation $a_0^\dagger \approx N^{1/2}$ and $a_0 \approx N^{1/2}$, thus replacing these operators with numbers. Further, since we assume that most of the particles are in the condensate ($\mathbf{p} = 0$ state), we keep in the Hamiltonian only terms up to second order with respect to $a^\dagger_{\mathbf{p}}$, $a_{\mathbf{p}}$ with $\mathbf{p} \neq 0$. This yields:

$$\widehat{H} = \frac{N_0^2 U_0}{2V} + \sum_{\mathbf{p}\neq 0}(\epsilon_p^{(0)} + 2n_0U_0)a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + \frac{n_0U_0}{2}\sum_{\mathbf{p}\neq 0}(a^\dagger_{\mathbf{p}}a^\dagger_{-\mathbf{p}} + a_{\mathbf{p}}a_{-\mathbf{p}})\,, \tag{2.85}$$

where $n_0 = N_0/V$.

The total number of particles is $N = N_0 + \sum_{\mathbf{p}\neq 0} a^\dagger_{\mathbf{p}}a_{\mathbf{p}}$, so that, within the same approximation as above , $N^2 \simeq N_0^2 + 2N_0\sum_{\mathbf{p}\neq 0} a^\dagger_{\mathbf{p}}a_{\mathbf{p}}$. Using this in the first term in Eq. (2.85), we get

$$\begin{aligned}
\widehat{H} &= \frac{N^2U_0}{2V} + \sum_{\mathbf{p}\neq 0}\left[(\epsilon_p^{(0)} + n_0U_0)a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + \frac{n_0U_0}{2}(a^\dagger_{\mathbf{p}}a^\dagger_{-\mathbf{p}} + a_{\mathbf{p}}a_{-\mathbf{p}})\right] \\
&= \frac{N^2U_0}{2V} + {\sum_{\mathbf{p}\neq 0}}'\left[(\epsilon_p^{(0)} + n_0U_0)(a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + a^\dagger_{-\mathbf{p}}a_{-\mathbf{p}}) + n_0U_0(a^\dagger_{\mathbf{p}}a^\dagger_{-\mathbf{p}} + a_{\mathbf{p}}a_{-\mathbf{p}})\right].
\end{aligned} \tag{2.86}$$

In the last form, the prime on the sum means that the summation goes over half of the momentum space $\mathbf{p} \neq 0$, i.e., that each pair $\mathbf{p}, -\mathbf{p}$ is counted only once.

2.4.2 Bogoliubov transformation

The structure of $\widehat{H}$ in Eq. (2.86) is simple as it decouples in a sum of independent terms corresponding each to only a pair of momenta $\mathbf{p}, -\mathbf{p}$. What is special, however, is that it contains not only usual terms of the type $a^\dagger_{\mathbf{p}}a_{\mathbf{p}}$ but also products of two creation operators or two annihilation operators, $a^\dagger_{\mathbf{p}}a^\dagger_{-\mathbf{p}}$ and $a_{\mathbf{p}}a_{-\mathbf{p}}$. There is a number of very important problems in physics where such Hamiltonians arise, for either bosons or fermions, including, in particular, superfluidity, antiferromagnetism, and superconductivity. The way to treat them was pioneered by Bogoliubov, and the corresponding canonical transformation described below bears his name. We present a general analysis first (for bosons) and then apply it to the Hamiltonian (2.86).

Consider a Hamiltonian

$$\widehat{H} = \epsilon_0(a_1^\dagger a_1 + a_2^\dagger a_2) + \lambda(a_1^\dagger a_2^\dagger + a_2 a_1)\,, \qquad \epsilon_0 > 0\,, \tag{2.87}$$

with canonical Bose commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$ and $[a_1, a_2] = [a_1^\dagger, a_2^\dagger] = 0$. (We will later apply it to Eq. (2.86) with $a_1 \to a_{\mathbf{p}}$ and $a_2 \to a_{-\mathbf{p}}$.) The idea is to diagonalize the Hamiltonian. For this purpose, we introduce new operators

$$b_1 = ua_1 + va_2^\dagger\,, \qquad b_2 = ua_2 + va_1^\dagger\,, \tag{2.88}$$

with coefficients u and v that remain to be specified. In general, u and v can be complex but we take them real as it will be sufficient for our purposes. Calculating the commutators, we get

$$[b_1, b_1^\dagger] = [b_2, b_2^\dagger] = u^2 - v^2 \qquad [b_1, b_2] = [b_1, b_2^\dagger] = 0\,. \tag{2.89}$$

We require that the operators b_i satisfy bosonic canonical commutation relations. This is fulfilled if u and v satisfy

$$u^2 - v^2 = 1\,. \tag{2.90}$$

The inverse transformation then reads

$$a_1 = ub_1 - vb_2^\dagger\,, \qquad a_2 = ub_2 - vb_1^\dagger\,. \tag{2.91}$$

Substituting this in Eq. (2.87), we find

$$\widehat{H} = 2v^2\epsilon_0 - 2uv\lambda + [\epsilon_0(u^2+v^2) - 2uv\lambda](b_1^\dagger b_1 + b_2^\dagger b_2) + [\lambda(u^2+v^2) - 2uv\epsilon_0](b_1^\dagger b_2^\dagger + b_2 b_1)\,. \tag{2.92}$$

We require now that the term proportional to $b_1^\dagger b_2^\dagger + b_2 b_1$ vanishes, i.e.,

$$\lambda(u^2 + v^2) - 2uv\epsilon_0 = 0\,. \tag{2.93}$$

In view of Eq. (2.90), we can parametrize u and v via

$$u = \cosh\theta\,, \qquad v = \sinh\theta\,. \tag{2.94}$$

Equation (2.93) then becomes

$$\tanh 2\theta = \frac{\lambda}{\epsilon_0}\,. \tag{2.95}$$

It follows that

$$\cosh 2\theta = (1 - \tanh^2 2\theta)^{-1/2} = \left[\frac{1}{1 - (\lambda/\epsilon_0)^2}\right]^{1/2} = \frac{\epsilon_0}{\epsilon}\,, \tag{2.96}$$

where we have defined

$$\epsilon = \sqrt{\epsilon_0^2 - \lambda^2}\,, \tag{2.97}$$

where the positive branch of square root should be taken, $\epsilon > 0$. Note that we should have $|\lambda| < \epsilon_0$ in the initial Hamiltonian; otherwise there will be an instability in the theory.

From Eqs. (2.94) and (2.96) we obtain

$$u^2 = \frac{1}{2}(\cosh 2\theta + 1) = \frac{1}{2}\left(\frac{\epsilon_0}{\epsilon} + 1\right)\,, \qquad v^2 = \frac{1}{2}(\cosh 2\theta - 1) = \frac{1}{2}\left(\frac{\epsilon_0}{\epsilon} - 1\right)\,, \tag{2.98}$$

and thus

$$u^2 + v^2 = \frac{\epsilon_0}{\epsilon}\,, \qquad 2uv = \frac{\lambda}{\epsilon}\,. \tag{2.99}$$

Substituting this in (2.92), we obtain the final result for the Hamiltonian after the Bogoliubov transformation:

$$\widehat{H} = \epsilon - \epsilon_0 + \epsilon(b_1^\dagger b_1 + b_2^\dagger b_2)\,, \tag{2.100}$$

with ϵ given by Eq. (2.97). This fully solves the problem, since the Hamiltonian has now a standard form with two independent kinds of non-interacting bosons. The ground state energy is $\epsilon - \epsilon_0$, and the ground state is determined by the conditions $b_i|0\rangle = 0$ for $i = 1, 2$. The excited states are obtained by acting on the ground state with operators $b_1^\dagger$ and $b_2^\dagger$; they are characterized by the numbers n_1 and n_2 of the two kinds of bosons. Each excitation adds energy ϵ.

2.4.3 Elementary excitations in the weakly interacting Bose gas

We apply now the results of Sec. 2.4.2 to the Hamiltonian (2.86). For every pair of momenta $\mathbf{p}, -\mathbf{p}$, we have a contribution of the type (2.87) in the Hamiltonian, with $a_1 \to a_{\mathbf{p}}$ and $a_2 \to a_{-\mathbf{p}}$, and with $\epsilon_0 \to \epsilon_p^{(0)} + n_0 U_0$ and $\lambda \to n_0 U_0$. The Bogoliubov transformation (2.91) reads

$$b_{\mathbf{p}} = u_p a_{\mathbf{p}} + v_p a_{-\mathbf{p}}^\dagger\,, \qquad b_{-\mathbf{p}} = u_p a_{-\mathbf{p}} + v_p a_{\mathbf{p}}^\dagger\,, \tag{2.101}$$

with the inverse transformation

$$a_{\mathbf{p}} = u_p b_{\mathbf{p}} - v_p b_{-\mathbf{p}}^\dagger\,, \qquad a_{-\mathbf{p}} = u_p b_{-\mathbf{p}} - v_p b_{\mathbf{p}}^\dagger\,, \tag{2.102}$$

where

$$u_p^2 = \frac{1}{2}\left(\frac{\epsilon_p^{(0)} + n_0 U_0}{\epsilon_p} + 1\right)\,, \qquad v_p^2 = \frac{1}{2}\left(\frac{\epsilon_p^{(0)} + n_0 U_0}{\epsilon_p} - 1\right)\,, \tag{2.103}$$

and

$$\epsilon_p = \sqrt{\left(\epsilon_p^{(0)} + n_0 U_0\right)^2 - (n_0 U_0)^2} = \sqrt{\left(\epsilon_p^{(0)}\right)^2 + 2\epsilon_p^{(0)} n_0 U_0}\,. \tag{2.104}$$

The Hamiltonian takes the form

$$\widehat{H} = \frac{N^2 U_0}{2V} - \frac{1}{2}\sum_{\mathbf{p}\neq 0}\left[\epsilon_p^{(0)} + n_0 U_0 - \epsilon_p\right] + \sum_{\mathbf{p}\neq 0}\epsilon_p b_{\mathbf{p}}^\dagger b_{\mathbf{p}}\,, \tag{2.105}$$

so that the system possesses bosonic excitations with the famous Bogoliubov dispersion law ϵ_p,

$$\epsilon_p = \sqrt{\left(\frac{p^2}{2m}\right)^2 + \frac{n_0 U_0}{m} p^2}\,. \tag{2.106}$$

These excitations are created by operators $b_{\mathbf{p}}^\dagger = u_p a_{\mathbf{p}}^\dagger + v_p a_{-\mathbf{p}}$. The ground state $|0\rangle$ satisfies $b_{\mathbf{p}}|0\rangle = 0$ for all $\mathbf{p} \neq 0$ and has the energy

$$E_0 = \frac{N^2 U_0}{2V} - \frac{1}{2}\sum_{\mathbf{p}\neq 0}\left[\epsilon_p^{(0)} + n_0 U_0 - \epsilon_p\right]\,. \tag{2.107}$$

Let us analyze the dispersion law (2.106). For sufficiently large momenta, it is close to the quadratic free-particle dispersion:

$$\epsilon_p \simeq \frac{p^2}{2m} + n_0 U_0\,, \qquad p \gg \sqrt{2m n_0 U_0}\,, \tag{2.108}$$

with the second term being a relatively small correction to the dominant term $p^2/2m$. On the other hand, for low momenta, the dispersion law is linear,

$$\epsilon_p \simeq cp \qquad \text{with} \quad c = \sqrt{\frac{n_0 U_0}{m}}\,, \qquad p \ll \sqrt{2mn_0U_0}\,. \tag{2.109}$$

Thus, for low momenta p (equivalently, low wave vectors $k = p/\hbar$, or large wave length $2\pi k^{-1} = 2\pi\hbar/p$), the excitations have collective character. These low-momenta collective excitations can be viewed as phonons, which are quantized sound waves, with $c = \sqrt{n_0U_0/m}$ being the sound velocity. The crossover between these collective phonon excitations with linear dispersion and quadratic free-particle dispersion of excitations takes place at wave vector $k \sim \sqrt{2mn_0U_0}/\hbar$ or, equivalently, at length scale of order of

$$\xi = \frac{\hbar}{\sqrt{2mn_0U_0}}\,. \tag{2.110}$$

The length ξ, which is called "coherence length" or "healing length", thus determines the characteristic scale for the collective behavior of the system.

The ground state energy E_0 is dominated by the first term in Eq. (2.107) under the condition of weak interaction or, equivalenty, diluteness of the gas,

$$\frac{U_0 m}{\hbar^2} \ll n^{-1/3}\,. \tag{2.111}$$

The l.h.s. of this inequality is the characteristic length associated with the interaction potential U_0 (known as scattering length), while the r.h.s. is a typical distance between particles. Under this condition,

$$E_0 \simeq \frac{N^2U_0}{2V}\,. \tag{2.112}$$

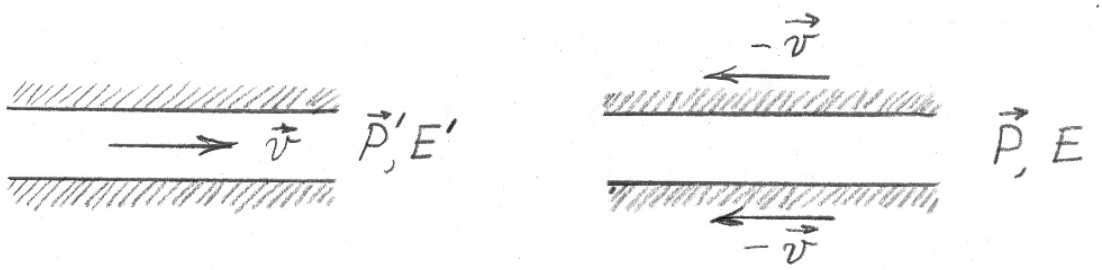
Consequently, the chemical potential is given by

$$\mu = \left(\frac{\partial E_0}{\partial N}\right)_{V,T} \simeq U_0\frac{N}{V} = U_0 n\,. \tag{2.113}$$

Note that, at variance with the non-interacting Bose gas, for which $\mu = 0$ at zero temperature, in the presence of interaction we have $\mu > 0$.

2.5 Landau criterion of superfluidity

To explain that the dispersion (2.106) of elementary excitations leads to superfluidity, we invoke the Landau criterion of superfluidity. Consider a fluid flowing in a pipe at zero temperature. In the resting ("laboratory") reference frame, the pipe is at rest, and the fluid moves with a velocity $\boldsymbol{v}$. One wants to find out whether any friction (i.e., energy dissipation) occurs. For this purpose, it is useful first to consider the whole system in a moving frame, in which the fluid is at rest and the pipe moves with the velocity $-\boldsymbol{v}$.



