



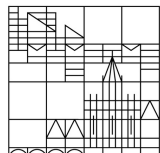
Proximity Effects *in* *Altermagnetic Systems*

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a bachelor thesis.

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Acknowledgment

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1 Theoretical Background

In order to describe the superconductors we are going to introduce the second quantisation formalism. It allows us to describe the wavefunction of a system using creation and annihilation operators over energystates of the system and simplify a lot the notation. The mathematical fundation of this formalism lays in the Hilbert space, its dual space and furthermore we are going to introduce the Fock space.

It's also relevant for our study that we are going to work on fermions. The formalism stays the same for bosons but the results are fundamentally different. One can mention the Pauli principle as an exemple which only applies on fermion is can be derived with the help of the second quantisation.

1.1 Bosons and fermions

We consider without loss of generality the following hamiltonian.

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

with the single particle operator \hat{H}_0 and the interaction operator \hat{H}_I :

$$\hat{H}_0 = \sum_{i \in \llbracket N \rrbracket} \hat{h}_i(x_i), \quad \hat{h}_i(x_i) = -\frac{\hbar^2}{2m} \nabla_i^2 + \hat{U}(x_i)$$

Where we introduce the notation $\llbracket N \rrbracket = \{n \in \mathbb{N} : n \leq N\}$. We call it single particle operator because the operator only applies on a particle. It may depend from the particle's position \mathbf{r} or spin s : $x_i := (\mathbf{r}, s) \in \mathcal{X} \subseteq \mathbb{R}^3 \times \mathbb{S}$. For exemple we have for an electron $\mathbb{S} = -\frac{1}{2}, \frac{1}{2}$. A single particle operator is in this case the sum of the kinetic- and potential energy operators.

Further we describe a quantum state that a particle can occupy with a wavefunction $\phi_\nu(x)$, which own a certain energy $\epsilon_\nu \in \mathbb{R}$. This energy depends on the wavevector and the spin of the particle: $\nu = (\mathbf{k}, \sigma)$. The fundamental equation of quantum mechanics relates the wave function with the hamiltonian using the energy of the state:

$$\hat{h}\phi_\nu(x) = \epsilon_\nu \phi_\nu(x)$$

The wave function lay in the Hilbert space [more details?]. Therefor $\phi_\nu(x)$ are eigenfunction or -states of the Hamiltonian with eigenvalues ϵ_ν . Further the wavefunction should build an orthonormal basis:

$$\int_{\mathcal{X}} \phi_{\nu'}(x) \phi_\nu(x) dx = \delta_{\nu'\nu}.$$

ν and ν' are two different states. We introduced here the korenker delta $\delta_{\nu'\nu}$ which is one when the two indicies are equal and zero otherwise. Because the spin s is not continuous one can understand the integral in the following way:

$$\int_{\mathcal{X}} dx = \sum_{s \in \mathbb{S}} \int_{\mathbb{R}^3} d^3r$$

where $\int_{\mathbb{R}^3} d^3r = \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} dr_1 dr_2 dr_3$. We integrate over all possible states.

Now that we can describe one particle we want to describe a system containing many instance of that particle. The wavefunction sums up all possible combination of wavefunction in the system and should stay normalized. A combination is discribed as the product of the wavefunction of the particle in a certain state. These particle can be swaped and therefore we need to consider all combinations. We restrict ourselves to fermions and bosons. We admit having $N \in \mathbb{N}$ paricles in the system.

Bosons The many-particle wavefunction of the bosons is a symetric (exponent S) under swap of two particles.

$$\Phi^{(S)}(x_1, \dots, x_N) = \left(N! \prod_N (n_\nu)! \right)^{-\frac{1}{2}} \sum_{P \in S_n} P \phi_{\nu_1}(x_1) \dots \phi_{\nu_N}(x_N)$$

This represents the an eigenfunction of the non interacting bosonic-Hamiltonian. We used n_ν , which represents the number of particle in the state ν . Therefor we usaly call it the occupation number of the state ν . For fermion this integer has no constrain in general. The permutation set S_n contains all the possbile combinations of x_i in the state ν_j for $i, j \in \llbracket N \rrbracket$.

Fermions Fermions are a bit different, their many-particle fermion wavefunction is antisymmetric under swap of two particles. We denote it as

$$\Phi^{(A)}(x_1, \dots, x_N) = (N!)^{-\frac{1}{2}} \sum_{P \in S_n} \text{sgn}(P) \cdot P \phi_{\nu_1}(x_1) \dots \phi_{\nu_N}(x_N).$$

which is an eigenfunction of the non interacting fermionic-Hamiltonian. sgn represents the signum function. Applied on a permutation P it is one if P is even and minus one if P is even.

We already know that the Pauli principle implies that it can be up to one particle in each energy state. We therefore have $n_\nu \in \{0, 1\}$. The normalisization factor is the same but the product over the ones vanishes.

At this point one might have recognised the formula of the determinant

$$\Phi^{(A)}(x_1, \dots, x_N) = (N!)^{-\frac{1}{2}} \det \begin{pmatrix} \varphi_{\nu_1}(x_1) & \dots & \varphi_{\nu_1}(x_N) \\ \vdots & & \vdots \\ \varphi_{\nu_N}(x_1) & \dots & \varphi_{\nu_N}(x_N) \end{pmatrix},$$

which vanishes if two rows or columns are identic. We usaly describe this expression as the Slatter determinant. This means that the probability of finding two fermions in the same state is zero. This is the Pauli principle. Only one or no particle may occupy each state.

Further we entcounter a major problem. The many-particle wave function of fermions is defined up to a sign. For instance if we consider two particles “having” x_1 and x_2 , we have two possible state ν_1 and ν_2 . To possible solttuion are

$$\begin{aligned} \Phi^{(A_1)} &= \frac{1}{\sqrt{2}} (\varphi_{\nu_1}(x_1) \varphi_{\nu_2}(x_2) - \varphi_{\nu_1}(x_2) \varphi_{\nu_2}(x_1)) \\ \text{or } \Phi^{(A_2)} &= \frac{1}{\sqrt{2}} (\varphi_{\nu_1}(x_2) \varphi_{\nu_2}(x_1) - \varphi_{\nu_1}(x_1) \varphi_{\nu_2}(x_2)) \\ &= -\Phi^{(A_1)}. \end{aligned}$$

This sign difference may lead to computation errors. We aim to give a labeling to our states when we count them and keep it when it comes to build the Slater determinant.

