# Microscopic Theory of Superconductivity

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# 1 Introduction

The microscopic theory of superconductivity was formulated by John Bardeen, Leon N. Cooper, and J. Robert Schrieffer[1, 2]. It is among the most beautiful and successful theories in physics. The BCS-theory starts from an effective Hamiltonian of fermionic quasiparticle excitations that interact via a weak attractive interaction. It yields a ground-state many-body wave function and thermal excitations to describe superconductivity. Historically, the first underlying microscopic mechanism that lead to such an attraction was the exchange of lattice vibrations. In the meantime ample evidence exists, in particular in case of the copper-oxide high-temperature superconductors, for superconductivity that is caused at least predominantly by electronic interactions. Other materials that are candidates for electronically induced pairing are the heavy electron systems, organic charge transfer salts and the iron based superconductors.

The BCS-theory and its generalizations have been summarized in numerous lecture notes and books. This leads to the legitimate question: Why write another manuscript on this topic? My answer is twofold: i) It was my personal experience as a student that after I followed step-by-step the manipulations of the BCS-theory, a lot more new puzzles and worries emerged than old ones got resolved. The troubling issues range from the electrodynamics and collective excitations of superconductors to the question of the order parameter and symmetry breaking. To collect some of the insights that have been obtained in this context over the years and that occur less frequently in textbooks seemed sensible. ii) There are many developments in the theory of superconductivity that took place during the last decade and that deserve to be summarized in a consistent form. Examples are superconductivity in non-Fermi liquids, unconventional pairing due to electronic interactions, topological superconductivity, and superconducting quantum criticality. The hope is that taken together there is sufficient need for a monograph that takes a new look at the microscopic theory of superconductivity.

From the very beginning of this monograph, we stress that the theory of superconductivity cannot be confined to a description of the electronic degrees of freedom alone. This important aspect was vividly summarized by Bohm in 1949 and originally goes back to Bloch[3]: Suppose a finite momentum $\langle \mathbf{P} \rangle = \left\langle \Psi | \widehat{\mathbf{P}} | \Psi \right\rangle \neq 0$ in the ground state $\Psi$ of a purely electronic system, which leads to a finite current $\langle \mathbf{j} \rangle = e \langle \mathbf{P} \rangle / m$. Let the Hamiltonian

$$H = \sum_i \left( -\frac{\hbar^2 \nabla^2}{2m} + U(\mathbf{r}_i) \right) + \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j) \tag{1}$$

consist of the kinetic energy, the potential $U(\mathbf{r}_i)$ due to the electron-ion coupling and the electron-electron interaction $V(\mathbf{r}_i - \mathbf{r}_j)$. One then finds that the wave function

$$\Phi = \exp\left( i \delta \mathbf{p} \cdot \sum_i \mathbf{r}_i / \hbar \right) \Psi \tag{2}$$

has a lower energy than $\Psi$ if the variational parameter $\delta\mathbf{p}$ points opposite to $\langle\mathbf{P}\rangle$. Thus, $\Psi$ cannot be the ground state unless $\langle\mathbf{j}\rangle = 0$ for the electronic problem, Eq.1. Super-currents necessarily require an analysis of the electromagnetic properties of superconductors.

These notes do not provide the reader with the necessary tools in many-body theory that are required to read them. There are many excellent books on second quantization, Green's functions, Feynman diagrams etc. and it would be foolish to try to repeat them here. Our notation will be defined where it appears and is quite standard. If needed we will give references such that further details can be looked up. Thus, we pursue an application oriented approach. At the same time we only briefly repeat the main experimental facts about superconductivity. Once again, there are excellent monographs on the subject that offer a thorough discussion, in particular of conventional superconductors. The last disclaimer is that we do not offer a theory of superconductivity of the copper-oxide or organic or any other real material with strong electronic correlations and what seems to be an electronic pairing mechanism. While I believe that the cuprates are superconducting because of a magnetic pairing-mechanism, forming $d_{x^2-y^2}$-Cooper pairs, a concise description of the key observations in the normal and superconducting states does not exist. Instead we summarize theoretical concepts and models, like weak coupling approaches, the RVB theory, or quantum critical pairing that have been developed to describe systems like the cuprates. Whether these approaches are detailed descriptions of a specific correlated material known today is not our primary concern. Instead we are rather interested in offering theoretical statements that are internally consistent and correct within the assumtions made. Such an approach should have the potential to inspire further research on the exciting topic of strongly correlated superconductors.

# References


[1] J. Bardeen, L. N. Cooper, J. R. Schrieffer, Phys. Rev.**106**, 162 (1957).

[2] J. Bardeen, L. N. Cooper, J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[3] D. Bohm, Phys. Rev. **75**, 502 (1949).

# Part I
# Off-Diagonal Long Range Order

The initial observation of superconductivity was made by measuring the resistivity $\rho(T)$ of mercury as function of temperature. Below the superconducting transition temperature, $T_c$, $\rho(T) = 0$ with very high precision. Understanding this drop in the resistivity is a major challenge in a theory of superconductivity. We will return to this problem later. Arguably even more fundamental than the vanishing voltage drop are two central experiments: the Meissner effect and the quantization of the magnetic flux in multiply connected superconductors. The Meissner effect implies that a weak magnetic field is expelled from the bulk of a superconductor. The effect occurs regardless of whether the external field is switched on for temperatures below $T_c$ or before the system is cooled down to enter the superconducting state. This strongly supports the view that a superconductor is in thermal equilibrium. Multiply connected superconducting geometries such as a ring, can however lead to a subtle memory effects. Switching off an external magnetic field for $T < T_c$ leads to magnetic flux trapped in non-superconducting holes. This flux takes values that are integer multiples of the flux quantum

$$\Phi_0 = \frac{h}{2e} \approx 2.067833758(46) \times 10^{-15}\ \mathrm{Tm}^2, \tag{3}$$

where $h$ is Planck's constant and $e$ the magnitude of the electron charge $e$. By discussing in some detail the concept of off-diagonal long range order we give precise microscopic criteria that lead to the Meissner effect and to flux quantization. A theory of superconductivity consistent with these criteria is therefore guaranteed to correctly describe these fundamental experimental observations. As we will see later, the BCS theory is such a theory.

Off-diagonal long-range order (ODLRO) is a natural generalization of the Bose-Einstein condensation of free bosons to the regime of interacting systems. It was introduced to capture the nontrivial physics of superfluid $^4$He[1, 2] and later generalized to describe superconductivity and superfluidity of fermions[3]. The formal definition is based on the single-particle and two-particle density matrix $\rho^{(1)}$ and $\rho^{(2)}$, respectively:

$$\begin{aligned} \rho^{(1)}_{\alpha\alpha'}(\mathbf{r},\mathbf{r}') &= \left\langle \psi^\dagger_\alpha(\mathbf{r})\,\psi_{\alpha'}(\mathbf{r}')\right\rangle, \\ \rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}'_1,\mathbf{r}'_2) &= \left\langle \psi^\dagger_\alpha(\mathbf{r}_1)\,\psi^\dagger_\beta(\mathbf{r}_2)\,\psi_{\beta'}(\mathbf{r}'_2)\,\psi_{\alpha'}(\mathbf{r}'_1)\right\rangle. \end{aligned} \tag{4}$$

$\psi^\dagger_\alpha(\mathbf{r})$ and $\psi_\alpha(\mathbf{r})$ are the creation and annihilation operators of a boson or fermion at position $\mathbf{r}$ and with spin $\alpha$, respectively. The operators are in the Schrödinger picture such that the $\rho^{(n)}$ are independent on time in thermal equilibrium. Generalizations to an $n$-particle density matrix $\rho^{(n)}$ with $n > 2$ or averages with respect to a non-equilibrium scenario are straightforward. Before we define ODLRO, we summarize a few properties of these density matrices.

It is useful to relate the above definitions to the many body wave eigenfunctions $|\nu\rangle$ with eigenvalues $E_\nu$ of the system. The partition function of the problem is $Z = \sum_\nu e^{-\beta E_\nu}$ with inverse temperature $\beta = 1/(k_B T)$. To simplify our notation we use the index $1 = (\mathbf{r}_1, \gamma_1)$ etc. It holds:

$$\begin{aligned}\rho^{(1)}(l,m) &= \sum_\nu \frac{e^{-\beta E_\nu}}{Z} \left\langle \nu \left| \psi_l^\dagger \psi_m \right| \nu \right\rangle \\ &= \int_{1\cdots N} \sum_\nu \frac{e^{-\beta E_\nu}}{Z} \left\langle \nu \left| \psi_l^\dagger \psi_m \right| 1\cdots N \right\rangle \langle 1\cdots N|\, \nu\rangle \end{aligned} \tag{5}$$

The fully (anti)symmetrized many-body wave function is

$$\Psi_\nu(\mathbf{r}_1\gamma_1\cdots\mathbf{r}_N\gamma_N) = \langle \mathbf{r}_1\gamma_1\cdots\mathbf{r}_N\gamma_N|\, \nu\rangle\,, \tag{6}$$

which corresponds in our compact notation to

$$\Psi_\nu(1\cdots N) = \langle 1\cdots N|\, \nu\rangle\,. \tag{7}$$

At the same time, we have

$$|\mathbf{r}_1\gamma_1\cdots\mathbf{r}_N\gamma_N\rangle = \psi_{\gamma_1}^\dagger(\mathbf{r}_1)\cdots\psi_{\gamma_N}^\dagger(\mathbf{r}_N)\,|0\rangle\,, \tag{8}$$

expressed in terms of field operators. Compactly written this corresponds to

$$|1\cdots N\rangle = \psi_1^\dagger\cdots\psi_N^\dagger\,|0\rangle\,. \tag{9}$$

It follows

$$\psi_l^\dagger\psi_m\,|1\cdots N\rangle = \sum_{t=1}^N \delta(t,m)\,|1\cdots t-1, l, t+1\cdots N\rangle\,, \tag{10}$$

where we used the canonical commutation relations

$$\left[\psi_l, \psi_m^\dagger\right]_\pm = \delta(l,m) \tag{11}$$

of bosons and fermions, respectively. With these results we obtain for the single-particle density matrix:

$$\begin{aligned}\rho^{(1)}(l,m) &= \int_{1\cdots N} \sum_\nu \frac{e^{-\beta E_\nu}}{Z} \sum_{t=1}^N \delta(t,m) \\ &\quad \times\Psi_\nu^*(1\cdots t-1, l, t+1\cdots N)\,\Psi_\nu(1\cdots N) \\ &= N\int_{2\cdots N} \sum_\nu \frac{e^{-\beta E_\nu}}{Z} \Psi_\nu^*(l, 2\cdots N)\,\Psi_\nu(m, 2\cdots N)\,. \end{aligned} \tag{12}$$

Let us write this for completeness in our original formulation:

$$\begin{aligned}\rho^{(1)}_{\alpha\alpha'}(\mathbf{r},\mathbf{r}') &= N\int d^d r_2\cdots d^d r_N \sum_{\gamma_2\cdots\gamma_N} \sum_\nu \frac{e^{-\beta E_\nu}}{Z} \\ &\times \Psi_\nu^*(\mathbf{r}\alpha, \mathbf{r}_2\gamma_2, \cdots, \mathbf{r}_N\gamma_N) \\ &\times \Psi_\nu(\mathbf{r}'\alpha', \mathbf{r}_2\gamma_2, \cdots, \mathbf{r}_N\gamma_N)\,. \end{aligned} \tag{13}$$

A similar analysis for the two-particle density matrix gives

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}'_1,\mathbf{r}'_2\right) &= N\left(N-1\right)\int d^dr_3\cdots d^dr_N\sum_{\gamma_3\cdots\gamma_N}\sum_{\nu}\frac{e^{-\beta E_\nu}}{Z}\\ &\times\ \Psi^*_\nu\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta,\mathbf{r}_3\gamma_3,\cdots,\mathbf{r}_N\gamma_N\right)\\ &\times\ \Psi_\nu\left(\mathbf{r}'_1\alpha',\mathbf{r}'_2\beta',\mathbf{r}_3\gamma_3,\cdots,\mathbf{r}_N\gamma_N\right).\end{aligned}\tag{14}$$

We obtain immediately the expected normalization

$$\mathrm{tr}\rho^{(1)}=\int d^dr\sum_\alpha\rho^{(1)}_{\alpha\alpha'}\left(\mathbf{r},\mathbf{r}'\right)=N\tag{15}$$

as well as

$$\mathrm{tr}\rho^{(2)}=\int d^dr_1d^dr_2\sum_{\alpha\beta}\rho^{(2)}_{\alpha\beta\alpha\beta}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_2\right)=N\left(N-1\right).\tag{16}$$

# 2 Single particle ODLRO of charged bosons

We first concentrate on spin-less bosons in a translation invariant system and analyze $\rho^{(1)}$. It is a hermitian matrix with respect to the matrix indices $\mathbf{r}$ and $\mathbf{r}'$. If $n_p$ is the $p$-th real eigenvalue of $\rho^{(1)}$ with eigenvector $\phi_p\left(\mathbf{r}\right)$, we can expand[1]

$$\rho^{(1)}\left(\mathbf{r},\mathbf{r}'\right)=\sum_p n_p\phi^*_p\left(\mathbf{r}'\right)\phi_p\left(\mathbf{r}\right).\tag{17}$$

As we showed earlier, it holds $\mathrm{Tr}\rho^{(1)}=\int d^dr\rho^{(1)}\left(\mathbf{r},\mathbf{r}\right)=N$ with total number of bosons $N$.

A macroscopic occupation of a single-particle state occurs if there exists one eigenvalue, say $n_0$, that is of order of the particle number $N$ of the system. This is a natural generalization of Bose-Einstein condensation to interacting systems. Off-diagonal long range order occurs if for large distances $|\mathbf{r}-\mathbf{r}'|$ the expansion,

[1]Consider a hermitian matrix $A$ with eigenvectors $\mathbf{x}_{(n)}$ and eigenvalues $\lambda_{(n)}$, i.e.

$$\sum_j A_{ij}x_{(n)j}=\lambda_{(n)}x_{(n)i}.$$

We can consider the matrix $A_{ij}$ for given $j$ as vector with components labelled by $i$ and expand with respect to the complete set of eigenvectors. The same can be done for the other index. This implies

$$A_{ij}=\sum_{pq}\alpha_{(p,q)}x_{(p)i}x^*_{(q)j}.$$

Inserting this expansion into the eigenvalue equation and using the orthogonality and normalization of the eigenvectors ($\sum_j x^*_{(p)j}x_{(q)j}=\delta_{pq}$) it follows

$$\sum_j A_{ij}x_{(n)j}=\sum_p\alpha_{(p,n)}x_{(n)i}.$$

Since the $\mathbf{x}_{(n)}$ are eigenvectors it follows $\alpha_{(p,n)}=\lambda_{(n)}\delta_{p,n}$.

Eq.17, is dominated by a single term (the one with the macroscopic eigenvalue $n_0$ and eigenfunction $\phi_0(\mathbf{r})$). The condition for ODLRO is therefore

$$\rho^{(1)}(\mathbf{r},\mathbf{r}')\Big|_{|\mathbf{r}-\mathbf{r}'|\to\infty} \to n_0\phi_0^*(\mathbf{r}')\,\phi_0(\mathbf{r})\,. \tag{18}$$

For a translation invariant system further holds that $\rho^{(1)}(\mathbf{r},\mathbf{r}') = \rho^{(1)}(\mathbf{r}-\mathbf{r}')$, i.e. the quantum number $p$ corresponds to the momentum vector $\mathbf{p}$. In the thermodynamic limit holds that $\lim_{\mathbf{r}\to\infty}\rho^{(1)}(\mathbf{r}) = \alpha N/V$ with $\alpha$ a generally complex coefficient where $|\alpha|$ is of order unity. Here $V$ is the volume of the system and we used $\phi_0 \approx \frac{1}{\sqrt{V}}$.

We first consider the case of free bosons where $\phi_p(\mathbf{r}) = \frac{1}{\sqrt{V}}e^{i\mathbf{p}\cdot\mathbf{r}}$ and the eigenvalues are given by the Bose-Einstein distribution function:

$$n_{\mathbf{p}} = \frac{1}{e^{\beta(\epsilon(\mathbf{p})-\mu)}-1}. \tag{19}$$

We consider the regime above the Bose-Einstein condensation temperature with

$$k_B T_{\mathrm{BEC}} = 2\pi\varsigma\left(\frac{3}{2}\right)^{-2/3}\frac{\hbar^2}{m}\left(N/V\right)^{2/3}, \tag{20}$$

where $\mu < 0$ and the occupation of all single-particle states behaves in the thermodynamic limit as $\lim_{N\to\infty} n_{\mathbf{p}}/N = 0$. $n_{\mathbf{p}}$ decays for increasing momenta exponentially on the scale $2\pi/\lambda_T$ with thermal de Broglie wave length

$$\lambda_T = \sqrt{\frac{2\pi\hbar^2}{k_B T m}}. \tag{21}$$

It follows

$$\rho^{(1)}(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{p}} n_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} = \int \frac{d^3p}{(2\pi)^3} n_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} \tag{22}$$

decays exponentially like $e^{-r/\lambda_T}$, implying no ODLRO. On the other hand, in case of a macroscopic occupation $n_{\mathbf{0}} = \alpha N$ of the lowest energy state, i.e. for $\mathbf{p} = \mathbf{0}$, below $T_{BEC}$ follows

$$\rho^{(1)}(\mathbf{r}) = \alpha\frac{N}{V} + \frac{1}{V}\sum_{\mathbf{p}>0} n_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} \tag{23}$$

The second term decays exponentially, with the same reasoning as for $T > T_{BEC}$ while the first term gives rise to ODLRO. Our reasoning is in fact more general. In case of a macroscopic occupation of a momentum state, i.e. $n_{\mathbf{p}_0} = \alpha_0 N$ holds

$$\lim_{\mathbf{r}\to\infty}\rho^{(1)}(\mathbf{r}) = \alpha_0\frac{N}{V}e^{i\mathbf{p}_0\cdot\mathbf{r}} \tag{24}$$

as long as the occupation of all other momentum states decays sufficiently fast for large momenta, they will not contribute in the limit of large $\mathbf{r}$. Thus, we have established that the macroscopic occupation of states is rather generally related to large distant correlations of the one particle density matrix.

## 2.1 Meissner effect of condensed, charged bosons

Next we discuss some physical implications of this observation and demonstrate that charged bosons with ODLRO are subject to the Meissner effect and flux quantization. The discussion is adapted from Refs.[4, 5] where fermionic systems were discussed. We start from the Hamiltonian of a system of bosons in a uniform magnetic field $\mathbf{B}$:

$$H = \sum_j \frac{\left(\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}\left(\mathbf{r}_j\right)\right)^2}{2m} + \sum_{i\neq j} V\left(\mathbf{r}_i - \mathbf{r}_j\right). \tag{25}$$

The vector potential can be written as

$$\mathbf{A}\left(\mathbf{r}\right) = \mathbf{A_0}\left(\mathbf{r}\right) + \nabla\varphi\left(\mathbf{r}\right), \tag{26}$$

where $\mathbf{A}_0\left(\mathbf{r}\right) = \frac{1}{2}\mathbf{B}\times\mathbf{r}$ and $\varphi$ is an arbitrary function. The many-body wave function of the problem is $\Psi_\nu\left(\mathbf{r}_1,\cdots,\mathbf{r}_N\right) = \Psi_\nu\left(\mathbf{r}_j\right)$.

