Majorana Fermions in topological superconducting quantum wire and wells

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Abstract

Topological state of matter is one of the ultimate discovery by condensed matter physicists, pursuing a deeper understanding of condensed matter systems. This manner of classifying the various phase of matter. In this work we report some of our latest study of topological phase of matter. In these notes we have present a summary of our understanding of topological superconductors and Majorana Fermions.

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Majorana Fermions in 1D spinless p-wave superconductors

Majorana fermions are fundamental particles proposed by Etore Majorana [1] in 1937, that possess the peculiar property of being their own antiparticles. In high energy experiments, nevertheless, such exotic type particles have never been found. Recently, quasi-particle excitations with this exquisite properties have attracted a great deal of attention in condensed matter physics[2, 3, 4]. In this context, however, what is found are quasi-particle excitations composed of electrons and holes. Therefore, if Majorana fermions are to be found in condensed matter system it must appear as some kind of zero mode excitations. Finding such an excitation is one of the most challenging tasks within the condensed matter community in the recent years.

More formally, a particle being its own antiparticle means that the corresponding creator operator $\gamma^\dagger$ and annihilation operators γ are equal: $\gamma = \gamma^\dagger$. Designing experimental setups and and achieving the appropriate conditions for the observation of Majorana quasi-particle is a very complex matter[5, 6, 7].

The simplest and most promising proposal for the formation and observation of Majorana excitations is related to the Cooper pairs induced in quantum wires in close proximity to a superconductors[8, 9, 10, 11, 12] . In this system the Majorana modes are localized at the ends of the quantum wire. Similarly, in a two dimensional electron gas with a $p_x + ip_y$ superconducting Majorana modes are predicted to be bound at the core of superconducting vortices[13].

The increasing interest in studying Majorana fermions in condensed matter relies on two interesting aspects: (1) The possibility of observing such an exotic quasi-particle provides a convenient platform for investigating the statistical properties of such particles[14](“braiding”). (2) The existence of such Majorana modes is intimately associated to highly non-local electronic states, that have been proposed as possibly relevant to quantum computation[15].

Despite the difficulties in practical realization of Majorana modes in condensed matter experiments, in 2001 Yu Kitaev[16] has proposed a toy model Hamiltonian that contains unpaired Majorana modes. Basically, the Kitaev model describes a finite tight-binding chain with a nearest neighbor hopping term plus a superconducting pairing term.

Although Kitaev has discussed possible connections of his model to real systems, his focus was his focus was on the investigations of the excitation properties of the model. Nowadays, one of the strategies in the search for Majorana modes is to design a real physical setup whose Hamiltonian can be mapped onto the Kitaev model in some parameter range. In our project we propose to investigate the Majorana Fermions in a generalized version of the Kitaev model and their emergence in more realistic wire systems.

1.0.1 1D Kitaev model

Lets start our study of Majorana fermions within a toy model proposed by Kitaev[16] in 2001. The Kitaev model is described by the spinless Hamiltonian

$$H = \mu \sum_j c_j^\dagger c_j - \frac{1}{2} \sum_j \left(t c_j^\dagger c_{j+1} + \Delta e^{i\phi} c_j c_{j+1} + H.c. \right), \tag{1.1}$$

where c_j^+ (c_j) creates (annihilates) an electron in the j-th site of the chain, μ is the chemical potential of the chain, t is the hoping between the nearest neighbor sites, Δ is the pairing potential and ϕ is a superconductor phase. We should not worry, at least for now, with the physical origin of the parameters Δ and ϕ (which will be given latter). Here we rather want to understand in detail how Majorana modes emerge within this simplified model.

Lets define the Fourier transform

$$c_k = \frac{1}{\sqrt{\mathcal{N}}} \sum_j e^{ikx_j} c_j \tag{1.2}$$

$$c_j = \frac{1}{\sqrt{\mathcal{N}}} \sum_k e^{-ikx_j} c_k. \tag{1.3}$$

Replacing in the Hamiltonian we obtain

$$\begin{aligned} H \;=\; & \mu \frac{1}{\mathcal{N}} \sum_j \sum_{kk'} e^{-ix_j(k-k')} c_k^\dagger c_{k'} - \frac{1}{2\mathcal{N}} t \sum_j \sum_{kk'} e^{-ix_j(k-k')} e^{ik'a} c_k^\dagger c_{k'} \\ & - \frac{t}{2\mathcal{N}} \sum_j \sum_{kk'} e^{-ix_j(k'-k)} e^{-ik'a} c_{k'}^\dagger c_k - \frac{\Delta e^{i\phi}}{2\mathcal{N}} \sum_j \sum_{kk'} e^{ix_j(k+k')} e^{ik'a} c_k c_{k'} \\ & - \frac{\Delta e^{-i\phi}}{2\mathcal{N}} \sum_j \sum_{kk'} e^{-ix_j(k'+k)} e^{-ik'a} c_{k'}^\dagger c_k^\dagger \end{aligned} \tag{1.4}$$

$$
\begin{aligned}
H &= -\mu \sum_{kk'} c_k^\dagger c_{k'} \delta_{k,k'} - \frac{1}{2} t \sum_{kk'} e^{ik'a} c_k^\dagger c_{k'} \delta_{k,k'} - \frac{t}{2} \sum_{kk'} e^{-ik'a} c_{k'}^\dagger c_k \delta_{k,k'} \\
&\quad - \frac{\Delta e^{i\phi}}{2} \sum_{kk'} e^{ik'a} c_k c_{k'} \delta_{k',-k} - \frac{\Delta e^{-i\phi}}{2} \sum_{kk'} e^{ik'a} c_{k'}^\dagger c_k^\dagger \delta_{k,-k'} \\
&= \sum_k \left[-\mu - t \left(\frac{e^{ika} + e^{-ika}}{2} \right) \right] c_k^\dagger c_k - \frac{\Delta e^{i\phi}}{2} \sum_k e^{ika} c_k c_{-k} - \frac{\Delta e^{-i\phi}}{2} \sum_k e^{-ika} c_{-k}^\dagger c_k^\dagger \\
&= -\sum_k \left[\mu + t \cos(ka) \right] c_k^\dagger c_k - \frac{\Delta e^{i\phi}}{2} \sum_k e^{ika} c_k c_{-k} - \frac{\Delta e^{-i\phi}}{2} \sum_k e^{-ika} c_{-k}^\dagger c_k^\dagger \qquad (1.5)
\end{aligned}
$$

Notice that

$$
\begin{aligned}
\sum_k e^{ika} c_k c_{-k} &= \sum_{k<0} e^{ika} c_k c_{-k} + \sum_{k>0} e^{ika} c_k c_{-k} = \sum_{k<0} e^{ika} c_k c_{-k} + \sum_{k<0} e^{-ika} c_{-k} c_k \\
&= \sum_{k<0} \left(e^{ika} - e^{-ika} \right) c_k c_{-k} = \sum_{k<0} 2i \sin(ka) c_k c_{-k} \qquad (1.6)
\end{aligned}
$$

Also

$$
\begin{aligned}
\sum_k e^{ika} c_k c_{-k} &= \sum_{k<0} e^{ika} c_k c_{-k} + \sum_{k>0} e^{ika} c_k c_{-k} = \sum_{k>0} e^{-ika} c_{-k} c_k + \sum_{k>0} e^{ika} c_k c_{-k} \\
&= \sum_{k>0} \left(e^{ika} - e^{-ika} \right) c_k c_{-k} = \sum_{k>0} 2i \sin(ka) c_k c_{-k}. \qquad (1.7)
\end{aligned}
$$

From the last two expressions we have

$$
2 \sum_k e^{ika} c_k c_{-k} = \sum_{k<0} 2i \sin(ka) c_k c_{-k} + \sum_{k>0} 2i \sin(ka) c_k c_{-k} \qquad (1.8)
$$

or

$$
\sum_k e^{ika} c_k c_{-k} = \sum_k i \sin(ka) c_k c_{-k}. \qquad (1.9)
$$

Analogously,

$$
\begin{aligned}
\sum_k e^{-ika} c_k^\dagger c_{-k}^\dagger &= \sum_{k<0} e^{-ika} c_k^\dagger c_{-k}^\dagger + \sum_{k>0} e^{-ika} c_k^\dagger c_{-k}^\dagger = \sum_{k<0} e^{-ika} c_k^\dagger c_{-k}^\dagger + \sum_{k<0} e^{ika} c_{-k}^\dagger c_k^\dagger \\
&= \sum_{k<0} \left(e^{ika} - e^{-ika} \right) c_{-k}^\dagger c_k^\dagger = \sum_{k<0} 2i \sin(ka) c_{-k}^\dagger c_k^\dagger \qquad (1.10)
\end{aligned}
$$

Also

$$
\begin{aligned}
\sum_k e^{-ika} c_k^\dagger c_{-k}^\dagger &= \sum_{k<0} e^{-ika} c_k^\dagger c_{-k}^\dagger + \sum_{k>0} e^{-ika} c_k^\dagger c_{-k}^\dagger = \sum_{k>0} e^{ika} c_{-k}^\dagger c_k^\dagger + \sum_{k>0} e^{-ika} c_k^\dagger c_{-k}^\dagger \\
&= \sum_{k>0} \left(e^{ika} - e^{-ika} \right) c_{-k}^\dagger c_k^\dagger = \sum_{k>0} 2i \sin(ka) c_{-k}^\dagger c_k^\dagger. \qquad (1.11)
\end{aligned}
$$

Hence

$$\sum_k e^{-ika} c_k^\dagger c_{-k}^\dagger = \sum_k i\sin(ka) c_{-k}^\dagger c_k^\dagger. \tag{1.12}$$

and

$$\sum_k e^{-ika} c_{-k}^\dagger c_k^\dagger = -\sum_k i\sin(ka) c_{-k}^\dagger c_k^\dagger. \tag{1.13}$$

Therefore we can write

$$\begin{aligned} H &= -\sum_k \left[\mu + t\cos(ka)\right] c_k^\dagger c_k - \frac{i\Delta e^{i\phi}}{2}\sum_k \sin(ka) c_k c_{-k} + \frac{i\Delta e^{-i\phi}}{2}\sum_k \sin(ka) c_{-k}^\dagger c_k^\dagger \\ &\quad -\sum_k \left[\mu + t\cos(ka)\right] c_k^\dagger c_k - \frac{1}{2}\sum_k \left[i\Delta e^{i\phi}\sin(ka) c_k c_{-k} - i\Delta e^{-i\phi}\sin(ka) c_{-k}^\dagger c_k^\dagger\right] \\ &= \frac{1}{2}\sum_k \left\{-2\left[\mu + t\cos(ka)\right] c_k^\dagger c_k + i\Delta e^{i\phi}\sin(ka) c_k c_{-k} - i\Delta e^{-i\phi}\sin(ka) c_{-k}^\dagger c_k^\dagger\right\}. \end{aligned} \tag{1.14}$$

1.0.2 Bogoliubov-de Gennes Hamiltonian

Lets define now the operator $C_k^\dagger = [c_k^\dagger, c_{-k}]$ and its hermitian conjugate. Lets try to write the Hamiltonian above in the form

$$H = \frac{1}{2}\sum_k C_k^\dagger \mathcal{H}_k C_k, \tag{1.15}$$

where $\mathcal{H}_k$ is a 2×2 matrix to be determined. Suppose the matrix in the form

$$\mathcal{H}_k = \begin{pmatrix} a_k & b_k \\ d_k & e_k \end{pmatrix}. \tag{1.16}$$

Then

$$\begin{aligned} \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \mathcal{H}_k \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} &= \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \begin{pmatrix} a_k & b_k \\ d_k & e_k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \\ &= a_k c_k^\dagger c_k + b_k c_k^\dagger c_{-k}^\dagger + d_k c_{-k} c_k + e_k c_{-k} c_{-k}^\dagger \\ &= a_k c_k^\dagger c_k + b_k c_k^\dagger c_{-k}^\dagger + d_k c_{-k} c_k + e_k (1 - c_{-k}^\dagger c_{-k}) \end{aligned} \tag{1.17}$$

and

$$\begin{aligned} \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \mathcal{H}_k \begin{pmatrix} a_k \\ b_k \end{pmatrix} &= \sum_k \left[a_k c_k^\dagger c_k + b_k c_k^\dagger c_{-k}^\dagger + d_k c_{-k} c_k + e_k (1 - c_{-k}^\dagger c_{-k})\right] \\ &= \sum_k \left[a_k c_k^\dagger c_k + b_k c_k^\dagger c_{-k}^\dagger + d_k c_{-k} c_k + e_{-k} (1 - c_k^\dagger c_k)\right] \\ &= \sum_k \left[(a_k - e_{-k}) c_k^\dagger c_k + b_k c_k^\dagger c_{-k}^\dagger + d_k c_{-k} c_k + e_{-k}\right]. \end{aligned} \tag{1.18}$$

Notice that we can chose $e_{-k} = -a_k$ we can write

$$\sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \mathcal{H}_k \begin{pmatrix} a_k \\ b_k \end{pmatrix} = \sum_k \left[2a_k c_k^\dagger c_k + b_k c_k^\dagger c_{-k}^\dagger + d_k c_{-k} c_k \right] + \sum_k e_{-k}. \quad (1.19)$$

Finally, we can identify

$$2a_k = -2\left[\mu + t\cos(ka)\right] = 2\varepsilon_k, \quad (1.20)$$

$$d_k = i\Delta e^{i\phi} \sin(ka) = \tilde{\Delta}_k \quad (1.21)$$

and

$$b_k = -i\Delta e^{-i\phi} \sin(ka) = \tilde{\Delta}_k^*. \quad (1.22)$$

Since $e_{-k} = -a_k = -\varepsilon_k$, we obtain

$$\mathcal{H}_k = \begin{pmatrix} \varepsilon_k & \tilde{\Delta}_k^* \\ \tilde{\Delta}_k & -\varepsilon_k \end{pmatrix}. \quad (1.23)$$

$$\begin{aligned} \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \mathcal{H}_k \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} &= \sum_k \Big\{ -2[\mu + t\cos(ka)] c_k^\dagger c_k - i\Delta e^{-i\phi} \sin(ka) c_k^\dagger c_{-k}^\dagger \\ &\quad + i\Delta e^{i\phi} \sin(ka) c_{-k} c_k \Big\} - \sum_k \varepsilon_k. \end{aligned} \quad (1.24)$$

Notice that the last terms is just a constant. Comparing this expression with Eq. (1.14) (after omitting the additive constant) we finally obtain

$$H = \frac{1}{2} \sum_k C_k^\dagger \mathcal{H}_k C_k, \quad (1.25)$$

which is the Bogoliubov- de Gennes form. The next step is to diagonalize the Hamiltonian (1.23). Before doing so let us discuss the implication of the form of the Eq. (1.23).

