# 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 try to "recycle" the mean-field Hamiltonian that we previously used to derive the Usadel equation. This ensures that the conventions and notations we use 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 scattering and mean-field ferromagnetism. The second term covers the two-particle interactions that give rise to superconductivity.

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,

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

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 $\boldsymbol{r}$:

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

[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.

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:

$$\mathcal{H} = \sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r}\, \psi^\dagger_\sigma(\boldsymbol{r}) H_{\sigma\sigma'}(\boldsymbol{r})\, \psi_{\sigma'}(\boldsymbol{r}) \tag{4}$$

$$= \sum_{ij\sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma'} \int \mathrm{d}\boldsymbol{r}\, w^*(\boldsymbol{r} - \boldsymbol{R}_i) H_{\sigma\sigma'}(\boldsymbol{r})\, w(\boldsymbol{r} - \boldsymbol{R}_j) \tag{5}$$

$$\equiv \sum_{i\sigma\sigma'} \epsilon_i^{\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'} - \sum_{\langle ij\rangle\sigma\sigma'} t_{ij}^{\sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma'} + \cdots . \tag{6}$$

This procedure provides the rigorous connection between the original model and the lattice model. In this case, we only included local terms $\epsilon_i$ and nearest-neighbour hopping integrals $t_{ij}$, but we could in theory also include e.g. next-nearest-neighbour interactions in this series expansion. The spin indices again allow for spin-dependent processes, e.g. spin-flip and spin-orbit scattering.

## 1.1 Non-interacting electrons

Using the above, let us now translate the Hamiltonian used to derive the Usadel equation to the lattice model. Translating eq. (3.3) in my project thesis [3] to the notation of eq. (1), and neglecting 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 described above then provides spin-independent contributions to the Hamiltonian describing the chemical potential $\mu$ 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.

## 1.2 Electromagnetic fields

Let us now consider electromagnetic fields. Eq. (3.2) in my project thesis [3] is:

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

Written out explicitly, 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 $\mu_i$ 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 give a kinetic energy contribution. The associated hopping integral is:

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

Let us now consider the inverse hopping $\tau_{ji}$. 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 $\tau_{ij}$ above, and this parameter still satisfies the property $t_{ji}' = t_{ij}'^*$. Note that if the orbitals $w(\boldsymbol{r})$ can be chosen to be purely real, then the hopping coefficients $t_{ij}'$ would be purely real for $\boldsymbol{A} = 0$ and get imaginary contributions when $\boldsymbol{A} \neq 0$. In the following subsections, we will refer to the chemical potential $\mu_i$ and hopping integrals $t_{ij}$ without primes, but will keep in mind the shifts above that incorporate electromagnetic fields.

## 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 a 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 $\tau_{ji}^{\sigma'\sigma} = (\tau_{ij}^{\sigma\sigma'})^*$. From here on, we include these spin-orbit effects into the regular hopping terms $t_{ij}^{\sigma\sigma'} \equiv t'_{ij} + \tau_{ij}^{\sigma\sigma'}$, which we will denote without explicit primes.

## 1.4 Ferromagnetism

Based on eq. (3.18) in my project thesis [3], we can write the Hamiltonian contribution for an itinerant ferromagnet treated via the mean-field approach:

$$H_{\sigma\sigma'} = -\big[\boldsymbol{h}(\boldsymbol{r}) \cdot \boldsymbol{\sigma}\big]_{\sigma\sigma'}. \tag{17}$$

From this, we can write the lattice Hamiltonian for such a ferromagnet as

$$\mathcal{H}_F = -\sum_{i\sigma\sigma'} \big[\boldsymbol{h}_i \cdot \boldsymbol{\sigma}\big]_{\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'}, \tag{18}$$

where the exchange field $\boldsymbol{h}_i \equiv \int \mathrm{d}\boldsymbol{r}\, \boldsymbol{h}(\boldsymbol{r})|w(\boldsymbol{r} - \boldsymbol{R}_i)|^2 \approx \boldsymbol{h}(\boldsymbol{R}_i)$, 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 $\mu'_{i\sigma\sigma'} \equiv \mu_i + [\boldsymbol{h}_i \cdot \boldsymbol{\sigma}]_{\sigma\sigma'}$. It is also worth noting that $[\boldsymbol{h}_i \cdot \boldsymbol{\sigma}]_{\sigma'\sigma} = [\boldsymbol{h}_i \cdot \boldsymbol{\sigma}^*]_{\sigma\sigma'}$, which we will use later.