Let us perform a spatial displacement $\mathbf{r}_j \to \mathbf{r}_j - \mathbf{a}$ with some length scale $\mathbf{a}$. The boson-boson interaction is invariant with respect to this transformation, while the vector potential transforms as

$$\begin{aligned}\mathbf{A}\left(\mathbf{r}\right) &\to \mathbf{A}\left(\mathbf{r}-\mathbf{a}\right)\\ &= \mathbf{A}\left(\mathbf{r}\right) - \frac{1}{2}\mathbf{B}\times\mathbf{a} + \nabla\left(\varphi\left(\mathbf{r}-\mathbf{a}\right) - \varphi\left(\mathbf{r}\right)\right)\\ &= \mathbf{A}\left(\mathbf{r}\right) + \nabla\chi_{\mathbf{a}}\left(\mathbf{r}\right),\end{aligned} \tag{27}$$

with

$$\chi_{\mathbf{a}}\left(\mathbf{r}\right) = \mathbf{a}\cdot\mathbf{A}_0\left(\mathbf{r}\right) + \varphi\left(\mathbf{r}-\mathbf{a}\right) - \varphi\left(\mathbf{r}\right).$$

The displacement can be understood as a gauge transformation. Thus, we can write the Schrödinger equation as it emerges after the transformation:

$$\left(\sum_j \frac{\left(\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}\left(\mathbf{r}_j-\mathbf{a}\right)\right)^2}{2m} + \sum_{i\neq j} V\left(\mathbf{r}_i-\mathbf{r}_j\right)\right)\Psi_\nu\left(\mathbf{r}_j-\mathbf{a}\right) = E_\nu\Psi_\nu\left(\mathbf{r}_j-\mathbf{a}\right)$$

alternatively as

$$\begin{aligned}\left(\sum_j \frac{\left(\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}\left(\mathbf{r}_j\right)\right)^2}{2m} + \sum_{i\neq j} V\left(\mathbf{r}_i-\mathbf{r}_j\right)\right) e^{i\frac{e}{\hbar c}\sum_j \chi_{\mathbf{a}}\left(\mathbf{r}_j\right)}\Psi_\nu\left(\mathbf{r}_j-\mathbf{a}\right)&\\ = E_\nu e^{i\frac{e}{\hbar c}\sum_j \chi_{\mathbf{a}}\left(\mathbf{r}_j\right)}\Psi_\nu\left(\mathbf{r}_j-\mathbf{a}\right),&\end{aligned}$$

with $\chi_{\mathbf{a}}\left(\mathbf{r}\right)$ given above. In addition to the many-body wave functions $\Psi_\nu\left(\mathbf{r}_j\right)$ we have the alternative choice

$$\Psi'_\nu\left(\mathbf{r}_j\right) = e^{i\frac{e}{\hbar c}\sum_j \chi_{\mathbf{a}}\left(\mathbf{r}_j\right)}\Psi_\nu\left(\mathbf{r}_j-\mathbf{a}\right). \tag{28}$$

The density matrix can therefore we evaluated using the original or the primed wave functions. For the density matrix expressed in terms of the primed wave functions follows

$$\begin{aligned}\rho^{(1)}(\mathbf{r},\mathbf{r}') &= e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r})-\chi_{\mathbf{a}}\left(\mathbf{r}'\right)\right)}N\int d^dr_2\cdots d^dr_N\sum_\nu\frac{e^{-\beta E_\nu}}{Z}\\ &\times\ \Psi_\nu^*(\mathbf{r}-\mathbf{a},\mathbf{r}_2-\mathbf{a},\cdots,\mathbf{r}_N-\mathbf{a})\\ &\times\ \Psi_\nu(\mathbf{r}'-\mathbf{a},\mathbf{r}_2-\mathbf{a},\cdots,\mathbf{r}_N-\mathbf{a}).\end{aligned}\tag{29}$$

All other phase factors $\propto\chi_{\mathbf{a}}(\mathbf{r}_j)$ for $j=2\cdots N$ cancel. Using periodic boundary conditions we can shift the integration variables $\mathbf{r}_j\to\mathbf{r}_j-\mathbf{a}$ and obtain

$$\rho^{(1)}(\mathbf{r},\mathbf{r}')=e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r})-\chi_{\mathbf{a}}\left(\mathbf{r}'\right)\right)}\rho^{(1)}(\mathbf{r}-\mathbf{a},\mathbf{r}'-\mathbf{a}).\tag{30}$$

Let us now assume ODLRO, i.e. for large distance between $\mathbf{r}$ and $\mathbf{r}'$ holds Eq.18. This implies

$$\phi_0^*(\mathbf{r}')\,\phi_0(\mathbf{r})=e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r})-\chi_{\mathbf{a}}\left(\mathbf{r}'\right)\right)}\phi_0^*(\mathbf{r}'-\mathbf{a})\,\phi_0(\mathbf{r}-\mathbf{a})\tag{31}$$

which implies for the eigenfunction of the density operator

$$\phi_0(\mathbf{r})=f_{\mathbf{a}}e^{-i\frac{e}{\hbar c}\chi_{\mathbf{a}}(\mathbf{r})}\phi_0(\mathbf{r}-\mathbf{a}),\tag{32}$$

where $f_{\mathbf{a}}$ is a phase factor that is $\mathbf{r}$-independent but displacement dependent. We now perform two successive transformations

$$\begin{aligned}\phi_0(\mathbf{r}) &= f_{\mathbf{b}}e^{-i\frac{e}{\hbar c}\chi_{\mathbf{b}}(\mathbf{r})}\phi_0(\mathbf{r}-\mathbf{b})\\ &= f_{\mathbf{a}}f_{\mathbf{b}}e^{-i\frac{e}{\hbar c}\chi_{\mathbf{b}}(\mathbf{r})}e^{-i\frac{e}{\hbar c}\chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b})}\phi_0(\mathbf{r}-\mathbf{a}-\mathbf{b})\end{aligned}\tag{33}$$

Of course, we can also change the order of the displacements:

$$\phi_0(\mathbf{r})=f_{\mathbf{a}}f_{\mathbf{b}}e^{-i\frac{e}{\hbar c}\chi_{\mathbf{a}}(\mathbf{r})}e^{-i\frac{e}{\hbar c}\chi_{\mathbf{b}}(\mathbf{r}-\mathbf{a})}\phi_0(\mathbf{r}-\mathbf{a}-\mathbf{b}).\tag{34}$$

Since the wave function is single valued, the two phase factors that relate the two wave functions must be the same and we find the condition:

$$e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{b}}(\mathbf{r})+\chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b}))}=e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{a}}(\mathbf{r})+\chi_{\mathbf{b}}(\mathbf{r}-\mathbf{a}))},\tag{35}$$

It follows from the above definition of $\chi_{\mathbf{a}}(\mathbf{r})$ that

$$\chi_{\mathbf{b}}(\mathbf{r})+\chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b})=\chi_{\mathbf{a}+\mathbf{b}}(\mathbf{r})+\frac{1}{2}\mathbf{B}\cdot(\mathbf{a}\times\mathbf{b}).\tag{36}$$

Here, we used:

$$\begin{aligned}\chi_{\mathbf{b}}(\mathbf{r}) &= \mathbf{b}\cdot\mathbf{A}_0(\mathbf{r})+\varphi(\mathbf{r}-\mathbf{b})-\varphi(\mathbf{r})\\ \chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b}) &= \mathbf{a}\cdot\mathbf{A}_0(\mathbf{r}-\mathbf{b})+\varphi(\mathbf{r}-\mathbf{a}-\mathbf{b})-\varphi(\mathbf{r}-\mathbf{b})\\ &= \mathbf{a}\cdot\mathbf{A}_0(\mathbf{r})-\frac{1}{2}\mathbf{a}\cdot(\mathbf{B}\times\mathbf{b})+\varphi(\mathbf{r}-\mathbf{a}-\mathbf{b})-\varphi(\mathbf{r}-\mathbf{b}).\end{aligned}$$

The result

$$\chi_{\mathbf{a}}(\mathbf{r}) + \chi_{\mathbf{b}}(\mathbf{r}-\mathbf{a}) = \chi_{\mathbf{a}+\mathbf{b}}(\mathbf{r}) - \frac{1}{2}\mathbf{B}\cdot(\mathbf{a}\times\mathbf{b}) \tag{37}$$

follows immediately by switching $\mathbf{a}$ and $\mathbf{b}$. Combining the two terms we obtain

$$\begin{aligned}\chi_{\mathbf{b}}(\mathbf{r}) + \chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b}) - \chi_{\mathbf{a}}(\mathbf{r}) - \chi_{\mathbf{b}}(\mathbf{r}-\mathbf{a}) &= \frac{1}{2}\mathbf{B}\cdot(\mathbf{a}\times\mathbf{b}) - \frac{1}{2}\mathbf{B}\cdot(\mathbf{b}\times\mathbf{a}) \\ &= \mathbf{B}\cdot(\mathbf{a}\times\mathbf{b}),\end{aligned} \tag{38}$$

which is independent on the position $\mathbf{r}$. Our condition for the above phases can therefore be written as:

$$\frac{e}{\hbar c}\mathbf{B}\cdot(\mathbf{a}\times\mathbf{b}) = 2\pi n, \tag{39}$$

where $n$ is an integer.

The displacement vectors $\mathbf{a}$ and $\mathbf{b}$ are arbitrary. Thus, we can continuously vary the vectors $\mathbf{a}$ and $\mathbf{b}$ on the left hand side. On the other hand, since $n$ is an integer, we cannot continuously vary the right hand side. The only acceptable uniform field is therefore

$$\mathbf{B} = 0. \tag{40}$$

This is the Meissner effect of charged bosons with ODLRO. A system with ODLRO cannot support a uniform magnetic field.

This derivation of the Meissner effects makes very evident the importance of macroscopic condensation. Without condensation, we could still perform a similar analysis for the density operator and obtain the condition

$$\begin{aligned}2\pi n\frac{\hbar c}{e} &= \chi_{\mathbf{b}}(\mathbf{r}) + \chi_{\mathbf{a}}(\mathbf{r}-\mathbf{b}) - \chi_{\mathbf{a}}(\mathbf{r}) - \chi_{\mathbf{b}}(\mathbf{r}-\mathbf{a}) \\ &- \left(\chi_{\mathbf{b}}(\mathbf{r}') + \chi_{\mathbf{a}}(\mathbf{r}'-\mathbf{b}) - \chi_{\mathbf{a}}(\mathbf{r}') - \chi_{\mathbf{b}}(\mathbf{r}'-\mathbf{a})\right).\end{aligned} \tag{41}$$

Inserting our above expression for the sum of the phases the right hand side gives a zero, i.e. we merely obtain the condition $n = 0$, without restriction on $\mathbf{B}$. In other words, as long as the density matrix is determined by a sum over many eigenstates, no Meissner effect occurs. Only the condensation in one state and a density matrix

$$\rho^{(1)}(\mathbf{r},\mathbf{r}') \to n_0\phi_0^*(\mathbf{r}')\,\phi_0(\mathbf{r}). \tag{42}$$

for large $|\mathbf{r}-\mathbf{r}'|$ yields a vanishing $\mathbf{B}$-field. We conclude, that macroscopic condensation and Meissner effect are closely related.

## 2.2 Flux quantization of condensed, charged bosons

In order to demonstrate flux quantization we perform an infinite sequence of infinitesimal displacements along a path. Let us first consider a finite sequence. It follows for the accumulated phases after one step: $\chi_{\mathbf{a_1}}(\mathbf{r})$, after two steps: $\chi_{\mathbf{a}_2}(\mathbf{r}) + \chi_{\mathbf{a}_1}(\mathbf{r}-\mathbf{a}_2)$, after three steps:$\chi_{\mathbf{a}_3}(\mathbf{r}) + \chi_{\mathbf{a}_2}(\mathbf{r}-\mathbf{a}_2) + \chi_{\mathbf{a}_1}(\mathbf{r}-\mathbf{a}_2-\mathbf{a}_3)$,

etc. Thus after $S$-steps we have accumulated the phase:$\sum_{i=1}^{S}\chi_{\mathbf{a}_i}\left(\mathbf{r}+\sum_{j=2}^{i}\mathbf{a}_i\right)$, such that

$$\phi_0(\mathbf{r}) = e^{i\frac{e}{\hbar c}\sum_{i=1}^{S}\chi_{\mathbf{a}_i}\left(\mathbf{r}-\sum_{j=2}^{i}\mathbf{a}_i\right)}\phi_0\left(\mathbf{r}-\sum_{i=1}^{S}\mathbf{a}_i\right). \tag{43}$$

If we go to the continuum's limit with $\mathbf{r}_0 = \mathbf{r}-\sum_{i=1}^{S}\mathbf{a}_i$ and $\mathbf{r}' = \mathbf{r}-\sum_{j=2}^{i}\mathbf{a}_i$

$$\begin{aligned}\sum_{i=1}^{S}\chi_{\mathbf{a}_i}\left(\mathbf{r}-\sum_{j=2}^{i}\mathbf{a}_i\right) &\rightarrow \int di\chi_{\mathbf{a}_i}(\mathbf{r}'(i))\\ &= \int_{\mathbf{r}_0}^{\mathbf{r}}\mathbf{A}_0(\mathbf{r}')\cdot d\mathbf{r}+\varphi(\mathbf{r}_2)-\varphi(\mathbf{r}_1)\\ &= \int_{\mathbf{r}_1}^{\mathbf{r}_2}\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}.\end{aligned} \tag{44}$$

For the phase factor $f_{\mathbf{a}}$ follows after $S$ infinitesimal steps $f_{\sum_i^S\mathbf{a}_i}$ which becomes $f_{\int_{\mathbf{r}_1}^{\mathbf{r}_2}\mathbf{dr}}$.[2] For an arbitrary path follows therefore

$$\phi_0(\mathbf{r}) = f_{\int_{\mathbf{r}_0}^{\mathbf{r}}\mathbf{dr}'}e^{-i\frac{e}{\hbar c}\int_{\mathbf{r}_0}^{\mathbf{r}}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'}\phi_0(\mathbf{r}_0). \tag{45}$$

If we now consider a closed loop, it hold with $\oint\mathbf{dr}=0$ and $f_{\mathbf{0}}=1$ that

$$\phi_0(\mathbf{r}) = e^{-i\frac{e}{\hbar c}\oint\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}}\phi_0(\mathbf{r}). \tag{46}$$

This gives for the magnetic flux

$$\Phi = \oint\mathbf{A}(\mathbf{r})\cdot d\mathbf{r} = \frac{\hbar c}{e}2\pi n = n\Phi_{0,bos}, \tag{47}$$

with flux quantum $\Phi_{0,bos}=\frac{hc}{e}$. This is of course only relevant in situations where the Bose condensed region is not simply connected. Then, in a region without Bose condensate, the Meissner effect doesn't matter and the field can be finite. The enclosed flux must be a multiple of the flux quantum.

We conclude that the Meissner effect and flux quantization can occur in bosonic systems, provided the bosons are condensed and ODLRO is present. The ODLRO occurred in the single particle density matrix. One can easily convince one-selves that single particle ODLRO cannot occur in a fermionic system: One can always diagonalize the density operator $\rho^{(1)}$. In the diagonalizing basis holds

$$\rho^{(1)}_{lm} = \delta_{lm}\left\langle c_l^\dagger c_l\right\rangle. \tag{48}$$

Because of the Pauli principle $0\leq\left\langle c_l^\dagger c_l\right\rangle\leq 1$, i.e. the largest eigenvalue is equal to or smaller than unity and can never be of the order of the system size.

[2]Performing a displacement $\mathbf{a}+\mathbf{b}$ one finds $f_{\mathbf{a}+\mathbf{b}} = e^{i\frac{e}{\hbar c}\mathbf{B}\cdot(\mathbf{a}\times\mathbf{b})}f_{\mathbf{a}}f_{\mathbf{b}}$. If the two displacements are in a region of ODLRO it holds $\mathbf{B}=\mathbf{0}$ and thus $f_{\mathbf{a}+\mathbf{b}} = f_{\mathbf{a}}f_{\mathbf{b}}$.

To investigate ODLRO in fermionic systems is however possible if one considers two-particle density matrices $\rho^{(2)}$.

The relation Eq.30 between the density matrix $\rho^{(1)}(\mathbf{r},\mathbf{r}')$ and the corresponding matrix at displaced coordinates can easily be derived in the formalism of second quantization as well. The logic is very similar to the one used above in the many-body wave function description: Performing a displacement $\mathbf{r}\to\mathbf{r}-\mathbf{a}$ we recognize for the vector potential that $\mathbf{A}(\mathbf{r}-\mathbf{a})=\mathbf{A}(\mathbf{r})+\nabla\chi_{\mathbf{a}}(\mathbf{r})$ is a gauge transformation, i.e. the two field operators obey

$$\psi(\mathbf{r})=e^{i\frac{e}{\hbar c}\chi_{\mathbf{a}}(\mathbf{r})}\psi(\mathbf{r}-\mathbf{a}). \tag{49}$$

Inserting this relation into the definition of the density operator we obtain Eq.30 immediately. The consequences like Meissner effect and flux quantization follow accordingly.

