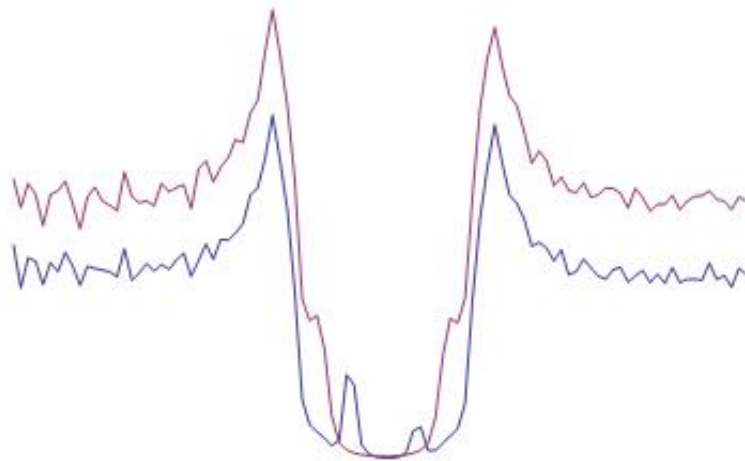


Bachelor Thesis
The Green's Function Solution to Orbital Alterations Due
to Impurities in Superconductors

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Abstract

This bachelor thesis is about investigating the properties of impurities in superconductors. By introducing tools like the Green's function method and with that the spectral function, it takes a look inside the superconductor, to see what happens to the density of states when affected by said impurity. Further, it looks into which specific orbitals are affected the most by this impurity, and it finds that it is only three of five orbitals whose density of states are worsened. Two remain superconducting properties (however, the material itself has sustained too much damage to be superconducting), and one orbital is even improved by the impurity.

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1 Introduction

In this paper, we will be looking into the whole superconductor-ordeal, which includes the tight-binding model for condensed matter with a twist of perturbed Hamiltonian. This problem quickly becomes large and time-consuming, if not dealt with in a simple manner, so it would be favourable to introduce a few tools for solving the problem in exactly such a manner. These tools include the second quantization formalism, the Green's function method and the spectral function derived from this. Through these tools, the problem has been dealt with by using numerical analysis. This might sound data heavy and not really simple at all, but don't worry, sit back, and keep on reading.

1.1 Why Superconductivity?

Everything that happens in a superconducting material sounds cool. There is the name of it, superconducting, which is pretty cool in itself. It means that this material can conduct electric currents without loss of energy. But this is old news, we've known that for quite some time. Then there is something called screening currents, which are currents that the superconductor makes with its super currents, to screen out any magnetic fields attempting to penetrate the material. This is what causes the materials to expel the magnetic field, and simply float inside it as quite a few people have seen on youtube by now. It just sticks there, until it warms back up, and the superconducting properties are lost again. When affected by a strong enough magnetic field, however, the superconductor also loses its properties, 'quenched' by the magnetic field. Sometimes, though, in the proper type of superconductor, it becomes energetically favourable for the superconductor to form vortices (also pretty cool) inside the material, allowing some magnetic fieldlines through, and retaining its properties. All in all, it sounds a lot cooler (and probably is cooler, too) than fuel cells or whatever else one could have chosen as subject for a bachelor thesis. So, there's one reason for choosing it.

Everything that you could do with a superconductor working at room temperature is cool. There is the whole 'save the world with no energy-spill in wires' thing, which alone should cause everyone to focus their attention to this field. Then, there is the fact that the superconductors fly, or, at least they glide, in magnetic fields, with no added energy other than what's needed to get moving, and to make up for the wind resistance. That's the safe way to get to the flying car, without all those giant propellers that has been seen attempted. It is also the way in to the hoverboard, and most other things we've seen in science fiction that can fly or float or glide, call it what you want. This is just the stuff that I've been thinking about, what lies in the minds of all the real superconductor research-giants i can't say. But i can say that it's probably pretty cool. There's another reason.

With two darn good reasons to choose superconductivity as a field of research, I begin the

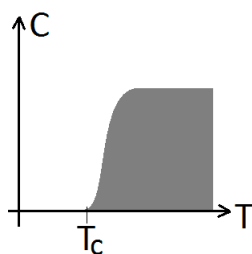


Figure 1: *At first, the conductance of metals was estimated to be constant for all temperatures. This turned out not to be the entire truth - for even though the conductance is pretty constant at high temperatures, it goes to zero when the temperature becomes low enough. This is what gives rise to the entire field of research on superconductivity, as it is attempted to find materials for which the temperature does not have to be so low in order to induce the superconducting properties.*

description of my own research. It has, however, not been all cool all the way, since the theory behind all this coolness takes some time getting into. It has been hard to see through all the equations and into the places it could be used, because the equations of my research does not really describe the floating/flying properties of the superconductors, nor does it directly have to do with conducting electricity without energy-loss. What it does do, is try to help and improve what we already know. This process is long, and you don't really get to see if you've helped before someone makes the breakthrough into something that's actually useful, with the help of your research. This is the daily life of many scientists, and it's tough going. But we have to keep it up, otherwise we'll never get those flying cars out in time for our children to use. A small step for a man, and all that. With these humble words, I begin my bachelor thesis*.

1.2 Second Quantization

The second quantization representation is all about simplifying. It works from the concept that we can describe any many-particle system from a basis, consisting entirely of single-particle states. All that matters is that we consider enough states to fill the system. Strictly speaking, it builds on the fact that in quantum mechanics, all particles that are the same in spin, mass, charge and so on, act the same. As such they can't be told apart or marked, without changing the properties of the particle. Furthermore, it utilizes the fact that we can create a basis of N-particle states for the Hilbert space, by using (Slater)determinants and permanents of single-particle states. These two physical notions allow us to use this second quantization.

N	Fermion basis states $ n_{s_1}, n_{s_2}, n_{s_3}, \dots\rangle$
0	$ 0, 0, 0, \dots\rangle$
1	$ 1, 0, 0, 0, \dots\rangle, 0, 1, 0, 0, \dots\rangle, 0, 0, 1, 0, \dots\rangle, \dots$
2	$ 1, 1, 0, 0, \dots\rangle, 1, 0, 1, 0, \dots\rangle, 0, 0, 1, 1, \dots\rangle, \dots$
\vdots	...

Table 1: *A few examples of building the system from a basis of single-particle states.*

The space spanned with this occupation number basis is called the Fock space. Now that we have a picture of what's going on, we can go on to looking at the number operator \hat{n}_{s_j} . What it does is to look into the states it's used on, and tell you if that exact state s_j is occupied or not. At least, this is the case for fermions. For bosons, the number operator also tell you the number of particles occupying the state.

$$\hat{n}_{s_1} |n_{s_1}\rangle = n_{s_1} |n_{s_1}\rangle \quad (1)$$

$$\hat{n}_{s_j} = \begin{cases} 0, 1 & \text{for fermions} \\ 0, 1, 2, \dots & \text{for bosons} \end{cases}$$

Since we now have an operator that can count the number of particles, it is natural to take into consideration two new operators. These are the creation and annihilation operators. The rules for these differ some between fermions and bosons, so, for brevity, we will be looking solely at the fermion case from here on. Here, we start by looking at the creation operator:

$$c_{s_j}^\dagger |\dots, n_{s_{j-1}}, n_{s_j}, n_{s_{j+1}}, \dots\rangle = C_+(n_{s_j}) |\dots, n_{s_{j-1}}, n_{s_j} + 1, n_{s_{j+1}}, \dots\rangle, \quad (2)$$

*This introduction to superconductors was inspired by a course i followed in the spring, textbook by [Solyom, 2010]

where $C_+(n_{s_j})$ is a constant of normalization, which still is to be determined. The operator is here working on a large number of states, but only one element of the operator yields something different than zero. This is where $\langle n_{s_j} + 1 | c_{s_j}^\dagger | n_{s_j} \rangle$. To find c_{s_j} we take the adjoint of $c_{s_j}^\dagger$:

$$\langle n_{s_j} + 1 | c_{s_j}^\dagger | n_{s_j} \rangle^* = \langle n_{s_j} | (c_{s_j}^\dagger)^\dagger | n_{s_j} + 1 \rangle \quad (3)$$

And thereby revealing the annihilation operator, $c_{s_j} \equiv (c_{s_j}^\dagger)^\dagger$, which does exactly as it's name suggests: It reduces the occupation number of state $|s_j\rangle$ by 1

$$c_{s_j} | \dots, n_{s_{j-1}}, n_{s_j}, n_{s_{j+1}}, \dots \rangle = C_-(n_{s_j}) | \dots, n_{s_{j-1}}, n_{s_j} - 1, n_{s_{j+1}}, \dots \rangle. \quad (4)$$

In terms of these two operators of creation and annihilation, there are few operators that can't be expressed. They are the fundamental operators of the second quantization formalism, and the next step in understanding them further, is to look at their properties.