We have here neglected a mean-field contribution that is proportional to $\boldsymbol{h}^2$ [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.

## 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:[2]

$$\mathcal{H}_S = -\int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r})\, \psi^\dagger_\downarrow(\boldsymbol{r})\psi^\dagger_\uparrow(\boldsymbol{r})\psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r}). \tag{19}$$

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 [5]:

$$\mathcal{H}_S = -\int \mathrm{d}\boldsymbol{r}\, \Big\{\Delta(\boldsymbol{r})\, \psi^\dagger_\downarrow(\boldsymbol{r})\psi^\dagger_\uparrow(\boldsymbol{r}) + \Delta^*(\boldsymbol{r})\, \psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r})\Big\}. \tag{20}$$

[2] 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 [5].

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:

$$\begin{aligned}\mathcal{H}_S &= -\sum_{ij} c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} \int \mathrm{d}\boldsymbol{r}\, \Delta(\boldsymbol{r})\, w^*(\boldsymbol{r}-\boldsymbol{R}_i)\, w^*(\boldsymbol{r}-\boldsymbol{R}_j) + \text{h.c.} \\ &\equiv -\sum_{ij} \Delta_{ij} c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} + \text{h.c.}\end{aligned} \tag{21}$$

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:

$$\mathcal{H}_S = -\sum_i \left\{ \Delta_i c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} + \Delta^*_i c_{i\uparrow} c_{i\downarrow} \right\}. \tag{22}$$

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:

$$E_0 = \int \mathrm{d}\boldsymbol{r}\, U \langle \psi^\dagger_\downarrow \psi^\dagger_\uparrow \rangle \langle \psi_\uparrow \psi_\downarrow \rangle = \int \mathrm{d}\boldsymbol{r}\, U \frac{\Delta^*}{U} \frac{\Delta}{U} = \int \mathrm{d}\boldsymbol{r}\, \frac{|\Delta|^2}{U}. \tag{23}$$

Performing the tight-binding transformation, this readily transforms into

$$E_0 = \sum_i \frac{|\Delta_i|^2}{U_i}. \tag{24}$$

This matches eq. (4) in Atousa's paper [6]. More such terms must be added we are to e.g. treat magnetism self-consistently [cf. eq. (3.14) in my project thesis].

## 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 previously used to derive the Usadel equation, all notations and conventions should be compatible.

$$\begin{aligned}\mathcal{H} = E_0 &- \sum_{i\sigma} \mu_i c^\dagger_{i\sigma} c_{i\sigma} - \sum_{\langle ij\rangle \sigma\sigma'} t^{\sigma\sigma'}_{ij} c^\dagger_{i\sigma} c_{j\sigma'} \\ &- \sum_{i\sigma\sigma'} \left[\boldsymbol{h}_i \cdot \boldsymbol{\sigma}\right]_{\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'} - \sum_i \left\{ \Delta_i c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} + \Delta^*_i c_{i\uparrow} c_{i\downarrow} \right\}.\end{aligned} \tag{25}$$

This result seems consistent with eq. (2.5) in Ref. [1], eqs. (10–11) in Atousa's paper [6], and eqs. (1) and (3) in Lina's paper [7]. 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.

# 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:

$$\hat{c}_i \equiv (c_{i\uparrow}, c_{i\downarrow}, c^\dagger_{i\uparrow}, c^\dagger_{i\downarrow}). \tag{26}$$

This corresponds to the $D_i$ operators in Terrade's thesis [8] 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 $\{c^\dagger_{i\sigma}, c_{i\sigma}\} = 1$, so we can write the term as

$$\sum_{i\sigma} \mu_i c^\dagger_{i\sigma} c_{i\sigma} = \frac{1}{2}\sum_{i\sigma} \mu_i \left\{ c^\dagger_{i\sigma} c_{i\sigma} - c_{i\sigma} c^\dagger_{i\sigma} \right\} + \frac{1}{2}\sum_{i\sigma} \mu_i. \tag{27}$$

Correspondingly, for the hopping term we get

$$\sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} = \frac{1}{2}\sum_{\langle ij\rangle\sigma} t_{ij} \left\{ c^\dagger_{i\sigma} c_{j\sigma} - c_{j\sigma} c^\dagger_{i\sigma} \right\} = \frac{1}{2}\sum_{\langle ij\rangle\sigma} \left\{ t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - t_{ji} c_{i\sigma} c^\dagger_{j\sigma} \right\}. \tag{28}$$

