Proximity Effects in Altermagnetic Systems

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a bachelor thesis.

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1 Theoretical Background

In order to describe the superconductors we are going the introduce the second quantisation formalism. It allows us to describe the wavefunction of a system using creation and anihinaltion 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 Foch 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 fundamentaly 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.

$$\hat{H} = \hat{H}_0 + \hat{H}_I \tag{1}$$

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

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

Where we introduce the notation $[\![N]\!] = \{n \in \mathbb{N} : n \leq N\}$. We call it single particle operator because the operator only applies on a particle. It may depend from the particle's postion $\boldsymbol{r}$ or spin s: $x_i := (\boldsymbol{r}, s) \in \mathcal{X} \subseteq \mathbb{R}^3 \times \mathbb{S}$. 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 $\epsilon_n \in \mathbb{R}$. This energy depends on the wavevector and the spin of the particle: $\nu = (\boldsymbol{k}, \sigma)$. 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:

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

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:

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

where $\int_{\mathbb{R}^3} \mathrm{d}r^3 = \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} \mathrm{d}r_1 \mathrm{d}r_2 \mathrm{d}r_3$. 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 normalsized. A combination is discribed as the product of the wavefunction of the particle in a certain state. These particle can be swaped and therfore 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.

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

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 $i, j \in [\![N]\!]$.

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

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

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 therfore have $n_\nu \in \{0, 1\}$. The normalsization factor is the same but the product over the ones vanishes.

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

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

which vanishes if two rows or columms 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 soltutuion are

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

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 Slatter 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:

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

Therfore we can expend any many-particle wavefunction Ψ as the linear combination of these:

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

where f_a is a coefficent and a a labeling.

What we just discused 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. $|\boldsymbol{k}, \sigma, ..\rangle$. Then we need operators that act on these states to allow interactions in the system. We need an operator that creates a states and another that anihilates a state.

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

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

1.2.1 Second quantisation for fermions

Creation operator $c_\nu^\dagger$ The creation operatortor adds a particle in the state that is concernd and rephase the state:

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

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 appling this operator after another on the vaccum 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:

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

Annihilation operator c_ν Likewise the anihinaltion operator destroys a particle in the corresponding state. The operator reads

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

We can easly 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 compution rules that are going to help us later.

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

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

$$[c_\nu, c_\mu]_+ = 0 \tag{$\mathfrak{Fer}_1$}$$

$$[c_\nu^\dagger, c_\mu^\dagger]_+ = 0 \tag{$\mathfrak{Fer}_2$}$$

$$[c_\nu^\dagger, c_\mu]_+ = \delta_{\mu,\nu} \tag{$\mathfrak{Fer}_3$}$$

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

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

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

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

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 Slatter determinant and the single particle state to understand the following. First we introduce two basis element —$\Phi_\alpha\rangle$ and $|\Phi_\beta\rangle$, which can be many-particles eigenstate of the system. We can also call them Slatter 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, potental, interactions,..). This is described by the matrix element $\langle\Phi_\alpha|A|\Phi_\beta\rangle$ which involves the single particle states $|\alpha_1\rangle, .., |\alpha_N\rangle$ of $|\Phi_\alpha\rangle$ and $|\beta_1\rangle, .., |\beta_N\rangle$ 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 overlapp of the two configurations, after that we modified $|\Phi_\beta\rangle$ with A. On the right hand side (r.h.s) we introduced the braket scalar product notation. The bra $\langle\alpha|$ lives in the dual space of the Hilbert space. One reads it as the complexe transpose of $|\alpha\rangle$.

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

$$\hat{H}_0 = \sum_{i\in[\![N]\!]} \hat{h}(x_i) \rightsquigarrow \sum_{\alpha,\beta} \langle\alpha|\hat{h}|\beta\rangle c_\alpha^\dagger c_\beta \tag{2}$$

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

$$\langle\alpha|\hat{h}|\beta\rangle = \int \varphi_\alpha^*(x)\hat{h}(x)\varphi_\beta(x)\mathrm{d}x \tag{3}$$

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 slatter determinant $|\Phi\rangle$ and $|\Phi'\rangle$ differs in more than two state, there are some scattering that we can't describe, so the overlapp must be zero. We allow only two states to be modified. Otherwise the single-particle states differ and due to their orthonal properties, we get a zero.

Similarly for the two-particle operator we have

$$\hat{H}_I = \frac{1}{2}\sum_{i\neq j\in[\![N]\!]} \hat{v}(x_i, x_j) \rightsquigarrow \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \tag{4}$$

involving a more nested overlap of the four states:

$$\langle\alpha\beta|\hat{v}|\gamma\delta\rangle = \int\int \varphi_\alpha^*(x)\varphi_\beta^*(x')\hat{v}(x,x')\varphi_\gamma(x)\varphi_\delta(x')\mathrm{d}x\mathrm{d}x'. \tag{5}$$

which modifies four states so the overlapp 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.

1.2.2 Second quantisation for bosons

1.3 Basis transformation

Until now considerd the wavefunction in a restricted basis $\{\varphi_\alpha(x)\}$. A wave function is defined as the overlapp between the basis and the state:

$$\phi(x) = \langle x|\alpha\rangle.$$

Let us now define a more general new operator that create a states $|\alpha\rangle = a_\alpha|0\rangle$ for fermion and bosons. We asume that we have another basis $\{|\tilde{\alpha}\rangle\}$. We now want to show, that the new operator a_α can be expressed as a linear combination of the other operator $a_{\tilde{\alpha}}$. This will be a usefull too to jump from a basis to another. We first notice the following identity relations:

$$\mathbb{I} = \sum_\alpha |\alpha\rangle\langle\alpha| = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle\langle\tilde{\alpha}|$$

this allow us to write

$$a_\alpha^\dagger|0\rangle = |\alpha\rangle = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle \underbrace{\langle\tilde{\alpha}|\alpha\rangle}_{\text{scalar}} = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle|\tilde{\alpha}\rangle$$

inverting the indicies leads to the same result, which leads to the transformation rules

$$a_\alpha^\dagger = \sum_{\tilde{\alpha}} \langle \tilde{\alpha} | \alpha \rangle a_{\tilde{\alpha}}^\dagger$$
$$a_\alpha = \sum_{\tilde{\alpha}} \langle \alpha | \tilde{\alpha} \rangle a_{\tilde{\alpha}}.$$

Further we can use these relations to express a wavefunction in the basis of another wavefunction. We have

$$\phi_\alpha(x) = \langle x|\alpha\rangle = \langle x| \left(\sum_{\tilde{\alpha}} \langle \tilde{\alpha}|\alpha\rangle |\tilde{\alpha}\rangle \right) = \sum_{\tilde{\alpha}} \langle \tilde{\alpha}|\alpha\rangle \langle x|\tilde{\alpha}\rangle = \sum_{\tilde{\alpha}} \langle \tilde{\alpha}|\alpha\rangle \varphi_{\tilde{\alpha}}(x).$$

Inverting α and $\tilde{\alpha}$ leads as well $\varphi_{\tilde{\alpha}}(x) = \sum_\alpha \langle \alpha|\tilde{\alpha}\rangle \phi_\alpha(x)$.

Morover we can show that the basis transformation is unitary. This is an important feature because we can simplify the calculation by changing the basis but the result we seek for would remain the same after the unitary transformation. Such transformations plays a major role later in the thesis. We can save the $\langle \tilde{\alpha}|\alpha\rangle$ in a matrix D and prove that this matrix is unitary. We have

$$\begin{aligned} \langle \tilde{\alpha}|\tilde{\beta}\rangle &= \sum_\gamma \langle \tilde{\alpha}|\gamma\rangle \langle \gamma|\beta\rangle = \sum_\gamma \langle \tilde{\alpha}|\gamma\rangle \langle \beta|\gamma\rangle^* \\ &= \sum_\gamma D_{\alpha\gamma} D_{\beta\gamma}^* = \sum_\gamma D_{\alpha\gamma} D_{\gamma\beta}^\dagger = (DD^\dagger)_{\alpha\beta}. \end{aligned}$$

meanwhile $\langle \tilde{\alpha}|\tilde{\beta}\rangle = \delta_{\tilde{\alpha}\tilde{\beta}}$ so that $DD^\dagger = \mathbb{I}$. The matrix D is therfore unitary. but do we also have the orthonormality of if we take two different basis?.

The last important step is to show that the basis transformation keeps the anti-, commutation relations. Let us for the seek of readability use the notation $[A, B]_\xi = AB + \xi BA$ where $\xi = -$ for bosons and $\xi = +$ for fermions. We have for exemple using $[a_\alpha, a_{\alpha'}^\dagger]_\xi = \delta_{\alpha\alpha'}$

$$[a_{\tilde{\alpha}}, a_{\tilde{\alpha}'}^\dagger]_\xi = \sum_{\tilde{\alpha}\tilde{\alpha}'} \langle \tilde{\alpha}|\alpha\rangle \langle \alpha'|\tilde{\alpha}'\rangle [a_\alpha, a_{\alpha'}^\dagger]_\xi = \langle \tilde{\alpha}|\tilde{\alpha}'\rangle = \delta_{\tilde{\alpha}\tilde{\alpha}'}.$$

The first step follows after spliting the commutator in two parts, insert the transformation and recombine the new commutator. The last step involves the orthonormality of the basis. On the same way one can prove $[a_{\tilde{\alpha}}, a_{\tilde{\alpha}'}] = [a_{\tilde{\alpha}}^\dagger, a_{\tilde{\alpha}'}^\dagger] = 0$.

1.3.1 Field operators

Later in this thesis we are going to use field opertors to describe an order parameter of a superconductive system. These are creation and annihilation operators that are defined in the $|x\rangle$-space-spin basis regarding antoher basis $\{|\alpha\rangle\}$. We here give the state as an argument an not as an index anymore. Despite the notation the following operators musn't be confused with a wavefunction.

$$\hat{\psi}^\dagger(x) = \sum_\alpha \langle \alpha|x\rangle a_\alpha^\dagger = \sum_\alpha \varphi_\alpha^*(x) a_\alpha^\dagger \tag{6}$$
$$\hat{\psi}(x) = \sum_\alpha \langle \alpha|x\rangle a_\alpha = \sum_\alpha \varphi_\alpha(x) a_\alpha^\dagger \tag{7}$$

involving fermonic or bosonic operators a. We can then annihilation and create a particle at a spin-space location x. Beacause these operators are involded, the commutations property respects which particle we are describing. Using the result we had for $[a_\alpha, a_{\alpha'}]_\xi, [a_\alpha, a_{\alpha'}^\dagger]_\xi$ and $[a_\alpha^\dagger, a_{\alpha'}^\dagger]_\xi$ where $\xi = -$ for the bosons and $+$ for the fermions. We find the following commutation relations:

$$\left[\hat{\psi}(x), \hat{\psi}(x')\right]_\xi = \left[\hat{\psi}(x)^\dagger, \hat{\psi}^\dagger(x)\right]_\xi = 0$$
$$\left[\hat{\psi}(x), \hat{\psi}^\dagger(x')\right]_\xi = \delta(x - x')$$

In the last expression we obtain a $\langle x|x'\rangle$ which cant normalsize the $\{|x\rangle\}$-basis so instead of a Korenker delta $\delta_{xx'}$ we get a delta distribution $\delta(x-x')$. The goal is now to describe the Hamiltonian using this fields operators. Thefore we rebuild the fields operator in the Hamiltonian using a $\{|x\rangle\}$ basis

$$\hat{H}_0 = \int \hat{\psi}^\dagger(x)\hat{h}(x)\hat{\psi}(x)\mathrm{d}x$$
$$\hat{H}_I = \frac{1}{2}\int\int \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')\hat{v}(x,x')\hat{\psi}(x')\hat{\psi}(x)\mathrm{d}x'\mathrm{d}x$$

We already know that the first and second quantisation are equivalent. We could now insert the definition of the field operators 6 and 7 in the Hamiltonian and obtain a wave function description. Then we can just use the first to second quantisation translation 3 and 5 to a the second quantised representation. The reulst is a generlisation of the experession with the operators a.

1.4 Interactive electron gas

As we are later going to study, the electron are allowed to interact with each other. During such processes a photon is usaly carying the momentum transfert of the scattering. We're going to use the formalism we introduced to find a second quantisation representation of the interacting Hamiltonian.

The system we're stying is a cube of side length L with wolume $\Omega = L^3$ with N electrons. Further we consider a periodic boundary condition for an arbitrary position vector $\boldsymbol{r} = (x,y,z)$:

$$(L,y,z) = (0,y,z)\ ,\ (x,L,z) = (x,0,z)\ ,\ (x,y,L) = (x,y,0).$$

We use the general form of the Hamiltonian 1 introduced in the beggining. We have a Coulomb potential and a kinetic energy term.

$$H_0 = T + U = -\sum_{i\in[\![N]\!]}\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i\in[\![N]\!]}u(x_i) \tag{8}$$
$$H_I = V = \sum_{i\neq j\in[\![N]\!]}v(x_i,x_j) \tag{9}$$

Where the pairwise potential is just a Coulomb potential $v(x_i,x_j) = \frac{e^2}{4\pi\epsilon_0|x_i-x_j|} = v(|x_i-x_j|)$. drop of the hat? We aim to describe the Hamiltonian in the momentum space, which is more convenient for the second quantisation. Therfore we first need to find an expression for the wavevector $\boldsymbol{k}$. We describe a state $\alpha = (\boldsymbol{k},\sigma)$ at a spin-space coordinate $x = (\boldsymbol{r},s)$. First we take a plane wave solution of the Schrödinger equation:

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\chi_\sigma(s)$$

The periodicity of the system allows us to write $\psi(x=0) = \psi(x=L)$ using the boundary condition and obtain $1 = e^{\mathrm{i}k_xL}$ as well as for the two other coordinates. The results reflects in the wavevector $\boldsymbol{k}$:

$$\boldsymbol{k} = \frac{2\pi}{L}(n_x,n_y,n_z)\ ,\quad n_i\in\mathbb{Z}.$$

As we saw earlier the eigenfunctions build a complete basis:

$$\begin{aligned}\int \psi^*_{\alpha'}(x)\psi_\alpha(x)\mathrm{d}x &= \int\sum_s \psi^*_{\alpha'}(x)\psi_\alpha(x)\mathrm{d}x\\ &= \frac{1}{\Omega}\int e^{\mathrm{i}\boldsymbol{r}(\boldsymbol{k}-\boldsymbol{k}')}\underbrace{\sum_s\delta_{s\sigma}\delta_{s\sigma'}}_{\delta_{\sigma\sigma'}}\,\mathrm{d}x\\ &= \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\sigma\sigma'} = \delta_{\alpha\alpha'}.\end{aligned}$$

where the integaral over the exponential function diverges if $\boldsymbol{k} \neq \boldsymbol{k}'$ so we use the case $\boldsymbol{k} = \boldsymbol{k}'$ and the integaral is zero otherwise.
The kinetic energy operator is a single particle operator so we have according to 2 we have:

$$T = \sum_{\alpha,\alpha'} \langle\alpha|\frac{\hat{\boldsymbol{p}}^2}{2m}|\alpha'\rangle c_\alpha^\dagger c_{\alpha'}.$$

Now we can juste use $\hat{\boldsymbol{p}} = \mathrm{i}\hbar\nabla$ and to compute this expression we use its first quantised form (see 3) indvolving the $\delta_{\sigma\sigma'}$ trick we introduced in the derivation of the complete basis. We also use $\boldsymbol{k}' = \boldsymbol{k}$ and hide the $\frac{1}{\Omega}$ is the $\delta_{\boldsymbol{k}\boldsymbol{k}'}$. The result is

$$T = \sum_{\alpha,\alpha'} \delta_{\alpha\alpha'} \frac{\hbar\boldsymbol{k}^2}{2m} c_{\alpha'}^\dagger c_\alpha = \sum_\alpha \underbrace{\frac{\hbar\boldsymbol{k}^2}{2m}}_{=:\epsilon_{\boldsymbol{k}}} c_\alpha^\dagger c_\alpha \tag{10}$$

we recognise the occupation number operator $\hat{n}_\alpha = c_\alpha^\dagger c_\alpha$ and the energy of the state $\epsilon_{\boldsymbol{k}}$. This variable plays a central role later. We obtain a quite meaningfull result, the non-interacting energy part of the system is the product of the energy of a state with the number of particle within that state, summed over all states.

We don't consider the single particle external potental for now.

For the interaction potential , we have a two-particle operator. This is described by eqaution 4 and requiers 5 to be solved.

$$V = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \langle\alpha\beta|v|\gamma\delta\rangle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

Introducing these in V using $v(\boldsymbol{r},\boldsymbol{r}') = v(\boldsymbol{r}-\boldsymbol{r}')$ leads to:

$$\langle\alpha\beta|v|\gamma\delta\rangle = \frac{1}{\Omega^2}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta} \int\int e^{\mathrm{i}\boldsymbol{r}(\boldsymbol{k}_\gamma-\boldsymbol{k}_\alpha)} e^{\mathrm{i}\boldsymbol{r}'(\boldsymbol{k}_\delta-\boldsymbol{k}_\beta)} v(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}\boldsymbol{r}'\mathrm{d}\boldsymbol{r}$$

we can make a substitution $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$, add and substract a $(\boldsymbol{k}_\gamma - \boldsymbol{k}_\alpha)\boldsymbol{r}'$ and obtain

$$\langle\alpha\beta|v|\gamma\delta\rangle = \frac{1}{\Omega^2}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta} \underbrace{\int e^{-\mathrm{i}\boldsymbol{R}(\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta)} v(\boldsymbol{R})\mathrm{d}\boldsymbol{R}}_{v_{\boldsymbol{k}_\delta-\boldsymbol{k}_\alpha}} \underbrace{\int e^{\mathrm{i}\boldsymbol{r}'(\boldsymbol{k}_\gamma-\boldsymbol{k}_\beta+\boldsymbol{k}_\delta-\boldsymbol{k}_\alpha)}\mathrm{d}\boldsymbol{r}'}_{=\delta_{\boldsymbol{k}_\gamma-\boldsymbol{k}_\beta+\boldsymbol{k}_\delta,\boldsymbol{k}_\alpha}}.$$

Almost finished, we derive a combursom equation

$$V = \frac{1}{2\Omega} \sum_{\substack{\boldsymbol{k}_\alpha\boldsymbol{k}_\beta\boldsymbol{k}_\gamma\boldsymbol{k}_\delta \\ \sigma_\alpha\sigma_\beta\sigma_\gamma\sigma_\delta}} \delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\delta_{\boldsymbol{k}_\alpha,\boldsymbol{k}_\gamma-\boldsymbol{k}_\beta+\boldsymbol{k}_\delta} v_{\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta} c_{\boldsymbol{k}_\alpha\sigma_\alpha}^\dagger c_{\boldsymbol{k}_\beta\sigma_\beta}^\dagger c_{\boldsymbol{k}_\gamma\sigma_\gamma} c_{\boldsymbol{k}_\delta\sigma_\delta}.$$

we can sum over the $\boldsymbol{k}_\alpha$, rename $\sigma_\alpha \to \sigma$ and $\sigma_\beta \to \sigma'$ and sum up over σ_γ and σ_δ to simplify the Kroneker deltas.

$$V = \frac{1}{2\Omega}\sum \sigma\sigma' \sum_{\boldsymbol{k}_\beta\boldsymbol{k}_\gamma\boldsymbol{k}_\delta} v_{\boldsymbol{k}_\gamma-\boldsymbol{k}_\beta} c_{\boldsymbol{k}_\delta+\boldsymbol{k}_\gamma-\boldsymbol{k}_\beta,\sigma}^\dagger c_{\beta\sigma'}^\dagger c_{\gamma\sigma'} c_{\delta\sigma'}$$

where using $\boldsymbol{k}_\alpha = \boldsymbol{k}_\gamma - \boldsymbol{k}_\beta + \boldsymbol{k}_\delta$ from the Kroneker delta we get $v_{\boldsymbol{k}_\alpha-\boldsymbol{k}_\delta} = v_{\boldsymbol{k}_\gamma-\boldsymbol{k}_\beta+\cancel{\boldsymbol{k}_\delta-\boldsymbol{k}_\delta}}$. Then we can introduce the following variable transformations:

$$\boldsymbol{k}_\delta \to \boldsymbol{k}\ , \quad \boldsymbol{k}_\gamma \to \boldsymbol{k}'\ , \quad \boldsymbol{k}_\beta \to \boldsymbol{k}' - \boldsymbol{q}$$

which yields

$$\begin{aligned} \boldsymbol{k}_\delta + \boldsymbol{k}_\gamma - \boldsymbol{k}_\beta &= \boldsymbol{k} + \boldsymbol{q} \\ \boldsymbol{k}_\gamma - \boldsymbol{k}_\beta &= -\boldsymbol{q} \end{aligned}$$

and we finaly get our second quantised interaction operator

$$V = \frac{1}{2\Omega}\sum_{\boldsymbol{q}} v_q \sum_{\substack{\boldsymbol{k}\sigma \\ \boldsymbol{k}'\sigma'}} c_{\boldsymbol{k}+\boldsymbol{q},\sigma}^\dagger c_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}^\dagger c_{\boldsymbol{k}'\sigma'} c_{\boldsymbol{k}\sigma}.$$

This describes an electron transfering a momentum $\boldsymbol{q}$ to another electron. The fornula tells that we kill the electron we had before the interaction and create two in states where one loosed some momentum, that has been transferd the other electron. As we saw earlier this depends on the distance $\boldsymbol{r} - \boldsymbol{r}'$ between the electrons, but not $\boldsymbol{r}$ and $\boldsymbol{r}'$ respectivly, so this process is translation invariant. The following diagramm is a good illustration of this effect.