## 2.3 the order parameter

In case of ODLRO, we have

$$\rho^{(1)}(\mathbf{r},\mathbf{r}',t)\Big|_{|\mathbf{r}-\mathbf{r}'|\to\infty}=n_0(t)\,\phi_0^*(\mathbf{r}',t)\,\phi_0(\mathbf{r},t), \tag{50}$$

where we allowed for an explicit time dependence of the density matrix, that exists in out-of-equilibrium situations. This suggest to introduce the quantity

$$\Psi(\mathbf{r},t) \quad = \quad \sqrt{n_0(t)}\phi_0(\mathbf{r},t). \tag{51}$$

A definition that immediately implies

$$\int d^dr\,|\Psi(\mathbf{r},t)|^2=n_0(t), \tag{52}$$

which follows from the normalization to unity of the eigenfunction $\phi_0(\mathbf{r},t)$. The behavior of the eigenfunction $\phi_0$ under gauge transformations, suggests that the function $\Psi(\mathbf{r},t)$ behaves in many ways like a condensate wave function. Frequently, the order parameter of a Bose condensate is also defined via the expectation value of the field operator

$$\Psi(\mathbf{r},t)=\langle\psi(\mathbf{r},t)\rangle. \tag{53}$$

Then, Bose condensation is associated with a spontaneous breaking of the global $U(1)$ symmetry $\psi(\mathbf{r})\to e^{i\theta}\psi(\mathbf{r})$. At first glance these two statements seem contradictory. $\Psi(\mathbf{r},t)$ was defined for a system with fixed particle number and, more importantly, for a Hamiltonian with conserved particle number. Breaking the global $U(1)$ symmetry implies that the particle number conservation is spontaneously broken, which seems at first glance rather odd. Notice that merely using a grand-canonical ensemble does not resolve the issue. Particle number conservation implies that the density matrix is block-diagonal with respect to the number of particles. In such a situation it must hold that $\langle\psi(\mathbf{r},t)\rangle=0$ even

for a grand-canonical description. The two definitions of the order-parameter can, however, be reconciled. This is done by explicitly breaking particle conservation and adding a term

$$H_\eta = -\int d^d r \left(\eta\left(\mathbf{r}\right)\psi^\dagger\left(\mathbf{r}\right) + \eta^*\left(\mathbf{r}\right)\psi\left(\mathbf{r}\right)\right) \tag{54}$$

to the Hamiltonian and taking the limit $\eta \to 0$ after the thermodynamic limit. It turns out that $\langle\psi\left(\mathbf{r},t\right)\rangle \neq 0$ when the system establishes ODLRO. The density matrix can be decomposed as

$$\begin{aligned}\rho^{(1)}\left(\mathbf{r},\mathbf{r}',t\right) &= \left\langle\psi^\dagger\left(\mathbf{r},t\right)\right\rangle\langle\psi\left(\mathbf{r},t\right)\rangle \\ &+ \left\langle\left(\psi^\dagger\left(\mathbf{r},t\right) - \left\langle\psi^\dagger\left(\mathbf{r},t\right)\right\rangle\right)\left(\psi\left(\mathbf{r}',t\right) - \langle\psi\left(\mathbf{r}',t\right)\rangle\right)\right\rangle,\end{aligned} \tag{55}$$

where the first term remains finite for large $\mathbf{r}-\mathbf{r}'$, while the second one decays. We will not demonstrate this here, but rather perform the corresponding analysis when we discuss fermionic systems.

While the definition $\Psi\left(\mathbf{r},t\right)$ in terms of the condensate eigenfunctions of the density matrix is conceptually more satisfying, the usage of $\langle\psi\left(\mathbf{r},t\right)\rangle$ is very convenient in mean-field theories like the Bogoliubov theory of dilute or weakly interacting condensed bosons.

# 3 ODLRO, Meissner effect, and flux quantization of fermions

The analysis of ODLRO in fermionic systems proceeds in close analogy to the bosonic case discussed in the previous section[3]. It is, however, based upon the two-particle density matrix

$$\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2'\right) = \left\langle\psi^\dagger_\alpha\left(\mathbf{r}_1\right)\psi^\dagger_\beta\left(\mathbf{r}_2\right)\psi_{\beta'}\left(\mathbf{r}_2'\right)\psi_{\alpha'}\left(\mathbf{r}_1'\right)\right\rangle.$$

We consider the combined index $(\mathbf{r}_1\alpha,\mathbf{r}_2\beta)$ that describes the two-particle matrix. Expanding $\rho^{(2)}$ with respect to its eigenfunctions

$$\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2'\right) = \sum_p n_p \phi^*_p\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right)\phi_p\left(\mathbf{r}_1'\alpha',\mathbf{r}_2'\beta'\right), \tag{56}$$

with eigenvalues $n_p$. ODLRO is again a state where the largest eigenvalue $n_0$ is of the order of the particle number $N$. In this case holds

$$\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2'\right) \to n_0\phi^*_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right)\phi_0\left(\mathbf{r}_1'\alpha',\mathbf{r}_2'\beta'\right) \tag{57}$$

in the limit where $|\mathbf{r}_i - \mathbf{r}_i'| \to \infty$ while $|\mathbf{r}_1-\mathbf{r}_2|$ and $|\mathbf{r}_1'-\mathbf{r}_2'|$ remain finite.

From the antisymmetry of the fermionic wave function follows

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2'\right) &= -\rho^{(2)}_{\beta\alpha\alpha'\beta'}\left(\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_1',\mathbf{r}_2'\right) \\ &= -\rho^{(2)}_{\alpha\beta\beta'\alpha'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_2',\mathbf{r}_1'\right).\end{aligned} \tag{58}$$

This implies for the eigenfunction

$$\phi_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right)=-\phi_0\left(\mathbf{r}_2\beta,\mathbf{r}_1\alpha\right) \tag{59}$$

as expected for a genuine two particle wave function.

A displacement $\mathbf{a}$ can again be thought of as a gauge transformation[4, 5]. Thus, one can use either the wave functions $\Psi_\nu\left(\mathbf{r}_j,\gamma_j\right)$ (here $\gamma_j$ stands for the spin and other quantum numbers) or the alternative functions

$$\Psi'_\nu\left(\mathbf{r}_j,\gamma_j\right)=e^{i\frac{e}{\hbar c}\sum_j\chi_{\mathbf{a}}(\mathbf{r}_j)}\Psi_\nu\left(\mathbf{r}_j-\mathbf{a},\gamma_j\right).$$

As our magnetic field is assumed to be homogeneous, the displacement will not affect the coupling of the magnetic field to the spin. Expressing $\rho^{(2)}$ in terms of both sets of wave functions, we find the relationship

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}'_1,\mathbf{r}'_2\right) &= e^{-i\frac{e}{\hbar c}\left(\chi_{\mathbf{a}}(\mathbf{r}_1)+\chi_{\mathbf{a}}(\mathbf{r_2})-\chi_{\mathbf{a}}\left(\mathbf{r}'_1\right)-\chi_{\mathbf{a}}\left(\mathbf{r}'_2\right)\right)}\\ &\times\ \rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\mathbf{r}_1-\mathbf{a},\mathbf{r}_2-\mathbf{a},\mathbf{r}'_1-\mathbf{a},\mathbf{r}'_2-\mathbf{a}\right).\end{aligned} \tag{60}$$

For the eigenfunction follows from Eq.60 that

$$\phi_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right)=f_{\mathbf{a}}e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{a}}(\mathbf{r}_1)+\chi_{\mathbf{a}}(\mathbf{r}_2))}\phi_0\left(\mathbf{r}_1-\mathbf{a}\alpha,\mathbf{r}_2-\mathbf{a}\beta\right). \tag{61}$$

This is the two particle generalization of our earlier result Eq.32 for bosons. Meissner effect and flux quantization followed rather directly from this result. The Meissner effect follows from two consecutive displacements in alternate order:

$$\begin{aligned}\phi_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right) &= e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{b}}(\mathbf{r}_1)+\chi_{\mathbf{b}}(\mathbf{r}_2))}e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{a}}(\mathbf{r}_1-\mathbf{b})+\chi_{\mathbf{a}}(\mathbf{r}_2-\mathbf{b}))}\\ &\times\ f_{\mathbf{a}}f_{\mathbf{b}}\phi_0\left(\mathbf{r}_1-\mathbf{a}-\mathbf{b}\alpha,\mathbf{r}_2-\mathbf{a}-\mathbf{b}\beta\right)\end{aligned} \tag{62}$$

and

$$\begin{aligned}\phi_0\left(\mathbf{r}_1\alpha,\mathbf{r}_2\beta\right) &= e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{a}}(\mathbf{r}_1)+\chi_{\mathbf{a}}(\mathbf{r}_2))}e^{-i\frac{e}{\hbar c}(\chi_{\mathbf{b}}(\mathbf{r}_1-\mathbf{a})+\chi_{\mathbf{b}}(\mathbf{r}_2-\mathbf{a}))}\\ &\times\ f_{\mathbf{a}}f_{\mathbf{b}}\phi_0\left(\mathbf{r}_1-\mathbf{a}-\mathbf{b}\alpha,\mathbf{r}_2-\mathbf{a}-\mathbf{b}\beta\right),\end{aligned} \tag{63}$$

which requires that the two phase factors must be the same. We already found that

$$\chi_{\mathbf{b}}\left(\mathbf{r}\right)+\chi_{\mathbf{a}}\left(\mathbf{r}-\mathbf{b}\right)-\chi_{\mathbf{a}}\left(\mathbf{r}\right)-\chi_{\mathbf{b}}\left(\mathbf{r}-\mathbf{a}\right)=\mathbf{B}\cdot\left(\mathbf{a}\times\mathbf{b}\right). \tag{64}$$

The condition of identical phases then corresponds to

$$\frac{2e}{\hbar c}\mathbf{B}\cdot\left(\mathbf{a}\times\mathbf{b}\right)=2\pi n. \tag{65}$$

The only difference to the case of single-particle ODLRO is the new factor 2 that is a consequence of the two-particle ODLRO considered here. In case one were to analyze ODLRO in $\rho^{(l)}$ one would have a coefficient $\frac{le}{\hbar c}$. The argumentation which implied that a homogeneous magnetic field must vanish is now the same

as before: The left hand side of the above condition can be continuously varied while the right hand side cannot and the only solution is:

$$\mathbf{B} = \mathbf{0}. \tag{66}$$

The reasoning for flux-quantization also follows in full analogy to the bosonic case. We perform an infinite sequence of infinitesimal displacements along a path.

$$\phi_0\left(\mathbf{r}_1'\alpha, \mathbf{r}_2'\beta\right) = f_{\int_{\mathbf{r}_1}^{\mathbf{r}_2}\mathbf{dr}} e^{-i\frac{e}{\hbar c}\left(\int_{\mathbf{r}_1}^{\mathbf{r}_1'}\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}+\int_{\mathbf{r}_2}^{\mathbf{r}_2'}\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}\right)}\phi_0\left(\mathbf{r}_1\alpha, \mathbf{r}_2\beta\right). \tag{67}$$

Here, the path that connects $\mathbf{r}_1$ with $\mathbf{r}_1$' must be the same as the one that connects $\mathbf{r}_2$ with $\mathbf{r}_2$'. In case of a closed loop follows

$$\phi_0\left(\mathbf{r}_1\alpha, \mathbf{r}_2\beta\right) = e^{-i\frac{2e}{\hbar c}\oint\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}}\phi_0\left(\mathbf{r}_1\alpha, \mathbf{r}_2\beta\right). \tag{68}$$

The corresponding result for the quantization of the flux is

$$\Phi = \oint \mathbf{A}\left(\mathbf{r}\right)\cdot d\mathbf{r} = \frac{\hbar c}{2e}2\pi n = n\Phi_0, \tag{69}$$

with flux quantum $\Phi_0 = \frac{hc}{2e}$. Once again the additional factor of 2 in the flux quantum is a consequence of the two-particle ODLRO. If we consider a path surrounding a region without ODLRO, the argumentation that lead to the Meissner effect doesn't apply and the field can be finite. The enclosed flux must however be a multiple of the flux quantum.

Macroscopic coherence in fermionic systems, reflected in a single large eigenvalue $n_0$ of $\rho^{(2)}$ of the order of the system size, is the crucial ingredient that leads to the Meissner effect and to flux quantization.

## 3.1 the order parameter

In full analogy to the case of charged bosons, the natural choice of the order parameter of a fermionic system with ODLRO is the condensate wave function

$$\Psi\left(\mathbf{R}, \mathbf{r}, \alpha, \beta, t\right) = \sqrt{n_0\left(t\right)}\phi_0\left(\mathbf{r}_1\alpha, \mathbf{r}_2\beta\right), \tag{70}$$

where we use instead of the individual particle coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center of gravity coordinate $\mathbf{R} = \frac{1}{2}\left(\mathbf{r}_1 + \mathbf{r}_2\right)$, respectively. An alternative approach is motivated by the theory of magnetism.

Consider a magnet with global $SU\left(2\right)$ spin-rotation invariance. Applying a finite magnetic field $\mathbf{B}\left(\mathbf{r}\right)$, the symmetry is spontaneously broken if the expectation value

$$\mathbf{s_0}\left(\mathbf{r}\right) = \frac{1}{2}\lim_{\mathbf{B}\to 0}\lim_{N,V\to\infty}\sum_{\alpha\beta}\left\langle\psi_\alpha^\dagger\left(\mathbf{r}\right)\boldsymbol{\sigma}_{\alpha\beta}\psi_\beta\left(\mathbf{r}\right)\right\rangle \tag{71}$$

is finite. Without the external magnetic field, multiple degenerate configurations would cancel each other, leading to a zero magnetization. The same is true if one

performs the limit $\mathbf{B} \to 0$ for a finite system as there is still a finite macroscopic tunneling probability between degenerate states. This is the reason why the zero field limit must be performed after the thermodynamic limit.

In the context of superconductivity, spontaneous symmetry breaking can be analyzed if we add to the Hamiltonian a source term

$$H = -\int d^d r_1 d^d r_2 \sum_{\alpha\beta} \left( \eta_{\alpha\beta} \left( \mathbf{r}_1, \mathbf{r}_2 \right) \psi_\alpha^\dagger \left( \mathbf{r}_1 \right) \psi_\beta^\dagger \left( \mathbf{r}_2 \right) + h.c. \right). \tag{72}$$

A physical realization of the source field $\eta_{\alpha\beta} \left( \mathbf{r}_1, \mathbf{r}_2 \right)$ is the coupling to another superconductor via a weak Josephson junction (see below). Just like in case of a magnet, we perform the limit $\eta \to 0$ after the thermodynamic limit. One expects ODLRO to be identical to a finite expectation value

$$\Psi \left( \mathbf{R}, \mathbf{r}, \alpha, \beta, t \right) = \lim_{\eta \to 0} \lim_{N,V \to \infty} \left\langle \psi_\beta \left( \mathbf{r}_2 \right) \psi_\alpha \left( \mathbf{r}_1 \right) \right\rangle. \tag{73}$$

While a general proof for the equivalence between these two definitions does not seem to exist, we will later show that they are identical within the BCS theory. This formulation makes evident the statement that at a superconducting transition the global $U\left(1\right)$ symmetry

$$\psi_\alpha \left( \mathbf{r} \right) \to e^{i\theta} \psi_\alpha \left( \mathbf{r} \right) \tag{74}$$

is spontaneously broken. Breaking the global $U\left(1\right)$ symmetry implies that the particle number conservation is spontaneously broken. While one frequently encounters the notion that at the superconducting transition the electromagnetic gauge symmetry is spontaneously broken, it seems more adequate to simply refer to a global $U\left(1\right)$ symmetry as the same symmetry is also broken in neutral fermionic superfluids. What is unique about charged superfluids is however associated with the condensed matter realization of the Higgs mechanism in superconductors that we will discuss later. For a lucid discussion of the issue of gauge symmetry breaking at the superconducting transition, see Ref.[6].

The source field $\eta_{\alpha\beta} \left( \mathbf{r}_1, \mathbf{r}_2 \right)$ has well defined behavior upon exchanging particles. Fermi statistics implies that

$$\psi_\alpha^\dagger \left( \mathbf{r}_1 \right) \psi_\beta^\dagger \left( \mathbf{r}_2 \right) = -\psi_\beta^\dagger \left( \mathbf{r}_2 \right) \psi_\alpha^\dagger \left( \mathbf{r}_1 \right). \tag{75}$$

If we now relabel the indices $\mathbf{r}_1 \alpha \longleftrightarrow \mathbf{r}_2 \beta$ the source field must compensate for the minus sign to recover the original Hamiltonian, i.e.

$$\eta_{\alpha\beta} \left( \mathbf{r}_1, \mathbf{r}_2 \right) = -\eta_{\beta\alpha} \left( \mathbf{r}_2, \mathbf{r}_1 \right). \tag{76}$$

The $(2 \times 2)$ matrix form of $\eta$ suggests an expansion in terms of Pauli matrices $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ and the unit matrix $\sigma^0$. Out of those for matrices. $\sigma^y$ is the only one that is antisymmetric ($\sigma^y_{\alpha\beta} = -\sigma^y_{\beta\alpha}$). All other are symmetric. This suggests an expansion (the additional factor $i$ is for convenience):

$$\eta_{\alpha\beta} \left( \mathbf{r}_1, \mathbf{r}_2 \right) = \eta_s \left( \mathbf{r}_1, \mathbf{r}_2 \right) \left( i\sigma^y \right)_{\alpha\beta} + \boldsymbol{\eta}_t \left( \mathbf{r}_1, \mathbf{r}_2 \right) \cdot \left( i\sigma^y \boldsymbol{\sigma} \right)_{\alpha\beta}. \tag{77}$$

The first term behaves like a singlet two particle wave function; it is antisymmetric with respect to the spin indices, i.e. it must be symmetric with respect to the spatial indices. The opposite is the case for the second term that describes the triplet part of the source field.

The same is of course true for the order parameter itself, i.e. we expand

$$\Psi\left(\mathbf{R},\mathbf{r},\alpha,\beta\right)=\Psi_{s}\left(\mathbf{R},\mathbf{r}\right)\left(i\sigma^{y}\right)_{\alpha\beta}+\mathbf{\Psi}_{t}\left(\mathbf{R},\mathbf{r}\right)\cdot\left(i\sigma^{y}\boldsymbol{\sigma}\right)_{\alpha\beta}, \tag{78}$$

where the singlet and triplet part obey:

$$\begin{aligned}\Psi_{s}\left(\mathbf{R},\mathbf{r}\right) &= \Psi_{s}\left(\mathbf{R},-\mathbf{r}\right),\\ \mathbf{\Psi}_{t}\left(\mathbf{R},\mathbf{r}\right) &= -\mathbf{\Psi}_{t}\left(\mathbf{R},-\mathbf{r}\right).\end{aligned} \tag{79}$$

Consider now a three dimensional system with inversion symmetry. Then each operator should either be even or odd under $\mathbf{r}\rightarrow-\mathbf{r}$. The spin is a pseudovector, i.e. it does not change under parity. Thus, it must hold that

$$\Psi\left(\mathbf{R},\mathbf{r},\alpha,\beta\right)=\pm\Psi\left(\mathbf{R},-\mathbf{r},\alpha,\beta\right). \tag{80}$$

It follows that a superconducting state with inversion symmetry must either form ODLRO of triplets or of singlets. For a combination of the singlet and triplet pairing, the total wave function would have no well defined parity eigenvalue. It is interesting that our proof is valid even if one includes spin orbit interaction. In crystals without inversion symmetry or on the surface of a three dimensional crystal, both pairing states can of course exist simultaneously.