These bosonic and fermionic wavefunctions are eigenstate of the Hamiltonian \hat{H}_0 and the corresponding eigenvalue E_ν is given by summing the energy of each state times its occupation number: $E_\nu = \sum_\nu \epsilon_\nu n_\nu$. For this reason it's important that they build an orthonormal basis:

$$\int_{\mathcal{X}^N} \Phi_a^*(x_1, \dots, x_N) \Phi_b(x_1, \dots, x_N) d^N x = \delta_{ab}.$$

Therefore we can expand any many-particle wavefunction Ψ as the linear combination of these:

$$\Psi = \sum_a f_a \Phi_a(x_1, \dots, x_N)$$

where f_a is a coefficient and a a labeling.

What we just discussed is the so called first quantisation- or wave function formalism. Now we intend to introduce a better way of describing our system.

1.2 The second quantisation

For a better description of the many-particle system we introduce a simpler notation. The second quantisation lays on three important objects. States described as “ket”. We put any relevant information between the ket e.g. $|\mathbf{k}, \sigma, \dots\rangle$. Then we need operators that act on these states to allow interactions in the system. We need an operator that creates a state and another that annihilates a state.

States In this section we describe a state as the number of particle that occupies each single-particle state. Therefore we order the state $1 < 2 < \dots < N$. We then can describe the wave function as follow $|n_1, \dots, n_N\rangle$.

Further the state where no particle are present is called the vacuum state and we denote it as $|0_{\nu_1}, \dots, 0_{\nu_N}\rangle = |0\rangle$.

1.2.1 Second quantisation for fermions

Creation operator c_ν^\dagger The creation operator adds a particle in the state that is concerned and rephase the state:

$$c_\nu^\dagger |n_1, \dots, n_\nu, \dots\rangle = (-1)^{\sum_{\mu < \nu} n_\mu} (1 - n_\nu) |n_1, \dots, n_\nu + 1, \dots\rangle$$

We notice the $(1 - n_\nu)$ term which avoid to create a particle at the state, if one already exist. This is the expression of the Pauli-principle. and we can then construct a state by applying this operator after another on the vacuum state. To avoid the minus one to add a negative sign, we start from the end and add the particle backwards in the order of the state:

$$|n_1, \dots, n_N\rangle = (c_1^\dagger)^{n_1} \cdot \dots \cdot (c_N^\dagger)^{n_N} |0\rangle$$

Anihilation operator c_ν Likewise the anihilation operator destroys a particle in the corresponding state. The operator reads

$$c_\nu |n_1, \dots, n_\nu, \dots\rangle = (-1)^{\sum_{\mu < \nu} n_\mu} (n_\nu) |n_1, \dots, n_\nu - 1, \dots\rangle.$$

We can easily recognise that due to the n_ν -term, destroying a particle that doesn't exist gives zero, so it's only possible to destroy particle that exist. Further we intend to introduce some few computation rules that are going to help us later.

The anticommutator of two operator reads $[A, B]_+$ or $\{A, B\} := AB + BA$ and is an operator as well. We're going to stick with $[A, B]_+$ since it's more consistent with the commutator notation $[A, B]_-$ (or simply $[A, B]$).

The following results are obtained by separating the $\nu = \mu$ from the $\nu \neq \mu$. We must also say that the dagger \dagger should be understood as the complex transpose of the operator and $(AB)^\dagger = B^\dagger A^\dagger$.

$$\begin{aligned}[c_\nu, c_\mu]_+ &= 0 \\ [c_\nu^\dagger, c_\mu^\dagger]_+ &= 0 \\ [c_\nu^\dagger, c_\mu]_+ &= \delta_{\mu, \nu}\end{aligned}$$

We can then combine the creation and annihilation operator to count the number of particles in a state:

$$c_\nu^\dagger c_\nu |n_1, \dots, n_\nu, \dots\rangle = n_\nu |n_1, \dots, n_\nu, \dots\rangle.$$

From this we can define the number operator $\hat{n}_\nu := c_\nu^\dagger c_\nu$ which we can combine in the total number operator

$$\hat{N} = \sum_\nu \hat{n}_\nu, \quad \text{where logically } N = \sum_\nu n_\nu$$

if we apply the operator on a state.

Second quantisation description of the single- and two- particle operators We first need to make an important observation between the Slater determinant and the single particle state to understand the following. First we introduce two basis elements $|\Phi_\alpha\rangle$ and $|\Phi_\beta\rangle$, which can be many-particles eigenstate of the system. We can also call them Slater determinant. Further we introduce the probability of the configuration $|\Phi_\alpha\rangle$ to scatter into the $|\Phi_\beta\rangle$ due to the action of an operator A (momentum, potential, interactions,...). This is described by the matrix element $\langle\Phi_\alpha|A|\Phi_\beta\rangle$ which involves the single particle states $|\alpha_1\rangle, \dots, |\alpha_N\rangle$ of $|\Phi_\alpha\rangle$ and $|\beta_1\rangle, \dots, |\beta_N\rangle$ of $|\Phi_\beta\rangle$.

$$\langle\Phi_\alpha|A|\Phi_\beta\rangle = \sum_{i,j} C_{ij} \langle\alpha_i|A|\beta_j\rangle$$

involving some constants C_{ij} . This describes the overlap of the two configurations, after that we modified $|\Phi_\beta\rangle$ with A . On the right hand side (r.h.s) we introduced the bracket scalar product notation. The bra $\langle\alpha|$ lives in the dual space of the Hilbert space. One reads it as the complex transpose of $|\alpha\rangle$.