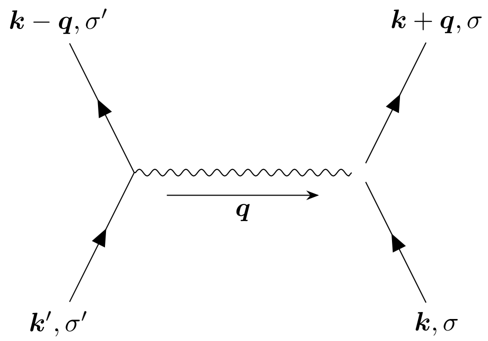


Figure 2: The interaction of two electrons modulated by a photon of momentum $\boldsymbol{q}$.

This closes the introduction theorie on the second quantisation. We saw how we can express integaral over wavefunctions as bra-kets scalarproducts. This allowed us to introduce some operators that creates and annihilates particles in a certain state. Using this formalism we were able to compute the Hamiltonian of the system in the momentum sapce. We found that the non interacting-part relies on the energy of each state times there occupation number and that an interaction between two electrons can be described as a momentum transfert between them wich is modulated by the fourier transform of the Coulomb potential.

Now we can move on to the descirption of a superconductive state.

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 araise 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 araise 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.

Along the derivation of the superconductivity formalism we are going to follow closely the work of Fossheim and Sudbø [1] from chapter 2 to 4. For readability reason we set the reducted Planck constant $\hbar = 1$ in the following. Furhter they added the chemical potential to the energy of the state such that now $\epsilon_k + \mu \to \epsilon_k$ from eq. 10.

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.

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

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

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

We have m and M as the mass of the electron and the ion. $\boldsymbol{r}$ and $\boldsymbol{R}$ 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. Usely the potential of a lattice is periodic. If so the wavefunction o f a particle moving in the system is a plane wave modulated by a periodic function. Eigenstates of the corresponding hamiltonian are called Bloch state.

2.1.1 The non-interacting electron gas

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

$$H = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c_{\boldsymbol{k},\sigma}^\dagger c_{\boldsymbol{k},\sigma}. \tag{11}$$

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 $\boldsymbol{k}_F$, 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.

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

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

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} \quad , \quad \Theta(-x) = 1 - \Theta(x). \tag{12}$$

This means that if we count the particle that have an energy heigher than the Fermi-energy ($\boldsymbol{k} > \boldsymbol{k}_F$) 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 $|\boldsymbol{k}',\sigma\rangle$ at t' know it at $|\boldsymbol{k},\sigma\rangle$, t. An important fact is that without interaction, the particle shouldn't scatter in another state due to energy conservation. Therfore

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

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.

$$G_0(\boldsymbol{k},\omega) = \int_{\mathbb{R}} e^{\mathrm{i}\omega t} G_0(\boldsymbol{k},t)\mathrm{d}t = \frac{1}{\omega - \epsilon_{\boldsymbol{k}} + \mathrm{i}\delta_{\boldsymbol{k}}} \tag{13}$$

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

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

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 excitation 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 abscence 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.

$$\begin{aligned} A(\boldsymbol{k},\omega) = -\frac{1}{\pi}\mathcal{I}m\left[G_0(\boldsymbol{k},\omega)\right] &= \frac{1}{\pi}\frac{\delta_{\boldsymbol{k}}}{(\omega-\epsilon_{\boldsymbol{k}})^2+\delta_{\boldsymbol{k}}} \\ &= \delta(\omega-\epsilon_{\boldsymbol{k}}) \end{aligned} \tag{14}$$

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

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

and for the density of state

$$D(\omega) = \int A(\boldsymbol{k},\omega)\mathrm{d}^3k \ , \quad \text{or for discontinuous state} \ \sum_{\boldsymbol{k}} A(\boldsymbol{k},\omega). \tag{15}$$

2.1.2 Fermi-Liquid - the interacting case

Now that we've described the non interacting system, let us complexify the model by introducing the interactions. In an earlyer section we saw how

$$H = \sum_{\boldsymbol{k},\sigma}\epsilon_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\sigma,\boldsymbol{k}',\sigma'} V_{\boldsymbol{k}\boldsymbol{k}',\boldsymbol{q}}c^\dagger_{\boldsymbol{k}-\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma'}c_{\boldsymbol{k},\sigma}c_{\boldsymbol{k}',\sigma'} \tag{16}$$

represent the pairwise interaction of multiple electrons and their respective energy.

To extend the model we now want to introduce two new quantities, the propagator G and the one-particle irreductible self-energy Σ. The propagator maps in the complex space and sgives the probability amplitude of finding a the particle in the state $|\boldsymbol{k},\sigma\rangle$ at a time t. On the other hand $\Sigma = \Sigma_R + \mathrm{i}\Sigma_I$ contains the lifetime of the particle in this state and shift of energy of the particle due to the interaction with the surroundings. The frameworks defines the non-interacting energy of the particle as $\epsilon_{\boldsymbol{k}}$. Whene put in an interacting system the spectrum shifts and becomes $\tilde{\epsilon}_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} + \Sigma_R$. Due to the interactions, the particle then has a much smaller lifetime. Σ_I is antiproportional to the particle's lifetime $\tau_{\boldsymbol{k}}$. We therfore expect Σ_I to be realy small in the non interacting case. These two quantities are linked trough the Dyson equation, which reads

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

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 13 we obtain

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

This function has a pole at $\omega = \epsilon_{\boldsymbol{k}} + \Sigma_R + \mathrm{i}\Sigma_I$, where in the none interacting case $\omega = \epsilon_{\boldsymbol{k}} + \mathrm{i}\Sigma_I$. It makes makes sense, the particle spectrum is now shifted due to the finite lifetime of the particle as a result of the interaction.
The pole yields to an expression for the spectrum

$$\omega - \epsilon_{\boldsymbol{k}} - \left(\Sigma_R(\boldsymbol{k},\omega) + \mathrm{i}\Sigma_I(\boldsymbol{k},\omega)\right) = 0 \tag{17}$$

In complexe analysis the order of a pole is given as n if $f(z)$ is meromorphic and has a pole at z_0 where

$$(z-z_0)^n f(z)$$

is also meromorphic in the neighbourhood of z_0. In our case we're interested in the 0.th order of the pole *why?*. We therfore ignore the imaginary part of the pole and we get

$$\omega = \epsilon_{\boldsymbol{k}} + \Sigma_R(\boldsymbol{k}, \epsilon_{\boldsymbol{k}}) = \tilde{\epsilon}_{\boldsymbol{k}}.$$

If we take into account a tiny imaginary part of Σ we obtain a shifted pole. Performing a Taylor expension of Σ_R in the neighbourhood of $\omega = \tilde{\epsilon}_{\boldsymbol{k}}$ will help us.

$$\Sigma_R(\boldsymbol{k}, \omega) = \Sigma_R(\boldsymbol{k}, \tilde{\epsilon}_{\boldsymbol{k}}) + (\omega - \tilde{\epsilon}_{\boldsymbol{k}}) \frac{\partial \Sigma_R}{\partial \omega}\bigg|_{\omega = \tilde{\epsilon}_{\boldsymbol{k}}} + \mathcal{O}(\omega^2)$$

We aim to compute to the first order in Σ_I such that we evaluate it at $\omega = \tilde{\epsilon}_{\boldsymbol{k}}$. This leads to starting from 17 and, after inserting the Taylor expension for Σ_R

$$\begin{aligned} \omega - \underbrace{\left(\epsilon_{\boldsymbol{k}} + \Sigma_R(\boldsymbol{k}, \tilde{\epsilon}_{\boldsymbol{k}})\right)}_{=\tilde{\epsilon}_{\boldsymbol{k}}} - (\omega - \tilde{\epsilon}_{\boldsymbol{k}}) \frac{\partial \Sigma_R}{\partial \omega}\bigg|_{\omega = \tilde{\epsilon}_{\boldsymbol{k}}} - \mathrm{i}\Sigma_I(\boldsymbol{k}, \tilde{\epsilon}_{\boldsymbol{k}}) = 0 \\ \iff \quad (\omega - \tilde{\epsilon}_{\boldsymbol{k}}) \left(1 - \frac{\partial \Sigma_R}{\partial \omega}\bigg|_{\omega = \tilde{\epsilon}_{\boldsymbol{k}}}\right) - \mathrm{i}\Sigma_I(\boldsymbol{k}, \tilde{\epsilon}_{\boldsymbol{k}}) = 0 \end{aligned} \tag{18}$$

We define the residue of the propagator as

$$z_{\boldsymbol{k}} = \frac{1}{1 - \frac{\partial \Sigma}{\partial \omega}\big|_{\omega = \tilde{\epsilon}_{\boldsymbol{k}}}} \tag{19}$$

which we can insert in the inverse lifetime of the electron occupying the state $|\boldsymbol{k}, \sigma\rangle$

$$\frac{1}{\tau_{\boldsymbol{k}}} = -z_{\boldsymbol{k}} \Sigma_I(\boldsymbol{k}, \tilde{\epsilon}_{\boldsymbol{k}}). \tag{20}$$

This justifies the statement $\Sigma_I \propto 1/\tau_{\boldsymbol{k}}$ This residue is a decreasing function of the energy, which means that its influence is more important for low energies. An interpretation could be that the slow moving electrons have less time to interact with their fast homologues, which results in a longer lifetime.

We recall once again the difference of the propagators to conclude this section:

Free electron	Interacting electron
$G_0(\boldsymbol{k}, \omega) = \dfrac{1}{\omega - \epsilon_{\boldsymbol{k}} + \mathrm{i}\delta_{\boldsymbol{k}}}$	$G(\boldsymbol{k}, \omega) = \dfrac{1}{\omega - \tilde{\epsilon}_{\boldsymbol{k}} + \mathrm{i}\frac{1}{\tau_{\boldsymbol{k}}}}$

Interacting electrons are degraded version of the non-interacting case. There remains a $z_{\boldsymbol{k}} < 1$.

Quasi-particles The main question we have now is how does the residue look like on the fermi surface? We set us in the context of a low energy electron, close to the Fermi-surface and once we had a interaction. It turns out that if there is a $z_{\boldsymbol{k}_F} > 0$ we find a precise low energy single particle excitation. This excitation is very close to the exact eigenfunction of an non-interacting Hamiltonian. We call this state akin to the free electron a quasi-particle.

This is it, a Fermi-liquid is a system of interacting electrons and quasi-particles. These quasi-particles are not eigenstates of the interacting Hamiltonian anymore. We can't consider them as an electron like excitation in the interaction context. The interactions allows to scatter some states in and out of the Bloch-State.

The above expression for the momentum distribution $n(\boldsymbol{k})$ can be ploted and we can recognise a gap of $z_{\boldsymbol{k}_F} < 1$. This wich is an inportant feature of the Fermi-liquid. Whereas for the non interacting system the momentum distribution has a discontinuity from one to zero when crossing the Fermi surface.

An important feature to mention that is the key understanding of the Fermi-liquid and revealed itself to be very correct for metals, is the on-to-one correspondance of quantum numbers between the interactinf and non-interacting electrons. This means we can start with simple Hamiltonian like Eq. 11 and add new particles by introducing some perturbations. The obtained quasi-particles are a result of the excitation of the non-interacting system. We then observe this one-to-one correspondance.

The last question one can ask is why does this approximation work so well in the most case? The answer lays in the reference system we choose to perturb arround. Keeping in mind the Pauli-principle, we notice that the added particle are restricted in their scattering. This is so strong that it almost cancels out the "switching-on" of the interactions. It's a good decision to perturb arround the free system. Due to the fact that we are limitted in the number of ground states, thermodynamic quantites moves in a smooth manner when perturbating.

We want to emphasize one last time that the Fermi-liquid formalism work because of the momentum restrictions due to the Pauli exclusion principle.

Repulsive interactions In condensed matter physics the dominant effect is the repulsive interactions between the electrons due to the coulomb potential. We already described it in the Hamiltonian $H_{e^-e^-}$ using some pairwise interactions in 16. Therfore the goal is now to find an expression for the potential $V_{\boldsymbol{k}\boldsymbol{k}',\boldsymbol{q}}$.

As we can see in eq. 16 the system is describe in the momentum-space. For this reason we need to consider the Fourier-transform of the real-sapce potential. We start with the coulomb potential which is predominant in the solid state physics. However the integral is going to diverge for $r \to 0$. To solve this problem We introduce the Yakuma potential which exponentialy modulates the coulomb potential:

$$V_\lambda(r) = \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}e^{-r\lambda} \tag{21}$$

this is a solid approximation since we can the fourier transform and let $\lambda \to 0$ in the result. Result in appendix?. The result we get is

$$V_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} = V_{\mathrm{el}}(\boldsymbol{q}) := \frac{1}{4\pi\epsilon_0}\frac{2\pi e^2}{\boldsymbol{q}^2} \tag{22}$$

with $\boldsymbol{q}$ the momentum transfert during the interaction. The Fermi-liquid remains stable to the repulsive processes.

However as we're going to see in the next section, attractive interactiosn also takes place due to an exchange of phonons between two electrons. This will be the ground stone to our description of the Meissner state.

2.1.3 Instability due to attractive Interactions

Hier we are going to show how the attractive interactions destabilise the Fermi-liquid. In other words we are going to show that new ground states open.
Leon Cooper introduced a very specific context of attraction that has a huge influence on the stability. Taking this exemple we are going to make clear that attractive interaction can in some cases exeed the Coulomb force resulting in unexpected new eigenstates.

Let's asume we have an impotent Fermi sea where the electrons as considered non interacting. Adding to electrons requiers to place them above the sea. The exotic context lays into the interactions. They can only interact if they are withing a small cover ω_0 over the Fermi surface, one on each side, facing them trough the complete surface. If this is not the case the interaction vanishes.
Fossheim and Sudbø derivated a methode in [1] from p.67 to 69. They conclude with the fact that allowing such interaction leads to a total energy of the interacting system E smaller than $2\epsilon_F$. This means in the attraction of the electrons shift them in a state that lays under the Fermi sea. Further they showed that if the Fermi sea vanishes (one could take electrons out of the system) then this attractive pairing disapears. The same is observed as we approche

the classical limit. By forming a pair the electron share their fermionic properties and act as bosons. The Pauli principle doesn't rule their energies anymore.

We now understand why attractive processes create instabilities. An engery gap opens next to the surface, reflecting the energy needed to break the new formed Cooper pair. The shell ω_0 is the maximum frequency delivering the "adesive" that allows the electron to pair. Now that we showed the influence of attractive interactions, we seek some candidate process that are attractive.

2.1.4 Phonon-mediated attractive interactions reformulate

As known from condensed matter physics, the lattice can have some intern oscillations called phonons resulting from the spring coupling between the ions. Now we can imagine that due to the Coulomb interactions, an electron can shift an ions producing a phonon. If this phonon travels and influences another electron on it way, we result in an effective electron-electron interaction thanks to the phonon. A similar case would be the exchange of a photon between two electrons. We are going to show how this exchange can lead to an attractive interaction.

Tn a dense lattice the ions moves much slowly around their equilibrium positions than the lights electrons who pass by. The electron moves the charges of the ions resulting in a small dipol moment. A second electron that also passes in the surounding is going to feel the dipol moment and will be attracted. Then the ion shifts back in its new equilibrium position and the dipol moment vanishes long after the first electron passed.

Morover due to the Coulomb interaction, the electrons aim to put as most distance as they can between them in a minimal amount of time. Therfore we can say that the $\boldsymbol{k}$-quantum number should be opposite between the two electron. If we target to put these concepts in a mathematical form, we use our previous Hamiltonian and add an electron-phonon interaction term.

$$H = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\sigma,\boldsymbol{k}',\sigma'} V_{\boldsymbol{k}\boldsymbol{k}',\boldsymbol{q}} c^{\dagger}_{\boldsymbol{k}-\boldsymbol{q},\sigma} c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma'} c_{\boldsymbol{k},\sigma} c_{\boldsymbol{k}',\sigma'} + V_{e^-\text{phonon}}$$

where $V_{e^-\text{phonon}}$ usely depends on the sum of the phonons-modes λ. These modes are similar to the oscillations modes we have in a CO_2-molecule. The expression form the phonon-depend potential in momentum space reads

$$V_{e^-\text{phonon}} = \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} M_{\boldsymbol{q}} \left(a_{-\boldsymbol{q}^\dagger} + a_{\boldsymbol{q}}\right) c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma}. \tag{23}$$

$M_{\boldsymbol{q}} \left(a_{-\boldsymbol{q}^\dagger} + a_{\boldsymbol{q}}\right)$ is a matrix element of the coupling between the electron and the phonon. The $a_{\boldsymbol{q}}$ and $a_{\boldsymbol{q}^\dagger}$ are annihilation and creation operators of the phonon with wavevector $\boldsymbol{q}$. Further researches have shown that source

$$\left[a_{\boldsymbol{q}}, a_{\boldsymbol{q}^\dagger}\right] = \delta_{\boldsymbol{q},\boldsymbol{q}'}$$

and therefor phonons act like bosons. Their number is however not conserved in a solid. The matrix element M is a function of the eigenfrequency or energy? of the phonon $\omega_{\boldsymbol{q}}, \lambda$ and the fourier tramsform $\tilde{V}$ of the electrostatic potential $V_\lambda(\boldsymbol{q})$ between the electron and the phonon of mode λ, if included. more details?

$$M_{\boldsymbol{q},\lambda} = \mathrm{i}(\boldsymbol{q} \cdot \boldsymbol{\xi}_\lambda) \sqrt{\frac{\hbar}{2M\omega_{\boldsymbol{q},\lambda}}} \tilde{V}_\lambda(\boldsymbol{q}).$$

M can't be realy computed due to its complexity, we hold it as a parameter here. This pairing is much waker than the electron-photon interaction. An other important fact ist than for $\boldsymbol{q} \to 0$ the matrix element M vanishes. M is proportional to $\boldsymbol{q}$ which illustrate the the electron-phonon interaction happens between a point charge and a dipol.

