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Tight-binding theory of superconductivity

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Abstract

The focus of this report is the derivation of the Bogoliubov-de Gennes equations for superconductors from a tight-binding model, restricting ourselves to the case of s-wave superconductors.

Contents

1 Introduction

In condensed matter physics, tight-binding models are commonly used to study different phenomena. One such phenomena is superconductivity, which can be modeled microscopically using Bogoliubov-de Gennes (BdG) theory. The goal of this project has been to gain a better theoretical understanding of BdG theory of superconductors. The first section of this report will attempt to give a brief overview of the basics of superconductivity, while the second section will give a detalied derivation of the BdG equations for an s-wave superconductor from a tight-binding model.

2 Superconductivity

Superconductivity was first discovered in mercury by H. Kamerlingh Onnes in 1911 [1]. Three years prior he had managed to liquify helium which made it possible to reach the low temperatures necessary to observe superconductivity in elemental solids. Later, superconductivity was also found in other elemental solids like lead and tin. The two characteristic phenomenas of superconductivity [1] are *perfect conductivity*, i.e. zero resistivity, and *perfect diamagnetism*, where any magnetic field is expelled from the solid, also called the *Meissner effect*. In order for the material to exhibit these properties it must be cooled down below a critical temperature T_c, specific to the material.

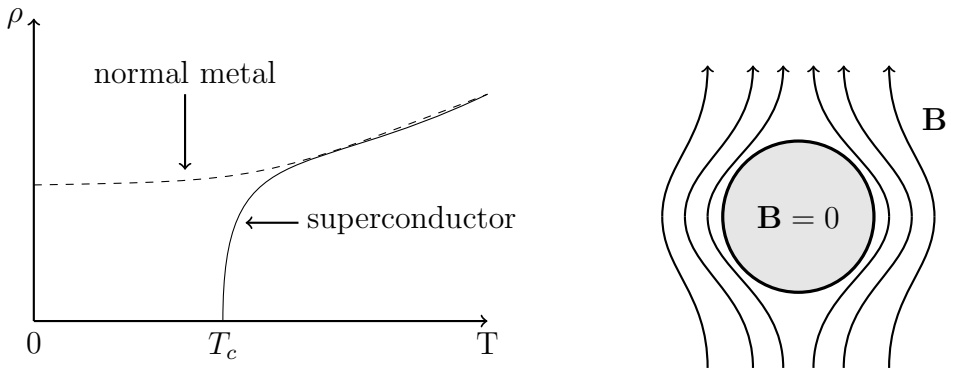

Figure 1: Left: Characteristic for superconductivity is that the electrical resistivity drops to zero as the temperature goes below a critical temperature T_c. Right: As the temperature goes below T_c a superconductor will expel magnetic fields, acting as a perfect diamagnet. This is called the *Meissner effect*.

The Ginzburg-Landau theory for superconductors [1] provides a phenomenological explanation of superconductivity. For a microscopic description of conventional super-

conductivity one can turn to BCS [2] theory which was developed by John Bardeen, Leon Cooper and John Schrieffer. It describes that electrons pair up in so called *Cooper pairs*, which opens up a gap at the Fermi surface. The only way for all of the electrons in a conventional superconductor to have a "friend" to pair up with, is for the two electrons pairing up to have opposite momentum, frequency, and spin. In a conventional superconductor, the *pairing mechanism* is electron-phonon interaction, i.e. the attractive interaction coupling the Cooper pairs is mediated by lattice vibrations, phonons. Electrons on their own are fermions, but when they are bound together in Cooper pairs they form bosonic quasiparticles, which are allowed to occupy the same quantum state, thus leading to superconductivity. In order to break a Cooper pair you have to overcome the quasiparticle excitation gap, or *the superconducting gap*, Δ. This gap can have different symmetries and structures depending on the properties of the material. A conventional superconductor has what is called s-wave symmetry, meaning that the superconducting gap is uniform, see figure (2).