For fermions, the listing of occupation numbers is not just a list. Each difference between states represents some change of property, and so we must demand that the fundamental fermionic antisymmetry be maintained,

$$| \dots, n_{s_j} = 1, \dots, n_{s_k} = 1, \dots \rangle = - | \dots, n_{s_k} = 1, \dots, n_{s_j} = 1, \dots \rangle. \quad (5)$$

As a consequence we must demand that $c_{s_j}^\dagger$ and $c_{s_k}^\dagger$ anti-commute, and by Hermitian conjugation, so must c_{s_j} and c_{s_k} . The anti-commutator for two operators A and B is defined as

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

which means that

$$\{A, B\} = 0 \Rightarrow BA = -AB. \quad (6)$$

For $j \neq k$, c_{s_j} and $c_{s_j}^\dagger$ must also anti-commute, as this ensures the antisymmetry of eq. (6). However, if $j = k$, we're in unexplored territory again. If the annihilation operator acts on an empty state, we must demand that the entire basis is ruined, since this is out of the physical picture. With the physical understanding and the mathematics of the anti-commutation, we can set down some definitions for the factors of normalization:

$$c_{s_j} | \dots, 0, \dots \rangle = 0 \Rightarrow C_-(0) = 0, \quad (7)$$

and likewise for the creation operator trying to create a particle in a state already occupied:

$$c_{s_j}^\dagger | \dots, 1, \dots \rangle = 0 \Rightarrow C_+(0) = 0. \quad (8)$$

For operations that are allowed, we put the constants equal to 1:

$$c_{s_j} | \dots, 1, \dots \rangle = | \dots, 0, \dots \rangle \Rightarrow C_-(1) = 1 \quad (9)$$

$$c_{s_j}^\dagger | \dots, 0, \dots \rangle = | \dots, 1, \dots \rangle \Rightarrow C_+(0) = 1 \quad (10)$$

From this we clearly see that there is a difference between $c_{s_j}^\dagger c_{s_j} | 0 \rangle = 0$ and $c_{s_j} c_{s_j}^\dagger | 0 \rangle = | 0 \rangle$, the first of the two completely destroying the basis. Clearly, $c_{s_j}^\dagger$ and c_{s_j} do not anti-commute. However, in the case of $j \neq k$, they do. Summing up, we have gathered these rules for the creation and annihilation operators of fermions:

$$\{c_{s_j}^\dagger, c_{s_k}^\dagger\} = 0, \quad \{c_{s_j}, c_{s_k}\} = 0, \quad \{c_{s_j}, c_{s_k}^\dagger\} = \delta_{s_j, s_k}. \quad (11)$$

What follows from this is that

$$(c_{s_j}^\dagger)^2 = 0, \quad (c_{s_j})^2 = 0 \quad (12)$$

Since double-creating in a state will always result in breaking the system, and likewise for double-annihilating.

Now we're at a point where we can express the number operator in terms of the creation- and annihilation-operators. Looking further into the commutation relations between the creation/annihilation operators, we find these two important relations:

$$\begin{aligned} [c_{s_k}^\dagger c_{s_k}, c_{s_j}] &= c_{s_k}^\dagger c_{s_k} c_{s_j} - c_{s_j} c_{s_k}^\dagger c_{s_k} = -c_{s_k}^\dagger c_{s_j} c_{s_k} - c_{s_j} c_{s_k}^\dagger c_{s_k} = -(c_{s_k}^\dagger c_{s_j})^\dagger c_{s_k} - c_{s_j} c_{s_k}^\dagger c_{s_k} \\ &= -(\delta_{j,k} - c_{s_j} c_{s_k}^\dagger) c_{s_k} - c_{s_j} c_{s_k}^\dagger c_{s_k} = -\delta_{j,k} c_{s_k} + c_{s_j} c_{s_k}^\dagger c_{s_k} - c_{s_j} c_{s_k}^\dagger c_{s_k} = -\delta_{j,k} c_{s_k} = -c_{s_j}, \end{aligned} \quad (13)$$

and with the same math we find that

$$[c_{s_j}^\dagger c_{s_j}, c_{s_k}^\dagger] = c_{s_j}^\dagger \quad (14)$$

Showing that $c_{s_j}^\dagger$ and c_{s_j} must share the eigenvalues of $c_{s_j}^\dagger c_{s_j}$, else we would not have been able to get these two results. As we've seen, the eigenvalues of both $c_{s_j}^\dagger$ and c_{s_j} are 0 and 1, so if they are the same for $c_{s_j}^\dagger c_{s_j}$, we could be closing in on the number operator (which also shares those exact eigenvalues). Proving that

$$(c_{s_j}^\dagger c_{s_j})^2 = c_{s_j}^\dagger (c_{s_j} c_{s_j}^\dagger)^\dagger c_{s_j} = c_{s_j}^\dagger (1 - c_{s_j}^\dagger c_{s_j}) c_{s_j} = c_{s_j}^\dagger c_{s_j} - (c_{s_j}^\dagger c_{s_j})^2 = c_{s_j}^\dagger c_{s_j} \quad (15)$$

results in

$$c_{s_j}^\dagger c_{s_j} (c_{s_j}^\dagger c_{s_j} - 1) = 0. \quad (16)$$

This last result comes from the fact that we've just shown $(c_{s_j}^\dagger c_{s_j})^2 = c_{s_j}^\dagger c_{s_j}$, so naturally $(c_{s_j}^\dagger c_{s_j})^2 - c_{s_j}^\dagger c_{s_j} = 0$. Pulling $c_{s_j}^\dagger c_{s_j}$ out, and placing it outside the parenthesis like in (16), leads us to conclude that if this is true, then the only values possible for $c_{s_j}^\dagger c_{s_j}$ are 0 and 1. And that is pretty solid proof of the eigenvalues. This supports the simple normalization for the operators that we saw in eqs. (7) through (10), and it looks a whole lot like the values we allowed for the number operator. Concluding:

$$c_{s_j}^\dagger c_{s_j} = \hat{n}_{s_j}, \quad c_{s_j}^\dagger c_{s_j} |n_{s_j}\rangle = n_{s_j} |n_{s_j}\rangle, \quad n_{s_j} = 0, 1 \quad (17)$$

$$c_s |0\rangle = 0, \quad c_s^\dagger |1\rangle = 0, \quad c_s |1\rangle = |0\rangle, \quad c_s^\dagger |0\rangle = |1\rangle \quad (18)$$

1.3 Green's Functions and the Spectral Function

1.3.1 Introducing the Green's Function

The Green's function method begins as an idea on solving differential equations. The best way to introduce it, I believe, is to use it in an example. We could take Poisson's equation of finding the electrical potential, given a fixed charge distribution

$$\nabla^2 \phi(\mathbf{r}) = \frac{-1}{\epsilon_0} \rho_e(\mathbf{r}). \quad (19)$$

[†]From (11), $\{c_{s_j}, c_{s_k}^\dagger\} = c_{s_j} c_{s_k}^\dagger + c_{s_k}^\dagger c_{s_j} = \delta_{j,k} \Rightarrow c_{s_k}^\dagger c_{s_j} = \delta_{j,k} - c_{s_j} c_{s_k}^\dagger$

[‡]Like before, $c_{s_j} c_{s_j}^\dagger - c_{s_j}^\dagger c_{s_j} = 1 \Rightarrow c_{s_j} c_{s_j}^\dagger = 1 - c_{s_j}^\dagger c_{s_j}$

Using the Green's function method, we now have to rewrite this equation a little, into a related but simpler version

$$\nabla_{\mathbf{r}}^2 G(\mathbf{r}) = \delta(\mathbf{r}). \quad (20)$$

Here, the Green's function $G(\mathbf{r})$ is acting as the Green's function for the Laplace operator, $\nabla_{\mathbf{r}}^2$. The $\delta(\mathbf{r})$ is the Dirac delta function. At this moment, we don't really know anything about this Green's function. In order to find out about it, we have to Fourier transform it into k-space

$$\int \nabla_{\mathbf{r}}^2 G(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} d\mathbf{r} = \int \delta(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} d\mathbf{r}. \quad (21)$$

The right-hand side immediately equals 1, and the left-hand side becomes

$$-k^2 \int G(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} d\mathbf{r} = 1. \quad (22)$$

All that's left now is for the transformation to take place. This causes $\int G(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} d\mathbf{r} = G(\mathbf{k})$, which means that

$$G(\mathbf{k}) = -\frac{1}{k^2}. \quad (23)$$

But k-space doesn't really tell us much about the electrical potential we set out to find. So, we are going to transform back into real-space with another Fourier transformation, and see if this doesn't reveal something about $G(\mathbf{r})$

$$G(\mathbf{r}) = \frac{1}{2\pi^3} \int e^{i\mathbf{k}\mathbf{r}} G(\mathbf{k}) d\mathbf{k} = -\frac{1}{2\pi^3} \int e^{i\mathbf{k}\mathbf{r}} \frac{1}{k^2} d\mathbf{k} = -\frac{1}{4\pi\mathbf{r}}. \quad (24)$$

