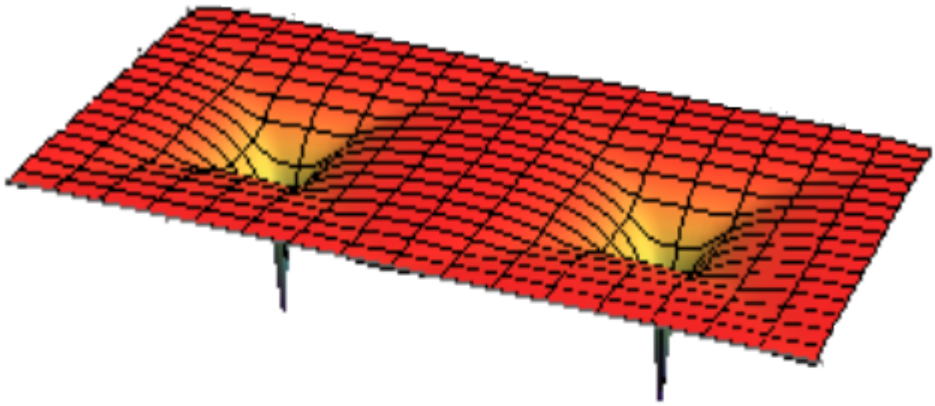
THE EFFECTS OF MAGNETIC FIELD IN LATTICE PERIODIC HAMILTONIANS AND VORTICES IN TYPE II SUPERCONDUCTORS



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Contents

Abstract

The motivation for this project was it to serve as a starting point to study vortices in Iron based superconductors. Thus, this project had two main goals. First, two understand the effects of the magnetic field in the sense that the presence of the vector potential in the Hamiltonian, breaks translational symmetry.Then it is crucial to understand it to still take advantage of the symmetries and to apply the correct boundary conditions. This theory has been used to compute the well known $Hofstadter\ butterfly$ and to study the s-wave superconductors using the $BCS\ theory$ and by solving numerically the $Bogoliubov-de\ Gennes$ equations, i.e. we study the superconductors from a microscopical point of view. The second goal was to understand the effect of magnetic fields in s-wave type II superconductors, i.e. the vortices.

Chapter 1

Introduction

When physical systems are studied and simulated computationally, boundary conditions must be chosen. When the Hamiltonian is translational invariant, *Bloch* boundary conditions are a physically correct choice. When a magnetic field is applied, this translational invariance is broken and one has to be careful with choosing the physically correct boundary conditions. We will see that the formulation of a $Magnetic\ Bloch\ theorem$ will give the solution to this problem.

When studying electrons in a lattice, a good starting point is the so called "Tight-binding" Hamiltonian. When apart of a potential, a magnetic field is present, the Hamiltonian Eq.3.2 describes the system. This Hamiltonian describes electrons on a two-dimensional square lattice with nearest-neighbour hopping in a perpendicular uniform magnetic field. We have seen that, as expected from other the work of other authors[1], plotting the spectra versus magnetic-flux through each placket, one gets the well known$Hostadter - butterfly$.

$J.Bardeen$, $L.N.Cooper$, and $J.R.Schrieffer$ elaborated the microscopic theory of superconductivity by 1957. This theory was named after their names' initials as the BCS theory. One of the most important assumption of the BCS theory is that below T_c a fraction of the electrons are condensed into Cooper pairs in the ground state of superconductors, this fact leading to superconductivity. Many interesting phenomena arise in this new state, among them, the mixed state of the superconductors of kind II, where superconductivity is suppressed in certain areas by the magnetic field, this leading to the creation of a vortex lattice.

1.1 Tools and concepts

1.1.1 Second quantization

Many-particle physics is formulated in terms of the so-called second quantization representation. Thus, one deals with the so called creation and annihilation operators constantly, which add or remove a particle (boson or fermion) to many-body wave functions. The convention used in this thesis is the following:

$c^\dagger_{k\sigma}$: creates an electron in state k with spin σ	(1.1)
$c_{k\sigma}$: annihilates an electron in state k with spin σ	(1.2)
$\gamma^\dagger_{k\sigma}$: creates a Bogoliubon in state k with spin σ	(1.3)
$\gamma_{k\sigma}$: annihilates a Bogoliubon in state k with spin σ	(1.4)

And they act as following in the many-body wave-functions $|\psi\rangle = |n_1 n_2 ... n_k ... n_N\rangle$, n_k being the number of particles in state k:

$$c_i^\dagger |n_1 ... n_i ...\rangle = (-1)^{\sum_i}(1 - n_i) |n_1 ... n_i + 1 ...\rangle \tag{1.5}$$

$$c_i |n_1 ... n_i ...\rangle = (-1)^{\sum_i} n_i |n_1 ... n_i - 1 ...\rangle \tag{1.6}$$

where,

$$(-1)^{\sum_i} = (-1)^{n_1 + ... + n_{i-1}} \tag{1.7}$$

Anti-commutation relations that fulfil this operators are the following:

$$\{c_{\nu_j}^\dagger, c_{\nu_k}^\dagger\} = 0 \tag{1.8}$$

$$\{c_{\nu_j}, c_{\nu_k}\} = 0 \tag{1.9}$$

$$\{c_{\nu_j}, c_{\nu_k}^\dagger\} = \delta_{\nu_j \nu_k} \tag{1.10}$$

where

$$\{A, B\} = AB + BA \tag{1.11}$$

1.1.2 Mean-Field approximation

In mean-field approximation, one assumes that certain operators deviate only little from their average values. As an example to give insight to it, let us take the following Hamiltonian

$$H = H_0 + H_{int} \tag{1.12}$$

$$H_0 = \Sigma_\nu \xi_\nu^a a_\nu^\dagger a_\nu + \Sigma_\mu \xi_\mu^b b_\mu^\dagger b_\mu \tag{1.13}$$

$$H_{int} = \Sigma_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} a_\nu^\dagger b_\mu^\dagger b_{\mu'} a_{\nu'} \tag{1.14}$$

Now, we define the deviation operators

$$d_{\nu\nu'} = a_\nu^\dagger a_{\nu'} - \left\langle a_\nu^\dagger a_{\nu'} \right\rangle \tag{1.15}$$

$$e_{\mu\mu'} = b_\mu^\dagger b_{\mu'} - \left\langle b_\mu^\dagger b_{\mu'} \right\rangle \tag{1.16}$$

and insert them into Eq.(12),which gives

$$H = H_0 + V_{MF} + \Sigma_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} d_{\nu\nu'} e_{\mu\mu'}, \tag{1.17}$$

where

$$V_{MF} = \Sigma_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} (a_\nu^\dagger a_{\nu'} \left\langle b_\mu^\dagger b_{\mu'} \right\rangle + b_\mu^\dagger b_{\mu'} \left\langle a_\nu^\dagger a_{\nu'} \right\rangle) - \Sigma_{\nu\nu',\mu\mu'} V_{\nu\mu,\nu'\mu'} \left\langle a_\nu^\dagger a_{\nu'} \right\rangle \left\langle b_\mu^\dagger b_{\mu'} \right\rangle \tag{1.18}$$

Because $d_{\nu\nu'}$ and $e_{\mu\mu'}$ are small, last term in equation (17) is neglected.