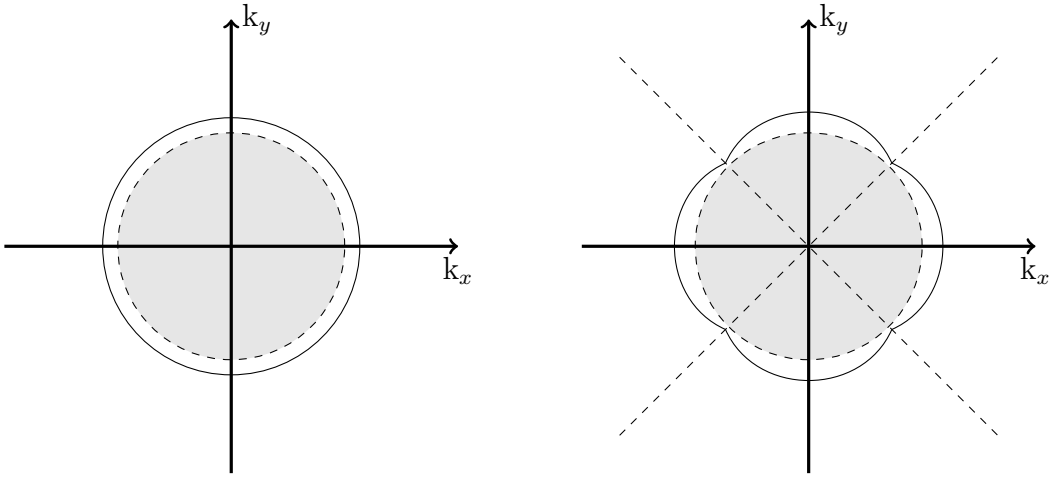

Figure 2: Schematic of the superconducting gap. Left: s-wave pairing superconductor. Right: d-wave pairing superconductor.

Unconventional superconductors are superconductors for which the electron-phonon interaction is too weak to be able to explain the observed superconductivity, instead some other mechanism is causing the attractive interaction in the Cooper pairs. One such class is high T_c cuprate superconductors, which were discovered in 1986 by Bednorz and Müller [3]. Superconductors in this class are d-wave superconductors, meaning that the superconducting gap is not uniform, but instead have nodes, see Figure (2). Another class of unconventional superconductors which were discovered in 2008 [4] are Fe-based superconductors. The symmetry and structure of the su-

perconducting gap in this class is still an open research question. One gap structure that is commonly suggested is called s^{+-} [5], but it might be that not all Fe-based superconductors have the same one. As previously mentioned, the superconductivity in unconventional superconductors can not be explained by just the electron-phonon interaction, but require some different pairing mechanism. One common suggestion for such a mechanism is spin fluctuation pairing [5].

3 Bogoliubov-de Gennes equations

In this section we will derive the Boboliubov-de Gennes equations for superconductors from a tight-binding model. This section is largely based on the second chapter of *Bogoliubov-de Gennes Method and Its Applications* [6] by J.-X. Zhu. We will restrict ourselves to finding the BdG equations for an s-wave superconductor, starting from the single-particle part of the Hamiltonian

$$H_0 = \iint d\mathbf{r}d\mathbf{r}'\psi^\dagger_\alpha(\mathbf{r})h_{\alpha\beta}(\mathbf{r},\mathbf{r}')\psi_\beta(\mathbf{r}') \tag{1}$$

where non-local and spin-flip effects are included in $\mathrm{h}_{\alpha\beta}(\mathbf{r},\mathbf{r}')$ and

$$\begin{aligned}\psi_\alpha(\mathbf{r}) &= \sum_i w(\mathbf{r}-\mathbf{R}_i)c_{i\alpha},\\ \psi^\dagger_\alpha(\mathbf{r}) &= \sum_i w^*(\mathbf{r}-\mathbf{R}_i)c^\dagger_{i\alpha}\end{aligned} \tag{2}$$