Let $\boldsymbol{P}$ and E be the momentum and energy of the fluid in this reference frame. Further, let the spectrum of excitations consist of quasiparticles with momentum and energy $\{\boldsymbol{p}\,,\,\varepsilon(\boldsymbol{p}\,)\}$. Then, excitation of a quasiparticle in the frame, in which the fluid rests, leads to change of momentum and energy of the fluid:

$$\Delta\boldsymbol{P}\,=\boldsymbol{p}\,,\qquad \Delta E=\varepsilon(\boldsymbol{p}\,)\,. \tag{2.114}$$

Now we make a Galilei transformation to the laboratory frame (in which the pipe rests). The momentum and energy transform according to relations known from classical mechanics:

$$\boldsymbol{P}\,'=\boldsymbol{P}\,+M\boldsymbol{v}\,,\qquad E'=E+\boldsymbol{P}\,\boldsymbol{v}\,+\frac{Mv^2}{2}\,, \tag{2.115}$$

where M is the mass of the fluid. (These formulas follow from summing the momenta and kinetic energies of particles: $\boldsymbol{p}\,'=m\boldsymbol{u}\,'=m(\boldsymbol{u}\,+\boldsymbol{v}\,)$ and $\epsilon'=m(\boldsymbol{u}\,')^2/2=m(\boldsymbol{u}\,+\boldsymbol{v}\,)^2/2$; potential energy is not affected by the transformation). Thus, the change of the energy in the laboratory frame associated with the quasiparticle excitation (2.114) is

$$\Delta E'=\Delta E+\Delta\boldsymbol{P}\,\cdot\boldsymbol{v}\,=\varepsilon(\boldsymbol{p}\,)+\boldsymbol{v}\,\boldsymbol{p}\,. \tag{2.116}$$

Since the pipe is at rest in the laboratory frame, it cannot provide energy to the fluid. Therefore, the quasiparticle can be excited only if its excitation lowers the energy of the system, i.e., if $\Delta E'<0$. If this is the case for some of possible excitations, they will be excited, so that there will be a finite friction, i.e., there will be no superfluidity. Let us assume an isotropic dispersion $\varepsilon(\boldsymbol{p}\,)=\varepsilon(p)$. Then, for a given $p=|\boldsymbol{p}\,|$, the minimal value of $\Delta E'$ is reached for $\boldsymbol{p}$ directed opposite to $\boldsymbol{v}\,$:

$$\Delta E'=\varepsilon(p)-vp\,,\qquad p=|\boldsymbol{p}\,|>0\,. \tag{2.117}$$

The system is thus superfluid if $\Delta E'$ as given by Eq. (2.117) is positive for any $p>0$. This can be equivalently rewritten as

$$v<\min_p\left(\frac{\varepsilon(p)}{p}\right)\equiv v_c\,, \tag{2.118}$$

which is the famous Landau criterion for superfluidity. Here v_c is the critical velocity. For $v<v_c$, no excitations will be created, implying superfluidity. Only for $v>v_c$ excitations with $\Delta E'<0$ appear, and dissipation (i.e., friction) emerges. Thus, as long as $v_c>0$, the system is superfluid for sufficiently small flow velocities, $v<v_c$.

Application to a (weakly-interacting) Bose system

For the Bogoliubov excitation spectrum (2.106), the critical velocity v_c as determined by Eq. (2.118) is given by the sound velocity, $v_c=c>0$, implying superfluidity for flow velocitiy $v<c$. Note that the sound velocity is $c=(U_0n_0/m)^{1/2}$, Eq. (2.109), so that for a free Bose gas ($U_0=0$), we have $v_c=0$. i.e., no superfluidity.

Application to a Fermi system

The Landau criterion of superfluidity can be also applied to an interacting Fermi system that may become superconducting, as will be discussed in Sec. 2.8.

2.6 Long-range order, symmetry breaking, and order parameter for a Bose fluid

2.6.1 Wave function of condensate

Consider one-particle correlation function (density matrix) for bosons

$$G(\mathbf{r}-\mathbf{r}') = \langle \Phi_0 | \widehat{\Psi}^\dagger(\mathbf{r}) \widehat{\Psi}(\mathbf{r}') | \Phi_0 \rangle \,. \tag{2.119}$$

Obviously, $G(0) = n$ (density of particles). To analyze the dependence on distance, we go the momentum representation:

$$\widehat{\Psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{p}} e^{i\boldsymbol{p}\,\mathbf{r}/\hbar}\, a_{\boldsymbol{p}} \,. \tag{2.120}$$

For high temperatures, for which there is no Bose-Einstein condensation, i.e., no macroscopic occupation of the $\boldsymbol{p} = 0$ state, the sum can be replaced by an integral, yielding

$$G(\mathbf{r}-\mathbf{r}') = \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{i\boldsymbol{p}\,(\mathbf{r}-\mathbf{r}')/\hbar}\, \langle n_p \rangle \,, \tag{2.121}$$

where $\langle n_p \rangle = \langle \Phi_0 | a^\dagger_{\boldsymbol{p}}\, a_{\boldsymbol{p}} | \Phi_0 \rangle$ is the distribution of particles over momenta. This leads to

$$G(\mathbf{r}-\mathbf{r}') \to 0 \qquad \text{at} \qquad |\mathbf{r}-\mathbf{r}'| \to \infty \,, \tag{2.122}$$

cf. an analogous calculation for fermions in Sec. 2.3.1. On the other hand, for low T there is Bose-Einstein condensation, so that the term with $\boldsymbol{p} = 0$ is crucially important,

$$\widehat{\Psi}(\mathbf{r}) = \frac{1}{\sqrt{V}}\, a_0 + \frac{1}{\sqrt{V}} \sum_{\boldsymbol{p}\neq 0} e^{i\boldsymbol{p}\,\mathbf{r}/\hbar}\, a_{\boldsymbol{p}} \,. \tag{2.123}$$

The $\boldsymbol{p} = 0$ term gives now a constant contribution to $G(\mathbf{r}-\mathbf{r}')$ equal to the condensate density $n_0 = \langle \Phi_0 | a_0^\dagger a_0 | \Phi_0 \rangle$, so that the correlation function remains nonzero at infinite separation:

$$G(\mathbf{r}-\mathbf{r}') \to n_0 \qquad \text{at} \qquad |\mathbf{r}-\mathbf{r}'| \to \infty \,, \tag{2.124}$$

This is frequently called "off-diagonal long-range order" (and abbreviated as ODLRO), since the long-range order here manifests itself in off-diagonal components ($\boldsymbol{r} \neq \boldsymbol{r}\,'$) of one-particle density matrix.

Equation (2.123) has the form

$$\widehat{\Psi}(\mathbf{r}) = \widehat{\Psi}_0(\mathbf{r}) + \delta\widehat{\Psi}(\mathbf{r}) \,, \tag{2.125}$$

with the first term corresponding to the condensate and the second term to the rest. Since number of particles in the condensate is large, $N_0 = n_0 V$, we can consider $\Psi_0(\mathbf{r})$ as a number rather than an operator, as was done above in the Bogoliubov approximation (Sec. 2.4.1). More accurately, $\widehat{\Psi}(\mathbf{r})$ changes the number of particles in the condensate by one, and we can define

$$\langle N-1 | \widehat{\Psi}_0(\mathbf{r}) | N \rangle \equiv \Psi_0(\mathbf{r}) \,, \qquad \langle N | \widehat{\Psi}_0^\dagger(\mathbf{r}) | N-1 \rangle \equiv \Psi_0^*(\mathbf{r}) \,, \tag{2.126}$$

where $|N\rangle$ and $|N-1\rangle$ differ only by a number of particles in the condensate (N_0 vs. $N_0 - 1$) and thus are physically equivalent up to $1/N_0$ corrections. In this sense, we can replace $\widehat{\Psi}(\mathbf{r})$ by $\Psi_0(\mathbf{r})$. The function $\Psi_0(\mathbf{r})$ is called **"wave function of condensate"**. In Eq. (2.123), it

is $\Psi_0(\mathbf{r}) = N_0^{1/2} V_0^{-1/2} = n_0^{1/2}$, but, more generally (e.g., in spatially varying fields, or if the fluid flows), $\Psi_0(\mathbf{r})$ may vary:

$$\Psi_0(\mathbf{r}) = n_0^{1/2}(\mathbf{r}) e^{iS(\mathbf{r})} \,. \tag{2.127}$$

The wave function of condensate plays the role of the **order parameter** for the superfluid state (distinguishing it from the normal state).

For stationary states, the time-dependence of the condensate wave function is

$$\Psi_0(\mathbf{r}, \mathbf{t}) = \langle N-1 | e^{i\widehat{H}t/\hbar} \widehat{\Psi}_0(\mathbf{r}) e^{-i\widehat{H}t/\hbar} | N \rangle = e^{-i(E_N - E_{N-1})t/\hbar} \langle N-1 | \widehat{\Psi}_0(\mathbf{r}) | N \rangle = e^{-i\mu t/\hbar} \Psi_0(\mathbf{r}) \,, \tag{2.128}$$

where we have used

$$\mu = \frac{\partial E_0(N)}{\partial N} = E_0(N) - E_0(N-1) \,. \tag{2.129}$$

2.6.2 Gross-Pitaevskii equation

To derive an equation for the condensate wave function, we begin with the evolution equation (2.69) for the Heisenberg operator $\widehat{\Psi}(\mathbf{r}, t)$,

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \widehat{\Psi}(\mathbf{r}, t) = \left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + U_{\mathrm{ext}}(\mathbf{r}, t) + \int \mathrm{d}r' \, \widehat{\Psi}^\dagger(\mathbf{r}', t) V(\mathbf{r} - \mathbf{r}') \widehat{\Psi}(\mathbf{r}', t) \right] \widehat{\Psi}(\mathbf{r}, t) \,. \tag{2.130}$$

where $U_{\mathrm{ext}}(\mathbf{r}, t)$ is an external potential (which can be in general also time-dependent) and $V(\mathbf{r} - \mathbf{r}')$ two-particle interaction. As above, we consider a weak local interaction $V(\mathbf{r} - \mathbf{r}') = U_0 \delta(\mathbf{r} - \mathbf{r}')$, see the Hamiltonian Eq. (2.83). Further, we focus on low temperatures, when nearly all particles are in the condensate, $n_0 \approx n$, and thus replace the operator $\widehat{\Psi}$ by the condensate wave function Ψ_0. Equation (2.130) then becomes

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \Psi_0(\mathbf{r}, t) = \left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + U_{\mathrm{ext}}(\mathbf{r}, t) + U_0 |\Psi_0(\mathbf{r}, t)|^2 \right] \Psi_0(\mathbf{r}, t). \tag{2.131}$$

Equation (2.131) is the **Gross-Pitaevskii equation** for the wave function of the condensate (sometimes also called "non-linear Schrödinger equation"). This equation has proven to be very useful in describing various aspects of the physics of superfluids, including superfluid hydrodynamics, excitations (vortices, solitons, small-amplitude oscillations), various geometries, etc.

2.6.3 Stationary solutions and U(1) symmetry breaking

Assume that the external potential U_{ext} is time-independent. In this situation, we may look for stationary solutions of the Gross-Pitaevskii equation. According to Eq. (2.128), the t-dependence of the condensate wave function in a stationary state is

$$\Psi_0(\mathbf{r}, \mathbf{t}) = \Psi_0(\mathbf{r}) e^{-i\mu t/\hbar} \,. \tag{2.132}$$

Substituting this in Eq. (2.131), we obtain the stationary form of this equation:

$$\left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + U_{\mathrm{ext}}(\mathbf{r}) - \mu + U_0 |\Psi_0(\mathbf{r})|^2 \right] \Psi_0(\mathbf{r}) = 0 \,. \tag{2.133}$$

This equation can be presented in the form

$$\frac{\delta}{\delta \Psi_0^*(\mathbf{r})} E'\{\Psi_0, \Psi_0^*\} = 0 \,, \tag{2.134}$$

where E' is the (grand-canonical) energy functional

$$E'\{\Psi_0, \Psi_0^*\} = E - \mu \int dr |\Psi_0|^2 = \int dr \left[\frac{\hbar^2}{2m} |\boldsymbol{\nabla} \Psi_0|^2 + U_{\rm ext}(\mathbf{r}) |\Psi_0|^2 - \mu |\Psi_0|^2 + \frac{U_0}{2} |\Psi_0|^4 \right]. \tag{2.135}$$

The solution of the Gross-Pitaevskii equation thus corresponds to a minimum of the energy E'.

Consider the case $U_{\rm ext}(\mathbf{r}) = 0$. The minimum of E' is the provided by a spatially uniform ($\mathbf{r}$-independent) configuration $\Psi_0(\mathbf{r}) = \Psi_0$. The energy functional on such configurations takes the form

$$E' = V \left(-\mu |\Psi_0|^2 + \frac{U_0}{2} |\Psi_0|^4 \right). \tag{2.136}$$

We recall that $\mu > 0$ and $U_0 > 0$. The function (2.136) has the form of a "mexican hat" potential. It is of the same form as in the Ginzburg-Landau theory on the broken-symmetry side. Let us emphasize a difference, however: the Ginzburg-Landau theory is formulated for the vicinity of a phase transition, while here we deal with the system at zero (or very low) temperature, i.e., deeply in the superfluid (broken-symmetry) phase. Near the transition, the Landau functional will have a similar structure but the coefficients will be very different.

The minimum of the functional (2.136) is achieved at

$$|\Psi_0|^2 = \mu / U_0 \,, \tag{2.137}$$

in agreement with Eq. (2.113). Importantly, Eq. (2.137) fixes the amplitude but not the phase of Ψ_0. Thus, there is the whole family of solutions,

$$\Psi_0 = |\Psi_0| e^{i\alpha} = (\mu/U_0)^{1/2} \, e^{i\alpha} \,, \tag{2.138}$$

with arbitrary phase α. This is a manifestation of the $U(1)$ symmetry of the theory corresponding to the particle number conservation. Choosing one particular α **breaks this symmetry**. All solutions with a constant α are physically equivalent (since multiplication of a wave function by a constant phase factor does not have any implications for physical observables). Nevertheless, the symmetry breaking is of crucial importance: allowing the phase α to change in space and time yields excitations, see below.

2.6.4 Small-amplitude oscillations. Long-wave-length oscillations as Goldstone mode.

We consider now small-amplitude oscillations with respect to a stationary configuration (2.132). (This is a classical analysis; upon quantising, we should get low-lying excitations of the system, as we discuss in the end.) We look for a solution of the Gross-Pitaevskii equation (2.131) in the form

$$\Psi_0(\mathbf{r}, t) = \Psi'(\mathbf{r}, t) e^{-i\mu t/\hbar} = \left[\Psi_0(\mathbf{r}) + \chi(\mathbf{r}, t) \right] e^{-i\mu t/\hbar} \,, \tag{2.139}$$

with a small $\chi(\mathbf{r}, t)$. Equation for $\Psi'(\mathbf{r}, t)$ is obtained by substituting Eq. (2.139) into Eq. (2.131) (with a time-independent external potential $U_{\rm ext}$):

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \Psi'(\mathbf{r}, t) = \left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + U_{\rm ext}(\mathbf{r}) - \mu + U_0 |\Psi'(\mathbf{r}, t)|^2 \right] \Psi'(\mathbf{r}, t) \,. \tag{2.140}$$

This equation can be presented in the form

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \Psi'(\mathbf{r}, t) = \frac{\delta E'}{\delta \Psi'^*(\mathbf{r}, t)} \,, \tag{2.141}$$

where E' is the functional (2.135). We substitute $\Psi'(\mathbf{r},t) = \Psi_0(\mathbf{r}) + \chi(\mathbf{r},\mathbf{t})$ in Eq. (2.140) and linearize with respect to a small term $\chi(\mathbf{r},t)$. Further, we look for a solution oscillating with a certain frequency ω. Since the non-linear term in Eq. (2.140) gives rise not only to $\chi(\mathbf{r},t)$ but also to $\chi^*(\mathbf{r},t)$, we should look for a solution of the form

$$\chi(\mathbf{r},t) = u(\mathbf{r})e^{-i\omega t} + v^*(\mathbf{r})e^{i\omega t}\,. \tag{2.142}$$

Substituting this ansatz and separating terms proportional to $e^{-i\omega t}$ and to $e^{i\omega t}$, we obtain a system of two equations:

$$\begin{aligned} \hbar\omega u &= \left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + U_{\rm ext}(\mathbf{r}) - \mu + 2U_0|\Psi_0(\mathbf{r})|^2\right) u + U_0\Psi_0^2(\mathbf{r})\, v\,, \\ -\hbar\omega v &= \left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + U_{\rm ext}(\mathbf{r}) - \mu + 2U_0|\Psi_0(\mathbf{r})|^2\right) v + U_0\Psi_0^2(\mathbf{r})\, u\,. \end{aligned} \tag{2.143}$$

We focus now on a situation of a uniform gas: $U_{\rm ext}(\mathbf{r}) = 0$, so that $|\Psi_0(\mathbf{r})|^2 = n_0 \approx n$. We further use the relation $\mu = U_0 n$. Without restricting generality, we can choose the condensate Ψ_0 around which oscillations are considered as real, $\Psi_0 = \sqrt{n}$. Since equations are now translationally-invariant, the solutions have the form of plane waves:

$$u(\mathbf{r}) = u\, e^{i\mathbf{kr}}\,, \qquad v(\mathbf{r}) = v\, e^{i\mathbf{kr}}\,. \tag{2.144}$$

This yields the following system of equations for the amplitudes u and v:

$$\begin{aligned} \hbar\omega u &= \frac{\hbar^2k^2}{2m}\, u + U_0 n(u+v)\,, \\ -\hbar\omega v &= \frac{\hbar^2k^2}{2m}\, v + U_0 n(u+v)\,, \end{aligned} \tag{2.145}$$

or, in the matrix form

$$\begin{pmatrix} -\hbar\omega + \dfrac{\hbar^2k^2}{2m} + U_0 n & U_0 n \\ U_0 n & \hbar\omega + \dfrac{\hbar^2k^2}{2m} + U_0 n \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0\,. \tag{2.146}$$

For a non-trivial solution to exist, the determinant should be zero, which yields

$$(\hbar\omega)^2 = \left(\frac{\hbar^2k^2}{2m}\right)^2 + \frac{\hbar^2k^2}{m}\, U_0 n\,. \tag{2.147}$$

Equation (2.147) is the final result for the frequency of oscillations as a function of the wave vector k. In the quantum language, the momentum and energy of excitations are related to k and ω via $p = \hbar k$ and $\epsilon_p = \hbar\omega$. Equation (2.147) then becomes identical to the Bogoliubov dispersion law (2.106). Thus, Bogoliubov excitations correspond to quantized oscillations described by the Gross-Pitaevskii equation.