1.1.3 Bogoliubov transformation

Any second-quantization quadratic Hamiltonian can be diagonalized by the so called *Bogoliubov transformation*. For example, if one takes the *BCS* Hamiltonian Eq.4.1 and decouples the quartic term by performing a mean-field approximation, the following steps would lead to a diagonal Hamiltonian: First, perform the *Bogoliubov transformation*:

$$c_{i\sigma} = \sum_n (u_{i\sigma}^n \gamma_{n\sigma} + v_{i\sigma}^{n*} \gamma_{n\bar{\sigma}}^\dagger) \tag{1.19}$$

$$c_{i\sigma}^{\dagger} = \sum_{n} (u_{i\sigma}^{n*} \gamma_{n\sigma}^{\dagger} + v_{i\sigma}^{n} \gamma_{n\bar{\sigma}}) \tag{1.20}$$

Then, by requiring that the full Hamiltonian assumes the diagonal form

$$H = GS + \sum_{n\sigma} E_{n\sigma} \gamma_{n\sigma}^{\dagger} \gamma_{n\sigma} \tag{1.21}$$

the complex functions u and v are determined. All these calculations will be show in detail in section 6.

Chapter 2

Boundary conditions

2.1 Bloch boundary conditions

The fact that a Hamiltonian is lattice-periodic, may not be possible to see in the wave-function, which is not an observable. Evenso, Bloch's theorem applies to the solutions of the Schrdinger equation with a lattice periodic potential. Bloch's theorem says that: the eigenfunctions of a lattice-periodic Hamiltonian may be characterized by a wave-vector quantum number k, which is defined in the primitive cell of the reciprocal lattice. The values of the eigenfunctions ψ_k evaluated at different primitive cells differ just by a phase factor:

$$\psi_k(\vec{r}+\vec{T}) = e^{i\vec{k}.\vec{T}}\psi_k(\vec{r}) \tag{2.1}$$

2.2 Magnetic Bloch boundary conditions

The mentioned *Bloch* form of the eigenvectors of lattice periodic Hamiltonians, is a consequence of translational invariance under periodic translations. When a magnetic field is present, this is not true anymore. In this case, this is included in the kinetic energy by substituting the canonical momentum $\vec{p}$ with the kinetic momentum $(\vec{p}-q\vec{A})$. Thus, the Hamiltonian and the translation operator no longer commute, since the translation operator shifts the argument of the vector potential. Evenso, periodicity is not destroyed by a uniform magnetic field.. Since the vector potential $\vec{A}$ describing the homogeneous magnetic field is linear in $\vec{r}$, this shift can be compensated by a gauge transformation $\varepsilon_R = exp(\frac{ie}{\hbar}\vec{r}.\vec{A}(\vec{R}))$(See section 6.3) and the Hamiltonian commutes with the "magnetic translation operators" $M_R = \varepsilon_R T_R$. In general the magnetic translations do not commute with each other. For instance, for the basis vectors $\vec{a_1}$ and $\vec{a_2}$, by using the $BakerCampbellHausdorff\ formula$(section 6.2) is easy to show that

$$M_{\vec{a_1}} M_{\vec{a_2}} = M_{\vec{a_2}} M_{\vec{a_1}} exp(-2\pi i \frac{\Phi_p}{\Phi_0}) \tag{2.2}$$

where $\vec{a_1} = (a_1, 0)$, $\vec{a_2} = (0, a_2)$, Φ_p is the magnetic flux per unit cell and $\Phi_0 = \frac{h}{e}$, namely, the flux quanta. Thus, if we choose the flux such that, the flux through each unit cell is an integer number of flux quanta, magnetic translations through a unit cell commute with each other. But, we are interested having magnetic translations of the whole system that commute with each other. If $\frac{\Phi}{\Phi_0} = \frac{p}{q}$, $\frac{p}{q}$ being a rational number, one can consider the system made of "magnetic" unit cells with basis $q\vec{a}$ and $\vec{b}$. This unit cells will then be penetrated by an integer number p of flux quanta. Doing so, we ensure that that every magnetic translation $\vec{R'} = n(q\vec{a}) + m\vec{b}$ commute with each other. Thus, the eigenvectors of the

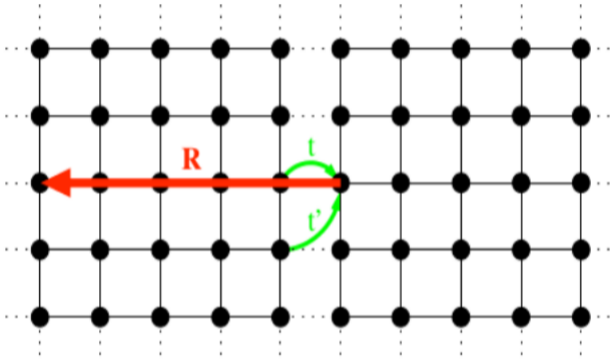


Figure 2.1: Hopping between supercells. A particle, which hops from the left supercell into the right supercell, is translated to the left supercell through the thranlation vector $\vec{R}$. As result, as we know from the Bloch theorem, u and v get an extra phase factor.

BdG(see below Eq. 6.21) matrix must fulfil the so called *Magnetic Bloch* theorem,

$$\begin{pmatrix} u_k(\hat{T}_R\vec{r}) \\ v_k(\hat{T}_R\vec{r}) \end{pmatrix} = e^{i\vec{k}.\vec{R}} \begin{pmatrix} e^{i\frac{2\pi}{\Phi_0}\vec{A}(\vec{R}).\vec{r}} u_k(\vec{r}) \\ e^{-i\frac{2\pi}{\Phi_0}\vec{A}(\vec{R}).\vec{r}} v_k(\vec{r}) \end{pmatrix} \tag{2.3}$$

where,

$$\vec{k} = (k_x, k_y) \text{ and } k_\alpha = 0, ..., \frac{M_\alpha - 1}{M_\alpha}\frac{2\pi}{M_\alpha a} \tag{2.4}$$

2.2.1 Application of the (Magnetic)Bloch theorem to our problem

Because we are solving the *BdG* Eq.6.17 matrix numerically, it is quite useful to use Bloch's theorem in order to diagonalize smaller matrices. To maximize the size of the system for which the *BdG* matrix can be diagonalized numerically, we use the fact that our Hamiltonian is lattice periodic, thus we can apply Bloch's theorem. Same as other authors have done before[2],we divide the lattice in M_x x M_y identical *supercells*, each one of these having N_x x N_y sites. This reduces the eigenvalue problem from, diagonalizing a matrix of dimensions $2M_xN_x$ x $2M_yN_y$ to a problem where we just have to diagonalize M_x x M_y matrices of size N_x x N_y, which is a lot faster. The way this works is, that each time a particle in the boundary jumps outside, because there is not such point, using the fact that the value of the eigenvector in the opposite site differs just by a phase factor from this "non-existing" point, we translate it back to the opposite side, and the eigenvector gets a phase. This is illustrated in Fig.2.1.

Chapter 3

Two-dimensional electron gas subjected to a weak 2D lattice potential and a magnetic field

3.1 Tight-binding model

When doing calculations of physical systems and simulating their behaviour, one has to use numerical methods to approach the continuity of space for example, i.e. space has to be discretized. One such example, is the $tight-binding$ model where the Hamiltonian is discretized in a lattice. The smaller the lattice constant is chosen, the nearer to the continuous limit we are. In the discretization, each lattice point does not represent an atom but a certain region, which might or might not have many atoms inside. This region should be small compared the the physically relevant quantities such as the Fermi wavelength.