Now we know what $G(\mathbf{r})$ is. To get back to the electrical potential and charge distribution, we use the formula given in [*Bruus and Flensberg, 2004*]

$$\phi(\mathbf{r}) = \frac{-1}{\epsilon_0} \int G(\mathbf{r} - \mathbf{r}') \rho_e(\mathbf{r}') d\mathbf{r}'. \quad (25)$$

$$\Rightarrow \phi(\mathbf{r}) = \frac{-1}{4\pi\epsilon_0} \int \frac{\rho_e(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'. \quad (26)$$

Which happens to be the potential felt by a charge at a distance $\mathbf{r} - \mathbf{r}'$ from the center of the distribution. All this illustrates that it's possible to use the Green's functions as a shortcut through problems on differential equations. However, this classical way of solving the problems is hardly needed when looking into the superconductor problem. Here, we need some Green's functions that allow us to use the quantum mechanical formalism. In the general case, we get two Green's functions, that can be used to describe two other Green's functions. For fermions, they look like this

$$\begin{aligned} G^>(s, t, t') &\equiv -i \langle c_s(t) c_s^\dagger(t') \rangle \\ G^<(s, t, t') &\equiv i \langle c_s^\dagger(t') c_s(t) \rangle, \end{aligned} \quad (27)$$

called the greater and lesser Green's functions, they are used to describe these two

$$\begin{aligned} G^R(s, t, t') &= \theta(t - t') [G^>(s, t, t') - G^<(s, t, t')] \\ G^A(s, t, t') &= \theta(t' - t) [G^<(s, t, t') - G^>(s, t, t')] \\ \theta(x) &= \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x > 0 \end{cases}. \end{aligned} \quad (28)$$

The two letters R and A are there to describe when to use the particular Green's function. The R is for 'retarded', this function is used when we want to propagate a particle forward in time. We know where it's been at time t , and we are projecting it into time t' . The 'advanced' Green's function (the A), predicts where a particle must have been at time t , given a known position at a later time t' . These particular Green's functions have no real spacial dependence, since that is out of the immediate scope of this thesis. For now, we will settle for a dependence on the state and time that we are in.

1.3.2 Chasing the Spectral Function

Expanding eqs. (27) into the basis of single-particle states that we were using in the section 1.2, we find that:

$$G^>(s, t, t') \equiv -i \langle c_s(t) c_s^\dagger(t') \rangle$$

when using the formula[§] for thermal averaging of quantum operators becomes

$$= -i \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | c_s(t) c_s^\dagger(t') | n \rangle,$$

then, using the fact that $\sum_n |n\rangle \langle n| = 1$, and 1 we can insert anywhere, we get

$$= -i \frac{1}{Z} \sum_{n n'} e^{-\beta E_n} \langle n | c_s(t) | n' \rangle \langle n' | c_s^\dagger(t') | n \rangle. \quad (29)$$

From here we have to write the time-dependant creation and annihilation operators as they are, in order to get the time-invariant operators. They are defined as

$$\begin{aligned} c_s^\dagger(t) &\equiv e^{iHt} c_s^\dagger e^{-iHt} \\ c_s(t) &\equiv e^{iHt} c_s e^{-iHt}. \end{aligned} \quad (30)$$

When inserting (30) into (29), and remembering that when the Hamilton operators in the exponential functions of the time-dep. operators get to act on the states $|n\rangle$, we get the specific energies of that state, we find that (29) becomes

$$\begin{aligned} &= \frac{-i}{Z} \sum_{n n'} e^{-\beta E_n} \langle n | e^{iHt} c_s e^{-iHt} | n' \rangle \langle n' | e^{iHt'} c_s^\dagger e^{-iHt'} | n \rangle \\ &= \frac{-i}{Z} \sum_{n n'} e^{-\beta E_n} \langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle e^{i(E_n - E_{n'})(t - t')} \end{aligned} \quad (31)$$

We can do the same thing for $G^<$, which yields

$$G^<(s, t, t') = \frac{-i}{Z} \sum_{n n'} \langle n | c_s^\dagger | n' \rangle \langle n' | c_s | n \rangle e^{-i(E_n - E_{n'})(t - t')} \quad (32)$$

Now, putting those two together as a $G^R(s, t, t')$, we can Fourier transform to the frequency domain, in order to better make use of the function. Doing this, we go to a slightly tweaked

[§] $\langle A \rangle = \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | A | n \rangle$

frequency space, using $\omega + i\eta$ for our new frequency. Here, η is a positive infinitesimal, so we can treat the space as if it was purely a frequency space.

$$G^R(s, \omega) = -i \int_{-\infty}^{\infty} \theta(t-t') e^{i(\omega+i\eta)(t-t')} \frac{1}{Z} \sum_{n n'} e^{-\beta E_n} \\ \times \left(\langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle e^{i(E_n - E_{n'})(t-t')} + \langle n | c_s^\dagger | n' \rangle \langle n' | c_s | n \rangle e^{-i(E_n - E_{n'})(t-t')} \right) dt.$$

Now, letting the step function $\theta(t-t')$ do its thing with the limits, and substituting $u = (t-t') \Rightarrow du = dt$ while checking that the limits of the substitution keep up, $u(t') = 0$, and $u(\infty) = \infty$, we find

$$= \frac{-i}{Z} \sum_{n n'} e^{-\beta E_n} \int_0^{\infty} \langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle e^{ui(\omega+i\eta+E_n-E_{n'})} \\ + \langle n | c_s^\dagger | n' \rangle \langle n' | c_s | n \rangle e^{ui(\omega+i\eta-E_n+E_{n'})} du.$$

At this point, we see that there is a slight problem in the integral. u is at the moment in the imaginary space, so putting the ∞ there, will only result in endless spinning to no avail. This is where η shines, because taking the i into the parenthesis, lets η become real, and hence we have a term in which the ∞ can go berserk, and reduce the exponential function to zero. So, doing the integral gets us to

$$= \frac{-i}{Z} \sum_{n n'} e^{-\beta E_n} \left[\frac{\langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle}{i(\omega + i\eta + E_n - E_{n'})} e^{u(i\omega - \eta + i(E_n - E_{n'}))} \right. \\ \left. + \frac{\langle n | c_s^\dagger | n' \rangle \langle n' | c_s | n \rangle}{i(\omega + i\eta - E_n + E_{n'})} e^{u(i\omega - \eta + i(E_{n'} - E_n))} \right] \Big|_0^{\infty} \\ = \frac{-i}{Z} \sum_{n n'} e^{-\beta E_n} \left(\frac{\langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle}{i(\omega + i\eta + E_n - E_{n'})} + \frac{\langle n | c_s^\dagger | n' \rangle \langle n' | c_s | n \rangle}{i(\omega + i\eta - E_n + E_{n'})} \right) (e^{-\infty} - e^0) \\ = \frac{1}{Z} \sum_{n n'} e^{-\beta E_n} \left(\frac{\langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle}{\omega + i\eta + E_n - E_{n'}} + \frac{\langle n | c_s^\dagger | n' \rangle \langle n' | c_s | n \rangle}{\omega + i\eta - E_n + E_{n'}} \right) \\ = \frac{1}{Z} \sum_{n n'} \frac{\langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle}{\omega + i\eta + E_n - E_{n'}} (e^{-\beta E_n} + e^{-\beta E_{n'}}). \quad (33)$$

Now, recalling the relation between the denominator and a delta function,

$$(\omega + i\eta)^{-1} = \mathcal{P} \frac{1}{\omega} - i\pi\delta(\omega), \quad (34)$$

where \mathcal{P} is the principal value, avoiding any singularities the denominator might cause. With this, and taking the imaginary part of eq. (33), we get

$$\frac{1}{\pi} \text{Im} G^R(s, \omega) = -\frac{1}{Z} \sum_{n n'} \langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle (e^{-\beta E_n} + e^{-\beta E_{n'}}) \delta(\omega + E_n - E_{n'}) \quad (35)$$

The $1/\pi$ factor is solely for normalization. The result of this long and tedious calculation is important for this thesis, since it is used to prove that the spectral function obeys the sum rule, and as such is a probability distribution. This will be done in section 1.3.3.

1.3.3 The Spectral Function

This function of spectrality, better known as the spectral function, is part of what makes the Green's functions so beautiful, and simple to use. It builds on the imaginary part of the retarded Green's function, and immediately transforms it into something that is passable for the density of states. This remarkable feature allows you to have enormous matrices in your Green's function, and with a simple calculation done thousands of times (depending on the size of the matrix, of course) it gives you the density. The bigger the matrix, the better is the resolution.