We recall the single particle Hamiltonian we introduced earlier. Its second quantisation representation reads

$$\hat{H}_0 = \sum_{i \in \llbracket N \rrbracket} \hat{h}(x_i) \rightsquigarrow \sum_{\alpha, \beta} \langle\alpha|\hat{h}|\beta\rangle c_\alpha^\dagger c_\beta$$

where α and β are single-particle states of the system. $c_\alpha^\dagger c_\beta$ tries to transfer a fermion from the state $|\beta\rangle$ to the state $|\alpha\rangle$. We have

$$\langle\alpha|\hat{h}|\beta\rangle = \int \varphi_\alpha^*(x) \hat{h}(x) \varphi_\beta(x) dx$$

where x still represents the position and the spin of the particle.

\hat{h} is a single particle operator, it means it acts on one particle at a time. Two states are going to be changed. $|\alpha\rangle$ loses a particle and $|\beta\rangle$ gains one. We say for instance, that the configuration before the scattering is $|\Phi\rangle$ and after the scattering is $|\Phi'\rangle$. This means, if our two Slater determinant $|\Phi\rangle$ and $|\Phi'\rangle$ differs in more than two states, there are some scattering that we can't describe, so the overlap must be zero. We allow only two states to be modified. Otherwise the single-particle states differ and due to their orthonormal properties, we get a zero.

Similarly for the two-particle operator we have

$$\hat{H}_I = \frac{1}{2} \sum_{i \neq j \in \llbracket N \rrbracket} \hat{v}(x_i, x_j) \rightsquigarrow \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

involving a more nested overlap of the four states:

$$\langle\alpha\beta|\hat{v}|\gamma\delta\rangle = \int \int \varphi_\alpha^*(x) \varphi_\beta^*(x') \hat{v}(x, x') \varphi_\gamma(x) \varphi_\delta(x') dx dx'.$$

which modifies four states so the overlap of two slatter determinant vanishes if the determinant differ in at least four states.

The l.h.s of the equation is the matrix element $\langle \Phi_\alpha | \hat{v} | \Phi_\beta \rangle$ of the the operator \hat{v} , which involves two basis state $|\Phi_\alpha\rangle$ and $|\Phi_\beta\rangle$. On the r.h.s we have a description with wavefunctions, which own to the first quantisation. What we have here is the bridge between the first and the second quantisation. One could compute each side separately and notice that both formalism lead to the same result.

A useful tool that one can use is gives a wavefunction of a single-particle state:

$$\varphi_\alpha(x) = \langle x | \alpha \rangle$$

1.2.2 Second quantisation for bosons

1.3 Basis transformation

1.4 Interactive electron gas

The main transformation between the second quantisation to the first are the followings:

$$\langle \alpha | V | \beta \rangle = \int \varphi_\alpha^*(x) V(x) \varphi_\beta(x) dx$$

2 Superconductivity

Superconductivity can be illustrated as a phase transition of a meterial under a crital temperature. In the superconductive state the material become a perfect diamaget and its resistivity vanishes. We then observe some shielding currents that arise on it's surface and we can let flew a current for a very long time without loosing energy. The superconductive state is also described as Meissner state.

Suppose that we heat the material to the critical temperature T_c , some fluctuation effects arise and break the superconductive state. The shielding effects reacts different on the material. We usely distinguish type I and type II superconductors. The type I superconductor loose abruplty their magnetisation over T_c . Type II have a mixed state where the magnetisation slowly decreases until we can't measure it anymore.

The break of the superconductive state can be described as letting more and more filed flew inside of the material. Asuming that some particle are responsible for the superconductivity, the field achieve to penetrate where wo observe a lower density of these particles. The penetration is described as some magnetic field vortecies reaching a certain depth in the material.

The Meissner state is a thermodynamical state. We can show that the free energy of the superconductive state is higher than the normal state. This results in a lower entropy compered to the normal state.

2.1 Theoretical framework and BCS theory

The Hamiltonian of the system is discribed by the solid state physics. The consider the energy of the electrons and the ions in a lattice.

$$H = H_{e^-e^-} + H_{e^-ion} + H_{ion ion}$$

Each term consist of a kinetik and potential energy term. For a more mathematical approach we consider a system of N electrons and L ions.

$$\begin{aligned} H_{e^-e^-} &= \sum_{i \in [N]} \frac{p_i^2}{2m} + \sum_{i,j \in [N]} V_{\text{Coulomb}}^{e^-e^-}(\mathbf{r}_i - \mathbf{r}_j) \\ H_{ion ion} &= \sum_{i \in [M]} \frac{p_i^2}{2M} + \sum_{i,j \in [L]} V_{\text{Coulomb}}^{\text{ion-ion}}(\mathbf{R}_i - \mathbf{R}_j) \\ H_{e^-ion} &= \sum_{i \in [N], j \in [L]} V_{\text{Coulomb}}^{e^-ion}(\mathbf{r}_i - \mathbf{R}_j) \end{aligned}$$

We have m and M as the mass of the electron and the ion. \mathbf{r} and \mathbf{R} are the position of the electron and the ion. The ion-ion potential freezes the ions into the lattice. We first going to introduce some concepts by describing a non-interacting electron and then improve it to include the interactions.

2.1.1 The non-interacting electron gas

In this case of study the Hamiltonian only include a kinetic term

$$H = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma}.$$

We asume that it exist a the ground state $|0\rangle$, where the system is filled up with a certain amount of electron until the Fermi-energy ϵ_F is reached. Associated with this energy we find a wave vector \mathbf{k}_F , the Fermi-momentum. The set of enery up to ϵ_F is called the Fermi-sea, as an analogy to the level zero of the topographic maps.

$$\hat{n}_{\mathbf{k}, \sigma} |0\rangle = \Theta(\epsilon_F - \epsilon_{\mathbf{k}}) |0\rangle.$$

We introduced here a very useful tool called the Heavyside-step function wich is defined as:

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases}, \quad \Theta(-x) = 1 - \Theta(x).$$

This means that if we count the particle that have an energy heigher than the Fermi-energy ($\mathbf{k} > \mathbf{k}_F$) than we get zero.