For small wave vectors, $k \to 0$, we have $\omega \to 0$ according to Eq. (2.147). Let's inspect the character of these long-wave-length excitations. From Eq. (2.146), we immediately see that $u \approx -v$ at small k and ω. This means that $\chi(\mathbf{r},t)$ as given by Eq. (2.142) is purely imaginary. Since $\Psi'(\mathbf{r},t) = \Psi_0 + \chi(\mathbf{r},\mathbf{t})$ with a real Ψ_0, this corresponds to oscillations of the **phase** of the condensate. These excitations have $\omega \to 0$ at $k \to 0$ because the energy E' is invariant with respect to the transformation $\Psi_0 \mapsto \Psi_0 e^{i\alpha}$ with a constant α. Therefore, the long-wave-length excitations represent a **Goldstone mode** associated with spontaneous breaking of the U(1) symmetry.

Goldstone modes of excitations (Goldstone bosons) are generically associated with spontaneously broken continuous symmetries. A paradigmatic example is spin waves (magnons) in einem Heisenberg ferromagnet.

2.6.5 Superfluid velocity

Multiplying the Gross-Pitaevskii equation (2.131) by $\Psi_0^*(\mathbf{r},t)$ and subtracting the complex conjugate, one obtains

$$\frac{\partial|\Psi_0|^2}{\partial t} + \boldsymbol{\nabla}\left[\frac{\hbar}{2mi}(\Psi_0^*\boldsymbol{\nabla}\Psi_0 - \Psi_0\boldsymbol{\nabla}\Psi_0^*)\right] = 0\,. \tag{2.148}$$

(Note that the non-linear term cancels, so that this is the same equation as for the conventional Schrödinger equation.) This is the continuity equation, with the density $n = |\Psi_0|^2$. The expression in square brackets is thus the current, which can be written in the form $\boldsymbol{j} = n\boldsymbol{v}$, with velocity

$$\boldsymbol{v} = \frac{\hbar}{2mi}\,\frac{\Psi_0^*\boldsymbol{\nabla}\Psi_0 - \Psi_0\boldsymbol{\nabla}\Psi_0^*}{|\Psi_0|^2}\,. \tag{2.149}$$

Separating the absolute value and the phase of the condensate wave function,

$$\Psi_0(\mathbf{r},t) = n^{1/2}(\mathbf{r},t)e^{iS(\mathbf{r},t)}\,, \tag{2.150}$$

we obtain from Eq. (2.149)

$$\boldsymbol{v} = \frac{\hbar}{m}\boldsymbol{\nabla}S\,. \tag{2.151}$$

Thus, the superfluid velocity is proportional to the gradient of the phase of the condensate wave function.

2.7 Fermi gas with an attractive interaction: Cooper instability

2.7.1 Attractive interaction between electrons mediated by lattice

As discussed in previous sections, bosons experience at low temperatures Bose-Einstein condensation, which can be understood as spontaneous U(1) symmetry breaking. In presence of repulsive interaction at short distances (always present in physical systems), this leads to superfluidity.

Now we consider a system of interacting fermions. The most important realization of such a system is electron gas in a metal. The phenomenon analogous to superfluidity in this case is **superconductivity**, i.e., vanishing of electric resistance. It was discovered experimentally by H. Kamerlingh Onnes in 1911. While the superconductivity is certainly one of most important phenomena in condensed matter physics, it has taken almost half a century to develop a microscopic theory of this phenomenon. This was done in 1957 by Bardeen, Cooper, and Schrieffer (BCS theory, see below). An important step towards this theory was understanding of an instability of the conventional (filled Fermi see) ground state of a gas of fermions in the presence of **attractive interaction** between fermions (Cooper instability, 1956).

The most conventional interaction between electrons is Coulomb interaction, which is of course repulsive. Where does attractive come from in physical systems? Within the most standard mechanism, which is operative in conventional superconductors, the electron-electron attraction originates from electron-phonon interaction, i.e., the interaction between electrons and ions forming the lattice. A simple way to understand the physics of the electron-electron attraction mediated by lattice is as follows. An electron (which is negatively charged) attracts ions, creating a positively-charged lattice density perturbation around the position of the electron. This positive charge attracts another electron, thus leading to an effective electron-electron attraction. Importantly, ions are much heavier than electrons and thus move relatively

slowly. The characteristic frequency of ion vibrations is the Debye frequency ω_D. Since the frequency of a harmonic oscillator with a mass M scales $\propto M^{-1/2}$, we can estimate

$$\hbar\omega_D \sim \sqrt{\frac{m}{M}}\,\epsilon_F\,, \tag{2.152}$$

where m is electron mass, M is ion mass, and ϵ_F is Fermi energy (which is the characteristic electronic energy scale), so that $\hbar\omega_D$ is roughly two orders of magnitude smaller than ϵ_F. Typical values for metals are $\epsilon_F \sim 2$ – 10 eV and $\hbar\omega_D \sim 0.01$ – 0.1 eV.

In view of this, the effective attractive interaction between electrons is operative only at sufficiently low energies of electrons (counted from from Fermi energy),

$$|\epsilon_{\boldsymbol{k}} - \epsilon_F| \lesssim \hbar\omega_D\,. \tag{2.153}$$

Translated to time domain, the effective attractive interaction is retarded, with a characteristic retardation time $t_D \sim \omega_D^{-1}$.

2.7.2 Cooper instability and Cooper pairs

Consider an exactly solvable model problem that consists of a Fermi see of free (non-interacting) electrons and two electrons with attractive interaction. The role of the Fermi see is in blocking of all states with energies $\varepsilon < \varepsilon_F$.

We thus look for a wave function in the form

$$|\Phi\rangle = \sum_{|\boldsymbol{k}_1|>k_F,\,\sigma_1,\,|\boldsymbol{k}_2|>k_F,\,\sigma_2} \phi(\boldsymbol{k}_1,\boldsymbol{k}_2,\sigma_1,\sigma_2)\; c^\dagger_{\boldsymbol{k}_1,\sigma_1} c^\dagger_{\boldsymbol{k}_2,\sigma_2}|\Phi_0\rangle\,, \tag{2.154}$$

where

$$|\Phi_0\rangle = \prod_{|\boldsymbol{k}|\le k_F,\,\sigma} c^\dagger_{\boldsymbol{k},\sigma}|0\rangle \tag{2.155}$$

is the filled Fermi see. Here $\boldsymbol{k}_i$ are electron momenta and σ_i are spin projections (either $\uparrow$ of $\downarrow$, as we deal with electrons, i.e., spin-$\frac{1}{2}$ fermions). The total momentum $\boldsymbol{K} = \boldsymbol{k}_1 + \boldsymbol{k}_2$ is a conserved quantity. The ground state is expected to be at $\boldsymbol{K} = 0$, so that $\boldsymbol{k}_1 = -\boldsymbol{k}_2$. Further, the interaction does not couple spin and orbital degrees of freedom, so that we look for a function ϕ in the form

$$\phi(\boldsymbol{k}, -\boldsymbol{k}, \sigma_1, \sigma_2) = \psi(\boldsymbol{k})\chi(\sigma_1,\sigma_2)\,. \tag{2.156}$$

The following model interaction is considered:

$$g_{\boldsymbol{k},-\boldsymbol{k},\boldsymbol{k}',-\boldsymbol{k}'} = \begin{cases} -g\,, & 0 < \xi_k,\ \xi_{k'} < \hbar\omega_D\,, \\ 0, & \text{sonst.} \end{cases} \tag{2.157}$$

Here $\boldsymbol{k}$, $-\boldsymbol{k}$ are initial electron momenta, while $\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{q}$ and $-\boldsymbol{k}' = -\boldsymbol{k} - \boldsymbol{q}$ are final-state electron momenta. Further, $\xi_k = \varepsilon_k - \varepsilon_F$. Finally, $g > 0$ is a constant. This interaction models the phonon-induced attraction within the shell of the width $\hbar\omega_D$ near the Fermi energy. The Hamiltonian thus reads

$$H = H_0 + H_{\text{ee}}\,; \qquad H_{\text{ee}} = -\frac{g}{2V} \sum_{\boldsymbol{k},\boldsymbol{k}':\,0<\xi_k,\,\xi_{k'}<\hbar\omega_D;\,\sigma_1,\sigma_2} c^\dagger_{\boldsymbol{k}',\sigma_1}\, c^\dagger_{-\boldsymbol{k}',\sigma_2}\, c_{-\boldsymbol{k},\sigma_2}\, c_{\boldsymbol{k},\sigma_1}. \tag{2.158}$$

Since the interaction is only operative in the shell $0 < \xi_k < \hbar\omega_D$, the function $\psi(\boldsymbol{k})$ will be non-zero only within this shell.

The Schrödinger equation $H|\Phi\rangle = E|\Phi\rangle$ yields

$$\sum_{\boldsymbol{k},\sigma_1,\sigma_2} 2\varepsilon_k \psi(\boldsymbol{k})\chi(\sigma_1,\sigma_2) c^\dagger_{\boldsymbol{k},\sigma_1} c^\dagger_{-\boldsymbol{k},\sigma_2}|\Phi_0\rangle - \frac{g}{V}\sum_{\boldsymbol{k},\boldsymbol{k}',\sigma_1,\sigma_2} \psi(\boldsymbol{k})\chi(\sigma_1,\sigma_2) c^\dagger_{\boldsymbol{k}',\sigma_1} c^\dagger_{-\boldsymbol{k}',\sigma_2}|\Phi_0\rangle$$
$$= E\sum_{\boldsymbol{k},\sigma_1,\sigma_2} \psi(\boldsymbol{k})\chi(\sigma_1,\sigma_2) c^\dagger_{\boldsymbol{k},\sigma_1} c^\dagger_{-\boldsymbol{k},\sigma_2}|\Phi_0\rangle\,, \tag{2.159}$$

where the sums over $\boldsymbol{k}$ and $\boldsymbol{k}'$ go over the shell $0 < \xi_k,\, \xi_{k'} < \hbar\omega_D$, and the energy E is counted from the energy of the filled Fermi sea. Equating the coefficients in front of $c^\dagger_{\boldsymbol{k},\sigma_1} c^\dagger_{-\boldsymbol{k},\sigma_2}|\Phi_0\rangle$, we get

$$\boxed{2\varepsilon_k \psi(\boldsymbol{k}) - \frac{g}{V}\sum_{\boldsymbol{k}':\, 0<\xi_{k'}<\hbar\omega_D} \psi(\boldsymbol{k}') = E\psi(\boldsymbol{k})\,.} \tag{2.160}$$

We denote

$$C \equiv \frac{1}{V}\sum_{\boldsymbol{k}:\, 0<\xi_k<\hbar\omega_D} \psi(\boldsymbol{k})\,. \tag{2.161}$$

Equation (2.160) yields

$$\psi(\boldsymbol{k}) = \frac{gC}{2\varepsilon_k - E}\,. \tag{2.162}$$

Summing this equation over $\boldsymbol{k}$ in the shell $0 < \xi_k < \hbar\omega_D$ and dividing by volume V, we get

$$C = \frac{1}{V}\sum_{\boldsymbol{k}:\, 0<\xi_k<\hbar\omega_D} \frac{gC}{2\varepsilon_k - E}\,. \tag{2.163}$$

We thus have obtained an equation for E:

$$1 = \frac{g}{V}\sum_{\boldsymbol{k}:\, \varepsilon_F<\varepsilon_k<\varepsilon_F+\hbar\omega_D} \frac{1}{2\varepsilon_k - E}\,. \tag{2.164}$$

The sum over momenta can be rewritten in the usual way as an integral over energy:

$$1 = g\int\limits_{\varepsilon_F}^{\varepsilon_F+\hbar\omega_D} d\varepsilon\, \nu(\varepsilon)\,\frac{1}{2\varepsilon - E}\,, \tag{2.165}$$

where $\nu(\varepsilon)$ is the density of states per spin projection. Approximating the density of states by its value at the Fermi energy $\nu(\epsilon) \simeq \nu(\varepsilon_F) \equiv \nu_0$, we obtain

$$\frac{1}{g\nu_0} = \frac{1}{2}\ln\frac{2\varepsilon_F + 2\hbar\omega_D - E}{2\varepsilon_F - E} \tag{2.166}$$

Thus

$$\frac{2\varepsilon_F + 2\hbar\omega_D - E}{2\varepsilon_F - E} = e^{\frac{2}{g\nu_0}} \tag{2.167}$$

and, therefore,

$$\delta E \equiv E - 2\varepsilon_F = -\frac{2\hbar\omega_D}{e^{\frac{2}{g\nu_0}} - 1} \simeq -2\hbar\omega_D\, e^{-\frac{2}{g\nu_0}} < 0\,. \tag{2.168}$$

On the last step, we assumed a weak interaction, $g\nu_0 \ll 1$.

We have thus obtained a reduction of energy due to interaction ($\delta E < 0$), i.e., a bound state of two electrons: a **Cooper pair**. The binding energy per electron is

$$\boxed{\Delta = \frac{1}{2}|\delta E| = \hbar\omega_D\, e^{-\frac{2}{g\nu_0}}.} \tag{2.169}$$

Comments:

(i) We have assumed that the interaction $g_{\boldsymbol{k},-\boldsymbol{k},\boldsymbol{k}',-\boldsymbol{k}'}$ is independent of the directions $\hat{k}$, $\hat{k}'$ and obtained, as a result, that the Cooper-pair wave function $\psi(\boldsymbol{k})$ is independent on $\hat{k}$, i.e., s-wave pairing (angular momentum $L = 0$ of the Cooper pair). The total wave function $\phi(\boldsymbol{k}, -\boldsymbol{k}, \sigma_1, \sigma_2) = \psi(\boldsymbol{k})\chi(\sigma_1, \sigma_2)$ should be antisymmetric (since electrons are fermions): $\phi(\boldsymbol{k}, -\boldsymbol{k}, \sigma_1, \sigma_2) = -\phi(-\boldsymbol{k}, \boldsymbol{k}, \sigma_2, \sigma_1)$. Since the orbital part is symmetric, $\psi(\boldsymbol{k}) = \psi(-\boldsymbol{k})$, the spin part $\chi(\sigma_1, \sigma_2)$ should be antisymmetric, i.e. the Cooper pair is in spin-singlet state, with total spin $S = 0$.