Let us start introducing the spectral function by beginning with a Green's function suited for use in a conducting material:

$$G_0^R(\mathbf{k}\sigma, t - t') = -i\theta(t - t')e^{-i\xi_{\mathbf{k}}(t-t')}. \quad (36)$$

This retarded propagator has been calculated for a translational invariant system of free electrons. $\xi_{\mathbf{k}}$ represents the energy of the system, and the σ represents the spin of the state \mathbf{k} . In this form, the propagator is not much use to us. This time-dependence is not optimal, so we transform into the frequency-space. As in section 1.3.2, we use the slightly tweaked frequency space, in order to more easily get out of the integral. However, this will later reveal itself to be not the only use we get of the infinitesimal η .

$$G_0^R(\mathbf{k}\sigma, \omega) = -i \int_{-\infty}^{\infty} \theta(t - t') e^{i\omega(t-t')} e^{-i\xi_{\mathbf{k}}(t-t') - \eta(t-t')} dt$$

substituting $u = (t - t') \Rightarrow du = dt$, again as in section 1.3.2, and letting the theta function work on the limits, we can write the integral as

$$\begin{aligned} &= -i \int_0^{\infty} e^{i\omega u - i\xi_{\mathbf{k}}u - \eta u} du = -i \int_0^{\infty} e^{-u(-i\omega + i\xi_{\mathbf{k}} + \eta)} du \\ &= \frac{-i}{-(-i\omega + i\xi_{\mathbf{k}} + \eta)} \left[e^{-u(-i\omega + i\xi_{\mathbf{k}} + \eta)} \right]_{u=0}^{u=\infty} = \frac{i}{i - i\omega + i\xi_{\mathbf{k}} + \eta} (e^{-\infty} - e^0) \\ &= \frac{-1}{\omega - \xi_{\mathbf{k}} + i\eta} (-1) = \frac{1}{\omega - \xi_{\mathbf{k}} + i\eta}. \end{aligned} \quad (37)$$

Now we're ready for the spectral function.

$$A_0(\mathbf{k}\sigma, \omega) = -\frac{1}{\pi} \text{Im} G_0^R(\mathbf{k}\sigma, \omega) = \delta(\omega - \xi_{\mathbf{k}}). \quad (38)$$

This delta function can be interpreted to mean that the only possible way of exciting an electron with the energy ω , is to add an electron to state \mathbf{k} , with the appropriate energy $\xi_{\mathbf{k}} = \omega$. Recalling statistical physics, we know that the density of states is

$$g(\omega) = \sum_{\mathbf{k}} \delta(\omega - \xi_{\mathbf{k}}), \quad (39)$$

which means that all we have to do to the spectral function is to sum over all the states

$$g(\omega) = \sum_{\mathbf{k}\sigma} A_0(\mathbf{k}\sigma, \omega) = \sum_{\mathbf{k}} \delta(\omega - \xi_{\mathbf{k}}). \quad (40)$$

All in all, supplying us with a reasonably easy access to the density of states for large systems.

When dealing with large systems, we could have a Hamiltonian such as the one for non-interacting systems:

$$H_0 = \sum_s \xi_s c_s^\dagger c_s, \quad (41)$$

where the s nominates the eigenstates of the system, and insert this in place of $\xi_{\mathbf{k}}$ in eq. 37. When using the spectral function we would run through all the states in the system, and resulting in the density of the states in this system. This is what it's been used for in this thesis, however the Hamiltonian does grow a little more advanced when dealing with superconductivity. Before going any further, though, we should make us of all the hard work done in section 1.3.2, and prove the spectral function to have properties of a probability distribution. Doing so, means solving the integral

$$\pi \int_{-\infty}^{\infty} A(s, \omega) d\omega = 1 \quad (42)$$

Using the math from eq. (35), we jump right into the imaginary part of $G^R(s, \omega)$:

$$\begin{aligned} \pi \int_{-\infty}^{\infty} A(s, \omega) d\omega &= \int_{-\infty}^{\infty} \frac{1}{Z} \sum_{n n'} \langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle (e^{-\beta E_n} + e^{-\beta E_{n'}}) \delta(\omega + E_n - E_{n'}) \\ &= \frac{1}{Z} \sum_{n n'} \langle n | c_s | n' \rangle \langle n' | c_s^\dagger | n \rangle (e^{-\beta E_n} + e^{-\beta E_{n'}}) \\ &= \langle c_s c_s^\dagger \rangle + \langle c_s^\dagger c_s \rangle = \langle c_s c_s^\dagger + c_s^\dagger c_s \rangle = 1. \end{aligned}$$

Stripping the Green's function apart with the same rules that built it in section 1.3.2. The last equality is the operator algebra deduced in eq. (11). This final proof, together with the fact that eq. (33) ensures that the spectral function can never be negative, solidifies the spectral function's properties in regard as to whether or not it can be treated as a probability distribution. However great this all is, the spectral function in itself is much more than just a tool for the density of states. The other uses for it eludes this thesis, however, so i will not go further into those.

This wraps up all the tools needed for the continued research in this thesis. As we progress through the sections, the retarded Green's function will advance with the complicity of the Hamiltonian it builds on, and the spectral function will practically disappear into the math done. However, it should be apparent for the reader when the spectral function is in effect.

2 The Research

2.1 Atomic Structure

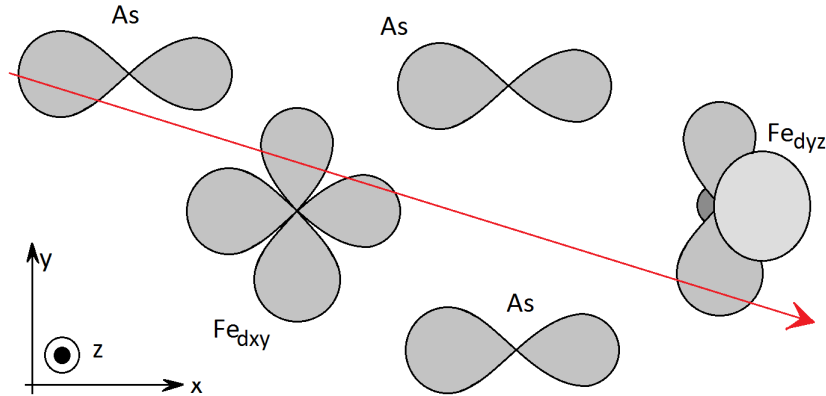


Figure 2: *This is a simplified version of what it looks like inside a superconductor. This material is constructed from iron (Fe) and arsenic (As), and in the picture we have to differently aligned iron atoms. The 'bubbles' on each atom represents the probability distribution of the wavefunction. The red line through the image represents the 'cut' we choose when plotting the bands of the structure. However, in real materials the distributions overlap, allowing for electron transfer.*

Reaching the actual research of this thesis, we will start slowly by looking into how these tools work in the basic tight-binding model. This model is used for metals, and represents the electrons as being tightly bound to the ions. However, there is the fermisurface to consider. Here, on the outermost orbital of the atom, the electrons roam free between the atoms, resulting in the heightened conductivity of metals. Figure (2) attempts picturing the atomic view on a material, in this case a superconducting material. The space between the probability distributions of each atom has been overestimated in this view, as they should be overlapping - at least in some places. The overlaps are what makes it possible for the electron of one atom to reach a different atom, e.g. in the process of conducting. From this rises the band-structure of a material, based on the orbitals of each atom. We can calculate these by taking the Hamiltonian of the non-interacting system

$$H_0 = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}, \quad (43)$$

For five orbitals we would have a 5×5 matrix that, when summing over \mathbf{k} gives us the eigenenergies. These have been plotted in figure (3), showing three routes through the brillouin zone in the lattice of the material. The bands are constructed of the energies of the orbitals in the atoms of the lattice. Whatever energy the bands have for each value of \mathbf{k} comes from the orbitals. In much the same way, we can take a look at bands from a 'top down' point of view, looking down on the fermisurface they create. This has been done in figure (??). When reading a fermisurface it is important to remember the boundary-nature of the lines that are the bands in figure (3). Below the upper line, all energies have states in which to contain a particle of the given energy. This is also the case in the fermisurface view, only here the allowed states are those on the corner side of each 'banana'.

Both the bands structure and the fermisurface of a material are products of the orbitals of

the atoms the material consists of. In section 2.2 we will see how an impurity can affect these orbitals, thereby also affecting both the band structure and the fermisurface. These new bands and surface will not be shown in this thesis, but the impact these alterations have are still a matter to keep in mind when reading the figures of the next sections.

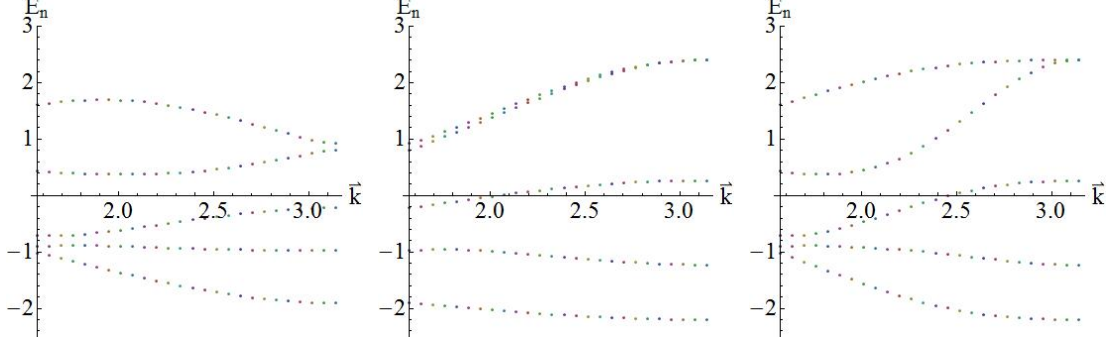


Figure 3: A view into the k -space band structure of the tight-binding model, these graphs picture the bands for 3 different 'cuts' through the Brillouin zone of the lattice.

