Bogoliubov–de Gennes equations

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Abstract

This is a derivation of the Bogoliubov–de Gennes equations from a tight-binding model. While many such derivations take the Hubbard model as their starting point, I here reuse the mean-field Hamiltonian that we previously used to derive the Usadel equation. This ensures the conventions and notations used in the two formalisms are as compatible as possible.

1 Tight-binding model

One way to derive the Bogoliubov–de Gennes (BdG) equations is via a so-called *tight-binding model*.[1] We can start with a regular second-quantized Hamiltonian:

$$\begin{aligned}\mathcal{H} = &\sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r}\, \psi_\sigma^\dagger(\boldsymbol{r}) H_{\sigma\sigma'}(\boldsymbol{r}) \psi_{\sigma'}(\boldsymbol{r}) \\ &+ \sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{r'}\, \psi_\sigma^\dagger(\boldsymbol{r}) \psi_{\sigma'}^\dagger(\boldsymbol{r'})\, V_{\sigma\sigma'}(\boldsymbol{r},\boldsymbol{r'})\, \psi_{\sigma'}(\boldsymbol{r'}) \psi_\sigma(\boldsymbol{r}).\end{aligned} \tag{1}$$

The first term here is a general one-particle Hamiltonian of the same form as we used in my project thesis to derive the Usadel equation [3]. The spin indices on $H_{\sigma\sigma'}$ permit e.g. spin-flip and spin-orbit scattering. The second term covers the two-particle interactions that give rise to superconductivity and ferromagnetism; which one depends on the sign of V, as well as what particular combinations of primes are placed on the positions and spins (direct vs. exchange interactions).

We can then select a basis of localized *Wannier orbitals* $w(\boldsymbol{r} - \boldsymbol{R}_i)$. These orbitals are localized in the sense that they are large when $\boldsymbol{r} \to \boldsymbol{R}_i$, where $\boldsymbol{R}_i$ is the location of atom number i. They should also form an orthonormal basis,

$$\int \mathrm{d}\boldsymbol{r}\, w^*(\boldsymbol{r} - \boldsymbol{R}_i)\, w(\boldsymbol{r} - \boldsymbol{R}_j) = \delta_{ij}. \tag{2}$$

[1] Ref. [1] presents two derivations: ch. 1 is a continuum model derivation and ch. 2 a tight-binding model derivation. The continuum approach is more similar to the original derivation presented in de Gennes' textbook [2], while the tight-binding approach appears to be more common in modern literature. I'm therefore focusing on the tight-binding approach herein.

In terms of these orbitals, we can then define a new set of creation and annihilation operators that operate on lattice sites i rather than continuous space $\boldsymbol{r}$:

$$\psi_\sigma(\boldsymbol{r}) \equiv \sum_i w(\boldsymbol{r}-\boldsymbol{R}_i)\, c_{i\sigma}, \qquad \psi^\dagger_\sigma(\boldsymbol{r}) \equiv \sum_i w^*(\boldsymbol{r}-\boldsymbol{R}_i)\, c^\dagger_{i\sigma}. \tag{3}$$

The transition from a continuum model to tight-binding model can then be formalized by calculating matrix elements and taking advantage of the orthonormality of the orbitals. For example, in eq. (1), the single-particle term becomes:

$$\begin{aligned}
\mathcal{H} &= \sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r}\, \psi^\dagger_\sigma(\boldsymbol{r}) H_{\sigma\sigma'}(\boldsymbol{r})\, \psi_{\sigma'}(\boldsymbol{r}) && (4)\\
&= \sum_{ij\sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma'} \int \mathrm{d}\boldsymbol{r}\, w^*(\boldsymbol{r}-\boldsymbol{R}_i) H_{\sigma\sigma'}(\boldsymbol{r})\, w(\boldsymbol{r}-\boldsymbol{R}_j) && (5)\\
&\equiv \sum_{i\sigma\sigma'} \epsilon_i^{\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'} - \sum_{\langle ij\rangle\sigma\sigma'} t_{ij}^{\sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma'} + \cdots . && (6)
\end{aligned}$$

This procedure provides the rigorous connection between the original continuum model and the discretized lattice model. In this example, we have only included local terms ϵ_i and nearest-neighbour hopping integrals t_{ij}, but we could in theory continue expanding e.g. the next-nearest-neighbour interactions in this series.