In a similar way, one can assume an attraction in a channel with orbital angular momentum $L = 1, 2, \ldots, ..$:

$L = 0$	s-wave	$S = 0$	spin-singlet
$L = 1$	p-wave	$S = 1$	spin-triplet
$L = 2$	d-wave	$S = 0$	spin-singlet

etc.

(ii) The binding energy Δ depends on the interaction strength g in a non-analytic way. Thus, this result cannot be obtained by means of a perturbative expansion in g.

(iii) Without the effect of the Fermi-see blocking, there is no bound states for a weak potential in 3D.

2.8 Superconductivity: BCS theory

J. Bardeen, L. Cooper, and R. Schrieffer, 1957

Now we consider the full many-body problem.

2.8.1 BCS Hamiltonian

We work in the grand canonical ensemble. The grand canonical partition function:

$$Z_G = \sum_{n,N} e^{-\beta(E_{n,N} - \mu N)} \,. \tag{2.170}$$

At $T = 0$ one has to find the ground state of the grand canonical Hamiltonian $H_G = H - \mu N$, which is given by

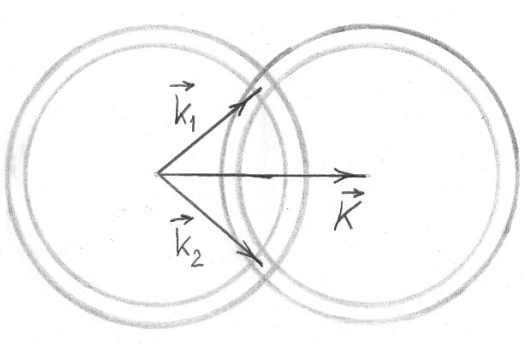
$$H_G = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k},\sigma}\, c_{\boldsymbol{k},\sigma} - \frac{1}{2}\,\frac{g}{V} \sum_{\boldsymbol{k}_1,\sigma_1,\boldsymbol{k}_2,\sigma_2,\boldsymbol{q}} c^\dagger_{\boldsymbol{k}_1+\boldsymbol{q},\sigma_1}\, c^\dagger_{\boldsymbol{k}_2-\boldsymbol{q},\sigma_2}\, c_{\boldsymbol{k}_2,\sigma_2}\, c_{\boldsymbol{k}_1,\sigma_1} \,, \tag{2.171}$$

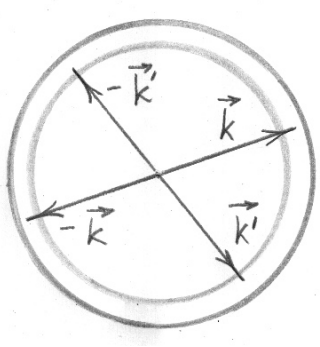
where $\xi_k = \varepsilon_k - \mu$. Here $g > 0$, implying attraction. To model the attraction induced by phonons, the summation in the second term goes over such momenta that all involved electrons are in the $\hbar\omega_D$ shell around the Fermi energy:

$$|\xi_{\boldsymbol{k}_1}|, |\xi_{\boldsymbol{k}_2}|, |\xi_{\boldsymbol{k}_1+\boldsymbol{q}}|, |\xi_{\boldsymbol{k}_2-\boldsymbol{q}}| < \hbar\omega_D \,. \tag{2.172}$$

Electrons outside of this shell are thus characterized by a free Hamiltonian and totally decouple, so that we only consider the electrons within the shell (2.172) below.

We further notice that the attraction is much more efficient for electron pairs satisfying $\boldsymbol{k}_1 + \boldsymbol{k}_2 \simeq 0$ (Cooper pairs). Indeed, if $\boldsymbol{K} = \boldsymbol{k}_1 + \boldsymbol{k}_2$, the momentum of an electron $\boldsymbol{k}' = \boldsymbol{k}_1 + \boldsymbol{q}$ created by interaction term should satisfy $|\boldsymbol{k}'| \simeq k_F$ and $|\boldsymbol{K} - \boldsymbol{k}'| \simeq k_F$. For a generic (large) $\boldsymbol{K}$, the corresponding phase space (intersection of two shifted narrow shells) is very small. It is strongly enhanced when $\boldsymbol{K} \simeq 0$.





We thus keep only terms with $\boldsymbol{k}_1 + \boldsymbol{k}_2 = 0$. Further, since we consider the s-wave pairing, the Cooper pairs are spin singlets, i.e. $\sigma_1 = -\sigma_2$ in Eq. (2.171), see a comment in the end of Sec. 2.7. We thus get a reduced Hamiltonian: **BCS Hamiltonian**

$$\boxed{H_{\rm BCS} = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k},\sigma}\, c_{\boldsymbol{k},\sigma} - \frac{g}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} c^\dagger_{\boldsymbol{k}',\uparrow}\, c^\dagger_{-\boldsymbol{k}',\downarrow}\, c_{-\boldsymbol{k},\downarrow}\, c_{\boldsymbol{k},\uparrow}\,,} \qquad (2.173)$$

$-\hbar\omega_D < \xi_k, \xi_{k'} < \hbar\omega_D\,.$

2.8.2 Mean-field solution

We perform now the mean-field approximation for the interaction term; symbolically (omitting indices):

$$c^\dagger c^\dagger c c \quad \mapsto \quad \langle c^\dagger c^\dagger\rangle cc + c^\dagger c^\dagger \langle cc\rangle - \langle c^\dagger c^\dagger\rangle\langle cc\rangle\,. \qquad (2.174)$$

Here we take into account only anomalous averages. This yields the effective (mean-field) Hamiltonian

$$H_{\rm eff} = \sum_{\boldsymbol{k},\sigma} \xi_k c^\dagger_{\boldsymbol{k},\sigma}\, c_{\boldsymbol{k},\sigma} - \Delta^* \sum_{\boldsymbol{k}} c_{-\boldsymbol{k},\downarrow}\, c_{\boldsymbol{k},\uparrow} - \Delta \sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\uparrow}\, c^\dagger_{-\boldsymbol{k},\downarrow} + V\frac{|\Delta^2|}{g}\,, \qquad (2.175)$$

where

$$\Delta = \frac{g}{V}\sum_{\boldsymbol{k}'} \langle c_{-\boldsymbol{k}',\downarrow}\, c_{\boldsymbol{k}',\uparrow}\rangle\,, \qquad \Delta^* = \frac{g}{V}\sum_{\boldsymbol{k}'} \langle c^\dagger_{\boldsymbol{k}',\uparrow}\, c^\dagger_{-\boldsymbol{k}',\downarrow}\rangle. \qquad (2.176)$$

In general, Δ can be complex but it is sufficient to take it real at this stage. The Hamiltonian $H_{\rm eff}$ is similar to the bosonic Hamiltonian in (2.86). Specifically, $H_{\rm eff}$ contains anomalous terms of the type $c^\dagger c^\dagger$ and cc. Further it represents a sum of decoupled terms, each of which involves operators corresponding only to $\boldsymbol{k}\,,\sigma$ and $-\boldsymbol{k}\,,-\sigma$. The essential difference compared to (2.86) is that we now deal with fermions. We thus need a **fermionic version of Bogoliubov transformation**. To understand it, we consider first, in analogy with Sec. 2.4.2, a Hamiltonian (which is the fermionic counterpart of Eq. (2.87))

$$\widehat{H} = \epsilon_0(c^\dagger_1 c_1 + c^\dagger_2 c_2) - \lambda(c^\dagger_1 c^\dagger_2 + c_2 c_1)\,, \qquad (2.177)$$

with real ϵ_0 and λ. Without restricting generality, we assume $\lambda > 0$. (One can always change the sign of λ by renaming $c_1 \leftrightarrow c_2$.) The operators c_j satisfy canonical fermionic anticommutation relations $\{c_i, c^\dagger_j\} = \delta_{ij}$ and $\{c_1, c_2\} = \{c^\dagger_1, c^\dagger_2\} = 0$. (We will later apply it to Eq. (2.175) with $c_1 \to c_{\boldsymbol{k},\uparrow}$ and $c_2 \to c_{-\boldsymbol{k},\downarrow}$.) The idea is to diagonalize the Hamiltonian. For this purpose, we introduce new operators

$$b_1 = uc_1 - vc^\dagger_2\,, \qquad b_2 = uc_2 + vc^\dagger_1\,, \qquad (2.178)$$

with coefficients u and v that remain to be specified. In general, u and v can be complex but we take them real as it will be sufficient for our purposes. We require that the operators b_i

satisfy fermionic canonical anticommutation relations. Calculating the anticommutators, we get

$$\{b_1, b_1^\dagger\} = \{b_2, b_2^\dagger\} = u^2 + v^2\,, \qquad \{b_1, b_2\} = \{b_1, b_2^\dagger\} = 0\,. \tag{2.179}$$

Note that opposite signs in Eqs. (2.178) are crucial for getting $\{b_1, b_2\} = 0$. The anticommutation relations have the canonical form if u and v satisfy

$$u^2 + v^2 = 1\,. \tag{2.180}$$

The inverse transformation then reads

$$c_1 = ub_1 + vb_2^\dagger\,, \qquad c_2 = ub_2 - vb_1^\dagger\,. \tag{2.181}$$

Substituting this in Eq. (2.177), we find

$$\widehat{H} = 2v^2\epsilon_0 - 2uv\lambda + [\epsilon_0(u^2 - v^2) + 2uv\lambda](b_1^\dagger b_1 + b_2^\dagger b_2) - [\lambda(u^2 - v^2) - 2uv\epsilon_0](b_1^\dagger b_2^\dagger + b_2 b_1)\,. \tag{2.182}$$

We require now that the term proportional to $b_1^\dagger b_2^\dagger + b_2 b_1$ vanishes, i.e.,

$$\lambda(u^2 - v^2) - 2uv\epsilon_0 = 0\,. \tag{2.183}$$

In view of Eq. (2.180), we can parametrize u and v via

$$u = \cos\theta\,, \qquad v = \sin\theta\,. \tag{2.184}$$

Equation (2.183) then becomes

$$\tan 2\theta = \frac{\lambda}{\epsilon_0}\,. \tag{2.185}$$

We take its solution $2\theta \in [0, \pi]$, so that $\theta \in [0, \pi/2]$ and thus $u, v > 0$. It follows that

$$\cos 2\theta = (1 + \tan^2 2\theta)^{-1/2} = \left[\frac{1}{1 + (\lambda/\epsilon_0)^2}\right]^{1/2} = \frac{\epsilon_0}{\epsilon}\,, \tag{2.186}$$

where we have defined

$$\epsilon = \sqrt{\epsilon_0^2 + \lambda^2} > 0\,. \tag{2.187}$$

From Eqs. (2.184) and (2.186) we obtain

$$u^2 = \frac{1}{2}(1 + \cos 2\theta) = \frac{1}{2}\left(1 + \frac{\epsilon_0}{\epsilon}\right)\,, \qquad v^2 = \frac{1}{2}(1 - \cos 2\theta) = \frac{1}{2}\left(1 - \frac{\epsilon_0}{\epsilon}\right)\,, \tag{2.188}$$

and thus

$$u^2 - v^2 = \frac{\epsilon_0}{\epsilon}\,, \qquad 2uv = \frac{\lambda}{\epsilon}\,. \tag{2.189}$$

Substituting this in (2.182), we obtain the final result for the Hamiltonian after the Bogoliubov transformation:

$$\widehat{H} = \epsilon_0 - \epsilon + \epsilon(b_1^\dagger b_1 + b_2^\dagger b_2)\,, \tag{2.190}$$

with ϵ given by Eq. (2.187). This fully solves the problem, since the Hamiltonian has now a standard form with two "flavors" of non-interacting fermions. The ground state energy is $\epsilon_0 - \epsilon$, and the ground state is determined by the conditions $b_i|0\rangle = 0$ for $i = 1, 2$. The excited states are obtained by acting on the ground state with operators $b_1^\dagger$ and $b_2^\dagger$; they are characterized by the numbers n_1 and n_2 of the two kinds of fermions. Since we deal with fermions, n_i take values 0 or 1. Each excitation adds energy ϵ.

Now we apply these results to the Hamiltonian $H_{\rm eff}$, Eq. (2.175) (with real Δ) by substituting $c_1 \to c_{\boldsymbol{k},\uparrow}$ and $c_2 \to c_{-\boldsymbol{k},-\downarrow}$. The correspondence between parameters is $\epsilon_0 \mapsto \xi_k$ and $\lambda \mapsto \Delta$. We use $\sigma = +1$ equivalently to $\sigma = \uparrow$, and $\sigma = -1$ equivalently to $\sigma = \downarrow$. The transformation (2.178) then becomes

$$b_{\boldsymbol{k},\sigma} = u_{\boldsymbol{k}}\, c_{\boldsymbol{k},\sigma} - \sigma v_{\boldsymbol{k}}\, c^\dagger_{-\boldsymbol{k},-\sigma}\,, \qquad b^\dagger_{\boldsymbol{k},\sigma} = u_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k},\sigma} - \sigma v_{\boldsymbol{k}}\, c_{-\boldsymbol{k},-\sigma}\,, \tag{2.191}$$

which is the fermionic counterpart of the bosonic Bogoliubov transformation (2.101). Here $u_{-\boldsymbol{k}} = u_{\boldsymbol{k}}$ and $v_{-\boldsymbol{k}} = v_{\boldsymbol{k}}$ are real (and positive); in fact, $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ depend only on $k = |\boldsymbol{k}\,|$.

The formulas below essentially repeat the derivation that we have performed for Eq. (2.177), and the final result (2.201) for the Hamiltonian (after diagonalization) is Eq. (2.190), with summation over momenta.

Requiring the fermionic (anticommutation) relations

$$\left\{ b_{\boldsymbol{k},\sigma}, b^\dagger_{\boldsymbol{k}',\sigma'} \right\} = \delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\sigma,\sigma'}\,, \tag{2.192}$$

we get a condition on the coefficients:

$$u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2 = 1\,. \tag{2.193}$$

A second condition on the coefficients $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ comes from the requirement that the Hamiltonian in terms of new operators has the form

$$H = \sum_{\boldsymbol{k},\sigma} E_{\boldsymbol{k}}\, b^\dagger_{\boldsymbol{k},\sigma}\, b_{\boldsymbol{k},\sigma} + \text{const}\,, \tag{2.194}$$

i.e. terms of the type $b^\dagger b^\dagger$ and bb cancel.