2.1.1 The Density of States

There is a short word to be said for the density of states, before we venture out into the superconductor version thereof. The orbitals of the atoms lie closer and closer, the higher the energy of the occupying electrons get. So it is natural for the density to rise with energy, peaking where the specific atom has its outermost orbital. For this non-interaction system it would have been nice to have a plot of the density of states calculated with the spectral function, to show and compare to the superconducting DOS that will be shown later in this thesis. This didn't work out entirely the way it was supposed to, probably due to the lack of resolution. It sounds like a small thing, but the resolution was one of the big issues of this math, and getting it to work on the superconductors took a lot of time. So, instead, figure (5) shows what it ended up as, and what it should have looked like. What the superconductor does to this we're about to see in the following sections.

2.2 The Superconductor

Moving into the theory behind expanding our Green's functions to account for superconducting systems, we find that it is useful to go to a matrix-formalism. This formalism is known as the Nambu-formalism. Consider the superconducting Hamiltonian:

$$H_{sc} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger - \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \quad (44)$$

where Δ is the gap-coefficient, not to be delved deeper into in this thesis. We accept that it's there, and what it does. This Hamiltonian can be written on matrix form:

$$H_{sc} = C \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}\uparrow}^\dagger \\ c_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{bmatrix} \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & -\xi_{-\mathbf{k}} \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix}. \quad (45)$$

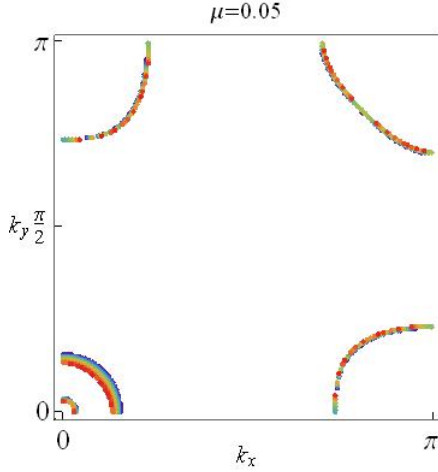


Figure 4: This figure presents the Fermi surface in the Brillouin zone of the same system presented in figure (3). What we see are the bands themselves, only this time it's from a 'top down' look, as if we were above the bands, looking down on their surfaces. The coloring on the dots shows how deep the dot is, compared to the others, in order of the visible light spectrum; red first, blue and purple last, purple being the deepest points. This third dimensional effect comes from taking a cut with some breadth to it, instead of cutting in a line like in figure (3)

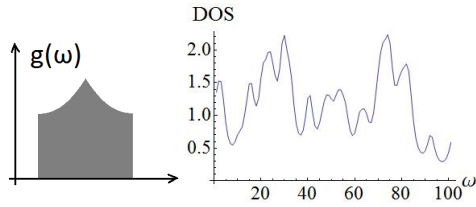


Figure 5: To the left is a figure of how the density of states for the non-interacting system should have looked, using the Green's function. To the right is how it ended up looking. The two being quite dissimilar, the plot was quickly abandoned to focus the research on the superconducting systems.

Which is quickly seen to be a hermitian matrix. But can the Hamiltonian be presented in this way? We'll make a quick proof:

$$\begin{aligned}
H_{sc} &= C \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}\uparrow}^\dagger \\ c_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{bmatrix} \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & -\xi_{-\mathbf{k}} \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} \\
&= C \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}\uparrow}^\dagger \\ c_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}} c_{\mathbf{k}\uparrow} + \Delta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger \\ \Delta_{\mathbf{k}}^* c_{\mathbf{k}\uparrow} - \xi_{-\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} \\
&= C \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} - \sum_{\mathbf{k}} \xi_{-\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{-\mathbf{k}\downarrow} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger + \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow},
\end{aligned}$$

finding the normalization factor to be $C = -1$, and using the operator algebra for the creation/annihilation operators in the first term

$$= \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} + \xi_{-\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}\downarrow} \right) - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger - \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}. \quad (46)$$

The matrix representation comes in handy when the Hamiltonian is already on a 5×5 form, such as the one treated during this thesis. The gap-coefficient is then likewise a 5×5 matrix, and they can be put together in a 10×10 full Hamiltonian matrix by following the representation of H_{sc} . This is how the math got done, by inserting the newly found Hamiltonian in the Green's function from section 1.3.3, eq. (37)

$$\mathcal{G}^{(0)}(\mathbf{k}\sigma, \omega) = \frac{1}{I(\omega + i\eta) - H_{sc}}, \quad (47)$$

writing H_{sc} as

$$H_{sc} = \begin{pmatrix} H_0(\mathbf{k}, \uparrow) & H_{\Delta}(\mathbf{k}, \uparrow, \downarrow) \\ H_{\Delta}^*(\mathbf{k}, \downarrow, \uparrow) & -H_0(-\mathbf{k}, \downarrow) \end{pmatrix}, \quad (48)$$

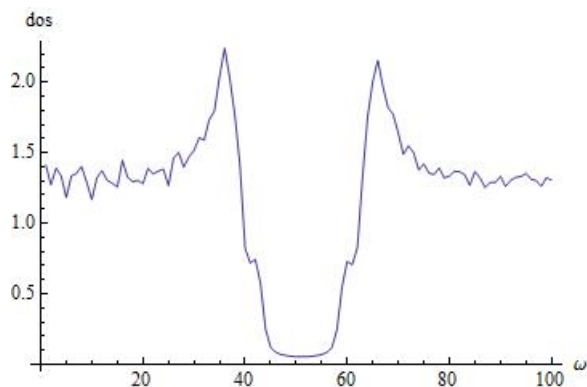


Figure 6: *This figure plots the density of states (dos) for the clean superconductor (no impurities yet). What we see here, is that there are very few states available for the electrons in the energy gap from $\omega = 45$ to $\omega = 58$. This is what makes the material superconducting. If this partitioning of the states break down, the superconducting properties are lost.*

we get the Nambu matrix-formalism Green's function \mathcal{G} . The I is a 10×10 identity matrix, making sure all the dimensions fit. Since we got this far, we might as well take a look at the density of states for this system. Using the spectral function and summing over \mathbf{k} gets us the density, as plotted on figure (6). This form of density of states is what creates the whole superconductivity property in a material. Somehow, that gap squeezes the electrons, and forces them to choose other states to occupy. This results in some of them becoming able of carrying the super current through the material. How this exactly happens, we don't know yet.

With the DOS for 'clean' systems, we are ready to investigate what happens when adding an impurity to the Green's function. To do this, we must first find the full Green's function, as this is the one that allows for such impurities. This will be done in the following section.

2.2.1 Inserting the Impurity

For calculating the influence of an impurity in our superconductor, we need the full Green's function, because it takes any potential impurities into consideration. We begin by introducing the two equations of motion, as presented in [Andersen, 2004]

$$[-\partial_{\tau_a} - H_0(a)]\mathcal{G}^{(0)}(a, b) = \delta_{a,b}, \quad (49)$$

$$[-\partial_{\tau_a} - H(a)]\mathcal{G}(a, b) = \delta_{a,b}. \quad (50)$$

These we can use to find a way of introducing an impurity potential $H_{imp} = V$, using the fact that $-H_0 = -H + H_{imp}$

$$\begin{aligned} [-\partial_{\tau_a} - H(a)]\mathcal{G}(a, b) &= [-\partial_{\tau_a} - H(a) + V(a)]\mathcal{G}^{(0)}(a, b) \\ &= [-\partial_{\tau_a} - H(a)]\mathcal{G}^{(0)}(a, b) + V(a)\mathcal{G}^{(0)}(a, b) \\ &= [-\partial_{\tau_a} - H(a)]\mathcal{G}^{(0)}(a, b) + \sum_c \delta_{a,c}V(c)\mathcal{G}^{(0)}(c, b). \end{aligned}$$

On that last equation we pull in a new variable, which we use to define the position of the impurity in the material. If we now act with a $[-\partial_{\tau_a} - H(a)]^{-1}$ matrix from the left, we will get an equation consisting only of the Green's functions and the impurity potential:

$$\mathcal{G}(a, b) = \mathcal{G}^{(0)}(a, b) + \sum_c \mathcal{G}(a, c)V(c)\mathcal{G}^{(0)}(c, b). \quad (51)$$

From this it is possible to go to real-space coordinates $a = i$ and $b = j$. The c , as noted above, now defines the location of our impurity. Setting this to be the origin and thereby considering the impurity as some sort of delta-function (since it only exists in one place) to get rid of the sum, we get

$$\mathcal{G}(i, j) = \mathcal{G}^{(0)}(i - j) + \mathcal{G}(i, 0)V(0)\mathcal{G}^0(0 - j). \quad (52)$$