The two-particle density matrix $\rho^{(2)}$ is an equal-time correlation function. Using the fluctuation-dissipation theorem we can therefore relate it to a retarded Green's function (we use the abbreviation $\{\mathbf{r}_i\}=(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}'_1,\mathbf{r}'_2)$

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}\left(\{\mathbf{r}_i\}\right) &= \left\langle\psi^{\dagger}_{\alpha}\left(\mathbf{r}_1\right)\psi^{\dagger}_{\beta}\left(\mathbf{r}_2\right)\psi_{\beta'}\left(\mathbf{r}'_2\right)\psi_{\alpha'}\left(\mathbf{r}'_1\right)\right\rangle\\ &= -\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\mathrm{Im}\chi_{\alpha\beta\alpha'\beta'}\left(\{\mathbf{r}_i\},\omega+i0^{+}\right)}{e^{\beta\omega}-1},\end{aligned}$$

where $\chi$ us the Fourier transform ($\chi\left(\omega\right)=\int_{-\infty}^{\infty}dt\chi\left(t\right)e^{i\omega t}$) of the retarded function

$$\chi_{\alpha\beta\alpha'\beta'}\left(\{\mathbf{r}_i\},t\right)=-i\theta\left(t\right)\left\langle\left[\psi^{\dagger}_{\alpha}\left(\mathbf{r}_1,t\right)\psi^{\dagger}_{\beta}\left(\mathbf{r}_2,t\right),\psi_{\beta'}\left(\mathbf{r}'_2,0\right)\psi_{\alpha'}\left(\mathbf{r}'_1,0\right)\right]_{-}\right\rangle,$$

where the operators are now in the Heisenberg picture. $\chi$ is the pair-susceptibility of the system, i.e. the change of the expectation value $\left\langle\psi^{\dagger}_{\beta}\left(\mathbf{r}_2,t\right)\psi^{\dagger}_{\alpha}\left(\mathbf{r}_1,t\right)\right\rangle$ with respect to a rime dependent source field $\eta_{\alpha'\beta'}\left(\mathbf{r}'_1,\mathbf{r}'_2,t'\right)$:

$$\chi_{\alpha\beta\alpha'\beta'}\left(\{\mathbf{r}_i\},t-t'\right)=\left.\frac{\delta\left\langle\psi^{\dagger}_{\beta}\left(\mathbf{r}_2,t\right)\psi^{\dagger}_{\alpha}\left(\mathbf{r}_1,t\right)\right\rangle}{\delta\eta^{*}_{\alpha'\beta'}\left(\mathbf{r}'_1,\mathbf{r}'_2,t'\right)}\right|_{\eta,\eta^{*}\rightarrow0}. \tag{81}$$

As before, the limit of vanishing source fields must be taken after the thermodynamic limit.

## 3.2 density matrix of free fermions

We are now in the position to test whether a given system establishes ODLRO. Let us first consider a system of noninteracting particles. We use the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center of gravity coordinate $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$. It follows ($\mathbf{r}_{1,2} = \mathbf{R} \pm \frac{\mathbf{r}}{2}$ and $\mathbf{r}'_{1,2} = \mathbf{R}' \pm \frac{\mathbf{r}'}{2}$

$$\rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{R},\mathbf{r},\mathbf{R}',\mathbf{r}') = \left\langle \psi^\dagger_\alpha(\mathbf{r}_1)\,\psi^\dagger_\beta(\mathbf{r}_2)\,\psi_{\beta'}(\mathbf{r}'_2)\,\psi_{\alpha'}(\mathbf{r}'_1)\right\rangle.$$

We perform a Fourier transformation

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{R},\mathbf{r},\mathbf{R}',\mathbf{r}') &= \frac{1}{V^2}\sum_{\mathbf{k}_1\cdots\mathbf{k}'_2}\left\langle \psi^\dagger_{\mathbf{k}_1\alpha}\psi^\dagger_{\mathbf{k}_2\beta}\psi_{\mathbf{k}'_2\beta'}\psi_{\mathbf{k}'_1\alpha'}\right\rangle \\ &\times\ e^{-i\left((\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{R}+(\mathbf{k}_1-\mathbf{k}_2)\cdot\frac{\mathbf{r}}{2}-\left(\mathbf{k}'_1+\mathbf{k}'_2\right)\cdot\mathbf{R}'-\left(\mathbf{k}'_1-\mathbf{k}'_2\right)\cdot\frac{\mathbf{r}'}{2}\right)}.\end{aligned}$$

This expectation value for a free fermion can be evaluated using the Wick expansion

$$\begin{aligned}\left\langle \psi^\dagger_{\mathbf{k}_1\alpha}\psi^\dagger_{\mathbf{k}_2\beta}\psi_{\mathbf{k}'_2\beta'}\psi_{\mathbf{k}'_1\alpha'}\right\rangle &= \left\langle \psi^\dagger_{\mathbf{k}_1\alpha}\psi_{\mathbf{k}'_1\alpha'}\right\rangle\left\langle \psi^\dagger_{\mathbf{k}_2\beta}\psi_{\mathbf{k}'_2\beta'}\right\rangle \\ &- \left\langle \psi^\dagger_{\mathbf{k}_1\alpha}\psi_{\mathbf{k}'_2\beta'}\right\rangle\left\langle \psi^\dagger_{\mathbf{k}_2\beta}\psi_{\mathbf{k}'_1\alpha'}\right\rangle \\ &= n_{\mathbf{k}_1}n_{\mathbf{k}_2}\left(\delta_{\mathbf{k}_1,\mathbf{k}'_1}\delta_{\mathbf{k}_2,\mathbf{k}'_2}\delta_{\alpha\alpha'}\delta_{\beta\beta'} - \delta_{\mathbf{k}_1,\mathbf{k}'_2}\delta_{\mathbf{k}_2,\mathbf{k}'_1}\delta_{\alpha\beta'}\delta_{\beta\alpha'}\right)\end{aligned}$$

We write

$$\begin{aligned}\delta_{\alpha\alpha'}\delta_{\beta\beta'} &= \langle\alpha\beta|\alpha'\beta'\rangle = \sum_{S,m}\chi^{S,m*}_{\alpha'\beta'}\chi^{S,m}_{\alpha\beta} \\ \delta_{\alpha\beta'}\delta_{\beta\alpha'} &= \langle\alpha\beta|\beta'\alpha'\rangle = \sum_{S,m}\chi^{S,m*}_{\beta'\alpha'}\chi^{S,m}_{\alpha\beta}\end{aligned} \tag{82}$$

The spin eigenfunctions $\chi^{S,m}_{\alpha\beta}$ are the singlet

$$\chi^{0,0}_{\alpha\beta} = \frac{1}{\sqrt{2}}\left(\delta_{\alpha,+}\delta_{\beta,-} - \delta_{\alpha,-}\delta_{\beta,+}\right) \tag{83}$$

and the triplets

$$\chi^{1,m}_{\alpha\beta} = \begin{cases} \delta_{\alpha,+}\delta_{\beta,+} & \text{if} \quad m=1 \\ \frac{1}{\sqrt{2}}\left(\delta_{\alpha,+}\delta_{\beta,-} + \delta_{\alpha,-}\delta_{\beta,+}\right) & \text{if} \quad m=0 \\ \delta_{\alpha,-}\delta_{\beta,-} & \text{if} \quad m=-1 \end{cases}. \tag{84}$$

It follows with the symmetry of the spin wave function: $\chi^{S,m}_{\beta'\alpha'} = -(-1)^S\chi^{S,m}_{\alpha'\beta'}$ and after eliminating the $\delta$-functions in momentum space that:

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{R},\mathbf{r},\mathbf{R}',\mathbf{r}') &= \frac{1}{V^2}\sum_{\mathbf{k}_1\mathbf{k}_2} n_{\mathbf{k}_1}n_{\mathbf{k}_2}\chi^{S,m}_{\alpha\beta}\chi^{S,m*}_{\alpha'\beta'}e^{-i(\mathbf{k}_1+\mathbf{k}_2)\cdot\left(\mathbf{R}-\mathbf{R}'\right)} \\ &\times\ \left(e^{-i(\mathbf{k}_1-\mathbf{k}_2)\cdot\frac{\mathbf{r}-\mathbf{r}'}{2}} + (-1)^S e^{-i(\mathbf{k}_1-\mathbf{k}_2)\cdot\frac{\mathbf{r}+\mathbf{r}'}{2}}\right).\end{aligned}$$

We use the total momentum $\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2$ and the relative momentum $\mathbf{k} = (\mathbf{k}_1 - \mathbf{k}_2)/2$, and symmetrize the sum over $\mathbf{k}$ according to $\sum_{\mathbf{k}} a_{\mathbf{k}} = \frac{1}{2}\sum_{\mathbf{k}} (a_{\mathbf{k}} + a_{-\mathbf{k}})$ such that with

$$\begin{aligned}\rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{R},\mathbf{r},\mathbf{R}',\mathbf{r}') &= \frac{1}{2V^2}\sum_{\mathbf{Kk}} n_{\frac{1}{2}\mathbf{K}+\mathbf{k}} n_{\frac{1}{2}\mathbf{K}-\mathbf{k}} \chi^{S,m*}_{\alpha\beta}\chi^{S,m}_{\alpha'\beta'} e^{-i\mathbf{K}\cdot(\mathbf{R}-\mathbf{R}')} \\ &\times \left\{ e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} + e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \right. \\ &\left. + (-1)^S \left( e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{r}')} + e^{i\mathbf{k}\cdot(\mathbf{r}+\mathbf{r}')} \right) \right\}. \end{aligned} \tag{85}$$

We write the term in curly brackets as

$$\left(e^{i\mathbf{k}\cdot\mathbf{r}} + (-1)^S e^{-i\mathbf{k}\cdot\mathbf{r}}\right)^* \left(e^{i\mathbf{k}\cdot\mathbf{r}'} + (-1)^S e^{-i\mathbf{k}\cdot\mathbf{r}'}\right)$$

and finally obtain

$$\rho^{(2)}_{\alpha\beta\alpha'\beta'}(\mathbf{R},\mathbf{r},\mathbf{R}',\mathbf{r}') = \sum_{\mathbf{Kk},SM} n^{(2)}_{\mathbf{K},\mathbf{k},S,m} \phi^*_{\mathbf{K},\mathbf{k},S,m}(\mathbf{R},\mathbf{r},\alpha,\beta)\,\phi_{\mathbf{K},\mathbf{k},S,m}(\mathbf{R}',\mathbf{r}',\alpha',\beta')$$

with eigenfunctions of the density matrix

$$\phi_{\mathbf{K},\mathbf{k},S,m}(\mathbf{R},\mathbf{r},\alpha,\beta) = \frac{1}{\sqrt{V}} e^{i\mathbf{K}\cdot\mathbf{R}} \varphi_S(\mathbf{k}\cdot\mathbf{r})\,\chi^{S,m}_{\alpha\beta}. \tag{86}$$

The relative wave function of the singlet is

$$\varphi_0 = \sqrt{\frac{2}{V}}\cos(\mathbf{k}\cdot\mathbf{r}) \tag{87}$$

for the singlet and (we drop a trivial phase factor $i$)

$$\varphi_1 = \sqrt{\frac{2}{V}}\sin(\mathbf{k}\cdot\mathbf{r}) \tag{88}$$

for the triplet. The wave functions are chosen to be normalized to unity, allowing us to determine the eigenvalues of the two particle density matrix:

$$n^{(2)}_{\mathbf{K},\mathbf{k},S,m} = n_{\frac{1}{2}\mathbf{K}+\mathbf{k}} n_{\frac{1}{2}\mathbf{K}-\mathbf{k}} \leq 1. \tag{89}$$

Obviously, no eigenvalue of $\rho^{(2)}$ is of the order of the system size and a system of non-interacting fermions will not undergo ODLRO. This is relevant in view of the fact that the conductivity of a gas of free fermions with full translation invariance is infinite. This perfect conductance is therefore distinct from the macroscopic coherence of a supercondctor that is associated with ODLRO.

### 3.3 The effects of a discrete lattice

Our analysis ignored the effects of lattice periodicity, relevant to electrons in crystals. In case of a periodic lattice, the allowed displacements are only

$$\mathbf{a} = l_1\mathbf{e}_1 + l_2\mathbf{e}_2 + l_3\mathbf{e}_3, \tag{90}$$

where the $\mathbf{e}_i$ refer to the unit vectors along the crystal axes (i.e. they are not necessarily orthogonal). The arguments that lead to the Meissner effect in a system with full translation invariance apply and we find the criterion

$$\frac{2e}{\hbar c}\mathbf{B}\cdot(\mathbf{e}_i\times\mathbf{e}_j) = 2\pi n_{ij} \tag{91}$$

for all combinations $i$ and $j$ and with integers $n_{ij}$. In case where $n_{ij} = 0$ for all $i$ and $j$, we have again $\mathbf{B} = 0$. The smallest values for the integers are $|n_{ij}| = 1$ for some pair $i$, $j$. Then we obtain a typical amplitude of the field of $B \approx \frac{hc}{2e}a_0^2 = \Phi_0 a_0^2$, where $a_0$ is the interatomic distance. Thus we could have a field strength that yields a flux quantum per area $a_0^2$. Such fields are about $10^9$G which is significantly larger (by about six orders of magnitude) than the typical external magnetic fields supported by superconductors. Currently no laboratory exists that can generate magnetic fields of this magnitude, so it is an open question whether an exotic superconducting state could emerge in such fields. For external field values smaller than this value, the magnetic field in the superconductor must, however, vanish.

The reasoning for the flux quantization can also be generalized to closed loops that consist of discrete steps on the crystalline lattice. The condition for flux quantization is now:

$$\sum_{\mathcal{C}} \mathbf{A}(\mathbf{r})\cdot\Delta\mathbf{r} = n\Phi_0. \tag{92}$$

Except that closed paths are made up of discrete lattice translation is the substance of this result the same as the continuous version discussed earlier.

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# Part II
# The Pairing Instability

The analysis of ODLRO revealed that a condensation in the two-particle density matrix with macroscopic occupation of a two-particle bound state explains the key observation of superconductors, the Meissner effect and fluz quantization. Motivated by those considerations we perform now an analysis of fermions with weak attractive interaction in a many-body system. To demonstrate that such an attractive interaction can be realized despite the repulsive electron-electron Coulomb interaction, we first discuss the effective interaction due to the exchange of lattice vibrations. While this is not the only route to superconductivity it the accepted microscopic pairing mechanism for so called conventional superconductors. These considerations are followed by a discussion of the Cooper instability using several alternative approaches.

## 4 Attraction due to the exchange of phonons

### 4.1 Integrating out phonons

In what follows we derive an effective electron-electron interaction mediated by the electron-phonon coupling. We will see that such an interaction leads to an effective coupling between electrons that is attractive. We start from the Hamoltonian

$$\begin{aligned} H &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \psi^\dagger_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} a^\dagger_{\mathbf{q}} a_{\mathbf{q}} \\ &+ \sum_{\mathbf{q}} g_{\mathbf{q}} \rho_{\mathbf{q}} \left( a_{\mathbf{q}} + a^\dagger_{-\mathbf{q}} \right). \end{aligned} \tag{93}$$

Here $\epsilon_{\mathbf{k}}$ is the electronic band dispersion and $\omega_{\mathbf{q}}$ are phonon frequencies. $\psi_{\mathbf{k}\sigma}$ is the electron annihilation operator for spin $\sigma$ and momentum $\mathbf{k}$ and $a_{\mathbf{q}}$ annihilates a phonon with momentum $\mathbf{q}$. The last term is the electron phonon coupling where the electron density

$$\rho_{\mathbf{q}} = \sum_{\mathbf{k}\sigma} \psi^\dagger_{\mathbf{k}\sigma} \psi_{\mathbf{k}+\mathbf{q}\sigma}$$

couples to the phonon displacement $u_{\mathbf{q}} \propto \left( a_{\mathbf{q}} + a^\dagger_{-\mathbf{q}} \right)$. $g_{\mathbf{k},\mathbf{q}}$ is the matrix element of the electron-phonon coupling. It is straightforward to generalize the approach and include more than one phonon branch and to allow for a $\mathbf{k}$, dependence of the electron-phonon matrix element, i.e. $g_{\mathbf{q}} \to g_{\mathbf{k},\mathbf{q}}$. In the latter case one has to write the coupling term as

$$H_{el-ph} = \sum_{\mathbf{k},\mathbf{q}\sigma} g_{\mathbf{k},\mathbf{q}} \psi^\dagger_{\mathbf{k}\sigma} \psi_{\mathbf{k}+\mathbf{q}\sigma} \left( a_{\mathbf{q}} + a^\dagger_{-\mathbf{q}} \right)$$

The fastest way to perform this analysis is to express the partition function as a coherent state functional integral on the imaginary time axis

$$Z = \int D\psi^{\dagger} D\psi D a^{\dagger} D a e^{-S} \tag{94}$$

with action[3]

$$\begin{aligned} S &= \int_0^{\beta} \left( \sum_{\mathbf{k}\sigma} \overline{\psi}_{\mathbf{k}\sigma}(\tau) \left(\partial_\tau + \epsilon_{\mathbf{k}}\right) \psi_{\mathbf{k}\sigma}(\tau) + \sum_{\mathbf{q}} \overline{a}_{\mathbf{q}}(\tau) \left(\partial_\tau + \omega_{\mathbf{q}}\right) a_{\mathbf{q}}(\tau) \right) \\ &+ \int_0^{\beta} d\tau \sum_{\mathbf{q}} g_{\mathbf{q}} \rho_{\mathbf{q}}(\tau) \left( a_{\mathbf{q}}(\tau) + \overline{a}_{-\mathbf{q}}(\tau) \right). \end{aligned} \tag{95}$$

The electron-phonon interaction can formally be eliminated by performing the Gaussian integration over the complex bosonic coherent states. One can do this by shifting the phonon variables according to

$$\begin{aligned} a_{\mathbf{q}}(\tau) &\rightarrow b_{\mathbf{q}}(\tau) = a_{\mathbf{q}}(\tau) - g_{\mathbf{q}} \int_0^{\beta} d\tau' G_{\mathbf{q}}^{(ph)}(\tau - \tau') \rho_{\mathbf{q}}(\tau') \\ \overline{a}_{\mathbf{q}}(\tau) &\rightarrow \overline{b}_{\mathbf{q}}(\tau) = \overline{a}_{\mathbf{q}}(\tau) - g_{\mathbf{q}} \int_0^{\beta} d\tau' \rho_{\mathbf{q}}(\tau') G_{\mathbf{q}}^{(ph)}(\tau' - \tau). \end{aligned} \tag{96}$$

Here $G_{\mathbf{q}}^{(ph)}(\tau - \tau')$ is the bare phonon Green's function which obeys

$$\left(\partial_\tau + \omega_{\mathbf{q}}\right) G_{\mathbf{q}}^{(ph)}(\tau - \tau') = -\delta(\tau - \tau'). \tag{97}$$