The relations inverse to Eq. (2.191) read:

$$c_{\boldsymbol{k},\sigma} = u_{\boldsymbol{k}}\, b_{\boldsymbol{k},\sigma} + \sigma v_{\boldsymbol{k}}\, b^\dagger_{-\boldsymbol{k},-\sigma}\,, \qquad c^\dagger_{\boldsymbol{k},\sigma} = u_{\boldsymbol{k}}\, b^\dagger_{\boldsymbol{k},\sigma} + \sigma v_{\boldsymbol{k}}\, b_{-\boldsymbol{k},-\sigma}\,. \tag{2.195}$$

Substituting them in Eq. (2.175), we get

$$\begin{aligned} H_{\rm eff} &= \sum_{\boldsymbol{k}\,\sigma} \xi_k [u_{\boldsymbol{k}}\, b^\dagger_{\boldsymbol{k},\sigma} + \sigma v_{\boldsymbol{k}}\, b_{-\boldsymbol{k},-\sigma}][u_{\boldsymbol{k}}\, b_{\boldsymbol{k},\sigma} + \sigma v_{\boldsymbol{k}}\, b^\dagger_{-\boldsymbol{k},-\sigma}] \\ &- \left\{ \Delta \sum_{\boldsymbol{k}} [u_{\boldsymbol{k}}\, b_{-\boldsymbol{k},\downarrow} - v_{\boldsymbol{k}}\, b^\dagger_{\boldsymbol{k},\uparrow}][u_{\boldsymbol{k}}\, b_{\boldsymbol{k},\uparrow} + v_{\boldsymbol{k}}\, b^\dagger_{-\boldsymbol{k},\downarrow}] + \text{h.c.} \right\} + \text{const.} \end{aligned} \tag{2.196}$$

Inspecting the coefficient of the term $b_{-\boldsymbol{k},\downarrow} b_{\boldsymbol{k},\uparrow}$ and requiring that it is equal to zero, we get the condition

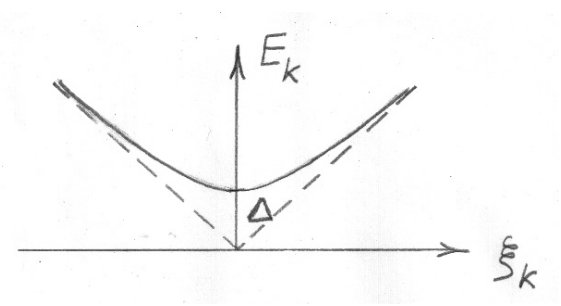
$$2\xi_k v_{\boldsymbol{k}}\, u_{\boldsymbol{k}} - \Delta(u_{\boldsymbol{k}}^2 - v_{\boldsymbol{k}}^2) = 0\,. \tag{2.197}$$

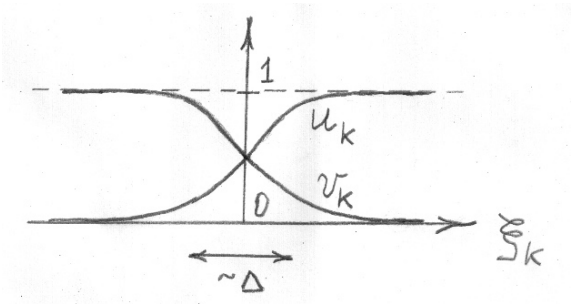
Solving it together with Eq. (2.193), we get

$$u_{\boldsymbol{k}} = \sqrt{\frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right)}\,, \qquad v_{\boldsymbol{k}} = \sqrt{\frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right)}\,, \tag{2.198}$$

where

$$E_k = \sqrt{\xi_k^2 + \Delta^2}\,. \tag{2.199}$$





Collecting now the coefficient in front of $b^\dagger_{\boldsymbol{k}\,\sigma} b_{\boldsymbol{k}\,\sigma}$ in Eq. (2.196), we find

$$\xi_k(u_k^2 - v_k^2) + \Delta \cdot 2u_k v_k = \xi_k \frac{\xi_k}{E_k} + \Delta \frac{\Delta}{E_k} = \frac{\xi_k^2 + \Delta^2}{E_k} = E_k \,. \tag{2.200}$$

Thus, the Hamiltonian has the form

$$H = \sum_{\boldsymbol{k},\sigma} E_k b^\dagger_{\boldsymbol{k},\sigma}\, b_{\boldsymbol{k},\sigma} + \text{const}\,, \tag{2.201}$$

with E_k given by Eq. (2.199). This is exactly Eq. (2.190), with summation over momenta and with $\epsilon \mapsto E_k$. The excitations are **Bogoliubov quasiparticles** (for which $b^\dagger_{\boldsymbol{k},\sigma}$, $b_{\boldsymbol{k},\sigma}$ are creation and annihilation operators), with the spectrum E_k. The key property of this spectrum is the **energy gap** Δ (to be determined below). The "const" in Eq. (2.201) is the ground-state energy; we will also determine it below.

The ground state $|\Phi_{\rm BCS}\rangle$ is determined by the condition

$$b_{\boldsymbol{k},\sigma}|\Phi_{\rm BCS}\rangle = 0 \tag{2.202}$$

for all $\boldsymbol{k}\,,\sigma$. It is given by

$$|\Phi_{\rm BCS}\rangle = \prod_{\boldsymbol{k}} (u_k + v_k c^\dagger_{\boldsymbol{k},\uparrow} c^\dagger_{-\boldsymbol{k},\downarrow})|0\rangle. \tag{2.203}$$

Using $b_{\boldsymbol{k},\sigma} = u_{\boldsymbol{k}}\, c_{\boldsymbol{k},\sigma} - \sigma v_{\boldsymbol{k}}\, c^\dagger_{-\boldsymbol{k},-\sigma}$ [Eq. (2.191)], it is easy to see that Eq. (2.202) is indeed satisfied.

Self-consistency equation

To determine the gap Δ, we derive the self-consistency equation:

$$\begin{aligned} \Delta &= \frac{g}{V}\sum_{\boldsymbol{k}} \langle c_{-\boldsymbol{k},\downarrow}\, c_{\boldsymbol{k},\uparrow}\rangle = \frac{g}{V}\langle [u_k b_{-\boldsymbol{k},\downarrow} - v_k b^\dagger_{\boldsymbol{k},\uparrow}][u_k b_{\boldsymbol{k},\uparrow} + v_{\boldsymbol{k}}\, b^\dagger_{-\boldsymbol{k},\downarrow}]\rangle \\ &\overset{T=0}{=} \frac{g}{V}\sum_{\boldsymbol{k}} u_k v_k \underbrace{\langle b_{-\boldsymbol{k},\downarrow} b^\dagger_{-\boldsymbol{k},\downarrow}\rangle}_{=1} = \frac{g}{V}\sum_{\boldsymbol{k}} u_k v_k \,. \end{aligned} \tag{2.204}$$

Substituting here expressions for u_k and v_k, Eq. (2.198), we obtain

$$\boxed{\Delta = \frac{g}{2V}\sum_{\boldsymbol{k}} \frac{\Delta}{\sqrt{\xi_k^2 + \Delta^2}}\,.} \tag{2.205}$$

After a replacement of the summation by an integral, the equation takes the form

$$1 = \frac{g\nu_0}{2}\int\limits_{-\hbar\omega_D}^{\hbar\omega_D} d\xi \frac{1}{\sqrt{\Delta^2 + \xi^2}} = g\nu_0 \int_0^{\hbar\omega_D} d\xi \frac{1}{\sqrt{\Delta^2 + \xi^2}}$$

$$= g\nu_0 \int_0^{\hbar\omega_D/\Delta} dx \frac{1}{\sqrt{1+x^2}} = g\nu_0 \, \ln(\sqrt{1+x^2}+x)\Big|_0^{\hbar\omega_D/\Delta} \simeq g\nu_0 \ln\frac{2\hbar\omega_D}{\Delta} \qquad (2.206)$$

On the last step, we have assumed $\Delta \ll \hbar\omega_D$, which is the case for weak interaction, $g\nu_0 \ll 1$. Thus, we find the **gap at** $T = 0$:

$$\boxed{\Delta = 2\hbar\omega_D \, e^{-\frac{1}{\nu_0 g}} \, .} \qquad (T = 0) \qquad (2.207)$$

2.8.3 Ground state energy

Let us show that the energy of the BCS ground state $|\Phi_{\rm BCS}\rangle$ is lower than the energy of the normal state $|\Phi_0\rangle$ (filled Fermi sea, which can be obtained from the BCS state by setting $\Delta = 0$). The energy of the BCS state is (subscript "s" for "superconductor")

$$E_s = \langle\Phi_{\rm BCS}|H_{\rm eff}|\Phi_{\rm BCS}\rangle = V\frac{\Delta^2}{g} + \sum_{\boldsymbol{k}}(\xi_k - E_k) \, , \qquad (2.208)$$

where the first term is the constant term from Eq. (2.175) and the second term is a sum of constant terms in Eq. (2.190), with substitution $\epsilon_0 - \epsilon \mapsto \xi_k - E_k$. The energy of the normal state $|\Phi_0\rangle$ is (subscript "n" for "normal")

$$E_n = \langle\Phi_0|H_{\rm eff}|\Phi_0\rangle = 2\sum_{|\boldsymbol{k}|<k_F} \xi_k \, . \qquad (2.209)$$

The difference is

$$E_s - E_n = V\frac{\Delta^2}{g} + \sum_{|\boldsymbol{k}|>k_F}(\xi_k - E_k) + \sum_{|\boldsymbol{k}|<k_F}(-\xi_k - E_k) = V\frac{\Delta^2}{g} + 2\sum_{|\boldsymbol{k}|>k_F}(\xi_k - E_k) \, , \quad (2.210)$$

where, in the last step, we used the symmetry around the Fermi energy (ξ_k is odd, and E_k is even). Replacing summation by an integral, we obtain

$$\begin{aligned} E_s - E_n &= V\frac{\Delta^2}{g} + 2V\nu_0 \int_0^{\hbar\omega_D} d\xi \, (\xi - \sqrt{\xi^2+\Delta^2}) \\ &= V\frac{\Delta^2}{g} + 2V\nu_0\Delta^2 \int_0^{\hbar\omega_D/\Delta} dx \, (x - \sqrt{x^2+1}) \\ &= V\frac{\Delta^2}{g} - V\nu_0\Delta^2\left(\frac{1}{2} + \ln\frac{2\hbar\omega_D}{\Delta}\right) = V\frac{\Delta^2}{g} - V\nu_0\Delta^2\left(\frac{1}{2} + \frac{1}{\nu_0 g}\right) \end{aligned} \qquad (2.211)$$

On the last step we used Eq. (2.207) for the gap Δ. We thus see that the term $V\Delta^2/g$ cancels, and the final result for the difference between the energy of the BCS state and the normal state (per unit volume) is

$$\frac{E_s - E_n}{V} = -\frac{1}{2}\nu_0 \, \Delta^2 < 0 \, . \qquad (2.212)$$

Importantly, $E_s - E_n < 0$. i.e., BCS state has lower energy than the Fermi see. This is another confirmation of the fact that the BCS state is the ground state of the Hamiltonian. Equation (2.212) is the **condensation energy**. Its magnitude can be understood in a simple way: electrons within the energy window $\sim \Delta$ gain an energy $\sim \Delta$ due to pairing.

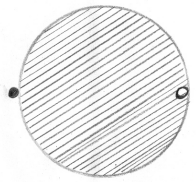
2.8.4 Superconductivity: Landau criterion

We recall the Landau criterion for superfluidity (2.118)

$$v < \min_p \left(\frac{\varepsilon(p)}{p} \right) \equiv v_c \,, \tag{2.213}$$

Here v_c is the critical velocity. For $v < v_c$, no excitations will be created, implying superfluidity. Only for $v > v_c$ excitations with $\Delta E' < 0$ appear, and dissipation (i.e., friction) emerges. Thus, as long as $v_c > 0$, the system is superfluid for sufficiently small flow velocities, $v < v_c$.

In a Fermi liquid, excitations are particle-hole pairs. Their momentum is $p \in [0, 2p_F]$, and the energy can be arbitrarily small. Therefore, $v_c = 0$, i.e., there is a finite friction (resistance) for any velocity of the flow (i.e., for any current).



On the other hand, in the presence of weak attractive interaction, the ground state and the spectrum of excitations around it are given by the BCS theory. Crucially, there is a gap 2Δ for creation of quasiparticle pairs. Therefore,

$$v_c = \frac{2\Delta}{2p_F} = \frac{\Delta}{p_F} > 0 \,, \tag{2.214}$$

so that there is no friction, i.e., no resistance, for $v < v_c$. The system is thus a superfluid. In the case of charged fermions—most importantly, electrons—it is a **superconductor**. The critical velocity v_c implies the critical current density

$$j_c = nev_c = ne\,\frac{\Delta}{p_F} \,, \tag{2.215}$$

where n is the electron density and e the electron charge. For $j < j_c$ the current flows without resistance, i.e., the system is superconducting.

2.8.5 Extension to finite temperature

The BCS theory can be extended to a finite temperature T. The difference will be in the self-consistency equation, since the average in Eq. (2.204) should be then taken not over the ground state but over the thermal state. We omit here details of the calculation and only present the results.

The self-consistency equation at finite T takes the form

$$\boxed{\Delta = \frac{g}{2V} \sum_k \frac{\Delta}{E_k} \tanh \frac{\beta E_k}{2} \,, \qquad E_k = \sqrt{\Delta^2 + \xi_k^2} \,.} \tag{2.216}$$

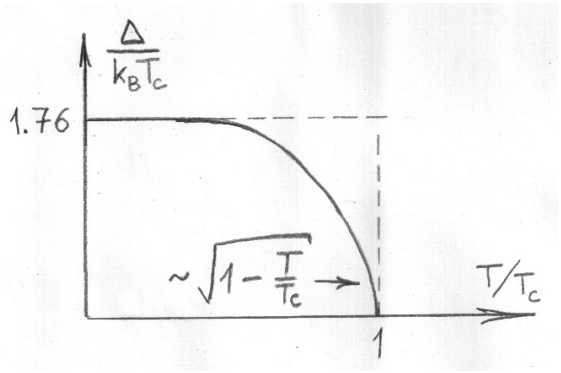
A non-trivial solution $\Delta(T)$ of this equation is found for temperatures $T < T_c$, with the critical temperature T_c given by

$$\boxed{k_{\rm B} T_c = \frac{2e^\gamma}{\pi}\, \hbar\omega_D\, e^{-\frac{1}{\nu_0 g}} \simeq 1.14\, \hbar\omega_D\, e^{-\frac{1}{\nu_0 g}}} \,, \tag{2.217}$$

where $\gamma \simeq 0.5772$ is the Euler constant. Comparing this with Eq. (2.207) for the gap at $T = 0$, we get a universal ratio

$$\boxed{\frac{\Delta(T=0)}{k_B T_c} = \frac{\pi}{e^\gamma} \simeq 1.76 \,.} \tag{2.218}$$

With increasing T, the gap $\Delta(T)$ monotonically decreases:



The behavior for temperatures $T < T_c$ close to T_c is

$$\boxed{\Delta(T) \simeq \left(\frac{8\pi^2}{7\zeta(3)}\right)^{1/2} k_{\rm B}\, T_c \sqrt{1-\frac{T}{T_c}} \simeq 3.06\, k_{\rm B} T_c \sqrt{1-\frac{T}{T_c}}\,.} \tag{2.219}$$

We see the scaling $\Delta(T) \propto (T_c - T)^{1/2}$ with the familiar mean-field value of the exponent $\beta = 1/2$.