1.1 Non-interacting electrons

Using the above, let us now translate the Hamiltonian used to derive the Usadel equation to the lattice model. Rewriting eq. (3.3) of my project thesis to the notation of eq. (1), and disregarding any electromagnetic fields, we get:

$$H_{\sigma\sigma'} = -\left(\frac{1}{2m}\nabla^2 + \mu(\boldsymbol{r})\right)\delta_{\sigma\sigma'}. \tag{7}$$

The procedure outlined above yields a Hamiltonian that describes a normal metal with chemical potential μ and hopping amplitude t,

$$\mathcal{H}_N = -\sum_{i\sigma} \mu_i c^\dagger_{i\sigma} c_{i\sigma} - \sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}, \tag{8}$$

where the hopping amplitude could in theory be calculated from the orbitals,

$$\begin{aligned}
t_{ij} &= -\frac{1}{2m}\int \mathrm{d}\boldsymbol{r}\, w^*(\boldsymbol{r}-\boldsymbol{R}_i)\nabla^2 w(\boldsymbol{r}-\boldsymbol{R}_j)\\
&= +\frac{1}{2m}\int \mathrm{d}\boldsymbol{r}\, [\nabla w(\boldsymbol{r}-\boldsymbol{R}_i)]^*[\nabla w(\boldsymbol{r}-\boldsymbol{R}_j)],
\end{aligned} \tag{9}$$

the second form following from an integration by parts using $w(\pm\infty) = 0$. Note that this result explicitly shows that $t_{ji} = t^*_{ij}$, which will be useful later on. In practice, the hopping amplitudes t_{ij} are usually taken to be positive and real, and it is often used as the base unit that other energies are measured against.

1.2 Electromagnetic fields

Let us now consider electromagnetic fields. Eq. (3.2) in my project thesis is:

$$H_{\sigma\sigma'} = \left\{ -\frac{1}{2m}[\nabla - ie\boldsymbol{A}(\boldsymbol{r})]^2 + e\phi(\boldsymbol{r}) - \mu(\boldsymbol{r}) \right\} \delta_{\sigma\sigma'}. \tag{10}$$

Expanding the square and assuming a Coulomb gauge $\nabla \cdot \boldsymbol{A} = 0$, this becomes:

$$H_{\sigma\sigma'} = \left\{ -\frac{1}{2m}\nabla^2 + \frac{ie}{m}\boldsymbol{A}(\boldsymbol{r}) \cdot \nabla + \frac{e^2}{2m}\boldsymbol{A}^2(\boldsymbol{r}) + e\phi(\boldsymbol{r}) - \mu(\boldsymbol{r}) \right\} \delta_{\sigma\sigma'}. \tag{11}$$

The non-derivative terms can be treated as shifts to the chemical potential. In other words, they enter into the Hamiltonian like an effective chemical potential

$$\mu_i' \equiv \mu_i - e\phi_i - \frac{e^2}{2m}\boldsymbol{A}_i^2. \tag{12}$$

From here on, we only explicitly include μ_i in the equations, but refer back to this substitution if we need to include e.g. electrostatic potentials in the model.

The remaining term is the $\boldsymbol{A} \cdot \nabla$ contribution, which as a derivative term should yield a kinetic energy contribution. The associated hopping integral is:

$$\begin{aligned} \tau_{ij} &= \frac{ie}{m} \int \mathrm{d}\boldsymbol{r}\, w^*(\boldsymbol{r} - \boldsymbol{R}_i) \left[\boldsymbol{A}(\boldsymbol{r}) \cdot \nabla\right] w(\boldsymbol{r} - \boldsymbol{R}_j) \\ &= \frac{ie}{m} \int \mathrm{d}\boldsymbol{r}\, \boldsymbol{A}(\boldsymbol{r}) \cdot [w^*(\boldsymbol{r} - \boldsymbol{R}_i)\nabla w(\boldsymbol{r} - \boldsymbol{R}_j)], \end{aligned} \tag{13}$$

which is generally imaginary when the hopping amplitudes t_{ij} are purely real. Let us now consider the inverse hopping τ_{ji}. Using the Coulomb gauge $\nabla \cdot \boldsymbol{A} = 0$, and the fact that $w(\pm\infty) = 0$, and performing an integration by parts, we get:

$$\begin{aligned} \tau_{ji} &= +\frac{ie}{m} \int \mathrm{d}\boldsymbol{r}\, \boldsymbol{A}(\boldsymbol{r}) \cdot w^*(\boldsymbol{r} - \boldsymbol{R}_j)[\nabla w(\boldsymbol{r} - \boldsymbol{R}_i)] \\ &= -\frac{ie}{m} \int \mathrm{d}\boldsymbol{r}\, \boldsymbol{A}(\boldsymbol{r}) \cdot [\nabla w^*(\boldsymbol{r} - \boldsymbol{R}_j)] w(\boldsymbol{r} - \boldsymbol{R}_i) \\ &= -\frac{ie}{m} \int \mathrm{d}\boldsymbol{r}\, \boldsymbol{A}(\boldsymbol{r}) \cdot w(\boldsymbol{r} - \boldsymbol{R}_i)[\nabla w^*(\boldsymbol{r} - \boldsymbol{R}_j)] \\ &= \tau_{ij}^*. \end{aligned} \tag{14}$$

Thus, we can define an effective hopping coefficient $t_{ij}' \equiv t_{ij} + \tau_{ij}$, where t_{ij} was defined in the previous subsection and τ_{ij} above, and this parameter still satisfies the property $t_{ji}' = t_{ij}'^*$. From here on, we refer to t_{ij} without primes, but will take this to be a complex number to accommodate electromagnetic fields.