We now want to study how the electron can scatter in different states. The function that we're using is called the propagator and gives the probailty to find the particle at $|\mathbf{k}', \sigma\rangle$ at t' know it at $|\mathbf{k}, \sigma\rangle$, t . An important fact is that without interaction, the particle shouldn't scatter in another state due to energy conservation. Therefore

$$G_0(\mathbf{k}, \mathbf{k}', t' - t) = G_0(\mathbf{k}, t' - t) \delta_{\mathbf{k}, \mathbf{k}'},$$

which is zero if the wave-vectors between the two timepoint differs. We observe that only the past time $t' - t$ is relevant. This is due to the time independent property of the Hamiltonian. We are going to use the representation in the frequency space, using a Fourier-transformation.

$$G_0(\mathbf{k}, \omega) = \int_{\mathbb{R}} e^{i\omega t} G_0(\mathbf{k}, t) dt = \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}}$$

where $\delta_{\mathbf{k}} = \delta \cdot \text{sgn}(\epsilon_{\mathbf{k}} - \epsilon_F)$ involving a very small non zero number δ . We observe that this analytical function has a pole given by

$$\begin{aligned} \omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}} &= 0 \\ \iff \omega &= \epsilon_{\mathbf{k}} - i\delta_{\mathbf{k}} \end{aligned}$$

where we denote i as the imaginary unit to avoid confusion with the index i . The frequency ω gives the so called spectrum of the exitation from the unique-particle system. The imaginary part serves as a damping term and is inversly proportional to the lifetime of the particle. δ is a small number due to the infinitely long lifetime. This is a direct result of the absence of scattering.

Further the propagator yields important informations on the system when considering the integration over its different arguments. First we take the imaginary part of the propagator called the single particle spectral weight.

$$\begin{aligned} A(\mathbf{k}, \omega) &= -\frac{1}{\pi} \text{Im} [G_0(\mathbf{k}, \omega)] = \frac{1}{\pi} \frac{\delta_{\mathbf{k}}}{(\omega - \epsilon_{\mathbf{k}})^2 + \delta_{\mathbf{k}}^2} \\ &= \delta(\omega - \epsilon_{\mathbf{k}}) \end{aligned}$$

which informs us about the occupation of a state $|\mathbf{k}\rangle$ with energy ω . We can find a form for the momentum distribution $n(\mathbf{k})$

$$n(\mathbf{k}) = \int A(\mathbf{k}, \omega) d\omega$$

and for the density of state

$$D(\omega) = \int A(\mathbf{k}, \omega) d^3k, \quad \text{or for discontinuous state } \sum_{\mathbf{k}} A(\mathbf{k}, \omega).$$

2.1.2 Fermi-Liquid

In an earlier section we saw how

$$H = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} + \sum_{\mathbf{k}, \sigma, \mathbf{k}', \sigma'} V_{\mathbf{k} \mathbf{k}', \mathbf{q}} c_{\mathbf{k}-\mathbf{q}, \sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q}, \sigma'}^{\dagger} c_{\mathbf{k}, \sigma} c_{\mathbf{k}', \sigma'}$$

represent the pairwise interaction of multiple electrons and their respective energy. To extend the model we now want to introduce two new [measures], the propagator G and the one-particle irreducible self-energy Σ .

The propagator [bildet ab] in the complex space and gives the probability amplitude of finding a the particle in the state $|\mathbf{k}, \sigma\rangle$ at a time t . On the other hand $\Sigma = \Sigma_R + i\Sigma_I$ contains the lifetime of the particle in this state and shift of energy of the particle due to the interaction with the surroundings. The framework defines the non-interacting energy of the particle as $\epsilon_{\mathbf{k}}$. When put in an interacting system the spectrum shifts and becomes $\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma_R$. Due to the interactions, the particle then has a much smaller lifetime. Σ_I is antiproportional to the particle's lifetime $\tau_{\mathbf{k}}$. We therefore expect Σ_I to be really small in the non interacting case. These two *Größe* are linked through the Dyson equation, which reads

$$(G(\mathbf{k}, \omega))^{-1} = (G_0(\mathbf{k}, \omega))^{-1} - \Sigma(\mathbf{k}, \omega).$$

sigma R One can use a Fourier-transformation to switch from the time representation to the frequency representation ω . Reordering the equation and using the result from 2.1.1 we obtain

$$G(\mathbf{k}, \omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma}.$$

3 Bogoliubov-de Gennes Formalism

The Bogoliubov-de Gennes transformation allows us to express the hamiltonian in a diagonal way and finding some quantities by looking at the eigenvectors of the hamiltonian. The resulting matrix is expressed in a huge space and is very sparse.

To give a taste of it, it will allow us to rewrite our hamiltonian as following

$$H = E_0 - \frac{1}{2} \tilde{c}^{\dagger} \tilde{H} \tilde{c}, \quad (1)$$

involving $\tilde{c} = (\hat{c}_1, \dots, \hat{c}_N)$, where each \hat{c}_i is a vector containing the creation and annihilation operators of a lattice site i : $\hat{c}_i = (c_{i,\uparrow}, c_{i,\downarrow}, c_{i,\uparrow}^{\dagger}, c_{i,\downarrow}^{\dagger})$.

As we see we just describe each site with the four possible c -operators. This means for each lattice site, we have a 4×4 -submatrix that reflects the possible combinations of creation and annihilation operators of both spins. For the readability we are going to drop the comma between the site and spin indices.