Discretization of the Hamiltonian

Let us consider the Hamiltonian of a spin less electron, moving in a two-dimensional lattice,

$$H = \frac{1}{2m^*}\left(i\hbar\vec{\nabla} - e\vec{A}\right)^2 \tag{3.1}$$

where m^* is the effective mass of the electron. As mentioned in section 2.2, in the presence of magnetic a magnetic field, canonical momentum $\vec{p}$ has to be substituted with the kinetic momentum $(\vec{p} - q\vec{A})$. The procedure to discretize the Hamiltonian is the following. First, one has to discretize space into points and the coordinates of each point will be $(x, y) = (ia, ja)$,a being the lattice constant. Then, using finite differences, one has to approach the first derivative by $\frac{\partial\psi_k}{\partial\alpha} = 1/[\psi_k(\alpha + a/2) - \psi_k(\alpha - a/2)]$, where $\alpha = x, y$. Afterwards, by substituting the wave-functions $\psi_k(\alpha)$ by $\langle 0|c_\alpha c_k^\dagger|0\rangle$ and at the end using that $c_k c_k^\dagger|0\rangle = |0\rangle$, one can show that the Hamiltonian (ref), can be mapped onto a nearest-neighbours tight-binding Hamiltonian(reference)

$$H = \sum_{\langle i,j\rangle} t_{i,j} c_i^\dagger c_j \tag{3.2}$$

The quantity $t_{i,j}$ gives the hopping amplitude. In the absence of magnetic field we have that

$$t_{ij}^x = t_{ij}^y = -t = -\frac{\hbar^2}{2m^* a^2} \tag{3.3}$$

Instead, when we have a perpendicular magnetic field, we have introduce the $Peierls factors$, thus the hopping amplitude becomes dependent of the vector potential,

$$t_{ij} = -te^{\frac{-ie}{\hbar}\int \vec{A}\cdot\vec{dl}} \tag{3.4}$$

where $\int \vec{A} \cdot \vec{dl}$ is the integral of the vector potential along the path $i \to j$.

3.1.1 The Hofstadter butterfly

If we place a two-dimensional electron gas in an applied magnetic field, the quantum mechanical solution gives that electronic energy levels are the so called $Landau\ levels$, which have degeneracy $N_p = \frac{eB}{2\pi\hbar}L_xL_y$ and separation $\Delta E = \hbar\frac{eB}{m_e}$. When lattice interaction is included, the degeneracy of the LL is lifted and leads to $Landau\ bands$ with an oscillatory width and a rather complex band internal structure. The plotting of the energy spectrum versus placket flux density, gives rise to the well known $Hofstadter\ butterfly$. As explained by[1], when the system is exposed to a perpendicular magnetic field, there are some commensurability problems due to the interplay of the two length scales of the lattice constant a and magnetic length $l = \sqrt{\frac{\hbar}{eB}}$. As explained in [1], we need the following condition be fulfilled,

$$\frac{\Phi}{\Phi_0} = \frac{a^2}{2\pi l^2} = \frac{p}{q} \tag{3.5}$$

p and q being coprime. This a commensurability condition for the lattice period a and magnetic length l.

Chapter 4

The superconducting system

4.1 Vortices in type II superconductors

An important feature of superconductors is that in the superconducting phase(below temperature dependent critical field $H_{c1}(T)$), they are perfect diamagnets, they expel magnetic field(this also called the $Meissner - Ochsenfeld\ Effect$). In *type I* superconductors, transition between superconducting and normal state takes place abruptly at H_c. Instead, in *type II* superconductors, the change is not abrupt. There are two critical temperatures, such that when $H_{c1} \leq H \leq H_{c2}$, magnetic field penetrates in certain regions, which are in the normal state. This state is called the $mixed - state$.

In 1950, Ginzburg and Landau created a phenomenological theory where they generalized the Landau theory of second-order phase transitions to the normal-superconducting transition. They assumed that the superconducting phase can be characterized by an order parameter that takes a finite value in the superconducting phase and goes to zero in the normal state. They also assumed that this order parameter was related to the wave function of the superconducting electrons. In this theory, there are two characteristic lengths; the *coherence length* ξ which characterizes the length of the region where order parameter varies in an normal-superconducting interface and the *penetration depth* λ_L which characterizes the length of the region where magnetic field can penetrate the superconductor. In this theory, the two types of superconductors are divided by the $Ginzburg - Landau(G-L)$ parameter κ. When $\kappa < \frac{1}{\sqrt{2}}$, the surface energy of normal-superconducting interface is positive and we have a *type I* superconductor. When $\kappa > \frac{1}{\sqrt{2}}$, the energy of the interface is negative and we have a *type II* superconductor. Tn $G-L$ *theory* it is also showed that the flux penetrating in each vortex is equal to an integer number of superconducting flux quanta $\Phi_0 = \frac{h}{2e}$. Actually, each vortex is penetrated by a single Φ_0 because, being the energy of the interface between normal and superconducting state negative, it is energetically favorable to have as many vortexes as possible.

4.2 BCS theory

4.2.1 Cooper pair formation

Probably the most important concept in BCS theory is the Cooper pair. Cooper found that an arbitrarily weak attraction between electrons would lead to a rearrangement of the Fermi surface and the formation of quasi-bound electron pairs, namely Cooper pairs. The attractive interaction leading to the creation of Cooper pairs is mediated by phonons(in conventional superconductors). An electron attracts the positively charged ions, polarizing the surrounding. When the electrons moves out, the ions still keep being there because they are much heavier than the electrons and their time scale is much slower. So,

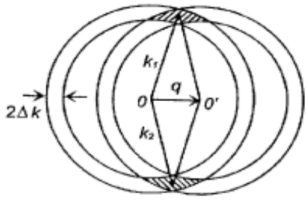


Figure 4.1: If coupled electrons have a total momentum q, the interaction involves only the electrons occupying k states within the dashed area.

this net positive charge, attracts another electron. This is how electrons have an effective attractive interaction despite the Coulomb repulsion. They basically avoid the Coulomb repulsion by being at the same place at different times.

At T=0, without interactions, the lowest energy state corresponds to the state where all the states below the Fermi surface are filled and the ones above are empty. This corresponds to the state where the kinetic energy is minimum and the potential energy zero. When interactions are present, namely, the attractive interactions between electrons, the contribution of this potential energy is negative, i.e. it lowers the energy. But this can only be possible if the pair is allowed to scatter from state (k_1, k_2) to $(k_1^{'}, k_2^{'})$, i.e. if state (k_1, k_2) is filled and state $(k_1^{'}, k_2^{'})$ empty before the scattering. Thus, the Fermi sphere with all the states below filled and all sates above empty is not the ground state anymore. When the states above the Fermi surface are being filled up, it happens in pairs $k_\uparrow$ and $-k_\downarrow$. This happens to be the most favorable way of coupling. When a transition from (k_1, k_2) to $(k_1^{'}, k_2^{'})$ happens, there must be conservation of momenta, i.e. $k_1 + k_2 = k_1^{'} + k_2^{'}$. The more Cooper pairs are created the more the energy is lowered. Now consider, for example, $k_1 + k_2 = q$ as illustrated in Fig.4.1. Here only the electrons occupying the k states in the dashed areas of momentum space are allowed to participate in the transitions. Now if we reduce q, the dashed areas will grow larger. Finally, at $q = 0$, all states within a band of width $2\hbar w_D$ around the Fermi surface will contribute to the reduction of the energy.