TODO: Add discussion of the Peierls substitution here.

1.3 Spin-orbit coupling

Let us now consider a spin-orbit coupling that is linear in spin and momentum, which covers e.g. Rashba and Dresselhaus spin-orbit coupling. This approach is based on sec. 3.4 in my project thesis, which was in turn based on Bergeret and Tokatly's paper [4]. The spin-dependent Hamiltonian was then parametrized as

$$H_{\sigma\sigma'} = \frac{i}{m}\boldsymbol{\mathcal{A}}_{\sigma\sigma'} \cdot \nabla, \tag{15}$$

where we did not include the artificial $\boldsymbol{\mathcal{A}}^2$ term required to get SU(2) symmetry, and we only consider spin-orbit couplings that are constant within each material. Going through the same kind of derivation as for the electromagnetic gauge field, we find that spin-orbit coupling produces a spin-dependent hopping term:

$$\tau_{ij}^{\sigma\sigma'} = \frac{i}{m}\boldsymbol{\mathcal{A}}_{\sigma\sigma'} \cdot \int \mathrm{d}\boldsymbol{r}\, w^*(\boldsymbol{r} - \boldsymbol{R}_i)\nabla w(\boldsymbol{r} - \boldsymbol{R}_j). \tag{16}$$

Since $\boldsymbol{\mathcal{A}}$ is Hermitian we have $\boldsymbol{\mathcal{A}}_{\sigma\sigma'} = \boldsymbol{\mathcal{A}}^*_{\sigma'\sigma}$ which implies that $\tau_{ji}^{\sigma'\sigma} = (\tau_{ij}^{\sigma\sigma'})^*$.

Check more carefully derivation of $\boldsymbol{d}_{ij}$.

One can show that the integral above is proportional to hopping distance $\boldsymbol{d}_{ij} \equiv \boldsymbol{R}_i - \boldsymbol{R}_j$. Moreover, the easiest spin-orbit coupling to experimentally realize is Rashba coupling, so we will likely focus on $\boldsymbol{\mathcal{A}} \sim \boldsymbol{n} \times \boldsymbol{\sigma}$ where $\boldsymbol{n}$ is the direction of broken inversion symmetry. Performing all these adjustments, and using the triple product identity, we obtain $\tau_{ij} \sim i(\boldsymbol{n} \times \boldsymbol{\sigma}) \cdot \boldsymbol{d}_{ij} \sim -i(\boldsymbol{n} \times \boldsymbol{d}_{ij}) \cdot \boldsymbol{\sigma}$. This motivates the following simplified form of the spin-orbit hopping amplitude,

$$\tau_{ij} = -i(\boldsymbol{\alpha} \times \boldsymbol{d}_{ij}) \cdot \boldsymbol{\sigma}, \tag{17}$$

where $\boldsymbol{\alpha}$ is proportional to the standard Rashba coupling but has different units. Just like t_{ij}, this amplitude can be neglected except for nearest neighbours $\langle ij \rangle$.

1.4 Ferromagnetism

Based on eq. (3.18) in my project thesis, we can write the Hamiltonian for an itinerant ferromagnet treated via the mean-field approach as follows:

$$H_{\sigma\sigma'} = -\big[\boldsymbol{m}(\boldsymbol{r}) \cdot \boldsymbol{\sigma}\big]_{\sigma\sigma'}. \tag{18}$$

We can thus write the lattice Hamiltonian for a ferromagnet as $\mathcal{H}_N + \mathcal{H}_F$, where

$$\mathcal{H}_F = -\sum_{i\sigma\sigma'} \big[\boldsymbol{m}_i \cdot \boldsymbol{\sigma}\big]_{\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'}. \tag{19}$$

The exchange field $\boldsymbol{m}_i \equiv \int \mathrm{d}\boldsymbol{r}\, \boldsymbol{m}(\boldsymbol{r})|w(\boldsymbol{r} - \boldsymbol{R}_i)|^2 \approx \boldsymbol{m}(\boldsymbol{R}_i)$, where the last approximation follows from that the exchange field varies slowly cf. the orbitals. This shows that the effect of ferromagnetism on the system is similar to if we had

introduced a spin-dependent effective chemical potential $\mu'_{i\sigma\sigma'} \equiv \mu_i + [\boldsymbol{m}_i \cdot \boldsymbol{\sigma}]_{\sigma\sigma'}$. It is also worth noting that $[\boldsymbol{m}_i \cdot \boldsymbol{\sigma}]_{\sigma'\sigma} = [\boldsymbol{m}_i \cdot \boldsymbol{\sigma}^*]_{\sigma\sigma'}$, which we will use later.