For example if one has (without loss of generality) a chemical potential at the site i , then the hamiltonian is described in the following way:

$$H_{\text{chem}, i} = \sum_{\sigma} \mu_i c_{i, \sigma}^{\dagger} c_{i, \sigma}$$

If we want to describe it in terms of \hat{c}_i we have:

$$H_{\text{chem}, i} = \hat{c}_i^{\dagger} \cdot \mu_i \mathbb{I}_4 \cdot \hat{c}_i = \begin{pmatrix} c_{i,\uparrow}^{\dagger} \\ c_{i,\downarrow}^{\dagger} \\ c_{i,\uparrow} \\ c_{i,\downarrow} \end{pmatrix} \cdot \mu_i \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} c_{i,\uparrow} \\ c_{i,\downarrow} \\ c_{i,\uparrow}^{\dagger} \\ c_{i,\downarrow}^{\dagger} \end{pmatrix}$$

Depending on the interaction we wish to describe, we can figure out what combination of operators we want and design the 4×4 matrix accordingly. To achieve a full description of the system we can consider the interaction between sites i, j as a 4×4 matrix involving the \hat{c}_i^{\dagger} and c_j operators. Then we can build a huge matrix \tilde{H} based on 4×4 matrices at $\tilde{H}_{i,j}$ and the vector we multiply it to is just the \hat{c}_i^{\dagger} and c_j operators stacked above one and other forming the above-introduced \tilde{c} vector. As a result, one gets the first formula introduced in this section 1.

3.1 Tigh Binding Model

Our goal is now to fix our particle on lattice sites and describe their interactions. We are therefore going to translate our wavefunction formalism in an on site plus nearest neighbour description.

For the generalities, assume we have the Hamiltonian in the second quantisation formalism:

$$H = \sum_{\sigma\sigma'} \int \phi_{\sigma}^{\dagger}(\mathbf{r}) H_{\sigma\sigma'}(\mathbf{r}) \psi_{\sigma'}(\mathbf{r}) d^3r \\ + \sum_{\sigma\sigma'} \int \int \phi_{\sigma}^{\dagger}(\mathbf{r}) \phi_{\sigma'}^{\dagger}(\mathbf{r}') V_{\sigma\sigma'}(\mathbf{r}, \mathbf{r}') \phi_{\sigma'}(\mathbf{r}') \phi_{\sigma}(\mathbf{r}) d^3r' d^3r$$

We introduce a basis of so called Wannier orbitals $w(\mathbf{r} - \mathbf{R}_i)$ with \mathbf{R}_i an atom location. They should be large in the neighbourhood of \mathbf{R}_i and vanishes when the distance tends to infinity. They are therefore called “localised”. The basis is complete, the orbitals verify the orthonormality condition:

$$\int w^*(\mathbf{r} - \mathbf{R}_i) w(\mathbf{r} - \mathbf{R}_j) d^3r = \delta_{ij}.$$

therefore we can define some field operator in this basis, based on creation and annihilation operators that acts on a lattice site i :

$$\phi_{\sigma}(\mathbf{r}) := \sum_i w(\mathbf{r} - \mathbf{R}_i) c_{i\sigma} \quad \phi_{\sigma}^{\dagger}(\mathbf{r}) := \sum_i w^*(\mathbf{r} - \mathbf{R}_i) c_{i\sigma}^{\dagger} \quad (2)$$

which is not a continuous description anymore. Inserting these operators back into our above Hamiltonian and using the orthonormality allows us to have an on site/nearest neighbour Hamiltonian. Taking for instance the first part of the Hamiltonian:

$$H = \sum_{\sigma\sigma'} \int \psi_{\sigma}^{\dagger}(\mathbf{r}) H_{\sigma\sigma'}(\mathbf{r}) \psi_{\sigma'}(\mathbf{r}) d^3r \\ = \sum_{ij\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} \int w^*(\mathbf{r} - \mathbf{R}_i) H_{\sigma\sigma'}(\mathbf{r}) w(\mathbf{r} - \mathbf{R}_j) d^3r \\ := \sum_{i\sigma\sigma'} \epsilon_i^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{\langle ij \rangle \sigma\sigma'} t_{ij}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} + \dots$$

In the last line we include a local energy term ϵ and the so called hopping term t_{ij} , which is the interaction with the nearest neighbour sites j of i . For a more precise description one could consider more neighbours. The spin dependent term can be used to describe spin orbit coupling or spin-flip processes.

We now aim to define the useful process for this thesis using this formalism.

3.1.1 Non-interacting electrons

The two main components of the non-interacting system Hamiltonian H_N are the chemical potential μ_i which is specific to each site and the hopping term t_{ij} . The chemical potential is modulated by the number of particles on the site i and the hopping term gives the amplitudes of moving an electron from site i to j . We assume it as spin-independent here.

$$H_N = - \sum_{i\sigma} \mu_i c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} \quad (3)$$

where $\langle ij \rangle$ is a commonly-used notation to sum over i and its nearest neighbours j , skipping $i = j$. We label it the normal Hamiltonian.

The hopping amplitude can be computed from the overlap of the orbitals under a kinetic operator $-\nabla^2/(2m)$, which explains the meaning “hopping”:

$$t_{ij} = - \int w^*(\mathbf{r} - \mathbf{R}_i) \frac{\nabla^2}{2m} w(\mathbf{r} - \mathbf{R}_j) d^3r \\ = + \frac{1}{2m} \int (\nabla w(\mathbf{r} - \mathbf{R}_i))^* (\nabla w(\mathbf{r} - \mathbf{R}_j)) d^3r.$$

We used a partial integration considering the boundary conditions of the Wannier orbitals $w(\pm\infty) = 0$. Therefore one part of the partial integration vanishes and we integrate/differentiate the integrands in the other integral, leading to two ∇ s. Further we see that $t_{ij} = t_{ji}^*$ by swapping the two integrands.

3.1.2 Superconductivity

Previous study of ours on the superconductivity have led us to the following Hamiltonian:

$$H_S = - \int U(\mathbf{r}) \psi_{\downarrow}^{\dagger}(\mathbf{r}) \psi_{\uparrow}^{\dagger}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) d^3r \quad (4)$$

on which we can apply a mean field approximation $\Delta(\mathbf{r}) = U(\mathbf{r}) \langle \psi_{\uparrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) \rangle$. This yields to a common BCS-Hamiltonian for regular superconductors.

$$H_S = - \int \left(\Delta(\mathbf{r}) \psi_{\downarrow}^{\dagger}(\mathbf{r}) \psi_{\uparrow}^{\dagger}(\mathbf{r}) + \Delta(\mathbf{r})^* \psi_{\uparrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) \right) d^3r. \quad (5)$$

we see that the second integrand is just the complex conjugate of the first one. To spare some place, we are going to focus ourselves on the first one and denoted its homologue with *h.c.* "hermitian conjugate".