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:

$$\sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} = \frac{1}{2}\sum_{\langle ij\rangle\sigma} \left\{ t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - t^*_{ij} c_{i\sigma} c^\dagger_{j\sigma} \right\}. \tag{29}$$

For the ferromagnetic contribution, we get a similar derivation, where we again can use that $\boldsymbol{\sigma}_{\sigma'\sigma} = \boldsymbol{\sigma}^*_{\sigma\sigma'}$ to end up with a complex conjugation. The result is:

$$\sum_{i\sigma} h_{i\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'} = \frac{1}{2}\sum_{i\sigma} \left\{ h_{i\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'} - h^*_{i\sigma\sigma'} c_{i\sigma} c^\dagger_{i\sigma'} \right\}, \tag{30}$$

where we have introduced the notation $h_{i\sigma\sigma'} \equiv [\boldsymbol{h}_i \cdot \boldsymbol{\sigma}]_{\sigma\sigma'}$ for brevity. Regarding 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. The total Hamiltonian of the system can now be written as:

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

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

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

$$\hat{H}_{ij} = \begin{pmatrix}(\mu_i + \boldsymbol{h}_i\cdot\boldsymbol{\sigma})\delta_{ij} + t_{ij} & \Delta(-i\sigma_2)\delta_{ij} \\ \Delta^*(+i\sigma_2)\delta_{ij} & -(\mu_i + \boldsymbol{h}_i\cdot\boldsymbol{\sigma}^*)\delta_{ij} - t^*_{ij}\end{pmatrix} \tag{34}$$

We have here not bothered explicitly restricting the $t_{ij}$ sum to nearest-neighbour pairs, instead relying on those parameters being set to zero for non-neighbours. The $t_{ij}$ may be complex (gauge fields) and spin-dependent (spin-orbit coupling). Note that this result follows a more general pattern mentioned by e.g. Nagai [9],

$$\hat{H}_{ij} = \begin{pmatrix}H_{ij} & \Delta_{ij} \\ \Delta^\dagger_{ij} & -H^*_{ij}\end{pmatrix}. \tag{35}$$

## 2.2 Lattice space

It is now convenient to define another set of operators in Lattice⊗Nambu⊗Spin space,[3] which allows us to compress eq. (33) even more. Defining the operator

$$\check{c} \equiv (\hat{c}_1, \hat{c}_2, \ldots, \hat{c}_N), \tag{36}$$

along with a corresponding Hamiltonian matrix

$$\check{H} \equiv \begin{pmatrix}\hat{H}_{11} & \cdots & \hat{H}_{1N} \\ \vdots & \ddots & \vdots \\ \hat{H}_{N1} & \cdots & \hat{H}_{NN}\end{pmatrix}, \tag{37}$$

we can now finally write the Hamiltonian of the system as

$$\mathcal{H} = E_0 - \frac{1}{2}\check{c}^\dagger\check{H}\check{c}. \tag{38}$$

[3] Nagai [9] uses Nambu⊗Lattice⊗Spin space, so the matrix structure depends on the author.

$\check{H}$ is in general 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 single index is used to represent 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 $i = 1 + (i_x - 1) + N_x(i_y - 1)$. 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:

$$\check{H}\check{\chi}_n = E_n\check{\chi}_n. \tag{39}$$

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

$$\sum_j \hat{H}_{ij}\hat{\chi}_{nj} = E_n\hat{\chi}_{ni}. \tag{40}$$

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

$$\sum_j \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^\dagger & -H_{ij}^* \end{pmatrix} \begin{pmatrix} u_{nj} \\ v_{nj} \end{pmatrix} = E_n \begin{pmatrix} u_{nj} \\ v_{nj} \end{pmatrix}. \tag{41}$$

We now write the electron and hole equations separately,

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

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

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

$$\sum_j \big( H_{ij}u_{nj} + \Delta_{ij}v_{nj} \big) = +E_n u_{nj}, \tag{44}$$

$$\sum_j \big( H_{ij}v_{nj}^* + \Delta_{ij}u_{nj}^* \big) = -E_n v_{nj}^*. \tag{45}$$

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 one with eigenvalue $-E_n$.