The goal is now the implicitly express the phonon exchange with an effective electron-electron process. If we consider two diagrams, one aiming to describe the absorption of a phonon and one the emission of a phonon, we can combine them to get a new effective interaction like the photon exchange case.

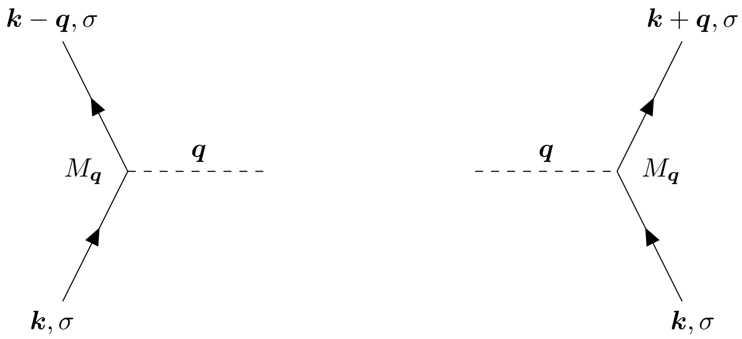


Figure 3: The emission (left) and absorption (right) digramm of a phonon of wavevector $\boldsymbol{q}$ by an electron.

If we represent this inderaction by linking both $\boldsymbol{q}$-edges. The energy of phonon is simply defined as

$$H_{\text{phonon}} = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} a^\dagger_{\boldsymbol{q}} a_{\boldsymbol{q}}$$

and we can write a propagator which describes the dashed line in a connected context similar to to photon case described in the figure **??**.

$$D_0(\boldsymbol{q}, \omega) = \frac{2\omega_{\boldsymbol{q}}}{\omega^2 - \omega_{\boldsymbol{q}}^2 + i\eta}$$

involving a very small quantity η. From this we obtain an expression for the phonon-mediated interaction of two electrons. This is performed using $V^{(ph)}_{\text{eff}}(\boldsymbol{q}, \omega) = \mathcal{R}\text{e}\left(|M_{\boldsymbol{q}}|^2 D_0(\boldsymbol{q}, \omega)\right)$ and discarding the second order η term which is very small.

$$V^{(ph)}_{\text{eff}}(\boldsymbol{q}, \omega) = \frac{2|M_{\boldsymbol{q}}|^2 \omega_{\boldsymbol{q}}}{\omega^2 - \omega_{\boldsymbol{q}}^2} \tag{24}$$

with $\boldsymbol{q}$ the momentum transfert. We can now use a more complete potential in the Hamiltonian involving both the electrostatic 22 and effective phonon-mediated interactions 24.

$$V_{\text{eff}}(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{q}) = V_{\text{el}}(\boldsymbol{q}) + V^{(ph)}_{\text{eff}}(\boldsymbol{q}, \omega) = \frac{1}{4\pi\epsilon_0} \frac{2\pi e^2}{\boldsymbol{q}^2} + \frac{2|M_{\boldsymbol{q}}|^2 \omega_{\boldsymbol{q}}}{\omega^2 - \omega_{\boldsymbol{q}}^2} \tag{25}$$

Here we have reached a very important point. This new potential can be in some case negative, which means we result in an attractive interaction between the electrons. With other word, in some cases the phonon exchage can be attractive and even overcome the strong repulsive coulomb potential. Graph of V and the simplified version of it, which is also a very good predication.

2.1.5 Contraction of the effective Hamiltonian

We want to restrict ourselves in the case where the effective Hamiltonian is attractive. This happens in a small shell around the Fermi-surface. If we want to maximise the phase space for the scattering, the state before and after the scattering have to be in this shell. A good idea is to consider that the two electrons have opposite wavevectors. The folowing figure illustrates this process.

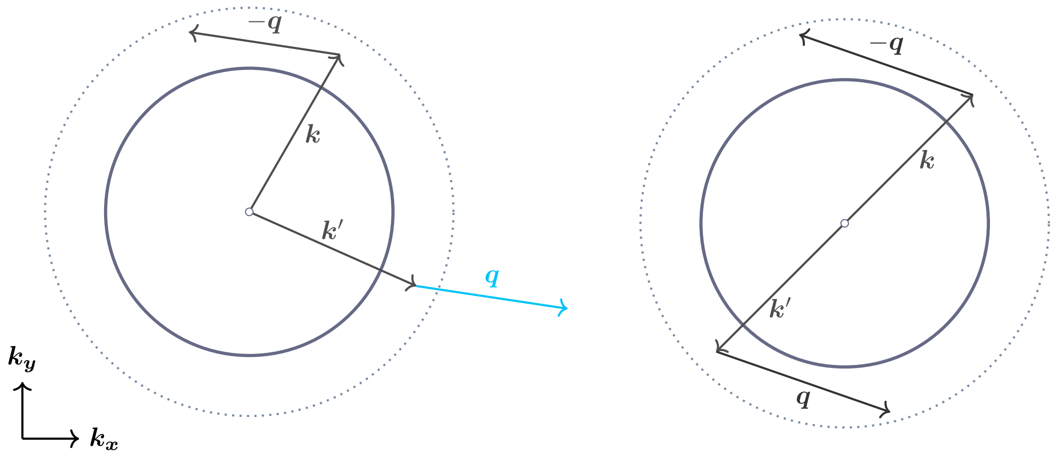


Figure 4: The scattering process of two electrons with opposite wavevectors $\boldsymbol{k}$ and $\boldsymbol{k}'$. We have a momentum transfert $\boldsymbol{q}$ between them. The thick line illustrates the Fermi-surface and the dotted one the thin shell. As we see if the electrons have opposite wavevectors, and the $\boldsymbol{k}$ electrons scatters into the shell, then the $\boldsymbol{k}'$ electron scatters in the shell as well. This is not allways the case if the wavevectors don't agree as we can see on the left figure. The right figure points out the maximisation process. With opposite wavevectors, we get the largest possbility spectrum for the scattering.

Further the attractivity is a short range effect, so if we want to consider it, we must think that the electrons are very close to eachother. This requires the electrons to have opposite spins due to the Pauli principle. This is a same as a lattice site. This is the only possbility for them to cohabit the same neighbourhood. check The approximation turns out to be a good model.

Now we allow us to rename some variables:

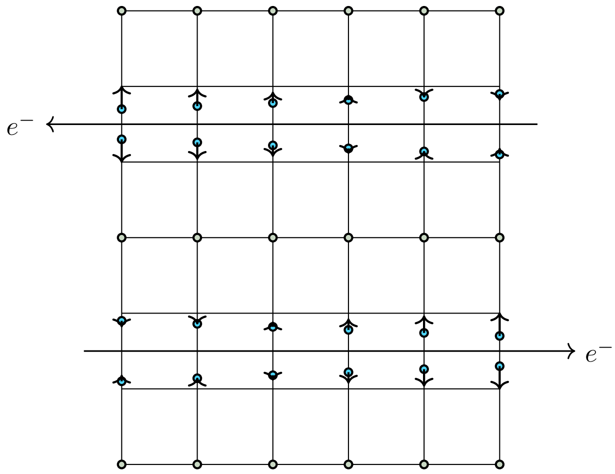
$$\boldsymbol{k}+\boldsymbol{q} \longrightarrow \boldsymbol{k}\ ,\quad \boldsymbol{k} \longrightarrow \boldsymbol{k}'$$

The Hamiltonian that follows from these transformations is called the BCS-reduced Hamiltonian

$$H = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\sigma,\boldsymbol{k}} V_{\boldsymbol{k}\boldsymbol{k}'} c^{\dagger}_{\boldsymbol{k},\sigma} c^{\dagger}_{-\boldsymbol{k},-\sigma} c_{-\boldsymbol{k}',-\sigma} c_{\boldsymbol{k}',\sigma} \tag{26}$$

$V_{\boldsymbol{k}\boldsymbol{k}'}$ is now a matrix element that acts if the wavevectors are close to the Fermi-surface. The electrons have to move in opposite directions with opposite spins. Due to the retardation processes we introduced earlier, there remains a distortion in the lattice long after the electrons passed. Due to the inducting dipol moment, the other electron is attracted towards the distortion with $M_{\boldsymbol{q}}$?. As we also saw, the coulomb repulsion causes a colinear displacement, close to the distortion of the homologue. This phenomenon is called the Cooper-pairing and is a coupling that happens in momentum space.

The reader might want to see a picture of what is happing in the real space. To achieve a representation two simple statements are enough. First, the Coulomb force aims to maximize the distance between the electrons in minimal time. This is achieved by moving them collinearly in opposite directions. Second, due to the retardation process, it's energetically more favourable for the electron to move along the distortion of the lattice. The result is illustrated in the figure **??**.



Here the moved ions in blue are shifting back to their equilibrium position but it is important to remember that when the other electron passes, it expriences almost the same distortion everywhere. An interacting fact is that these interactions are the source of the superconductivity but they are also the main origin of resistivity in clean materials.

2.1.6 On our way to the BCS-theory

After this introduction on the phonon coupling between the electrons in the momentum space, or Cooper-pairing, we aim to describe the energy of the superconductor in a mean-field approach. The goal of it is to reduce the description with the neighbours to the description of a site, in the mean field of the other sites. Thefore we are going to describe a one-boby problem which is easier to compute. As known mean-fiels approches requier self-consistent equations that will as well follow.

The first step is to introduce the following epexctation values:

$$b_{\boldsymbol{k}} = \langle c_{-\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\uparrow} \rangle \tag{27}$$

$$b_{\boldsymbol{k}}^{\dagger} = \langle c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger} \rangle \tag{28}$$

wich lead to a new expression for the c operators:

$$c_{-\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\uparrow} = b_{\boldsymbol{k}} + \underbrace{c_{-\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\uparrow} - b_{\boldsymbol{k}}}_{\delta_{b_{\boldsymbol{k}}}} \tag{29}$$

where we can see the $\delta_{b_{\boldsymbol{k}}}$ as a deviation, or fluctuation term. If we introduce it back into the Hamiltonian, we can write

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} \left(b_{\boldsymbol{k}}^{\dagger} + \delta_{b_{\boldsymbol{k}}}^{\dagger}\right)\left(b_{\boldsymbol{k}} + \delta_{b_{\boldsymbol{k}}}\right).$$

We can compute the product of the two terms in parenthesis and forget the $\mathcal{O}\left(\delta_{b_{\boldsymbol{k}}}^2\right)$ because the fluctuation are small. We then obtain the following expression

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} \left(b_{\boldsymbol{k}}^{\dagger} c_{-\boldsymbol{k}'\downarrow} c_{\boldsymbol{k}'\uparrow} + b_{\boldsymbol{k}'}^{\dagger} c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger} - b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}'}\right).$$

The next step is to define the superconduction gap parameter Δ:

$$\Delta_{\boldsymbol{k}} := -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} b_{\boldsymbol{k}}^{\dagger} \tag{30}$$

$$\Delta_{\boldsymbol{k}}^{\dagger} := -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} b_{\boldsymbol{k}'} \tag{31}$$

wich brings our Hamiltonian in another form:

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma} - \sum_{\boldsymbol{k}} \left(\Delta_{\boldsymbol{k}}^{\dagger} c_{-\boldsymbol{k}'\downarrow} c_{\boldsymbol{k}'\uparrow} + \Delta_{\boldsymbol{k}}^{\dagger} c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger} - b_{\boldsymbol{k}}^{\dagger} \Delta_{\boldsymbol{k}}^{\dagger}\right). \tag{32}$$

We took the liberty to spilt the sum, rename the $\boldsymbol{k}'$ to $\boldsymbol{k}$ and recombine the sum. We notice that this form involves a lot of creation and annihilation terms that are not commun for an effective non-interacting electron gaz. We remeber that we aim a one particle descirption in a mean field of its neighbours. This complexity will lead to some difficulties to express the quais-particle spectrum. A good soltution is to rotate the basis of the c operators to land in a basis that diagonalises the Hamiltonian and therfore minimises the number of operators.

The transformation involves two new fermionic operator η and γ that therfore respect $\mathfrak{Fer}_1$ to $\mathfrak{Fer}_3$ and reads

$$\begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} \eta_{\boldsymbol{k}} \\ \gamma_{\boldsymbol{k}} \end{pmatrix} \tag{33}$$

along with the conjugate transpose of each component of the l.h.s vector rebuild into a matrix-vector equation

$$\begin{pmatrix} c^\dagger_{\boldsymbol{k}\uparrow} \\ c_{-\boldsymbol{k}\downarrow} \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} \eta^\dagger_{\boldsymbol{k}} \\ \gamma^\dagger_{\boldsymbol{k}} \end{pmatrix}. \tag{34}$$

We can reintroduce these into the Hamiltonian 32. Some of the multiplication involves $\cos(\theta)^2 - \sin(\theta)^2 = \cos(2\theta)$ and $\cos(\theta)^2 + \sin(\theta)^2 = 1$. Further due to the anticommutations we have $\eta\gamma^\dagger = -\gamma^\dagger\eta$ and so on for $\gamma\eta^\dagger = -\eta^\dagger\gamma$. We obtain the following expression

$$\begin{aligned} H =& \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} \cdot 1 + \Delta_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}} \\ &+ \sum_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} \cos(2\theta) - \cos(\theta)\sin(\theta)\left(\Delta^\dagger_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}}\right)\right] \eta^\dagger_{\boldsymbol{k}}\eta_{\boldsymbol{k}} \\ &- \sum_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} \cos(2\theta) - \sin(\theta)\cos(\theta)\left(\Delta^\dagger_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}}\right)\right] \gamma^\dagger_{\boldsymbol{k}}\eta_{\boldsymbol{k}} \\ &- \sum_{\boldsymbol{k}} \left[\Delta_{\boldsymbol{k}} \cos(\theta)^2 - \Delta^\dagger_{\boldsymbol{k}} \sin(\theta)^2 + 2\epsilon_{\boldsymbol{k}}\cos(\theta)\sin(\theta)\right] \eta^\dagger_{\boldsymbol{k}}\gamma_{\boldsymbol{k}} \\ &- \sum_{\boldsymbol{k}} \left[\Delta_{\boldsymbol{k}} \cos(\theta)^2 - \Delta^\dagger_{\boldsymbol{k}} \sin(\theta)^2 + 2\epsilon_{\boldsymbol{k}}\cos(\theta)\sin(\theta)\right] \gamma^\dagger_{\boldsymbol{k}}\eta_{\boldsymbol{k}}. \end{aligned} \tag{35}$$

The goal is to diagonalise the Hamiltonian in the (γ, η) basis. Thefore have to rotate with θ such that the terms with $\gamma^\dagger\eta$ and $\eta^\dagger\gamma$ vanish. A difficulty that we may entcounter along with this idea is that Δ is an order parameter and own a complex phase fluctuation. With other words one can write $\Delta = |\Delta|e^{\mathrm{i}\tau}$ where τ has has some fluctuations. We are going to ignore them.

We can set

$$\Delta_{\boldsymbol{k}} = \Delta^\dagger_{\boldsymbol{k}} \quad \text{and} \quad \tan(2\theta) = -\frac{\Delta_{\boldsymbol{k}}}{\epsilon_{\boldsymbol{k}}}$$

and introduce two new variables called the coherence factors

$$v^2_{\boldsymbol{k}} := \sin(\theta)^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right), \tag{36}$$

$$u^2_{\boldsymbol{k}} := \cos(\theta)^2 = \frac{1}{2}\left(1 + \frac{\epsilon_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right) \tag{37}$$

along with a new energy $E_{\boldsymbol{k}} = \sqrt{\epsilon^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2}$. Historical context? These factors play an important role in NMR as well as in the ultra sound propagation in superconductors. Cooper and Schrieffer made some corrrect predictions in an advanced many-body system. This is labeld as one of the greates achievements in condensed matter physics in the 20th century.
source
We obtain a Hamiltonian that looks very similar to a free fermion qusiparticle gas source?

$$H = \underbrace{\sum_{\boldsymbol{k}} \left(\epsilon_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}}\right)}_{\substack{=:H_0 \text{ constant} \\ \text{mean-field term}}} + \underbrace{\sum_{\boldsymbol{k}} E_{\boldsymbol{k}} \left(\eta^\dagger_{\boldsymbol{k}}\eta_{\boldsymbol{k}} - \gamma^\dagger_{\boldsymbol{k}}\gamma_{\boldsymbol{k}}\right)}_{\substack{\text{Spinless fermion system with} \\ \text{two types of fermions of} \\ \text{energies } E_{\boldsymbol{k}} \text{ and } -E_{\boldsymbol{k}}.}}. \tag{38}$$

where we dont describe any interaction, but two types of particles in a mean field. As [1] described it in chapter 3, p.83-84, one can note that we don't have any spins involved. This is due to the fact that we describe the quasiparticles as a linear combiantion of electrons and holes with opposite spins. source Therfore talking about degrees of freedom the two electron-hole singlets replace the $\uparrow, \downarrow$ degrees of freedom and they are preserved.

The ernegy $E_{\boldsymbol{k}}$ shows up a gap in the energy of the qusiparticle whene looking at the fermi-surface $\epsilon_{\boldsymbol{k}} = 0$ We count relative to it? But the way it is define in a non interacting Ham. is not relative to it right?. This is due to the fact that the exepectation values we introduced in 27 and 28 are not zero. The gap is a result of the Cooper-pairing. These expections values are the order parameters of the Meissner state and should be confused with the superconducting gap Δ. They are however zero at the same time.

This context of a free case is a good oportnity to introduce the grand chanonical ensemble of the Hamiltonian. Even if we could give the direct result, deriving this ensemble involves a lot of important step, so for the seek of completeness we are going to derive it.