4.2.2 BCS Hamiltonian and BCS ground state

Due to the physical arguments previously discussed, only those processes in which singlet pairs with total momentum zero are scattered into singlet pairs are considered. The BCS Hamiltonian acting in this restricted Hilbert space of $\mathbf{q} = 0$ singlet pairs states has the form

$$H_{BCS} = \sum_k \xi_k (c_{k\uparrow}^\dagger c_{k\uparrow} + c_{-k\downarrow}^\dagger c_{-k\downarrow}) + \frac{1}{\Omega} \sum_{kk'} V_{kk'} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow} \tag{4.1}$$

where $\xi_k = \varepsilon_k - \mu$ is the energy of electrons measured from the chemical potential and

$$V_{kk'} = \begin{cases} -V_0 & \text{for } \varepsilon_F - \hbar\omega_D < \varepsilon_k,\, \varepsilon_{k'} < \varepsilon_F + \hbar\omega_D \\ 0 & \text{otherwise} \end{cases} \tag{4.2}$$

It is assumed that the potential weakly depends on k and $k^{'}$. Another important assumption of the BCS theory is that all electrons are condensed into Cooper pairs in the ground state of superconductors. *Bardeen*, *Cooper*, and *Schrieffer* proposed the following ground state:

$$|\Psi_{BCS}\rangle = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger)\,|0\rangle \tag{4.3}$$

According to the probabilistic interpretation of the wavefunction, $|u_k|^2$ is the probability of finding the pair in the system and $|v_k|^2$ gives the probability of its absence. The relation

$$|u_k|^2+|v_k|^2= 1 \tag{4.4}$$

has to be satisfied, which is at the same time the normalization condition of the wavefunction. In the BCS ground state, the number of particles is not fixed; the wavefunction is a linear combination of states with 0,2,4,...,N,... electrons. That is why it is necessary to work with a grand canonical ensemble.

In order to get the ground-state energy, it is necessary to do approximations. One possible way to do it is to apply the $Variational-principle$, minimizing the expectation value of the BCS Hamiltonian,

$$E^0_{BCS} = \langle \Psi_{BCS}| H_{BCS} |\Psi_{BCS}\rangle = \sum_k \xi_k(1 - |u_k|^2+|v_k|^2) + \frac{1}{\Omega}\sum_{kk'} V_{kk'} v^*_k u^*_{k'} u_k v_{k'} \tag{4.5}$$

with respect to u_k and v_k and with the constraint that $|u_k|^2+|u_k|^2= 1$. This can be carried out by using the method of $Lagrange-multipliers$. This calcualtions are done in detail in [3]. Solving the problem leads to,

$$|u_k|^2= \frac{1}{2}\left[1 + \frac{\xi_k}{\sqrt{\xi_k^2 + |\Delta_k|^2}}\right] \tag{4.6}$$

$$|v_k|^2= \frac{1}{2}\left[1 - \frac{\xi_k}{\sqrt{\xi_k^2 + |\Delta_k|^2}}\right] \tag{4.7}$$

$$u^*_k v_k = \frac{\xi_k}{2\sqrt{\xi_k^2 + |\Delta_k|^2}} \tag{4.8}$$

where,

$$\Delta_k = -\frac{1}{\Omega}\sum_{k'} V_{kk'} u^*_{k'} v_{k'} \tag{4.9}$$

Now, substitution of Eq.4.8 in Eq.4.9, leads to the *gap equation*,

$$\Delta_k = -\frac{1}{\Omega_k}\sum_{k'} \frac{V_{kk'}\Delta_{k'}}{2\sqrt{\xi_{k'}^2 + |\Delta_{k'}|^2}} \tag{4.10}$$

The quantity Δ_k is k independent taking Eq.(ref) as the interaction potential, it can be denoted as Δ_0. Changing from a sum over wave vector to an integral in energy, approximating the density of states by a constant (it's value at the Fermi energy) and taking Eq.(ref) as the potential, one gets the following gap value;

$$\Delta_0 = \hbar\omega_D sinh^{-1}\left(-\frac{2}{V_0\rho(\varepsilon_F)}\right) \tag{4.11}$$

If it is assumed that $V_0\rho(\varepsilon_F) << 1$ and $\Delta_0 << \hbar\omega_D$

$$\Delta_0 = 2\hbar\omega_D exp\left(-\frac{2}{V_0\rho(\varepsilon_F)}\right) \tag{4.12}$$

which is very similar(up to a factor 2 in the exponent) to the binding energy for the Cooper pairs found by Cooper.

The superconducting *gap* depends on temperature. The expression will not be derived here, but it is thoroughly done in [3], thus,

$$\Delta(T) \approx 3.06 K_B T_c\sqrt{1 - \frac{T}{T_c}} \tag{4.13}$$

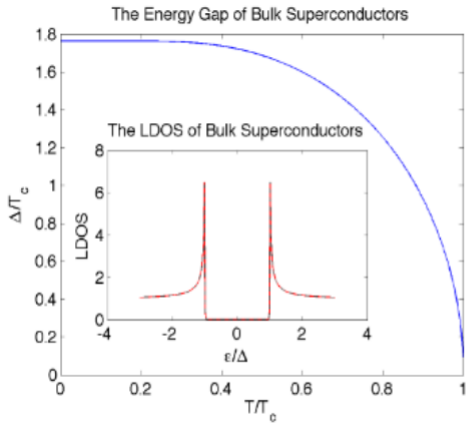


Figure 4.2: Temperature dependence of the gap and LDOS for s-wave superconductors.

4.2.3 Quasiparticles in the Superconducting state

The new operators introduced in Eq.6.8 (γ) can be understood as the creation annihilation operators of the quasiparticles of the superconducting state, also called *Bogoliubons*. They are a superposition of electron and hole. They are electronlike above the Fermi energy and holelike below it.They correspond to particles whose pair is missing. The expression for the excited states of the diagonal Hamiltonian, i.e. Bogoliubon eigen-energies is

$$E_k = \sqrt{\xi_k^2 + |\Delta_k|^2} \tag{4.14}$$

The minimum energy of these excitations is Δ_k. That means that there are forbidden state around the Fermi energy and Δ_k characterizes the width of this gap. The local density of states(LDOS) looks like Fig.4.2. For homogeneous superconductors, the local density of states looks the same in every lattice point, i.e. the LDOS is proportional to the density of states(DOS). Instead, for type II superconductors, when $H_{c1} \leq H \leq H_{c2}$, in the mixed state, magnetic flux will penetrate the superconductor and form an Abrikosov vortex lattice. As predicted by Caroli, de Gennes and Matricon[4], low-lying quasiparticle excitations will exist, and for S-wave superconductors, will be bound to the vortex core where the order parameter vanishes. Thus, far away from the vortex the LDOS looks like in the homogeneous superconductors but in the vortex core the situation is not trivial. What happens in the vortex core is that the center region is surrounded by an energy gap, so it is intuitive that there should be low energy bound states there.

4.2.4 Supercurrents around vortices

The shape of the density of the supercurrents $j_s$around the vortices is characterized by penetration length λ and coherence length ξ. The magnitude of j_s rises linearly from the vortex center to $\xi_1 \approx \xi\frac{T}{T_c}$, where it dies off, with an exponential decay of length λ. The maximum value of j_s depends on temperature and approaches the vortex core as temperature goes to zero. This is known as the $Kramer - Pesch$ effect.

The current between two neighbour sites for a system described by the Hamiltonian Eq.6.1 is given by,

$$j_{ij} = (\frac{-iet}{\hbar}) \sum_{\sigma} \left[e^{i\varphi_{ij}} \left\langle c_{i\sigma}^{\dagger} c_{j\sigma} \right\rangle - e^{i\varphi_{ji}} \left\langle c_{j\sigma}^{\dagger} c_{i\sigma} \right\rangle \right] \tag{4.15}$$

where,

$$\varphi_{ji} = \frac{2\pi}{\Phi_0} \int_j^i \vec{A}(\vec{r}) \cdot d\vec{r} \tag{4.16}$$

The expression for the current flow in each lattice site is derived in detail in section 6.4.