We insert 2 and obtain:

$$\begin{aligned} H_S &= - \sum_{ij} c_{i\downarrow}^{\dagger} c_{i\uparrow}^{\dagger} \int \Delta(\mathbf{r}) w^*(\mathbf{r} - \mathbf{R}_i) w^*(\mathbf{r} - \mathbf{R}_j) d^3r + \text{h.c.} \\ &:= - \sum_{ij} \Delta_{ij} c_{i\downarrow}^{\dagger} c_{i\uparrow}^{\dagger} + \text{h.c.} \end{aligned}$$

$\Delta(\mathbf{r})$ is an order parameter and doesn't vary to much in the coherence length, which is much bigger than the atomic length. Therefore we can say that the orbitals vary faster than the gap. Moreover these orbitals are peaked in the neighbourhood of the atomic location \mathbf{R}_i and \mathbf{R}_j . Achieving the integral we get $\Delta_{ij} = \Delta_i \delta_{ij}$. We can from then reintroduce the *h.c.* and we get

$$H_S = - \sum_i \Delta_i c_{i\downarrow}^{\dagger} c_{i\uparrow}^{\dagger} + \Delta_i^* c_{i\uparrow} c_{i\downarrow}. \quad (6)$$

We however we're missing the mean field term E_0 :

$$E_0 = \int U \langle \psi_{\downarrow}^{\dagger} \psi_{\uparrow}^{\dagger} \rangle \langle \psi_{\uparrow} \psi_{\downarrow} \rangle d^3r = \int U \frac{\Delta^*}{U} \frac{\Delta}{U} d^3r = \int \frac{|\Delta|^2}{U} d^3r.$$

and after applying the tight binding formalism we get:

$$E_0 = \sum_i \frac{|\Delta_i|^2}{U},$$

which is a term we can add to the Hamiltonian 6. From these equations we have the final Hamiltonian for the superconducting system:

$$H = E_0 + H_N + H_S$$

3.2 A more symmetric Hamiltonian

As we introduced it while motivating the Bogoliubov-de Gennes formalism, we aspire to describe each state as a vector-matrix-vector product of

$$\hat{c}_i = \left(c_{i\uparrow}, c_{i\downarrow}, c_{i\uparrow}^{\dagger}, c_{i\downarrow}^{\dagger} \right).$$

For more clarity we briefly bring the Hamiltonian in a more diagonal form.

The chemical potential term can be expressed using the anticommutation relations of the fermionic operators $[c_{i\sigma}^{\dagger}, c_{i\sigma}]_+ = 1$:

$$\sum_{i\sigma} \mu_i c_{i\sigma}^{\dagger} c_{i\sigma} = \frac{1}{2} \sum_{i\sigma} \mu_i \left(c_{i\sigma}^{\dagger} c_{i\sigma} - c_{i\sigma} c_{i\sigma}^{\dagger} + 1 \right) \quad \text{why?} \quad (7)$$

and in the same way the hopping term can be expressed as:

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

we can take the liberty to reorder the indicies in a term of a sum and use the fact that $t_{ij} = t_{ji}^*$:

$$\sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} = \frac{1}{2} \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - t_{ji} c_{i\sigma} c_{j\sigma}^\dagger = \frac{1}{2} \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - t_{ji}^* c_{i\sigma} c_{j\sigma}^\dagger. \quad (8)$$

We then finish this section by using 7 and 8 in the Hamiltonian and obtain the following form:

$$H = E_0 - \frac{1}{2} \sum_{i\sigma} \left(c_{i\sigma}^\dagger c_{i\sigma} - c_{i\sigma} c_{i\sigma}^\dagger \right) - \frac{1}{2} \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - t_{ji}^* c_{i\sigma} c_{j\sigma}^\dagger.$$

We can now rewrite the Hamiltonian in a more compact way:

$$H = E_0 - \frac{1}{2} \sum_{i,j} \hat{c}_i^\dagger \hat{H}_{ij} \hat{c}_j \quad (9)$$

where the on site matrix reads

$$\hat{H}_{ij} = \begin{pmatrix} \mu_i \mathbb{I}_2 \delta_{ij} + t_{ij} & -i\sigma_2 \Delta_i \delta_{ij} \\ i\sigma_2 \Delta_i^* \delta_{ij} & -\mu_i \mathbb{I}_2 \delta_{ij} - t_{ij}^* \end{pmatrix} = \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^\dagger & -H_{ij}^* \end{pmatrix} \quad (10)$$

where we haven't explicitly described the sum over the nearest neighbours. This causes t_{ij} to vanish in case i and j are not neighbours. At this point it's interesting to note that if we wish to build some periodic boundary conditions, it might be the case that a site on side is neighbour with a site on the other side.

We can further compress our \hat{c}_i operator by introducing

$$\check{c} = (\hat{c}_1, \dots, \hat{c}_N)$$

along with the system Hamiltonian-matrix $\check{H}_{ij} := \hat{H}_{ij}$ which allows us to rewrite the Hamiltonian 9 as:

$$H = E_0 - \frac{1}{2} \check{c}^\dagger \check{H} \check{c}. \quad (11)$$

3.3 Eigenvalues

We now have a look at the following eigenvalue problem, which later helps from the diagonalization of the Hamiltonian:

$$\check{H} \check{\chi}_n = E_n \check{\chi}_n$$

n runs over the number of the eigenvalue and $\check{\chi}_n$ is the corresponding eigenvector. we can decompose the $\check{\chi}_n$ to reflect each lattice site: $\check{\chi}_n = (\hat{\chi}_{n1}, \dots, \hat{\chi}_{nN})$. This means $\chi_{n,i}$ refers to a 4×4 block, i.e. the one on the submatrix we had earlier talked about. Therefore this $\chi_{n,i}$ contains four values, grouped in two vectors of length two, one for each spin: $\chi_{n,i} = (u_{ni}, v_{ni})$. Further $u_{ni} = (u_{ni\uparrow}, u_{ni\downarrow})$ couples to the two first components ($c_{i\uparrow}, c_{i\downarrow}$) we had in \hat{c} and similarly $v_{ni} = (v_{ni\uparrow}, v_{ni\downarrow})$ to the two last components ($c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger$) of the four operator \hat{c} .