2.8.6 Density of states of Bogoliubov quasiparticles

Consider first quasiparticles with momenta $\boldsymbol{k}$ satisfying $\xi_k > 0$. The number of quasiparticles in the volume d^3k is the same in the normal state and the superconducting state. Thus, we can write for the number of quasiparticles in the interval $d\xi$:

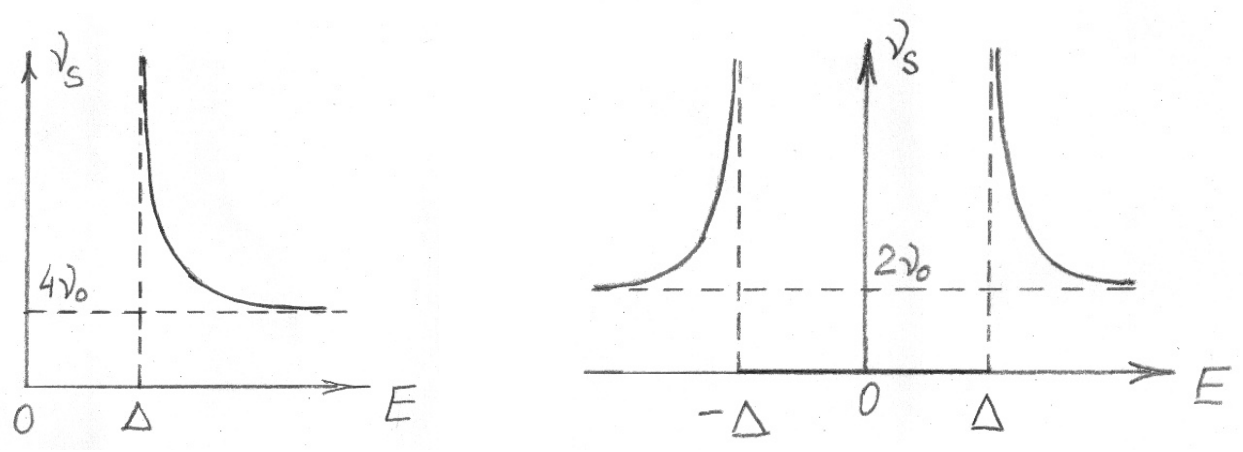
$$\nu_s(E)dE = \underbrace{\nu_n(\xi)}_{\simeq 2\nu_0} d\xi\,, \qquad E = \sqrt{\xi^2+\Delta^2}\,, \tag{2.220}$$

where the subscripts "s" and "n" refer to superconductor and normal state, respectively, and factor 2 in $2\nu_0$ is due to spin. Thus, we have for quasiparticles with $\xi > 0$:

$$\nu_s(E) = 2\nu_0 \frac{d\xi}{dE} = 2\nu_0 \times \begin{cases} \frac{E}{\sqrt{E^2-\Delta^2}}\,, & E > \Delta\,; \\ 0\,, & E < \Delta\,. \end{cases} \tag{2.221}$$

Quasiparticles with $\xi_k < 0$ yield the same contribution, so that the total $\nu_s(E)$ is twice that given by Eq. (2.221), see left figure below. Note that here E is the excitation energy above the ground state that is by definition positive.

To make a closer contact with the picture of a normal metal, in which we have a constant density of states $2\nu_0$, with states with negative energy (counted from μ) filled and states with positive energy empty, one frequently represents the density of states in a "symmetrized" form, with $\nu_s(-E) = \nu_s(E)$ given by Eq. (2.221) with $E \mapsto |E|$, see the right figure below. Such density of states can be directly measured by measuring the differential conductance dI/dV in a tunneling experiment (from a normal metal to a superconductor), with bias voltage V translating into the energy E. Such a representation visualizes in a particularly clear way the gap 2Δ for excitation of a quasiparticle pair.



2.9 Electrodynamics of superconductors: London equations and Meissner effect

We first present a phenomenological theory as developed by F. London and H. London in 1935. Later we discuss its derivation from the microscopic (BCS) theory.

Consider first electrons (with charge $-e$) that move without friction (resistance) in an electric field. (For a normal system, this would be the case if the electrons would not interact with lattice and impurities.)

$$m\dot{\boldsymbol{v}} = -e\boldsymbol{E} \,. \tag{2.222}$$

Since the current is given by $\boldsymbol{j} = -ne\boldsymbol{v}$, where n is the electron density, we obtain then

$$\frac{\partial \boldsymbol{j}}{\partial t} = \frac{ne^2}{m}\boldsymbol{E} \,. \tag{2.223}$$

In terms of the scalar and vector potentials, the electric field is $\boldsymbol{E} = -\frac{1}{c}\dot{\boldsymbol{A}} - \boldsymbol{\nabla}\phi$. We choose the gauge $\phi = 0$ and $\boldsymbol{\nabla}\cdot\boldsymbol{A} = 0$ (Coulomb gauge or, in the superconductivity context, London gauge). Then, if we allow ourselves to remove time derivatives, Eq. (2.223) takes the form

$$\boldsymbol{j} = -\frac{ne^2}{mc}\boldsymbol{A} \,. \tag{2.224}$$

Taking the curl of this equation, we get

$$\boldsymbol{\nabla}\times\boldsymbol{j} = -\frac{ne^2}{mc}\boldsymbol{B} \,. \tag{2.225}$$

The London ansatz postulates that these equations hold for a superconducting system, with a replacement $n \mapsto n_s$, where n_s is the "density of superconducting electrons",

$$\boxed{\boldsymbol{j} = -\frac{n_s e^2}{mc}\boldsymbol{A} \,.} \tag{2.226}$$

An important assumption here is that Eq. (2.226) holds also for static fields. For $T = 0$, when the system is in the ground state, all electrons are superconducting, so that $n_s = n$. At finite temperature, $0 < T < T_c$, one has

$$0 < n_s(T) < n \,, \qquad n_s(T) + n_n(T) = n \,, \tag{2.227}$$

where $n_n(T)$ is the density of the normal component of the electron system. Equation (2.226) yields, in analogy with Eqs. (2.223) and (2.225),

$$\frac{\partial \boldsymbol{j}}{\partial t} = \frac{n_s e^2}{m} \boldsymbol{E} \ , \tag{2.228}$$

$$\boldsymbol{\nabla} \times \boldsymbol{j} \ = -\frac{n_s e^2}{mc} \boldsymbol{B} \ . \tag{2.229}$$

Comment: Note that Eq. (2.226) can be equivalently written in terms of Cooper pairs. Indeed, it is invariant under the substitution $n_s \mapsto n_s/2$, $m \mapsto 2m$, and $e \mapsto 2e$.

2.9.1 Static fields

Assume a static (time-independent) situation. The inhomogeneous Maxwell equation for $\boldsymbol{B}$ then reads

$$\boldsymbol{\nabla} \times \boldsymbol{B} \ = \frac{4\pi}{c} \boldsymbol{j} \ . \tag{2.230}$$

Note that we consider induced currents explicitly and thus use the microscopic Maxwell equation. Taking the curl of this equation, we obtain

$$\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{B}\,) = \frac{4\pi}{c} \boldsymbol{\nabla} \times \boldsymbol{j} \ \overset{(2.229)}{=} \ -\frac{4\pi n_s e^2}{mc^2} \boldsymbol{B} \ . \tag{2.231}$$

The l.h.s. can be transformed via the identity

$$\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{B}\,) = \boldsymbol{\nabla} \ (\underbrace{\boldsymbol{\nabla} \cdot \boldsymbol{B}}_{=0}) - \boldsymbol{\nabla}^{\,2} \boldsymbol{B} \ = -\boldsymbol{\nabla}^{\,2} \boldsymbol{B} \ . \tag{2.232}$$

Thus, Eq. (2.231) yields

$$\boxed{\boldsymbol{\nabla}^{\,2} \boldsymbol{B} \ = \frac{4\pi n_s e^2}{mc^2} \boldsymbol{B} \ .} \tag{2.233}$$

Consider a boundary between the vacuum and a superconductor, with axis x transverse to the boundary, so that $x < 0$ corresponds to the vacuum and $x > 0$ to the superconductor. The magnetic field will locally depend on x only, so that Eq. (2.233) takes the form

$$\frac{\partial^2 \boldsymbol{B}}{\partial x^2} = \frac{4\pi n_s e^2}{mc^2} \boldsymbol{B} \qquad (x > 0). \tag{2.234}$$

The solution reads

$$\boxed{\boldsymbol{B}\,(x) = \boldsymbol{B}_{\,0}\, e^{-x/\lambda_L} \,,} \tag{2.235}$$

where $\boldsymbol{B}_{\,0}$ is the field at the boundary and

$$\boxed{\lambda_L = \sqrt{\frac{mc^2}{4\pi n_s e^2}}} \tag{2.236}$$

is the London **penetration depth**. The result (2.235) is a manifestation of the **Meißner effect** (also called **Meißner-Ochsenfeld effect**): the magnetic field is expelled from the superconductor and is sizeable only in a narrow layer (of depth $\sim \lambda_L$) at the surface. The Meißner effect is, along with the vanishing of the resistance, one of main hallmarks of superconductivity.

Comment: The Meißner effect in a superconductor is a paradigmatic example of the **Higgs**

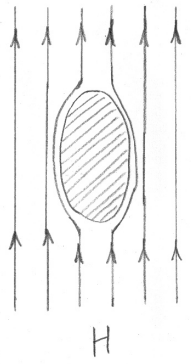
mechanism (also called **Anderson-Higgs mechanism**) for generation of mass of gauge bosons coupled to a field that exhibits a spontaneous symmetry breaking. Its counterpart in the particle physic is generation of mass of W and Z bosons due to coupling to the Higgs field. We will return to it below in Sec. 2.11.6.

In the same way as Eq. (2.233) is derived above, we get from Eqs. (2.229) and (2.230):

$$\boldsymbol{\nabla}^2 \boldsymbol{j} = \frac{4\pi n_s e^2}{mc^2} \boldsymbol{j} \; . \tag{2.237}$$

It follows from this equation that currents in the superconducting state also flow in the narrow layer of depth λ. In particular, these currents create magnetization that screens the external magnetic field.

2.9.2 Critical magnetic field



The Meißner effect (and more generally, the superconductivity) holds as long as the external magnetic field $\boldsymbol{H}$ is not too strong and the system gains energy by expelling the magnetic field. There is a critical field H_c such that for $H > H_c$ this is not the case any more and, as a result, the magnetic field penetrates the system and the superconductivity is destroyed. Let us find H_c.

The total magnetic field $\boldsymbol{B} = 0$ inside the superconductor is a sum of the external field and the field induced by the magnetisation current:

$$\boldsymbol{B} = \underbrace{\boldsymbol{B}_{\rm ext}}_{=\boldsymbol{H}} + \underbrace{\boldsymbol{B}_{\rm ind}}_{=4\pi\boldsymbol{M}} = 0 \qquad \Longrightarrow \qquad \boldsymbol{B}_{\rm ind} = -\boldsymbol{H} \; . \tag{2.238}$$

The total free-energy density of a superconductor consists of the zero-field free energy F_s and the energy of the induced currents screening the external magnetic field. The latter is given by $B_{\rm ind}^2/(8\pi)$. Therefore, the superconducting state "wins" as long as

$$F_s + \frac{B_{\rm ind}^2}{8\pi} < F_n \qquad \Longleftrightarrow \qquad F_s + \frac{H^2}{8\pi} < F_n \, , \tag{2.239}$$

where F_n is the normal-state free-energy density. At the critical field H_c, Eq. (2.239) becomes an equality, i.e.,

$$\boxed{H_c^2 = 8\pi (F_n - F_s) \, .} \tag{2.240}$$

At zero temperature, $T = 0$, F_s and F_n are the ground state energies E_s and E_n (per unit volume) that were calculated in Sec. 2.8.3.

Equivalent derivation: Thermodynamics in a magnetic field

$\boldsymbol{H}$ — external field, $\boldsymbol{B} = \boldsymbol{H} + 4\pi\boldsymbol{M}$ – total field. Free energy:

$$F(T, V, \boldsymbol{B}) ; \qquad dF = \underbrace{-S dT - P dV}_{dF_0} + \int d^3 r \, \frac{1}{4\pi} \boldsymbol{H} \, d\boldsymbol{B} \; , \tag{2.241}$$

where F_0 is the free energy in the absence of the field. Since it is not $\boldsymbol{B}$ but rather the external field $\boldsymbol{H}$ that is fixed, one should perform Legendre transformation:

$$F(T,V,\boldsymbol{B}) \quad \longrightarrow \quad F_H(T,V,\boldsymbol{H}) = F - \int d^3r\, \frac{\boldsymbol{H}\,\boldsymbol{B}}{4\pi}\,. \tag{2.242}$$

This is similar to a Legendre transformation $V \mapsto P$, and in this sense F_H is analogous to free enthalpy (or, equivalently, Gibbs free energy). The differential of F_H reads (per unit volume)

$$dF_H = dF_0 - \frac{1}{4\pi}\boldsymbol{B}\,d\boldsymbol{H}\ , \tag{2.243}$$

where F_0 and F_H are now defined per unit volume (i.e., they are densities of the corresponding thermodynamic potentials). Note that

$$-\frac{1}{4\pi}\boldsymbol{B}\,d\boldsymbol{H} = -\frac{1}{4\pi}\boldsymbol{H}\,d\boldsymbol{H} - \boldsymbol{M}\,d\boldsymbol{H}\ ,$$

where the first term depends only on the external field $\boldsymbol{H}$ and thus does not influence the comparison of F_H in the normal and superconducting states. For this reason, it is frequently omitted in the expression for dF_H. We use below dF_H as given by Eq. (2.243). If $\boldsymbol{B} = \mu\boldsymbol{H}$, where μ is magnetic permeability, we have

$$F_H = F_0 - \frac{\mu H^2}{8\pi}\,. \tag{2.244}$$

The point $H = H_c$ of the phase transition between normal (n) and superconducting (s) states is determined by the condition

$$F_{H,n} = F_{H,s}\,. \tag{2.245}$$

In the normal state we have $\mu = 1$ (i.e., $\boldsymbol{M} = 0$), so that

$$F_{H,n} = F_{0,n} - \frac{H^2}{8\pi}\,. \tag{2.246}$$

In the superconducting state $\boldsymbol{B} = 0$, i.e., $\mu = 0$, so that

$$F_{H,s} = F_{0,s}\,. \tag{2.247}$$

Thus, the condition for the critical field H_c reads

$$F_{0,n} - \frac{H_c^2}{8\pi} = F_{0,s} \qquad \Longrightarrow \qquad \boxed{\frac{H_c^2}{8\pi} = F_{0,n} - F_{0,s}\,,} \tag{2.248}$$

in agreement with Eq. (2.240).

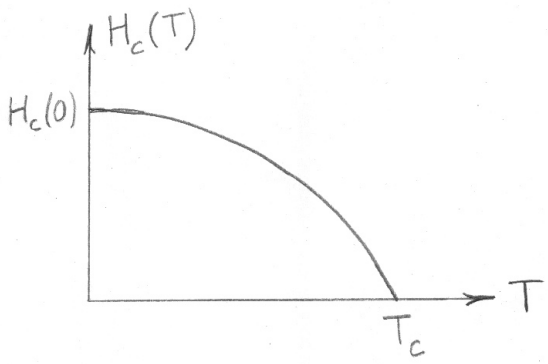
2.9.3 Critical field in the BCS theory

We calculate H_c according to Eq. (2.240), $H_c^2 = 8\pi(F_n - F_s)$, in the BCS theory at zero temperature, $T = 0$. In this case the free energy F reduces to the energy E, so that $F_n = E_n$ and $F_s = E_s$. Substituting the result (2.212) for $E_n - E_s$ into the formula $H_c^2 = 8\pi(E_n - E_s)$, where energies are defined per unit volume, we find the zero-temperature critical field

$$\boxed{H_c(T=0) = 2\sqrt{\pi\nu_0}\,\Delta(T=0)\,.} \tag{2.249}$$

For $T \to T_c - 0$ one obtains (we do not provide a derivation here)

$$H_c(T) \simeq 1.735\, H_c(0) \left(1 - \frac{T}{T_c}\right) . \quad (2.250)$$



2.9.4 Derivation of London equations from the BCS theory

We consider, within the BCS theory, coupling of the superconductor to an external electromagnetic field described by a vector potential $\boldsymbol{A}$. Since the dominant effect comes from the coupling to the orbital motion, we neglect the spin coupling. The kinetic-energy part of the Hamiltonian reads, in the second-quantized form,

$$H_{\rm kin} = \sum_\sigma \int d^3r\, \widehat{\Psi}^\dagger_\sigma(\boldsymbol{r}\,) \frac{\left(-i\hbar\boldsymbol{\nabla} + \frac{e}{c}\boldsymbol{A}\right)^2}{2m} \widehat{\Psi}_\sigma(\boldsymbol{r}\,) . \quad (2.251)$$

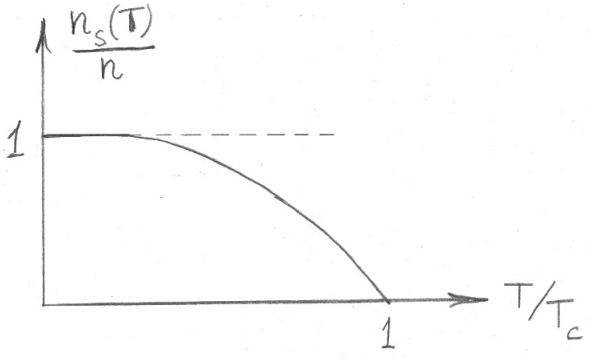
One can now calculate the current within the BCS theory by considering the vector potential as a perturbation (i.e., to the linear order in $\boldsymbol{A}$). We omit the derivation and directly present the result. It has exactly the form of the London equation (2.226),

$$\boxed{\boldsymbol{j} = -\frac{n_s e^2}{mc}\boldsymbol{A}\,,} \quad (2.252)$$

with the superconducting density n_s given by

$$\boxed{n_s = n\left[1 - \int_{-\infty}^{\infty} d\xi \left(-\frac{\partial f}{\partial E}\right)\right],} \qquad f(E) = \frac{1}{e^{\beta E}+1}\,, \qquad E = \sqrt{\Delta^2 + \xi^2}\,. \quad (2.253)$$

The temperature dependence $n_s(T)$ that is determined by Eq. (2.253) looks as follows:



$\underline{\mathbf{T > T_c}}$

In this case $\Delta = 0$ and $E = \xi$. Thus,

$$\int d\xi \left(-\frac{\partial f}{\partial E}\right) = \int d\xi \left(-\frac{\partial f}{\partial \xi}\right) = 1\,, \quad (2.254)$$

so that

$$n_s = 0 \quad (2.255)$$

as expected. The system is in normal state, there is no superconductivity.