Chapter 5

Results

5.1 Hofstadter butterfly

As explained, if the energy spectrum of the $tight-binding$ Hamiltonian is plotted for different α values, this being the number of flux-quanta per each placket, the result is the $Hofstadter-butterfly$. This part of the thesis, served as a check-point that we were putting the correct phases.

5.2 Order parameter for s-wave superconductors

5.2.1 Without magnetic field

As explained before, in the absence of magnetic field one expects the order parameter to be homogeneous. This calculations have been carried out by solving the $Bogoliubov-deGennes$ equations numerically. It has been computed in two different ways. First using a single system and applying $Born-VonKarman$ boundary conditions, and secondly using the $Super-cells\ method$. It has been probed that one gets exact same results with both methods.

5.2.2 With magnetic field

For type II superconductors, when $H_{c1} \leq H \leq H_{c2}$, the flux penetrates creating the vortex lattice. In this case, we chose to put a magnetic field such that the flux is equal to two half flux quanta $\Phi = 2\Phi_0^*$, thus we get two vortices.

5.2.3 The Vortex Core Size

It has been seen that as expected, the the order parameter decreases with increasing temperature, which was already shown in Fig.4.2. Furthermore, it has been shown also that the slope of the order parameter in the core increases with decreasing temperature. Hence, the system reaches the critical temperature, the order parameter vanishes, that is the gap vanishes, since gap and order parameter are proportional to each other.

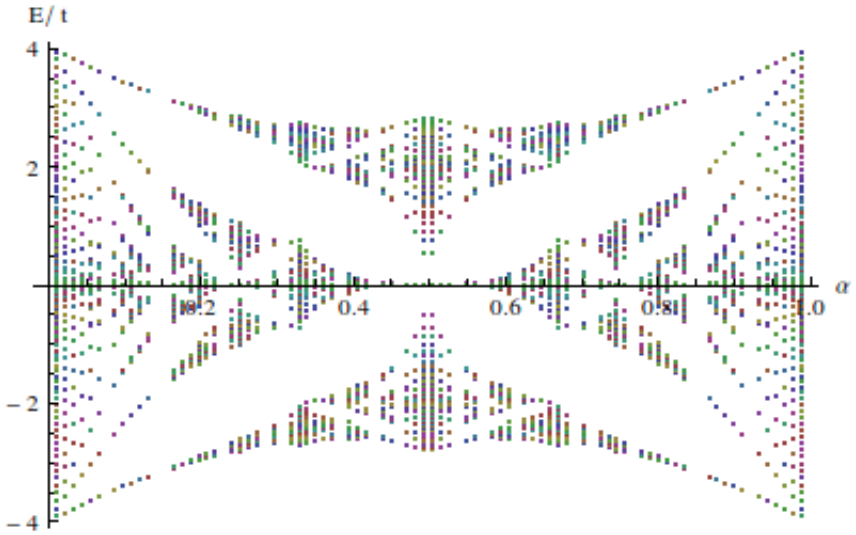


Figure 5.1: The Hofstadter butterfly, for a $91a$x$91a$ square lattice with hopping parameter t=1.

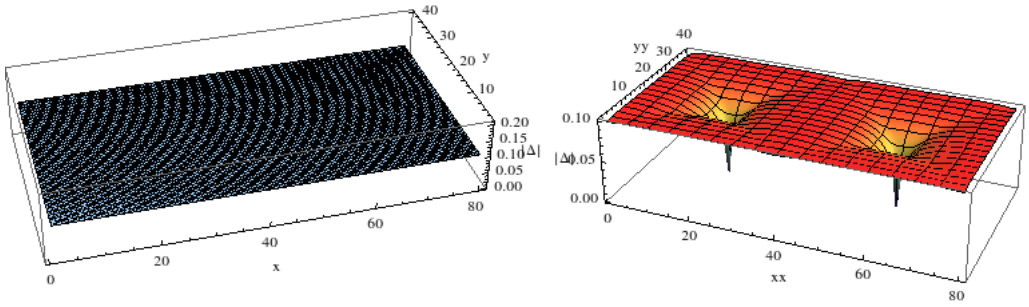


Figure 5.2: Superconducting order parameter for homogeneous sytem and system subject to a magnetic magnetic flux $\Phi = \Phi_0$. The lattice size is $80a$x$20a$, hopping parameter t=1 and attractive potential of electrons $V(r) = 1.2t$.

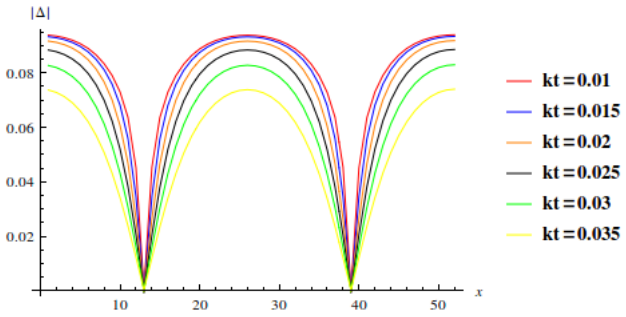
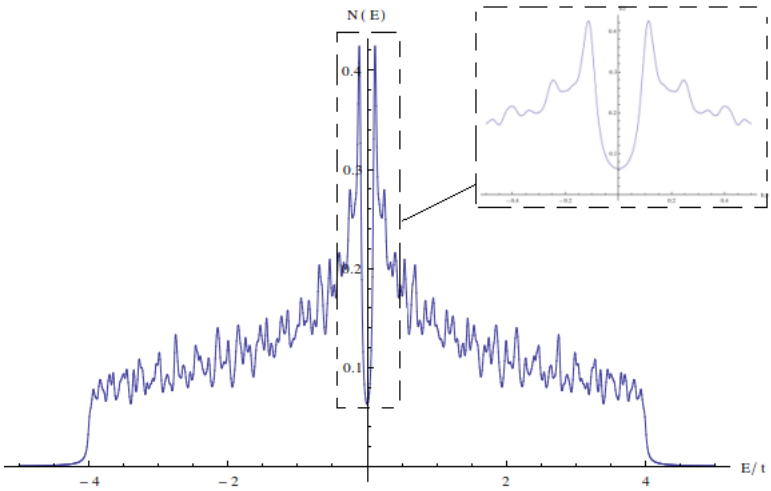
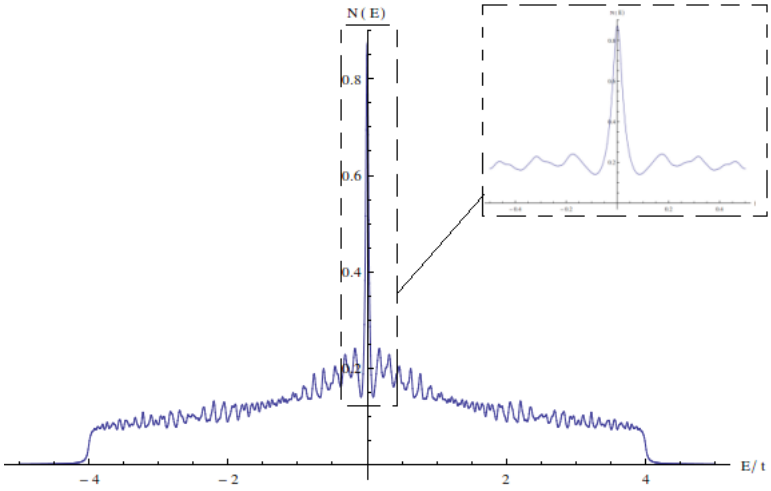


Figure 5.3: Shrinkage of the core radius with decreasing temperature. The lattice size is $52a$x$26a$, hopping parameter t=1, attractive potential of electrons $V(r) = 1.2t$ and magnetic flux $\Phi = \Phi_0$.