We define the particle number operator $N = \sum_{\boldsymbol{k}} \mu \left(n_{\eta \boldsymbol{k}} + n_{\gamma \boldsymbol{k}}\right)$ where the index $\boldsymbol{k}$ is proper to this equation. Further the possible states $\boldsymbol{k}$ are in a "continous" set $\mathfrak{K} = \{\boldsymbol{k}_1, \boldsymbol{k}_2, ..\}$. $\{n_{\boldsymbol{k}}\}$ is the set of the diffent occupation numbers of all the states $\boldsymbol{k}$. Further we consider fermions so the occupation numbers of the particle type η or γ in state $\boldsymbol{k}$ are labeled $n_{\eta \boldsymbol{k}}$ and $n_{\gamma \boldsymbol{k}}$ and equals either 0 or 1.

$$
\begin{aligned}
Z_G &= \operatorname{Tr}\left(e^{-\beta(H+\mu N)}\right) \\
&= \sum_{\{n_{\boldsymbol{k}}\}} e^{-\beta H_0} \langle \{n_{\boldsymbol{k}}\}| \exp\left(\sum_{\boldsymbol{k}'} -\beta E_{\boldsymbol{k}'} \eta^\dagger_{\boldsymbol{k}'} \eta_{\boldsymbol{k}'} + \beta E_{\boldsymbol{k}'} \gamma^\dagger_{\boldsymbol{k}'} \gamma_{\boldsymbol{k}'}\right) \exp\left(-\beta \mu N\right) |\{n_{\boldsymbol{k}}\}\rangle \\
&= \sum_{\{n_{\eta \boldsymbol{k}}\}} \sum_{\{n_{\gamma \boldsymbol{k}}\}} e^{-\beta H_0} \exp\left(\sum_{\boldsymbol{k}} -\beta \left[E_{\boldsymbol{k}} \eta^\dagger_{\boldsymbol{k}} \eta_{\boldsymbol{k}} + \mu\right] + \beta \left[E_{\boldsymbol{k}} \gamma^\dagger_{\boldsymbol{k}} \gamma_{\boldsymbol{k}} - \mu\right]\right) \\
&= e^{-\beta H_0} \sum_{\substack{n_{\eta \boldsymbol{k}_1}, \\ n_{\eta \boldsymbol{k}_2}, ..}} \sum_{\substack{n_{\gamma \boldsymbol{k}_1}, \\ n_{\gamma \boldsymbol{k}_2}, ..}} \exp\left(\sum_{\boldsymbol{k}} -\beta \left[E_{\boldsymbol{k}} n_{\eta \boldsymbol{k}} + \mu\right] + \beta \left[E_{\boldsymbol{k}} n_{\gamma \boldsymbol{k}} - \mu\right]\right) \\
&= e^{-\beta H_0} \sum_{\substack{n_{\eta \boldsymbol{k}_1}, \\ n_{\eta \boldsymbol{k}_2}, ..}} \prod_{\boldsymbol{k}} \exp\left(-\beta \left[E_{\boldsymbol{k}} n_{\eta \boldsymbol{k}} + \mu\right]\right) \sum_{\substack{n_{\gamma \boldsymbol{k}_1}, \\ n_{\gamma \boldsymbol{k}_2}, ..}} \prod_{\boldsymbol{k}} \exp\left(\beta \left[E_{\boldsymbol{k}} n_{\gamma \boldsymbol{k}} - \mu\right]\right) \\
&= e^{-\beta H_0} \sum_{n_{\eta \boldsymbol{k}_1}} \exp\left(-\beta \left[E_{\boldsymbol{k_1}} n_{\eta \boldsymbol{k}_1} + \mu\right]\right) \sum_{n_{\eta \boldsymbol{k}_2}} \exp\left(-\beta \left[E_{\boldsymbol{k_2}} n_{\eta \boldsymbol{k}_2} + \mu\right]\right) \cdot .. \\
&\quad \sum_{n_{\gamma \boldsymbol{k}_1}} \exp\left(\beta \left[E_{\boldsymbol{k}_1} n_{\gamma \boldsymbol{k}_1} - \mu\right]\right) \sum_{n_{\gamma \boldsymbol{k}_2}} \exp\left(\beta \left[E_{\boldsymbol{k}_2} n_{\gamma \boldsymbol{k}_2} - \mu\right]\right) \cdot .. \\
&= e^{-\beta H_0} \prod_{\boldsymbol{k}} \left(1 + e^{-\beta(E_{\boldsymbol{k}} + \mu)}\right) \left(1 + e^{\beta(E_{\boldsymbol{k}} - \mu)}\right)
\end{aligned}
$$

This partition function isn't very useful like this in our case. But we can derive the free energy which will help us to solve the self consitency eqution for the gap.
According to [3] p.99 the free engery can be derived from the partition function as (Appendix for more details?)

$$
F = -\frac{1}{\beta} \ln(Z_G) = H_0 - \frac{1}{\beta} \sum_{\boldsymbol{k}} + \ln\left(1 + e^{-\beta E_{\boldsymbol{k}}}\right) \ln\left(1 + e^{\beta E_{\boldsymbol{k}}}\right)
$$

According to [1] we obtain in the limit of low temperatures ($\beta \to \infty$)

$$
\begin{aligned}
F &= H_0 + \sum_{\boldsymbol{k}} E_{\boldsymbol{k}} \theta\left(-E_{\boldsymbol{k}}\right) + E_{\boldsymbol{k}} \theta\left(E_{\boldsymbol{k}}\right) \\
&= H_0 + \sum_{\boldsymbol{k}} E_{\boldsymbol{k}} - E_{\boldsymbol{k}} \theta\left(E_{\boldsymbol{k}}\right) + E_{\boldsymbol{k}} \theta\left(E_{\boldsymbol{k}}\right) \\
&= \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}} E_{\boldsymbol{k}}.
\end{aligned}
$$

whee we used the properties from the Heavyside step-function described in 12. The minimation of the free energy F should self-consitently determine the gap $\Delta_{\boldsymbol{k}}$. This is a statement that depends neither on the momentum space structure nor on the attractivity of the potential [1]. $E_{\boldsymbol{k}}$ has an implicit $\Delta_{\boldsymbol{k}}$-dependence. We compute the derivation $\frac{\partial F}{\partial \Delta_{\boldsymbol{k}}}$ and search the argument of the zero-postion. Derivating one $\boldsymbol{k}$ from the sum is enough. We demand the following to be satisfied:

$$\frac{\partial F}{\partial \Delta_{\boldsymbol{k}}} = 0 \ , \quad \frac{\partial F}{\partial \Delta_{\boldsymbol{k}}^{\dagger}} = 0 \tag{39}$$

This leads to Appendix?

$$b_{\boldsymbol{k}}^{\dagger} = \Delta_{\boldsymbol{k}} \underbrace{\frac{\tanh(\beta E_{\boldsymbol{k}}/2)}{E_{\boldsymbol{k}}}}_{\chi(\boldsymbol{k})}$$

$\chi(\boldsymbol{k})$ is the pair- suzeptibility and gives how capapble the system is to create Cooper-pairs [1]. If we allow us to relabel $\boldsymbol{k} \to \boldsymbol{k}'$ then multiply on both sides with $-\sum_{\boldsymbol{k}} V_{\boldsymbol{k}\boldsymbol{k}'}$ and introduce 31 we obtain the self-consitency equation for the gap. This usely denominated as the BCS gap equation.

$$\Delta_{\boldsymbol{k}} = -\sum_{\boldsymbol{k}} V_{\boldsymbol{k}\boldsymbol{k}'} \Delta_{\boldsymbol{k}'} \frac{\tanh(\beta E_{\boldsymbol{k}'}/2)}{E_{\boldsymbol{k}'}}. \tag{40}$$

Fossheim and Sudbø [1] emphasize that this eqution is not limited to phonon mediated interaction, as long we don't specify the potential. Further Cooper-pairs can condensate because in the pair the electron involed have opposite spins and this adds up to zero. The pair is not ruled anymore by the Pauli principle and can take part into the superconducting condensate. Even if the formation temperature of Cooper-pairs in higher than the critical temperature T_C, this mean field approch makes this temperatures agree.

As we introduced earlier the gap has a complex phase fluctuation. This phase is hard to vary in good metals because the number of carrier electrons is high. On the other side in poor metals the fluctuations that break the pair are more easely reched, i.e. at a lower temperature than in good metal. Supercomductivity is therfore more stable in metals of good value.

In this section we saw how to reduce the many body Hamiltonian to a single-body problem in the means field of its neighbours. The system that follows from this is a non interacting gas of a type electrons and holes. This involves the introduction of the superconducting gap parameter that we can thanks to the statistical mechanics formalism express a in a self-consitent way.

2.1.7 Generalized gap equation, s-wave and d-wave superconductivity

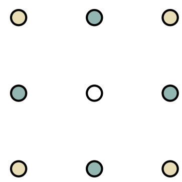
As we introduced in an earlier section, the formalism follows from the attractive phonon exchange but can be generalized. The superconductivity is the result of the pairing of the electrons into Cooper-pairs. These pairs shift into a condensate of take part of a coherent matter-wave. Making the analogy with the coherent light wave, superconductivity can be viewed as the *analogos* of lasers like Fossheim and Sudbø highlight it in [1].

To achieve such generlisation we let the formalism be open to other kind of interactions and don't restrict it to the thin shell around the Fermi-surface. The potential matrix-element can therefor take a complexer form than introduced in 25.

We recall that the electrons move into a lattice. We can asume that this crystal owns some symmetries that are reflected in its crysalographic (complete) basis $\{g_\eta(\boldsymbol{k})\}$. Similar to the Bloch state, we could imagine that the symmetries emphasize some physical quantities. Asuming this we propose a form for the potential:

$$V_{\boldsymbol{k}\boldsymbol{k}'} = \sum_{\eta} \lambda_\eta g_\eta(\boldsymbol{k}) g_\eta(\boldsymbol{k}')$$

η is also often labeld as the channel [1]. Asuming we have a square lattice,



with interaction strengh $U/2$ on site, for nearest neighbours $2V$ and $4W$ for second-nearest neighbours. need of more details from Jacob. Taking the fourier transform of this leads:

$$f(k,k') = \cos(k)\cos(k') + \sin(k)\sin(k')$$

$$\begin{aligned} V_{\boldsymbol{kk'}} = &U + 2V\left(f(k_x,k_x') + f(k_y,k_y')\right) \\ &+ 4W\left(f(k_x,k_x')\cdot f(k_y,k_y')\right) \end{aligned}$$

We can then introduce the basis-functions $\{g_\eta(\boldsymbol{k})\}$ we talked about a few paragraphs ago.

$$\begin{aligned} g_1(\boldsymbol{k}) =&\frac{1}{2\pi} \\ g_2(\boldsymbol{k}) =&\frac{1}{2\pi}\left(\cos(k_x)+\cos(k_y)\right) && \text{(s-wave)} \\ g_3(\boldsymbol{k}) =&\frac{1}{2\pi}\cos(k_x)\cos(k_y) \\ g_4(\boldsymbol{k}) =&\frac{1}{2\pi}\left(\cos(k_x)-\cos(k_y)\right) && \text{(d-wave)} \\ g_5(\boldsymbol{k}) =&\frac{1}{2\pi}\sin(k_x)\sin(k_y) \end{aligned}$$

from which involves the following lambdas $\lambda_1 = 2U\pi^2,\ \lambda_2 = \lambda_4 = 4V\pi^2,\ \lambda_3 = \lambda_5 = 4W\pi^2$ and for greater η ge set $\lambda_{\eta\geq 6} = 0$.

For $\eta \in \{1,2\}$, the corresponding g is the identity under all symmteries of C_{v4} and for $\eta \in \{3,4,5\}$ we observe a change of sign under $\pi/2$ rotations. The same behaviour is found in the spherical harmonics for resp. the quantum numbers $l = 0$ and $l = 2$. From this we can deduct the use of the terms s-wave and d-wave. Does this need a source?

Furhter we can reintroduce the BCS gap equation 40 and obtain a lattice-dependent form for the gap:

$$\begin{aligned} \Delta_{\boldsymbol{k}} &= -\sum_{\boldsymbol{k'}} V_{\boldsymbol{kk'}}\Delta_{\boldsymbol{k'}}\chi(E_{\boldsymbol{k}}) \\ &= -\sum_{\eta\in[\![5]\!]} \lambda_\eta g_\eta(\boldsymbol{k}) \underbrace{\sum_{\boldsymbol{k'}} g_\eta(\boldsymbol{k'})\Delta_{\boldsymbol{k'}}\chi(E_{\boldsymbol{k'}})}_{=:\Delta_\eta/\lambda_\eta} \\ &= \sum_{\eta\in[\![5]\!]} \Delta_\eta g_\eta(\boldsymbol{k}) \end{aligned} \tag{41}$$

This is a nice form to have as Fossheim and Sudbø [1] point out p.92. The gap is a linear combination of the physical quantites $g_\eta(\boldsymbol{k})$ which gives a physical quantities as well. The newly introduced Δ_η are independent from the wavevector $\boldsymbol{k}$ but are function if the temperature. We can express them in the basis of antoher η':

$$\begin{aligned} \Delta_\eta =& \sum_{\eta'\in[\![5]\!]} \Delta_{\eta'}\mathcal{M}_{\eta,\eta'} \\ \mathcal{M}_{\eta,\eta'} =& -\lambda_\eta \sum_{\boldsymbol{k}} g_\eta(\boldsymbol{k}) g_{\eta'}(\boldsymbol{k})\chi(E_{\boldsymbol{k}}). \end{aligned}$$

These nummericaly combuersom to compiute but taking $U > 0$, $V < 0$ and $W = 0$ in the square lattice we obtain no attraction $V_{\boldsymbol{kk'}\eta=1} > 0$? in the λ_1-channel but atraction in the s- and d-wave channels. This tells us a lot like [1] analised it. First the gap is highly associated to the Fourier transform of the wavefunction of the Cooper-pairss Which variable describes their wavefunction? Further the gap accomodate itself to be zero in the channel where the wavefucntion is non-zero "for zero separation between the electrons". The s- and d-wave channels are prefered which as consequence avoid the on site coulomb repulsion (i.e the Coulomb froce between the two members of the pair). This can be put in comparasion with the special case of the phonon pairing. In the latest the electrons used retardation processes to cancel out the repulsion. They avoided themselves in time. Here the avoidance takes place in space. (How to recognise the angluar momentum coupeling here?)

The manifestation of the retardation effects are acctualy a direct consequence of restricting ourselves to a thin shell ouround the Fermi-surface. But members of a Cooper pairs must have oposite spin and momenta. The opposite mometum is a result of the shell so is this statement valid in general?. This means without restrictions, the whole Brillouin zone is taken into account to compute the gap.

Further we can express the Fourier transform of the gap as $\Delta(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}}$ which leads $\Delta(0) = \sum_{\boldsymbol{k}} \delta_{\boldsymbol{k}}$. However a repulsive interaction is obtained for $\Delta(\boldsymbol{0}) \neq 0$ so we need to find $\Delta_{\boldsymbol{k}}$s whose sum satisfy this. This can be done using the s-wave and d-wave channels, i.e $\Delta_{\boldsymbol{k}} = \Delta_0(T)g_2(\boldsymbol{k})$ and $\Delta_{\boldsymbol{k}} = \Delta_0(T)g_4(\boldsymbol{k})$. We already motivated superconductivity and its difficulty to maintain due to the phase fluctuations above the (freezing) critical temperature T_c. However superconductivity involving d-wave channels is belived [1] p.92 to be found in materials with high T_c. $\Delta_{\boldsymbol{k}} = \Delta_0(T)g_4(\boldsymbol{k})$ is therfore a good case of study.

Density of Meisnner states

We imaging some fluctuation in? $g(\boldsymbol{k})$ that only depend on $E_{\boldsymbol{k}} = \sqrt{\epsilon_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2}$. Further we asume Δ beeing $\boldsymbol{k}$- independent for now. We can introduce the normal density of states.

$$D_n(\epsilon) = \frac{1}{N} \sum_{\boldsymbol{k}} \delta(\epsilon - \epsilon_{\boldsymbol{k}})$$

with N the number of Fourier modes. This is the same as the number of lattice sites for us [1] p.93.

$$\sum_{\boldsymbol{k}} g(\boldsymbol{k}) = \int D_n(\epsilon) g\left(\sqrt{\epsilon^2 - \Delta^2}\right) \mathrm{d}\epsilon$$

as well as a variable transformation $E = \sqrt{\epsilon^2 + \Delta^2}$ which leads to

$$\mathrm{d}E = \frac{\epsilon}{\sqrt{\epsilon^2 + \Delta^2}} \mathrm{d}\epsilon \quad \Longleftrightarrow \quad \mathrm{d}\epsilon = \frac{E}{\epsilon} \mathrm{d}E,$$

$$\sum_{\boldsymbol{k}} g(\boldsymbol{k}) = \int D_n(\epsilon) g(E) \frac{E}{\epsilon} \mathrm{d}E.$$

Further we have $\frac{\partial \epsilon}{\partial E} = \frac{E}{\sqrt{E^2 - \Delta^2}} = \frac{E}{\epsilon}$ so that

$$\sum_{\boldsymbol{k}} g(\boldsymbol{k}) = \int g(E) \underbrace{D_n(\epsilon) \frac{\partial \epsilon}{\partial E}}_{D_s(E)} \mathrm{d}E. \qquad \text{(take total or partial derivative?)}$$

Then we use a methode we alread used (sure?) to simplify the expression. We asume that $D_n(\epsilon)$ is slowly varying so that $D_n(\epsilon) \approx D_n(0)$ where ϵ is measured relative to the Fermi-sruface. Hopefully we don't have any sharpness arround the Fermi-surface [1] p.93. We can therfore exclude the Van Hove singularities close to the Fermi-surface.

$$\frac{D_s(E)}{D_n(0)} \frac{E}{\sqrt{E^2 - \Delta^2}} = \frac{E}{\sqrt{E^2 - \Delta^2}} \underbrace{\frac{D_n(\epsilon)}{D_n(0)}}_{=\Theta(E - |\Delta|)} .$$

For the $\boldsymbol{k}$ dependence of the gap we can use the spectral weight introduced in 14. In analogy to the propagator or Green function introduced in **??** for the electrons, we can define one for the superconducting condensate that involves time-dependent fermionic oeprators.

$$G(\boldsymbol{k}, t; \sigma) = -\mathrm{i} \langle 0 | c_{\boldsymbol{k}\sigma}(t) c^{\dagger}_{\boldsymbol{k}\sigma}(0) | 0 \rangle$$

involving the BCS superconducting ground state $|0\rangle$ which an eigenstate of 38. As before we can consider the fourier transform of the propagator $G(\boldsymbol{k},\omega;\sigma)$

$$G(\boldsymbol{k},\omega;\sigma) = \frac{1}{2\pi}\int e^{\mathrm{i}\omega t} G(\boldsymbol{k},\omega;\sigma)\mathrm{d}t$$

We recall that Cooper pairs are two made of two electrons with opposite spin. We can first take a look at the density of state of the pair-member with $\sigma = \uparrow$. However are only considering spin singlet pairing so proving that the spectral weight A is spin independent should show that computing it for $\sigma = \uparrow$ is enough as Fossheim and Sudbø argued in [1] p.94.

So without loss of generality we set $\sigma = \uparrow$ and reintroduce the rotation of the basis of the c operators we performed in 33 and 34.

$$\begin{aligned} G(\boldsymbol{k},t;\uparrow) = -\mathrm{i}\langle 0|\ &\left(\cos(\theta)\eta^\dagger_{\boldsymbol{k}}(t) - \sin(\theta)\gamma^\dagger_{\boldsymbol{k}}(t)\right) \\ &\cdot\left(\cos(\theta)\eta_{\boldsymbol{k}}(0) - \sin(\theta)\gamma_{\boldsymbol{k}}(0)\right)|0\rangle \end{aligned}$$

The goal of these rotated operators was to diagonalise the hamiltonian. It follows

$$\langle 0|\eta^\dagger_{\boldsymbol{k}}\gamma^\dagger_{\boldsymbol{k}}|0\rangle = 0 = \langle 0|\eta_{\boldsymbol{k}}\gamma_{\boldsymbol{k}}|0\rangle$$

and therfore

$$\begin{aligned} G(\boldsymbol{k},t;\uparrow) =& -\mathrm{i}\cos(\theta)^2\langle 0|\eta^\dagger_{\boldsymbol{k}}(t)\eta_{\boldsymbol{k}}(0)|0\rangle \\ &-\mathrm{i}\sin(\theta)^2\langle 0|\eta^\dagger_{\boldsymbol{k}}(t)\eta_{\boldsymbol{k}}(0)|0\rangle. \end{aligned} \tag{42}$$

We can nicely split the propagator in the sum of free η- and γ-particles in the superconducting state. Employing to coherence factors 37 and 36 in the Fourier transform of we obtain

$$G(\boldsymbol{k},\omega;\uparrow) = \frac{u^2_{\boldsymbol{k}}}{\omega - E_{\boldsymbol{k}} + \mathrm{i}\delta_{\boldsymbol{k}}} + \frac{v^2_{\boldsymbol{k}}}{\omega + E_{\boldsymbol{k}} - \mathrm{i}\delta_{\boldsymbol{k}}}.$$

which gives the spectral weight

$$A(\boldsymbol{k},\omega;\uparrow) = u^2_{\boldsymbol{k}}\delta(\omega - E_{\boldsymbol{k}}) + v^2_{\boldsymbol{k}}\delta(\omega + E_{\boldsymbol{k}}).$$

This value is spin independent and using the arguments we've just given in such a case, we find

$$\begin{aligned} D_s(\omega) =& \frac{1}{N}\sum_{\boldsymbol{k}} A(\boldsymbol{k},\omega) \\ =& \frac{1}{N}\sum_{\boldsymbol{k}}\left(u^2_{\boldsymbol{k}}\delta(\omega - E_{\boldsymbol{k}}) + v^2_{\boldsymbol{k}}\delta(\omega + E_{\boldsymbol{k}})\right). \end{aligned}$$

The density of state of the superconductive condensate D_s is also spin independent since we're considering spin-singlet pairings.