Inserting this into the action $S$ we obtain for the bare phonon term

$$\begin{aligned} S_0^{(ph)} &= \int_0^{\beta} d\tau \sum_{\mathbf{q}} \overline{a}_{\mathbf{q}}(\tau) \left(\partial_\tau + \omega_{\mathbf{q}}\right) a_{\mathbf{q}}(\tau) \\ &= \int_0^{\beta} d\tau \sum_{\mathbf{q}} \overline{b}_{\mathbf{q}}(\tau) \left(\partial_\tau + \omega_{\mathbf{q}}\right) b_{\mathbf{q}}(\tau) \\ &- \int_0^{\beta} d\tau \sum_{\mathbf{q}} g_{\mathbf{q}} \rho_{\mathbf{q}}(\tau) \left( b_{\mathbf{q}}(\tau) + \overline{b}_{-\mathbf{q}}(\tau) \right) \end{aligned} \tag{98}$$

For the interaction term we obtain

$$\begin{aligned} S_{int} &= \int_0^{\beta} d\tau \sum_{\mathbf{q}} g_{\mathbf{q}} \rho_{\mathbf{q}}(\tau) \left( b_{\mathbf{q}}(\tau) + \overline{b}_{-\mathbf{q}}(\tau) \right). \\ &+ \int_0^{\beta} d\tau' d\tau' \sum_{\mathbf{q}} V_{\mathbf{q}}^{\text{eff}}(\tau - \tau') \rho_{\mathbf{q}}(\tau) \rho_{-\mathbf{q}}(\tau') \end{aligned}$$

[3] As usual $\psi$, $\overline{\psi}$ are anticommuting Grassmann variables and $a$ and $\overline{a}$ are complex numbers.

with

$$V_{\mathbf{q}}^{\text{eff}}(\tau-\tau') = g_{\mathbf{q}}^2\left(G_{\mathbf{q}}^{(ph)}(\tau'-\tau) + G_{\mathbf{q}}^{(ph)}(\tau-\tau')\right).$$

When we add all terms we find that there is no direct interaction between the operators $b$ and the fermions, i.e. we have

$$\begin{aligned} S &= \int_0^\beta \left(\sum_{\mathbf{k}\sigma} \overline{\psi}_{\mathbf{k}\sigma}(\tau)\left(\partial_\tau + \epsilon_{\mathbf{k}}\right)\psi_{\mathbf{k}\sigma}(\tau) + \sum_{\mathbf{q}} \overline{b}_{\mathbf{q}}(\tau)\left(\partial_\tau + \omega_{\mathbf{q}}\right) b_{\mathbf{q}}(\tau)\right) \\ &+ S_{\text{int}}\left[\overline{\psi},\psi\right] \end{aligned} \tag{99}$$

with purely electronic interaction:

$$S_{\text{int}}\left[\overline{\psi},\psi\right] = \int_0^\beta d\tau' d\tau' \sum_{\mathbf{q}} V_{\mathbf{q}}^{\text{eff}}(\tau-\tau')\,\rho_{\mathbf{q}}(\tau)\,\rho_{-\mathbf{q}}(\tau') \tag{100}$$

Thus, one can exactly map the system of electrons coupled to phonons onto a problem free phonons that completely decouple from the electronic system and of electrons that only interact with each other. This interaction is however a retarded (not instantaneous) interaction, caused by the fact that phonons are dynamic degrees of freedom. Such a retarded interaction cannot be expressed in terms of a purely electronic Hamiltonian. However, there is no problem within the coherent state functional integral. In case of an alectron phonon coupling $g_{\mathbf{k},\mathbf{q}}$ that depends on the fermionic momentum, one only needs to replace $g_{\mathbf{q}}\rho_{\mathbf{q}}$ by $\tilde{\rho}_{\mathbf{q}} = \sum_{\mathbf{k}\sigma} g_{\mathbf{k},\mathbf{q}}\psi_{\mathbf{k}\sigma}^\dagger\psi_{\mathbf{k}+\mathbf{q}\sigma}$.

To interpret the obtained effective interaction we Fourier transform and obtain

$$S_{\text{int}}\left[\overline{\psi},\psi\right] = T\sum_{\mathbf{q},n} V_{\mathbf{q}}^{\text{eff}}(i\omega_n)\,\rho_{\mathbf{q}}(i\omega_n)\,\rho_{-\mathbf{q}}(-i\omega_n) \tag{101}$$

with bosonic Matsubara frequency $\omega_n = 2n\pi T$. For the phonon Green's function holds for imaginary frequencies:

$$G_{\mathbf{q}}^{(ph)}(i\omega_n) = \frac{1}{i\omega_n - \omega_{\mathbf{q}}} \tag{102}$$

and we find

$$\begin{aligned} V_{\mathbf{q}}^{\text{eff}}(i\omega_n) &= g_{\mathbf{q}}^2\left(\frac{1}{i\omega_n-\omega_{\mathbf{q}}} + \frac{1}{-i\omega_n-\omega_{\mathbf{q}}}\right) \\ &= -g_{\mathbf{q}}^2\frac{2\omega_{\mathbf{q}}}{\omega_n^2+\omega_{\mathbf{q}}^2}. \end{aligned} \tag{103}$$

For a physical interpretation of this result it is more appropriate to return to real frequency axis $i\omega_n \to \omega + i0^+$ and consider retarded Green's functions. It follows

$$V_{\mathbf{q}}^{\text{eff}}\left(\omega+i0^+\right) = -g_{\mathbf{q}}^2\frac{2\omega_{\mathbf{q}}}{\omega_{\mathbf{q}}^2-\left(\omega+i0^+\right)^2}. \tag{104}$$

Thus, for interactions $\omega$ smaller than the phonon frequencies, one obtains a density-density interaction that is attractive

$$\mathrm{Re}V_{\mathbf{q}}^{\mathrm{eff}}\left(\omega+i0^{+}\right)\big|_{|\omega|<\omega_{\mathbf{q}}}<0. \tag{105}$$

## 4.2 The role of the Coulomb interaction

The effective attractive interaction mediated by phonons is interesting. A natural question is, however, whether there remains such an interaction if one includes the Coulomb repulsion of electrons. We add to the Hamiltonian the direct Coulomb interaction:

$$\begin{aligned} H &= \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}\psi_{\mathbf{k}\sigma}^{\dagger}\psi_{\mathbf{k}\sigma}+\sum_{\mathbf{q}}\omega_{\mathbf{q}}a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}} \\ &+ \sum_{\mathbf{q}}\left(g_{\mathbf{q}}\rho_{\mathbf{q}}\left(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger}\right)+V_{\mathbf{q}}^{(0)}\rho_{\mathbf{q}}\rho_{-\mathbf{q}}\right), \end{aligned} \tag{106}$$

where

$$V_{\mathbf{q}}^{(0)}=\frac{4\pi e^{2}}{q^{2}} \tag{107}$$

is the Fourier transform of the Coulomb interaction $V^{(0)}(\mathbf{r})=e^{2}/r$. It is well established that this interaction is screened by highly mobile electrons, an effect that can be expressed in terms of a momentum and frequency dependent dielectric function $\varepsilon(\mathbf{q},\omega)$:

$$V_{\mathbf{q}}^{\mathrm{eff}}(\omega)=\frac{4\pi e^{2}}{q^{2}\varepsilon(\mathbf{q},\omega)}. \tag{108}$$

In what follows we determine this dielectric function. In this derivation of the effective interaction between electrons that is mediated by the crystalline lattice, we follow Bardeen and Pines and analyze a so called jellium model, where the ions are described in terms of a structureless positive background of fluctuating charge densities. We consider an external charge $\rho_{\mathrm{ext.}}(\mathbf{r},t)$ that leads to induced screening charges $\rho(\mathbf{r},t)$ in the system. The Maxwell equation that determines the electric field that results from a charge redistribution is:

$$\begin{aligned} \nabla\cdot\mathbf{E} &= 4\pi\left(\rho+\rho_{\mathrm{ext.}}\right) \\ \nabla\cdot\mathbf{D} &= 4\pi\rho_{\mathrm{ext.}}, \end{aligned} \tag{109}$$

where we introduced the displacement field

$$\begin{aligned} \mathbf{D}(\mathbf{r},t) &= \int d^{3}r'dt'\varepsilon(\mathbf{r}-\mathbf{r}',t-t')\,\mathbf{E}(\mathbf{r}',t') \\ &= \mathbf{E}(\mathbf{r},t)+4\pi\mathbf{P}(\mathbf{r},t) \end{aligned} \tag{110}$$

i.e.

$$\nabla \cdot \mathbf{P} = -\rho_{\text{ext.}}. \tag{111}$$

In Fourier space follows

$$\begin{aligned} i\mathbf{q} \cdot \mathbf{D}(\mathbf{q},\omega) &= i\mathbf{q} \cdot \mathbf{E}(\mathbf{q},\omega)\varepsilon\left(\mathbf{q},\omega\right) \\ &= 4\pi\rho_{\text{ext.}}(\mathbf{q},\omega). \end{aligned} \tag{112}$$

and

$$i\mathbf{q} \cdot \mathbf{E}(\mathbf{q},\omega) = 4\pi\left(\rho\left(\mathbf{q},\omega\right) + \rho_{\text{ext.}}(\mathbf{q},\omega)\right). \tag{113}$$

Thus, the total charge $\rho + \delta\rho$ is related to the external charge $\delta\rho$ via

$$\rho\left(\mathbf{q},\omega\right) + \rho_{\text{ext.}}\left(\mathbf{q},\omega\right) = \frac{1}{\varepsilon\left(\mathbf{q},\omega\right)}\rho_{\text{ext.}}\left(\mathbf{q},\omega\right). \tag{114}$$

We first consider the classical motion of a charge density governed by Newton's law:

$$m\frac{d^2\mathbf{r}}{dt^2} = e\mathbf{E} \tag{115}$$

and express the velocity of the carriers in terms of the charge current

$$\mathbf{j} = en_0\frac{d\mathbf{r}}{dt}, \tag{116}$$

where $n_0$ is the particle density of charge $e$. It follows

$$m\frac{d\mathbf{j}}{dt} = e^2 n_0\mathbf{E}. \tag{117}$$

The current is related to the charge density via the continuity equation

$$\partial_t\rho + \nabla \cdot \mathbf{j} = 0, \tag{118}$$

which yields (assuming $\frac{\partial \mathbf{j}}{\partial t} = \frac{d\mathbf{j}}{dt}$ which is correct at linear response to the external electric field):

$$\begin{aligned} \frac{\partial^2\rho}{\partial t^2} &= -\nabla \cdot \frac{\partial \mathbf{j}}{\partial t} = -\frac{e^2 n_0}{m}\nabla \cdot \mathbf{E} \\ &= -\frac{4\pi e^2 n_0}{m}\left(\rho + \rho_{\text{ext.}}\right) \end{aligned} \tag{119}$$

This is the equation of a forced oscillator with resonance frequency

$$\omega_p = \sqrt{\frac{4\pi e^2 n_0}{m}}.$$

$\omega_p$ is the plasma frequency of a system of movable charges. Such plasma oscillations do indeed occur in metals where the plasma frequency corresponds to

several electrons volts, depending obviously on the electron density. In Fourier space the above result becomes

$$\rho = \frac{\omega_p^2}{\omega^2}\left(\rho + \rho_{\text{ext.}}\right), \tag{120}$$

which leads to the dielectric constant

$$\varepsilon\left(\omega\right) = 1 - \frac{\omega_p^2}{\omega^2}. \tag{121}$$

A vanishing dielectric constant implies an infinite response to an arbitrarily small ecternal charge density, confirming our expectation that $\omega_p$ is a resonance frequency of the charge density. A natural question arises: Do ions also undergo plasma oscillations? If so it seems to be in conflict with the emergence of acoustic sound modes where the frequency vanishes in the long wavelength limit.

To this end we consider a system that consists of electrons and ions. We write the total induced charge as sum of the charge densitied of both components

$$\rho\left(\mathbf{q},\omega\right) = \rho_e\left(\mathbf{q},\omega\right) + \rho_i\left(\mathbf{q},\omega\right). \tag{122}$$

If we treat the ion dynamics as classical, we use Newton's law

$$M\frac{d^2\mathbf{r}}{dt^2} = e\mathbf{E} \tag{123}$$

and express the veocity of the carriers in terms of the ion-charge current

$$\mathbf{j} = eZn_0\frac{d\mathbf{r}}{dt} \tag{124}$$

which yields

$$M\frac{d\mathbf{j}_i}{dt} = e^2Zn_0\mathbf{E} \tag{125}$$

From the continuity equation of the ion charge and current densities

$$\partial_t\rho_i + \nabla\cdot\mathbf{j}_i = 0 \tag{126}$$

follows in analogy to our earlier calculation

$$\begin{aligned}\frac{\partial^2\rho_i}{\partial t^2} &= -\nabla\cdot\frac{\partial\mathbf{j}_i}{\partial t} = -\frac{e^2Zn_0}{M}\nabla\cdot\mathbf{E}\\ &= -\frac{4\pi Ze^2n_0}{M}\left(\rho_i + \rho_e + \rho_{\text{ext.}}\right)\end{aligned} \tag{127}$$

This corresponds in Fourier space to

$$\rho_i = \frac{\omega_i^2}{\omega^2}\left(\rho_i + \rho_e + \rho_{\text{external}}\right) \tag{128}$$

with the ion-plasma frequency

$$\omega_i = \sqrt{\frac{4\pi Z e^2 n_0}{M}}. \tag{129}$$

The key difference to the case of a single component plasma is that now the dynamic electron charge plays the role of an addition "external" charge. Thus, $\omega_i$ is not necessarily the resonance frequency of the charge distribution.

To address this issue we need to develop a model for the induced electron density. To solve this issue we take advantage of the fact that the on the time scale of the ionic motion, electrons react almost instantaneously. Suppose there is a potential $\phi(\mathbf{r})$, caused by the total electric field $\mathbf{E} = -\nabla\phi$. If this potential varies slowly in space we can assume that it only modified locally the chemical potential

$$\mu \to \mu + e\phi. \tag{130}$$

For a three dimensional gas of free fermions,the electron concentration without potential is related to the Fermi energy according to $n_e(\mu) = C\mu^{3/2}$with constant $C$. More generally we can simply assume some form $n_e(\mu)$ and expand

$$n_e(\mu + e\phi) \approx n_e(\mu) + \kappa e\phi \tag{131}$$

with compressibility

$$\kappa = \frac{\partial n}{\partial \mu}. \tag{132}$$

The induced electron charge is then

$$\begin{aligned} \rho_e &= -\left(e n_e(\mu + e\phi) - e n_e(\mu)\right) \\ &\simeq -\kappa e^2 \phi. \end{aligned} \tag{133}$$

Since

$$\nabla^2\phi = -4\pi\left(\rho_e + \rho_i + \rho_{\text{external}}\right) \tag{134}$$

we obtain yields

$$\nabla^2\rho_e = 4\pi\kappa e^2\left(\rho_e + \rho_i + \rho_{\text{external}}\right) \tag{135}$$

In Fourier space follows

$$\rho_e = -\frac{k_{TF}^2}{q^2}\left(\rho_e + \rho_i + \rho_{\text{external}}\right) \tag{136}$$

where we introduced the Thomas Fermi screening wave number

$$k_{TF}^2 = 4\pi\kappa e^2. \tag{137}$$

If we ignore for the moment the ion charge, it follows $\rho = \rho_e = -\frac{k_{TF}^2}{q^2}\left(\rho + \rho_{\text{ext.}}\right)$ which leads to the dielectric constant

$$\varepsilon(q) = \frac{\rho_{\text{external}}}{\rho + \rho_{\text{external}}} = \frac{k_{TF}^2 + q^2}{q^2} \tag{138}$$

The potential energy of a point charge is affected by this dielectric constant

$$V(q) = \frac{4\pi e^2}{q^2} \rightarrow V_{\text{eff}}(q) = \frac{1}{\varepsilon(q)} \frac{4\pi e^2}{q^2} = \frac{4\pi e^2}{q^2 + k_{TF}^2}, \tag{139}$$

which yields after Fourier transformation

$$V_{\text{eff}}(r) = \frac{e^2}{r} \exp(-k_{TF} r). \tag{140}$$

Thus, the induced charge density in response to a test charge will effectively weaken the Coulomb interaction at long distances. This electrostatic screening effect leads to an effective short range interaction between charges.

The above analysis ignored the inclusion of the ion charge dynamics. However, combining Eq.136 and 127 leads to an dielectric constant

$$\varepsilon(q, \omega) = \frac{\omega^2 \left(k_{TF}^2 + q^2\right) - \omega_i^2 q^2}{\omega^2 q^2} \tag{141}$$

This result combines the static screening of the electron interaction with Thomas Fermi screeniing length in the limit $\omega_i = 0$ (frozen ions) with the plasma edge resonance of ions in the limit $k_{TF} = 0$ (no electrons). However the actual resonance frequency of the combined system results from $\varepsilon(q, \omega) = 0$ and yields

$$\omega_{phon}(q) = \frac{\omega_i}{\sqrt{k_{TF}^2 + q^2}} q \tag{142}$$

which does indeed reproduce the behavior of an acoustic vibration as $q \rightarrow 0$. Thus, in case of the coupled ion-electron systems, the ion plasma frequency is strongly modified by screening due to electrons, leading to acoustic sound.

Finally we can analyze the effective interaction between electrons coupled to dynamic charge distribrutions

$$\begin{aligned} V_{eff}(q, \omega) &= \frac{1}{\varepsilon(q, \omega)} \frac{4\pi e^2}{q^2} \\ &= \frac{4\pi e^2}{k_{TF}^2 + q^2} \frac{\omega^2}{\omega^2 - \omega_{phon}^2(q)} \end{aligned} \tag{143}$$

The crucial aspect of this result is that $V_{eff}(q, \omega)$ changes its sign for $\omega < \omega_{phon}(q)$, i.e. the interaction between equally charged point charges with frequencies below the phonon frequencies is attractive. This is the attractive interaction between electrons that is mediated by phonons. We can also rewrite this result as:

$$V_{\text{eff}}(q, \omega) = \frac{4\pi e^2}{k_{TF}^2 + q^2} \left(1 - \frac{\omega_{phon}^2(q)}{\omega_{phon}^2(q) - \omega^2}\right). \tag{144}$$

The second term is identical to the one we obtained without inclusion of the electron-electron repulsion. The latter adds a positive term yo the effective interaction. The key result that

$$\text{Re} V_{\mathbf{q}}^{\text{eff}}\left(\omega + i0^+\right)\big|_{|\omega| < \omega_{\mathbf{q}}} < 0 \tag{145}$$

is however not affected by the Coulomb interaction. The reason for the surprising result is the retarded, i.e. delayed in time, nature of the interaction induced by electron-phonon coupling.