Redundancy of the Bogoliubov-de Gennes form

There is a redundancy of the Bogoliubov de Gennes Hamitonian (1.23). To see this, suppose for a moment that there is no superconductivity ($\Delta_k = 0$). In this case the Hamiltonian (1.23) becomes

$$\mathcal{H}_k = \begin{pmatrix} \varepsilon_k & 0 \\ 0 & -\varepsilon_k \end{pmatrix}. \quad (1.26)$$

This is a Hamiltonian that possesses two copies of the energy ε_k with different signs. we can interpret ε_k as the energy of electrons while $-\varepsilon_k$ are the energy of holes. Since it is enough to specify ε_k, the appearance of $-\varepsilon_k$ in the Hamiltonian is redundant. Let us analyze more closely the origin of this redundancy. Suppose we had considered $e_{-k} = 0$ in Eq. (1.18). Then the Eq. (1.19) would becomes

$$\sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \mathcal{H}_k \begin{pmatrix} a_k \\ b_k \end{pmatrix} = \sum_k \left[a_k c_k^\dagger c_k + b_k c_k^\dagger c_{-k}^\dagger + d_k c_{-k} c_k \right]. \tag{1.27}$$

By comparing this expression with Eq. (1.14) we would obtain precisely the form

$$\mathcal{H}_k = \begin{pmatrix} \varepsilon_k & \tilde{\Delta}_k^* \\ \tilde{\Delta}_k & 0 \end{pmatrix}, \tag{1.28}$$

without any additive constant, unlike in the previous choice. Now, for $\Delta_k = 0$ Eq. (1.28) has no redundancy. Therefore, the redundancy built-in Eq. (1.23) results from the choice of e_k. As we have seen, the price payed for the choice $e_k = -\varepsilon_k$ the appearance of a constant in the Hamiltonian. This by no means alter the physics of the problem. The advantage of that the Bogoliubov-de Gennes form introduces an adequate form for studying the problem from a topological perspective, as we will see latter.

Diagonalization of the Bogoliubov-de Gennes Hamitonian

In order to diagonalize the Bogoliubov-de Gennes Hamiltonian (1.23) we define another annihilation operator

$$\alpha_k = u_k c_k + v_k c_{-k}^\dagger \tag{1.29}$$

with its corresponding hermitian conjugate,

$$\alpha_k^\dagger = u_k^* c_k^\dagger + v_k^* c_{-k}, \tag{1.30}$$

where $|u_k|^2 + |v_k|^2 = 1$ and try to write Eq. (1.23) in a simpler form as

$$H = \sum_k E_k \alpha_k^\dagger \alpha_k. \tag{1.31}$$

The dispersion E_k is the eigenvalue of $\mathcal{H}_k$,

$$E_k = \sqrt{\varepsilon_k^2 + |\tilde{\Delta}_k|^2}. \tag{1.32}$$

There is another eigenvalue with negative signal but we do not need to worry about is for now. The coefficients u_k and v_k can be determined by

$$\begin{pmatrix} \varepsilon_k - E_k & \tilde{\Delta}_k^* \\ \tilde{\Delta}_k & -\varepsilon_k - E_k \end{pmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = 0 \tag{1.33}$$

from which we get

$$(\varepsilon_k - E_k)u_k + \tilde{\Delta}_k^* v_k = 0 \tag{1.34}$$

or

$$v_k = \frac{E_k - \varepsilon_k}{\tilde{\Delta}_k^*} u_k. \tag{1.35}$$

This expression shows that if we choice one of u_k and v_k to be even transforming $k \to -k$, the other has to be odd under such transformation.

$$|u_k|^2 = 1 - |v_k|^2 = 1 - \frac{(E_k - \varepsilon_k)^2}{|\tilde{\Delta}_k|^2}|u_k|^2 \tag{1.36}$$

$$\left[1 + \frac{(E_k - \varepsilon_k)^2}{|\tilde{\Delta}_k|^2}\right]|u_k|^2 = 1 \tag{1.37}$$

but

$$E_k^2 = \varepsilon_k^2 + |\tilde{\Delta}_k|^2 \Rightarrow E_k^2 - \varepsilon_k^2 = |\tilde{\Delta}_k|^2 \tag{1.38}$$

or

$$(E_k - \varepsilon_k)(E_k + \varepsilon_k) = |\tilde{\Delta}_k|^2 \Rightarrow (E_k - \varepsilon_k)^2 = \frac{|\tilde{\Delta}_k|^4}{(\varepsilon_k + E_k)^2} \tag{1.39}$$

therefore,

$$\left[1 + \frac{|\tilde{\Delta}_k|^2}{(\varepsilon_k + E_k)^2}\right]|u_k|^2 = 1 \tag{1.40}$$

$$\frac{(\varepsilon_k + E_k)^2 + |\tilde{\Delta}_k|^2}{(\varepsilon_k + E_k)^2}|u_k|^2 = 1 \tag{1.41}$$

$$\frac{\varepsilon_k^2 + E_k^2 + 2\varepsilon_k E_k + |\tilde{\Delta}_k|^2}{(\varepsilon_k + E_k)^2}|u_k|^2 = \frac{2E_k^2 + 2\varepsilon_k E_k}{(\varepsilon_k + E_k)^2}|u_k|^2 = \frac{2E_k}{(\varepsilon_k + E_k)}|u_k|^2 = 1 \tag{1.42}$$

$$\Rightarrow |u_k| = \frac{\sqrt{\varepsilon_k + E_k}}{\sqrt{2E_k}} \tag{1.43}$$

We can, clearly choose u_k to be complex and having the same symmetry of Δ_k,

$$u_k = \frac{\tilde{\Delta}_k}{|\tilde{\Delta}_k|}\frac{\sqrt{\varepsilon_k + E_k}}{\sqrt{2E_k}}. \tag{1.44}$$

Under this choice, v_k will be odd. It is interesting to expand the dispersion relation E_k

$$\begin{aligned} E_k &= \sqrt{[\mu + t\cos(ka)]^2 + \Delta^2 \sin^2(ka)} \\ &= \sqrt{(t^2 - \Delta^2)\cos^2(ka) + 2\mu t\cos(ka) + \Delta^2 + \mu^2}. \end{aligned} \tag{1.45}$$

In order to obtain gapless excitations we need

$$(t^2 - \Delta^2)\cos^2(ka) + 2\mu t\cos(ka) + \Delta^2 + \mu^2 = 0. \tag{1.46}$$

For the equation above to be satisfied for an arbitrary value of Δ we need that the terms $-\Delta^2\cos^2(ka)$ and Δ^2 to cancel out mutually. This is achieved only if $\cos(ka) = \pm 1$ which leads to $k = \pm\pi/a$. This conditions lead to the equations

$$\begin{cases} (\mu + t)^2 = 0, & \text{if } \cos(ka) = 1 \\ (\mu - t)^2 = 0, & \text{if } \cos(ka) = -1 \end{cases} \tag{1.47}$$

We conclude then that gapless excitations are possible only if $\mu = \pm t$, which is the border of the band. The particular k-points in the Brillouin zone where the gap closes are $k = \pm\pi/a$ for $\mu = t$ and $k = 0$ for $\mu = -t$.

1.0.3 $\mathbb{Z}_2$ topological invariant for the Kitaev model

The trivial and the topological phases in the Kitaev model are characterized by a well defined quantity called topological invariant. The concepts of topology is very useful in classifying superconductors as well as insulators. To illustrate this concept in practice, here we will present a simple way of calculating the $\mathbb{Z}_2$ topological invariant for the 1D Kitaev model.

We start by rewriting Eq. (2.43) as

$$\mathcal{H}_k = \begin{pmatrix} \varepsilon_k & \tilde{\Delta}_k^* \\ \tilde{\Delta}_k & -\varepsilon_k \end{pmatrix} = \varepsilon_k \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \texttt{Re}[\Delta_k] \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \texttt{Im}[\Delta_k] \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{1.48}$$

Notice that the matrices above are nothing else but the Pauli Matrices,

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \hat{\sigma}_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; \texttt{and} \; \hat{\sigma}_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.49}$$

With that we can write Eq. (1.48) as

$$\mathcal{H}_k = \mathbf{h}(k) \cdot \boldsymbol{\sigma}, \tag{1.50}$$

where we define

$$\mathbf{h}(k) = h_x(k)\hat{\mathbf{x}} + h_y(k)\hat{\mathbf{y}} + h_z(k)\hat{\mathbf{z}} \tag{1.51}$$

and

$$\boldsymbol{\sigma} = \hat{\sigma}_x\hat{\mathbf{x}} + \hat{\sigma}_y\hat{\mathbf{y}} + \hat{\sigma}_z\hat{\mathbf{z}}, \tag{1.52}$$

with

$$h_x(k) = \mathtt{Re}\Delta(k), \quad h_y(k) = \mathtt{Im}\Delta(k) \text{ and } \; h_z(k) = \varepsilon_k. \tag{1.53}$$

Suppose that $\mathbf{h}(k)$ is non zero over the fist Brilouin zone. Then we can define a unity vector $\hat{\mathbf{h}}(k)$ as

$$\hat{\mathbf{h}}(k) = \frac{\mathbf{h}(k)}{|\hat{\mathbf{h}}(k)|} \tag{1.54}$$

that maps the Hamiltonian on a unity sphere. From Eqs. (1.20), (1.21) and (1.22) we notice that

$$h_{x,y}(k) = -h_{x,y}(-k) \tag{1.55}$$

and

$$h_z(k) = h_z(-k). \tag{1.56}$$

The constraint (1.55) leads $h_{x,y}(0) = 0$. Moreover, directly from Eq. (1.21) we notice that $h_{x,y}(\pi) = 0$. Therefore, we can write

$$\hat{\mathbf{h}}(0) = s_0\hat{\mathbf{z}} \tag{1.57}$$

and

$$\hat{\mathbf{h}}(\pi) = s_\pi\hat{\mathbf{z}}. \tag{1.58}$$

Here, there are nothing special about s_0 or s_π, except that they are ± 1. What is really interesting is that the product $s_0 s_\pi$ is topologically invariant. This means that it remains unchanged by a smooth distortion of the Hamiltonian that does not close the gap. To get some more physical insight about this statement, remember that $h_z(k)$ is the kinetic energy. Then s_0 and s_π are the sign of the kinetic energy in the poles of the sphere. The topological invariant ν is defined as $(-1)^\nu = s_0 s_\pi$. Therefore, ν is defined only modulo 2, therefore has values 0 or 1. $\nu = 1$ then by some distortion of the Hamiltonian, the gap is necessarily closed at some point.

From Eqs. (1.53) and (1.20) we have (taking $a = 1$)

$$h_z(k) = -\mu + t\cos(k), \tag{1.59}$$

then, since $t > 0$,

$$s_0 = \frac{h_z(0)}{|h_z(0)|} = \frac{t-\mu}{|t-\mu|} = \begin{cases} +1, & \text{if } \mu < t \\ -1, & \text{if } \mu > t \end{cases} \tag{1.60}$$

and

$$s_\pi = \frac{h_z(\pi)}{|h_z(\pi)|} = \frac{-t-\mu}{|t-\mu|} = \begin{cases} +1, & \text{if } \mu > -t \\ -1, & \text{if } \mu < -t \end{cases} \tag{1.61}$$

therefore,

$$(-1)^\nu = s_0 s_\pi = -\frac{t^2-\mu^2}{|t-\mu|^2} = \begin{cases} -1, & \text{if } |\mu| < t \\ +1, & \text{if } |\mu| > t \end{cases}. \tag{1.62}$$

The region $\nu = 0$ corresponds to the *strong pairing trivial phase* while the region $\nu = 1$ is called *weak pairing topological phase*.

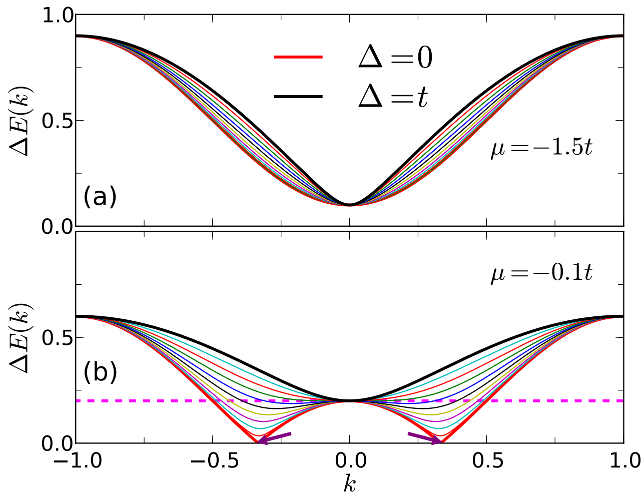

Figure 1.1: Energy difference between the upper and lower band of the Bogoliubov-de Gennes Hamiltonian for the Kitaev model. Panels (a) and (b) show the distortion of the Hamiltonian by slowly changing Δ in the trivial phase ($|\mu| = 0.75t > t$) and in the topological phase ($|\mu| = 0.1 < t$), respectively. Note that $\Delta E(k) = 0$ represents the closing gap in the topological phase.

Before proceeding with the investigation of the meaning of the strong and weak pairing phase. It is helpful for us to first take a close look at the physical consequence of the trivial and topological phase. Lets us take as a reference the point of the trivial phase of the Kitaev model $\Delta = t = 0$ and $\mu \neq 0$, in which case the dispersion are two horizontal lines place at $\pm\mu$. To show the difference between the two phases we will star with the Hamiltonian with some set of parameters ant then slowly vary some of then, trying to connect the trivial phase.

Suppose we start with $t > 0$ $\mu < -t$. We want to drive the Hamiltonian to the trivial phase $\Delta = t = 0$ and $\mu < 0$. We can do this pedagogically, we can do it in two steps. *step one*: we keep $t > 0$ fixed and slowly decrease Δ. This step is shown in Fig. 1.1(a) $\Delta E(k) = E_+(k) - E_-(k) = 2E_+(k)$, where we have fixed $t = 0.2$ $\mu = -1.5t$ and decrease Δ from $\Delta = 0.2$ to $\Delta = 0$ in ten steps. Notice that the gap $2|\mu|$ remains open during the process. *step two*: Once we get $\Delta = 0$ we then decrease t to zero, leading a straight horizontal line at 2μ. During this second step the gaps still remain open during the process.

Now, suppose we start with $t > 0$, $\Delta > 0$ and $-t < \mu < 0$. If we follow the same steps as before we will see that the gap will close already during the first step [see the two arrows in Fig. 1.1(b), indicating the points where the gap closes]. This is shown in Fig. 1.1(b). Moreover, we cannot find any other way to drive the system to the phase $\Delta = t = 0$ and $\mu < 0$. This is indeed the meaning of the topological difference between the two phases. This argument is also valid when we start from $\mu > 0$ and drive the Hamiltonian to the trivial phase characterized by $\Delta = t = 0$ and $\mu > 0$.