2.1.8 Transition temperature and energy gap

The goal of this discussion will to derive a unniversial ratio between Δ and the crital temperature. In the last section we already introduced some expressions for $\Delta_{\boldsymbol{k}}(T)$ and $V_{\boldsymbol{kk}}$. Let us consider the simplest case where $V_{\boldsymbol{kk}} = V$.
The phonon modulated interaction has a cover $\omega_0 = \omega_D$ the Debye-frequency. Inserting it back to the BCS gap equation 40 we see that the gap loses it's $\boldsymbol{k}$-dependence and results as the identity when applying the symmetries ruling the crystal:

$$1 = V\sum_{\boldsymbol{k}'}\frac{\tanh\left(\beta E_{\boldsymbol{k}'}\right)}{2E_{\boldsymbol{k}'}}.$$

This equation can be easely solved for $T = T_C$ or $T = 0$.

Considering T approching T_C from bellow, we can asume that the gap vanishes. We replace the $\boldsymbol{k}$-sum by an integral over the normal density of state $D_n(\epsilon)$. Due to the shell the sum occurs in a tiny volume arround the Fermi-Surface so that $D_n(\epsilon)$ is evaluated close to the surface. We asume that in this neighbourhood D_n varries slowly such that avoid some van Hove singularities we simply approximate $D_n(\epsilon) \to D_n(0)$ because ϵ is counted relative to the surface in our early toughts. We introduce $\lambda = VD_n(0)$. We get

$$\begin{aligned}1 =&\lambda \int_{[0,\omega_D]} \frac{\tanh(\beta\epsilon/2)}{\epsilon}\mathrm{d}\epsilon \\ =&\lambda \ln\left(\frac{2e^{\gamma}\beta\omega_D}{\pi}\right)\end{aligned}$$

using $\gamma := \lim_{\to m\to\infty} \left(\sum_{l\in[\![m]\!]} 1/l - \ln(m)\right)$ the Euler-Mascheroni constant. More details are provided in [1] p.88-89. We obtain

$$k_BT_C \approx 1.13 \cdot \omega_D e^{-1/\lambda}$$

For $T \to 0$ the gap equation takes a simpler form to solve:

$$1 = V\sum_{\boldsymbol{k}'} \frac{1}{2E_{\boldsymbol{k}'}} = \lambda \int_{[0,\omega_D]} \frac{1}{\sqrt{\epsilon^2+\Delta^2}}\mathrm{d}\epsilon$$

leads

$$\Delta(T=0) = 2\omega_D e^{-1/\lambda}$$

according to the same source. We see how these expressions are closely dependent on λ. Moreover we can interpret the essential singularity at $\lambda \to 0$ as following: The attractive processes are singular perturbations of the non interacting electron gas. m is very demending to solve even for simple metals and is a function of multiple small details of the system. We aim here to aquire a qualitative knowledge. Let us now bring the ratio

$$\frac{2\Delta(T=0)}{k_BT_C} = \frac{2\pi}{e^{\gamma}} \approx 3.52$$

which is a universial ratio and does not depend anymore on the properties of the material. Knowing the critical temperature one can know the gap at 0K.

3 Bogoliubov-de Gennes Formalism

The Bogoliubov-de Gennes transformation allows us to express the hamiltonian in a diagonal way and express our 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

$$H = E_0 - \frac{1}{2}\check{c}^\dagger \check{H}\check{c}, \tag{43}$$

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

As we see we just describe each site with the four possbile c-operators. This means for each lattice site, we have a 4×4-submatrix that reflects the possible combinations of creation and anihinaltion operators of both spins. For the readability we are going to drop the comma between the site and spin indices.
For exemple if one has (without loss of generality) a chemical potential at the site i, then the hamiltonian is discribed in the following way:

$$H_{\mu i} = -\sum_\sigma \mu_i c^\dagger_{i,\sigma} c_{i,\sigma}$$

If we want to discribe it in therm of $\hat{c}_i$ we have:

$$H_{\mu,i} = \hat{c}_i^\dagger \cdot \mu_i \mathbb{I}_4 \cdot \hat{c}_i = \begin{pmatrix} c^\dagger_{i\uparrow} \\ c^\dagger_{i\downarrow} \\ c_{i\uparrow} \\ c_{i\downarrow}\end{pmatrix} \cdot \mu_i \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \left(c_{i\uparrow}, c_{i\downarrow}, c^\dagger_{i\uparrow}, c^\dagger_{i\downarrow}\right)$$

Please not that in later discussions we will discuss about how the matrix must exhibit a kind of symmetry to respect the fermonic relations. This was just an exemple.

Depending on the interaction we wish to describe, we can figure out what combination of operatos we want and design the 4×4 matrix accordingly. To achieve a full description of the system we can consider the interaction between to site i, j as a 4×4 matrix involving the $\hat{c}_i^\dagger$ and c_j operators. Then we can build a huge matrix $\check{H}$ based on 4×4 matrices at $\check{H}_{ij}$ and the vector we multiply it to is juste the $\hat{c}_i^\dagger$ and c_j operators stack above one and other forming the above-introduced $\check{c}$ vector. As a result, one gets the first formula introduced in this section 43. We can then compute the eigenvalues and -vectors express the quantities we're interested in. This is what we call the Bogoliubov-de Gennes transformation.

Now that the motivation is clear, we need to bring our Hamiltonian in a form that involves the fermionic operators $c_{i\sigma}$ and $c_{i\sigma}^\dagger$.

3.1 Tigh Binding Model

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

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

$$\begin{aligned} H = &\sum_{\sigma\sigma'} \int \phi_\sigma^\dagger(\boldsymbol{r}) H_{\sigma\sigma'}(\boldsymbol{r}) \psi_{\sigma'}(\boldsymbol{r}) \mathrm{d}^3 r \\ &+ \sum_{\sigma\sigma'} \int \int \phi_\sigma^\dagger(\boldsymbol{r}) \phi_{\sigma'}^\dagger(\boldsymbol{r}') V_{\sigma\sigma'}(\boldsymbol{r}, \boldsymbol{r}') \phi_{\sigma'}(\boldsymbol{r}') \phi_\sigma(\boldsymbol{r}) \mathrm{d}^3 r' \mathrm{d}^3 r \end{aligned}$$

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

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

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

$$\phi_\sigma(\boldsymbol{r}) := \sum_i w(\boldsymbol{r} - \boldsymbol{R}_i) c_{i\sigma} \qquad \phi_\sigma^\dagger(\boldsymbol{r}) := \sum_i w^*(\boldsymbol{r} - \boldsymbol{R}_i) c_{i\sigma}^\dagger \tag{44}$$

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

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

In the last line we include a local energy term ϵ and the so called hopping term t_{ij}, wich is the interaction with the nearest neighbour sites j of i. For a more precise description one could consider more neighbour. The spin depent term can be use to describe spin orbit coupeling 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 wich 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 amptidudes of moving a electron from site i to j. We asume it as spin-independant here.

$$H_N = -\sum_{i\sigma} \mu_i c^\dagger_{i\sigma} c_{i\sigma} - \sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} \tag{45}$$

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

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

$$\begin{aligned} t_{ij} &= -\int w^*(\boldsymbol{r} - \boldsymbol{R}_i) \frac{\nabla^2}{2m} w(\boldsymbol{r} - \boldsymbol{R}_j) \mathrm{d}^3 r \\ &= +\frac{1}{2m} \int \left(\nabla w(\boldsymbol{r} - \boldsymbol{R}_i)\right)^* \left(\nabla w(\boldsymbol{r} - \boldsymbol{R}_j)\right) \mathrm{d}^3 r. \end{aligned}$$

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

3.1.2 Superconductivity

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

$$H_S = -\int U(\boldsymbol{r}) \psi^\dagger_\downarrow(\boldsymbol{r}) \psi^\dagger_\uparrow(\boldsymbol{r}) \psi_\uparrow(\boldsymbol{r}) \psi_\downarrow(\boldsymbol{r}) \mathrm{d}^3 r$$

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

$$H_S = -\int \Big(\Delta(\boldsymbol{r}) \psi^\dagger_\downarrow(\boldsymbol{r}) \psi^\dagger_\uparrow(\boldsymbol{r}) + \Delta(\boldsymbol{r})^* \psi_\uparrow(\boldsymbol{r}) \psi_\downarrow(\boldsymbol{r}) \Big) \mathrm{d}^3 r.$$

we see that we the second integrand is just the complexe 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 44 and obtain:

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

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

$$H_S = -\sum_i \Delta_i c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} + \Delta^*_i c_{i\uparrow} c_{i\downarrow}. \tag{46}$$

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

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

and after aplying the tight binding formalism we get:

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

wich is a term we can add to the Hamiltonian 46. Form these equations we have the final Hamiltonian for the superconducting system:

$$H = E_0 + H_N + H_S.$$

3.2 A more symmertic 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

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

However using the form we have in the superconducting 46 and normal 45 Hamiltonian will later not act as a fermionic operator upon the transformation we're about to do. We need to rewrite the Hamiltonian in a more symmertic way to later respect the anticommutation relations.

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

$$\sum_{i\sigma} \mu_i c^\dagger_{i\sigma} c_{i\sigma} = \frac{1}{2} \sum_{i\sigma} \mu_i \left(c^\dagger_{i\sigma} c_{i\sigma} - c_{i\sigma} c^\dagger_{i\sigma} + 1 \right) \tag{47}$$

The trick we used is quite straight forward but not obvious. Taking two different states α and γ we have:

$$c^\dagger_\alpha c_\gamma \;=\; \frac{1}{2} c^\dagger_\alpha c_\gamma + \frac{1}{2} c^\dagger_\alpha c_\gamma \;=\; \frac{1}{2} c^\dagger_\alpha c_\gamma + \underbrace{\frac{1}{2} c^\dagger_\alpha c_\gamma + \frac{1}{2} c_\gamma c^\dagger_\alpha}_{\frac{1}{2}\left[c^\dagger_\alpha, c_\gamma\right]_+ = \frac{1}{2}\delta_{\alpha\gamma}} - \frac{1}{2} c_\gamma c^\dagger_\alpha. \tag{$\mathfrak{Tr}1$}$$

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

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

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

$$\sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} = \frac{1}{2} \sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - t_{ji} c_{i\sigma} c^\dagger_{j\sigma} = \frac{1}{2} \sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - t^*_{ji} c_{i\sigma} c^\dagger_{j\sigma}. \tag{48}$$

The superconducting term for its part takes the form:

$$\sum_i \Delta_i c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} + \Delta^*_i c_{i\uparrow} c_{i\downarrow} = \frac{1}{2} \sum_i \Delta_i \left(c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} - c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \right) + \Delta^*_i \left(c_{i\uparrow} c_{i\downarrow} - c_{i\downarrow} c_{i\uparrow} \right). \tag{49}$$

We then finish this section by using Eq.47, 48 and 49 in the Hamiltonian and obtain the following form:

$$\begin{aligned} H = E_0 &- \frac{1}{2} \sum_{i\sigma} \mu_i \left(c^\dagger_{i\sigma} c_{i\sigma} - c_{i\sigma} c^\dagger_{i\sigma} \right) \\ &- \frac{1}{2} \sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - t^*_{ji} c_{i\sigma} c^\dagger_{j\sigma} \\ &- \frac{1}{2} \sum_i \Delta_i \left(c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} - c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \right) + \Delta^*_i \left(c_{i\uparrow} c_{i\downarrow} - c_{i\downarrow} c_{i\uparrow} \right). \end{aligned} \tag{50}$$

The constant term $\frac{1}{2}\sum_{i\sigma} \mu_i$ of the normal Hamiltonian just vanished in the E_0. right? We can now rewrite the Hamiltonian in a more compact way:

$$H = E_0 - \frac{1}{2} \sum_{i,j} \hat{c}^\dagger_i \hat{H}_{ij} \hat{c}_j \tag{51}$$

where the on site matrix reads

$$\hat{H}_{ij} = \begin{pmatrix} \mu_i \mathbb{I}_2 \delta_{ij} + t_{ij} & -\mathrm{i}\sigma_2 \Delta_i \delta_{ij} \\ \mathrm{i}\sigma_2 \Delta_i^* \delta_{ij} & -\mu_i \mathbb{I}_2 \delta_{ij} - t_{ij}^* \end{pmatrix} = \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^\dagger & -H_{ij}^* \end{pmatrix} \tag{52}$$

where we use $\mathbb{I}_n$ as an n-dimensional identity matrix. We havn't explicitely removed the t_{ij} if we're not concidering nearest neighbours. At this point it's intersting 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

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

along with the system Hamiltonian-matrix $\check{H}_{ij} := \hat{H}_{ij}$ wich allows us to rewrite the Hamiltonian 51 as:

$$H = E_0 - \frac{1}{2} \check{c}^\dagger \check{H} \check{c}. \tag{53}$$

3.3 Eigenvalues

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

$$\check{H} \check{\chi}_n = E_n \check{\chi}_n \tag{54}$$

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: $\check{\chi}_n = (\hat{\chi}_{n1}, .., \hat{\chi}_{nN})$. This means $\chi_{n,i}$ refers to a 4×4 block, i.e. the on the submatrix we had earlier talked about. Therfore 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 $\check{\chi}_n$:

$$\sum_{j \in [\![N]\!]} \hat{H}_{ij} \hat{\chi}_{nj} = E_n \hat{\chi}_{ni}.$$

We remember that $\check{H}_{ij}$ represent a complex scalar and $\hat{H}_{ij}$ is a 4×4 matrix with complexe entries. So it follows by reintroducing 52 the following set of equations:

$$\begin{cases} \sum_{j \in [\![N]\!]} H_{ij} u_{nj} + \Delta v_{nj} = & E_n u_{nj} \\ \sum_{j \in [\![N]\!]} \Delta^\dagger u_{nj} - H_{ij}^* v_{nj} = & E_n v_{nj}. \end{cases} \xrightarrow{(1)} \begin{cases} \sum_j H_{ij} u_{nj} + \Delta v_{nj} = & E_n u_{nj} \\ \sum_j H_{ij} v_{nj}^* + \Delta^\dagger u_{nj}^* = & -E_n v_{nj}^*. \end{cases} \tag{55}$$

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

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

3.4 Diagonalization

Our goal is now to express the Hamiltonian relative to its energy eigenvalues, which is more practicle to work with. As we have seen in the last section, eigenvectors χ_n allows us to compute the energies. Therfore 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 $\check{X} = [\check{\chi}_{\pm 1}, .., \check{\chi}_{\pm 2N}]$ and introduce a diagonal matrix $\check{D} = \text{diag}(E_{\pm 1}, .., E_{\pm 2N})$ 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 $\check{c} := \check{X}\check{\gamma}$

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

where $\mathcal{N} = \{\pm n : n \in [\![N]\!]\}$ Reagranging 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 wich is $2N$-dimensional:

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

and due to the symmerty we saw erlier,

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

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

$$\gamma^{\dagger}_{-n} = \sum_{i\sigma}\left(v^*_{ni\sigma}c^{\dagger}_{i\sigma} + u^*_{ni\sigma}c_{i\sigma}\right) = \gamma_n.$$

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 realted to eachother, 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: $\mathcal{N}_+ = \{n \in \mathcal{N} : n > 0\}$, $\mathcal{N}_- = \{n \in \mathcal{N} : n < 0\}$

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

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

Using this knowledge, we can express a final formula for the Hamiltonian by using the anti-commutation properties of the fermionic γ-operators: $\left[\gamma_n^\dagger, \gamma_n\right]_+ = 1$, so using the trick $\mathfrak{Tr}1$ and bringing the $\frac{1}{2}$ prefactor in the sum:

$$H = E_0 - \sum_{n \in [\![N]\!]} E_n \left(\gamma_n^\dagger \gamma_n - \frac{1}{2}\right). \tag{56}$$

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 $\Delta(\boldsymbol{r}) := U(\boldsymbol{r})\langle\psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r})\rangle$. 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:

$$\begin{aligned} c_{i\sigma} &= \sum_{n \in \mathcal{N}} u_{ni\sigma}\gamma_n \\ &= \sum_{n \in \mathcal{N}_+} u_{ni\sigma}\gamma_n + u_{-n,i\sigma}\gamma_{-n} \\ &= \sum_{n \in \mathcal{N}_+} u_{ni\sigma}\gamma_n + v_{ni\sigma}^*\gamma_n^\dagger \end{aligned} \tag{57}$$

$$\begin{aligned} c_{i\sigma}^\dagger &= \sum_{n \in \mathcal{N}_+} (u_{ni\sigma}\gamma_n)^\dagger + (v_{ni\sigma}^*\gamma_n^\dagger)^\dagger \\ &= \sum_{n \in \mathcal{N}_+} \gamma_n^\dagger u_{ni\sigma}^\dagger + \gamma_n (v_{ni\sigma}^*)^\dagger \\ &= \sum_{n \in \mathcal{N}_+} u_{ni\sigma}^*\gamma_n^\dagger + v_{ni\sigma}\gamma_n \end{aligned} \tag{58}$$

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

$$\begin{aligned} \langle c_{i\uparrow} c_{i\downarrow}\rangle &= \sum_{n,m \in \mathcal{N}_+} \left\langle \left(u_{ni\uparrow}\gamma_n + v_{ni\uparrow}^*\gamma_n^\dagger\right)\left(u_{mi\downarrow}\gamma_m + v_{mi\downarrow}^*\gamma_m^\dagger\right)\right\rangle \\ &= \sum_{n,m \in \mathcal{N}_+} \left\langle \left(u_{ni\uparrow}u_{mi\downarrow}\gamma_n\gamma_m + u_{ni\uparrow}v_{mi\downarrow}^*\gamma_n\gamma_m^\dagger + v_{ni\uparrow}^*u_{mi\downarrow}\gamma_n^\dagger\gamma_m + v_{ni\uparrow}^*v_{mi\downarrow}^*\gamma_n^\dagger\gamma_m^\dagger\right)\right\rangle \\ &\overset{(*)}{=} \sum_{n \in \mathcal{N}_+} \left\langle u_{ni\uparrow}v_{ni\downarrow}^*\gamma_n\gamma_n^\dagger\right\rangle + \left\langle v_{ni\uparrow}^*u_{ni\downarrow}\gamma_n^\dagger\gamma_n\right\rangle \\ &= \sum_{n \in \mathcal{N}_+} u_{ni\uparrow}v_{ni\downarrow}^*\left\langle\gamma_n\gamma_n^\dagger\right\rangle + v_{ni\uparrow}^*u_{ni\downarrow}\left\langle\gamma_n^\dagger\gamma_n\right\rangle \\ &= \sum_{n \in \mathcal{N}_+} u_{ni\uparrow}v_{ni\downarrow}^*\left(1 - f(E_n)\right) + v_{ni\uparrow}^*u_{ni\downarrow}f(E_n) \end{aligned} \tag{59}$$

where f is the Fermi-Dirac distribution. In $(*)$ we notice no $\gamma\gamma$ or $\gamma^\dagger\gamma^\dagger$ terms in the Hamiltonian, so their expectation value is zero [1].
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 onselves, we just take a look at the first quantisation expression of this braket. This result leads to the self consistency equation:

$$\Delta_i = U_i \sum_{n \in \mathcal{N}_+} u_{ni\uparrow}v_{ni\downarrow}^*\left(1 - f(E_n)\right) + u_{ni\downarrow}v_{ni\uparrow}^*f(E_n) \tag{60}$$

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.

[1] This is like the expectation value of killing twice a fermion in a state. It is not possbile, because we cant annihilate a state that has a possession number of zero. And in the same way due to the Pauli-principle we can't have more than one particle in the same state, so $\langle\gamma^\dagger\gamma^\dagger\rangle = 0$. We are not finding these terms in the Hamiltonian. Here we additionaly removed the indicies, in fact the diagonalty also takes place on the indicies so that we end just with n. The Hamiltonian is diagonal in $\gamma\gamma^\dagger$ and $\gamma^\dagger\gamma$ right?