Note that this symmetry implies that we would obtain the same energy spectrum whether we use $\mathcal{H} = E_0 - (1/2)\check{c}^\dagger \check{H} \check{c}$ or $\mathcal{H} = E_0 + (1/2)\check{c}^\dagger \check{H} \check{c}$. We can use this freedom to change to the more common (and more intuitive) definition

$$\mathcal{H} = E_0 + \frac{1}{2}\check{c}^\dagger \check{H} \check{c}. \tag{46}$$

## 2.4 Diagonalization

The eigenvalues $E_n$ and eigenvectors $\check{\chi}_n$ of the matrix $\check{H}$ were defined in eq. (39). Let us now define a matrix $\check{X} = \left[\check{\chi}_n\right]$ constructed from the eigenvectors and $\check{D} \equiv \mathrm{diag}(E_{-2N}, \ldots, E_{-1}, E_{+1}, \ldots, E_{+2N})$ from the eigenvalues. I here use the labeling $E_{-n} = -E_{+n}$, based on the previously derived symmetry. It is then known from linear algebra that the Hermitian matrix $\check{H}$ can be factorized as

$$\check{H} = \check{X}\check{D}\check{X}^{-1} = \check{X}\check{D}\check{X}^\dagger. \tag{47}$$

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

$$\mathcal{H} = E_0 + \frac{1}{2}\check{c}^\dagger \check{H} \check{c} = E_0 + \frac{1}{2}\check{\gamma}^\dagger \check{D} \check{\gamma} = E_0 + \frac{1}{2}\sum_n E_n \gamma_n^\dagger \gamma_n, \tag{48}$$

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 explicitly expand the $\check{\gamma}$ operators. The transformation equations are $\check{\gamma} = \check{X}^\dagger \check{c}$, which can be written out as

$$\begin{pmatrix} \gamma_{-2N} \\ \vdots \\ \gamma_{+2N} \end{pmatrix} = \begin{pmatrix} u_{-2N,1\uparrow} & \cdots & u_{+2N,1\uparrow} \\ u_{-2N,1\downarrow} & \cdots & u_{+2N,1\downarrow} \\ v_{-2N,1\uparrow} & \cdots & v_{+2N,1\uparrow} \\ v_{-2N,1\downarrow} & \cdots & v_{+2N,1\downarrow} \\ \vdots & \ddots & \vdots \\ u_{-2N,N\uparrow} & \cdots & u_{+2N,N\uparrow} \\ u_{-2N,N\downarrow} & \cdots & u_{+2N,N\downarrow} \\ v_{-2N,N\uparrow} & \cdots & v_{+2N,N\uparrow} \\ v_{-2N,N\downarrow} & \cdots & v_{+2N,N\downarrow} \end{pmatrix}^\dagger \begin{pmatrix} c_{1\uparrow} \\ c_{1\downarrow} \\ c_{1\uparrow}^\dagger \\ c_{1\downarrow}^\dagger \\ \vdots \\ c_{N\uparrow} \\ c_{N\downarrow} \\ c_{N\uparrow}^\dagger \\ c_{N\downarrow}^\dagger \end{pmatrix}, \tag{49}$$

or equivalently and more concisely,

$$\gamma_n = \sum_{i\sigma} (u_{n,i\sigma}^* c_{i\sigma} + v_{n,i\sigma}^* c_{i\sigma}^\dagger). \tag{50}$$

If $\gamma_n$ 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 $\gamma_{-n}$ with the eigenvalue $E_{-n}$, which can be written

$$\gamma_{-n} = \sum_{i\sigma} (v_{n,i\sigma} c_{i\sigma} + u_{n,i\sigma} c_{i\sigma}^\dagger). \tag{51}$$

Let us now take the Hermitian conjugate of this:

$$\gamma_{-n}^{\dagger} = \sum_{i\sigma} (v_{n,i\sigma}^{*} c_{i\sigma}^{\dagger} + u_{n,i\sigma}^{*} c_{i\sigma}). \tag{52}$$