We have here neglected a mean-field contribution that is proportional to $\boldsymbol{m}^2$ [see eq. (3.14) in my project thesis]. This term does not depend on the electron operators but may still be important when treating magnetism self-consistently.[2]

1.5 Superconductivity

We now get to the main ingredient of the BdG equations: superconductivity. In sec. 3.3 of my project thesis, we used the following two-particle Hamiltonian:[3]

$$\mathcal{H}_S = -\int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r})\, \psi_\downarrow^\dagger(\boldsymbol{r})\psi_\uparrow^\dagger(\boldsymbol{r})\psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r}). \tag{20}$$

We then performed a mean-field approximation using $\Delta(\boldsymbol{r}) \equiv U(\boldsymbol{r})\langle\psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r})\rangle$, producing the following BCS Hamiltonian for conventional superconductors [6]:

$$\mathcal{H}_S \approx -\int \mathrm{d}\boldsymbol{r}\, \left\{\Delta(\boldsymbol{r})\, \psi_\downarrow^\dagger(\boldsymbol{r})\psi_\uparrow^\dagger(\boldsymbol{r}) + \Delta^*(\boldsymbol{r})\, \psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r})\right\}. \tag{21}$$

The second term is the Hermitian conjugate of the first, so we only need to analyze the first term in detail. Substituting eq. (3) into the above, we find:

$$\begin{aligned}\mathcal{H}_S &= -\sum_{ij} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger \int \mathrm{d}\boldsymbol{r}\, \Delta(\boldsymbol{r})\, w^*(\boldsymbol{r}-\boldsymbol{R}_i)\, w^*(\boldsymbol{r}-\boldsymbol{R}_j) + \text{h.c.} \\ &\equiv -\sum_{ij} \Delta_{ij} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger + \text{h.c.}\end{aligned} \tag{22}$$

As $\Delta(\boldsymbol{r})$ varies slowly compared to the Wannier orbitals (atomic vs. coherence length), and the orbitals are strongly peaked near $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$, performing the integral results in $\Delta_{ij} \approx \Delta_i \delta_{ij}$. Using this observation and restoring the explicit Hermitian conjugates, we obtain this Hamiltonian for on-site singlet pairing:

$$\mathcal{H}_S = -\sum_i \left\{\Delta_i c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger + \Delta_i^* c_{i\uparrow} c_{i\downarrow}\right\}. \tag{23}$$

One part of the Hamiltonian is however missing: the mean field energy term. Going back to eq. (3.26) in my project thesis, we explicitly discarded this term:

$$E_0 = \int \mathrm{d}\boldsymbol{r}\, U\langle\psi_\downarrow^\dagger\psi_\uparrow^\dagger\rangle\langle\psi_\uparrow\psi_\downarrow\rangle = \int \mathrm{d}\boldsymbol{r}\, U\frac{\Delta^*}{U}\frac{\Delta}{U} = \int \mathrm{d}\boldsymbol{r}\, \frac{|\Delta|^2}{U}. \tag{24}$$

Performing the tight-binding transformation, this readily transforms into

$$E_0 = \sum_i \frac{|\Delta_i|^2}{U_i}. \tag{25}$$

This matches eq. (4) in Atousa's paper [7], and is needed to find the free energy.

[2] Note that my project thesis neglects electronic screening in metals $V(r) \sim \exp(-r/\lambda)/r$, which simplifies the calculation of the E_0 contribution. In fact, in this limit we get a Hubbard model with opposite sign from the superconducting case. For the details, see ch. 10 in Ref. [5].

[3] I here use the notation $-U(\boldsymbol{r})$ instead of $+\lambda(\boldsymbol{r})$ for the attractive interaction, and $\Delta(\boldsymbol{r})$ instead of $\zeta(\boldsymbol{r})$ for the complex order parameter. Sign conventions are as in my MSc thesis [6].

1.6 Summary

We started from the definition of a tight-binding model and derived a lattice model that describes normal metals, superconductors, and ferromagnets. Since this BdG model was derived from the same Hamiltonian as we used to derive the Usadel equation, all notations and conventions should be compatible. The Hamiltonian we obtained in the tight-binding and mean-field limits is as follows:

$$\begin{aligned}\mathcal{H} = E_0 &- \sum_{i\sigma} \mu_i c_{i\sigma}^\dagger c_{i\sigma} - \sum_{\langle ij\rangle\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \sum_{\langle ij\rangle\sigma\sigma'} \left[i(\boldsymbol{\alpha}\times\boldsymbol{d}_{ij})\cdot\boldsymbol{\sigma}\right]_{\sigma\sigma'} c_{i\sigma}^\dagger c_{j\sigma'} \\ &- \sum_{i\sigma\sigma'} \left[\boldsymbol{m}_i\cdot\boldsymbol{\sigma}\right]_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'} - \sum_i \left\{\Delta_i c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger + \Delta_i^* c_{i\uparrow} c_{i\downarrow}\right\}.\end{aligned} \tag{26}$$

This result seems consistent with eq. (2.5) in Ref. [1], eqs. (10–11) in Atousa's paper [7], and eqs. (1) and (3) in Lina's paper [8]. All of these sources, however, derived this result within various versions of the extended Hubbard model, while we derived it from the same Hamiltonian as we used to get the Usadel equation. The Rashba coupling is similar to eq. (1) in the corrected version of Ref. [9].