4 Altermagnetism

4.1 Introduction and overview

The reader might already be familiar with ferromagnets and all the regular magnetic models. Taking into account the spin and wave vector of each particle in a site, one can derive some symmetries under transform operations. For exemple a ferromagnet is symmetric under spin-flip (also called time reversal) and a rotation. In the exemple of the antiferromagnetism, we have two sub-lattice with opposite spins. In such systems the spin compensate eachother resulting in a null magnetism. The system is symmetric under spin-flip and translation and was theoretised in 1948 by Louis Néel as the Néel antiferromagnets. Allowing more complexity one could imagine multiple ions in a unit cell linked by rotation, screw, etc symmetries. The half ions of the cell owns an opposite spin from the other half. These material are labeled as zero q antiferromagnets. Both of these material keep the same electron spectra under such transformations. The spectra composente eachother resulting in a zero net magnetisation. This section summerises the historical work of [4].

Altermagnets implement two or more sub-lattice which are not related between eachother by translation nor inversion but rotation. These class of material was pinpointed in 2019.
These material are similar to complexer structure where the sublatticies aren't linked with the crystal symmetries. Therfore summing up the spin might not result in a trivial expression like the antiferromagnetic material. In fact the overall spin projection might almost be zero but not exactly.
However studying half metal and insulator leads to different result. Half metal can be seen as an insulator in one spin channel but not both [4]. The Quin Luttinger's theorem, showed that such substance must have an integer number of Bohr spin magnetic moment. Therfore structures with a small net magnetisation see these quantity be flooTamYellow to zero.

On the search of pratical applciation, reaseachers have found (an exaustive list is provided in [4]) that domain like tunneling magnetoresistance (TMR) are limited under the properties of the material. For instance the actual use of ferromagnets limits the frequency to the gigahertz range. This has to deal with the ferromagnetic resonance that connects the magnetisation with electromagnetic waves. The altermagnets could be used in the terahertz range. Mentioning that TMR is a key component of the magnetic random access memory (MRAM), the reader can easely estimate the performance improvment such upgrade could deliver in a computer.

In a more formal way, we can distinguish two types of altermagnet. In the first type, the altermagnet's lattice site have different distance to the neighbours depending on the linking axis and the spin of the particle in the site. This is illustrated in (***a***). On the other hand we can consider a unit cell beeing unsymmetric in its ion position. We consider a square lattice were each unit cell has a non magnetic ion and two magnetic ion with opposite spin. Please consider the second schema (***b***).

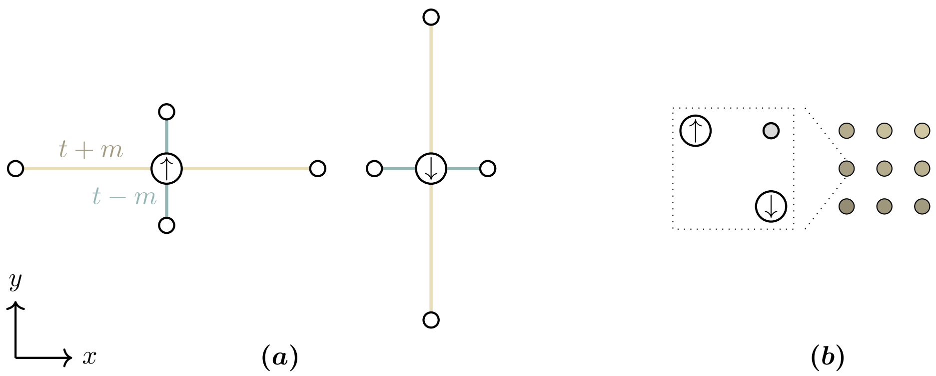


Figure 5: Altermagnet of type 1 and 2.

4.2 Symmetries

After giving an introduction on the geometric background of altermagnet we can now focus on the symmetries of the material. In this section we are going to focus on two simple transformation. The inversion P and the spin flip (time reversal) T.

$$\begin{aligned} P &: \boldsymbol{r} \mapsto -\boldsymbol{r} && \mathbb{R}^3 \to \mathbb{R}^3 \\ T &: t \mapsto -t \mathrel{\hat{=}} \sigma \mapsto -\sigma && \mathbb{R} \to \mathbb{R} \end{aligned}$$

We can first asume that the energy ϵ of the particle (or band structure) depends on the spin σ and the wave vector $\boldsymbol{k}$. Knowing $\boldsymbol{k} = \mathrm{d}\boldsymbol{r}/\mathrm{d}t$ leads to

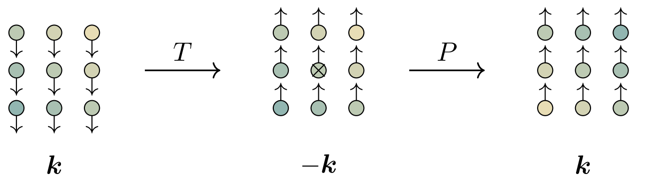
$$\begin{aligned} P\big(\epsilon(\boldsymbol{k}, \sigma)\big) &= \epsilon(-\boldsymbol{k}, \sigma) \\ T\big(\epsilon(\boldsymbol{k}, \sigma)\big) &= \epsilon(-\boldsymbol{k}, -\sigma) \end{aligned}$$

We observe the PT operation $P \circ T$. If the system is PT symetric one sould get $\epsilon(\boldsymbol{k}, \sigma) = P \circ T\big(\epsilon(\boldsymbol{k}, \sigma)\big)$. Asuming it's the case we can write

$$\epsilon(\boldsymbol{k}, \sigma) = P \circ T\big(\epsilon(\boldsymbol{k}, \sigma)\big) = \epsilon(\boldsymbol{k}, \downarrow)$$

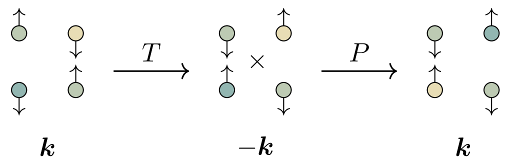
and therfore the PT-symmetric systems are spin-degenerated. We have the same energy for a given momentum at two opposite spins. Reciproquely this means that the existance of $\epsilon(\boldsymbol{k}, \sigma)$ is followed by an observation of $\epsilon(\boldsymbol{k}, -\sigma)$.

A few exemples We can imagine having a small section for the seek of readability. One should imagine the point where we apply the transformation in a the center of a 6×6 lattice, where we only show the second quadrant. We consider a ferromagnetic lattice where we apply the space inversion in the middle where the black cross is.

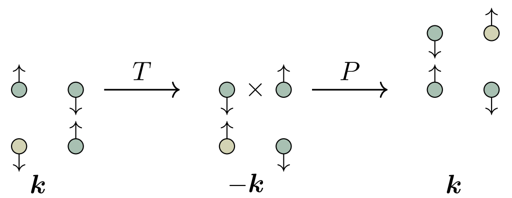


Letting the spin points upwards again will require to use another operation. Therfore the ferromagnet is not PT-symmetric and we observe no spin degenrancy as the equation shows it.

The antiferromagnet has an spin swich in every directions. If, as the ferromagnet, we pick a lattice point to apply the PT transformation to, we observe that this doesn't lead to a PT symmetry



However if we apply the inversion in the inbetween we observe something different.



This point we apply the P transformation arround makes the antiferromagnets having a PT symmetry. We see that the lattice site have moved but only the spin and the wave vector takes

part to the band ϵ. We therfore have a degenrancy in the energy spectrum.
Finding at least one point where the PT symmetry works makes the system PT symmetric.

If we now take a look at an altermagnets pictured in Fig.**??**, we have to different models to test. In the first one ***(a)*** the effect of the time reversal T makes the hopping change $m \to -m$. Then we find no point to invert the system around so that this first model doesn't have a PT symmetry. For the second one ***(b)*** we can first invert all spin but afterwards inverting the space doesn't brinng back the system in the original configuration. In fact neither applying the P after T on the lattice point nor on the space inbetween leads to a the lattice we began with. In both case the degenrancy is lifted, we have different eneries for the different spin-orientation.

Beyond the scope We refer as spin-orbit coupling (SOC) the interaction between the spin of the electron and the orbital motion. When this is disgarded we observe a rotation symmetry arround the spins. A rotation R can turn the spin back after the application of T resulting in a RT symmetry. $RT\big(\epsilon(\boldsymbol{k},\sigma)\big) = \epsilon(-\boldsymbol{k},\sigma)$ must equal $\epsilon(\boldsymbol{k},\sigma)$.

If we now consider a colinear magnet without SOC, we have a RT but no PT symmetry. Under such circumstances the spin-splitting must be symmetric under $\epsilon(-\boldsymbol{k},\sigma) = \epsilon(\boldsymbol{k},\sigma)$ wich describes an even band structure. Such systems are called inversion symetric altermagnets.

4.3 Implementation of an altermagnet

After introducing the basic propertires of an altermagnet we now aim to describe this system with the already introduced formalism. We are going to consider the first model involving a spin-dependent hopping. The Hamiltonian is given by

$$H_{AM} = -\sum_{\langle i,j\rangle\sigma\sigma'} (\boldsymbol{m}_{ij}\cdot\boldsymbol{\sigma})_{\sigma\sigma'}\, c^\dagger_{i\sigma} c_{j\sigma'}$$

involving $\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)^T$ the Pauli matricies. $\boldsymbol{m}_{ij}$ is the actual spin dependent hopping term. If the connection line between the two sites i and j lays on the $\boldsymbol{e}_x$ axis we have $\boldsymbol{m}_{ij} = m(0,0,1)$ and $\boldsymbol{m}_{ji} = m(0,0,-1)$ along $\boldsymbol{e}_y$ with m the desired hopping amplitude. $\boldsymbol{m}_{ij}$ scales and masks the pauli matricies.

Since the BdG formalism uses fermonic operators we again need to bring the matrix in a way that reflects the fermionic properties regarding to the $\check{c}$ opertor. We can remake use of Eq.$\mathfrak{Tr}$1:

$$H_{AM} = -\sum_{\langle i,j\rangle\sigma\sigma'} (\boldsymbol{m}_{ij}\cdot\boldsymbol{\sigma})_{\sigma\sigma'}\, \frac{1}{2}\left(c^\dagger_{i\sigma} c_{j\sigma'} - c_{i\sigma} c^\dagger_{j\sigma'}\right).$$

For the last summand we splitted the sum, exchanged the labeling of the states $i\sigma$ and $j\sigma'$ and recombined the sums. Bringing this Hamiltonian in the Nambu formalism we ontain by defining $(\boldsymbol{m}_{ij}\cdot\boldsymbol{\sigma})_{\sigma\sigma'} = \mathcal{M}_{\sigma\sigma'}$ the following Hamiltonian:

$$H^{(AM)}_{ij} = \frac{1}{2}\begin{pmatrix} -\mathcal{M} & \mathcal{O} \\ \mathcal{O} & \mathcal{M} \end{pmatrix}, \quad \text{where} \quad \mathcal{M} = \begin{pmatrix} \mathcal{M}_{\uparrow\uparrow} & \mathcal{M}_{\uparrow\downarrow} \\ \mathcal{M}_{\downarrow\uparrow} & \mathcal{M}_{\downarrow\downarrow} \end{pmatrix}.$$

Making use of this matrix in an altermagnetic lattice point, we can generate the according eigenvectors and -values. We can then study how the physical quantities behave in this material.

5 Simulations and ..

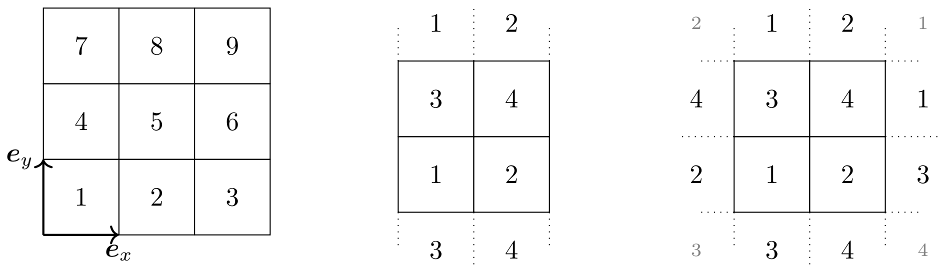
In the last chapters we introduced the theoretical background of superconductivity and altermagnets. The goal of this thesis is to use nummerical methodes to help us find some properties of the system. We remind here that all the code is avaliable on a GitHub repository at `https://github.com/Tamwyn001/Thesis`.

The repository contains the matlab code (.m) used to generates the datas in the a form of (coordinate, value) files (.dat). Gnuplot scripts (.gp) allow us to produce some plots that we can then directly link to the Latex source code of this thesis. Finaly some powershell scripts (.ps1) automate the gnuplot-latex process.

The matlab code contains two important files. The system.m file is a class that describes wich material we are using for the lattice, the physical context like the temperature and the chemical potential as well as the use or not of periodic boundary conditions. It contains also the Hamiltoninan of the system and keeps track of all lattice sites.
The LaticeSites.m describes the position of a lattice sites, stores its neighbours and monitorate the lattice site specific physical quantites. These quantites can be the superconducting gap or the current, etc.

We introduced earlier the need of a self consitent solution for the gap to correcly describe the Hamiltoninan. This is achieved in the GapEquation.m file which is the main script we run. We start with a guess for Δ_i and introduce it in the Hamiltoninan. This guess can depend on the material, or the site if we aim to introduce some phase shift at specific locations. We then derive a new site-dependent value using 60 for all site and reinsert it into the Hamiltonian. This requires to get eigenvectors and values of the Hamiltonian. This loop will be performed until the difference of each gap with its previous value reaches a treshhold. We then have a proper Hamiltonian and can start to derivate some values like the current. Matlab is a programm that works well with matricies so using it is a wise choice.

The site coordinate is stored as (x, y)-tuple as well as an index i that iterates over y-row and then starts again at the begining of the next row. This means that with different boundary conditions we get the following shape for the system:



Left we ahve a 3×3-system. The others are 2×2 with vertical periodic boundary conditions (PBC) and on the right with both vertical and horizontal PBC.

5.1 The non-trivial choice of the parameters

We want to describe a system including Cooper pairs. We already saw how the thermal fluctuations can break them. We pick a very low temperature of 10^{-3}K. For the chemical potential we need to pay closer attention. The band structure formula is given as

$$\epsilon_{\boldsymbol{k}} = -2t\left(\cos(k_x a) + \cos(k_y a)\right) - \mu$$

The fermi surface is given by $\epsilon_{\boldsymbol{k}} = 0$ when the chemical potential is included which means

$$-\frac{\mu}{2t} = \left(\cos(k_x a) + \cos(k_y a)\right)$$

We can fin a solution to this equaiton if

$$-4t \leq \mu \leq 4t.$$

in order to have a properly filled system we are going to choose $\mu = 3.75t$.

5.2 Currents

Using the charge conservation and the Heisenberg picture we are goning to derive an expression for the current in the lattice. The system we are taking into account is two dimensional.

The charge conservation reads

$$\partial_t \rho_i = -\nabla \boldsymbol{j}_i$$

and identifies the time variation of the charge density on the site i as the negative divergence of the current density. Now, performing some transformations, we bring this expression in a more useful form. The goal here is to integrate on both side over our two-dimensional surface Ω. For the charge density this yields to the charge at a site:

$$\int_\Omega \partial_t \rho_i \mathrm{d}\boldsymbol{r} = \partial_t Q_i.$$

For the current density we can use the Gauß law to change the integration set:

$$\int_\Omega \nabla \boldsymbol{j}_i \mathrm{d}\boldsymbol{r} = \int_{\partial\Omega} \boldsymbol{j}_i \boldsymbol{n} = \sum_n J_{i,n} a = \sum_n I_{i,n}$$

where $\partial\Omega$ is the boundary of Ω. The normal vector $\boldsymbol{n}$ points in the 2D-plane, outward from the boundary. Asuming we have a square lattice, we can asign to each lattice site a square unit cell with side lenght a. The sum over n happens to be over all the side.
Now introducing the Heisenberg picture with $\hbar = 1$ we get

$$\partial_t Q_i = \mathfrak{i}[H, Q_i].$$

Finlay we can introduce the second quantisation in the charge:

$$Q_i = \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} = \sum_\sigma n_{i,\sigma}$$

which is quite trivial, summing over all the particle at a site leads the charge of the site. After putting all together, this yields

$$I_i^{+x} + I_i^{+y} + I_i^{-x} + I_i^{-y} = -\mathfrak{i}\left[H, \sum_\sigma n_{i,\sigma}\right] \tag{61}$$

This mean the last step to perform is to compute the commutator of the different terms of the Hamiltonian with the chrage at a site i.
We reming here that our Hamiltonian contains a chemical potentail, a hopping, a superconduting and an altermagnetic term.

The hopping term We set remeber the use of a constant hopping amplitude $t_{ij} = t$.

$$\left[\sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma}, \sum_\sigma n_{l\sigma}\right] = \sum_{\langle ij\rangle\sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma} n_{l\sigma'} - n_{l\sigma'} c^\dagger_{i\sigma} c_{j\sigma}$$

We can then introduce a useful trick that involves the commutator $[n_\mu, c_\nu] = -\delta_{\mu\nu} c_\mu$

$$\begin{aligned} c^\dagger_{i\sigma} c_{j\sigma} n_{i,\sigma'} &= c^\dagger_{i\sigma}\big(\underbrace{c_{j\sigma} n_{l\sigma'} - n_{l\sigma'} c_{j\sigma}}_{-[n_{l\sigma'}, c_{j\sigma}]} + n_{l\sigma'} c_{j\sigma}\big) \\ &= c^\dagger_{i\sigma}\left(\delta_{\sigma'\sigma}\delta_{lj} c_{i\sigma'} + n_{l\sigma'} c_{j\sigma}\right). \end{aligned}$$

Following the same schema we derive the other part of the commutator. Here the expressions involves $[n_\mu, c^\dagger_\nu] = \delta_{\mu\nu} c^\dagger_\mu$:

$$\begin{aligned} n_{l\sigma'} c^\dagger_{i\sigma} c_{j\sigma} &= \big(\underbrace{n_{l\sigma'} c^\dagger_{i\sigma} - c^\dagger_{i\sigma} n_{l\sigma'}}_{[n_{l\sigma'}, c^\dagger_{i\sigma}]} + c^\dagger_{i\sigma} n_{l\sigma'}\big) c_{j\sigma} \\ &= \left(\delta_{\sigma'\sigma}\delta_{li} c^\dagger_{j\sigma'} + c^\dagger_{i\sigma} n_{l\sigma'}\right) c_{j\sigma} \end{aligned}$$

After substracting the second term from the first one we are left with

$$\left[\sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma}, \sum_\sigma n_{i\sigma}\right] = \sum_{\langle ij\rangle\sigma\sigma'} \delta_{\sigma'\sigma}\left(\delta_{lj}c^\dagger_{i\sigma}c_{j\sigma'} - \delta_{li}c^\dagger_{i\sigma'}c_{j\sigma}\right)$$
$$= \frac{1}{2}\sum_{i\boldsymbol{\delta}\sigma\sigma'} \delta_{\sigma'\sigma}\left(\delta_{l,i+\boldsymbol{\delta}}c^\dagger_{i\sigma}c_{i+\boldsymbol{\delta},\sigma'} - \delta_{li}c^\dagger_{i\sigma'}c_{i+\boldsymbol{\delta},\sigma}\right)$$

Because of the squared lattice we can summerise the neigbour set $\langle ij\rangle$ to $\{i+\delta_x, i-\delta_x, i+\delta_y, i-\delta_y\}$ involving δ_{axis} the displacemnt from the site to neighbour one along the given axis. This is abstracted in $i+\boldsymbol{\delta}$. We obtain after summing up over the σ' and i, and writing explicitely everything we obtain

$$\begin{aligned} = \frac{1}{2}\sum_\sigma & (c^\dagger_{l-\delta_x\sigma}c_{l,\sigma} - c^\dagger_{l\sigma}c_{l+\delta_x,\sigma}) + (c^\dagger_{l+\delta_x\sigma}c_{l,\sigma} - c^\dagger_{l\sigma}c_{l-\delta_x,\sigma}) \\ & + (c^\dagger_{l-\delta_y\sigma}c_{l,\sigma} - c^\dagger_{l\sigma}c_{l+\delta_y,\sigma}) + (c^\dagger_{l+\delta_y\sigma}c_{l,\sigma} - c^\dagger_{l\sigma}c_{l-\delta_y,\sigma}), \end{aligned} \tag{62}$$

where the one half factor avoids summing twice over the nearest neigbhours. This proportional to the current at a site l. The current of one side of the square unit cell is represnted by a pair of $c^\dagger_{l\pm\delta_x,\sigma}c_{l\sigma} - c^\dagger_{l\sigma}c_{l\pm\delta_x,\sigma}$ where the same displacement δ_x is involved. This will be an important consideration when coming to the altermagnet.