1.0.4 Meaning of the weak and strong pairing phases

To understand the terminology for the weak and strong pairing phase we need to return to the ground state solution of the Bogoliubov-de Gennes Hamiltonian (1.31). The form of Eq. (1.31) implies a ground state, $|g.s.\rangle$, such that

$$\alpha_k |g.s.\rangle = 0, \tag{1.63}$$

which means that the ground state has no Bogoliubov quasi-particles created by the operator $\alpha_k^\dagger$. Owing to the properties of the fermion operator $\alpha_k \alpha_k = 0$, we can construct the ground state as,

$$|g.s.\rangle = \sum_{0<k<\pi} \alpha_k \alpha_{-k} |0\rangle, \tag{1.64}$$

where $|0\rangle$ is the Fermi vacuum. From the defining expression (1.29) we can obtain the form

$$|g.s.\rangle = \sum_{0<k<\pi} u_k v_{-k} \left[1 + \varphi(k) c_{-k}^\dagger c_k^\dagger\right] |0\rangle, \tag{1.65}$$

where

$$\varphi(k) = \frac{v_k}{u_k} = \frac{E_k - \varepsilon_k}{\tilde{\Delta}_k^*}, \tag{1.66}$$

in which we have used the relation (1.35). It can be easily verified that any state of the form,

$$|g.s.\rangle \propto \sum_{0<k<\pi} \left[1 + \varphi(k) c^\dagger_{-k} c^\dagger_k\right] |0\rangle, \tag{1.67}$$

satisfy the condition (1.63), required for the ground state. From Eq. (1.66) and 1.45 we can write

$$\varphi(k) = \frac{\sqrt{[\mu + t\cos(ka)]^2 + \Delta^2 \sin^2(ka)} + \mu + t\cos(ka)}{-i\Delta e^{-i\phi} \sin{(ka)}}, \tag{1.68}$$

In the limit of small k we have

$$\varphi(k) \sim \frac{ie^{i\phi}}{\Delta} \frac{\sqrt{[\mu + t]^2 + \Delta^2 k^2} + \mu + t}{k}. \tag{1.69}$$

We can now expand the expression above in two different cases.

1. $\underline{\mu + t < 0}$ In this case the leading term in k is obtained by expanding the expression above, obtaining,

$$\varphi(k) \sim -\frac{ie^{\phi}}{2\Delta} \frac{k}{|\mu + t|}. \tag{1.70}$$

2. $\underline{\mu + t > 0}$ In this case the leading term is

$$\varphi(k) \sim \frac{2ie^{\phi}}{\Delta} \frac{|\mu + t|}{k}. \tag{1.71}$$

Bearing in mind that small-k corresponds to large distances we can interpret these results as: For $\mu + t < 0$, $\varphi(k)$ vanishes as $k \to 0$ or $\varphi(r)$ vanishes as $r \to \infty$. This means that the pair are strongly tight together, thereby the terminology **strong pairing regime**. On the other hand, for $\mu + t > 0$, $\varphi(k)$ diverges as $k \to 0$ or $\varphi(r)$ diverges as $r \to \infty$. This means that the pair are far apart from together, justifying then terminology **weak pairing regime**. For more formal discussion on this topic see Ref. [17]. Finally,combining these results with (1.72) we can summarize,

$$(-1)^\nu = s_0 s_\pi = -\frac{t^2 - \mu^2}{|t - \mu|^2} \Rightarrow \nu = \begin{cases} 1, & \text{if } |\mu| < t: \text{ weak pairing phase} \\ 0, & \text{if } |\mu| > t: \text{ strong pairing phase} \end{cases}. \tag{1.72}$$

2

2D electron gas with Rashba and Dresselhauss spin-orbit interaction

Lets consider the a two-dimensional electron gas with Rashba and Dresselhauss spin-orbit interaction,

$$H_0 = \int d^2k \psi_{\mathbf{k}}^{\dagger} \mathcal{H}_0(\mathbf{k}) \psi_{\mathbf{k}}, \tag{2.1}$$

where $\psi_{\mathbf{k}}$ is a field operators with spin degrees of freedom.

$$\begin{aligned} \mathcal{H}_0(\mathbf{k}) &= \left(\frac{k^2}{2m} - \mu\right) \mathbb{1} + \alpha(\sigma_x k_y - \sigma_y k_x) \\ &\quad + \beta(\sigma_x k_x - \sigma_y k_y) + V_Z \sigma_z, \end{aligned} \tag{2.2}$$

where k_x and k_y are the electron linear momentum along the x ([100]) and y ([010]) directions, respectively, m is the electron effective mass, α and β are the Rashba and Dresselhauss spin-orbit couplings, respectively, V_Z in a Zeeman energy induced by a magnetic field along the z-axis and $\sigma_{x,y}$ are the Pauli matrices. Inspired by Bernevig's work,[18] we shall restrict our study to the particular case of $\alpha = \beta$, for which the Hamiltonian (2.2) becomes

$$\mathcal{H}_0(\mathbf{k}) = \left(\frac{k^2}{2m} - \mu\right) \mathbb{1} + \alpha(k_x + k_y)(\sigma_x - \sigma_y) + V_Z \sigma_z, \tag{2.3}$$

where $\mathbb{1}$ denotes a 2×2 identity. Performing a rotation in the k-space, defined as

$$k_{\pm} = \frac{1}{\sqrt{2}}(k_x \pm k_y), \tag{2.4}$$

we can write in a matrix form

$$\mathcal{H}_0(\mathbf{k}) = \begin{bmatrix} \frac{k^2}{2m} + V_Z - \mu & \sqrt{2}\alpha(1+i)k_+ \\ \sqrt{2}\alpha(1-i)k_+ & \frac{k^2}{2m} - V_Z + \mu \end{bmatrix}, \tag{2.5}$$

where in Eq. (2.5), $k^2 = k_+^2 + k_-^2$. Hamiltonian (2.5) can be written in a diagonal form by defining the orthonormal wave vectors

$$\phi_{\mathbf{k}\pm} = \begin{pmatrix} a_{\mathbf{k}\pm} \\ b_{\mathbf{k}\pm} \end{pmatrix}, \tag{2.6}$$

for which,

$$\mathcal{H}_0(\mathbf{k})\phi_{\mathbf{k}\pm} = \varepsilon_{\mathbf{k}\pm}\phi_{\mathbf{k}\pm}. \tag{2.7}$$

The unitary matrix that diagonalizes the Hamiltonian can be written as

$$U_{\mathbf{k}} = \begin{pmatrix} a_{\mathbf{k}+} & b_{\mathbf{k}+} \\ a_{\mathbf{k}-} & b_{\mathbf{k}-} \end{pmatrix}. \tag{2.8}$$

The inverse transformation becomes then

$$\begin{pmatrix} \psi_{\mathbf{k}\uparrow} \\ \psi_{\mathbf{k}\downarrow} \end{pmatrix} = U_{\mathbf{k}}^{\dagger} \begin{pmatrix} \psi_{\mathbf{k}+} \\ \psi_{\mathbf{k}-} \end{pmatrix} = \begin{pmatrix} a_{\mathbf{k}+}^{*} & a_{\mathbf{k}-}^{*} \\ b_{\mathbf{k}+}^{*} & b_{\mathbf{k}-}^{*} \end{pmatrix} \begin{pmatrix} \psi_{\mathbf{k}+} \\ \psi_{\mathbf{k}-} \end{pmatrix}, \tag{2.9}$$

Solving the eigenvector equation (2.7) we find,

$$a_{\mathbf{k}+} = \frac{2\alpha|k_+|}{\sqrt{\sqrt{V_Z^2 + 4\alpha^2 k_+^2}\left[\sqrt{V_Z^2 + 4\alpha^2 k_+^2} - V_Z\right]}} \tag{2.10}$$

$$b_{\mathbf{k}+} = \frac{-\left[V_Z - \sqrt{V_Z^2 + 4\alpha^2 k_+^2}\right](1-i)k_+}{|k_+|\sqrt{2\sqrt{V_Z^2 + 4\alpha^2 k_+^2}\left[\sqrt{V_Z^2 + 4\alpha^2 k_+^2} - V_Z\right]}}. \tag{2.11}$$

$$a_{\mathbf{k}-} = \frac{\left[V_Z - \sqrt{V_Z^2 + 4\alpha^2 k_+^2}\right](1+i)k_+}{|k_+|\sqrt{2\sqrt{V_Z^2 + 4\alpha^2 k_+^2}\left[\sqrt{V_Z^2 + 4\alpha^2 k_+^2} - V_Z\right]}} \tag{2.12}$$

$$b_{\mathbf{k}-} = \frac{2\alpha|k_+|}{\sqrt{\sqrt{V_Z^2 + 4\alpha^2 k_+^2}\left[\sqrt{V_Z^2 + 4\alpha^2 k_+^2} - V_Z\right]}}, \tag{2.13}$$

whose eigenenergies are

$$\varepsilon_{\pm}(\mathbf{k}) = \frac{k^2}{2m} - \mu \pm \sqrt{V_Z^2 + 4\alpha^2 k_+^2}. \tag{2.14}$$

The Hamiltonian can be written in its diagonal form in terms of the operators $\psi_{\mathbf{k}+}$ and $\psi_{\mathbf{k}-}$, as

$$\mathcal{H}_0(\mathbf{k}) = \varepsilon_{\mathbf{k}+}\psi_{\mathbf{k}+}^{\dagger}\psi_{\mathbf{k}+} + \varepsilon_{\mathbf{k}-}\psi_{\mathbf{k}-}^{\dagger}\psi_{\mathbf{k}-} \tag{2.15}$$

Proximity to an s-wave superconductor

Suppose now that the system described above suffer a proximity effect to a s-wave superconductor. This effect can be translated as[7, 10]

$$H_{sup} = \frac{1}{2}\int d^2k \psi^\dagger_{\mathbf{k}} \mathcal{H}_{sup}(\mathbf{k}) \psi^\dagger_{\mathbf{k}}, \tag{2.16}$$

where

$$\mathcal{H}_{sup}(\mathbf{k}) = \Delta \psi^\dagger_{\mathbf{k}\uparrow}\psi^\dagger_{-\mathbf{k}\downarrow} + \Delta^* \psi_{-\mathbf{k}\downarrow}\psi_{\mathbf{k}\uparrow}, \tag{2.17}$$

in which $\psi^\dagger_{\mathbf{k}s}$ ($\psi_{\mathbf{k}s}$) creates (annihilates) an electron with momentum $\mathbf{k}$ and spin projection s along the z-axis. Using the Eq. (2.9) We can write the last expression in term of the new operators $\psi_{\mathbf{k}\pm}$ as

$$\begin{aligned}
\mathcal{H}_{sup}(\mathbf{k}) &= \Delta \left(a_{\mathbf{k}+}\psi^\dagger_{\mathbf{k}+} + a_{\mathbf{k}-}\psi^\dagger_{\mathbf{k}-}\right)\left(b_{-\mathbf{k}+}\psi^\dagger_{-\mathbf{k}+} + b_{-\mathbf{k}-}\psi^\dagger_{-\mathbf{k}-}\right) + H.c. \\
&= \Delta a_{\mathbf{k}+}b_{-\mathbf{k}+}\psi^\dagger_{\mathbf{k}+}\psi^\dagger_{-\mathbf{k}+} + \Delta a_{\mathbf{k}+}b_{-\mathbf{k}-}\psi^\dagger_{\mathbf{k}+}\psi^\dagger_{-\mathbf{k}-} \\
&\quad + \Delta a_{\mathbf{k}-}b_{-\mathbf{k}+}\psi^\dagger_{\mathbf{k}-}\psi^\dagger_{-\mathbf{k}+} + a_{\mathbf{k}-}b_{-\mathbf{k}-}\psi^\dagger_{\mathbf{k}-}\psi^\dagger_{-\mathbf{k}-}
\end{aligned} \tag{2.18}$$

or

$$\begin{aligned}
\mathcal{H}_{sup}(\mathbf{k}) &= \Delta a_{\mathbf{k}+}b_{-\mathbf{k}+}\psi^\dagger_{\mathbf{k}+}\psi^\dagger_{-\mathbf{k}+} + \Delta a_{\mathbf{k}-}b_{-\mathbf{k}-}\psi^\dagger_{\mathbf{k}-}\psi^\dagger_{-\mathbf{k}-} \\
&\quad + \Delta a_{\mathbf{k}+}b_{-\mathbf{k}-}\psi^\dagger_{\mathbf{k}+}\psi^\dagger_{-\mathbf{k}-} - \Delta a_{\mathbf{k}-}b_{-\mathbf{k}+}\psi^\dagger_{-\mathbf{k}+}\psi^\dagger_{\mathbf{k}-}.
\end{aligned} \tag{2.19}$$

Therefore,

$$\begin{aligned}
H_{sup} &= \frac{1}{2}\int d^2k \Big[\Delta a_{\mathbf{k}+}b_{-\mathbf{k}+}\psi^\dagger_{\mathbf{k}+}\psi^\dagger_{-\mathbf{k}+} + \Delta a_{\mathbf{k}-}b_{-\mathbf{k}-}\psi^\dagger_{\mathbf{k}-}\psi^\dagger_{-\mathbf{k}-} \\
&\quad + \Delta a_{\mathbf{k}+}b_{-\mathbf{k}-}\psi^\dagger_{\mathbf{k}+}\psi^\dagger_{-\mathbf{k}-} - \Delta a_{\mathbf{k}-}b_{-\mathbf{k}+}\psi^\dagger_{-\mathbf{k}+}\psi^\dagger_{\mathbf{k}-}\Big].
\end{aligned} \tag{2.20}$$

Notice that

$$a_{\mathbf{k}+}b_{-\mathbf{k}+} = \frac{-\sqrt{2}\alpha k_+(1-i)}{\sqrt{V_Z^2+4\alpha^2k_+^2}} \tag{2.21}$$

$$a_{\mathbf{k}-}b_{-\mathbf{k}-} = \frac{-\sqrt{2}\alpha k_+(1+i)}{\sqrt{V_Z^2+4\alpha^2k_+^2}} \tag{2.22}$$

$$a_{\mathbf{k}+}b_{-\mathbf{k}-} = \frac{4\alpha^2k_+^2}{\sqrt{V_Z^2+4\alpha^2k_+^2}\left[\sqrt{V_Z^2+4\alpha^2k_+^2}-V_Z\right]} \tag{2.23}$$

$$a_{\mathbf{k}-}b_{-\mathbf{k}+} = \frac{\left[V_Z-\sqrt{V_Z^2+4\alpha^2k_+^2}\right]^2}{\sqrt{V_Z^2+4\alpha^2k_+^2}\left[\sqrt{V_Z^2+4\alpha^2k_+^2}-V_Z\right]}. \tag{2.24}$$

From the last equation we can see that $a_{\mathbf{k}-}b_{-\mathbf{k}+} = a_{-\mathbf{k}-}b_{\mathbf{k}+}$, therefore Eq. (2.20) can be written as

$$\begin{aligned} H_{sup} &= \frac{1}{2}\int d^2k \Big[\Delta a_{\mathbf{k}+}b_{-\mathbf{k}+}\psi^{\dagger}_{\mathbf{k}+}\psi^{\dagger}_{-\mathbf{k}+} + \Delta a_{\mathbf{k}-}b_{-\mathbf{k}-}\psi^{\dagger}_{\mathbf{k}-}\psi^{\dagger}_{-\mathbf{k}-} \\ &\quad +\Delta\left(a_{\mathbf{k}+}b_{-\mathbf{k}-} - a_{\mathbf{k}-}b_{-\mathbf{k}+}\right)\psi^{\dagger}_{\mathbf{k}+}\psi^{\dagger}_{-\mathbf{k}-}\Big]. \end{aligned} \tag{2.25}$$