2 Matrix equations

2.1 Nambu space

Now that the basic Hamiltonian is in place, the next step is to organize it as a matrix equation. Similarly to our approach in the Usadel formalism, it is convenient to introduce operators in Nambu⊗Spin space to organize our equations:

$$\hat{c}_i \equiv (c_{i\uparrow}, c_{i\downarrow}, c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger). \tag{27}$$

This corresponds to the D_i operators in Terrade's thesis [10] and the B_i operators in Jacob's lecture notes. I'm here following the Usadel convention of putting hats on things with a Nambu-space structure.

Let us now rewrite the Hamiltonian in a more symmetric form before we fill out the corresponding matrix Hamiltonian. Starting with the chemical potential term, we have that $\{c_{i\sigma}^\dagger, c_{i\sigma}\} = 1$, so we can write the term as

$$\sum_{i\sigma} \mu_i c_{i\sigma}^\dagger c_{i\sigma} = \frac{1}{2}\sum_{i\sigma} \mu_i \left\{c_{i\sigma}^\dagger c_{i\sigma} - c_{i\sigma} c_{i\sigma}^\dagger\right\} + \sum_i \mu_i. \tag{28}$$

Correspondingly, for the hopping term we get

$$\sum_{\langle ij\rangle\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} = \frac{1}{2}\sum_{\langle ij\rangle\sigma} t_{ij}\left\{c_{i\sigma}^\dagger c_{j\sigma} - c_{j\sigma} c_{i\sigma}^\dagger\right\} = \frac{1}{2}\sum_{\langle ij\rangle\sigma}\left\{t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - t_{ji} c_{i\sigma} c_{j\sigma}^\dagger\right\}. \tag{29}$$

In the last step, we used our freedom to relabel the indices ij. However, going back to eq. (9), we see that by definition $t_{ji} = t_{ij}^*$. Thus, we can rewrite this as:

$$\sum_{\langle ij\rangle\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} = \frac{1}{2}\sum_{\langle ij\rangle\sigma}\left\{t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - t_{ij}^* c_{i\sigma} c_{j\sigma}^\dagger\right\}. \tag{30}$$

For spin-orbit coupling and ferromagnetism, we get very similar transformations as the above using the identities $i\boldsymbol{d}_{ji} = -i\boldsymbol{d}_{ij} = (+i\boldsymbol{d}_{ij})^*$ and $\boldsymbol{\sigma}_{\sigma'\sigma} = \boldsymbol{\sigma}^*_{\sigma\sigma'}$. As for the superconducting terms, we already have both particle and hole combinations, but they are not yet symmetrized wrt. spins. We can therefore again anticommute half of each term in the Hamiltonian, and then obtain:

$$\sum_i \left\{\Delta_i c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} + \Delta^*_i c_{i\uparrow} c_{i\downarrow}\right\} = \frac{1}{2}\sum_i \left\{\Delta_i (c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} - c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}) + \Delta^*_i (c_{i\uparrow} c_{i\downarrow} - c_{i\downarrow} c_{i\uparrow})\right\} \tag{31}$$

Let us now collect all the symmetrized contributions above. The total Hamiltonian of the system can now be written as:

$$\begin{aligned}
\mathcal{H} = E_0 &- \frac{1}{2}\sum_{i\sigma} \mu_i \left\{c^\dagger_{i\sigma} c_{i\sigma} - c_{i\sigma} c^\dagger_{i\sigma}\right\} \\
&- \frac{1}{2}\sum_{\langle ij\rangle\sigma} \left\{t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - t^*_{ij} c_{i\sigma} c^\dagger_{j\sigma}\right\} \\
&- \frac{1}{2}\sum_{\langle ij\rangle\sigma\sigma'} \left\{\left[(i\boldsymbol{\alpha}_i \times \boldsymbol{d}_{ij})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\right] c^\dagger_{i\sigma} c_{j\sigma'} - \left[(i\boldsymbol{\alpha}_i \times \boldsymbol{d}_{ij})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\right]^* c_{i\sigma} c^\dagger_{j\sigma'}\right\} \\
&- \frac{1}{2}\sum_{i\sigma\sigma'} \left\{\left[\boldsymbol{m}_i\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\right] c^\dagger_{i\sigma} c_{i\sigma'} - \left[\boldsymbol{m}_i\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\right]^* c_{i\sigma} c^\dagger_{i\sigma'}\right\} \\
&- \frac{1}{2}\sum_i \left\{\Delta_i (c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} - c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}) + \Delta^*_i (c_{i\uparrow} c_{i\downarrow} - c_{i\downarrow} c_{i\uparrow})\right\}
\end{aligned} \tag{32}$$