# 5 The Cooper instability

## 5.1 Two-particle bound states

We consider two particles that interact via an attractive potential $V(\mathbf{r}_1 - \mathbf{r}_2)$ with Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_1} - \frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_2} + V(\mathbf{r}_1 - \mathbf{r}_2)\right)\psi(\mathbf{r}_1\alpha, \mathbf{r}_2\beta) = E\psi(\mathbf{r}_1\alpha, \mathbf{r}_2\beta). \quad (146)$$

The spin wave function of this problem is either singlet or triplet, i.e. we can immediately go into the two-particle spin eigenbasis, labelled by $S$ and $m$, the quantum numbers of the total spin and its $z$-component, respectively. We further consider relative and center of gravity coordinates

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2, \\ \mathbf{R} &= \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \end{aligned} \quad (147)$$

which yields

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2_{\mathbf{R}} - \frac{\hbar^2}{2m_r}\nabla^2_{\mathbf{r}} + V(\mathbf{r})\right)\psi_{S,m}(\mathbf{R}, \mathbf{r}) = E\psi_{S,m}(\mathbf{R}, \mathbf{r}). \quad (148)$$

Here, $m^* = 2m$ is the total mass and $m_r = m/2$ the reduced mass. The center of gravity motion is unaffected by the potential leading to the ansatz

$$\psi_{S,m}(\mathbf{r}_1, \mathbf{r}_2) = \varphi_{S,m}(\mathbf{r})\, e^{i\mathbf{K}\cdot\mathbf{R}}. \quad (149)$$

The wave function it will be even in case of singlet pairing and odd in case of triplet pairing, i.e. $\varphi_{S,m}(\mathbf{r}) = (-1)^S \varphi_{S,m}(-\mathbf{r})$. Let us concentrate of the singlet channel first, i.e. $S = 0$ and $m = 0$. It follows

$$\left(-\frac{\hbar^2}{2m_r}\nabla^2_{\mathbf{r}} + V(\mathbf{r})\right)\varphi(\mathbf{r}) = \widetilde{E}\varphi(\mathbf{r}), \quad (150)$$

where $E = \widetilde{E} + \frac{\hbar^2\mathbf{K}^2}{2m^*}$. Obviously the lowest energy corresponds to the center of gravity momentum $\mathbf{K} = \mathbf{0}$, i.e. the individual momenta of the two particle that scatter are opposite. For $\mathbf{K} = \mathbf{0}$ we have $E = \widetilde{E}$.

It is useful to Fourier transform this equation with $\varphi(\mathbf{k}) = \int d^3r \varphi(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}}$ which yields

$$\int V(\mathbf{k} - \mathbf{k}')\varphi(\mathbf{k}')\frac{d^dk}{(2\pi)^d} = (E - 2\varepsilon_{\mathbf{k}})\varphi(\mathbf{k}), \quad (151)$$

where $\varepsilon_{\mathbf{k}} = \frac{\hbar^2}{2m}\mathbf{k}^2$ is the energy of a single free electron. This yields with $\Delta(\mathbf{k}) = (E - 2\varepsilon_{\mathbf{k}})\varphi(\mathbf{k})$ the equation

$$\Delta(\mathbf{k}) = -\int \frac{V(\mathbf{k}-\mathbf{k}')}{2\varepsilon_{\mathbf{k}'} - E}\Delta(\mathbf{k}')\frac{d^d k}{(2\pi)^d}. \tag{152}$$

A bound state occurs if $E < 2\varepsilon_{\mathbf{k}'}$.

Eq.150 and therefore the equivalent Eq.152 are identical to the Schrödinger equation of a single particle with potential $V(\mathbf{r})$. Suppose we have an attractive potential $V(\mathbf{r}) = -V_0$ for $|\mathbf{r}| < a$. It is known that for $d = 3$ the amplitude $V_0$ of the attractive potential must exceed the energy $\simeq \hbar^2/(2ma^2)$. Only then will a bound state form. In case of a many fermion system, states with momenta below the Fermi energy are all occupied and the integration over momenta starts with a magnitude $|\mathbf{k}| = k_F$ instead of $|\mathbf{k}| = 0$. Assuming for example that

$$V(\mathbf{k}-\mathbf{k}') = \begin{cases} -V_0 & |\varepsilon_{\mathbf{k}} - \varepsilon_F|, |\varepsilon_{\mathbf{k}'} - \varepsilon_F| < \omega_D \\ 0 & \text{otherwise} \end{cases}. \tag{153}$$

This yields in case of a constant $\Delta(\mathbf{k}) = \Delta$ (necessarily implying singlet pairing) that

$$\begin{aligned} \Delta &= \Delta V_0 \rho_F \int_{\varepsilon_F}^{\varepsilon_F + \omega_D} \frac{d\varepsilon'}{2\varepsilon' - E} \\ &= \Delta \frac{V_0 \rho_F}{2} \log\left(\frac{2\varepsilon_F - E}{2(\varepsilon_F + \omega_D) - E}\right). \end{aligned} \tag{154}$$

In the limit of small $\lambda = V_0\rho_F$ where $E$ must be close to $2\varepsilon_F$, the solution is

$$E = 2\varepsilon_F - 2\omega_D e^{-\frac{2}{\lambda}}, \tag{155}$$

which yields the binding energy

$$\varepsilon_b = 2\omega_D e^{-\frac{2}{\lambda}}. \tag{156}$$

To stress the distinction between the bound state formation in free space and with filled Fermi see once again, we go back to Eq.152 and vary the chemical potential:

$$\Delta = \Delta V_0 \int_{\varepsilon_F}^{\varepsilon_F + \omega_0} \frac{\rho(\varepsilon)}{2\varepsilon - E}\, d\varepsilon. \tag{157}$$

If indeed $\varepsilon_F \to 0$ it is not anymore allowed to approximate the density of states $\rho(\varepsilon)$ by a constant value at the Fermi level. One has to include the variation $\rho(\varepsilon) = A\sqrt{\varepsilon}$ near the band edge. In case of an empty Fermi see with $\varepsilon_F = 0$ we have

$$\Delta = \Delta V_0 A \int_0^{\omega_0} \frac{\sqrt{\varepsilon}}{2\varepsilon + \varepsilon_b}\, d\varepsilon. \tag{158}$$

As the integral is no longer divergent at the lower limit and for $\varepsilon_b \to 0$, we are back to the original result that one needs to have a threshold strength for the

potential $V_0$ to form a bound state. We conclude that the Cooper instability for infinitesimal interaction $V_0$ is a consequence of the fact that the number of low energy states is enhanced in case of a Fermi surface.

Finally we comment on the impact of a finite center of gravity momentum $\mathbf{K}$, that is naturally associated with a finite current density

$$j = \frac{n_e e\hbar}{m} |\mathbf{K}|, \tag{159}$$

where $n_e$ is the electron density and $\hbar |\mathbf{K}| /m$ the velocity of the pair. Repeating the above analysis for finite $\mathbf{K}$, it follows for the total energy

$$E = 2\varepsilon_F - \varepsilon_b + \frac{\hbar^2 \mathbf{K}^2}{2m^*} \tag{160}$$

with $\varepsilon_b$ of Eq.156. To get a bound state at finite current, it must hold that $E < 2\varepsilon_F$, which leads to the appearance of a critical current

$$j_c = 2n_e e\sqrt{\frac{\varepsilon_b}{m}}, \tag{161}$$

which is of the same order of magnitude as the result that follows from, BCS theory.

## 5.2 Instabilities of weakly interacting fermions

The analysis of the previous section revealed that there seems to be an instability of the Fermi surface with respect to a weak attractive interaction between fermions. For simplicity, we consider a model with weak attraction governed by the model Hamiltonian

$$\begin{aligned} H &= \sum_\alpha \int d^d r \psi_\alpha^\dagger (\mathbf{r}) \left( -\frac{\nabla^2}{2m} - \mu \right) \psi_\alpha (\mathbf{r}) \\ &- \int d^d r \psi_\uparrow^\dagger (\mathbf{r}) \psi_\downarrow^\dagger (\mathbf{r}) \psi_\downarrow (\mathbf{r}) \psi_\uparrow (\mathbf{r}) . \end{aligned} \tag{162}$$

We will see that the analysis of this continuum's model is ill defined without proper regularization. Therefore we consider a model where we restricts ourselves to an effective low energy theory, i.e. we consider a system where the fermionic excitations are confined to an energy scale $\pm\Lambda$ around the Fermi energy. We explore the behavior of this toy model.

In our Hamiltonian it suffices to consider a singlet wave function and to focus on $\mathbf{r}_1 = \mathbf{r}_2$ and $\mathbf{r}_1' = \mathbf{r}_2'$, i.e. we analyze the pairing susceptibility.

$$\chi (\mathbf{r}, \mathbf{r}', t) = -i\theta (t) \left\langle \left[ \psi_\uparrow^\dagger (\mathbf{r}, t) \psi_\downarrow^\dagger (\mathbf{r}, t), \psi_\downarrow (\mathbf{r}', 0) \psi_\uparrow (\mathbf{r}', 0) \right]_- \right\rangle . \tag{163}$$

Fourier transformation and Wick rotation to the imaginary time axis yields

$$\chi (\mathbf{r}, \mathbf{r}', \tau) = - \left\langle T_\tau \psi_\uparrow^\dagger (\mathbf{r}, \tau) \psi_\downarrow^\dagger (\mathbf{r}, \tau) \psi_\downarrow (\mathbf{r}', 0) \psi_\uparrow (\mathbf{r}', 0) \right\rangle . \tag{164}$$

In what follows we analyze this pairing susceptibility.

We first analyze the pair susceptibility of non-interacting electrons. The Fourier transform in momentum and frequency space is then given as

$$\chi_0\left(\mathbf{q}, i\nu_m\right) = T\sum_n \int \frac{d^dk}{\left(2\pi\right)^d} G_{\mathbf{k}}\left(i\omega_n\right) G_{-\mathbf{k}+\mathbf{q}}\left(-i\omega_n + i\nu_m\right), \tag{165}$$

where $\nu_m = 2m\pi T$ and $\omega_n = \left(2n+1\right)\pi T$ are bosonic and fermionic Matsubara frequencies, respectively.

$$G_{\mathbf{k}}\left(i\omega_n\right) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} \tag{166}$$

is the bare fermionic Green's function and $\epsilon_{\mathbf{k}} = \frac{k^2}{2m} - \mu$. Since we suspect that superconductivity is a homogeneous instability, without spatial and temporal modulations, we consider the limit $\mathbf{q} = 0$ and $\omega_n = 0$. It follows

$$\begin{aligned} \chi_0\left(T\right) &= T\sum_m \int \frac{d^dk}{\left(2\pi\right)^d} \frac{1}{\omega_n^2 + \epsilon_{\mathbf{k}}^2} \\ &= T\sum_m \int d\epsilon \frac{\rho\left(\epsilon\right)}{\omega_n^2 + \epsilon^2}, \end{aligned} \tag{167}$$

with density of states

$$\rho\left(\omega\right) = \int \frac{d^dk}{\left(2\pi\right)^d} \delta\left(\omega - \epsilon_{\mathbf{k}}\right). \tag{168}$$

We perform the Matsubara frequency sum and obtain

$$\chi_0\left(T\right) = \int_{-\infty}^{\infty} d\epsilon \frac{\rho\left(\epsilon\right)}{2\epsilon} \tanh\left(\frac{\epsilon}{2T}\right). \tag{169}$$

This expression makes evident that some appropriate cut off procedure is required to analyze the pairing susceptibility. While the above integral is well defined for any lattice model of a solid, where the density of states of individual bands has some upper and lower cut off, the continuum's theory diverges at the upper cut off. As mentioned above, an appropriate approach is to define the theory in an energy window $[\mu - \Lambda, \mu + \Lambda]$ around the Fermi energy and assume that the density of states is constant in this window. Then we have to evaluate:

$$\chi_0\left(T\right) = \rho_F \int_{-\Lambda}^{\Lambda} d\epsilon \frac{1}{2\epsilon} \tanh\left(\frac{\epsilon}{2T}\right). \tag{170}$$

We perform the integration to leading logarithmic accuracy:

$$\begin{aligned} \int_{-\Lambda}^{\Lambda} \frac{\tanh\left(\frac{\varepsilon}{2T}\right)}{2\varepsilon} d\varepsilon &= \int_0^{\beta\Lambda/2} \frac{\tanh\left(x\right)}{x} dx \\ &= -\int_0^{\beta\Lambda/2} \frac{\log\left(x\right)}{\cosh^2\left(x\right)} dx + \tanh\left(x\right)\log x\Big|_0^{\beta\Lambda/2} \end{aligned}$$

$$
\begin{aligned}
&= \gamma_E - \log\frac{\pi}{4} + \log\left(\frac{\Lambda}{2T}\right) + \mathcal{O}\left(\frac{T}{\Lambda}\right) \\
&= \log\left(\frac{2\Lambda e^{\gamma_E}}{\pi T}\right) + \mathcal{O}\left(\frac{T}{\Lambda}\right). \qquad (171)
\end{aligned}
$$

We obtain for the pairing susceptibility of a free electron gas

$$
\chi_0(T) = \rho_F \log\left(\frac{2\Lambda e^{\gamma_E}}{\pi T}\right).
$$

For any finite temperature the free electron pairing-susceptibility is finite. However the logarithmic increase of $\chi_0(T)$ for $T \to 0$ already indicates that a Fermi gas becomes increasingly susceptible if one adds an external pairing source $\eta_{\alpha\beta} = \eta_s i\sigma^y_{\alpha\beta}$.

Next we include electron-electron interactions. To this extend we sum ladder diagrams for the pairing susceptibility.

## 5.3 renormalization group approach

A more systematic expansion that demonstrated that the summation of ladder diagrams includes indeed the most dominant terms can be done in terms of a renormalization group calculation. We start the analysis from the action

$$
S = S_0 + S_{\text{int}} \qquad (172)
$$

that determines the partition function $Z = \int D\psi^\dagger D\psi e^{-S}$. The bare action is given as

$$
S_0 = \int_k^\Lambda \psi^\dagger_{k\alpha}\left(i\omega_n + \mu - \epsilon_{\mathbf{k}}\right)\psi_{k\alpha}, \qquad (173)
$$

where $k = (\omega_n, \mathbf{k})$ with fermionic Matsubara frequency $\omega_n = (2n+1)\pi T$ and momentum $\mathbf{k}$. $v_F\Lambda$ corresponds to an energy cut off such that only states with $|\epsilon_{\mathbf{k}} - \mu| < v_F\Lambda$ are included in the theory. $v_F$ is the Fermi velocity. For the interaction we write generally

$$
S_{\text{int}} = -\frac{1}{4}\int_{k_i}^\Lambda \psi^\dagger_{k_1\alpha}\psi^\dagger_{k_2\beta}\psi_{k_3\gamma}\psi_{k_4\delta}U^{\alpha\beta}_{\gamma\delta}(k_i)\,\delta(k_1 + k_2 - k_3 - k_4). \qquad (174)
$$

In case of $SU(2)$-invariance of the four-fermion interaction we can split it in a charge and spin contribution

$$
U^{\alpha\beta}_{\gamma\delta} = U_{ch}\delta_{\alpha\delta}\delta_{\beta\gamma} + U_{sp}\boldsymbol{\sigma}_{\alpha\beta}\cdot\boldsymbol{\sigma}_{\gamma\delta} \qquad (175)
$$

However, the usual antisymmetry of the interaction

$$
\begin{aligned}
U^{\alpha\beta}_{\gamma\delta}(k_1,k_2,k_3,k_4) &= -U^{\beta\alpha}_{\gamma\delta}(k_2,k_1,k_3,k_4) \\
&= -U^{\alpha\beta}_{\delta\gamma}(k_1,k_2,k_4,k_3) \qquad (176)
\end{aligned}
$$

makes it more efficient to split the interaction according to

$$U_{\gamma\delta}^{\alpha\beta} = U^A I_{\gamma\delta}^{\alpha\beta} + U^S T_{\gamma\delta}^{\alpha\beta} \tag{177}$$

where

$$\begin{aligned} I_{\gamma\delta}^{\alpha\beta} &= \delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta} \\ T_{\gamma\delta}^{\alpha\beta} &= \delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}. \end{aligned} \tag{178}$$

Now, $U^A$ is antisymmetric upon exchanging $k_1$ with $k_2$ or $k_3$ with $k_4$, while $U^S$ is symmetric.

We first perform a tree level analysis of the non-interacting part of the action. Integrating out states in the shells with $\Lambda/b < |\epsilon_{\mathbf{k}} - \mu| / v_F < \Lambda$ yields for the remaining low energy states

$$S_0^< = \int_k^{\Lambda/b} \psi_{k\alpha}^\dagger \left(i\omega_n + \mu - \epsilon_{\mathbf{k}}\right) \psi_{k\alpha}, \tag{179}$$

We linearize the fermion spetrum $\epsilon_{\mathbf{k}} = \mathbf{v}_{\mathbf{k}_F} \cdot (\mathbf{k} - \mathbf{k}_F)$ where $\mathbf{k}_F(\theta, \varphi)$ parametrizes the Fermi surface. In what follows we consider a spherical Fermi surface. Let $\mathbf{n} = \mathbf{v}_{\mathbf{k}_F}/v_F$ be the unit vector in the direction of $\mathbf{k}_F$ and

$$\mathbf{k} = (k_F + p)\, \mathbf{n}_i + \mathbf{k}_\perp, \tag{180}$$

where $\mathbf{k}_\perp$ refers to the momentum component perpendicular to $\mathbf{n}_i$. Then we have

$$\epsilon_{\mathbf{k}} = vp. \tag{181}$$

Rescaling $p' = bp$, $T' = bT$, $\mu' = b\mu$ and

$$\psi_{p\alpha} = b^{3/2} \psi'_{p'\alpha} \tag{182}$$

we obtain the original action in terms of the new, rescaled variables:

$$\begin{aligned} \int_k^\Lambda f_k &= T \sum_n \int \frac{d^d k}{(2\pi)^d} \theta\left(v_F\Lambda - |\epsilon_{\mathbf{k}} - \mu|\right) f\left(\mathbf{k}, \omega_n\right) \\ &= T \sum_n \int \frac{dn_d k^{d-1} dk}{(2\pi)^d} \theta\left(v_F\Lambda - |\epsilon_{\mathbf{k}}|\right) f\left(\mathbf{k}, \omega_n\right) \\ &\approx T k_F^{d-1} \sum_n \int \frac{dn_d dp}{(2\pi)^d} \theta\left(\Lambda - p\right) f\left(\mathbf{n}_d, p, \omega_n\right), \end{aligned} \tag{183}$$

To obtain this result we used that $\Lambda \ll k_F$ such that only the radial contribution of the fermion momenta enter the power counting in the integration.