Finally, we can define

$$\Delta_{++}(\mathbf{k}) = \Delta a_{\mathbf{k}+}b_{-\mathbf{k}+} = -\frac{\Delta\sqrt{2}\alpha k_{+}(1-i)}{\sqrt{V_Z^2 + 4\alpha^2 k_+^2}}, \tag{2.26}$$

$$\Delta_{--}(\mathbf{k}) = \Delta a_{\mathbf{k}-}b_{-\mathbf{k}-} = -\frac{\Delta\sqrt{2}\alpha k_{+}(1+i)}{\sqrt{V_Z^2 + 4\alpha^2 k_+^2}} \tag{2.27}$$

and

$$\Delta_{+-}(\mathbf{k}) = \Delta\left(a_{\mathbf{k}+}b_{-\mathbf{k}-} - a_{\mathbf{k}-}b_{-\mathbf{k}+}\right) = \frac{2\Delta V_Z}{\sqrt{V_Z^2 + 4\alpha^2 k_+^2}}, \tag{2.28}$$

allowing to write,

$$\begin{aligned} H_{sup} &= \frac{1}{2}\int d^2k \Big[\Delta_{++}(\mathbf{k})\psi^{\dagger}_{\mathbf{k}+}\psi^{\dagger}_{-\mathbf{k}+} + \Delta_{--}(\mathbf{k})\psi^{\dagger}_{\mathbf{k}-}\psi^{\dagger}_{-\mathbf{k}-} \\ &\quad +\Delta_{+-}(\mathbf{k})\psi^{\dagger}_{\mathbf{k}+}\psi^{\dagger}_{-\mathbf{k}-} + \Delta^*_{++}(\mathbf{k})\psi_{-\mathbf{k}+}\psi_{\mathbf{k}+} + \Delta^*_{--}(\mathbf{k})\psi_{-\mathbf{k}-}\psi_{\mathbf{k}-} + \Delta^*_{+-}(\mathbf{k})\psi_{-\mathbf{k}-}\psi_{\mathbf{k}+}\Big]. \end{aligned} \tag{2.29}$$

we can now define a four-component spinor, $\mathcal{C}^{\dagger}_{\mathbf{k}} = [\psi^{\dagger}_{\mathbf{k}-}, \psi_{-\mathbf{k}-}, \psi^{\dagger}_{\mathbf{k}+}, \psi_{-\mathbf{k}+}]$, such that

$$\mathcal{H}_{sup}(\mathbf{k}) = \begin{bmatrix} \varepsilon_{\mathbf{k}-} & \Delta_{--}(\mathbf{k}) & 0 & 0 \\ \Delta^*_{--}(\mathbf{k}) & -\varepsilon_{\mathbf{k}-} & \Delta^*_{+-}(\mathbf{k}) & 0 \\ 0 & \Delta_{+-}(\mathbf{k}) & \varepsilon_{\mathbf{k}+} & \Delta_{++}(\mathbf{k}) \\ 0 & 0 & \Delta^*_{++}(\mathbf{k}) & -\varepsilon_{\mathbf{k}+} \end{bmatrix}. \tag{2.30}$$

Effective 2×2 Bogoliubov-de Gennes Hamiltonian and topological analysis

In order to obtain a 2×2 Bogoliubov-de Gennes Hamiltonian from the 4×4 Hamiltonian (2.30), we will fold it down by separating the Hilbert space into two subspaces P and Q, corresponding to the two bands. Lets then rewrite the Hamiltonian as

$$\mathcal{H}_{sup}(\mathbf{k}) = \left[\begin{array}{cc|cc} \varepsilon_{\mathbf{k}-} & \Delta_{--}(\mathbf{k}) & 0 & 0 \\ \Delta^*_{--}(\mathbf{k}) & -\varepsilon_{\mathbf{k}-} & \Delta^*_{+-}(\mathbf{k}) & 0 \\ \hline 0 & \Delta_{+-}(\mathbf{k}) & \varepsilon_{\mathbf{k}+} & \Delta_{++}(\mathbf{k}) \\ 0 & 0 & \Delta^*_{++}(\mathbf{k}) & -\varepsilon_{\mathbf{k}+} \end{array}\right] = \left[\begin{array}{c|c} H_P & H_{PQ} \\ \hline H_{QP} & H_Q \end{array}\right], \tag{2.31}$$

where

$$H_P = \begin{bmatrix} \varepsilon_{\mathbf{k}-} & \Delta_{--}(\mathbf{k}) \\ \Delta^*_{--}(\mathbf{k}) & -\varepsilon_{\mathbf{k}-} \end{bmatrix}, \tag{2.32}$$

$$H_Q = \begin{bmatrix} \varepsilon_{\mathbf{k}+} & \Delta_{++}(\mathbf{k}) \\ \Delta^*_{++}(\mathbf{k}) & -\varepsilon_{\mathbf{k}+} \end{bmatrix}, \tag{2.33}$$

and

$$H_{PQ} = \begin{bmatrix} 0 & 0 \\ \Delta^*_{+-}(\mathbf{k}) & 0 \end{bmatrix} = H^\dagger_{QP}. \tag{2.34}$$

Following standard folding down procedure, we can write the effective Hamiltonian for the subspace P as

$$\begin{aligned} \tilde{\mathcal{H}}(\mathbf{k}) &= H_P + H_{PQ}\,(E - H_Q)^{-1}\,H_{QP} \\ &= H_P + \frac{H_{PQ}}{E}\left[1 + \frac{H_Q}{E} + \left(\frac{H_Q}{E}\right)^2 + \cdots\right]. \end{aligned} \tag{2.35}$$

Performing the matrix algebra we obtain,

$$\tilde{\mathcal{H}}(\mathbf{k}) = \begin{bmatrix} \varepsilon_{\mathbf{k}-} & \Delta_{--}(\mathbf{k}) \\ \Delta^*_{--}(\mathbf{k}) & -\varepsilon_{\mathbf{k}-} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \frac{|\Delta_{+-}|^2}{E} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \frac{|\Delta_{+-}|^2 \varepsilon_{\mathbf{k}+}}{E^2} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \frac{|\Delta_{+-}|^2 \varepsilon^2_{\mathbf{k}+}}{E^3} \end{bmatrix} + \cdots \tag{2.36}$$

Now, supposing

$$E \approx \varepsilon_{\mathbf{k}+} = \frac{k^2}{2m} - \mu + \sqrt{V_Z^2 + 4\alpha^2 k_+^2} \tag{2.37}$$

and having in mind that

$$|\Delta_{+-}|^2 = \frac{4\alpha^2 V_Z^2}{V_Z^2 + 4\alpha^2}, \tag{2.38}$$

for small $\mathbf{k}$ we obtain

$$\frac{|\Delta_{+-}|^2}{E} \approx 4\Delta \frac{\Delta}{V_Z - \mu}. \tag{2.39}$$

Considering $\Delta \ll |V_Z - \mu|$ we can safely keep only the first term of Eq. (2.36), obtaining

$$\tilde{\mathcal{H}}(\mathbf{k}) \approx \begin{bmatrix} \varepsilon_{\mathbf{k}-} & \Delta_{--}(\mathbf{k}) \\ \Delta^*_{--}(\mathbf{k}) & -\varepsilon_{\mathbf{k}-} \end{bmatrix}. \tag{2.40}$$

With the above we can replace Eq. (2.40) into Eq. (2.29) to obtain

$$H = \frac{1}{2}\int d^2k \left[\varepsilon_{\mathbf{k}-}\psi^\dagger_{\mathbf{k}-}\psi_{\mathbf{k}-} + \Delta_{--}(\mathbf{k})\psi^\dagger_{\mathbf{k}-}\psi^\dagger_{-\mathbf{k}-} + \Delta^*_{--}(\mathbf{k})\psi_{-\mathbf{k}-}\psi_{\mathbf{k}-}\right]. \tag{2.41}$$

Dropping the subindex, for simplicity, the Hamiltonian above can be written now in the Bogoliubov-de Gennes form, by reducing the four-component Nambu's operator to two-component one, $\mathcal{C}_{\mathbf{k}}^{\dagger} = [\psi_{\mathbf{k}}^{\dagger}, \psi_{-\mathbf{k}}]$, we can write

$$H = \frac{1}{2} \int d^2 k \mathcal{C}_{\mathbf{k}}^{\dagger} \mathcal{H}_{BdG}(\mathbf{k}) \mathcal{C}_{\mathbf{k}}, \tag{2.42}$$

where

$$\mathcal{H}_{BdG}(\mathbf{k}) = \begin{bmatrix} \varepsilon(\mathbf{k}) & \tilde{\Delta}_{\mathbf{k}}^{*} \\ \tilde{\Delta}_{\mathbf{k}} & -\varepsilon(\mathbf{k}) \end{bmatrix}, \tag{2.43}$$

with

$$\varepsilon(\mathbf{k}) = \frac{k^2}{2m} - \mu - \sqrt{V_Z^2 + 4\alpha^2 k_+^2}. \tag{2.44}$$

and

$$\tilde{\Delta}_{\mathbf{k}}^{*} = \Delta_{--}(\mathbf{k}) = -\frac{\Delta \sqrt{2}\alpha k_+ (1+i)}{\sqrt{V_Z^2 + 4\alpha^2 k_+^2}}. \tag{2.45}$$

One first important observation is that $\tilde{\Delta}_{\mathbf{k}} = -\tilde{\Delta}_{-\mathbf{k}}$, so that the superconductor pairing has a node at $k = 0$.

In order to analyze the topology of the Hamiltonian above, let us map it onto a unity sphere by writing the Bogoliubov-de Gennes Hamiltonian (2.43) as

$$\begin{aligned} \mathcal{H}_{BdG}(\mathbf{k}) &= \varepsilon(\mathbf{k}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \text{Re } \tilde{\Delta}_{\mathbf{k}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \text{Im } \tilde{\Delta}_{\mathbf{k}} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ &= \text{Re } \tilde{\Delta}_{\mathbf{k}} \sigma_x + \text{Im } \tilde{\Delta}_{\mathbf{k}} \sigma_y + \varepsilon(\mathbf{k}) \sigma_z \\ &= \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \end{aligned} \tag{2.46}$$

where, we have defined,

$$\mathbf{h}(k) = h_x(\mathbf{k})\hat{\mathbf{x}} + h_y(\mathbf{k})\hat{\mathbf{y}} + h_z(\mathbf{k})\hat{\mathbf{z}} \tag{2.47}$$

and

$$\boldsymbol{\sigma} = \hat{\sigma}_x \hat{\mathbf{x}} + \hat{\sigma}_y \hat{\mathbf{y}} + \hat{\sigma}_z \hat{\mathbf{z}}, \tag{2.48}$$

with $h_x(\mathbf{k}) = \text{Re } \tilde{\Delta}_{\mathbf{k}}$, $h_y(\mathbf{k}) = \text{Im } \tilde{\Delta}_{\mathbf{k}}$ and $h_z(\mathbf{k}) = \varepsilon(\mathbf{k})$. We can also define an unity vector

$$\hat{\mathbf{h}}(\mathbf{k}) = \frac{\mathbf{h}(\mathbf{k})}{|\mathbf{h}(\mathbf{k})|}. \tag{2.49}$$

Notice that

$$|\mathbf{h}(\mathbf{k})| = \sqrt{h_x^2+h_y^2+h_z^2} = \sqrt{\varepsilon(\mathbf{k})^2 + \frac{4\Delta^2\alpha^2k_+^2}{V_Z^2+4\alpha^2k_+^2}} \tag{2.50}$$

then

$$\hat{h}_x(\mathbf{k}) = \frac{-\frac{\Delta\sqrt{2}\alpha k_+}{\sqrt{V_Z^2+4\alpha^2k_+^2}}}{\sqrt{\varepsilon(\mathbf{k})^2+\frac{4\Delta^2\alpha^2k_+^2}{V_Z^2+4\alpha^2k_+^2}}} \tag{2.51}$$

$$\hat{h}_y(\mathbf{k}) = \frac{-\frac{\Delta\sqrt{2}\alpha k_+}{\sqrt{V_Z^2+4\alpha^2k_+^2}}}{\sqrt{\varepsilon(\mathbf{k})^2+\frac{4\Delta^2\alpha^2k_+^2}{V_Z^2+4\alpha^2k_+^2}}} \tag{2.52}$$

$$\hat{h}_z(\mathbf{k}) = \frac{\varepsilon(\mathbf{k})}{\sqrt{\varepsilon(\mathbf{k})^2+\frac{4\Delta^2\alpha^2k_+^2}{V_Z^2+4\alpha^2k_+^2}}}. \tag{2.53}$$

From Eq. (2.44) it is easy to see that $\hat{h}_{x,y} \to 0$ when $k \to 0, \infty$. Therefore we can write, $\hat{h}(\mathbf{k} \to 0) = s_0\hat{\mathbf{z}}$ and $\hat{h}(\mathbf{k} \to \infty) = s_\infty\hat{\mathbf{z}}$, where

$$s_0 = \lim_{k\to 0}\hat{h}_z(k) = \frac{-\mu - V_Z}{|\mu+V_Z|} = -1 \ \ (\text{if } \mu+V_z>0). \tag{2.54}$$

and

$$s_\infty = \lim_{k\to\infty}\hat{h}_z(k) = \lim_{k\to\infty}\frac{k^2/2m-2\alpha|k_+|}{|k^2/2m-2\alpha|k_+||} = 1. \tag{2.55}$$

Small-k: effective 1D behavior

Lets analyse the Hamiltonian in the small-$\mathbf{k}$ regime, where $k^2/2m \ll \mu$ and $4\alpha^2k^2 \ll V_Z$. In this regime we can take (up to first order in $\mathbf{k}_+$) $\varepsilon(\mathbf{k}) \approx -\mu - V_Z$ so that Eq. (2.43) becomes

$$\mathcal{H}_{BdG}(k_+) = \begin{bmatrix} -\mu - V_Z & \hat{\Delta}^* k_+ \\ \hat{\Delta}\ k_+ & \mu + V_Z \end{bmatrix}, \tag{2.56}$$

where $\hat{\Delta} = \sqrt{2}\Delta\alpha(1+i)/V_Z$. We notice that this Hamiltonian is one dimensional. It depends only on k_+. The Hamiltonian (2.56) has the same form of Eq. (1.23) for the Kitaev model for small-k.