Using the Nambu⊗Spin basis, this can be written in the compact form:

$$\mathcal{H} = E_0 + \frac{1}{2}\sum_{ij} \hat{c}^\dagger_i \hat{H}_{ij} \hat{c}_j, \tag{33}$$

$$\hat{H}_{ij} = \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta^\dagger_{ij} & -H^*_{ij} \end{pmatrix}, \tag{34}$$

where we defined $H_{ij} = -(\mu_i + \boldsymbol{m}_i\cdot\boldsymbol{\sigma})\delta_{ij} - t_{ij} - (i\boldsymbol{\alpha}_i \times \boldsymbol{d}_{ij})\cdot\boldsymbol{\sigma}$ and $\Delta_{ij} = \Delta\,\delta_{ij}\, i\sigma_2$. We have here not bothered explicitly restricting the sums to nearest-neighbour pairs, instead relying on t_{ij} and $\boldsymbol{d}_{ij}$ being set to zero for non-neighbour sites. In systems with electromagnetic fields, the t_{ij} become complex and μ_i are modified accordingly. Note that this matrix has the same symmetry as in e.g. Ref. [11].

2.2 Lattice space

It is now convenient to define another set of operators in Lattice⊗Nambu⊗Spin space,[4] which allows us to compress eq. (33) even more. Defining the operator

$$\check{c} \equiv (\hat{c}_1, \hat{c}_2, \ldots, \hat{c}_N), \tag{35}$$

[4] Nagai [11] uses Nambu⊗Lattice⊗Spin space, so the matrix structure depends on author.

along with the extended Hamiltonian matrix

$$\check{H} \equiv \begin{pmatrix} \hat{H}_{11} & \cdots & \hat{H}_{1N} \\ \vdots & \ddots & \vdots \\ \hat{H}_{N1} & \cdots & \hat{H}_{NN} \end{pmatrix}, \tag{36}$$

we can now finally write the Hamiltonian of the system as

$$\mathcal{H} = E_0 + \frac{1}{2}\check{c}^\dagger \check{H} \check{c}. \tag{37}$$

The matrix $\check{H}$ is very sparse. The diagonal blocks $\hat{H}_{ii}$ are generally nonzero, but the off-diagonal blocks $\hat{H}_{ij}$ are only nonzero when the hopping amplitudes t_{ij} are, i.e. when lattice sites i and j correspond to nearest neighbours. Although we only use one index i here, this index is used to represent both 2D and 3D systems; for example, in 2D we can use coordinates $1 \leq i_x \leq N_x, 1 \leq i_y \leq N_y$, which can be mapped to a single lattice index $i = 1 + (i_x - 1) + N_x(i_y - 1)$.[5] In such a situation, $t_{i,i+1}$ and $t_{i+1,i}$ would be nearest-neighbour hopping along the x-axis and $t_{i,i+N_x}$ and $t_{i+N_x,i}$ would be nearest-neighbour hopping along the y-axis, so $\check{H}$ would have only 5 nonzero diagonals in lattice space.

2.3 Particle-hole symmetry

We generally want to diagonalize the Hamiltonian $\mathcal{H}$, which we can accomplish by diagonalizing the $4N \times 4N$ matrix $\check{H}$. The eigenvalues E_n of this matrix can be defined as follows, where $\check{\chi}_n$ are the corresponding $4N$-element eigenvectors:

$$\check{H}\check{\chi}_n = E_n \check{\chi}_n. \tag{38}$$

Expanding this equation in lattice space, i.e. decomposing $\check{\chi}_n = (\hat{\chi}_{n1}, \ldots, \hat{\chi}_{nN})$ into one bispinor per lattice site $i \in \{1, \ldots, N\}$, we can rewrite the problem as

$$\sum_j \hat{H}_{ij}\hat{\chi}_{nj} = E_n \hat{\chi}_{ni}. \tag{39}$$

We can now decompose the bispinors $\hat{\chi}_{ni} = (u_{ni}, v_{ni})$ into constituent electron spinors u and a hole spinors v. Writing out the Nambu-space structure we find

$$\sum_j \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^\dagger & -H_{ij}^* \end{pmatrix} \begin{pmatrix} u_{nj} \\ v_{nj} \end{pmatrix} = E_n \begin{pmatrix} u_{nj} \\ v_{nj} \end{pmatrix}. \tag{40}$$

We now write the electron and hole equations separately,

$$\sum_j \big(+ H_{ij}u_{nj} + \Delta_{ij}v_{nj} \big) = E_n u_{nj}, \tag{41}$$

$$\sum_j \big(- H_{ij}^* v_{nj} + \Delta_{ij}^\dagger u_{nj} \big) = E_n v_{nj}, \tag{42}$$

[5] In a 0-indexed programming language this relation is simply $i = i_x + N_x i_y + N_x N_y i_z$.

and complex-conjugate the second equation using the fact that $\Delta_{ij}^\dagger = -\Delta_{ij}^*$,

$$\sum_j \big(H_{ij}u_{nj} + \Delta_{ij}v_{nj}\big) = +E_n u_{nj}, \tag{43}$$

$$\sum_j \big(H_{ij}v_{nj}^* + \Delta_{ij}u_{nj}^*\big) = -E_n v_{nj}^*. \tag{44}$$

This shows that if $\check{\chi}_n = (u_{n1}, v_{n1}, u_{n2}, v_{n2}, \ldots)$ is an eigenvector with eigenvalue $+E_n$, then $(v_{n1}^*, u_{n1}^*, v_{n2}^*, u_{n2}^*, \ldots)$ must be another with eigenvalue $-E_n$. Note that this symmetry implies that the two Hamiltonians $\mathcal{H} = E_0 \pm (1/2)\check{c}^\dagger \check{H}\check{c}$ should have the same energy spectrum and in practice describe the same physics.