are the field operators in terms of the localized-state basis. The operators $\mathrm{c}^\dagger_{i\alpha}$ and $\mathrm{c}_{i\alpha}$ creates and annihilates an electron at site i with spin α. The localized orbital around the atomic site $\mathbf{R}_i$ is denoted $w(\mathbf{r}-\mathbf{R}_i)$. One can think of these localized orbitals w as δ-functions centered at the atomic site $\mathbf{R}_i$. Substituting Eq. (2) into the single-particle Hamiltonian we get

$$\begin{aligned}H_0 &= \sum_{ij,\sigma\sigma'} c^\dagger_{i\sigma}h_{i\sigma,j\sigma'}c_{j\sigma}\\ &= -\sum_{i\neq j,\sigma\sigma'} t_{i\sigma,j\sigma'}c^\dagger_{i\sigma}c_{j\sigma'} + \sum_{i\sigma}\epsilon_i c^\dagger_{i\sigma}c_{i\sigma} + \sum_{i,\sigma\sigma'}\Omega_{i,\sigma\sigma'}c^\dagger_{i\sigma}c_{i\sigma'}\end{aligned} \tag{3}$$

where the first term is the kinetic energy, the second term is the on-site single-particle energy and the third term describes the effects of magnetic impurities. Similarly, the extended Hubbard model can be expressed using the same basis, resulting in the following Hamiltonian for superconductivity,

$$\begin{aligned}\mathscr{H} &= H_0 - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i \Big(n_{i\uparrow} - \frac{1}{2}\Big)\Big(n_{i\downarrow} - \frac{1}{2}\Big) - \frac{V}{2}\sum_{i\neq j} n_i n_j \\ &= \sum_{ij,\sigma\sigma'} c_{i\sigma}^\dagger \Big[h_{i\sigma,j\sigma'} - \Big(\mu + \frac{U}{2}\Big)\delta_{ij}\delta_{\sigma\sigma'}\Big] c_{j\sigma'} + U\sum_i n_{i\uparrow}n_{i\downarrow} - \frac{V}{2}\sum_{i\neq j} n_i n_j\end{aligned} \tag{4}$$

where the particle number operator is $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ and $n_i = \sum_\sigma n_{i\sigma}$. U is the on-site electron-electron interaction strength and V is the nearest neighbor electron-electron interaction strength. Repulsive interactions are defined with positive values for U and negative values for V. Subsequently, attractive interactions are defined using negative values for U and positive values for V. For s-wave superconducting we will neglect the electron-electron interactions between lattice sites and replace U by $-\mathrm{U}$ ($U > 0$), to get attractive on-site electron-electron interactions. The Hamiltonian then looks as follows,

$$\mathscr{H} = \sum_{ij,\sigma\sigma'} c_{i\sigma}^\dagger \Big[h_{i\sigma,j\sigma'} - \mu\delta_{ij}\delta_{\sigma\sigma'}\Big] c_{j\sigma'} - U\sum_i n_{i\uparrow}n_{i\downarrow} \tag{5}$$

Since it is complicated to work with terms with four field operators, we want to simplify the electron-electron interaction term so it becomes quadratic. We will therefore rewrite it using the mean-field approximation,

$$c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow} \approx \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\rangle c_{i\downarrow}c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \langle c_{i\downarrow}c_{i\uparrow}\rangle - \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\rangle\langle c_{i\downarrow}c_{i\uparrow}\rangle \tag{6}$$