3

Symmetry of the topological superconductors Hamiltonians

3.1 Particle-hole symmetry of the Bogoliubov-de Gennes Hamiltonian

In this section we will study some symmetry properties of the Bogoliubov-de Gennes Hamiltonian of the form (1.23), but now for arbitrary (one, two or three) dimensions [that is, the we replace k in Eq. (1.23) by a vector $\mathbf{k}$],

$$\mathcal{H}(\mathbf{k}) = \begin{bmatrix} \varepsilon(\mathbf{k}) & \Delta_{\mathbf{k}}^{*} \\ \Delta_{\mathbf{k}} & -\varepsilon(\mathbf{k}) \end{bmatrix}, \tag{3.1}$$

and discuss how they are important for the physical properties of the system. It is convenient to write

$$\varepsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu, \tag{3.2}$$

and

$$\Delta_{\mathbf{k}} = \Delta_0 f(\mathbf{k}), \tag{3.3}$$

where μ is the chemical potential, and Δ_0 is a complex constant and $f(\mathbf{k})$ is a real function. For a p-wave pairing $f(\mathbf{k})$ is a odd function of $\mathbf{k}$. Lets start by remembering that the Bolgoliubov-de Gennes Hamiltonian (3.1) is written in the Nambu's notation by the definition of the spinors

$$\mathcal{C}_{\mathbf{k}}^{\dagger} = \begin{pmatrix} \psi_{\mathbf{k}}^{\dagger} & \psi_{-\mathbf{k}} \end{pmatrix}, \tag{3.4}$$

and

$$\mathcal{C}_{\mathbf{k}} = \begin{pmatrix} \psi_{\mathbf{k}} \\ \psi^{\dagger}_{-\mathbf{k}} \end{pmatrix}. \tag{3.5}$$

Notice that

$$\sigma_x \mathcal{C}_{\mathbf{k}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_{\mathbf{k}} \\ \psi^{\dagger}_{-\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \psi^{\dagger}_{-\mathbf{k}} \\ \psi_{\mathbf{k}} \end{pmatrix} = \left(\mathcal{C}^{\dagger}_{-\mathbf{k}}\right)^{T}. \tag{3.6}$$

Notice that in this operation $\mathbf{k} \to -\mathbf{k}$. Since Eq. (3.4) and (3.5) corresponds, respectively to the creation and annihilation (creation of a hole) of a Bogoliubov-type of particle, Eq. 3.6 suggests a particle-hole symmetry of the form

$$\Xi = \sigma_x K, \tag{3.7}$$

where K is a complex conjugate operators and σ_x in the x-component of the Pauli matrix. Notice that

$$\Xi^2 = +1. \tag{3.8}$$

showing the Ξ is a unitary operator. Lets return to the Bogoliubov-de Gennes Hamiltonian (2.43). For $\Delta_{\mathbf{k}} = 0$ we have

$$\mathcal{H}_0(\mathbf{k}) = \begin{bmatrix} \varepsilon(\mathbf{k}) & 0 \\ 0 & -\varepsilon(\mathbf{k}) \end{bmatrix}. \tag{3.9}$$

Applying the particle-hole symmetry operator we obtain

$$\Xi \mathcal{H}_0(\mathbf{k}) \Xi^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{bmatrix} \varepsilon(\mathbf{k}) & 0 \\ 0 & -\varepsilon(\mathbf{k}) \end{bmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{bmatrix} -\varepsilon(\mathbf{k}) & 0 \\ 0 & \varepsilon(\mathbf{k}) \end{bmatrix} = -\mathcal{H}_0(\mathbf{k}). \tag{3.10}$$

Since in the particle hole transformation (3.6) $\mathbf{k} \to -\mathbf{k}$ we should expect the same in the transformation (3.10). Indeed, since $\varepsilon_{\mathbf{k}} - \varepsilon_{-\mathbf{k}}$, Eq. (3.10) can be written as

$$\Xi \mathcal{H}_0(\mathbf{k}) \Xi^{-1} = -\mathcal{H}_0(-\mathbf{k}). \tag{3.11}$$

This shows that in the absence of superconductivity ($\Delta_{\mathbf{k}} = 0$) the Bogoliubov-de Gennes has an intrinsic particle-hole symmetry expressed by Eq. (3.11).

In the general case of $\Delta_{\mathbf{k}} \neq 0$, the particle-hole operation gives,

$$\Xi \mathcal{H}(\mathbf{k}) \Xi^{-1} = \begin{pmatrix} 0 & K \\ K & 0 \end{pmatrix} \begin{bmatrix} \varepsilon(\mathbf{k}) & \Delta^{*}_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & -\varepsilon(\mathbf{k}) \end{bmatrix} \begin{pmatrix} 0 & K \\ K & 0 \end{pmatrix} = \begin{bmatrix} -\varepsilon(\mathbf{k}) & \Delta^{*}_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & \varepsilon(\mathbf{k}) \end{bmatrix}. \tag{3.12}$$

If we want the Eq. (3.12) to obey the same intrinsic particle-hole symmetry as expressed in

Eq. (3.11), i.e.

$$\Xi\mathcal{H}(\mathbf{k})\Xi^{-1} = -\mathcal{H}(-\mathbf{k}), \tag{3.13}$$

we see that $\Delta_{\mathbf{k}}$ must be of odd symmetry,

$$\Delta_{\mathbf{k}} = -\Delta_{-\mathbf{k}}. \tag{3.14}$$

One of the most important consequence of the particle-hole symmetry (3.13) is that each eigenstate with energy $+E_n(\mathbf{k})$ has a partner with energy $-E_n(\mathbf{k})$. Suppose $|u_{n,\mathbf{k}}\rangle$ is an egenstate of $H(\mathbf{k})$ with energy $E_n(\mathbf{k})$, i. e., $H(\mathbf{k})|u_{n,\mathbf{k}}\rangle = E_n(\mathbf{k})|u_{n,\mathbf{k}}\rangle$. Then,

$$\Xi H(\mathbf{k})\Xi^{-1}\Xi|u_{n,\mathbf{k}}\rangle = \Xi E_n(\mathbf{k})\Xi^{-1}\Xi|u_{n,\mathbf{k}}\rangle = E_n(-\mathbf{k})\Xi|u_{n,\mathbf{k}}\rangle \tag{3.15}$$

From Eq. (3.13) we can write

$$H(-\mathbf{k})\Xi|u_{n,\mathbf{k}}\rangle = -E_n(-\mathbf{k})\Xi|u_{n,\mathbf{k}}\rangle \to H(\mathbf{k})\Xi|u_{n,\mathbf{k}}\rangle = -E_n(\mathbf{k})\Xi|u_{n,\mathbf{k}}\rangle, \tag{3.16}$$

where $\Xi|u_{n,\mathbf{k}}\rangle$ is the particle-hole partiner of the state $|u_{n,\mathbf{k}}\rangle$.

To see the structure of the eigenstates associated to these energies, let us diagonalize the Hamiltonian (3.1) by introducing the Bogoliubov transformation,

$$\alpha_{\pm}(\mathbf{k}) = u_{\pm}(\mathbf{k})c_{\mathbf{k}} + v_{\pm}(\mathbf{k})c^{\dagger}_{-\mathbf{k}} \tag{3.17a}$$
$$\alpha^{\dagger}_{\pm}(\mathbf{k}) = u^{*}_{\pm}(\mathbf{k})c^{\dagger}_{\mathbf{k}} + v^{*}_{\pm}(\mathbf{k})c_{-\mathbf{k}}, \tag{3.17b}$$

such that in terms of these operators the Hamiltonian (3.1) acquires the form

$$\mathcal{H}(\mathbf{k}) = \sum_{\mathbf{k}} E_{\pm}(\mathbf{k})\alpha^{\dagger}_{\pm}(\mathbf{k})\alpha_{\pm}(\mathbf{k}), \tag{3.18}$$

where the energies are easily obtained and are

$$E_{\pm}(\mathbf{k}) = \pm\sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2} = \pm E(\mathbf{k}), \tag{3.19}$$

with $E(\mathbf{k}) = \sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}$. This means that each positive energy has its negative counterpart. With a little more we obtain,

$$u_{\pm}(\mathbf{k}) = \frac{\Delta_0}{|\Delta_0|}\sqrt{\frac{E_{\pm}(\mathbf{k}) + \varepsilon_{\mathbf{k}}}{2E_{\pm}(\mathbf{k})}} \tag{3.20}$$

and

$$v_{\pm}(\mathbf{k}) = \frac{E_{\pm}(\mathbf{k}) - \varepsilon_{\mathbf{k}}}{\Delta^{*}_{\mathbf{k}}}u_{\pm}(\mathbf{k}) \tag{3.21}$$

Since $\varepsilon_{\mathbf{k}} = \varepsilon_{-\mathbf{k}}$ and we suppose $\Delta_{\mathbf{k}} = -\Delta_{-\mathbf{k}}$, then

$$E_{\pm}(\mathbf{k}) = \pm E(-\mathbf{k}) = \pm E(-\mathbf{k}) = E_{\pm}(-\mathbf{k}), \tag{3.22}$$

$$u_{\pm}(-\mathbf{k}) = \frac{\Delta_0}{|\Delta_0|}\sqrt{\frac{E_{\pm}(-\mathbf{k}) + \varepsilon_{-\mathbf{k}}}{2E_{\pm}(-\mathbf{k})}} = u_{\pm}(\mathbf{k}) \tag{3.23}$$

and

$$v_{\pm}(-\mathbf{k}) = \frac{E_{\pm}(-\mathbf{k}) - \varepsilon_{-\mathbf{k}}}{\Delta^*_{-\mathbf{k}}} u_{\pm}(-\mathbf{k}) = -v_{\pm}(\mathbf{k}) \tag{3.24}$$

Eqs. (3.23) and (3.24) tells us that at $\mathbf{k} = 0$ $u_{\pm}(0) = u_{0\pm}$ and $v_{\pm}(0) = 0$. Therefore the operator $\alpha_{\pm} \sim c_0$ and $\alpha^{\dagger}_{\pm} \sim c^{\dagger}_0$ indicating that there are no Bogoliubov quasi particles (or Cooper pairs) at $\mathbf{k} = 0$.

However, a Bogoliubov quasi particle can be created with an infinitesimal energy. From Eq. (3.19) we can identify whether the system is gapped or not. Considere a model where

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m^*} - \mu - V_Z, \tag{3.25}$$

where m^* is the electron effective mass and V_Z can results from some external field. We see them that the system is fully gapped for all $\mu + V_Z > 0$. We will see however that the $\mu + V_Z > 0$ and $\mu + V_Z < 0$ constitutes two very distinct topological phases, separated by the point $\mu + V_Z = 0$. The passage from one to the other phase constitutes a topological quantum phase transition.

3.1.1 Compacting the notation

Lets return to the Bogoliubov-de Gennes Hamiltonian (3.1) and write it as

$$\mathcal{H}(\mathbf{k}) = \begin{bmatrix} \varepsilon(\mathbf{k}) & \mathtt{Re}\ \Delta_{\mathbf{k}} - i\mathtt{Im}\ \Delta_{\mathbf{k}} \\ \mathtt{Re}\ \Delta_{\mathbf{k}} + i\mathtt{Im}\ \Delta_{\mathbf{k}} & -\varepsilon(\mathbf{k}) \end{bmatrix} = \mathtt{Re}\ \Delta_{\mathbf{k}}\boldsymbol{\sigma}_x + \mathtt{Im}\ \Delta_{\mathbf{k}}\boldsymbol{\sigma}_y + \varepsilon_{\mathbf{k}}\boldsymbol{\sigma}_z. \tag{3.26}$$

where $\boldsymbol{\sigma}_i$'s are the components of the Pauli matrix $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_x, \sigma_y, \sigma_z)$. Defining now a vector

$$\boldsymbol{h}(\mathbf{k}) = (h_x, h_y, h_z) = (\mathtt{Re}\ \Delta_{\mathbf{k}}, \mathtt{Im}\ \Delta_{\mathbf{k}}, \varepsilon_{\mathbf{k}}) \tag{3.27}$$

we can write the Hamiltonian in a formidable form

$$\mathcal{H}(\mathbf{k}) = \boldsymbol{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \tag{3.28}$$

This has the same form of a Hamiltonian describing a magnetic moment in a magnetic field. Here however $\boldsymbol{h}(\mathbf{k})$ plays the role of a momentum dependent magnetic field acting on the pseudo spin $\boldsymbol{\sigma}$. We still define a unity vector,

$$\hat{\boldsymbol{h}}(\mathbf{k}) = \frac{\boldsymbol{h}(\mathbf{k})}{|\boldsymbol{h}(\mathbf{k})|} = \left[\frac{h_x(\mathbf{k})}{|\boldsymbol{h}(\mathbf{k})|}, \frac{h_y(\mathbf{k})}{|\boldsymbol{h}(\mathbf{k})|}, \frac{h_z(\mathbf{k})}{|\boldsymbol{h}(\mathbf{k})|}\right]. \tag{3.29}$$

Notice that

$$|\boldsymbol{h}(\mathbf{k})| = \sqrt{\varepsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} = E(\mathbf{k}), \tag{3.30}$$

then

$$\hat{\boldsymbol{h}}(\mathbf{k}) = \frac{1}{\sqrt{\varepsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}}(\texttt{Re}\ \Delta_{\mathbf{k}}, \texttt{Im}\ \Delta_{\mathbf{k}}, \varepsilon_{\mathbf{k}}). \tag{3.31}$$

The definition of $\hat{\boldsymbol{h}}(\mathbf{k})$ provides a mapping of the Hamiltonian on the surface of a unity Bloch sphere. In this way, as $\mathbf{k}$ varies continuously, the vector $\hat{\boldsymbol{h}}(\mathbf{k})$ travels on the surface of the sphere. We can define classes of Hamiltonians based upon the type of movements of the vector $\hat{\boldsymbol{h}}(\mathbf{k})$ when $\mathbf{k}$ is continuously varied. This type of classification of Hamiltonian is called *topological classification.* We finally add that the Hamiltonian (3.28) can also be rewritten as

$$\mathcal{H}(\mathbf{k}) = E(\mathbf{k})\hat{\boldsymbol{h}}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \tag{3.32}$$

Topological invariant

Suppose $\Delta_{\mathbf{k}}$ is a odd function of $\mathbf{k}$ and $\varepsilon_{\mathbf{k}}$ is of the type of the Eq. (3.25). In this case we see that

$$\lim_{\mathbf{k}\to 0} \varepsilon_{\mathbf{k}} = -\mu - V_Z \tag{3.33}$$

and

$$\lim_{\mathbf{k}\to 0} \Delta_{\mathbf{k}} = 0 \tag{3.34}$$

The last expression follows directly from the odd parity of $\Delta_{\mathbf{k}}$. Suppose, in addition that

$$\lim_{k\to\infty} \Delta_{\mathbf{k}} < \infty \tag{3.35}$$

independently of the direction of $\mathbf{k}$. We can see therefore that

$$\lim_{\mathbf{k}\to 0} \hat{\boldsymbol{h}}_{x,y}(\mathbf{k}) = \lim_{k\to\infty} \hat{\boldsymbol{h}}_{x,y}(\mathbf{k}) = 0, \tag{3.36}$$

so that $\hat{\boldsymbol{h}}(\mathbf{k})$ points along the z-direction in this two limits.