2.4 Diagonalization

The eigenvalues E_n and eigenvectors $\check{\chi}_n$ of the matrix $\check{H}$ were defined in eq. (38). Let us now define a matrix $\check{X} = \big[\check{\chi}_n\big]$ constructed from the eigenvectors and $\check{D} \equiv \mathrm{diag}(E_{-2N}, \ldots, E_{-1}, E_{+1}, \ldots, E_{+2N})$ from the eigenvalues. Inspired by the particle-hole symmetry we derived, we label the eigenvalues $E_{-n} = -E_{+n}$. It is then known from linear algebra that a Hermitian matrix $\check{H}$ can be factorized as

$$\check{H} = \check{X}\check{D}\check{X}^{-1} = \check{X}\check{D}\check{X}^\dagger. \tag{45}$$

Defining a new basis $\check{c} \equiv \check{X}\check{\gamma}$, we see that we can rewrite the Hamiltonian as

$$\mathcal{H} = E_0 + \frac{1}{2}\check{c}^\dagger\check{H}\check{c} = E_0 + \frac{1}{2}\check{\gamma}^\dagger\check{D}\check{\gamma} = E_0 + \frac{1}{2}\sum_n E_n \gamma_n^\dagger \gamma_n, \tag{46}$$

where we in the last step expanded the matrix multiplications of $\check{\gamma} = [\gamma_n]$ into a sum over the $4N$ components $n = \pm 1, \ldots, \pm 2N$.

Let us now take a closer look at the operator $\check{\gamma} = \check{X}^\dagger\check{c}$. Its components are:

$$\gamma_n = \sum_{i\sigma}(u_{n,i\sigma}^* c_{i\sigma} + v_{n,i\sigma}^* c_{i\sigma}^\dagger). \tag{47}$$

If γ_n is the eigenvector corresponding to a positive eigenvalue E_n, then the particle-hole symmetry from the previous subsection indicates that there must be another eigenvector γ_{-n} with the eigenvalue E_{-n}, which can be written

$$\gamma_{-n} = \sum_{i\sigma}(v_{n,i\sigma} c_{i\sigma} + u_{n,i\sigma} c_{i\sigma}^\dagger). \tag{48}$$

Let us now take the Hermitian conjugate of this:

$$\gamma_{-n}^\dagger = \sum_{i\sigma}(v_{n,i\sigma}^* c_{i\sigma}^\dagger + u_{n,i\sigma}^* c_{i\sigma}). \tag{49}$$

Thus, we conclude that $\gamma_{-n}^\dagger = \gamma_{+n}$. This means that the eigenvectors γ_{+n} corresponding to positive eigenvalues $E_{+n} = +E_n$ and the eigenvectors γ_{-n} corresponding to negative eigenvalues $E_{-n} = -E_n$ are not actually independent.

This conclusion can be understood as follows. We started with a Hamiltonian described in terms of $2N$ electron degrees of freedom $c_{i\sigma}$, but ended up with a Hamiltonian that have $4N$ electron and hole degrees of freedom $\hat{c}_i$. This change occurred when rewriting the equations in Nambu space at the beginning of this section. However, the number of physical degrees of freedom remains the same. The fact that γ_n for $n > 0$ ($E_n > 0$) and $n < 0$ ($E_n < 0$) are not independent resolves this issue: if we keep only $E_n > 0$, these correspond to $2N$ eigenvalues.

Let us now rewrite the Hamiltonian using only the independent operators:

$$\mathcal{H} = E_0 + \frac{1}{2}\sum_{n>0} E_{+n}\gamma^\dagger_{+n}\gamma_{+n} + \frac{1}{2}\sum_{n<0} E_{+n}\gamma^\dagger_{+n}\gamma_{+n} \tag{50}$$

$$= E_0 + \frac{1}{2}\sum_{n>0} E_{+n}\gamma^\dagger_{+n}\gamma_{+n} + \frac{1}{2}\sum_{n>0} E_{-n}\gamma^\dagger_{-n}\gamma_{-n} \tag{51}$$

$$= E_0 + \frac{1}{2}\sum_{n>0} E_{+n}\gamma^\dagger_{+n}\gamma_{+n} - \frac{1}{2}\sum_{n>0} E_{+n}\gamma_{+n}\gamma^\dagger_{+n} \tag{52}$$

$$= E_0 + \frac{1}{2}\sum_{n>0} E_n(\gamma^\dagger_n\gamma_n - \gamma_n\gamma^\dagger_n). \tag{53}$$