Thus, we conclude that $\gamma_{-n}^{\dagger} = \gamma_{+n}$. This means that the eigenvectors $\gamma_{+n}$ corresponding to positive eigenvalues $E_{+n} = +E_n$ and the eigenvectors $\gamma_{-n}$ 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 occured 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 $\gamma_n$ 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:

$$\mathcal{H} = E_0 + \frac{1}{2} \sum_{n>0} E_{+n} \gamma_{+n}^{\dagger} \gamma_{+n} + \frac{1}{2} \sum_{n<0} E_{+n} \gamma_{+n}^{\dagger} \gamma_{+n} \tag{53}$$

$$= E_0 + \frac{1}{2} \sum_{n>0} E_{+n} \gamma_{+n}^{\dagger} \gamma_{+n} + \frac{1}{2} \sum_{n>0} E_{-n} \gamma_{-n}^{\dagger} \gamma_{-n} \tag{54}$$

$$= E_0 + \frac{1}{2} \sum_{n>0} E_{+n} \gamma_{+n}^{\dagger} \gamma_{+n} - \frac{1}{2} \sum_{n>0} E_{+n} \gamma_{+n} \gamma_{+n}^{\dagger} \tag{55}$$

$$= E_0 + \frac{1}{2} \sum_{n>0} E_n (\gamma_n^{\dagger} \gamma_n - \gamma_n \gamma_n^{\dagger}). \tag{56}$$

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

$$\mathcal{H} = E_0 + \sum_{n>0} E_n (\gamma_n^{\dagger} \gamma_n - 1/2), \tag{57}$$

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

## 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

$$c_{i\sigma} = \sum_n u_{n,i\sigma} \gamma_n \tag{58}$$

$$= \sum_{n>0} (u_{+n,i\sigma} \gamma_{+n} + u_{-n,i\sigma} \gamma_{-n}) \tag{59}$$

$$= \sum_{n>0} (u_{+n,i\sigma} \gamma_{+n} + v_{+n,i\sigma}^{*} \gamma_{+n}^{\dagger}). \tag{60}$$

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:

$$\langle c_{i\uparrow} c_{i\downarrow} \rangle = \sum_{n,m>0} \left\{ v_{n,i\uparrow}^* u_{m,i\downarrow} \langle \gamma_n^\dagger \gamma_m + u_{n,i\uparrow} v_{m,i\downarrow}^* \langle \gamma_n \gamma_m^\dagger \rangle \rangle \right\} \tag{61}$$

$$= \sum_{n>0} \left\{ v_{n,i\uparrow}^* u_{n,i\downarrow} f(E_n) + u_{n,i\uparrow} v_{n,i\downarrow}^* [1 - f(E_n)] \right\}. \tag{62}$$

This produces the following self-consistency equation,

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

One more simplification can be performed by noting the particle-hole symmetry $1 - f(E_n) = f(-E_n)$. We can simplify this further using $1 - f(+E_n) = f(-E_n)$ and $f(\pm E_n) = [1 - \tanh(\pm E_n / 2T)]/2$. However, at this point, we may as well keep this general expression, which makes it easier to later update the distribution function $f(E)$ when we want to consider nonequilibrium systems.

Note that herein, I use the notation $\hat{\chi}_{ni} \equiv (u_{ni\uparrow}, u_{ni\downarrow}, v_{ni\uparrow}, v_{ni\downarrow})$, 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:

$$\Delta_i = U_i \sum_{n>0} \left\{ v_{in} w_{in}^* f(E_n) + u_{in} x_{in}^* [1 - f(E_n)] \right\}. \tag{64}$$

## 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:

$$\mathcal{H} = E_0 + \frac{1}{2} \check{c}^\dagger \check{H} \check{c}, \qquad \check{H} = \left[ \hat{H}_{ij} \right], \qquad \hat{H}_{ij} = \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^\dagger & -H_{ij}^* \end{pmatrix}. \tag{65}$$

We then just have to plug in the normal-state $H_{ij} = (\mu_i + \boldsymbol{h}_i \cdot \boldsymbol{\sigma}) \delta_{ij} + t_{ij}$ and superconducting $\Delta_{ij} = \Delta(-i\sigma_2)\delta_{ij}$ for a physical system. Later, we can generalize $H_{ij}$ and $\Delta_{ij}$ by deriving new terms from an extended Hubbard model. Note that we should only retain positive eigenvalues $E_n > 0$ of this Hamiltonian. These should be solved together with a self-consistency equation for the gap,

$$\Delta_i = U_i \sum_{n>0} \left\{ u_{n,i\downarrow} v_{n,i\uparrow}^* f(E_n) + u_{n,i\uparrow} v_{n,i\downarrow}^* [1 - f(E_n)] \right\}. \tag{66}$$

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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