(a) Local density of states in bulk, between the two vortices. The lattice size is $80a$x$40a$, hopping parameter t=1, attractive potential of electrons $V(r) = 1.2t$ and magnetic flux $\Phi = \Phi_0$.



(b) Local density of states in the vortex core, where order parameter is zero.

5.3 Local density of states

It has been measured, that for the inhomogeneous system, in bulk we have a full gap, i.e. a forbidden area around the Fermi energy ($E/t = 0$). Instead, when calculating $LDOS$ in the vortex core where the order parameter takes it's zero value, there are some states, namely, the low energy bound states explained previously. The resolution of the $LDOS$ has a very low quality, i.e. it is really spiky because of numerical constraint reasons. The system we have been working with it is not big enough as to get smooth curves. This might be the reason why we do not get two peaks as expected from other authors[6], in the low energy bound-states in the vortex core. It would have been possible to work with bigger systems using the $Magnetic\ Super-cells$ method, but we have not been able to make this code work so far; thus we have been forced to work with smaller systems.

5.4 Supercurrents

The result of the supercurrents are not correct, therefore they will not be shown.

Chapter 6

Appendices

6.1 Bogoliubov-de Gennes equations

In order to calculate the superconducting order parameter, we have solved the *Bogoliubov de Gennes* equations numerically. We have done the study in the real space representation because, we have studied vortexes, and the bound states inside vortexes, so it was crucial to work in real space. Here, the calculation are done for a system with out magnetic field. In the presence of a magnetic field, one has to include the *Peierls factors* in the tight-binding part of the Hamiltonian. The Hamiltonian:

$$H = H_0 + H_{BCS} \tag{6.1}$$

$$H_0 = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{ij,\sigma} c^\dagger_{i\sigma} c_{i\sigma} \tag{6.2}$$

$$H_{BCS} = -\sum_{ij} V(r) c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} c_{j\downarrow} c_{i\uparrow} \tag{6.3}$$

Then,we perform the *mean field* approximation. Because in the superconductor, the Cooper pairs are present in a macroscopic number, it assumable that the averages $\left\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right\rangle \langle c_{-k\downarrow} c_{k\uparrow} \rangle$ are non-zero. Moreover, it is assumed that these averaged operators do not deviate much from their average values. Thus,

$$H^{MF}_{BCS} = -\sum_{ij} (V(r) \langle c_{j\downarrow} c_{i\uparrow} \rangle c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} + H.c.) = -\sum_{ij} (\Delta_{ij} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} + H.c.) \tag{6.4}$$

where the superconducting order parameter has been defined as

$$\Delta_{ij} = V(r) \langle c_{j\downarrow} c_{i\uparrow} \rangle \tag{6.5}$$

As we wanted, we have a quadratic Hamiltonian now: $H^{MF} = H_0 + H^{MF}_{BCS}$, thus is possible two diagonalize it. In order to diagonalize the Hamiltonian, the first thing to do is to compute the commutator $\left[H^{MF}, c_{i\sigma}\right]$,

$$\begin{aligned} [H_0, c_{i\sigma}] &= \sum_{kl\sigma'} t_{kl} \left[c^\dagger_{k\sigma'} c_{l\sigma'} c_{i\sigma} \right] \\ &= -\sum_{kl\sigma'} t_{kl} \left\{ c^\dagger_{k\sigma'}, c_{i\sigma} \right\} c_{l\sigma'} \\ &= -\sum_{j} t_{ij} c_{j\sigma} \end{aligned} \tag{6.6}$$

$$\begin{aligned}\left[H_{BCS}^{MF}, c_{i\sigma}\right] &= -\sum_{kl}\Delta_{kl}\left[c_{k\uparrow}^{\dagger}c_{l\downarrow}^{\dagger}, c_{i\sigma}\right] \\ &= -\sum_{kl}\Delta_{kl}(c_{k\uparrow}^{\dagger}\left\{c_{l\downarrow}^{\dagger}, c_{i\sigma}\right\} - \left\{c_{k\uparrow}^{\dagger}, c_{i\sigma}\right\}c_{l\downarrow}^{\dagger}) \\ &= -\sum_{k}\Delta_{ki}c_{k\uparrow}^{\dagger}\delta_{\sigma\downarrow} + \sum_{l}\Delta_{il}c_{l\downarrow}^{\dagger}\delta_{\sigma\uparrow} \\ &= -\sum_{j}\Delta_{ji}c_{j\uparrow}^{\dagger}\delta_{\sigma\downarrow} + \sum_{j}\Delta_{ij}c_{j\downarrow}^{\dagger}\delta_{\sigma\uparrow}\end{aligned} \tag{6.7}$$

Then, the *Bogoliubov* transformation is performed,

$$c_{i\sigma} = \sum_{n}(u_{i\sigma}^{n}\gamma_{n\sigma} + v_{i\sigma}^{n*}\gamma_{n\bar{\sigma}}^{\dagger}) \tag{6.8}$$

$$c_{i\sigma}^{\dagger} = \sum_{n}(u_{i\sigma}^{n*}\gamma_{n\sigma}^{\dagger} + v_{i\sigma}^{n}\gamma_{n\bar{\sigma}}) \tag{6.9}$$

Now we require that the Hamiltonian has a diagonal form

$$H = GS + \sum_{n\sigma}E_{n\sigma}\gamma_{n\sigma}^{\dagger}\gamma_{n\sigma} \tag{6.10}$$

Then, compute the commutation relation $\left[H^{MF}, c_{i\sigma}\right]$, H being Eq.6.10 and $c_{i\sigma}$ being Eq.6.8,i.e. we require that H is diagonal.

$$\left[H^{MF}, c_{i\uparrow}\right] = \sum_{n}(-E_{n\uparrow}u_{i\uparrow}^{n}\gamma_{n\uparrow} + E_{n\downarrow}v_{i\uparrow}^{n*}\gamma_{n\downarrow}^{\dagger}) \tag{6.11}$$

$$\left[H^{MF}, c_{i\downarrow}\right] = \sum_{n}(E_{n\uparrow}v_{i\downarrow}^{n*}\gamma_{n\uparrow}^{\dagger} - E_{n\downarrow}u_{i\downarrow}^{n}\gamma_{n\downarrow}) \tag{6.12}$$

Now, we do the same thing but, instead of requiring a certain condition, we just carry out pure substitution Eq.6.8 and Eq.6.9 into Eq.6.7. This leads to the so called *Bogoliubov de Gennes* equations,

$$-E_{n\uparrow}u_{i\uparrow}^{n} = -\sum_{j}t_{ij}u_{j\uparrow}^{n} + \sum_{j}\Delta_{ij}v_{j\downarrow}^{n} \tag{6.13}$$

$$E_{n\uparrow}v_{i\downarrow}^{n*} = -\sum_{j}t_{ij}v_{j\downarrow}^{n*} - \sum_{j}\Delta_{ji}u_{j\uparrow}^{n*} \tag{6.14}$$

$$E_{n\downarrow}v_{i\uparrow}^{n*} = -\sum_{j}t_{ij}v_{j\uparrow}^{n*} + \sum_{j}\Delta_{ij}u_{j\downarrow}^{n*} \tag{6.15}$$

$$-E_{n\downarrow}u_{i\downarrow}^{n} = -\sum_{j}t_{ij}u_{j\downarrow}^{n} - \sum_{j}\Delta_{ji}v_{j\uparrow}^{n} \tag{6.16}$$