We used the above-mentioned symmetry to rewrite everything in terms of $n > 0$, which should be $2N$ independent operators. Using $\{\gamma^\dagger_n, \gamma_n\} = 1$, we conclude

$$\mathcal{H} = E_0 + \sum_{n>0} E_n(\gamma^\dagger_n\gamma_n - 1/2), \tag{54}$$

which has a similar form as the results in Jacob's notes on the BdG formalism.[6]

2.5 Self-consistency equation

We previously defined the superconducting gap as $\Delta(\boldsymbol{r}) \equiv U(\boldsymbol{r})\langle\psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r})\rangle$, which in the tight-binding formalism becomes $\Delta_i = U_i\langle c_{i\uparrow}c_{i\downarrow}\rangle$. Note that

$$c_{i\sigma} = \sum_n u_{n,i\sigma}\gamma_n \tag{55}$$

$$= \sum_{n>0}(u_{+n,i\sigma}\gamma_{+n} + u_{-n,i\sigma}\gamma_{-n}) \tag{56}$$

$$= \sum_{n>0}(u_{+n,i\sigma}\gamma_{+n} + v^*_{+n,i\sigma}\gamma^\dagger_{+n}). \tag{57}$$

[6] Note that if the BdG equation is solved via direct diagonalization, it may be more efficient to restrict the sum to positive momenta $\boldsymbol{k} > 0$ rather than positive energies $E_n > 0$.

Let us now calculate the expectation value $\langle c_{i\uparrow}c_{i\downarrow}\rangle$. Assuming a Fermi-Dirac distribution function $f(E)$, we get $\langle\gamma_n^\dagger\gamma_n\rangle = f(E_n)$ and $\langle\gamma_n\gamma_n^\dagger\rangle = 1 - f(E_n)$, so:

$$\langle c_{i\uparrow}c_{i\downarrow}\rangle = \sum_{n,m>0}\left\{v_{n,i\uparrow}^* u_{m,i\downarrow}\langle\gamma_n^\dagger\gamma_m + u_{n,i\uparrow}v_{m,i\downarrow}^*\langle\gamma_n\gamma_m^\dagger\rangle\rangle\right\} \tag{58}$$

$$= \sum_{n>0}\left\{v_{n,i\uparrow}^* u_{n,i\downarrow}f(E_n) + u_{n,i\uparrow}v_{n,i\downarrow}^*[1-f(E_n)]\right\}. \tag{59}$$

This produces the following self-consistency equation,

$$\Delta_i = U_i\sum_{n>0}\left\{u_{n,i\downarrow}v_{n,i\uparrow}^* f(E_n) + u_{n,i\uparrow}v_{n,i\downarrow}^*[1-f(E_n)]\right\}. \tag{60}$$

Further simplification is possible via particle-hole symmetry $1 - f(E_n) = f(-E_n)$ and the identities $f(\pm E_n) = [1-\tanh(\pm E_n/2T)]/2$. However, at this point, we may as well keep this version, which makes it easier to update the distribution function $f(E)$ if we want to generalize the equations to nonequilibrium systems.

Note that I have used the notation $\hat{\chi}_{ni} \equiv (u_{ni\uparrow}, u_{ni\downarrow}, v_{ni\uparrow}, v_{ni\downarrow})$ herein, while in Jacob's lecture notes $(u_{in}, v_{in}, w_{in}, x_{in})$ is used instead. Translating the notations I actually obtain the same result as eq. (10.50) in Jacob's lecture notes:

$$\Delta_i = U_i\sum_{n>0}\left\{v_{in}w_{in}^* f(E_n) + u_{in}x_{in}^*[1-f(E_n)]\right\}. \tag{61}$$

2.6 Summary

Let us now combine the results we have found so far. The Bogoliubov–de Gennes Hamiltonian can be expressed using the following set of matrices:

$$\mathcal{H} = E_0 + \frac{1}{2}\check{c}^\dagger\check{H}\check{c}, \qquad \check{H} = \left[\hat{H}_{ij}\right], \qquad \hat{H}_{ij} = \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^\dagger & -H_{ij}^* \end{pmatrix}. \tag{62}$$

We then just have to plug in the right H_{ij} and Δ_{ij} for a given system. Later, we can generalize these by deriving new terms from an extended Hubbard model. Note that we should only retain positive eigenvalues $E_n > 0$ of this Hamiltonian, which in our notation is indicated by restricting relevant eigenstate sums to $n > 0$. The above should be solved together with a self-consistency equation,

$$\Delta_i = U_i\sum_{n>0}\left\{u_{n,i\downarrow}v_{n,i\uparrow}^* f(E_n) + u_{n,i\uparrow}v_{n,i\downarrow}^*[1-f(E_n)]\right\}. \tag{63}$$

With this, we have derived a form of the BdG equations that is as consistent as possible with the version of the Usadel equation used during my PhD research.

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