$\mathbf{T < T_c}$

$E = \sqrt{\xi^2 + \Delta^2} \geq \Delta\,, \qquad \xi = \sqrt{E^2 - \Delta^2}.$

We thus have

$$\frac{n_s}{n} = 1 - 2\int_\Delta^\infty dE \left(-\frac{\partial f}{\partial E}\right) \frac{E}{\sqrt{E^2 - \Delta^2}}\,. \tag{2.256}$$

This formula can be used to obtain the dependence $n_s(T)$ at $T < T_c$.

$\mathbf{T = 0}$

$$-\frac{\partial f}{\partial E} = \delta(E) \qquad \Longrightarrow \qquad \int_\Delta^\infty dE \left(-\frac{\partial f}{\partial E}\right) \ldots = 0\,, \tag{2.257}$$

so that

$$n_s = n\,. \tag{2.258}$$

The "density of superconducting electrons" is equal to the total density.

$\mathbf{T \ll T_c}$

$$\int_\Delta^\infty dE \left(-\frac{\partial f}{\partial E}\right) \ldots \propto e^{-\Delta/T}\,, \tag{2.259}$$

and thus

$$1 - \frac{n_s}{n} \propto e^{-\Delta/T}\,. \tag{2.260}$$

$\mathbf{T \to T_c - 0}$

For temperatures in the superconducting phase ($T < T_c$) close to T_c, one finds from Eq. (2.256)

$$\frac{n_s}{n} \simeq 2\left(1 - \frac{T}{T_c}\right)\,. \tag{2.261}$$

London penetration depth

Using $n_s(T)$ obtained from the BCS theory, one immediately finds the temperature dependence of the London penetration depth given by Eq. (2.236)

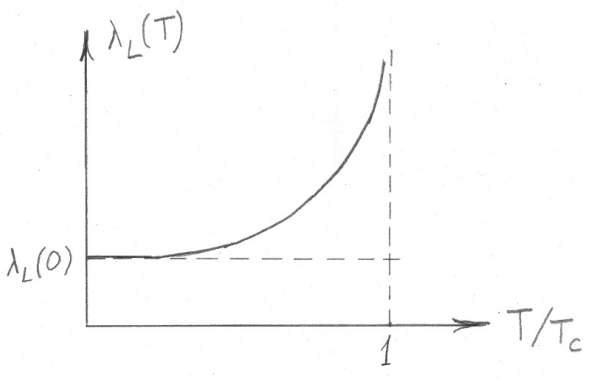
$$\lambda_L(T) = \sqrt{\frac{mc^2}{4\pi n_s(T) e^2}}\,. \tag{2.262}$$

For $T = 0$, we find, using Eq. (2.258),

$$\lambda_L(0) = \sqrt{\frac{mc^2}{4\pi n e^2}}\,. \tag{2.263}$$

Near T_c, the penetration depth diverges, according to Eq. (2.261), as follows:

$$\lambda_L(T) \simeq \frac{\lambda_L(0)}{\sqrt{2}} \left(1 - \frac{T}{T_c}\right)^{-1/2}\,. \tag{2.264}$$



2.10 Order parameter, phase of the condensate, and flux quantization

2.10.1 Superconducting condensate as order parameter, role of the phase

The superconducting state is distinguished from the normal state by a non-zero value of the **superconducting condensate**

$$\Delta = \frac{g}{V} \sum_{\boldsymbol{k}} \langle c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} \rangle = g \langle \widehat{\Psi}_{\downarrow}(\boldsymbol{r}\,) \widehat{\Psi}_{\uparrow}(\boldsymbol{r}\,) \rangle \,. \tag{2.265}$$

It plays thus the role of the **order parameter** for the transition from the normal state to the superconducting state.

Up to now, we considered the BCS ground state $|\mathrm{BCS}\rangle$ corresponding to real Δ. However, it is easy to construct an equivalent state with the same $|\Delta|$ and with arbitrary phase, $\Delta = |\Delta| e^{i\phi}$. To see this, we return to the BCS Hamitlonian and notice that it is invariant under the transformation

$$c^{\dagger}_{\boldsymbol{k},\sigma} \;\mapsto\; \tilde{c}^{\dagger}_{\boldsymbol{k},\sigma} = e^{i\phi/2} c^{\dagger}_{\boldsymbol{k},\sigma} \,, \qquad\qquad c_{\boldsymbol{k},\sigma} \;\mapsto\; \tilde{c}_{\boldsymbol{k},\sigma} = e^{-i\phi/2} c_{\boldsymbol{k},\sigma} \tag{2.266}$$

with arbitrary constant phase $\phi \in \mathbb{R}$:

$$\begin{aligned} H_{\mathrm{BCS}} &= \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}}\, c^{\dagger}_{\boldsymbol{k},\sigma}\, c_{\boldsymbol{k},\sigma} - \frac{g}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} c^{\dagger}_{\boldsymbol{k}',\uparrow}\, c^{\dagger}_{-\boldsymbol{k}',\downarrow}\, c_{-\boldsymbol{k},\downarrow}\, c_{\boldsymbol{k},\uparrow} \\ &= \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}}\, \tilde{c}^{\dagger}_{\boldsymbol{k},\sigma}\, \tilde{c}_{\boldsymbol{k},\sigma} - \frac{g}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} \tilde{c}^{\dagger}_{\boldsymbol{k}',\uparrow}\, \tilde{c}^{\dagger}_{-\boldsymbol{k}',\downarrow}\, \tilde{c}_{-\boldsymbol{k},\downarrow}\, \tilde{c}_{\boldsymbol{k},\uparrow} \,. \end{aligned} \tag{2.267}$$

We consider now the BCS ground state with $\Delta \in \mathbb{R}$ in terms of the operators $\tilde{c}^{\dagger}_{\boldsymbol{k},\sigma}, \tilde{c}_{\boldsymbol{k},\sigma}$:

$$\frac{g}{V} \sum_{\boldsymbol{k}} \langle \tilde{c}_{-\boldsymbol{k},\downarrow} \tilde{c}_{\boldsymbol{k},\uparrow} \rangle = \Delta \,. \tag{2.268}$$

Returning to the original operators $c^{\dagger}_{\boldsymbol{k},\sigma}, c_{\boldsymbol{k},\sigma}$, we find then

$$\frac{g}{V} \sum_{\boldsymbol{k}} \langle c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} \rangle = \Delta\, e^{i\phi} \,. \tag{2.269}$$

The corresponding ground state is obtained from

$$|\mathrm{BCS}\rangle = \prod_{\boldsymbol{k}} (u_k + v_k \tilde{c}^{\dagger}_{\boldsymbol{k},\uparrow} \tilde{c}^{\dagger}_{-\boldsymbol{k},\downarrow}) |0\rangle \tag{2.270}$$

by the transformation (2.266), which yields

$$|\mathrm{BCS}(\phi)\rangle = \prod_{\boldsymbol{k}} (u_k + e^{i\phi} v_k c^{\dagger}_{\boldsymbol{k},\uparrow} c^{\dagger}_{-\boldsymbol{k},\downarrow}) |0\rangle \,. \tag{2.271}$$

The general form of the self-consistency equation (2.216) (allowing for a complex Δ) is

$$\Delta = \frac{g}{2V} \sum_{k} \frac{\Delta}{E_k} \tanh \frac{\beta E_k}{2} \,, \qquad E_k = \sqrt{|\Delta|^2 + \xi_k^2} \,. \tag{2.272}$$

We have thus a family of degenerate ground states $|\mathrm{BCS}(\phi)\rangle$. The Hamiltonian is invariant under the transformation (2.266), see Eq. (2.267), but each ground state is not invariant. This is a situation of **spontaneous symmetry breaking**.

Any linear combination of ground states yields also a ground state. In particular, it is easy to construct a ground state wit a fixed number N of electrons (exercise: check this):

$$|\mathrm{BCS}(N)\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi} \, |\mathrm{BCS}(\phi)\rangle e^{-iN\phi/2} \, . \tag{2.273}$$

Equation (2.273) is a manifestation of the fact that the phase $\phi/2$ and number N are canonically conjugate variables (like coordinate and momentum).

Consider a quantum-mechanical gauge transformation (charge $-e$):

$$\boldsymbol{A} \;\mapsto\; \boldsymbol{A} + \boldsymbol{\nabla}\chi \equiv \boldsymbol{A}' \, , \qquad\qquad \chi = \chi(\boldsymbol{r}\,) \, , \tag{2.274}$$

$$\Psi \;\mapsto\; \Psi \exp\left\{ -\frac{ie}{\hbar c}\,\chi \right\} \equiv \Psi' \, . \tag{2.275}$$

According to Eq. (2.274), $\boldsymbol{A}' - \boldsymbol{\nabla}\chi$ is the invariant of the gauge transformation.

We compare now Eq. (2.275) with the transformation of the condensate $\Delta \;\mapsto\; \Delta\, e^{i\phi}$ and identify

$$\frac{\phi}{2} = -\frac{e}{\hbar c}\,\chi \, . \tag{2.276}$$

In the London equation for the gauge-invariant quantity (current), the gauge invariant combination should enter, i.e., in the case of a spatially varying phase of the condensate we should generalize the equation by replacing:

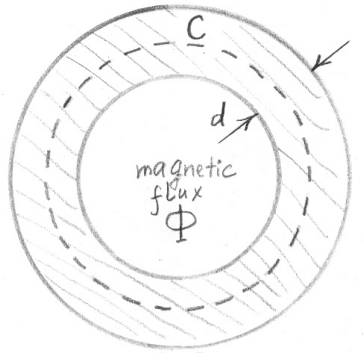
$$\boldsymbol{A} \;\mapsto\; \boldsymbol{A} + \frac{\hbar c}{2e}\,\boldsymbol{\nabla}\phi \, . \tag{2.277}$$

This yields the London equation for the supercurrent $\boldsymbol{j}_s$:

$$\boxed{\boldsymbol{j}_s = -\frac{e^2 n_s}{mc}\left(\boldsymbol{A} + \frac{\hbar c}{2e}\,\boldsymbol{\nabla}\phi \right) .} \tag{2.278}$$

The term proportional to the gradient of the phase is analogous to Eq. (2.151) for the superfluid velocity of a Bose gas.

2.10.2 Flux quantization



Consider a superconducting ring (cylinder) with a thickness $d \gg \lambda_L$.

Consider a closed path C deeply inside the ring. In the bulk of the superconductor $\boldsymbol{j}_s = 0$. On the other hand, integrating $\boldsymbol{j}_s$ over the path, we get

$$\underbrace{\oint_C d\boldsymbol{l} \cdot \underbrace{\boldsymbol{j}_s}_{=0}}_{=0} = -\frac{e^2 n_s}{mc}\left[\underbrace{\oint_C d\boldsymbol{l}\cdot\boldsymbol{A}}_{\text{magnetic flux } \Phi} + \frac{\hbar c}{2e} \underbrace{\oint_C d\boldsymbol{l}\cdot\boldsymbol{\nabla}\phi}_{2\pi n\,,\quad n\in\mathbb{Z}} \right] . \tag{2.279}$$

Thus, we get the **flux quantization**

$$\boxed{\Phi = \frac{2\pi\hbar\, c\, n}{2e} = n\,\Phi_0^{(s)}\,, \qquad n \in \mathbb{Z},} \tag{2.280}$$

where

$$\Phi_0^{(s)} = \frac{hc}{2e} \tag{2.281}$$

is the **superconducting flux quantum** (differs from the conventional flux quantum Φ_0 by a substitution $e \mapsto 2e$).

2.11 Ginzburg-Landau Theory

This is a phenomenological theory that was developed in 1950 (i.e., before the development of the microscopic BCS theory). Connection with the BCS theory will be discussed below.

One introduces a complex order parameter $\psi(\boldsymbol{r}\,)$ which is in general dependent on the spatial coordinate $\boldsymbol{r}$ (if there is an external magnetic field or spatial inhomogeneity of the problem):

$$\psi(\boldsymbol{r}\,) = \sqrt{\frac{n_s}{2}}\, e^{i\phi(\boldsymbol{r}\,)}\,, \tag{2.282}$$

On can view it as a wave function of the superconducting condensate. Here n_s is the density of superconducting electrons, and thus $n_s/2$ is the density of Cooper pairs.

Define a dimensionless parameter characterizing a distance from the transition point T_c:

$$\tau = \frac{T - T_c}{T_c}\,. \tag{2.283}$$

The theory is developed in the vicinity of T_c, i.e., for $|\tau| \ll 1$. The functional of the free-energy density can be then expanded in powers of ψ and of gradients. It is postulated to have the following form:

$$\boxed{F_H[\psi, \psi^*, \boldsymbol{A}\,](T, H) = F_H^{(n)}(T, 0) + a|\psi|^2 + \frac{b}{2}|\psi|^4 + \frac{1}{4m}\left|\left(-i\hbar\boldsymbol{\nabla} + \frac{2e}{c}\boldsymbol{A}\right)\psi\right|^2 + \frac{\boldsymbol{B}^2}{8\pi} - \frac{\boldsymbol{H}\cdot\boldsymbol{B}}{4\pi}\,.} \tag{2.284}$$

The total free energy is $\int d^3r F_H$. Here it was taken into account that the Cooper pair has a mass $2m$ and charge $-2e$. The field $\boldsymbol{H}$ is the given external field. The vector potential $\boldsymbol{A}$ is related to the magnetic field $\boldsymbol{B}$ in the usual way, $\boldsymbol{\nabla} \times \boldsymbol{A} = \boldsymbol{B}$. The free energy should be varied (minimized) with respect to ψ and $\boldsymbol{A}$. The result yields F_H, i.e., the Gibbs free energy (free enthalpy) with respect to magnetic field, cf. Sec. 2.9.2 for discussion of the thermodynamics in magnetic field.

Parameters a and b satisfy:

$$\boxed{a = \alpha\tau, \qquad \alpha > 0\,, \qquad\qquad b > 0\,,} \tag{2.285}$$

where α and b are constants.