Chemical potentail term For the chemical potential term it is useful to introduce that the commutator between two number operator vanishes. Since the charge and the chenical potential operators involves only number operator, we find that this term dont't take part to the current.

Superconducting term The superconduting term has a particlar behaviour. If one can sovle the gap (self consistently), this term doesn't contribute to the current as we are going to see. We first form the commutator between the Hubbard term and the charge operator:

$$\left[\sum_i\left(\Delta_i c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} + \Delta^*_i c_{i\uparrow}c_{i\downarrow}\right), \sum_\sigma n_{l,\sigma}\right]$$

again make the already introded commutator appear, we obtain

$$\begin{aligned} &= \sum_{i\sigma}\delta_{il}\left(\Delta^\dagger_i(\delta_{\sigma\downarrow}+\delta_{\sigma\uparrow})c_{i\downarrow}c_{i\uparrow} - \Delta_i(\delta_{\sigma\downarrow}+\delta_{\sigma\uparrow})c^\dagger_{i\downarrow}c^\dagger_{i\uparrow}\right) \\ &= 2\left(\Delta^\dagger_i c_{l\downarrow}c_{l\uparrow} - \Delta_i c^\dagger_{l\downarrow}c^\dagger_{l\uparrow}\right) \end{aligned}$$

This expression mixes creation and annihilation operators and makes it hard to recognise a current. One can view this term as a source need citation?meaning we havw a new term $\mathcal{C}_i$ that appears in the equation

$$-\partial_t Q_i = \mathcal{C}_i + \sum_n I_{i,n}.$$

To know the contribution to the current we can investigate the rate of charge generation of this term. This is achieved by taking the quantum expectation and the thermal average of the system.

$$\begin{aligned} & 2\left(\Delta^\dagger_l\langle c_{l\downarrow}c_{l\uparrow}\rangle - \Delta_l\langle c^\dagger_{l\downarrow}c^\dagger_{l\uparrow}\rangle\right) \\ &= 2\Delta_l\sum_n v_{nl\downarrow}u^*_{nl\uparrow}\left(1 - f\left(1/2E_n\right)\right) + 2\Delta^\dagger_l\sum_n u_{nl\downarrow}v^*_{nl\uparrow}f\left(1/2E_n\right) \\ &= \frac{2}{U_i}\left(\Delta^\dagger_l\Delta_l - \Delta_l\Delta^\dagger_l\right) = 0 \end{aligned}$$

Solving Δ self-consistently will lead to $\Delta\Delta^\dagger = \Delta^\dagger\Delta$ and therfore we find that the value vanishes.

Altermagnetic term As we introduced it in a previous discussion, the altermagnetic term is more complicated than the last one treated an need more work. In essence we describe an advanced hopping term, that changes regarding of the hopping axis. We can first bring the commutator where the matrix element $\left(\boldsymbol{m}_{ij}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}$ is a scalar:

$$
\begin{aligned}
\left[\sum_{\langle ij\rangle\sigma\sigma'}\left(\boldsymbol{m}_{ij}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\cdot c^\dagger_{i\sigma}c_{j\sigma'},\sum_{\tilde{\sigma}}n_{l,\tilde{\sigma}}\right] &= \sum_{\substack{\langle ij\rangle\\ \sigma\sigma'\tilde{\sigma}}}\left(\boldsymbol{m}_{ij}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\left(c^\dagger_{i\sigma}c_{j\sigma'}n_{l\tilde{\sigma}}-n_{l\tilde{\sigma}}c^\dagger_{i\sigma}c_{j\sigma'}\right)\\
&= \sum_{\substack{\langle ij\rangle\\ \sigma\sigma'\tilde{\sigma}}}\left(\boldsymbol{m}_{ij}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\delta_{\sigma\tilde{\sigma}}\left(\delta_{lj}c^\dagger_{i\sigma}c_{j\tilde{\sigma}}-\delta_{li}c^\dagger_{i\tilde{\sigma}}c_{j\sigma}\right)\\
&=\frac{1}{2}\sum_{i\boldsymbol{\delta}\sigma\sigma'}\left(\boldsymbol{m}_{i,i+\boldsymbol{\delta}}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\left(\delta_{l,i+\boldsymbol{\delta}}c^\dagger_{i\sigma}c_{i+\boldsymbol{\delta},\sigma}-\delta_{li}c^\dagger_{i\sigma}c_{i+\boldsymbol{\delta},\sigma}\right)
\end{aligned}
$$

Using the same transformation we made earlyer to introduce the commutator between n,c and $n,c^\dagger$ we obtain after summing over the $\tilde{\sigma}$ introducing a new set made of $\boldsymbol{\delta}$s as we did before. The summation over the $\boldsymbol{\delta}$ results in the following combersom expression

$$
\begin{aligned}
=\sum_{\sigma}\Bigg[&\left(c^\dagger_{l-\delta_x,\sigma}c_{l\sigma}-c^\dagger_{l\sigma}c_{l+\delta_x,\sigma}\right)\sum_{\sigma'}\left(\boldsymbol{m}_{l,l+\delta_x}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\\
&+\left(c^\dagger_{l+\delta_x,\sigma}c_{l\sigma}-c^\dagger_{l\sigma}c_{l-\delta_x,\sigma}\right)\sum_{\sigma'}\left(\boldsymbol{m}_{l,l-\delta_x}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\\
&+\left(c^\dagger_{l-\delta_y,\sigma}c_{l\sigma}-c^\dagger_{l\sigma}c_{l+\delta_y,\sigma}\right)\sum_{\sigma'}\left(\boldsymbol{m}_{l,l+\delta_y}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\\
&+\left(c^\dagger_{l+\delta_y,\sigma}c_{l\sigma}-c^\dagger_{l\sigma}c_{l-\delta_y,\sigma}\right)\sum_{\sigma'}\left(\boldsymbol{m}_{l,l-\delta_y}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\Bigg]
\end{aligned}
\tag{63}
$$

When it will come to identify the current on each side of the unit cell, we will have to take into account the displacement δ that is involved in the $c^\dagger_{l\pm\delta_x,\sigma}c_{l\sigma}-c^\dagger_{l\sigma}c_{l\pm\delta_x,\sigma}$. This has to be consitent with what we already did for the hopping term. This means each current side will be dependent on the spin hopping on both direction of the same axis. This will become clear in the derivation.

Side currents Each unit cell were introduced as a square. We can from the last derived equation identify the contribution of the current on each side of the cell. We have a side on each axis direction $+x,+y,-x,-y$ as introduced in Eq.61. Due to the symmetric properties of the current, we can abstract the notation for $r\in\{x,y\}$. Using Eq.62 and Eq.63 we can write the current on each side r as follow. We as well reintroduce the minus of every summand of the Hamiltonian (due to their attractive nature) we let aside for the commutator relations. This multiplies with the minus one from the Heisenberg picture resulting in a plus sign. Futher taking $\mathfrak{i}=-1/\mathfrak{i}$ we get:

$$\left(I_i^{\pm r}\right)_{hop}=-\frac{t}{2\mathfrak{i}}\sum_{\sigma}c^\dagger_{i\pm\delta_r,\sigma}c_{i\sigma}-c^\dagger_{i\sigma}c_{i\pm\delta_r,\sigma}\tag{64}$$

$$\left(I_i^{\pm r}\right)_{AM}=-\frac{1}{2\mathfrak{i}}\sum_{\sigma\sigma'}c^\dagger_{i\pm\delta_r,\sigma}c_{i\sigma}\left(\boldsymbol{m}_{i,i\mp\delta_r}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}-c^\dagger_{i\sigma}c_{i\pm\delta_r,\sigma}\left(\boldsymbol{m}_{i,i\pm\delta_r}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\tag{65}$$

In this sense the hopping and altermagnetic term are very similar from nature. However the altermagnetic term is scaled by the hopping amplitude t on each summand, which shows a spin-dependent behaviour.

However we're not quite finished. The way we difined the matrix element, is to be isotropic on each axis. By doing so we can asume that $\left(\boldsymbol{m}_{i,i-\delta_r}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}=\left(\boldsymbol{m}_{i,i+\delta_r}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}$ so that:

$$\left(I_i^{\pm r}\right)_{AM}=-\frac{1}{2\mathfrak{i}}\sum_{\sigma\sigma'}\left(\boldsymbol{m}_{i,i+\delta_r}\cdot\boldsymbol{\sigma}\right)_{\sigma\sigma'}\left(c^\dagger_{i\pm\delta_r,\sigma}c_{i\sigma}-c^\dagger_{i\sigma}c_{i\pm\delta_r,\sigma}\right).\tag{66}$$

Total currents Until now we are able to describe how the current flows trought each faces of the unit cell. For this we can simply split the term we derived. From this we now aim to derive the current flows on each axis. This can ealsy be done asuming that the current flowing in the $-x$ direction subtracted from the current in the positive x direction forms the total current in $\boldsymbol{e}_x$. From this we get for $r \in \{x, y\}$:

$$I_i^r = I_i^{+r} - I_i^{-r}.$$

The real current that we can measure can be obtained by taking the quantum expection value and the thermal average of the currents. Further we also introduce the BdG-transformed operators with the eigenvalues 79 and 80.

For the seak of readability we are going to stick with this r-notation. In fact the total currents takes a disproportionate size on the page so we abstract a bit. Further du to the linearity of the commutator one can split the current in different terms. We first start with the derivation of the physical current that comes from the hopping term.

$$\langle I_i^r \rangle_{\text{hop}} = \frac{t}{2\mathrm{i}} \left[\sum_\sigma \langle c^\dagger_{i-\delta_r,\sigma} c_{i\sigma} \rangle - \langle c^\dagger_{i\sigma} c_{i-\delta_r,\sigma} \rangle - \langle c^\dagger_{i+\delta_r,\sigma} c_{i\sigma} \rangle + \langle c^\dagger_{,\sigma} c_{i+\delta_r,\sigma} \rangle \right]$$

and after introducing the BdG-transformed operators we obtain for the first term:

$$\begin{aligned} \langle c^\dagger_{i-\delta_r,\sigma} c_{i\sigma} \rangle = \sum_{n,m \in \mathcal{N}_+} & u^*_{n,i-\delta_r,\sigma} u_{ni\sigma} \underbrace{\langle \gamma_n^\dagger \gamma_m \rangle}_{\delta_{mn} f(E_n)} + u^*_{n,i-\delta_r,\sigma} v^*_{mi\sigma} \underbrace{\langle \gamma_n^\dagger \gamma_m^\dagger \rangle}_{0} \\ & + v_{n,i-\delta_r,\sigma} u_{mi\sigma} \underbrace{\langle \gamma_n \gamma_m \rangle}_{0} + v_{n,i-\delta_r,\sigma} v^*_{mi\sigma} \underbrace{\langle \gamma_n \gamma_m^\dagger \rangle}_{\delta_{mn}(1-f(E_n))} . \end{aligned}$$

In the same way, we obtain for the other terms:

$$\begin{aligned} -\langle c^\dagger_{i\sigma} c_{i-\delta_r,\sigma} \rangle &= -\sum_{n \in \mathcal{N}_+} u^*_{ni\sigma} u_{n,i-\delta_r,\sigma} f(E_n) + v_{ni\sigma} v^*_{n,i-\delta_r,\sigma} \big(1 - f(E_n)\big), \\ -\langle c^\dagger_{i+\delta_r,\sigma} c_{i\sigma} \rangle &= -\sum_{n \in \mathcal{N}_+} u^*_{n,i+\delta_r,\sigma} u_{ni\sigma} f(E_n) + v_{n,i+\delta_r,\sigma} v^*_{ni\sigma} \big(1 - f(E_n)\big), \\ \langle c^\dagger_{i\sigma} c_{i+\delta_r,\sigma} \rangle &= \sum_{n \in \mathcal{N}_+} u^*_{ni\sigma} u_{n,i+\delta_r,\sigma} f(E_n) + v_{ni\sigma} v^*_{n,i+\delta_r,\sigma} \big(1 - f(E_n)\big). \end{aligned}$$

Here we can recognise a very usefull relation that is going to simplify everything. We have $\langle c^\dagger_{i\pm\delta_r,\sigma} c_{i\sigma} \rangle = \langle c^\dagger_{i\sigma} c_{i\pm\delta_r,\sigma} \rangle^*$. We can then recall a useful realtion that we can use in these expressions. Have z a complexe we obtain $\mathcal{I}\mathrm{m}(z) = \frac{1}{2\mathrm{i}}(z - z^*)$. Further $\mathcal{I}\mathrm{m}(z) + \mathcal{I}\mathrm{m}(z') = \mathcal{I}\mathrm{m}(z + z')$. After summing up the terms we obtain the following expression for current of the hopping term along the axis r:

$$\begin{aligned} \langle I_i^r \rangle_{\text{hop}} = t \cdot \mathcal{I}\mathrm{m} \Bigg[\sum_\sigma \sum_{n \in \mathcal{N}_+} & f(E_n) u_{ni\sigma} \left(u^*_{n,i-\delta_r,\sigma} - u^*_{n,i+\delta_r,\sigma} \right) \\ & + \big(1 - f(E_n)\big) v_{ni\sigma} \left(v^*_{n,i-\delta_r} - v^*_{n,i+\delta_r,\sigma} \right) \Bigg]. \end{aligned} \tag{67}$$

And inside the altermagnet we add the following term using the same derivation method. The matrix element is a constant regarding the states-brakets. In this sens the quantum expectation and thermal average leave this quantity unchanged. Finaly we obtain the exact same result than a t hopping but with a prefactor. This is consitent with the observation already made.

$$\begin{aligned} \langle I_i^r \rangle_{\text{AM}} = \mathcal{I}\mathrm{m} \Bigg[\sum_{\sigma\sigma'} (\boldsymbol{m}_{i,i+\delta_r} \cdot \boldsymbol{\sigma})_{\sigma\sigma'} \sum_{n \in \mathcal{N}_+} & f(E_n) u_{ni\sigma} \left(u^*_{n,i-\delta_r,\sigma} - u^*_{n,i+\delta_r,\sigma} \right) \\ & + \big(1 - f(E_n)\big) v_{ni\sigma} \left(v^*_{n,i-\delta_r} - v^*_{n,i+\delta_r,\sigma} \right) \Bigg]. \end{aligned} \tag{68}$$

6 An advanced superconductivity

6.1 Site dependend potential

In this section we are going to highlight how the neighbour-depending potential can lead to a new kind of superconductivity. These new superconductive states are label s, p and extended d-wave superconductivity. The derivations we are going to make are closely based on the work of A.H. Mjøs and J. Linder in [2].

The Hamiltonian beeing the groundstone of this disscusssion, we're going to beggin with it. It differs slightly from the symmertic one we derived in Eq.50. This extended version contains a neighbour-depending potential H_V that is going to produce the new superconductive Δ-part of the Hamiltonian. This potential is as well attractive such that $V > 0$, similar to the BCS theorie.

$$H = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} - \frac{V}{2} \sum_{\langle ij \rangle \sigma} n_{i\sigma} n_{j\bar{\sigma}}. \tag{69}$$

Here the $\bar{\sigma}$-notation means the opposite spin of σ. In other words the attraction finds only place between particles of opposite spin, mirroring the formation process of Cooper-pairs. We have a factor of one half to avoid counting twice the neighbours.

Trained eyes will recognise that H_V is not quadratic in the creation and annihilation operators which makes the Hamiltonian impossible to write in the BdG-formalism. For this reason we can use the so called Hartree-Fock mean field approximation $H_V \to H_V^{HF}$ defined as:

$$H_V^{HF} = \frac{1}{2} \sum_{\langle ij \rangle \sigma} V_{ij} \left(F_{ij}^{\sigma\bar{\sigma}} c^\dagger_{j\bar{\sigma}} c^\dagger_{i\sigma} + \text{h.c.} + |F_{ij}^{\sigma\bar{\sigma}}|^2 \right) \tag{70}$$

involving the pairing amplitude $F_{ij}^{\sigma\bar{\sigma}} = \langle c_{i\sigma} c_{j\bar{\sigma}} \rangle$ that we already introduced. The V_{ij} are the neighbour-depending potential. The last term is a constant energy term which we can discard during the diagonalization process. If one wanted to compute the free energy this must be included there. From this point simplifications can be made to reach out final Hamiltonian.

Using the fermionic property $[c^\dagger_{i\sigma}, c^\dagger_{j\sigma}]_+ = 0$ we have $c^\dagger_{i\sigma} c^\dagger_{j\sigma} = -c^\dagger_{i\sigma} c^\dagger_{j\sigma}$ which leads to $\langle c^\dagger_{i\sigma} c^\dagger_{j\sigma} \rangle = -\langle c^\dagger_{i\sigma} c^\dagger_{j\sigma} \rangle$. We can use this in the last step of the following simplification:

$$\begin{aligned}
H_V^{HF} =& \frac{1}{2} \sum_{\langle ij \rangle \sigma} V_{ij} \left(F_{ij}^{\sigma\bar{\sigma}} c^\dagger_{j\bar{\sigma}} c^\dagger_{i\sigma} + \text{h.c.} \right) \\
=& \frac{1}{2} \sum_{\langle ij \rangle} V_{ij} \left(F_{ij}^{\uparrow\downarrow} c^\dagger_{j\downarrow} c^\dagger_{i\uparrow} + F_{ij}^{\downarrow\uparrow} c^\dagger_{j\uparrow} c^\dagger_{i\downarrow} + \text{h.c.} \right) \\
=& \sum_{\langle ij \rangle} V_{ij} \left(F_{ij}^{\uparrow\downarrow} c^\dagger_{j\downarrow} c^\dagger_{i\uparrow} + \text{h.c.} \right)
\end{aligned} \tag{71}$$

Using the raltion $F_{ij}^{\uparrow\downarrow} = -F_{ij}^{\downarrow\uparrow}$ and the symmerty of the potential $V_{ij} = V_{ji}$ we can add the two terms up and remove the one half factor. The Hamiltonian is now ready to be diagonalized but first, we are going to discuss which advantages a Fourier transform of the Hamiltonian could bring us.

In an homogenous material we can consider a lattice and imagine some periodic boundary conditions in all directions. There is a translation invariance. In heterostructures however the material may vary, let's asume without loss of generality, in a direction. As we now, a periodic signal is a good candiade for a Fourier transform, which we can then express in a finite set of coeficient. This is very handfull. However the direction we want to transform on has to show a periodicty. For this reason an homogenous two-dimensional lattice involves a Fourier transformation in two space dimensions while a heterostructure we transform only in the direction where the material is the same. For instance a multilayer material in the x-direction can be described by combining a real space desciption in the x-axis combined to a Fourier transformation in the y-direction. In this thesis we are going to focus ourselves on a multilayer material in the x-direction.