It is readily seen, that these equations can be rewritten in a matrix form,

$$\begin{pmatrix}\hat{H} & \hat{\Delta}_{ij} \\ \hat{\Delta}_{ij}^{*} & -\hat{H}^{*}\end{pmatrix}\begin{pmatrix}u_{\uparrow}^{n} \\ v_{\downarrow}^{n}\end{pmatrix} = E_{n\uparrow}\begin{pmatrix}u_{\uparrow}^{n} \\ v_{\downarrow}^{n}\end{pmatrix} \tag{6.17}$$

and

$$\begin{pmatrix}\hat{H} & -\hat{\Delta}_{ji} \\ -\hat{\Delta}_{ij}^{*} & -\hat{H}^{*}\end{pmatrix}\begin{pmatrix}u_{\downarrow}^{n} \\ v_{\uparrow}^{n}\end{pmatrix} = E_{n\uparrow}\begin{pmatrix}u_{\downarrow}^{n} \\ v_{\uparrow}^{n}\end{pmatrix} \tag{6.18}$$

where,

$$\hat{H}u_{i} = \sum_{j}t_{ij}u_{j} \tag{6.19}$$

and

$$\hat{\Delta}_{ij}u_i = -\sum_j \Delta_{ij}u_j \tag{6.20}$$

Performing the following substitution in Eq.6.17 and taking the complex conjugate, one gets Eq.6.18.

$$\begin{pmatrix} u^n_\uparrow \\ v^n_\downarrow \\ E_{n\uparrow} \end{pmatrix} \mapsto \begin{pmatrix} v^{n*}_\uparrow \\ u^{n*}_\downarrow \\ -E_{n\downarrow} \end{pmatrix} \tag{6.21}$$

So it is enough to solve Eq.6.17 and account for all eigenvalues. We will refer to the matrix in Eq.6.17 as the *BdG* matrix. Using the *Bogoliubov* transformation, it is possible to write the self-consistent fields of the mean-field Hamiltonian in terms of $u^n_\uparrow$ and $v^n_\downarrow$ and the Fermi distribution of the *Bogoliubons*. Bogoliubons are fermions, that is why in thermal equilibrium,the occupation distribution is given by the Fermi function,

$$f(E_k) = \frac{1}{e^{\beta E_k}+1} \tag{6.22}$$

where E_k is the *Bogoliubon* energy.

6.1.1 Self-consistent fields

At this point, it is possible to express the self-consistent parameters of our mean-field Hamiltonian in terms of the eigenvectors and eigenvalues:

$$\begin{aligned} n_{i\uparrow} &= \left\langle c^\dagger_{i\uparrow}c_{i\uparrow}\right\rangle = \sum_n |u_{i\uparrow}|^2\left\langle \gamma^\dagger_{n\uparrow}\gamma_{n\uparrow}\right\rangle + \sum_n |v^n_{i\uparrow}|^2\left\langle \gamma_{n\downarrow}\gamma^\dagger_{n\downarrow}\right\rangle \\ &= \sum_n |u^n_{i\uparrow}|^2 f(E_{n\uparrow}) + \sum_n |v^n_{i\uparrow}|^2 f(-E_{n\downarrow}) \\ &= \sum_{n,E_{n\uparrow}>0} |u^n_{i\uparrow}|^2 f(E_{n\uparrow}) + \sum_{n,E_{n\uparrow}<0} |u^n_{i\uparrow}|^2 f(E_{n\uparrow}) \\ &= \sum_l |u^l_{i\uparrow}|^2 f(E_l) \end{aligned} \tag{6.23}$$

where $\sum_n$ sums only for those n values which have positive(or negative when specified) eigenvalues, $E_{n\sigma} > 0$, and $\sum_l$ sums over all positive and negative eigenvalues. The symmetry(reference) has been used. Following the same steps we get the expression for spin down density,

$$\begin{aligned} n_{i\downarrow} &= \left\langle c^\dagger_{i\downarrow}c_{i\downarrow}\right\rangle = \sum_n |u_{i\downarrow}|^2\left\langle \gamma^\dagger_{n\downarrow}\gamma_{n\downarrow}\right\rangle + \sum_n |v^n_{i\downarrow}|^2\left\langle \gamma_{n\uparrow}\gamma^\dagger_{n\uparrow}\right\rangle \\ &= \sum_n |u^n_{i\downarrow}|^2 f(E_{n\downarrow}) + \sum_n |v^n_{i\downarrow}|^2 f(-E_{n\uparrow}) \\ &= \sum_{n,E_{n\uparrow}<0} |v^n_{i\downarrow}|^2 f(-E_{n\uparrow}) + \sum_{n,E_{n\uparrow}>0} |v^n_{i\downarrow}|^2 f(-E_{n\uparrow}) \\ &= \sum_l |v^l_{i\downarrow}|^2 (1-f(E_l)) \end{aligned} \tag{6.24}$$

The order parameter:

$$\begin{aligned}\Delta_{ij} &= V(r)\left\langle c_{j\downarrow}c_{i\uparrow}\right\rangle \\ &= V(r)(\sum_n u^n_{j\downarrow}v^{n*}_{i\uparrow}\left\langle\gamma_{n\downarrow}\gamma^\dagger_{n\downarrow}\right\rangle + \sum_n v^{n*}_{j\downarrow}u^n_{i\uparrow}\left\langle\gamma^\dagger_{n\uparrow}\gamma_{n\uparrow}\right\rangle) \\ &= V(r)(\sum_{n,E_{n\uparrow}<0} v^{n*}_{j\downarrow}u^n_{i\uparrow}f(E_{n\uparrow}) + \sum_{n,E_{n\uparrow}>0} v^{n*}_{j\downarrow}u^n_{i\uparrow}f(E_{n\uparrow})) \\ &= \sum_l v^{l*}_{j\downarrow}u^l_{i\uparrow}f(E_l)\end{aligned} \tag{6.25}$$

6.1.2 LDOS

Spin resolved LDOS:

$$N_{i\sigma}(w) = -\frac{1}{\pi}Im\sum_n\left[\frac{|u^n_{i\sigma}|^2}{w-E_{n\sigma}+i\eta} + \frac{|v^n_{i\sigma}|^2}{w+E_{n\bar{\sigma}}+i\eta}\right] \tag{6.26}$$

So that,

$$N_{i\uparrow}(w) = -\frac{1}{\pi}Im\sum_n\left[\frac{|u^n_{i\uparrow}|^2}{w-E_{n\uparrow}+i\eta} + \frac{|v^n_{i\uparrow}|^2}{w+E_{n\downarrow}+i\eta}\right] \tag{6.27}$$

$$= -\frac{1}{\pi}Im\sum_n\left[\frac{|u^n_{i\uparrow}|^2}{w-E_{n\uparrow}+i\eta} + \frac{|u^n_{i\uparrow}|^2}{w-E_{n\uparrow}+i\eta}\right] \tag{6.28}$$

$$= -\frac{1}{\pi}Im\sum_l\left[\frac{|u^l_{i\uparrow}|^2}{w-E_{l\uparrow}+i\eta}\right]$$