3.1.2 Topological invariant and the Pfaffian in periodic systems

There is another interesting manner of analyzing the Bogoliubov-de Gennes Hamiltonians[?, 19]. It is based on the theory of the Pfaffians and determinants. Lets return to the Bogoliubov Hamiltonian (3.1) that under particle-hole symmetry transformation transforms as (3.13). In a periodic system, where the Bloch wave functions satisfy $|u_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r})\rangle = |u_{n,\mathbf{k}}(\mathbf{r})\rangle$, we may wonder whether if there are specific momenta $\mathbf{\Lambda}$ at which the Hamiltonian (3.1) is symmetric under the transformation $\mathbf{k} \to -\mathbf{k}$. This requirements can be written for the momentum $\mathbf{\Lambda}$

$$H(-\mathbf{\Lambda}) = \mathcal{H}(\mathbf{\Lambda}), \tag{3.37}$$

and from the periodicity of the of the system we also have

$$E_{n,\mathbf{\Lambda}+\mathbf{G}} = E_{n,\mathbf{\Lambda}}. \tag{3.38}$$

Therefore, from Eq. (3.37) that

$$E_{n,-\mathbf{\Lambda}}|u_{n,\mathbf{\Lambda}}(\mathbf{r})\rangle = H(-\mathbf{\Lambda})|u_{n,\mathbf{\Lambda}}(\mathbf{r})\rangle = H(\mathbf{\Lambda})|u_{n,\mathbf{\Lambda}}(\mathbf{r})\rangle = E_{n,\mathbf{\Lambda}}|u_{n,\mathbf{\Lambda}}(\mathbf{r})\rangle, \tag{3.39}$$

so that $E_{n,-\mathbf{\Lambda}} = E_{n,\mathbf{\Lambda}}$. From Eq. (3.38) we also have $E_{n,-\mathbf{\Lambda}} = E_{n,-\mathbf{\Lambda}+G} = E_{n,\mathbf{\Lambda}}$. Since from the toroidal structure of the periodic boundary condition we have $-\mathbf{\Lambda} + \mathbf{G} = \mathbf{\Lambda}$. Leading to $\mathbf{\Lambda} = 0$ and $\mathbf{\Lambda} = \mathbf{G}/2$.

Lets now define an anti-symmetric matrix $\mathbf{w}(\mathbf{\Lambda})$ as

$$\mathbf{w}(\mathbf{\Lambda}) = H(\mathbf{\Lambda})\sigma_x \tag{3.40}$$

Notice that

$$\mathbf{w}(\mathbf{\Lambda})^T = \sigma_x H^T(\mathbf{\Lambda}). \tag{3.41}$$

From the definition of the particle-hole symmetry operator, $\Xi = K\sigma_x$, and from (3.13) we notice that the Bogoliubov-de Gennes Hamiltonian obey

$$\sigma_x H(\mathbf{\Lambda})\sigma_x = -H^T(-\mathbf{\Lambda}). \tag{3.42}$$

Then the Eq. (3.41) becomes

$$\mathbf{w}^T(\mathbf{\Lambda}) = -\sigma_x\sigma_x H(-\mathbf{k})\sigma_x = -H(-\mathbf{\Lambda})\sigma_x = -H(\mathbf{\Lambda})\sigma_x = -\mathbf{w}(\mathbf{\Lambda}). \tag{3.43}$$

Where we have used Eq. (3.37) in the expression above. Eq. (3.43) shows that $\mathbf{w}(\mathbf{\Lambda})$ is indeed antisymmetric. Since $\Delta_{\mathbf{k}}$ is an odd function of $\mathbf{k}$ then in order for $H(-\mathbf{k}) = H(\mathbf{k})$ then $\Delta(\mathbf{\Lambda}) = 0$. Explicitly from Eq. (3.1)

$$\mathbf{w}(\mathbf{\Lambda}) = \begin{bmatrix} \varepsilon(\mathbf{\Lambda}) & 0 \\ 0 & -\varepsilon(\mathbf{\Lambda}) \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & \varepsilon(\mathbf{\Lambda}) \\ -\varepsilon(\mathbf{\Lambda}) & 0 \end{bmatrix}. \tag{3.44}$$

The Pfaffian reads

$$\mathrm{Pf}^2[\mathbf{w}(\mathbf{\Lambda})] = \det[\mathbf{w}(\mathbf{\Lambda})] = \varepsilon^2(\mathbf{\Lambda}). \tag{3.45}$$

The topological invariant ν is defined as

$$(-1)^\nu = \prod_i \frac{\mathrm{Pf}[\mathbf{w}(\mathbf{\Lambda}_i)]}{\sqrt{\det[\mathbf{w}(\mathbf{\Lambda}_i)]}} = \prod_i \mathrm{sign}\{\mathrm{Pf}[\mathbf{w}(\mathbf{\Lambda}_i)]\}. \tag{3.46}$$

We notice that $\nu = 0, 1$ modulo 2. $\nu = 0$ corresponds to a topologically trivial phase while $\nu = 1$ indicates a topologically non-trivial phase.

Applying these idea to the 1D Kitaev model written is the Bogoliubov-de Gennes form (1.23) with $\varepsilon_{\mathbf{k}} = -[\mu + t\cos(ka)]$ according to Eq. (1.20). The invariant momenta are $\Lambda_1 = 0$ and $\Lambda_2 = \pi/a$, at which we have $\varepsilon_0 = -(\mu + t)$ and $\varepsilon_\pi = -(\mu - t)$. Then

$$(-1)^\nu = \mathrm{sign}[\varepsilon_0]\mathrm{sign}[\varepsilon_\pi] = \frac{\varepsilon_0}{|\varepsilon_0|}\frac{\varepsilon_\pi}{|\varepsilon_\pi|} = \frac{\mu + t}{|\mu + t|}\frac{\mu - t}{|\mu - t|} = \frac{\mu^2 - t^2}{|\mu^2 - t^2|} = s_0 s_\pi \tag{3.47}$$

We conclude that $\nu = 0$ if $|\mu| > t$, corresponding to the (strong pairing) or trivial phase and $\nu = 1$ for $|\mu| < t$, corresponding to the (weak pairing) or topological phase. This is the same conclusion we have obtained in by Eq. (1.62) at the end of Sec. 1.0.3.

3.1.3 Dirac-like equation and Majorana bound states

Let us analyse the eigenvector-equation (3.1) at the low-momenta regime ($\mathbf{k} \to 0$) or, equivalently assuming $m \to \infty$. At this limit we can make

$$\varepsilon_{\mathbf{k}} = \frac{h^2 k^2}{2m} - \mu - V_Z \approx -(\mu + V_Z). \tag{3.48}$$

Here we will need to specify the form of $\Delta_{\mathbf{k}}$ for a 2D system. To avoid it for now we will instead consider the 1D case, for which, from odd parity of $\Delta_{\mathbf{k}}$ we can assume

$$\Delta(k_x) = \Delta_0 k_x. \tag{3.49}$$

Then we can write the Bogoliubov-de Gennes (1.23) as

$$\mathcal{H}(k_x) = \begin{pmatrix} -\mu - V_Z & \Delta_0^* k_x \\ \Delta_0 k_x & \mu + V_Z \end{pmatrix} = (\mathrm{Re}\Delta_0)p_x\sigma_x + (\mathrm{Im}\Delta_0)p_x\sigma_y + \tilde{\mu}\sigma_z. \tag{3.50}$$

If we can make Δ_0 real, then the equation above becomes

$$\mathcal{H}(k_x) = (\mathrm{Re}\Delta_0)p_x\sigma_x\tilde{\mu}\sigma_z = \mathtt{v}p_x\sigma_x + m\sigma_z, \tag{3.51}$$

This equations has precisely the form of the Dirac Hamiltonian[20], with the velocity $\mathtt{v} = \Delta_0$ playing the role of the light speed and the mass $\tilde{\mu} = \mu + V_Z$, corresponding to the mass of the quasi-particles (not to be confused with m, the mass of the electrons).

We can pass Eq. (3.51) to space position coordinate by writing $k = -id/dx$ and we will assume that $\tilde{\mu} = \mu + V_Z \to \tilde{\mu}(x)$. With that the the eigenvalue equation for Eq. (1.23) becomes

$$\begin{pmatrix} -\tilde{\mu}(x) & -i\Delta_0 \frac{d}{dx} \\ -i\Delta_0 \frac{d}{dx} & \tilde{\mu}(x) \end{pmatrix} \begin{pmatrix} u(x) \\ v(x) \end{pmatrix} = E \begin{pmatrix} u(x) \\ v(x) \end{pmatrix} = i\frac{d}{dt} \begin{pmatrix} u(x) \\ v(x) \end{pmatrix}. \tag{3.52}$$

Explictly, we have

$$i\frac{du}{dt} = -i\Delta_0 \frac{dv}{dx} - \tilde{\mu}(x)u, \tag{3.53}$$

$$i\frac{dv}{dt} = -i\Delta_0 \frac{du}{dx} + \tilde{\mu}(x)v. \tag{3.54}$$

The set of equation (3.53-3.54) has the form of the Dirac equation for the spinor (u, v). We now seek for zero-energy solutions for the Eq. (3.53). For the zero-energy case we have to solve the set of equations

$$i\Delta_0 \frac{dv}{dx} + \tilde{\mu}(x)u = 0, \tag{3.55}$$

$$i\Delta_0 \frac{du}{dx} - \tilde{\mu}(x)v = 0. \tag{3.56}$$

Suppose

$$\Psi(x) = \begin{pmatrix} u(x) \\ v(x) \end{pmatrix} \tag{3.57}$$

is a solution of the Eq (3.51) then we can write,

$$\left[i\Delta_0 \frac{d}{dx}\sigma_x - \tilde{\mu}(x)\sigma_z \right] \Psi(x) = 0 \tag{3.58}$$

Multiplying from the left by σ_x we have

$$\begin{aligned} \sigma_x \left[-i\Delta_0 \frac{d}{dx}\sigma_x + \tilde{\mu}(x)\sigma_z \right] \Psi(x) &= 0 \\ -i\Delta_0 \frac{d\Psi(x)}{dx} - i\tilde{\mu}(x)\sigma_y \Psi(x) &= 0. \end{aligned} \tag{3.59}$$

Or

$$\frac{d\Psi(x)}{dx} = \frac{\tilde{\mu}(x)}{\Delta_0}\sigma_y \Psi(x). \tag{3.60}$$

We notice that $\Psi(x)$ should be and eigenstate of σ_y such that $\sigma_y \Psi_\pm(x) = \pm\Psi_\pm(x)$. Then we can write

$$\frac{d\Psi_\pm(x)}{dx} = \pm\frac{\tilde{\mu}(x)}{\Delta_0}\Psi \pm (x). \tag{3.61}$$

Lets try the solution

$$\Psi_{\pm}(x) = \mathcal{A}\phi_{\pm} e^{\pm\frac{1}{\Delta_0}\int_0^x \tilde{\mu}(x')dx'} = \frac{\mathcal{A}}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix} e^{\pm\frac{1}{\Delta_0}\int_0^x \tilde{\mu}(x')dx'}, \tag{3.62}$$

where $\phi_{\pm} = (1, \pm i)$ is the eigenstates of σ_y with eigenvalues ± 1 and $\mathcal{A}$ a normalization constant. To check if this is indeed a solution, can derive it and find,

$$\frac{d\Psi_{\pm}(x)}{dx} = -\frac{\mathcal{A}\tilde{\mu}(x)}{\Delta_0} \begin{pmatrix} 1 \\ \pm i \end{pmatrix} e^{\pm\frac{1}{\Delta_0}\int_0^x \tilde{\mu}(x')dx'} = \pm\frac{m(x)}{\Delta_0}\Psi_{\pm}(x). \tag{3.63}$$

Showing that expression (3.63) is indeed a solution of the Eq. (3.61). We see here that if $\tilde{\mu}(x)$ is positive as $\to \infty$ the the only normalizable solution is $\Psi_{\pm}(x)$. So we will pick this one as our solution. We can introduce a global phase $e^{i\pi/4}$ in Ψ_-, such that

$$\Psi_- = e^{i\pi/4}\frac{\mathcal{A}}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{-\frac{1}{\Delta_0}\int_0^x \tilde{\mu}(x')dx'} = \frac{\mathcal{A}}{2} \begin{pmatrix} 1+i \\ 1-i \end{pmatrix} e^{-\frac{1}{\Delta_0}\int_0^x \tilde{\mu}(x')dx'} = \begin{pmatrix} u \\ v \end{pmatrix}, \tag{3.64}$$

where

$$u = (1+i)\frac{\mathcal{A}}{2} e^{-\frac{1}{\Delta_0}\int_0^x \tilde{\mu}(x')dx'} \tag{3.65}$$

and

$$v = (1-i)\frac{\mathcal{A}}{2} e^{-\frac{1}{\Delta_0}\int_0^x \tilde{\mu}(x')dx'}. \tag{3.66}$$

Notice that $u = v^*$. This is interesting because it suggests already a natural particle/antiparticle relation. Indeed, according to Dirac relativistic theory, while the wave function Ψ_- describes a particle, the charge-conjugate wave function Ψ_-^C describes its antiparticle. The relation between the particle and its antiparticle wave function is given by

$$\Psi_-^C = S_C \Psi_-^*, \tag{3.67}$$

where $S_C = \sigma_x$. With this we obtain

$$\Psi_-^C = \sigma_x \Psi^* = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u^* \\ v^* \end{pmatrix} = \begin{pmatrix} v^* \\ u^* \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} = \Psi_-. \tag{3.68}$$

The equation (3.68) shows that, indeed, the solution for the particle corresponds also to the solution for the antiparticle. This is one of the most striking property of a Majorana Fermion.

Another way to see this interesting property is by writing in the operator that annihilates the state Ψ_- in terms of the electron creation and annihilation operators as [see Eqs. (3.17)]

$$\gamma_0 = \mathcal{A} e^{i\pi/4} e^{-\frac{1}{\Delta_0}\int_0^x \tilde{\mu}(x')dx'} \frac{(c - ic^\dagger)}{\sqrt{2}}. \tag{3.69}$$

Note that

$$e^{i\pi/4}\frac{(c - ic^\dagger)}{\sqrt{2}} = \frac{1}{2}(1+i)(c - ic^\dagger) = \frac{1}{2}\left[(1+i)c + (1-i)c^\dagger\right]. \tag{3.70}$$

From the equation above we easily note that $[\gamma_0, \gamma_0]_+ = 1$, which corresponds to a fermion operator. Moreover, $\gamma_0 = \gamma_0^\dagger$, which is a translation of the property that a particle being its own antiparticle in terms Majorana creation operators. This second quantization language is equivalent to (3.68).

4

Geometrical description and Chern number

4.1 Geometrical phase

Consider a time independent Hamiltonian but dependent of a certain parameter $\mathbf{k}$, which in the present case is the linear momentum. In quantum mechanics we are interested in solving the Shrödinger equation

$$H(\mathbf{k})|\Psi(\mathbf{k})\rangle = E(\mathbf{k})|\Psi(\mathbf{k})\rangle, \tag{4.1}$$

where $E(\mathbf{k})$ is the eigenvalues associated to the eigenvector $|\Psi(\mathbf{k})\rangle$, supposed to be normalized. Lets take, for example, the band n denoted by $|\Psi_n(\mathbf{k})\rangle$, of the referred Hamiltonian. A given state of the Hamiltonian can be specified by its modulus and a phase. In general the phase plays no important role. Here, however it is an important ingredient and that it is useful to characterize fundamental physics of the system.