We can simplify the eigenvalue problem by taking a look only at a site i . We then only sum up over i .th row of \check{H}_{ij} with the components of $\check{\chi}_n$:

$$\sum_{j \in \llbracket N \rrbracket} \check{H}_{ij} \hat{\chi}_{nj} = E_n \hat{\chi}_{ni}.$$

we remember that $\check{H}_{ij} = \hat{H}_{ij}$ [SHOULD WE JUST USE H v ij?] so it follows by reintroducing 10 the following set of equations:

$$\begin{cases} \sum_{j \in \llbracket N \rrbracket} H_{ij} u_{nj} + \Delta v_{nj} = & E_n u_{nj} \\ \sum_{j \in \llbracket N \rrbracket} \Delta^\dagger u_{nj} - H_{ij}^* v_{nj} = & E_n v_{nj}. \end{cases} \xrightarrow{(1)} \begin{cases} \sum_j H_{ij} u_{nj} + \Delta v_{nj} = & E_n u_{nj} \\ \sum_j H_{ij} v_{nj}^* + \Delta^\dagger u_{nj}^* = & -E_n v_{nj}^*. \end{cases} \quad (12)$$

Where in (1) we took the conjugate of the second equation and used $\Delta^\dagger = -\Delta^*$. This is an important result, because it shows that if $\check{\chi}_n = (u_{n1}, v_{n1}, u_{n2}, v_{n2}, \dots)$ is an eigenvector with eigenvalue E_n , then so should be $(v_{n1}^*, u_{n1}^*, v_{n2}^*, u_{n2}^*, \dots)$ with the eigenvalue $-E_n$.

This leads to a symmetry in the energy spectrum of $H = E_0 \pm \frac{1}{2}\check{c}^\dagger \check{H} \check{c}$. This flexibility allows us to choose the version of H with the positive sign, which is more commonly used.

3.4 Diagonalization

Our goal is now to express the Hamiltonian relative to its energy eigenvalues, which is more practical to work with. As we have seen in the last section, eigenvectors χ_n allows us to compute the energies. Therefore we are going to diagonalize the Hamiltonian by using the eigenvectors χ_n to express the Hamiltonian according to its eigenvalues.

First we define a row-vector of our eigenstate $\check{X} = [\check{\chi}_{\pm 1}, \dots, \check{\chi}_{\pm 2N}]$ and introduce a diagonal matrix $\check{D} = \text{diag}(E_{\pm 1}, \dots, E_{\pm 2N})$ with the eigenvalues. Then we can write the Hamiltonian as:

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

we can then transform the Hamiltonian with $\check{c} := \check{X} \gamma$

$$\begin{aligned} H &= E_0 - \frac{1}{2} \check{c}^\dagger \check{H} \check{c} = E_0 - \frac{1}{2} \gamma^\dagger \check{X}^\dagger \check{H} \check{X} \gamma \\ &= E_0 - \frac{1}{2} \gamma^\dagger \underbrace{\check{X}^\dagger \check{X}}_{=\mathbb{I}} \underbrace{\check{D} \check{X}^{-1} \check{X}}_{=\mathbb{I}} \gamma \\ &= E_0 - \frac{1}{2} \gamma^\dagger \check{D} \gamma \\ &= E_0 - \frac{1}{2} \sum_{n \in \mathcal{N}} \end{aligned}$$

where $\mathcal{N} = \{\pm n : n \in \llbracket N \rrbracket\}$. Rearranging the transformation of \check{c} we get $\gamma = \check{X}^\dagger \check{c}$. Now that we've made the structure of the involved variables clear in the last section, we find the expression of the γ which is $2N$ -dimensional:

$$\begin{aligned} \gamma_n &= \sum_i \left(u_{ni\uparrow}^* c_{i\uparrow} + v_{ni\uparrow}^* c_{i\uparrow}^\dagger + u_{ni\downarrow}^* c_{i\downarrow} + v_{ni\downarrow}^* c_{i\downarrow}^\dagger \right) \\ &= \sum_{i\sigma} \left(u_{ni\sigma}^* c_{i\sigma} + v_{ni\sigma}^* c_{i\sigma}^\dagger \right) \end{aligned}$$

and due to the symmetry we saw earlier,

$$\gamma_{-n} = \sum_{i\sigma} \left(v_{ni\sigma} c_{i\sigma} + u_{ni\sigma} c_{i\sigma}^\dagger \right)$$

for $n \in \llbracket N \rrbracket$. We now take a look at the conjugate transpose of γ_{-n} . Because scalars are dimension 1×1 we have $(uc^\dagger)^\dagger = (c^\dagger)^\dagger u^\dagger = c^\dagger u^* = u^* c$ and it follows:

$$\gamma_{-n}^\dagger = \sum_{i\sigma} \left(v_{ni\sigma}^* c_{i\sigma}^\dagger + u_{ni\sigma}^* c_{i\sigma} \right) = \gamma_n.$$

Using this we can link each γ_i to the corresponding eigenvalue E_i : γ_n to the corresponding eigenvalue E_n and γ_{-n} to the corresponding eigenvalue $E_{-n} = -E_n$. We recall that we had $2N$ degrees of freedom $c_{i\sigma}$ due to the spins and after the transformation we get $4N$ degrees into \hat{c}_i . But because our energies E_n and E_{-n} are related to each other, we can keep the positive $2N$ eigenvalues and this maintain the total number of degree of freedom.