Using that

$$\begin{aligned} \mathcal{G}(i, 0) &= \mathcal{G}^{(0)}(i) + \mathcal{G}(i, 0)V(0)\mathcal{G}^0(0) \\ \Rightarrow \mathcal{G}^{(0)}(i) &= \mathcal{G}(i, 0) \left[1 - V(0)\mathcal{G}^{(0)}(0) \right] \\ \Rightarrow \mathcal{G}(i, 0) &= \mathcal{G}^{(0)}(i) \left[1 - V(0)\mathcal{G}^{(0)}(0) \right]^{-1}, \end{aligned}$$

and inserting it in place of $\mathcal{G}(i, 0)$ in eq. (52) gets us the exact solution thereof:

$$\mathcal{G}(i, j) = \mathcal{G}^{(0)}(i - j) + \mathcal{G}^{(0)}(i) \left[1 - V(0)\mathcal{G}^{(0)}(0) \right]^{-1} V(0)\mathcal{G}^{(0)}(-j). \quad (53)$$

Which is a nice solution, because it contains only the unperturbed Green's function \mathcal{G} on the right hand side. We now have the full Green's function for this system, based on the Green's function of our system without the impurity, and ready for use. To shorten the expression, we define the T-matrix:

$$\begin{aligned} T(0) &= \left[1 - V(0)\mathcal{G}^{(0)}(0) \right]^{-1} V(0) \\ \Rightarrow \mathcal{G}(i, j) &= \mathcal{G}^{(0)}(i - j) + \mathcal{G}^{(0)}(i)T(0)\mathcal{G}^{(0)}(-j). \end{aligned}$$

A decision is made here, to only look at the material directly on the impurity. We find $\mathcal{G}(0, 0)$ by simply inserting values

$$\mathcal{G}(0, 0) = \mathcal{G}^{(0)}(0) + \mathcal{G}^{(0)}(0)T(0)\mathcal{G}^{(0)}(0). \quad (54)$$

This gets us a view (by using the spectral function once again) into the density of states when it is affected by an impurity potential of a fixed value. The two figures (7) and (8) both contain a plot named "DOS V_{ALL} ", which are plots for an impurity $V = 2.0$. The plot is so named, because, considering that all the Green's functions are 10×10 matrices, we hit every single element of the matrices, and therefore every orbital, with the impurity potential. The difference between the two figures is that in figure (7) we slowly turn up the size of the impurity, starting at $V = 0.2$, and going all the way to $V = 1.0$. What we see in particular when doing this, is that a peak density forms on the left-hand peak of the zero-impurity plot, and then it moves slowly towards the middle of the gap as the size increases. We also see that the density falls drastically for the energies lower than those in the gap from $V = 1.0$ to $V = 2.0$. All in all, the impurity is bad for our superconductor, as it totally ruins both the density for the states at lower energies, and, most importantly, it messes with the gap, eventually causing it to close.

This business of hitting all the orbitals with the impurity is what makes the most sense from an experimental point of view. It would be straightforward to insert a material with all orbitals full, and whose outer shell would cost too much energy for the electrons of the surrounding states to occupy. This would create a site in the lattice, where the electrons were forbidden to go, not too dissimilar from what has been done in figure (7). In theory, however, we have a few more options since we don't have to consider the practical approach. We could, for example, investigate if the individual orbits have any particular influence on how the impurity affects the

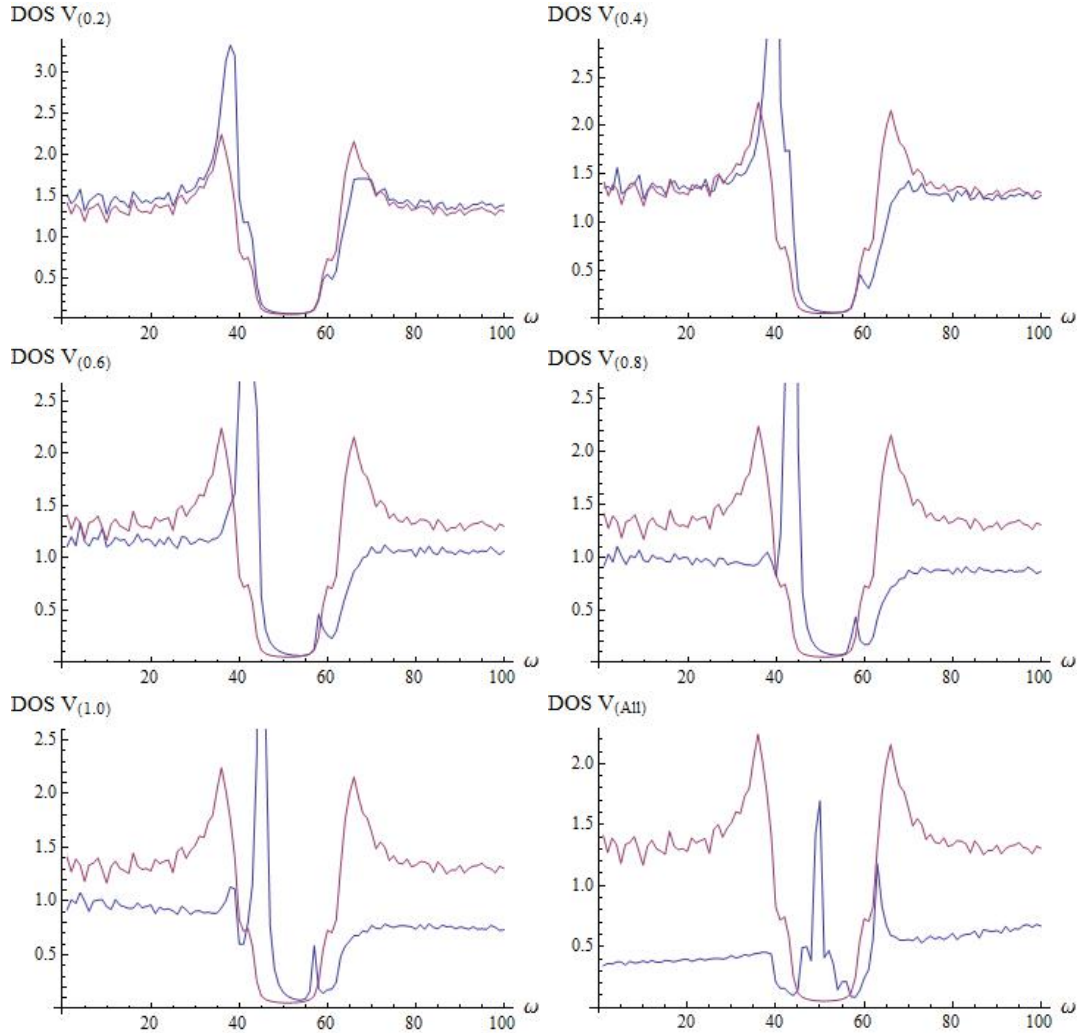


Figure 7: *These plots picture a gradually increasing impurity potential, showing it in 5 steps from $V = 0.2$ to $V = 1.0$. The last plot in the bottom right-hand corner is plotted for $V = 2$. All the plots are shown in blue line, with the 'clean' superconducting DOS of figure (6) in red line for comparison. We see that as the magnitude of the impurity increases, the general density of states decreases. Further, the peak generated by the impurity is moved closer and closer to the center of the gap, ruining the superconducting properties.*