2.11.1 No magnetic field, spatially uniform order parameter

One has then the Landau free energy

$$F(T) = F^{(n)}(T) + a|\psi|^2 + \frac{b}{2}|\psi|^4\,. \tag{2.286}$$

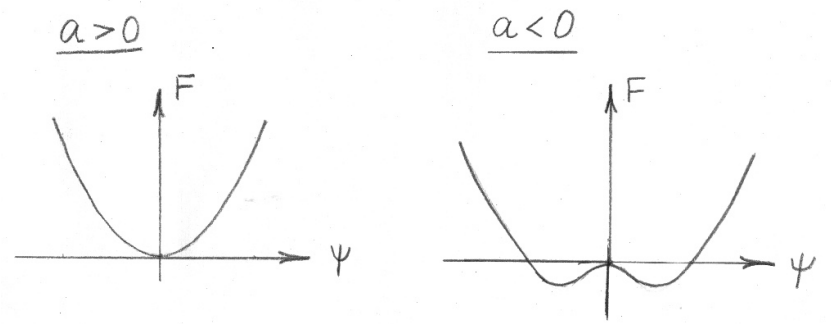
To find the thermodynamically stable state, we minimize with respect to ψ:

$$\frac{\partial F}{\partial \psi^*} = \psi \, (a + b|\psi|^2) = 0 \, . \tag{2.287}$$

For $\tau > 0$ (i.e., $T > T_c$) we have $a > 0$ and thus the trivial solution $\psi = 0$. On the other hand, for $\tau < 0$ (i.e., $T < T_c$) we have $a < 0$ and thus a non-trivial solution:

$$|\psi|^2 = \frac{-a}{b} = \frac{-\alpha\tau}{b} = \frac{\alpha}{b} \, \frac{T_c - T}{T_c} \, . \tag{2.288}$$

More precisely, there is a family of solutions for ψ (with different phases). This is a **spontaneous symmetry breaking.** The oder parameter ψ is proportional to Δ of the BCS theory; exact relation will be derived below.



2.11.2 Inhomogeneous situation

Now we consider the generic (inhomogeneous) situation, in the presence of magnetic field and current.

We have to minimize the free energy (2.284) with respect to ψ and $\boldsymbol{A}$. Varying with respect to ψ^* gives

$$\frac{\delta F_H}{\delta \psi^*} = 0 \qquad \Longrightarrow \qquad \frac{1}{4m} \left(-i\hbar \boldsymbol{\nabla} + \frac{2e}{c} \boldsymbol{A} \right)^2 \psi + a\psi + b|\psi|^2 \psi = 0 \, . \tag{2.289}$$

Varying (2.284) with respect to $\boldsymbol{A}$ gives the Maxwell equation

$$\frac{\delta F_H}{\delta \boldsymbol{A}} = 0 \qquad \Longrightarrow \qquad \nabla \times \boldsymbol{B} \, - \nabla \times \boldsymbol{H} \, = \frac{4\pi}{c} \boldsymbol{j} \, , \tag{2.290}$$

where $\boldsymbol{j}$ is the current (cf. Sec. 2.9.4)

$$\boldsymbol{j} \, = \frac{ie\hbar}{2m} \, (\psi^* \boldsymbol{\nabla} \, \psi - (\boldsymbol{\nabla} \, \psi^*)\psi) - \frac{2e^2}{mc} |\psi|^2 \boldsymbol{A} \, . \tag{2.291}$$

Using

$$\nabla \times \boldsymbol{H} \, = \frac{4\pi}{c} \boldsymbol{j}_{\,\mathrm{ext}} = 0 \, , \tag{2.292}$$

we reduce Eq. (2.290) to the form

$$\nabla \times \boldsymbol{B} \, = \frac{4\pi}{c} \boldsymbol{j} \, . \tag{2.293}$$

Substituting $\psi = |\psi| e^{i\phi}$ into Eq. (2.291), we obtain the London equation

$$\boldsymbol{j}_{\,s} = - \frac{e^2 n_s}{mc} \left(\boldsymbol{A} + \frac{\hbar c}{2e} \, \boldsymbol{\nabla} \, \phi \right) \, , \tag{2.294}$$

with

$$n_s = 2|\psi|^2 \,. \tag{2.295}$$

Thus, we find the London penetration depth

$$\lambda_{\rm L} = \sqrt{\frac{mc^2}{4\pi n_s e^2}} = \sqrt{\frac{mc^2}{8\pi|\psi|^2 e^2}} \,, \tag{2.296}$$

where $|\psi|^2$ is given by Eq. (2.288).

It is also not difficult to calculate the critical field H_c within the Ginzburg-Landau formalism (exercise).

2.11.3 Comparison between the Ginzburg-Landau and the BCS theory

We compare the Ginzburg-Landau theory to the microscopic BCS theory in the vicinity of the transition:

$$\tau \equiv \frac{T - T_c}{T_c} < 0 \,, \qquad |\tau| \ll 1 \,. \tag{2.297}$$

In the Ginzburg-Landau theory we have for the superconducting density n_s [Eqs. (2.295), (2.288)]:

$$n_s \;\; = \;\; 2|\psi|^2 = \frac{-2a}{b} = \frac{-2\alpha\tau}{b} \,. \tag{2.298}$$

On the other hand, in the BCS theory we have for n_s [Eq. (2.261)]

$$n_s \;\; = \;\; -2n_e\tau \,, \tag{2.299}$$

where n_e is the total electron density. We thus see that the Ginzburg-Landau theory yields correct dependence $n_s \propto |\tau|$. Similarly, one can verify that the scaling of H_c near the transition that follows from the Ginzburg-Landau theory is also in agreement with the BCS theory (exercise).

Comparing the results, one can express both phenomenological coefficients α and b of the Ginzburg-Landau theory in terms of microscopic parameters:

$$\alpha = \frac{12\pi^2}{7\zeta(3)}\, m \left(\frac{k_B T_c}{p_F}\right)^2 \,; \qquad\qquad b = \frac{\alpha}{n_e} \,. \tag{2.300}$$

2.11.4 Coherence length

Consider the case of $\boldsymbol{A} = 0$ and spatially varying order parameter $\psi(\boldsymbol{r})$. Equation (2.289) takes the form

$$-\frac{\hbar^2}{4m}\boldsymbol{\nabla}^2\psi + a\psi + b|\psi|^2\psi = 0 \,. \tag{2.301}$$

We consider a boundary of a metal (at $x < 0$) and superconductor (at $x > 0$), with x axis transverse to the boundary. We look for a solution $\psi(\boldsymbol{r}) = \psi(x)$, with $\psi \in \mathbb{R}$. Thus, the equation has the form

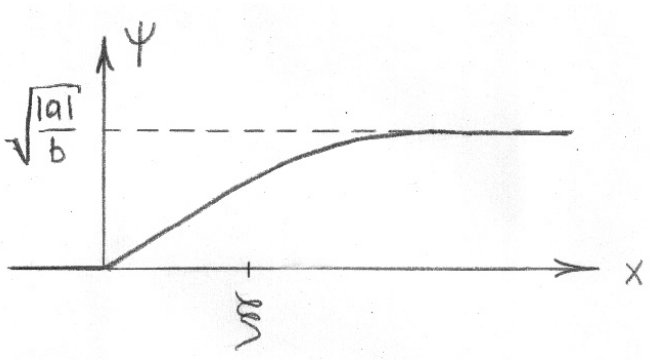
$$-\frac{\hbar^2}{4m}\frac{d^2\psi}{dx^2} + a\psi + b\psi^3 = 0 \,. \tag{2.302}$$

Since in the normal state (in a metal) $\psi = 0$, we set $\psi(x = 0) = 0$. (We slightly oversimplify with the boundary condition but it is sufficient for our purposes.) The solution of Eq. (2.301) with this boundary condition reads

$$\psi(x) = \sqrt{\frac{-a}{b}} \tanh \frac{x}{\sqrt{2}\xi}\,, \tag{2.303}$$

where ξ is the **coherence length** given by

$$\boxed{\xi = \frac{\hbar}{\sqrt{-4ma}} = \frac{\hbar}{\sqrt{4m\alpha|\tau|}}.} \tag{2.304}$$



The coherence length determines the characteristic scale at which the order parameter varies. An equivalent way to see the significance of ξ is to linearize Eq. (2.302) with respect to small deviations near the homogeneous solution $\psi = \sqrt{-a/b}$. One then finds that a small perturbation of ψ at $x = x_0$ decays as $e^{-\sqrt{2}|x-x_0|/\xi}$.

2.11.5 Relation of the Ginzburg-Landau order parameter and coherence length to the BCS gap Δ

In the BCS theory we had the gap

$$\Delta = g\langle \Psi_\downarrow(\boldsymbol{r}\,)\Psi_\uparrow(\boldsymbol{r}\,)\rangle\,, \tag{2.305}$$

with the result (2.219) close to T_c:

$$\Delta(T) = \left(\frac{8\pi^2}{7\zeta(3)}\right)^{1/2} k_{\rm B}\, T_c \sqrt{1 - \frac{T}{T_c}}\,, \tag{2.306}$$

i.e.,

$$|\Delta|^2 = \frac{8\pi^2}{7\zeta(3)}\, k_{\rm B}^2\, T_c^2 |\tau| \qquad\qquad (\tau < 0). \tag{2.307}$$

Comparing this with the result (2.288) of the Ginzburg-Landau theory,

$$|\psi|^2 = \frac{-a}{b} = n_e|\tau|\,, \tag{2.308}$$

we get a relation

$$\boxed{\psi(\boldsymbol{r}\,) = \left(\frac{7\zeta(3)}{8\pi^2}\right)^{1/2} n_e^{1/2}\, \frac{\Delta(\boldsymbol{r}\,)}{k_B T_c}\,.} \tag{2.309}$$

Furthermore, substituting Eq. (2.300) for the parameter α in Eq. (2.304) for the coherence length, we get

$$\xi = \frac{\hbar}{\sqrt{4m\alpha|\tau|}} = \hbar \left(\frac{48\pi^2}{7\zeta(3)}\right)^{-1/2} \frac{p_F}{mk_BT_c} |\tau|^{-1/2} . \tag{2.310}$$

Comparing this with Eq. (2.307), we express ξ in terms of the BCS gap Δ:

$$\boxed{\xi = \frac{1}{\sqrt{6}} \frac{\hbar v_F}{\Delta} .} \tag{2.311}$$

On a qualitative level, this relation has a meaning of the uncertainty relation: ξ sets the uncertainty in the coordinate of a Cooper pair and Δ/v_F the uncertainty in its momentum.

2.11.6 Meissner effect and Anderson-Higgs mechanism

We have already discussed the Meissner effect, and its relation to Higgs mechanism, in Sec. 2.9.1. Here we discuss it in the framework of the Ginzburg-Landau theory.

We know that for a superfluid Bose-gas, with the energy functional given by Eq. (2.135), fluctuations of the phase of the condensate give rise to Goldstone mode. This happens because, due to spontaneous symmetry breaking, phase fluctuations with large wave lengths cost almost no energy, thus giving rise to massless Goldstone bosons (Bogoliubov phonons). The same will happen for fermionic superfluid (BCS model) as long as it is charge neutral. However, the situation changes crucially for charged fermions—in particular, electrons. To clarify this, consider the Ginzburg-Landau free energy (2.284) for the condensate $\psi(\boldsymbol{r}) = \sqrt{n_s/2}\, e^{i\phi(\boldsymbol{r})}$ with fixed n_s and spatially varying phase. The term involving fluctuations of the phase now couples them to the vector potential $\boldsymbol{A}$. We thus consider this term together with the term corresponding to the energy of the magnetic field: $\mathcal{F}[\phi; \boldsymbol{A}] = \int d^3r\, F[\phi(\boldsymbol{r}); \boldsymbol{A}(\boldsymbol{r})]$ with

$$\begin{aligned} F[\phi(\boldsymbol{r}); \boldsymbol{A}(\boldsymbol{r})] &= \frac{1}{4m} \left| \left(-i\hbar\boldsymbol{\nabla} + \frac{2e}{c}\boldsymbol{A}\right)\psi \right|^2 + \frac{\boldsymbol{B}^2}{8\pi} \\ &= \frac{n_s}{8m} \left(\hbar\boldsymbol{\nabla}\phi + \frac{2e}{c}\boldsymbol{A}\right)^2 + \frac{(\boldsymbol{\nabla}\times\boldsymbol{A})^2}{8\pi}. \end{aligned} \tag{2.312}$$

The term proportional to $\boldsymbol{\nabla}\phi$ can be absorbed by a gauge transformation by defining $\boldsymbol{A}' = \boldsymbol{A} + (\hbar c/2e)\nabla\phi$. Further, $\boldsymbol{\nabla}\times\boldsymbol{A}' = \boldsymbol{\nabla}\times\boldsymbol{A}$ (which is gauge invariance of the magnetic field), so that the second term does not change its form under this transformation. To simplify notations, we denote the field $\boldsymbol{A}'$ again as $\boldsymbol{A}$. It is convenient to pass to the Fourier (momentum) space, $\boldsymbol{A}(\boldsymbol{r}) \to \boldsymbol{A}_{\boldsymbol{q}}$. Further, we split $\boldsymbol{A}_{\boldsymbol{q}}$ into components parallel and transverse to $\boldsymbol{q}$, which we denote as $\boldsymbol{A}^{\parallel}_{\boldsymbol{q}}$ and $\boldsymbol{A}^{\perp}_{\boldsymbol{q}}$, respectively. Upon Fourier transform,

$$\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A} \quad \mapsto \quad i\boldsymbol{q}\times\boldsymbol{A}_{\boldsymbol{q}} = i\boldsymbol{q}\times\boldsymbol{A}^{\perp}_{\boldsymbol{q}} , \tag{2.313}$$

i.e., the magnetic field depends only on transverse component. (For time-independent fields, the longitudinal components can be always gauged out.) Focussing thus on the transverse component, we obtain

$$\mathcal{F}[\boldsymbol{A}] = \sum_{\boldsymbol{q}} \left[\frac{n_s}{8m} \left(\frac{2e}{c}\right)^2 \boldsymbol{A}^{\perp}_{\boldsymbol{q}} \boldsymbol{A}^{\perp}_{-\boldsymbol{q}} + \frac{1}{8\pi}\boldsymbol{q}^2 \boldsymbol{A}^{\perp}_{\boldsymbol{q}} \boldsymbol{A}^{\perp}_{-\boldsymbol{q}} \right] = \frac{1}{8\pi} \sum_{\boldsymbol{q}} \left(\boldsymbol{q}^2 + \frac{4\pi n_s e^2}{mc^2}\right) \boldsymbol{A}^{\perp}_{\boldsymbol{q}} \boldsymbol{A}^{\perp}_{-\boldsymbol{q}} . \tag{2.314}$$

This calculation reveals two central features of the problem, where the Goldstone mode resulted from the spontaneous symmetry breaking is coupled to a gauge field. First, Goldstone

bosons (fluctuations of the condensate phase ϕ) are absorbed by the gauge field. There is no low-lying Goldstone mode in the spectrum. Second, the gauge field becomes massive. In the static limit, this manifests itself in the **Meissner effect**. Varying Eq. (2.314) with respect to $\boldsymbol{A}^{\perp}_{-\boldsymbol{q}}$ and using Eq. (2.313) leads exactly to Eq. (2.233) for the magnetic field and thus to the London penetration depth (2.236).

More generally, one can extend the Ginzburg-Landau theory by including in the action also time dependent terms and the scalar potential φ . Then the term involving $\partial_t\phi$ couples to the scalar potential φ and is absorbed into φ by a gauge transformation: $\boldsymbol{A}' = \boldsymbol{A} + (\hbar c/2e)\nabla\phi$ and $\varphi' = \varphi - (\hbar/2e)\partial_t\phi$.

This absorption of the would-be Goldstone boson by a gauge field, accompanied with generation of mass of the gauge boson is known as **Anderson-Higgs mechanism**. Here (superconductivity) it is implemented with the U(1) electromagnetic field. In particle physics (standard model), it is realized with non-abelian SU(2) gauge fields (W and Z gauge bosons) that are responsible for weak interactions.