The description of the creation and annihilation operators with a step in the momentum space for the y-direction can be expressed as follow:

$$c_{xy\sigma} = \frac{1}{\sqrt{N_y}} \sum_{k_y} c_{xk_y\sigma} e^{\mathrm{i}k_y y} \tag{72}$$

$$c^\dagger_{xy\sigma} = \frac{1}{\sqrt{N_y}} \sum_{k_y} c^\dagger_{xk_y\sigma} e^{-\mathrm{i}k_y y} \tag{73}$$

How do we find an expression for k_y? Well the periodicity (for ex. in the c operator) yields $c_{xy\sigma} = c_{x,y+N_x,\sigma}$ this means the following condition must be fullfilled:

$$\begin{aligned} c_{xy\sigma} = c_{x,y+N_x,\sigma} \Leftrightarrow & e^{\mathrm{i}k_y y} = e^{\mathrm{i}k_y(y+N_y)} \Leftrightarrow e^{\mathrm{i}k_y N_y} = 1 \\ \Leftrightarrow & k_y = \frac{2\pi n}{N_y}. \end{aligned}$$

We know that the momentum index should cover the entire first Brilloin zone. This covers the momentum from $-\pi/a$ to π/a where a is the lattice constant. Further due to the $2\pi/a$ periodicity we have the same k_y at $-\pi/a$ and π/a. For this reason we need to map k_y in $[-\pi/a; \pi/a)$. This means we have $n \in [-N_y/2; N_y/2 - 1]$ including 0. For $n = 4$ we then have $k_y \in \{-\pi, -\pi/2, 0, \pi/2\}$.

For the readebility we are going to use $k_y \to k$. Further to an index i can associate (x, y) and to j, (x', y'). We first want to transform the hopping term:

$$H_{\text{hop}} = -\sum_{\langle ij\rangle\sigma} t_{ij} \sum_{kk'} c^\dagger_{xk\sigma} c_{x'k'\sigma} e^{\mathrm{i}(k'y'-ky)}$$

Here we can use the neighbour shift properties $y' = y + \delta_y$ where $\delta_y = \pm 1$. Doing so we have

$$e^{\mathrm{i}(k'y'-ky)} = e^{\mathrm{i}(k'(y+\delta_y)-ky)} = e^{\mathrm{i}(k'-k)y} e^{\mathrm{i}k'\delta_y}$$

No wee need to express the neighbourhood sum. Precily we have

$$\begin{aligned} H_{\text{hop}} =& -\sum_{\langle ij\rangle\sigma} t_{ij} \sum_{kk'} c^\dagger_{xk\sigma} c_{x'k'\sigma} e^{\mathrm{i}(k-k')y} e^{\mathrm{i}k'\delta_y} \\ =& -\sum_{xy\sigma} \sum_{kk'} \Bigg(t_{x,x+1} \underbrace{c^\dagger_{xk\sigma} c_{x+1k'\sigma} e^{\mathrm{i}k'\cdot(0)}}_{+x \text{ hopping, no } \delta_y} + t_{x,x-1} \underbrace{c^\dagger_{xk\sigma} c_{x-1k'\sigma} e^{\mathrm{i}k'\cdot(0)}}_{-x \text{ hopping, no } \delta_y} \\ & + t_{x,y-1} \underbrace{c_{xk\sigma} c^\dagger_{xk'\sigma} e^{\mathrm{i}k'\cdot(-1)}}_{\delta_y=-1} + t_{x,y+1} \underbrace{c^\dagger_{xk\sigma} c_{xk'\sigma} e^{\mathrm{i}k'\cdot(1)}}_{\delta_y=1} \Bigg) e^{\mathrm{i}(k-k')y} \end{aligned}$$

As we see the y direction is now expressed in the k-index, which is unique for each lattice y-slice. The information is then conserved. We know that system have different material on the x axis. This means $t_{x,y-1} = t_{x,x} = t_{x,y+1}$ because the material are isotropic but every material has a different hopping term. Beside we can use the following realtion $1/N_y \sum_y e^{\mathrm{i}(k-k')y} = \delta_{kk'}$. Perfoming both expression leads after a summation over k' to

$$H_{\text{hop}} = -\sum_{xk\sigma} t_{x,x+1} c^\dagger_{xk\sigma} c_{x+1k\sigma} + t_{x,x-1} c^\dagger_{xk\sigma} c_{x+1k\sigma} + t_{x,x} c^\dagger_{xk\sigma} c_{xk\sigma} \left(e^{\mathrm{i}k} + e^{-\mathrm{i}k}\right)$$

And now we can reintroduce an arbitray second coordinate x' to describe the neighbours.

$$H_{\text{hop}} = -\sum_{xx'k\sigma} t_{x,x'} c^\dagger_{xk\sigma} c_{x'k\sigma} \left(\delta_{x+1,x'} + \delta_{x-1,x'} + \delta_{x,x'} 2\cos(k)\right) \tag{74}$$

The chemical potential term is more easly given. In fact the number opertor yields to use two operators $c^\dagger c$ at a same coordinate i.

$$H_\mu = -\mu \sum_{xkk'\sigma} c^\dagger_{xk\sigma} c_{xk'\sigma} e^{\mathrm{i}(k-k')y} = -\sum_{xx'k\sigma} \mu c^\dagger_{xk\sigma} c_{xk'\sigma} \delta_{xx'} \tag{75}$$

We finaly have for the terms involving $c^{\dagger}_{xx'\sigma}c_{xx'\sigma}$:

$$H_{\text{hop}} + H_{\mu} = \sum_{xx'k\sigma} \epsilon_{xx'k\sigma} c^{\dagger}_{xk\sigma} c_{x'k\sigma}$$

using

$$\epsilon_{xx'k\sigma} = -t_{xx'}\left(\delta_{x+1,x'} + \delta_{x-1,x'}\right) - \left(t_{xx'} 2\cos(k) + \mu\right)\delta_{xx'}$$

Moving on to the potential term we have to introduce a new notation. $i \pm \hat{x} = i \pm 1$ and $i \pm \hat{y} = i \pm N_x$. Write a single clear message at the beggining of the lattice introduction.. For the brevety we use $f(a) = V_{ia}F_{ia}c^{\dagger}_{a\downarrow}c^{\dagger}_{i\uparrow}$

$$\begin{aligned} H_V &= \sum_{\langle ij \rangle} V_{ij}F_{ij}c^{\dagger}_{i\downarrow}c^{\dagger}_{j\uparrow} + \text{h.c.} \\ &= \sum_{i} f(i-1) + f(i+1) + f(i+N_x) + f(i-N_x) + \text{h.c.} \end{aligned}$$

We can now insert our Fourier transformation introduced in Eq.73 and Eq.72 to obtain

$$\begin{aligned} H_V =& \sum_{xy} \frac{1}{N_y} \sum_{kk'} \Big(V_{x,x+1}F^{x+}_{x} c^{\dagger}_{x+1,k,\downarrow} c^{\dagger}_{xk'\uparrow} + V_{x,x-1}F^{x-}_{x} c^{\dagger}_{x+1,k,\downarrow} c^{\dagger}_{xk'\uparrow} \\ &+ V_{xx}\left(F^{y+}_{x}e^{-\mathrm{i}k} - F^{y-}_{x}e^{\mathrm{i}k}\right) c^{\dagger}_{xk\downarrow} c^{\dagger}_{xk'\uparrow} \Big) e^{-\mathrm{i}(k+k')y} + \text{h.c.} \end{aligned}$$

Defining a more general form for the summand involving two site i and j:

$$\begin{aligned} F_{xx'k} =& -V_{x,x'}\left(F^{x+}_{x}\delta_{x+1,x'} + F^{x-}_{x}\delta_{x-1,x'} \right. \\ &\left. + \left(F^{y+}_{x}e^{-\mathrm{i}k} - F^{y-}_{x}e^{\mathrm{i}k}\right)\delta_{xx'}\right), \end{aligned}$$

where we got $k' = -k$ from the sum over the y-direction. We can rewrite the expression of H_V as

$$H_V = \sum_{x}\sum_{kk'} F_{xx'k} c^{\dagger}_{xk\uparrow} c^{\dagger}_{x',-k,\downarrow} + F^{*}_{xx'k} c_{x',-k,\downarrow} c_{xk\uparrow}.$$

Now using H_{hop}, H_{μ} and H_V we can write the full Hamiltonian as

$$\begin{aligned} H &= \sum_{xx'k} D^{\dagger}_{xk} H_{xx'k} D_{x'k} \\ &= \sum_{xx'k} \begin{pmatrix} c^{\dagger}_{xk\uparrow} & c_{x,-k,\downarrow} \end{pmatrix} \begin{pmatrix} \epsilon_{xx'k\uparrow} & F_{xx'k} \\ F^{*}_{xx'k} & -\epsilon_{xx'k\downarrow} \end{pmatrix} \begin{pmatrix} c_{x'k\uparrow} \\ c^{\dagger}_{x',-k,\downarrow} \end{pmatrix}. \end{aligned} \tag{76}$$

The summation over all x, x' can be represented in a new matrix.

$$H = \sum_{k} D^{\dagger}_{k} H_k D_k$$

involving the $4Nx \times 4Nx$ matrix H_k and the $4Nx$-dimensional vector D_k.

$$H_k = \begin{pmatrix} H_{11k} & \dots & H_{1N_xk} \\ \vdots & \ddots & \\ H_{N_x1k} & & H_{N_xN_xk} \end{pmatrix}$$

As before the y information is stored in the k-index, which is unique for each lattice y-slice. This said, we can diagonalize N_y times a $4N_x \times 4N_x$ matrix. H_k represent the interaction of a y-line with itself. The eigenvalues are the same for each y-slices and physical quantities are going to be expressed with this summation over k and the eigenvalues, -vectors of each k (y-slice).

On the other hand the vector we use to carry the creation and annihilation operators is given as

$$D^{\dagger}_{k} = \begin{pmatrix} c^{\dagger}_{1k\uparrow} & c_{1,-k,\downarrow} & \dots & c^{\dagger}_{N_xk\uparrow} & c_{N_x,-k,\downarrow} \end{pmatrix} \in \mathbb{H}^{2N_x}$$

6.2 BdG-transformation

The eigenvalues equation is similar to Eq.54

$$H_k \mathfrak{X}_{nk} = E_{nk} \mathfrak{X}_{nk} \tag{77}$$

The eigenvectors and -values are given as

$$\mathfrak{X}_{nk} = \begin{pmatrix} \mathfrak{x}_{n1k} \\ \vdots \\ \mathfrak{x}_{nN_xk} \end{pmatrix}, \quad \mathfrak{x}_{nxk} = \begin{pmatrix} u_{nxk} \\ v_{nxk} \end{pmatrix}$$

if we stick to the formalism we already derived in the earlier Sec.3.4 we obtain similar eigenvectors where u_{nik} corresponds to c. We are now going to transform the c operators. First we need to define $\mathfrak{X}_k = [\mathfrak{X}_{1k}, .., \mathfrak{X}_{2N_xk}] \in \mathbb{H}^{2N_x \times 2N_x}$ storing the number of lattice sites times the number of spins (2) in the first dimension and the number of eigenvectors in the second dimension. Beside we have $\mathfrak{g}_k = (\mathfrak{g}_{1k}, .., \mathfrak{g}_{2N_xk})^T \in \mathbb{H}^{2N_x}$ along with $D_k = \mathfrak{X}_k \mathfrak{g}_k$, delivering $\mathfrak{g}_k = \mathfrak{X}_k^\dagger D_k$ which is equivalent to:

$$\mathfrak{g}_{nk} = \sum_{x \in N_x} u_{nxk} c_{xk\uparrow} + v_{nxk} c^\dagger_{x,-k,\downarrow}. \tag{78}$$

Looking at $D_k = \mathfrak{X}_k \mathfrak{g}_k$ we can derive two very usefull expressions:

$$c_{xk\uparrow} = \sum_{n \in [\![2N_x]\!]} u_{nxk} \mathfrak{g}_{nk} \tag{79}$$

$$c^\dagger_{x,-k,\downarrow} = \sum_{n \in [\![2N_x]\!]} v_{nxk} \mathfrak{g}_{nk}. \tag{80}$$

6.3 Pairing amplitudes

For the derivation of the pairing amplitudes on the axis $a \in \{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}\}$. Doing so, we will use our BdG-transformation as we did earlier to be able to solve these parameters self-consistently using the eigenvectors and -values.

$$F_i^{\pm a} = \langle c_{i\uparrow} c_{i\pm a,\downarrow} \rangle = \frac{1}{N_y} \sum_{kk'} \langle c_{i_xk\uparrow} c_{i_x\pm a,k',\downarrow} \rangle e^{\mathrm{i}(k+k')i_y} e^{\pm \mathrm{i}k'\delta_y}$$

using $y \pm a = y'$. Here for the brevety we have to sacrifice the notation. This is unformal and might be confusing so we clarify the point in first place.
So a describes a displacement in the x- or y-direction. On one hand $i + a$ refers to the lattice index when moving from i with a translation a. On the other hand, having "$i = (x, y)$", $x + a$ refers to the x-coordinate of the lattice site $i + a$. This is analogue for y.
This then means or $a = \hat{\boldsymbol{y}}$ we have $x \pm a = x$ and $k'_a = 0$.

The expectaion value is independant of the site vertical coordinate y. This means that we can achieve a site description by making the average of the value over a x-slice. In other words we can write:

$$F_i^{\pm a} = \frac{1}{N_y} \sum_{y \in [\![N_y]\!]} \frac{1}{N_y} \sum_{kk'} \langle c_{i_xk\uparrow} c_{i_x\pm a,k',\downarrow} \rangle e^{\mathrm{i}(k+k')\boldsymbol{r}_i} e^{\pm \mathrm{i}k'\delta_y}$$

which after the sumation over i results as we covered earlier as $1/N_y \sum_y e^{\mathrm{i}(k+k')i_y} = \delta_{k,-k'}$

$$F_i^{\pm x} = \frac{1}{N_y} \sum_k \langle c_{i_xk\uparrow} c_{i_x\pm a,k,\downarrow} \rangle e^{\mp \mathrm{i}k_a}$$

Now that we have simplifed the Fourier transform we can incorporate the BdG-transformation. The process is very similar to Eq.59 and yields

$$F_i^{\pm a} = \frac{1}{N_y} \sum_k \sum_{nn'} u_{ni_xk} v^*_{n',i_x\pm a,k} \langle \mathfrak{g}_{nk} \mathfrak{g}^\dagger_{n'k} \rangle e^{\mp \mathrm{i}k\delta_y} \tag{81}$$

where we can as well write $i_x = x$. Recalling the use of a to abstractise the axis we get:

$$F_i^{\pm x} = \frac{1}{N_y} \sum_{nk} u_{ni_xk} v^*_{n,i_x\pm x,k} \left(1 - f(E_{nk})\right) \tag{82}$$

$$F_i^{\pm y} = \frac{1}{N_y} \sum_{nk} u_{ni_xk} v^*_{ni_xk} \left(1 - f(E_{nk})\right) e^{\mp \mathrm{i}k}. \tag{83}$$

6.4 Advanced order parameters

In the more simple desciption of the superconductivity we outlied how the superconducting order parameter Δ depends on the pairing amplitude F. Because the potential was isotropic, we simply had $\Delta = U\langle c_{i\uparrow}c_{i\downarrow}\rangle$. Here however the potential is anisotropic and we obtain a linear combination of the pairing amplitudes in the different directions of the lattice. Achieving different combinations of the Fs we obtiain different superconducting states. Here is an exaustive list. repalce V with U for consistency?

$$\Delta_{s,i} = VF_{s,i} \quad = \frac{V}{4}\left(F_i^{x+(S)} + F_i^{x-(S)} + F_i^{y+(S)} + F_i^{y-(S)}\right) \tag{84}$$

$$\Delta_{d,i} = VF_{d,i} \quad = \frac{V}{4}\left(F_i^{x+(S)} + F_i^{x-(S)} - F_i^{y+(S)} - F_i^{y-(S)}\right) \tag{85}$$

$$\Delta_{p_x,i} = VF_{p_x,i} \quad = \frac{V}{2}\left(F_i^{x+(T)} - F_i^{x-(T)}\right) \tag{86}$$

$$\Delta_{p_y,i} = VF_{p_y,i} \quad = \frac{V}{2}\left(F_i^{y+(T)} - F_i^{y-(T)}\right) \tag{87}$$

F_s, F_d, F_{p_x} and F_{p_y} are the pairing amplitudes for the s, d (also called $d_{x^2-y^2}$ because of its expression), p_x and p_y-wave superconductivity. The S and T are the singlet and triplet expressions of the pairing amplitudes. More precily we define them as

$$F_{ij}^{(S)} = \frac{F_{ij} + F_{ji}}{2} \tag{88}$$

$$F_{ij}^{(T)} = \frac{F_{ij} - F_{ji}}{2} \tag{89}$$

Where we shorten the expression using $F_{ij}^{\uparrow\downarrow(S)} = F_{ij}^{(S)}$.

Symmetry discussion We see that these parameter depends on the spin and the momentum. Therfore it's a good idea to look at their respective behaviour under exchange of these variables.

The discussion for the spin echange is quite straight forward.

$$F_{ij}^{\uparrow\downarrow(S)} = \frac{F_{ij}^{\uparrow\downarrow} + F_{ji}^{\uparrow\downarrow}}{2} = \frac{\langle c_{i\uparrow}c_{j\downarrow}\rangle + \langle c_{j\uparrow}c_{i\downarrow}\rangle}{2}$$

$$F_{ij}^{\uparrow\downarrow(T)} = \frac{F_{ij}^{\uparrow\downarrow} - F_{ji}^{\uparrow\downarrow}}{2} = \frac{\langle c_{i\uparrow}c_{j\downarrow}\rangle - \langle c_{j\uparrow}c_{i\downarrow}\rangle}{2}$$

What's happening when we invert both spin? using $\langle c_{i\uparrow}c_{j\downarrow}\rangle = -\langle c_{i\downarrow}c_{j\uparrow}\rangle$. Using the linearity of the expression we obtain

$$F_{ij}^{\uparrow\downarrow(S)} = -F_{ij}^{\downarrow\uparrow(S)}$$

$$F_{ij}^{\uparrow\downarrow(T)} = F_{ij}^{\downarrow\uparrow(T)}.$$

This means that the singlet wave-pairing amplitude is antisymmetric under spin exchange and the triplet wave pairing is symmertic under spin excahnge. Their names find place in the analogy of the wavefunction formalism.

For the momentum exchange we re going to take a look at the Fourier transformation of the pairing amplitudes. Using the transformation we made to reach Eq.81 with any translation $x \to \boldsymbol{r}$, $r \in \{\boldsymbol{e}_x, \boldsymbol{e}_y\}$ we obtain

$$F_{i,i+\boldsymbol{r}} = \frac{1}{N}\sum_{\boldsymbol{k}} \langle c_{\boldsymbol{k}\uparrow}c_{-\boldsymbol{k},\downarrow}\rangle e^{-i\boldsymbol{kr}}.$$

Changing the sign of the momentum we obtain $\frac{1}{N}\sum_{\boldsymbol{k}}\langle c_{-\boldsymbol{k},\uparrow}c_{\boldsymbol{k},\downarrow}\rangle e^{i\boldsymbol{kr}} = F_{i,i-\boldsymbol{r}}$ because of the $\delta_{\boldsymbol{k},\boldsymbol{k}'}$ trick. For this reason $F_{i,i+\boldsymbol{r}} + F_{i,i-\boldsymbol{r}}$ is symmertic under momentum exchange while $F_{i,i+\boldsymbol{r}} - F_{i,i-\boldsymbol{r}}$ is antisymmetric.
Refering back to the order parameter definiton we see that the s and d-wave are symmertic under momentum exchange, where the p_x and p_y-wave are antisymmetric in such exchange.

6.5 Implementation of the advanced superconductivity

7 Literature

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