Consider two ground states $|\Psi_n(\mathbf{k}_1)\rangle$ and $|\Psi_n(\mathbf{k}_2)\rangle$. The projection of one of these states onto the other can be written as

$$\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle = |\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle|e^{i\Delta\phi_{12}}, \tag{4.2}$$

where $\Delta\phi_{12}$ is the phase difference between them. From the expression above we can write

$$e^{-i\Delta\phi_{12}} = \frac{\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle}{|\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle|}. \tag{4.3}$$

Taking the logarithm from both sides of the equation above we get

$$\begin{aligned} -i\Delta\phi_{12} &= \ln\left[\frac{\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle}{|\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle|}\right] \\ &= \ln\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle - \ln|\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle|. \end{aligned} \tag{4.4}$$

Since $-i\Delta\phi_{12}$ is a pure imaginary number and the second term of the equation above is real, then the unique imaginary contribution must come from the imaginary part of the first term. Therefore we can write

$$\Delta\phi_{12} \quad = \quad -\texttt{Imag}\left[\ln\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle\right]. \tag{4.5}$$

The phase difference is defined only modulo 2π, i. e., only the rest of the division of $\Delta\phi_{12}$ by 2π is unique, unless these states are mutually orthogonal. This can be checked easily. Suppose a phase difference $\Delta'_{12} = \Delta_{12} + 2\pi n$, where n in a positive integer. We can there write,

$$e^{-i\Delta\phi'_{12}} = e^{-i\Delta\phi_{12}}e^{-2\pi in} = e^{-i\Delta\phi_{12}} = \frac{\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle}{|\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle|}. \tag{4.6}$$

This expression is rigorously identical to Eq. (4.3).

It is useful to define the "distance" D_{12} between these states as

$$D_{12}^2 = 1 - |\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle|^2. \tag{4.7}$$

A different gauge would introduce an additional phase that is equal to all states. We can observe then that both the phase difference and the distance are gauge independent, once this additional phase is canceled out.

4.1.1 Berry Phase

Consideremos agora N estados fundamentais $|\Psi_n(\mathbf{k}_1)\rangle$, $|\Psi_n(\mathbf{k}_2)\rangle \cdots |\Psi_n(\mathbf{k}_N)\rangle$. A diferença de fase num circuito fechado formado por esses estados será dado por

$$\gamma = \Delta\phi_{12} + \Delta\phi_{23} + \cdots + \Delta\phi_{N1} \tag{4.8}$$

que, de acordo com a Eq. (4.5) temos

$$\begin{aligned}\gamma_n \quad &= \quad -\texttt{Imag}\left[\ln\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle\right] - \texttt{Imag}\left[\ln\langle\Psi_n(\mathbf{k}_2)|\Psi_n(\mathbf{k}_3)\rangle\right] - \cdots \\ &\quad\quad -\texttt{Imag}\left[\ln\langle\Psi_n(\mathbf{k}_N)|\Psi_n(\mathbf{k}_1)\rangle\right] \\ &= \quad -\texttt{Imag}\ln\left[\langle\Psi_n(\mathbf{k}_1)|\Psi_n(\mathbf{k}_2)\rangle\langle\Psi_n(\mathbf{k}_2)|\Psi_n(\mathbf{k}_3)\rangle\cdots\langle\Psi_n(\mathbf{k}_N)|\Psi_n(\mathbf{k}_1)\rangle\right] \end{aligned} \tag{4.9}$$

As in a different gauge choice an arbitrary phase cancel out in pairs, then γ has to be gouge independent.

Considere not two states $|\Psi_n(\mathbf{k})\rangle$ and $|\Psi_n(\mathbf{k}+d\mathbf{k})\rangle$ of a given band n that differ only by an infinitesimal change in $\mathbf{k}$. According to Eq. (4.5), the phase difference between these two states is given by

$$d\phi \quad = \quad -\texttt{Imag}\left[\ln\langle\Psi_n(\mathbf{k})|\Psi_n(\mathbf{k}+d\mathbf{k})\rangle\right]. \tag{4.10}$$

Expanding $|\Psi_n(\mathbf{k}+d\mathbf{k})\rangle$ in Taylor series we have

$$|\Psi_n(\mathbf{k}+d\mathbf{k})\rangle = |\Psi_n(\mathbf{k})\rangle + |\nabla\Psi_n(\mathbf{k})\rangle \cdot d\mathbf{k} + \cdots\,, \tag{4.11}$$

therefore

$$\begin{aligned}\langle\Psi_n(\mathbf{k})|\Psi_n(\mathbf{k}+d\mathbf{k})\rangle &= \langle\Psi_n(\mathbf{k})|\Psi_n(\mathbf{k})\rangle + \langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle\cdot d\mathbf{k} + \cdots \\ &= 1 + \langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle\cdot d\mathbf{k} + \cdots\,. \end{aligned}\tag{4.12}$$

Substituting the Eq. (4.12) up to first order in $d\mathbf{k}$ into Eq. (4.10) we obtain

$$d\phi \;=\; -\mathtt{Imag}\left[\ln\left(1 + \langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle\cdot d\mathbf{k}\right)\right]. \tag{4.13}$$

Using the approximation $\ln(1+x) = 1+x$ we get

$$\begin{aligned} d\phi &= -\mathtt{Imag}\left[1 + \langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle\cdot d\mathbf{k}\right] \\ &= -\mathtt{Imag}\langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle\cdot d\mathbf{k}. \end{aligned}\tag{4.14}$$

If we consider no a closed look C, the sum in Eq. (4.8) becomes an integral. Thus we can calculate the Berry phase by integrating $d\phi$ of Eq. (4.14) along the loop C, obtaining

$$\gamma_n = \oint_C -\mathtt{Imag}\langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle\cdot d\mathbf{k} \tag{4.15}$$

ou

$$\gamma_n = \oint_C \mathbf{A}_n(\mathbf{k})\cdot d\mathbf{k}, \tag{4.16}$$

where we define the Berry connection,

$$\mathbf{A}_n(\mathbf{k}) = -\mathtt{Imag}\langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle. \tag{4.17}$$

We note that the Berry fase (Eq. (4.16)) is a gauge invariant. It is also interesting to notice that that the Berry phase is defined only modulo 2π in the same way as we have proved in Sec. (4.1).

It is interesting to notice that the quantity $\langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle$ is purely imaginary. The reader should prove this by considering normalizable wave function $\Psi_n(\mathbf{k})\rangle$. That said, the expression above can be written as

$$\mathbf{A}_n(\mathbf{k}) = i\langle\Psi_n(\mathbf{k})|\nabla_k\Psi_n(\mathbf{k})\rangle. \tag{4.18}$$

4.1.2 Curvature

Suppose that the curl of $\mathbf{A}_n(\mathbf{k})$ is non vanishing. Thus we can make use of the Stokes theorem to write the Eq. (Eq. (4.16)) as

$$\gamma_n = \int_S \nabla \times \mathbf{A}_n(\mathbf{k}) \cdot d\mathbf{S}, \tag{4.19}$$

where $d\mathbf{S}$ is the oriented area element normal to the surface limited to by the curve C. We can also define a new vector $\boldsymbol{\Omega}$ named Berry curvature

$$\boldsymbol{\Omega}_n(\mathbf{k}) = \boldsymbol{\nabla}_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k}), \tag{4.20}$$

such that we can write

$$\gamma_n = \int_S \boldsymbol{\Omega}_n(\mathbf{k}) \cdot d\mathbf{S}. \tag{4.21}$$

Using the vector identity

$$\nabla \times f\mathbf{a} = \nabla f \times \mathbf{a} + f\nabla \times \mathbf{a} \tag{4.22}$$

and having in mind that the curl of a gradient is zero, we can write the Eq. (4.20) as

$$\boldsymbol{\Omega}_n(\mathbf{k}) = -\mathtt{Imag}\langle \nabla_k \Psi_n(\mathbf{k})| \times |\nabla_{\mathbf{k}} \Psi_n(\mathbf{k})\rangle. \tag{4.23}$$

The vector $\Omega_n(\mathbf{k})$ is called *Berry curvature*, whose modulus can be interpreted as the Berry phase per unity of area. A more physical picture can be drown here. From Eq. (4.20) we can interpret $\boldsymbol{A}(\mathbf{k})$ and $\boldsymbol{\Omega}(\mathbf{k})$, respectively, as a vector potential and the corresponding field, analogously to the situation in electromagnetism. Up to now we utilized the vector notation for the three-dimensional space ($d = 3$). In general, $\mathbf{k}$ represents a set of parameters in an arbitrary d-dimensional space. In that case the expression (4.23) has to be generalized.

4.1.3 Chern number

A quantity of great importance in the theory of topological insulators is the so called *Chern number*. Lets us consider again the Eq. (4.19), supposing now that the integration surface S is closed. Let us also assume that $\nabla_{\mathbf{k}}\Omega_n(\mathbf{k})$ is divergent free over the surface S. Thus we can

$$\oint_S \boldsymbol{\Omega}_n(\mathbf{k}) \cdot d\mathbf{S} = 2\pi\mathcal{C}_n, \tag{4.24}$$

where $\mathcal{C}_n$ is a quantized number and it is a robust topological invariant. The demonstration of this result is quite simple. Suppose that the surface S is an sphere. Let us divide the integral 4.24 just at the equator of the sphere ($z = 0$). The integral 4.24 can then be written as

$$\oint_S \mathbf{\Omega}_n(\mathbf{k}) \cdot d\mathbf{S} = \int_{S_+} \mathbf{\Omega}_n(\mathbf{k}) \cdot d\mathbf{S} + \int_{S_-} \mathbf{\Omega}_n(\mathbf{k}) \cdot d\mathbf{S}, \tag{4.25}$$

where, by construction, $S_+ = S_-$, but their normal vectors are opposite. Applying the Stokes theorem we can write

$$\oint_S \mathbf{\Omega}_n(\mathbf{k}) \cdot d\mathbf{S} = \oint_C \mathbf{A}_{n,+}(\mathbf{k}) \cdot d\mathbf{k} - \oint_C \mathbf{A}_{n,-}(\mathbf{k}) \cdot d\mathbf{k}, \tag{4.26}$$

The $\mathbf{A}_{n,+}(\mathbf{k})$ and $\mathbf{A}_{n,-}(\mathbf{k})$ are gauge potentials associated to the curvature $\mathbf{\Omega}_n(\mathbf{k})$ on north and south hemispheres, respectively. The rhs of the Eq. (4.26) is the difference between two Berry phases on the same close circuit C. Since the Berry phase is unique modulo 2π, then the difference has of two Berry phase along the same curve has to be multiple of 2π. With that we conclude that

$$\int_S \mathbf{\Omega}_n(\mathbf{k}) \cdot d\mathbf{S} = 2\pi \mathcal{C}_n, \tag{4.27}$$

where $\mathcal{C}_n$ is integer.

The total Chern number $\mathcal{C}$ is the sum of (4.24) over all occupied bands

$$\mathcal{C} = \sum_{n=1}^{N} \mathcal{C}_n. \tag{4.28}$$

4.2 Connection to the Bogoliubov-de Gennes Hamiltonian

The connection between all this discussion with the Bogoliubov-de Gennes Hamiltonian (3.28) is very beautiful. We can notice that the Eq. (4.17) is similar to the one we obtain for the Aharonov-Bohn effect, in which

$$\langle \Psi(\boldsymbol{R}) | \boldsymbol{\nabla}_{\boldsymbol{R}} \Psi(\boldsymbol{R}) \rangle = -\frac{iq}{\hbar} \boldsymbol{A}(\boldsymbol{R}), \tag{4.29}$$

or

$$i\boldsymbol{A}(\boldsymbol{R}) = -(\hbar/q) \langle \Psi(\boldsymbol{R}) | \boldsymbol{\nabla}_{\boldsymbol{R}} \Psi(\boldsymbol{R}) \rangle. \tag{4.30}$$

where $\boldsymbol{A}(\boldsymbol{R})$ is the electromagnetic vector potential. Making $q = \hbar = 1$ we obtain

$$\boldsymbol{A}(\boldsymbol{R}) = -\mathtt{Imag} \langle \Psi(\boldsymbol{R}) | \boldsymbol{\nabla}_{\boldsymbol{R}} \Psi(\boldsymbol{R}) \rangle, \tag{4.31}$$

Which is precisely the same form of Eq. (4.17). Isn't it wonderful?

We notice, however, from the definition of the curvature (4.17) that the corresponding curvature $\mathbf{\Omega}_n(\mathbf{k}) = \boldsymbol{\nabla}_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k})$ cannot be immediately identified with the $\mathbf{k}$-dependent effective magnetic field appearing the Bogoliubov-de Gennes Hamiltonian (3.28), since the $\mathbf{\Omega}(\mathbf{k})$ depends upon which band is been considered. For practical purpose we need, in principle, to determine $\mathbf{\Omega}_n(\mathbf{k})$ directly from Eq. (4.17).

We will now show a useful expression for the Chern number for Bogoliubov-de Gennes Hamiltonians of the form (3.26),

$$\mathcal{H}(\mathbf{k}) = \begin{bmatrix} \varepsilon(\mathbf{k}) & \texttt{Re}\ \Delta_{\mathbf{k}} - i\texttt{Im}\ \Delta_{\mathbf{k}} \\ \texttt{Re}\ \Delta_{\mathbf{k}} + i\texttt{Im}\ \Delta_{\mathbf{k}} & -\varepsilon(\mathbf{k}) \end{bmatrix} = h_x(\mathbf{k})\boldsymbol{\sigma}_x + h_y(\mathbf{k})\boldsymbol{\sigma}_y + h_z(\mathbf{k})\boldsymbol{\sigma}_z, \quad (4.32)$$

which can also be written in terms of new variables $\mathbf{R} = (x, y, z)$ as,

$$\mathcal{H}(\mathbf{R}) = \begin{bmatrix} z & x - iy \\ x + iy & -z \end{bmatrix} = \mathbf{R} \cdot \boldsymbol{\sigma}. \quad (4.33)$$

where $x = x(\mathbf{k}) = h_x(\mathbf{k})$, $y = y(\mathbf{k}) = h_y(\mathbf{k})$ and $z = z(\mathbf{k}) = h_z(\mathbf{k})$

By diagonalizing this Hamiltonian we find two eigenvalues $E_\pm = \pm R$, where $R = |\mathbf{R}|$. Following Sec. 3.1, the eigenvectors corresponding to these energies can be written as

$$|\mathbf{R}_+\rangle = \begin{pmatrix} u_+ \\ v_+ \end{pmatrix} \quad (4.34)$$

with

$$u_+ = \frac{x - iy}{\sqrt{x^2 + y^2}} \sqrt{\frac{z + E_+}{2E_+}} = \frac{x - iy}{\sqrt{x^2 + y^2}} \frac{1}{\sqrt{2}} \sqrt{\frac{z}{R} + 1}. \quad (4.35)$$

We have chosen $u_+(x, y)$ to be odd in the under the transform $(x, y) \rightarrow (-x, -y)$ such that $v_+(x, y)$ is even under this transformation. Moreover, we have followed the convention $u_+(x, y) \propto x - iy$, but $u_+(x, y) \propto x + iy$ would also work properly. The results will be different just by sign in the Chern number. This would not be a problem since the topological invariant is equal to the modulus of the Chern number. We can simplify the notation by introducing now the spherical coordinates, such that

$$\mathbf{R} = R \sin\theta \cos\phi \hat{\mathbf{x}} + R \sin\theta \sin\phi \hat{\mathbf{y}} + R \cos\theta \hat{\mathbf{z}}, \quad (4.36)$$

in which,

$$\cos\theta = \frac{z}{R}, \quad (4.37)$$

$$\cos\phi = \frac{x}{\sqrt{x^2 + y^2}} \quad (4.38)$$

and

$$\sin\phi = \frac{y}{\sqrt{x^2 + y^2}}. \quad (4.39)$$

Then

$$u_+ = \frac{1}{\sqrt{2}}\sqrt{\cos\theta + 1}(\cos\phi - i\sin\phi) = e^{-i\phi}\cos(\theta/2), \tag{4.40}$$

where we have used the identity $1 + \cos\theta = 2\cos^2(\theta/2)$. From normalization condition we find,

$$v_+ = \sin(\theta/2). \tag{4.41}$$

Therefore we have

$$|\mathbf{R}_+\rangle = \begin{bmatrix} e^{-i\phi}\cos(\theta/2) \\ \sin(\theta/2) \end{bmatrix}. \tag{4.42}$$