One might recognize this from Hartree-Fock, where a similar thing is done. The difference here is that we pair the annihilation operators with each other and the creation operators with each other, instead of having pairs of one annihilation operator and one creation operator, as one does in Hartree-Fock. Plugging eq. (6) into Eq. (5) we get that

$$\begin{aligned}\mathscr{H} &= \sum_{ij,\sigma\sigma'} c_{i\sigma}^\dagger \tilde{h}_{i\sigma,j\sigma'} c_{j\sigma'} - U\sum_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\downarrow}c_{i\uparrow} \\ &\approx \sum_{ij,\sigma\sigma'} c_{i\sigma}^\dagger \tilde{h}_{i\sigma,j\sigma'} c_{j\sigma'} - U\sum_i (\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\rangle c_{i\downarrow}c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\langle c_{i\downarrow}c_{i\uparrow}\rangle - \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\rangle\langle c_{i\downarrow}c_{i\uparrow}\rangle)\end{aligned} \tag{7}$$

where $\tilde{h}_{i\sigma,j\sigma'} = h_{i\sigma,j\sigma'} - \mu\delta_{ij}\delta_{\sigma\sigma'}$. By writing the singlet-pairing potentials as

$$\begin{aligned}\Delta_{ii} &= U\langle c_{i\downarrow}c_{i\uparrow}\rangle, \\ \Delta_{ii}^* &= U\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\rangle,\end{aligned} \tag{8}$$

we get the effective mean-field Hamiltonian,

$$\mathscr{H}_{eff} = \sum_{ij,\sigma\sigma'} c^\dagger_{i\sigma} \tilde{h}_{i\sigma,j\sigma'} c_{j\sigma'} - \sum_i \left[\Delta_{ii} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} + \Delta^*_{ii} c_{i\downarrow} c_{i\uparrow} \right] + E_{const} \tag{9}$$

where $E_{const} = U \sum_i \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle \langle c_{i\downarrow} c_{i\uparrow} \rangle$. The commutation relation for the annihilation operator $c_{i\uparrow}$ and the effective Hamiltonian can be obtained as

$$\begin{aligned} [c_{i\uparrow}, \mathscr{H}_{eff}] &= c_{i\uparrow} \mathscr{H}_{eff} - \mathscr{H}_{eff} c_{i\uparrow} \\ &= \sum_{j,\sigma'} \tilde{h}_{i\uparrow,j\sigma'} c_{j\sigma'} + \Delta_{ii} c^\dagger_{i\downarrow} \end{aligned} \tag{10}$$

Repeating the calculations for the remaining annihilation/creation operators we end up with the following commutation relations,

$$\begin{aligned} [c_{i\uparrow}, \mathscr{H}_{eff}] &= \sum_{j,\sigma'} \tilde{h}_{i\uparrow,j\sigma'} c_{j\sigma'} + \Delta_{ii} c^\dagger_{i\downarrow}, \\ [c^\dagger_{i\uparrow}, \mathscr{H}_{eff}] &= -\sum_{j\sigma'} \tilde{h}_{j\sigma',i\uparrow} c^\dagger_{j\sigma'} - \Delta^*_{ii} c_{i\downarrow}, \\ [c_{i\downarrow}, \mathscr{H}_{eff}] &= \sum_{j\sigma'} \tilde{h}_{i\downarrow,j\sigma'} c_{j\sigma'} - \Delta_{ii} c^\dagger_{i\downarrow}, \\ [c^\dagger_{i\downarrow}, \mathscr{H}_{eff}] &= -\sum_{j\sigma'} \tilde{h}_{j\sigma',i\downarrow} c^\dagger_{j\sigma'} + \Delta^*_{ii} c_{i\uparrow}. \end{aligned} \tag{11}$$

From this we can see that the electron field operators $c^\dagger_{i\sigma}$ and $c_{i\sigma}$ no longer constitute a good basis. What we instead would like to do is to express the electron field operators as linear combinations of electron- and hole-like quasiparticle excitations. This is done by performing a Bogoliubov canonical transformation,

$$c_{i\sigma} = {\sum_n}' (u^n_{i\sigma} \gamma_n - \sigma v^{n*}_{i\sigma} \gamma^\dagger_n), \quad c^\dagger_{i\sigma} = {\sum_n}' (u^{n*}_{i\sigma} \gamma^\dagger - \sigma v^n_{i\sigma} \gamma_n). \tag{12}$$