We can split the sum over the $n \in \mathcal{N}$ in two parts: $\mathcal{N}_+ = \{n \in \mathcal{N} : n > 0\}$, $\mathcal{N}_- = \{n \in \mathcal{N} : n < 0\}$

$$\begin{aligned}
H &= E_0 + \frac{1}{2} \sum_{n \in \mathcal{N}_+} E_n \gamma_n^\dagger \gamma_n + \frac{1}{2} \sum_{n \in \mathcal{N}_-} E_n \gamma_n^\dagger \gamma_n \\
&= E_0 + \frac{1}{2} \sum_{n \in \mathcal{N}_+} E_n \gamma_n^\dagger \gamma_n + \frac{1}{2} \sum_{n \in \mathcal{N}_+} E_{-n} \gamma_{-n}^\dagger \gamma_{-n} \\
&= E_0 + \frac{1}{2} \sum_{n \in \mathcal{N}_+} E_n \gamma_n^\dagger \gamma_n - \frac{1}{2} \sum_{n \in \mathcal{N}_+} E_n \gamma_{-n}^\dagger \gamma_{-n} \\
&= E_0 + \frac{1}{2} \sum_{n \in \mathcal{N}_+} E_n \gamma_n^\dagger \gamma_n - \frac{1}{2} \sum_{n \in \mathcal{N}_+} E_n \gamma_n \gamma_n^\dagger \\
&= E_0 + \frac{1}{2} \sum_{n \in \mathcal{N}_+} E_n (\gamma_n^\dagger \gamma_n - \gamma_n \gamma_n^\dagger)
\end{aligned}$$

where with used the energy symmetry and $\gamma_{-n}^\dagger = \gamma_n$, $\gamma_{-n} = \gamma_n^\dagger$.

Using this knowledge, we can express a final formula for the Hamiltonian by using the anticommutation properties of the fermionic γ -operators: $[\gamma_n^\dagger, \gamma_n] = 1$,

$$H = E_0 - \sum_{n \in \mathbb{N}} E_n \left(\gamma_n^\dagger \gamma_n - \frac{1}{2} \right). \quad (13)$$

This is the final form of the Hamiltonian in the Bogoliubov-de Gennes formalism. As a user one should build the Hamiltonian and computes its eigenvalues,-vector and transform them into the γ operators.

3.4.1 Superconducting Gap

We already covered how the superconducting gap Δ is a relevant property of the Meissner state. We now aim to use the mean field theorie in order to find the gap. This requires a self consistency equation, which we can be derived from the Hamiltonian.

The gap was defined as $\Delta(\mathbf{r}) := U(\mathbf{r}) \langle \psi_\uparrow(\mathbf{r}) \psi_\downarrow(\mathbf{r}) \rangle$. Back to the tight binding formalism, the gap now depends on the lattice site i and reads $\Delta_i = \langle c_{i\uparrow} c_{i\downarrow} \rangle$ and we can express $c_{i\sigma}$ in terms of the γ -operators:

$$\begin{aligned}
c_{i\sigma} &= \sum_{n \in \mathcal{N}} u_{ni\sigma} \gamma_n \\
&= \sum_{n \in \mathcal{N}_+} u_{ni\sigma} \gamma_n + u_{-n,i\sigma} \gamma_{-n} \\
&= \sum_{n \in \mathcal{N}_+} u_{ni\sigma} \gamma_n + v_{ni\sigma}^* \gamma_n^\dagger
\end{aligned}$$

where we used the symmetry of the eigenvectors. We can now compute expectation value involved in the gap:

$$\begin{aligned}
\langle c_{i\uparrow} c_{i\downarrow} \rangle &= \sum_{n,m \in \mathcal{N}_+} \langle (u_{ni\uparrow} \gamma_n + v_{ni\uparrow}^* \gamma_n^\dagger) (u_{mi\downarrow} \gamma_m + v_{mi\downarrow}^* \gamma_m^\dagger) \rangle \\
&= \sum_{n,m \in \mathcal{N}_+} \langle (u_{ni\uparrow} u_{mi\downarrow} \gamma_n \gamma_m + u_{ni\uparrow} v_{mi\downarrow}^* \gamma_n \gamma_m^\dagger + v_{ni\uparrow}^* u_{mi\downarrow} \gamma_n^\dagger \gamma_m + v_{ni\uparrow}^* v_{mi\downarrow}^* \gamma_n^\dagger \gamma_m^\dagger) \rangle \\
&= \text{why do the not cross term vanish? gamma orthogonal for the following sum } n, m \rightarrow n? \\
&= \sum_{n \in \mathcal{N}_+} \langle u_{ni\uparrow} v_{ni\downarrow}^* \gamma_n \gamma_n^\dagger \rangle + \langle v_{ni\uparrow}^* u_{ni\downarrow} \gamma_n^\dagger \gamma_n \rangle \\
&= \sum_{n \in \mathcal{N}_+} u_{ni\uparrow} v_{ni\downarrow}^* \langle \gamma_n \gamma_n^\dagger \rangle + v_{ni\uparrow}^* u_{ni\downarrow} \langle \gamma_n^\dagger \gamma_n \rangle \\
&= \sum_{n \in \mathcal{N}_+} u_{ni\uparrow} v_{ni\downarrow}^* (1 - f(E_n)) + v_{ni\uparrow}^* u_{ni\downarrow} f(E_n)
\end{aligned}$$

where f is the Fermi-Dirac distribution. The expectation value $\langle a\hat{A} \rangle_\Phi$ of a scalar times an operator reads $\langle \Phi | a\hat{A} | \Phi \rangle_\Phi = a \langle \Phi | \hat{A} | \Phi \rangle_\Phi = a \langle \hat{A} \rangle_\Phi$. To convince ourselves, we just take a look at the first quantisation expression of this bracket. This result leads to the self consistency equation:

$$\Delta_i = U_i \sum_{n \in \mathcal{N}_+} u_{ni\uparrow} v_{ni\downarrow}^* (1 - f(E_n)) + u_{ni\downarrow} v_{ni\uparrow}^* f(E_n)$$

We plan to solve this equation numerically, inserting some guess in the Hamiltonian, diagonalize it, update Δ_i and reinsert it into H and repeat until we reach a fixpoint.