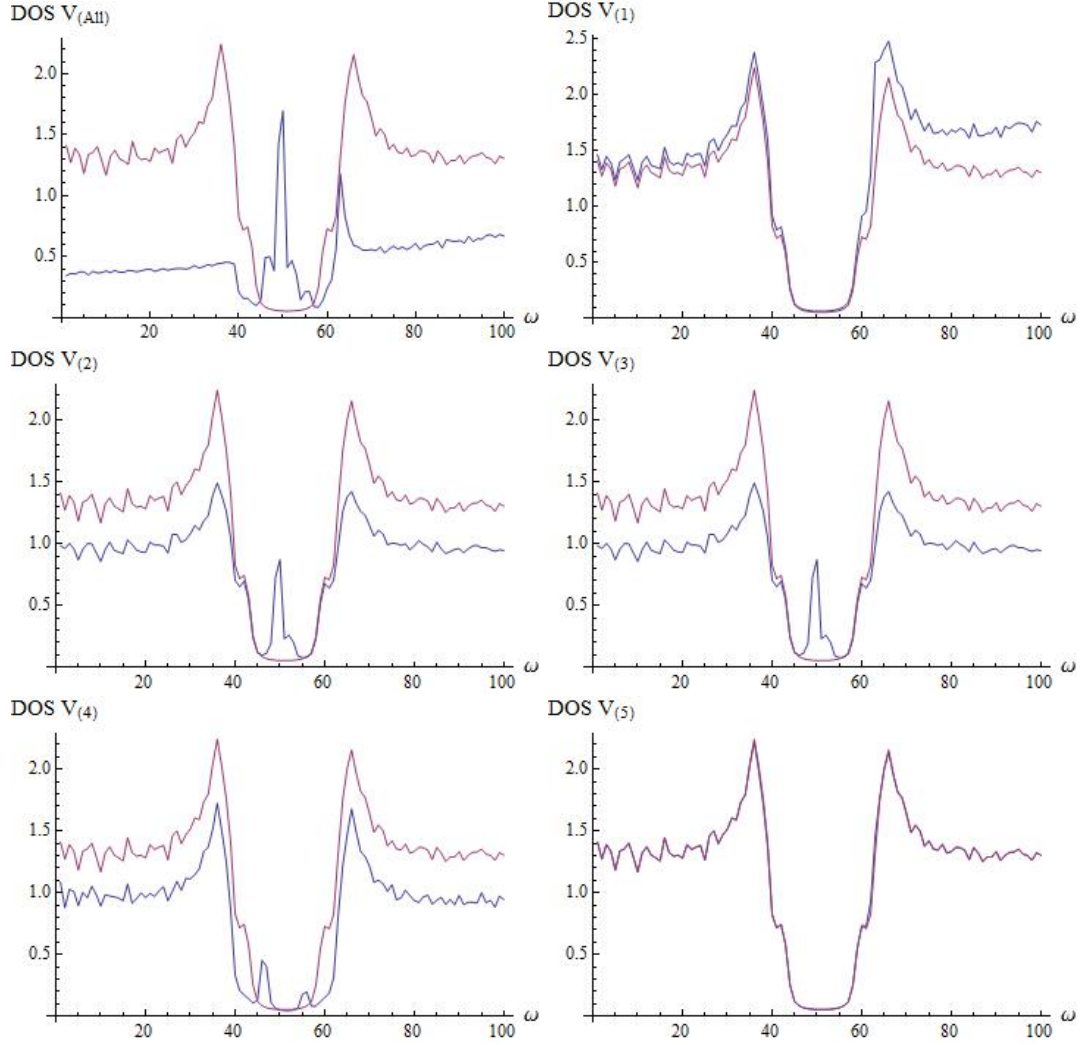


Figure 8: In blue line we have the impurity hitting the individual orbitals, again together with the plot for the impurity hitting them all. On all the plots in this figure, the impurity has a uniform magnitude, $V = 2$, and we have the DOS plot for the clean superconductor in red line for comparison. We see that the first orbital somehow looks to be improved by this impurity, and the fifth orbital hardly changes at all. The opposite goes for the second, third and fourth orbitals. The second and third look a lot alike, the properties of both heavily damaged by the impurity. The fourth at least retains some form of gap, even though it is overall lowered in value.

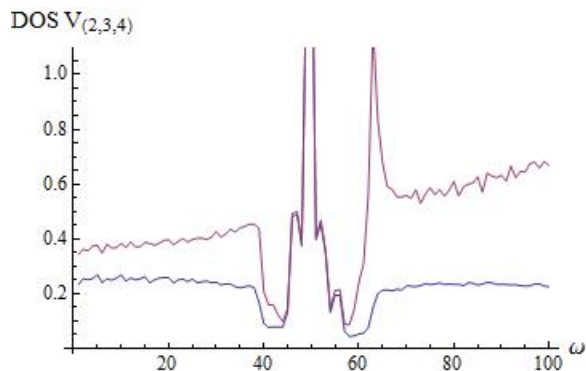


Figure 9: In this plot we compare the combined effect the impurity has on the second, third and fourth orbit (in blue) to the effect it has when hitting all the orbits (in red). We see that the center peak comes almost solely from the three middle orbits, and whatever remains of the gap in the red line is drastically diminished in the blue. This comes as no surprise, as we see in figure (8) that it is the first and fifth orbitals that are upholding the gap in the red line.

DOS. When attempting to place the impurity only in selected orbitals, we can start by looking at how a perturbation Hamiltonian would look, if it was to fit our needs.

$$H' = V \sum_{\mathbf{k}\mathbf{k}'\sigma} c_{i\mathbf{k}\sigma\vartheta}^\dagger c_{i\mathbf{k}'\sigma\vartheta}, \quad (55)$$

is a good candidate, since it allows for placement in the lattice (index i), for spin (σ) and for summing over \mathbf{k} , using ϑ for the orbital index. If we choose site $i = 0$ and orbital $\vartheta = 1$, then write it all in the Nambu formalism, we get

$$H' = \begin{pmatrix} c_{0\mathbf{k}\uparrow}^\dagger \\ c_{0\mathbf{k}\uparrow}^\dagger \\ c_{0\mathbf{k}\uparrow}^\dagger \\ c_{0\mathbf{k}\uparrow}^\dagger \\ c_{0\mathbf{k}\uparrow}^\dagger \\ c_{0-\mathbf{k}'\downarrow} \\ c_{0-\mathbf{k}'\downarrow} \\ c_{0-\mathbf{k}'\downarrow} \\ c_{0-\mathbf{k}'\downarrow} \\ c_{0-\mathbf{k}'\downarrow} \end{pmatrix} \begin{bmatrix} V & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -V & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{pmatrix} c_{0\mathbf{k}\uparrow} \\ c_{0\mathbf{k}\uparrow} \\ c_{0\mathbf{k}\uparrow} \\ c_{0\mathbf{k}\uparrow} \\ c_{0\mathbf{k}\uparrow} \\ c_{0-\mathbf{k}'\downarrow}^\dagger \\ c_{0-\mathbf{k}'\downarrow}^\dagger \\ c_{0-\mathbf{k}'\downarrow}^\dagger \\ c_{0-\mathbf{k}'\downarrow}^\dagger \\ c_{0-\mathbf{k}'\downarrow}^\dagger \end{pmatrix}, \quad (56)$$

leaving a minus sign on the [6,6]th element, just as we did in eq. (45). Introducing this matrix in $\mathcal{G}(0,0)$ in place of the other V -matrix (which was constructed similarly, but had V 's on all the diagonal elements) gives us figure (8). As noted, we have the DOS for when the impurity hits all the orbitals, for comparison to the other five plots. It is clear from the plots that the first and fifth orbitals more or less shake the impurity off. Orbitals two, three and four, however, are transformed into something that looks to be non-superconducting. Perhaps the fourth orbital still holds some properties, but the impurity has a strong effect on all three plots. If we were to 'attack' only the three middle orbitals, leaving the other two out, we would get figure (9). It is clear that the first and fifth are somehow 'defending' the superconductivity, but the three middle orbitals are just too affected by the impurity. However, it is remarkable to see this form of partitioning in which orbitals give in to the impurity, and which are able to uphold their properties.

3 Aftermath

This section is about what comes after the research done. Another way to put it is probably to call it a section for the research i didn't find the time to get done, so that it could have been in the actual research section. This name is rather long, however, so i choose to call it the aftermath section.

3.1 Next Step

After having looked into how the DOS behaves when under the effect of an impurity, it was the original idea to look at the situation from the same 'perspective' that we looked at the fermisurface, looking down on the surface from a higher place. This is figuratively speaking, of course. If we could map the real-space surface of the material, with the impurity in site $(0,0)$, we could investigate how an electron might scatter off of the impurity potential, and map this behaviour. We would, however, not be able to experimentally test the surface, so we would have to do it through what is known as the quasiparticle method. This method uses a purely theoretical particle with the desired properties, and sends it in to scatter off of the potential, just like we imagine an electron would (given that the quasiparticle has the same properties as the electron). We never got to the quasiparticle part, though, and this is why the method is not in the introduction with the other tools. What we do have, is an integration of the G_0^R with an exponential function, waiting to be Fourier transformed into realspace

$$G_0^R(\mathbf{r}, \omega) = \int_{-\infty}^{\infty} e^{i\mathbf{r}\mathbf{k}} G_0^R(\mathbf{k}\sigma, \omega) d\mathbf{k}. \quad (57)$$

It is still waiting, since it was keyed together with the process of spreading the green'sfunction over more sites, to make it into the map needed. Here we could have inserted the impurity, and then concocted a clever way of scattering the quasiparticles, all in all a larger process.

3.2 Conclusion

How did this project help researchers in the field of superconductivity. I am not sure that it did. What I am sure of, however, is that what it set off to do was a good idea, and not one that will be lost any time soon. The idea of the project was birthed from a German paper on the subject of quasiparticle scattering off of an impurity, meaning that there already has been people working on it, and I am sure there will be loads more.

The parts that did get done show some interesting features and properties in the orbitals of this superconductor. The fact that they are split the way that they are, into some that can resist the impurity, and some that cannot, must give grounds for further research. Also, we have shown the Green's function method to be a thorough and easily accessible tool, once one gets to know it.

Personally, I feel the project has given me a lot of insight into the field of theoretical research. How it's done, and how it's not done. It has taught me a great deal about handling a project on your own, and I intend to use this knowledge in the future.

3.3 Acknowledgements

First of all, I would like to thank my supervisor Brian M. Andersen for giving me the opportunity of writing a project on superconductors, and also for always being easy to talk to when I was confused and nothing made any sense.