Here the up and down spin orientations are denoted as $\sigma = \pm 1$. The Bogoliubov quasiparticle at state n is created and annihilated by $\gamma^\dagger_n$ and γ_n, respectively. The quasiparticle operators anti-commute, i.e. $\{\gamma_n, \gamma^\dagger_m\} = \delta_{nm}$ and $\{\gamma_n, \gamma_m\} = \{\gamma^\dagger_n, \gamma^\dagger_m\} = 0$. The prime sign over the summation indicates that we only count states which have a positive energy. By using this canonical transformation the Hamiltonian is diagonalized as

$$H_{eff} = \sum_n E_n \gamma^\dagger_n \gamma_n + E'_{const} \tag{13}$$

By substituting eq.(12) into eq.(11), using the following commutation relations

$$\begin{aligned}[\gamma_n^\dagger, H_{eff}] &= -E_n\gamma_n^\dagger, \\ [\gamma_n, H_{eff}] &= E_n\gamma_n\end{aligned} \tag{14}$$

and comparing the terms containing γ_n and $\gamma_n^\dagger$ we finally arrive at the BdG equations:

$$\begin{aligned}E_n u_{i\uparrow}^n &= \sum_{j\sigma'} \tilde{h}_{i\uparrow,j\sigma'} u_{j\sigma'}^n + \sigma_{ii} v_{i\downarrow}^n, \\ E_n u_{i\downarrow}^n &= \sum_{j\sigma'} \tilde{h}_{i\downarrow,j\sigma'} + \Delta_{ii} v_{i\uparrow}^n, \\ E_n v_{i\uparrow}^n &= -\sum_{j\sigma'} \sigma' \tilde{h}_{i\uparrow,j\sigma'} v_{j\sigma'}^n + \Delta_{ii}^* u_{i\downarrow}^n, \\ E_n v_{i\downarrow}^n &= \sum_{j\sigma'} \sigma' \tilde{h}_{j\sigma',i\downarrow} v_{j\sigma'}^n + \Delta_{ii}^* u_{i\uparrow}^n\end{aligned} \tag{15}$$

with the self-consistency condition:

$$\Delta_{ii} = \frac{U}{2} \sum_n{}' (u_{i\uparrow}^n v_{i\downarrow}^{n*} + u_{i\downarrow}^n v_{i\uparrow}^{n*}) \tanh\Big(\frac{E_n}{2k_BT}\Big). \tag{16}$$

From the BdG equations in Eq. (15) one can show that if $(u_{i\uparrow}^n, v_{i\downarrow}^n, u_{i\downarrow}^n, v_{i\uparrow}^n)$ solves the BdG equations for the eigenvalue E_n, then $(-v_{i\uparrow}^{n*}, u_{i\downarrow}^{n*}, v_{i\downarrow}^{n*}, -u_{i\uparrow}^{n*})$ is the solution corresponding to the eigenvalue $-E_n$. This can be used to simplify the self-consistency condition in Eq. (16) to

$$\Delta_{ii} = \frac{U}{2} \sum_n u_{i\uparrow}^n v_{i\downarrow}^{n*} \tanh\Big(\frac{E_n}{2k_BT}\Big). \tag{17}$$

Good to remember here is that Δ_{ii} is the order parameter which quantifies the superconductivity. This means that above the critical temperature T_c, Δ_{ii} will be zero. When solving the self-consistency, one way of doing it is to first guess what Δ_{ii} is and using that guess to solve the BdG equations, then plugging the solution into Eq. (17), comparing the new Δ_{ii} with the old. If they differ, you calculate the BdG equations again, but with the new Δ_{ii}, repeating the procedure until the difference between the new and old Δ_{ii} is "small enough", i.e. within some tolerance.