Next we analyze the tree level scaling of the electron-electron interaction. We write again

$$\mathbf{k}_i = (k_F + p_i)\, \mathbf{n}_i \tag{184}$$

where the unit vector sets the direction of the momenta. Momentum conservation implies

$$(k_F + p_1)\,\mathbf{n}_1 + (k_F + p_2)\,\mathbf{n}_2 = (k_F + p_3)\,\mathbf{n}_3 + (k_F + p_4)\,\mathbf{n}_4 \tag{185}$$

At some late stage of the renormalization procedure the $p_i$ will be negligible compared to $k_F$. Then we have the constraint

$$\mathbf{n}_1 + \mathbf{n}_2 = \mathbf{n}_3 + \mathbf{n}_4. \tag{186}$$

Consider a two-dimensional system where $\mathbf{n}_i = (\cos\theta_i, \sin\theta_i)$. It follows that for two vectors $\mathbf{n}_1$ and $\mathbf{n}_2$, which do not point in opposite directions, that either $\mathbf{n}_1 = \mathbf{n}_3$ and $\mathbf{n}_2 = \mathbf{n}_4$ or $\mathbf{n}_1 = \mathbf{n}_4$ and $\mathbf{n}_2 = \mathbf{n}_3$. If, on the other hand, $\mathbf{n}_1 = -\mathbf{n}_2$, then follows $\mathbf{n}_3 = -\mathbf{n}_4$.

As was pointed out by Shankar, a technical subtlety occurs if one wants to enforce the $\delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)$ constraint in a way that all four momenta are in the shell around the Fermi surface. In order to deal with this a soft cut off

$$\theta(\Lambda - p_4) \to e^{-|p_4|/\Lambda} \tag{187}$$

can be used. Thus, we write for the interaction

$$S_{\text{int}} - \frac{1}{4}\int_{k_1 k_2 k_3}^{\Lambda} \psi^{\dagger}_{k_1\alpha}\psi^{\dagger}_{k_2\beta}\psi_{k_3\gamma}\psi_{k_4\delta}U^{\alpha\beta}_{\gamma\delta}(k_i)\, e^{-|p_4|/\Lambda}, \tag{188}$$

where

$$p_4 = |k_F(\mathbf{n}_1 + \mathbf{n}_2 - \mathbf{n}_3) + p_1\mathbf{n}_1 + p_2\mathbf{n}_2 - p_3\mathbf{n}_3| - k_F. \tag{189}$$

Tus, upon rescaling holds

$$p_4 = b^{-1}\left(|bk_F(\mathbf{n}_1 + \mathbf{n}_2 - \mathbf{n}_3) + p_1'\mathbf{n}_1 + p_2'\mathbf{n}_2 - p_3'\mathbf{n}_3| - bk_F\right) \tag{190}$$

The momentum $p_4$ behaves properly if $p_4 = b^{-1}p_4'$. To avoid that the Fermi momentum diverges as $b$ grows, we find that only scattering processes with

$$|\mathbf{n}_1 + \mathbf{n}_2 - \mathbf{n}_3| = 1 \tag{191}$$

contribute, which is precisely what we already discussed above. The formal rescaling procedure now yields

$$U^{\alpha\beta}_{\gamma\delta}(\mathbf{k}_i.\omega_i) \to e^{-(b-1)\frac{k_F}{\Lambda}||\mathbf{n}_1+\mathbf{n}_2-\mathbf{n}_3|-1|}U^{\alpha\beta}_{\gamma\delta}(\mathbf{k}_i'.\omega_i'). \tag{192}$$

Thus, we can confine ourselves to the following cases:

$$\Phi^{A(S)}(\mathbf{n}_1, \mathbf{n}_2) = \rho_F U^{A(S)}(\mathbf{n}_1, \mathbf{n}_2; \mathbf{n}_1, \mathbf{n}_2) \tag{193}$$

which due to the antisymmetry (symmetry) of the interaction takes simultaneously care of $\mathbf{n}_1 = \mathbf{n}_3$ and $\mathbf{n}_2 = \mathbf{n}_4$ as well as $\mathbf{n}_1 = \mathbf{n}_4$ and $\mathbf{n}_2 = \mathbf{n}_3$. In addition we must consider

$$V^{A(S)}(\mathbf{n}_1, \mathbf{n}_3) = \rho_F U^{A(S)}(\mathbf{n}_1, -\mathbf{n}_1; \mathbf{n}_3, -\mathbf{n}_3). \tag{194}$$

The functions $\Phi^{S,A}$ and $V^{S,A}$ depend only on twho unit vectors. In case of a spherical Fermi surface they will then only depend on the angles $\theta = \arccos(\mathbf{n}_1 \cdot \mathbf{n}_2)$ and $\theta = \arccos(\mathbf{n}_1 \cdot \mathbf{n}_3)$, depending on whether we consider $\Phi$ or $V$. It is interesting to analyze the implications of antisymmetry of the interactions. In case of $V$ follows

$$V^{S,A}(\theta \pm \pi) = \pm V(\theta), \tag{195}$$

while for the coupling constant $\Phi$ holds

$$\Phi^{S,A}(-\theta) = \pm \Phi^{S,A}(\theta). \tag{196}$$

We can expand both functions according to

$$f(\theta) = \sum_{m=-\infty}^{\infty} e^{-im\theta} f_m \tag{197}$$

and obtain from the antisymmetry conditions that $\Phi_m^{S,A} = \pm \Phi_{-m}^{S,A}$ while for the interaction $V$ follows that $V_m^S = 0$ if $m$ is odd and $V_m^A = 0$ if $m$ is even.

The one loop correction of a generic fermionic theory is

$$\begin{aligned}
\Gamma_{\gamma\delta}^{\alpha\beta}(k_1,k_2,k_3,k_4) &= U_{\gamma\delta}^{\alpha\beta}(k_1,k_2,k_3,k_4) \\
&- \sum_{\sigma\sigma'} \int_{k_5 k_6} \Big( U_{\gamma\sigma}^{\alpha\sigma'}(k_1,k_5,k_3,k_6) U_{\sigma'\delta}^{\sigma\beta}(k_6,k_2,k_5,k_4) \\
&- U_{\gamma\sigma}^{\beta\sigma'}(k_2,k_5,k_3,k_6) U_{\sigma'\delta}^{\sigma\alpha}(k_6,k_1,k_5,k_4) \\
&- \frac{1}{2} U_{\sigma\sigma'}^{\alpha\beta}(k_1,k_2,k_6,k_5) U_{\gamma\delta}^{\sigma\sigma'}(k_6,k_5,k_3,k_4) \Big) G_{k_5} G_{k_6}
\end{aligned}$$

To proceed, we first ignore the spin indices and analyze the phase space of the various terms and how they contribute to the renormalization of the coupling functions $V$ and $\Phi$.

Let us first analyze contibutions to $\Phi(\mathbf{n}_1, \mathbf{n}_2)$. It holds

$$\delta\Phi(\mathbf{n}_1,\mathbf{n}_2) = -\frac{1}{\rho_F} \lim_{q\to 0} \int_k^> \Phi(\mathbf{n}_1,\mathbf{n}) \Phi(\mathbf{n},\mathbf{n}_2) G(k) G(k+q) \tag{198}$$

Here, we need to properly take the limit $q \to 0$, where $q = k_1 - k_3$. In other words, it is not possible to simply take the limit $k_1 = k_3$. Before we analyze this further, let us first discuss why only the first of the three diagrams contributes to the renormalization of $\Phi$. If we insert $\mathbf{k}_3 = \mathbf{k}_1$ and $\mathbf{k}_4 = \mathbf{k}_2$ in the second and third term, only very special configurations of the direction of the running momentum will yield the coupling constants $\Phi$ or $V$. Those contributions are of order $l^2$ and will be neglected if compared to terms of order $l$ that emerge from the term above. Let us now evaluate the integral

$$\int_k^> \cdots = T k_F^{d-1} \sum_n \int \frac{dn_d}{(2\pi)^d} \left( \int_{-\Lambda}^{-\Lambda/b} dk \cdots + \int_{\Lambda/b}^{\Lambda} dk \cdots \right) \tag{199}$$

The Matsubara sum yields

$$T\sum_n \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} \frac{1}{i\omega_n + i\Omega_m - \epsilon_{\mathbf{k}}} = \frac{1}{2} \frac{\tanh\left(\frac{\epsilon_{\mathbf{k}}}{2T}\right) - \tanh\left(\frac{\epsilon_{\mathbf{k}+\mathbf{q}}}{2T}\right)}{\epsilon_k - \epsilon_{k+q} + i\Omega_m}. \tag{200}$$

Now it becomes evident that the sum vanishes if one takes the limit $\mathbf{q} \to 0$ before the limit $\Omega_m \to 0$, while it is finite in the opposite limit. We consider the latter case. It follows

$$\delta\Phi\left(\mathbf{n}_1, \mathbf{n}_2\right) = -\frac{\beta l}{\cosh^2\left(\frac{1}{2}\beta v\Lambda\right)} \int \frac{d^2n}{2\pi} \Phi\left(\mathbf{n}_1, \mathbf{n}\right) \Phi\left(\mathbf{n}, \mathbf{n}_2\right). \tag{201}$$

The flow equation can be solved in one takes into account that $\Phi(\theta)$ only depends on the angle between the two unit vectors. Expanding

yields

$$\frac{d\Phi_m}{dl} = \frac{\frac{1}{2}v\Lambda\beta}{\cosh^2\left(\frac{1}{2}\beta v\Lambda\right)} \Phi_m^2 \tag{202}$$

The flow equation for the inverse temperature is still

$$\frac{d\beta}{dl} = -\beta \tag{203}$$

Introducing the variable $\tau = \tanh\left(\frac{1}{2}\beta v\Lambda\right)$ we can write the flow equation as

$$\frac{d\Phi_m}{d\tau} = -\Phi_m^2. \tag{204}$$

Let us now return to the spinful case:

We use the identities

$$\begin{aligned} I^{\alpha\sigma'}_{\gamma\sigma} I^{\sigma\beta}_{\sigma'\delta} &= \frac{5}{2} I^{\alpha\beta}_{\gamma\delta} - \frac{3}{2} T^{\alpha\beta}_{\gamma\delta} \\ I^{\alpha\sigma'}_{\gamma\sigma} T^{\sigma\beta}_{\sigma'\delta} &= -\frac{1}{2} I^{\alpha\beta}_{\gamma\delta} + \frac{3}{2} T^{\alpha\beta}_{\gamma\delta} \\ T^{\alpha\sigma'}_{\gamma\sigma} T^{\sigma\beta}_{\sigma'\delta} &= \frac{1}{2} I^{\alpha\beta}_{\gamma\delta} + \frac{1}{2} T^{\alpha\beta}_{\gamma\delta} \end{aligned}$$

and the properties

$$\begin{aligned} I^{\alpha\beta}_{\mu\nu} I^{\nu\mu}_{\gamma\delta} &= 2 I^{\alpha\beta}_{\gamma\delta} \\ T^{\alpha\beta}_{\mu\nu} T^{\nu\mu}_{\gamma\delta} &= -2 T^{\alpha\beta}_{\gamma\delta} \\ T^{\alpha\beta}_{\mu\nu} I^{\nu\mu}_{\gamma\delta} &= 0 \end{aligned}$$

and obtain

$$\frac{d\Phi_m^{A,S}}{dl} = \frac{\frac{1}{2}v\Lambda\beta}{\cosh^2\left(\frac{1}{2}\beta v\Lambda\right)} P_m^{A,S}$$

where

$$\begin{aligned} P_m^A &= 3\left(\Phi_m^A\right)^2 - 2\Phi_m^S\Phi_m^A + \left(\Phi_m^S\right)^2 \\ P_m^S &= -2\left(\Phi_m^A\right)^2 + 4\Phi_m^S\Phi_m^A \end{aligned} \tag{205}$$

The most efficient way to folve these equations is by introducing

$$\begin{aligned} F^{sp,ch} &= 2\Phi^S - 4\Phi^A \\ F^{sp,ch} &= -\Phi^S - \Phi^A \end{aligned} \tag{206}$$

which leads to the flow equations

$$\frac{dF^{sp,ch}}{d\tau} = \left(F^{sp,ch}\right)^2. \tag{207}$$

The solution is

$$F^{sp,ch}(\tau) = \frac{F_0^{sp,ch}}{1-(\tau-\tau_0)F_0^{sp,ch}}, \tag{208}$$

where $\tau_0 = \tanh\left(\frac{1}{2}\beta v\Lambda\right)$ and $\tau = \tanh\left(\frac{1}{2}\beta e^{-l}v\Lambda\right)$. If we send $l \to \infty$ it holds that $\tau \to 0$ and the coupling constants approach finite fixed point values

$$F_*^{sp,ch}(T) = \frac{F_0^{sp,ch}}{1+\tau_0 F_0^{sp,ch}}. \tag{209}$$

If we now take the limit $T \to 0$, we find that

$$F_*^{sp,ch}(T \to 0) = \frac{F_0^{sp,ch}}{1+F_0^{sp,ch}}. \tag{210}$$

Thus, as long as $F_0^{sp,ch} > -1$ the fixed pint value of the interaction is finite. Most important for pour consideration is that there is no coupling between the coupling constants $\Phi$ and $V$.

Let is now analyze the couplings $V^S$and $V^A$. Only the BCS-type diagram (the last term in the above expression for $\Gamma$) will contribute to the renormalization of this interaction. The Matsubara sum yields

$$T\sum_n \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}}\frac{1}{-i\omega_n - \epsilon_{\mathbf{k}}} = \frac{\tanh\left(\frac{\epsilon_{\mathbf{k}}}{2T(l)}\right)}{2\epsilon_k} \tag{211}$$

and it follows

$$\delta V^{A,S}(\mathbf{n}_1,\mathbf{n}_2) = \pm\tanh\left(\frac{\beta(l)v\Lambda}{2}\right) l\int\frac{d^2n}{2\pi}V^{A,S}(\mathbf{n}_1,\mathbf{n})V^{A,S}(\mathbf{n},\mathbf{n}_2) \tag{212}$$

This yields the flow equation

$$\begin{aligned}\frac{dV_m^A(l)}{dl} &= \tanh\left(\frac{\beta(l)v\Lambda}{2}\right)\left(V_m^A(l)\right)^2 \\ \frac{dV_m^S(l)}{dl} &= -\tanh\left(\frac{\beta(l)v\Lambda}{2}\right)\left(V_m^S(l)\right)^2\end{aligned} \tag{213}$$

Of course we have to keep in mind that $V_m^A$ is only finite if $m$ is odd and $V_m^S$ finite if $m$ is even, as follows from the antisymmetry of the four particle interaction. The corresponding flow equation for the inverse temperature is, of course,

$$\frac{d\beta(l)}{dl} = -\beta(l). \tag{214}$$

The solution of these flow equations are

$$V_m^{A,S}(l) = \frac{V_m^{A,S(0)}}{1 \mp V_m^{A,S(0)} \int_0^l \tanh\left(\frac{1}{2}\beta v\Lambda e^{-l'}\right) dl'}. \tag{215}$$

Thus, we find that for $V_m^A < 0$ or $V_m^S > 0$ areduced, renormalized coupling constant occurs for increasing flow variable $l$. On the opther hand, we find that for $V_m^A > 0$ or $V_m^S < 0$ the coupling constant grows and a divergent renormalized coupling constant occurs when the denominator vanishes. The highest temperature $T_c = \beta_c^{-1}$ where the divergence happens is determined by the condition

$$\frac{1}{\lambda_m} \equiv \frac{1}{\left|V_m^{A,S(0)}\right|} = \int_0^\infty \tanh\left(\frac{1}{2}\beta_c v\Lambda e^{-l'}\right) dl', \tag{216}$$

where the flow goes all the way to infinity and the contribution of the intagral becomes largest. Introducing $x = \frac{1}{2}\beta_c v\Lambda e^{-l}$ the integral can also be written as

$$\begin{aligned}\int_0^\infty \tanh\left(\frac{1}{2}\beta_c v\Lambda e^{-l'}\right) dl' &= \int_0^{\beta_c\Lambda/2} \frac{\tanh(x)}{x} dx \\ &= \log\left(\frac{2v\Lambda e^{\gamma_E}}{\pi T_c}\right) + \mathcal{O}\left(\frac{T}{\Lambda}\right),\end{aligned} \tag{217}$$

where we used our earlier result, already obtained in the context of the superconducting susceptibility. As a result we obtain the condition for the instability temperature

$$T_c = \frac{2e^{\gamma_E}}{\pi} v\Lambda e^{-\frac{1}{\lambda_m}}. \tag{218}$$

Thus we find that the instability occurs for the largest $\left|V_m^{A,S(0)}\right|$ which then determines whether we have singlet ($m$ even) or triplet ($m$ odd) pairing. Most importantly, we established that in case of a spherical Fermi surface, it is sufficient to sum up ladder diagrams if one wants to determine the Cooper instability.

Other diagrams do not lead to a renormalization of the pairing interaction. This behavior will be different if we consider non-generic Fermi surfaces.

Our renormalization groupo analysis was performed at finite temperatures. Sometimes it is more convenient to set $T = 0$ and then analyze the simplified flow equations

$$\frac{dV_m^{A,S}}{dl} = \pm \left(V_m^{A,S}\right)^2 \tag{219}$$

with solution

$$V_m^{A,S}(l) = \frac{V_m^{A,S(0)}}{1 \mp V_m^{A,S(0)} l}. \tag{220}$$

Now the coupling constant diverges at a scale $l_c = \frac{1}{\lambda_m}$ and one can estimate the transition temperature via $l_c = \log \frac{v\Lambda}{T_c}$ which gives the correct behavior, except for the numerical prefactor in front of the $e^{-1/\lambda_m}$ term.

There is an interessting application of this approach that allows to simultaneously include a repulsive interaction at high energies and an attractive interaction at lower energies, as was found earlier in our analysis of the electron-phonon coupling with screened electron-electron interaction. Thus, we consider a repulsive interaction for all energies up to the Fermi energy:

$$V_{rep} = \mu > 0, \tag{221}$$

and an additional attractive interaction for energies below the Debye energy $\omega_D$

$$V_{attr.} = -\lambda < 0. \tag{222}$$

Since we consider angular independent interactions, we only have the coupling in the $m = 0$ channel. If we now perform the RG decimation of states between $\omega_D$ and $E_F$ then only the repulsive part of the interaction is affected by our analysis and we obtain at the scale $l^* = \log \frac{E_F}{\omega_D}$ the result

$$\mu \to \mu^* = \frac{\mu}{1 + \mu l^*} = \frac{\mu}{1 + \mu \log \frac{E_F}{\omega_D}}. \tag{223}$$

The subsequent flow starts therefore with an effective coupling constant

$$\lambda_{\text{eff}} = \lambda - \mu^*. \tag{224}$$

If $\lambda_{\text{eff}} > 0$ we have a net attractive interaction at the scale $\omega_D$ and can continue our analysis with the initial coupling constant $\lambda_{\text{eff}}$ and with a cut-off scale $\omega_D$. Thus, we obtain

$$\begin{aligned} T_c &= \frac{2e^{\gamma_E}}{\pi} \omega_D e^{-\frac{1}{\lambda_{\text{eff}}}} \\ &= \frac{2e^{\gamma_E}}{\pi} \omega_D e^{-\frac{1}{\lambda - \mu^*}}. \end{aligned} \tag{225}$$

This analysis demonstrates, that for $E_F \gg \omega_D$, the reduction of a repulsive interaction at high energies can be significant. The net interaction at low energies is attractive as long as $\lambda > \mu^*$, even if $\mu > \lambda$, i.e. the bare interaction is repulsive all the way down to lowest energies.