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4 Mathematica Code

```
(*Gathering data into Hamiltonian and finding eigenvalues*)
H0u = {{\[\Epsilon][1, 1][Re[kx], Re[ky], kz] -
  Re[\[\Mu]], \[\Epsilon][1, 2][Re[kx], Re[ky],
  kz], \[\Epsilon][1, 3][Re[kx], Re[ky], kz], \[\Epsilon][1, 4][
  Re[kx], Re[ky], kz], \[\Epsilon][1, 5][Re[kx], Re[ky],
  kz]}, {\([\Epsilon][1, 2][Re[kx], Re[ky],
  kz])\[Conjugate], \[\Epsilon][2, 2][Re[kx], Re[ky], kz] -
  Re[\[\Mu]], \[\Epsilon][2, 3][Re[kx], Re[ky],
  kz], \[\Epsilon][2, 4][Re[kx], Re[ky], kz], \[\Epsilon][2, 5][
  Re[kx], Re[ky],
  kz]}, {\([\Epsilon][1, 3][Re[kx], Re[ky],
  kz])\[Conjugate], (\[\Epsilon][2, 3][Re[kx], Re[ky],
  kz])\[Conjugate], \[\Epsilon][3, 3][Re[kx], Re[ky], kz] -
  Re[\[\Mu]], \[\Epsilon][3, 4][Re[kx], Re[ky],
  kz], \[\Epsilon][3, 5][Re[kx], Re[ky],
  kz]}, {\([\Epsilon][1, 4][Re[kx], Re[ky],
  kz])\[Conjugate], (\[\Epsilon][2, 4][Re[kx], Re[ky],
  kz])\[Conjugate], (\[\Epsilon][3, 4][Re[kx], Re[ky],
  kz])\[Conjugate], \[\Epsilon][4, 4][Re[kx], Re[ky], kz] -
  Re[\[\Mu]], \[\Epsilon][4, 5][Re[kx], Re[ky],
  kz]}, {\([\Epsilon][1, 5][Re[kx], Re[ky],
  kz])\[Conjugate], (\[\Epsilon][2, 5][Re[kx], Re[ky],
  kz])\[Conjugate], (\[\Epsilon][3, 5][Re[kx], Re[ky],
  kz])\[Conjugate], (\[\Epsilon][4, 5][Re[kx], Re[ky],
  kz])\[Conjugate], \[\Epsilon][5, 5][Re[kx], Re[ky], kz] -
  Re[\[\Mu]]}}};
H0u == ConjugateTranspose[H0u];

\[\Mu] = 0.05;
kz = 0.0;
kx = 1;
ky = 1;
Eigensystem[H0u][[1]];

(*Summing up and plotting the bands*)
nk = 200;
klist = Table[i*Pi/nk, {i, 0, nk}];
En0 = Table[Eigensystem[H0u][[1]], {kx, klist}, {ky, klist}];
Grid[{{ListPlot[
  Table[Table[{klist[[kx]], En0[[kx, nk/2 + 1, \[\Mu]]}], {\[\Mu], 1,
  Nband}], {kx, nk/2 + 1, nk + 1}], AspectRatio -> 1,
  PlotRange -> {-2.5, 3}],
ListPlot[
  Table[Table[{klist[[ky]], En0[[nk + 1, ky, \[\Mu]]}], {\[\Mu], 1,
  Nband}], {ky, nk/2 + 1, nk + 1}], AspectRatio -> 1,
  PlotRange -> {-2.5, 3}],
```

```

ListPlot[
  Table[
    Table[{klist[[ky]], En0[[ky, ky, \[Mu]]}], {\[Mu], 1,
      Nband}], {ky, nk/2 + 1, nk + 1}], AspectRatio -> 1,
  PlotRange -> {-2.5, 3}]]]

(*Plotting fermisurface*)
emin = 0.01;
FS = {};
Table[Flatten[
  Table[If[En0[[kx, ky, \[Mu]]] <= emin && En0[[kx, ky, \[Mu]]] > 0,
    AppendTo[
      FS, {klist[[kx]], klist[[ky]], En0[[kx, ky, \[Mu]]}]], {kx, 1,
      nk}, {ky, 1, nk}], 1], {\[Mu], 1, Nband}];
ferms = ListPointPlot3D[FS, PlotLabel -> Style["\[Mu]=0.05", 20],
  ViewPoint -> {0, 0, Infinity}, ColorFunction -> "Rainbow",
  PlotStyle -> PointSize[Medium],
  Ticks -> {{0, Pi}, {0, Pi/2, Pi}, None},
  LabelStyle -> Directive[Large],
  AxesLabel -> {Style[Subscript[k, x], 20],
  Style[Subscript[k, y], 20]}]

(*Creating G and summing up for the spectral function*)

Gbase[px-, py-, w-] :=
  Inverse[IdentityMatrix[10]*(w + I*\[Eta]) -
  ArrayFlatten[{{Hbase[px, py],
    Hstube[px, py]}, {Conjugate[Hstube[px, py]],
    Conjugate[-Hbase[-px, -py]]}]]];

Gbasereal[Nx-, Ny-, x-] :=
  Module[{tmp, tot, kx, ky}, tmp = 0.0;
  For[kx = -Pi, kx <= Pi - 2 Pi/Nx, kx += 2 Pi/Nx,
  For[ky = -Pi, ky <= Pi - 2 Pi/Ny, ky += 2 Pi/Ny,
  tmp += Gbase[kx, ky, x]]; tot = tmp/(Nx*Ny)];

ProgressIndicator[Dynamic[i], {0, 120}]
MEGA2 = Table[Gbasereal[100, 100, -0.06 + 0.001*i], {i, 0, 120}];

(*Creating the T-matrix and inserting it into full Green's*)

T[V-, w-] := Inverse[IdentityMatrix[10] - (ID[V]).G00bma[[w]].(ID[V]);

Gsumimp[V-, x-] := G00bma[[x]] + G00bma[[x]].T[V, x].G00bma[[x]]

(*Using an open identity matrix (ID) to better specify which orbitals \
get hit*)

ID[V-] :=

```



```

V {{1, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, 0, 0, 0, 0, 0, 0, 0, 0},
   {0, 0, 1, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, 0, 0, 0, 0, 0, 0},
   {0, 0, 0, 0, 1, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 0, 0, 0, 0},
   {0, 0, 0, 0, 0, 0, 1, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 1, 0, 0},
   {0, 0, 0, 0, 0, 0, 0, 0, 1, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 1}};
ID[V] // MatrixForm;

(*Summing and plotting*)

ProgressIndicator[Dynamic[i], {1, 100}]
MEGAV = Table[Gsumimp[2, i], {i, 1, 100}];

listGsumimp =
Table[{-0.05 + 0.001*(i - 1), -Im[MEGAV[[i]][[1, 1]]]/
  Pi, -Im[MEGAV[[i]][[2, 2]]]/Pi, -Im[MEGAV[[i]][[3, 3]]]/
  Pi, -Im[MEGAV[[i]][[4, 4]]]/Pi, -Im[MEGAV[[i]][[5, 5]]]/
  Pi, -Im[MEGAV[[i]][[6, 6]]]/Pi, -Im[MEGAV[[i]][[7, 7]]]/
  Pi, -Im[MEGAV[[i]][[8, 8]]]/Pi, -Im[MEGAV[[i]][[9, 9]]]/
  Pi, -Im[MEGAV[[i]][[10, 10]]]/Pi}, {i, 1, 100}];

Impplot =
ListPlot[{listGsumimp[[All, 2]] + listGsumimp[[All, 3]] +
  listGsumimp[[All, 4]] + listGsumimp[[All, 5]] +
  listGsumimp[[All, 6]],
  listG00bma[[All, 2]] + listG00bma[[All, 3]] +
  listG00bma[[All, 4]] + listG00bma[[All, 5]] +
  listG00bma[[All, 6]]}, Joined -> True]

(*readying for real space map*)

Gbase[px_, py_, w_] :=
Inverse[IdentityMatrix[10]*(w + I*\[Eta]) -
  ArrayFlatten[{{Hbase[px, py],
    Hstube[px, py]}, {Conjugate[Hstube[px, py]],
    Conjugate[-Hbase[-px, -py]]}}]];

Gallsites[Nx_, Ny_, rx_, ry_, x_] :=
Total[1/(Nx*Ny)*
  ParallelTable[
    Exp[I*rx*kx + I*ry*ky]*Gbase[kx, ky, x], {kx, -Pi,
    Pi, (2*Pi)/Nx}, {ky, -Pi, Pi, (2*Pi)/Ny}]]

ProgressIndicator[Dynamic[j], {0, 1}]
ProgressIndicator[Dynamic[i], {0, 1}]
MEGAcheck =
  ParallelTable[Gallsites[100, 100, i, j, 0], {i, 0, 1}, {j, 0, 1}];

```

References

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- [3] J. Solyom: *Fundamentals of the Physics of Solids*. Springer, 2010.