If we do not have spin-orbit coupling and spin-flip scattering, i.e. $\tilde{h}_{i\uparrow,j\downarrow} = \tilde{h}_{i\downarrow,j\uparrow} = 0$, then the BdG equations can be further simplified to the following to sets of equations, making the BdG equations block-diagonalized,

$$
\begin{aligned}
E_{\tilde{n}1} u_{i\uparrow}^{\tilde{n}1} &= \sum_j \tilde{h}_{i\uparrow,j\uparrow} u_{j\uparrow}^{\tilde{n}1} + \Delta_{ii} v_{i\downarrow}^{\tilde{n}1}, \\
E_{\tilde{n}1} v_{i\downarrow}^{\tilde{n}1} &= -\sum_j \tilde{h}_{i\downarrow,j\downarrow}^{*} v_{j\downarrow}^{\tilde{n}1} + \Delta_{ii}^{*} u_{i\uparrow}^{\tilde{n}1}
\end{aligned}
\tag{18}
$$

and

$$
\begin{aligned}
E_{\tilde{n}2} u_{i\downarrow}^{\tilde{n}2} &= \sum_j \tilde{h}_{i\downarrow,j\downarrow} u_{j\downarrow}^{\tilde{n}2} + \Delta_{ii} v_{i\uparrow}^{\tilde{n}2}, \\
E_{\tilde{n}2} v_{i\uparrow}^{\tilde{n}2} &= -\sum_j \tilde{h}_{i\uparrow,j\uparrow}^{*} v_{j\uparrow}^{n} + \Delta_{ii}^{*} u_{i\downarrow}^{\tilde{n}2}.
\end{aligned}
\tag{19}
$$

Given the block-diagonalization and the symmetry we saw earlier for the solutions of the BdG equations with eigenvalue E_n and $-E_n$ respectively, it is enough to solve the first set of equations, Eq. (18), with the following self-consistency condition

$$
\Delta_{ii} = \frac{U}{2} \sum_{\tilde{n}} u_{i\uparrow}^{\tilde{n}1} v_{i\downarrow}^{\tilde{n}1*} \tanh\Big(\frac{E_{\tilde{n}1}}{2k_B T}\Big). \tag{20}
$$

This diagonalization takes us from a $4N$ by $4N$ matrix to a $2N$ by $2N$ matrix, which of course improves the computational efficiency greatly.

Once one has solved the BdG equations and found a solution $(u_{i\uparrow}^n, v_{i\downarrow}^n, u_{i\downarrow}^n, v_{i\uparrow}^n)$ with eigenvalue E_n, these can be used to calculate the charge density, the density of states and the band structure. For example, the charge density is calculated as

$$
\begin{aligned}
n_{i\uparrow} &= \sum_n |u_{i\uparrow}^n|^2 f(E_n), \\
n_{i\downarrow} &= \sum_n |v_{i\downarrow}|^2 f(-E_n),
\end{aligned}
\tag{21}
$$

where $f(E)$ is the Fermi-Dirac distribution, $f(E) = 1/(\exp(E/k_B T) + 1)$, and the local density of states is calculated as

$$
\rho_{i\sigma}(E) = \sum_n{}' (|u_{i\sigma}^n|^2 \delta(E_n - E) + |v_{i\sigma}|^2 \delta(E_n + E)). \tag{22}
$$

Now we have only looked at the case of s-wave superconductors, i.e. an on-site attractive interaction U, but the same procedure can be done for a d-wave superconductor. Then one would instead pick a repulsive on-site interaction, and include an attractive nearest-neighbour electron-electron interaction V in the Hamiltonian in Eq. (4).

4 Conclusion

We have now seen how one can arrive at the BdG equations for an s-wave superconductor from a tight-binding model. These can then be applied when studying superconductivity. In the case that spin-orbit coupling and/or spin-flip scattering are present one will use the BdG equations in Eq. (15) and the self-consistency conditions in Eq. (17). If spin-orbit coupling and spin-flip scattering are both absent, one can instead just solve the BdG equations in Eq. (18) with the self-consistency condition in Eq. (20).

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