And following the same line,

$$N_{i\downarrow}(w) = -\frac{1}{\pi}Im\sum_n\left[\frac{|u^n_{i\downarrow}|^2}{w-E_{n\downarrow}+i\eta} + \frac{|v^n_{i\downarrow}|^2}{w+E_{n\uparrow}+i\eta}\right] \tag{6.29}$$

$$= -\frac{1}{\pi}Im\sum_l\left[\frac{|v^l_{i\downarrow}|^2}{w+E_{l\uparrow}+i\eta}\right] \tag{6.30}$$

6.2 Baker-Cambell-Hausdorff formula

If $[\hat{x},[\hat{x},\hat{y}]] = [\hat{y},[\hat{x},\hat{y}]] = 0$, then :

$$e^{\hat{x}+\hat{y}} = exp\left(-\frac{1}{2}\left[\hat{x},\hat{y}\right]\right)e^{\hat{x}}e^{\hat{y}} = exp\left(\frac{1}{2}\left[\hat{x},\hat{y}\right]\right)e^{\hat{y}}e^{\hat{x}} \tag{6.31}$$

6.3 Gauge transformation in magnetic translation operators

Let us consider that the Hamiltonian of a single electron is the following,

$$H = H_0 + U(\vec{r}) = \frac{1}{2m}(\vec{p}+e\vec{A}(\vec{r}))^2 + U(\vec{r}) \tag{6.32}$$

where $\vec{A}(\vec{r}) = (-By, 0)$, namely, the Landau gauge. Thus, when a magnetic field is turned on, the Hamiltonian is not lattice periodic anymore, i.e. it does not commute with translation operator anymore because tarantion operators shift the vector potential,

$$T_R^\dagger \vec{A}(\vec{r}) T_R = \vec{A}(\vec{r} - \vec{R}) = \vec{A}(\vec{r}) - \vec{A}(\vec{R}) \tag{6.33}$$

Thus, one has to make a gauge transformation,

$$\vec{A}(\vec{r}) \to \vec{A}(\vec{r}) + (\vec{\nabla}\chi(\vec{r})) \tag{6.34}$$
$$\chi(\vec{r}) = \vec{r} \cdot \vec{A}(\vec{R})$$

And introduce the *Magnetic translation operators*

$$M_R = T_R e^{\frac{ie}{\hbar}\vec{r}\cdot\vec{A}(\vec{R})} \tag{6.35}$$

So now,

$$M_R^\dagger \vec{A}(\vec{r}) M_R = e^{-\frac{ie}{\hbar}\vec{r}\cdot\vec{A}(\vec{R})} T_R^\dagger \vec{A}(\vec{r}) T_R e^{\frac{ie}{\hbar}\vec{r}\cdot\vec{A}(\vec{R})} = \vec{A}(\vec{r}) - \vec{A}(\vec{R}) \tag{6.36}$$

and

$$\begin{aligned} M_R^\dagger \vec{p} M_R &= e^{-\frac{ie}{\hbar}\vec{r}\cdot\vec{A}(\vec{R})} T_R^\dagger \vec{p}(\vec{r}) T_R e^{\frac{ie}{\hbar}\vec{r}\cdot\vec{A}(\vec{R})} \\ &= \left(\sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{ie}{\hbar}\vec{r}\cdot\vec{A}(\vec{R})\right)^n\right)\vec{p}\left(\sum_{m=0}^{\infty}\frac{1}{m!}\left(-\frac{ie}{\hbar}\vec{r}\cdot\vec{A}(\vec{R})\right)^m\right) \\ &= \vec{p} + \frac{ie}{\hbar}\left[\vec{p}, \vec{r}\cdot\vec{A}(\vec{R})\right] \\ &= \vec{p} + e\vec{A}(\vec{R}) \end{aligned} \tag{6.37}$$

Thus

$$M_R^\dagger(\vec{p} + e\vec{A}(\vec{r}))M_R = \vec{p} + e\vec{A}(\vec{r}) \tag{6.38}$$

and therefore, the Hamiltonian does commute with magnetic translations. This done in[5].

6.4 Supercurrents

To get the currents, one has to start from the continuity equation,

$$-e\dot{n}_k + \vec{\nabla}\cdot\vec{j} = 0 \tag{6.39}$$

$$\dot{n}_k = \frac{i}{\hbar}[H, n_k] \tag{6.40}$$

$$n_k = \sum_\sigma n_{k\sigma} \tag{6.41}$$

Thus, one has to commute each of the terms of the Hamiltonian(reference), with the current density operator,

$$[H_0, n_k] = \sum_{ij\sigma} t\left[e^{i\varphi_{ij}} c_{i\sigma}^\dagger c_{k\sigma}\delta_{jk} - e^{i\varphi_{ij}} c_{k\sigma}^\dagger c_{j\sigma}\delta_{ik}\right] \tag{6.42}$$

Because we have nearest neighbours hopping, if we write explicitly the for nearest neighbours of the site j (i=j-1(left),i=j+1(right),i=j+2n(up),i=j-2n(down)),

$$\begin{aligned} [H_0, n_k] = -(iet/\hbar)\sum_\sigma [&\left(e^{i\varphi_{k+1,k}} c_{k+1,\sigma}^\dagger c_{k\sigma} - e^{i\varphi_{k,k+1}} c_{k\sigma}^\dagger c_{k+1,\sigma}\right) + \\ &\left(e^{i\varphi_{k-1,k}} c_{k-1,\sigma}^\dagger c_{k\sigma} - e^{i\varphi_{k,k-1}} c_{k\sigma}^\dagger c_{k-1,\sigma}\right) + \\ &\left(c_{k+2n,\sigma}^\dagger c_{k\sigma} - c_{k\sigma}^\dagger c_{k+2n,\sigma}\right) + \\ &\left(c_{k-2n,\sigma}^\dagger c_{k\sigma} - c_{k\sigma}^\dagger c_{k-2n,\sigma}\right)] \end{aligned} \tag{6.43}$$

$$\left[H_{BCS}^{MF}, n_k\right] = \sum_j (\Delta_{kj} c_{k\uparrow}^{\dagger} c_{j\downarrow} - \Delta_{jk}^{*} c_{j\downarrow} c_{k\uparrow} + \Delta_{kj} c_{j\uparrow} c_{k\downarrow}) \tag{6.44}$$

This terms are neglected, because if one commutes instead of H_{BCS}^{MF} H_{BCS}, this terms vanish. Thus,

$$< \vec{\nabla}\vec{j} >=< -(-e\dot{n}) >=< j_{i,i+1} > + < j_{i,i-2} > + < j_{i,i+2n} > + < j_{i,i-2n} > \tag{6.45}$$

Now, performing the $Bogoliubov - transformation$ in Eq.4.15, one gets that, the current between two neighbour sites is,

$$< j_{ij} >= (-iet/\hbar) \sum_l (e^{i\varphi_{i,j}} u_{i\uparrow}^{l*} u_{j\uparrow}^{l} - e^{i\varphi_{j,i}} u_{j\uparrow}^{l*} u_{i\uparrow}^{l}) f(E_{l\uparrow}) + (e^{i\varphi_{i,j}} v_{i\downarrow}^{l} v_{j\downarrow}^{l*} - e^{i\varphi_{j,i}} v_{j\downarrow}^{l} v_{i\downarrow}^{l*}) f(-E_{l\uparrow}) \tag{6.46}$$

Chapter 7

Conclusions

In this thesis, rather than draw conclusions, different previously known things have been checked as showed in section 5. There is no new discovery in this thesis, it is just the beginning of a bigger project about vortices in iron based superconductors, which will take place throughout the next whole year and for which it was necessary to learn and deal with all the basics that have been shown in this thesis. Therefore, this is a work in progress.

Chapter 8

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