# Part III
# BCS theory

## 6 The BCS ground-state

The BCS theory gives an answer to the open question that emerges as consequence of the Cooper instability: What happens with an entire Fermi-sea of attractively interacting electrons? Based on the insight that the leading instability occurs at zero center of mass momentum we model the attractive interaction between electrons, mediated by phonons via he BCS or pairing Hamiltonian:

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{V_0}{N} \sum_{\mathbf{k},\mathbf{k}'} \gamma_{\mathbf{k},\mathbf{k}'}\, c^\dagger_{\mathbf{k}',\uparrow}\, c^\dagger_{-\mathbf{k}',\downarrow}\, c_{-\mathbf{k},\downarrow}\, c_{\mathbf{k},\uparrow} \tag{226}$$

It consists of the usual kinetic energy with band dispersion

$$\varepsilon_{\mathbf{k}} = \frac{k^2}{2m} - \mu \tag{227}$$

and an interaction term. The choice of the parabolic spectrum is for specificity. The subsequent analysis will reveal that it is trivial to generalize the approach to different dispersions. The sign in front of the interaction $V_0$ was chosen such that $V_0 > 0$ corresponds to an attractive coupling. The matrix element

$$\gamma_{\mathbf{k},\mathbf{k}'} = \begin{cases} 1 & |\varepsilon_{\mathbf{k}}|, |\varepsilon_{\mathbf{k}'}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

takes into account that only fermionic states that have energies relative to the Fermi energy below the phonon frequency interact.

### 6.1 Mean field theory and ground state energy

To find an approximate solution of this problem we perform the Hartree-Fock decoupling

$$AB = (A - \langle A\rangle)(B - \langle B\rangle) + A\langle B\rangle + B\langle A\rangle - \langle A\rangle\langle B\rangle \tag{228}$$

with

$$\begin{aligned} A &= c^\dagger_{\mathbf{k}',\uparrow}\, c^\dagger_{-\mathbf{k}',\downarrow} \\ B &= c_{-\mathbf{k},\downarrow}\, c_{\mathbf{k},\uparrow}. \end{aligned} \tag{229}$$

This choice for $A$ and $B$ is motivated by the expectation, that $\langle A\rangle \neq 0$ and $\langle B\rangle \neq 0$ amount to pairing of electrons, as discussed earlier. Performing the mean field decoupling yields:

$$H_{\mathrm{BCS}}^{\mathrm{MF}} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left( \Delta_{\mathbf{k}}^{*} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} + \Delta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\uparrow}^{\dagger} \right) + \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}^{2}}{V_0}, \tag{230}$$

where we introduced the abbreviation

$$\Delta_{\mathbf{k}} = \frac{V_0}{N} \sum_{\mathbf{k}} \gamma_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle. \tag{231}$$

The form of this Hamiltonian is similar to an effective free-electron problem in the sense that it only contains terms that are products of two operators $c_{\mathbf{k}\sigma}^{\dagger}$ or $c_{\mathbf{k}\sigma}$, respectively. However, the appearance terms like $\Delta_{\mathbf{k}}^{*} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}$ and $\Delta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\uparrow}^{\dagger}$ has no analog in the free electron limit. An expectation value $\left\langle c_{\mathbf{k}',\uparrow}^{\dagger} c_{-\mathbf{k}',\downarrow}^{\dagger} \right\rangle \neq 0$ must be understood as consequence of an external source field that couples to the operators $A$ and $B$ and is switched off after the thermodynamic limit has been taken. Within a mean field theory such source field would only be an infinitesimal addition to the mean field anyway. Thus, we never actually have to include the mentioned source field since we broke the symmetry "by hand" already. Those anomalous terms are obviously the ones that explicitly violate charge conservation at the mean field level. In order to bring this Hamiltonian into the desired form, we introduce the Nambu spinor

$$c_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix}, \tag{232}$$

which allows us to express $H_{\mathrm{BCS}}^{\mathrm{MF}}$ in a form that resembles more the usual free fermion problem:

$$H_{\mathrm{BCS}}^{\mathrm{MF}} = \sum_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} h_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{k}} \left( \varepsilon_{\mathbf{k}} + \frac{\Delta_{\mathbf{k}}^{2}}{V_0} \right), \tag{233}$$

with $2 \times 2$-matrix

$$h_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^{*} & -\varepsilon_{\mathbf{k}} \end{pmatrix}. \tag{234}$$

The eigenvalues of $h_{\mathbf{k}}$ are determined by $(E - \varepsilon_{\mathbf{k}})(E + \varepsilon_{\mathbf{k}}) - |\Delta_{\mathbf{k}}|^2 = 0$, which yields

$$E_{\mathbf{k}\pm} = \pm E_{\mathbf{k}} \tag{235}$$

with

$$E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} > 0. \tag{236}$$

$h_{\mathbf{k}}$ is diagonalized by the unitary transformation $U_{\mathbf{k}}$. The columns of $U_{\mathbf{k}}$ are the eigenvectors $\mathbf{u}_{\mathbf{k}}^{(i)}$ of $h_{\mathbf{k}}$. Interestingly there is some nontrivial structure in

the matrix $h_{\mathbf{k}}$ that is worth exploring as it can be very helpful for more complex systems such as multi-band superconductors or inhomogeneous systems. It holds with $\gamma = i\sigma^y$ that

$$\gamma h_{\mathbf{k}}^* \gamma^{-1} = -h_{\mathbf{k}}. \tag{237}$$

Suppose one eigenvector of $h_{\mathbf{k}}$ is $\mathbf{u}_{\mathbf{k}}^{(1)} = (u_{\mathbf{k}}, v_{\mathbf{k}})^T$ and it corresponds, without restriction, to the eigenvalue $+E_{\mathbf{k}}$, i.e. $h_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}^{(1)} = E_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}^{(1)}$. We can now construct the another vector

$$\mathbf{u}_{\mathbf{k}}^{(2)} = -\gamma \mathbf{u}_{\mathbf{k}}^{(1)*} = (-u_{\mathbf{k}}^*, v_{\mathbf{k}}^*)^T \tag{238}$$

which obeys

$$\gamma \mathbf{u}_{\mathbf{k}}^{(2)*} = -\gamma^2 \mathbf{u}_{\mathbf{k}}^{(1)} = -\mathbf{u}_{\mathbf{k}}^{(1)} \tag{239}$$

$\mathbf{u}_{\mathbf{k}}^{(2)}$ is also an eigenvector but with eigenvalue $-E_{\mathbf{k}}$. To show that this is the case, we take the complex conjugate of the second eigenvalue equation $h_{\mathbf{k}}^*\mathbf{u}_{\mathbf{k}}^{(2)*} = -E_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}^{(2)*}$ and write it as $\gamma h_{\mathbf{k}}^*\gamma^{-1}\gamma\mathbf{u}_{\mathbf{k}}^{(2)*} = -\gamma E_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}^{(2)*}$ which yields $-h_{\mathbf{k}}\gamma\mathbf{u}_{\mathbf{k}}^{(2)*} = -\gamma E_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}^{(2)*}$ amd leads to the first eigenvalue equation $h_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}^{(1)} = E_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}^{(1)}$, proving our assertion. Thus, the eigenvalues of the mean field Hamiltonian occur in a pair of opposite sign and with eigenvalues related by the unimodular transformation $\gamma$. The unitary transformation that diagonalizes the above $2 \times 2$ matrix is

$$U_{\mathbf{k}} = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}}^* \\ v_{\mathbf{k}} & u_{\mathbf{k}}^* \end{pmatrix} \tag{240}$$

and it follows $U_{\mathbf{k}}^{-1}h_{\mathbf{k}}U_{\mathbf{k}} = \mathrm{diag}\,(E_{\mathbf{k}}, -E_{\mathbf{k}})$. It is straightforward to determine $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ from the eigenvalue equations. Unitarity, i.e. normalization of the eigenvectors implies $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ and it follows

$$u_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}} - \varepsilon_{\mathbf{k}}} v_{\mathbf{k}}. \tag{241}$$

This leads to:

$$\begin{aligned} u_{\mathbf{k}}^2 &= \frac{1}{2}\left(1 + \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \\ v_{\mathbf{k}}^2 &= 1 - u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right). \end{aligned} \tag{242}$$

as well as $u_{\mathbf{k}}v_{\mathbf{k}}^* = -\frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$.

The unitary transformation transforms the Nambu spinor $c_{\mathbf{k}}$ according to $a_{\mathbf{k}} = U_{\mathbf{k}}^{-1}c_{\mathbf{k}}$ with $a_{\mathbf{k}} = \left(a_{\mathbf{k}\uparrow}, a_{-\mathbf{k}\downarrow}^\dagger\right)^T$ and it follows

$$\begin{aligned} \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger h_{\mathbf{k}} c_{\mathbf{k}} &= \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger U_{\mathbf{k}} \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} U_{\mathbf{k}}^{-1} c_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} a_{\mathbf{k}} \end{aligned}$$

$$
\begin{aligned}
&= \sum_{\mathbf{k}} E_{\mathbf{k}} \left( a^{\dagger}_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} - a_{-\mathbf{k}\downarrow} a^{\dagger}_{-\mathbf{k}\downarrow} \right) \\
&= \sum_{\mathbf{k}} E_{\mathbf{k}} \left( a^{\dagger}_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} + a_{-\mathbf{k}\downarrow} a^{\dagger}_{-\mathbf{k}\downarrow} - 1 \right) \\
&= \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} E_{\mathbf{k}} \qquad (243)
\end{aligned}
$$

The mean field Hamiltonian is then given as:

$$
H^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \left( \frac{\Delta^2_{\mathbf{k}}}{V_0} + \varepsilon_{\mathbf{k}} - \sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2} \right). \qquad (244)
$$

Now, we managed to bring the Hamiltonian into the desired form of a free Fermi gas. In particular, it holds $\left\langle a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} \right\rangle = f\left(E_{\mathbf{k}}\right)$, where $f(\varepsilon) = \frac{1}{\exp(\beta\varepsilon)+1}$ is the usual Fermi function. Since $E_{\mathbf{k}} > 0$, we obtain $\left\langle a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} \right\rangle = 0$ at $T = 0$. The ground state energy is then given by the constant term in

$$
E_0 = \sum_{\mathbf{k}} \left( \frac{\Delta^2_{\mathbf{k}}}{V_0} + \varepsilon_{\mathbf{k}} - \sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2} \right). \qquad (245)
$$

The fermionic excitations only describe excitations above the ground state.

In order to determine $\Delta$ at $T = 0$ , we minimize $E_0$ with respect to $\Delta$. We perform the momentum integration via an integration over energy and subtract the value of the energy for $\Delta = 0$, i.e. $\delta E_0(\Delta) = E_0(\Delta) - E_0(\Delta = 0)$. It follows

$$
\begin{aligned}
\delta E_0 \quad /N = \quad & \frac{\Delta^2}{V_0} + \int_{-\infty}^{\infty} \rho(\epsilon)\, d\varepsilon \left( \varepsilon - \sqrt{\varepsilon^2 + \Delta^2} \right) - 2 \int_{-\infty}^{\infty} \rho(\epsilon)\, d\varepsilon \theta(-\varepsilon)\, \varepsilon \\
= \quad & \frac{\Delta^2}{V_0} + 2\rho \int_0^{\omega_D} d\varepsilon \left( \varepsilon - \sqrt{\varepsilon^2 + \Delta^2} \right) \\
= \quad & \frac{\Delta^2}{V_0} + \rho \Delta^2 \log\left( \frac{\Delta}{2\omega_D} \right) - \frac{\rho}{2} \Delta^2 \qquad (246)
\end{aligned}
$$

Minimizing the ground state energy with respect to $\Delta$ yields

$$
\frac{1}{N} \frac{\partial E_0}{\partial \Delta} = 2 \frac{\Delta}{V_0} + 2\rho\Delta \log\left( \frac{\Delta}{2\omega_D} \right) = 0,
$$

which has the trivial solution $\Delta = 0$ and the nontrivial solution

$$
\Delta(T = 0) = 2\omega_D \exp(-1/\lambda).
$$

Inserting the latter into the energy, we find

$$
E_0 = E_0(\Delta = 0) - 2N\rho_F \omega_D^2 e^{-2/\lambda} < E_0(\Delta = 0).
$$

The nontrivial solutions is indeed energetically lower.

## 6.2 The wave function

Next we want to determine the many body wave function that is associated with this new mean field state. To obtain the BCS wave function we use the fact that Eq.244 implies that the ground state wave function is the vacuum state of the Bogoliubov quasiparticles. Thus, it holds

$$a_{\mathbf{k}\sigma} \left|\Phi_{\mathrm{BCS}}\right\rangle = 0 \text{ for all } \mathbf{k}, \sigma. \tag{247}$$

To proceed, we assume

$$\left|\Phi_{\mathrm{BCS}}\right\rangle = C e^{\sum_{\mathbf{k}} \phi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{\mathbf{k}\downarrow}} \left|0\right\rangle = C \prod_{\mathbf{k}} e^{\phi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{\mathbf{k}\downarrow}} \left|0\right\rangle, \tag{248}$$

Here $|0\rangle$ is the vacuum state of the original operators, i.e. $c_{i\sigma}|0\rangle = 0$. We next determine $\phi_{\mathbf{k}}$ from the condition Eq.247. We write explicitly:

$$\begin{aligned} a_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\downarrow} \\ a_{\mathbf{k}\downarrow} &= v_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\uparrow} + u_{\mathbf{k}} c_{\mathbf{k}\downarrow}. \end{aligned} \tag{249}$$

Eq.247 is equivalent to

$$u_{\mathbf{k}} c_{\mathbf{k}\uparrow} \left|\Phi_{\mathrm{BCS}}\right\rangle = v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\downarrow} \left|\Phi_{\mathrm{BCS}}\right\rangle. \tag{250}$$

We first analyze $c_{\mathbf{k}\uparrow}\left|\Phi_{\mathrm{BCS}}\right\rangle$ . It is useful to introduce the operator

$$\theta = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \tag{251}$$

and it follows for the wave function

$$\left|\Phi_{\mathrm{BCS}}\right\rangle \propto \sum_{n=0}^{\infty} \frac{\theta^n}{n!} \left|0\right\rangle. \tag{252}$$

It is easy to show that $[c_{\mathbf{k}\uparrow}, \theta] = b^{\dagger}_{-\mathbf{k}\downarrow}$with operator $b^{\dagger}_{-\mathbf{k}\downarrow} = \phi_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\downarrow}$. Furthermore, it follows that $\left[b^{\dagger}_{-\mathbf{k}\downarrow}, \theta\right] = 0$. It is now easy to apply $c_{\mathbf{k}\uparrow}$ to each term in the sum of Eq.252 separately. It holds:

$$\begin{aligned} c_{\mathbf{k}\uparrow}\theta\left|0\right\rangle &= b^{\dagger}_{-\mathbf{k}\downarrow}\left|0\right\rangle \\ c_{\mathbf{k}\uparrow}\theta^2\left|0\right\rangle &= b^{\dagger}_{-\mathbf{k}\downarrow}\theta\left|0\right\rangle + \theta c_{\mathbf{k}\uparrow}\theta\left|0\right\rangle = 2\theta b^{\dagger}_{-\mathbf{k}\downarrow}\left|0\right\rangle \\ &\vdots \\ c_{\mathbf{k}\uparrow}\theta^n\left|0\right\rangle &= n\theta^{n-1} b^{\dagger}_{-\mathbf{k}\downarrow}\left|0\right\rangle. \end{aligned} \tag{253}$$

This result allows to sum-up the series Eq.252 and we obtain

$$c_{\mathbf{k}\uparrow}\left|\Phi_{\mathrm{BCS}}\right\rangle = b^{\dagger}_{-\mathbf{k}\downarrow}\left|\Phi_{\mathrm{BCS}}\right\rangle \tag{254}$$

The condition $a_{\mathbf{k}\sigma}\left|\Phi_{\mathrm{BCS}}\right\rangle = 0$ expressed in form of Eq.250 can now be expressed as

$$u_{\mathbf{k}}\phi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\downarrow}\left|\Phi_{\mathrm{BCS}}\right\rangle = v_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}\downarrow}\left|\Phi_{\mathrm{BCS}}\right\rangle. \tag{255}$$

This implies immediately $\phi_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}}$. It is easy to show that the condition $a_{-\mathbf{k}\downarrow}\left|\Phi_{\mathrm{BCS}}\right\rangle = 0$ leads to the same condition. It follows with normalization factor:

$$C = \prod_{\mathbf{k}} u_{\mathbf{k}}$$

for the wave function

$$\begin{aligned}\left|\Phi_{\mathrm{BCS}}\right\rangle &= \prod_{\mathbf{k}} u_{\mathbf{k}} e^{v_{\mathbf{k}}/u_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}}\left|0\right\rangle \\ &= \prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}\right)\left|0\right\rangle.\end{aligned}$$

The last step is a consequence of the fact that due to Pauli Principle $\left(c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}\right)^n = 0$ if $n > 1$. This approach allows to project the BCS-wave function into the space of fixed number of electrons $N$.

$$\left|\Psi_{\mathrm{BCS}}, N\right\rangle = C\left(\sum_{\mathbf{k}}\phi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}\right)^{2N}\left|0\right\rangle. \tag{256}$$

This projection can alternatively be realized if one starts from the BCS ground state and adds a global phase $\varphi$ of the function $\phi_{\mathbf{k}}$:

$$\left|\Psi_{\mathrm{BCS}}, N\right\rangle = \int_0^{2\pi}\frac{d\varphi}{2\pi}e^{-iN\varphi/2}\prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}}e^{i\varphi}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}\right)\left|0\right\rangle. \tag{257}$$

There exists an interesting relation between the phase $\varphi$ and the pair number operator $\hat{N}_p$ which should give $2N$ in case of $\left|\Psi_{\mathrm{BCS}}, N\right\rangle$. With phase $\varphi$ of $\phi_{\mathbf{k}}$ we have:

$$\begin{aligned}\left|\Psi_{\mathrm{BCS}}, N\right\rangle &= C\left(e^{i\varphi}\sum_{\mathbf{k}}\phi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}\right)^{N_p}\left|0\right\rangle \\ &= e^{i\varphi N_p}C\left(\sum_{\mathbf{k}}\phi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}\downarrow}\right)^{N_p}\left|0\right\rangle.\end{aligned} \tag{258}$$

This demonstrates immediately that

$$\hat{N}_p = -i\frac{\partial}{\partial\varphi}. \tag{259}$$

suggesting that particle number and phase are canonically conjugated variables, i.e. there should be a Heisenberg uncertainty relation between both quantities.