Analogously, we can find the other eigenvector,

$$|\mathbf{R}_-\rangle = \begin{bmatrix} e^{-i\phi}\sin(\theta/2) \\ -\cos(\theta/2) \end{bmatrix}, \tag{4.43}$$

that is orthogonal to $|\mathbf{R}_+\rangle$. We are not in position to calculate the Berry curvature from Eq. (4.17). With that we find,

$$A_\theta^{(+)} = i\langle\mathbf{R}_+|\frac{\partial}{\partial\theta}\mathbf{R}_+\rangle = -\frac{1}{2}\langle\mathbf{R}_+|\mathbf{R}_-\rangle = 0. \tag{4.44}$$

and

$$A_\phi^{(+)} = i\langle\mathbf{R}_+|\frac{\partial}{\partial\phi}\mathbf{R}_+\rangle = i\begin{bmatrix} e^{-i\phi}\cos(\theta/2) & \sin(\theta/2) \end{bmatrix}\begin{bmatrix} -ie^{-i\phi}\cos(\theta/2) \\ 0 \end{bmatrix} = \cos^2(\theta/2). \tag{4.45}$$

Similarly,

$$A_\theta^{(-)} = 0 \tag{4.46}$$

and

$$A_\phi^{(-)} = \sin^2(\theta/2). \tag{4.47}$$

We can now find the gauge field

$$\mathbf{\Omega}_n(R,\theta,\phi) = \boldsymbol{\nabla}\times\mathbf{A}_n(R,\theta,\phi), \tag{4.48}$$

from which we find

$$\mathbf{\Omega}_+(R,\theta,\phi) = -\frac{1}{2}\sin\theta\hat{\mathbf{R}}, \tag{4.49}$$

and

$$\boldsymbol{\Omega}_-(R,\theta,\phi) = +\frac{1}{2}\sin\theta\hat{\mathbf{R}}. \tag{4.50}$$

In order to go back to **k**-space, we should first transform these expressions back to the x, y, z-coordinates. To do so we use the Jacobian of the transform, that allows us to write us

$$\boldsymbol{\Omega}_\pm(x,y,z) = \frac{\partial(R,\theta,\phi)}{\partial(x,y,z)}\boldsymbol{\Omega}_\pm(R,\theta,\phi) = \frac{1}{\frac{\partial(x,y,z)}{\partial(R,\theta,\phi)}}\boldsymbol{\Omega}_\pm(R,\theta,\phi) = \frac{1}{R^2\sin\theta}\boldsymbol{\Omega}_\pm(R,\theta,\phi). \tag{4.51}$$

Or separately,

$$\boldsymbol{\Omega}_+(\mathbf{R}) = -\frac{1}{2}\frac{\mathbf{R}}{R^3} \tag{4.52}$$

and

$$\boldsymbol{\Omega}_-(\mathbf{R}) = \frac{1}{2}\frac{\mathbf{R}}{R^3}. \tag{4.53}$$

These fields corresponds to monopoles located at the origin. In rectangular coordinates the Chern number becomes

$$\mathcal{C} = \frac{1}{2\pi}\int_S \boldsymbol{\Omega}_-(\mathbf{R})\cdot d\mathbf{S} = \frac{1}{4\pi}\int_S \frac{\mathbf{R}}{R^3}\cdot\hat{\mathbf{n}}dxdy \tag{4.54}$$

Now, we remember that x, y and z are functions of $\mathbf{k}$. Since $\mathbf{R} = \mathbf{h}$, we can write

$$\mathcal{C} = -\frac{1}{4\pi}\int_S \frac{\mathbf{h}}{h^3}\cdot\hat{\mathbf{n}}dh_x dh_y. \tag{4.55}$$

We now need to write in terms of $\hat{\mathbf{n}}$, dh_x and dh_y in terms of $\mathbf{k}$-coordinates. We notice that the normal vector can be written as

$$\hat{\mathbf{n}} = \frac{\partial_{k_x}\mathbf{h}(\mathbf{k})\times\partial_{k_y}\mathbf{h}(\mathbf{k})}{|\partial_{k_x}\mathbf{h}(\mathbf{k})\times\partial_{k_y}\mathbf{h}(\mathbf{k})|} \tag{4.56}$$

and the element of area as

$$dh_x dh_y = |\partial_{k_x}\mathbf{h}(\mathbf{k})\times\partial_{k_y}\mathbf{h}(\mathbf{k})|dk_x dk_y. \tag{4.57}$$

replacing Eqs. (4.56) and (4.57) into Eq. (4.55) we obtain.

$$\mathcal{C} = \frac{1}{4\pi}\int_S \frac{\mathbf{h}}{h^3}\cdot\left[\partial_{k_x}\mathbf{h}(\mathbf{k})\times\partial_{k_y}\mathbf{h}(\mathbf{k})\right]dk_x dk_y. \tag{4.58}$$

This is one expression commonly found in the literature. It can also be written in terms of the unity vector $\hat{\mathbf{h}}$. To do so we notice that

$$\partial_{k_x}\mathbf{h} = \partial_{k_x}h\hat{\mathbf{h}} = h\partial_{k_x}\hat{\mathbf{h}} + (\partial_{k_x}h)\,\hat{\mathbf{h}} \tag{4.59}$$

and

$$\partial_{k_y}\mathbf{h} = \partial_{k_y} h\hat{\mathbf{h}} = h\partial_{k_y}\hat{\mathbf{h}} + \left(\partial_{k_y} h\right)\hat{\mathbf{h}}. \tag{4.60}$$

Then

$$\begin{aligned}\partial_{k_x}\mathbf{h} \times \partial_{k_y}\mathbf{h} &= \left(\partial_{k_x} h\right)\hat{\mathbf{h}} \times \left(\partial_{k_y} h\right)\hat{\mathbf{h}} + \left(\partial_{k_x} h\right)\hat{\mathbf{h}} \times h\partial_{k_y}\hat{\mathbf{h}} - \left(\partial_{k_y} h\right)\hat{\mathbf{h}} \times h\partial_{k_x}\hat{\mathbf{h}} \\ &\quad + h\partial_{k_x}\hat{\mathbf{h}} \times h\partial_{k_y}\hat{\mathbf{h}}. \end{aligned}\tag{4.61}$$

The first terms vanishes because it is a cross product between parallel vectors. The integrand of the Eq. (4.58) becomes

$$\begin{aligned}\frac{\mathbf{h}}{h^3} \cdot \left[\partial_{k_x}\mathbf{h}(\mathbf{k}) \times \partial_{k_y}\mathbf{h}(\mathbf{k})\right] &= \frac{\mathbf{h}}{h^3} \cdot \left[\left(\partial_{k_x} h\right)\hat{\mathbf{h}} \times h\partial_{k_y}\hat{\mathbf{h}} - \left(\partial_{k_y} h\right)\hat{\mathbf{h}} \times h\partial_{k_x}\hat{\mathbf{h}} + h\partial_{k_x}\hat{\mathbf{h}} \times h\partial_{k_y}\hat{\mathbf{h}}\right] \\ &= \hat{\mathbf{h}} \cdot \left[\partial_{k_x}\hat{\mathbf{h}} \times \partial_{k_y}\hat{\mathbf{h}}\right]. \end{aligned}\tag{4.62}$$

The passage from the firs to the second line of the equation above is made by noticing that the first and the second terms inside the brackets are both orthogonal to $\mathbf{h}$, so that their scalar product with $\mathbf{h}$ vanish. We can now replace Eq. (4.62) into Eq. (4.58) to finally obtain

$$\mathcal{C} = \frac{1}{4\pi}\int_S \hat{\mathbf{h}} \cdot \left[\frac{\partial\hat{\mathbf{h}}(\mathbf{k})}{\partial_{k_x}} \times \frac{\partial\hat{\mathbf{h}}(\mathbf{k})}{\partial_{k_y}}\right] dk_x dk_y. \tag{4.63}$$

5

Topological insulators and time reversal symmetry

We will describe here a powerfull theory for classifying the time-reversal invariant insulators based on topological analysis[21].

5.0.1 Short digression on time reversal symmetry

Classicaly a motion of a particle subject to to a given force $\boldsymbol{F}$ is governed by the Newton's law

$$m\frac{d^2\mathbf{k}}{dt^2} = \boldsymbol{F}(\mathbf{r}) = -\boldsymbol{\nabla}V(\mathbf{r}). \tag{5.1}$$

If $\mathbf{k}(t)$ is a solution of the equation (5.1), then $\mathbf{r}(-t)$ is also a solution of the equation. This means that if we transform $t \to -t$ the Newton's equation of motion remains unchanged. The motion is then time-reversible if we properly modify the initial conditions of the problem. Notice in addition that upon this transformation $\mathbf{p} = m(d\mathbf{r}/dt) \to m[d\mathbf{r}/d(-t)] = -d\mathbf{r}/dt = -\mathbf{p}$, meaning that $\mathbf{p} \to -\mathbf{p}$ upon time reversal transformation. In this sense, the time-reversal operation reverses the motion. Thereby it could be called more appropriately *motion reversal operation.*

In quantum mechanics the dynamics of a given system is described by the Schrödinger equation

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = H\Psi(\mathbf{r},t), \tag{5.2}$$

$$H\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right). \tag{5.3}$$

We notice that the Hamiltonian (5.3) is invariant upon transforming $t \to -t$. If $\Psi(\mathbf{r},t)$ is a solution for of the Eq. (5.2), $\Psi(\mathbf{r},-t)$ is not a solution of the equation because of the first order derivative on the left side of Eq. (5.2). But we see that $\Psi^*(\mathbf{r}, -t$ is a solution. We can easily check this assertion by considering the free particle solution $V(\mathbf{r}) = 0$. In this case $\Psi(\mathbf{r}, t) = ce^{i(\mathbf{p}\cdot\mathbf{r}-Et)/\hbar}$. Notice that $\Psi(\mathbf{r}, -t) = ce^{i(\mathbf{p}\cdot\mathbf{r}+Et)/\hbar}$ is also a solution but with the same momentum $\mathbf{p}$, while we should expect $-\mathbf{p}$ in the reversed motion, just like in the classical case. We can see that $\Psi^*(\mathbf{r}, -t) = ce^{-i(\mathbf{p}\cdot\mathbf{r}+Et)/\hbar} = ce^{i(-\mathbf{p}\cdot\mathbf{r}-Et)/\hbar}$ is the proper solution with the reversed linear momentum.

The discussion above suggest us some care with the definition of the time-reversal operator Θ. We first define an anti-unitary operation as

Anti-unitary transformation: Consider the transformation below:

$$|\alpha\rangle \to |\tilde{\alpha}\rangle = \theta|\alpha\rangle \tag{5.4a}$$

$$|\beta\rangle \to |\tilde{\beta}\rangle = \theta|\beta\rangle. \tag{5.4b}$$

This transformation is said to be anti-unitary if

$$\langle\tilde{\alpha}|\tilde{\beta}\rangle = \langle\alpha|\beta\rangle^* = \langle\beta|\alpha\rangle \tag{5.5a}$$

and

$$\theta\left[c_1|\alpha\rangle + c_2|\beta\rangle\right] = c_1^*\theta|\alpha\rangle + c_2^*\theta|\beta\rangle. \tag{5.5b}$$

It is convenient to write an anti-unitary operator as

$$\theta = UK, \tag{5.6}$$

where U is a unitary operator and K is the complex conjugation operator, that works as

$$K\phi = \phi^* K. \tag{5.7}$$

We stress for the fact that ϕ can be either a function or an operator.

Time reversal operator

Let us denote the time reversal operator as Θ. As a definition, the transformation

$$|\alpha\rangle \to \Theta|\alpha\rangle \tag{5.8}$$

time reverses the state $|\alpha\rangle$. Or, akin to the classical case, *time reverses* the state $|\alpha\rangle$. Analogously to the classical case, the action of the time reversal operator on a eigenstate $|\mathbf{p}\rangle$ reverses the momentum. Therefore,

$$\Theta|\mathbf{p}\rangle = |-\mathbf{p}\rangle, \tag{5.9}$$

apart from a possible phase factor. We can see that the operator Θ has to be anti-unitary. Consider a time reversal invariant quantum system described by the Shrödinger equation

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = H\Psi(\mathbf{r},t). \tag{5.10}$$

To see this we apply the time reversal operation on this equation we have

$$\begin{aligned}\Theta i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}\Theta^{-1} &= \Theta H\Psi(\mathbf{r},t)\Theta^{-1}\\ \Theta i\Theta^{-1}\Theta\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}\Theta^{-1} &= \Theta H\Theta^{-1}\Theta\Psi(\mathbf{r},t)\Theta^{-1}\\ \Theta i\Theta^{-1}\Theta\hbar\frac{\partial}{\partial t}\Theta^{-1}\Theta\Psi(\mathbf{r},t)\Theta^{-1} &= \Theta H\Theta^{-1}\Theta\Psi(\mathbf{r},t)\Theta^{-1}.\end{aligned} \tag{5.11}$$

Now, we know that

$$\Theta\hbar\frac{\partial}{\partial t}\Theta^{-1} = \hbar\frac{\partial}{\partial(-t)} = -\hbar\frac{\partial}{\partial t}, \tag{5.12}$$

$$\Theta\Psi(\mathbf{r},t)\Theta^{-1} = \Psi^*(\mathbf{r},-t) \tag{5.13}$$

and since the system is supposed to be time-reversal invariant,

$$\Theta H\Theta^{-1} = H. \tag{5.14}$$

Therefore

$$-\Theta i\Theta^{-1}\hbar\frac{\partial}{\partial t}\Psi^*(\mathbf{r},-t) = H\Psi^*(\mathbf{r},-t). \tag{5.15}$$

We notice then that in order for the equation (5.10) to be invariant we need to have $\Theta i\Theta^{-1} = -i$. Therefore the operator Θ possesses the anti-unitary properties. Moreover we have,

$$\Theta\mathbf{r}\Theta^{-1} = \mathbf{r} \tag{5.16}$$

$$\Theta\mathbf{p}\Theta^{-1} = -\mathbf{p} \tag{5.17}$$

and

$$\Theta\boldsymbol{J}\Theta^{-1} = \Theta(\mathbf{r}\times\mathbf{p})\Theta^{-1} = -\boldsymbol{J}. \tag{5.18}$$

Another important relations is

$$\langle\alpha|A|\beta\rangle = \langle\tilde{\beta}|A^\dagger|\tilde{\alpha}\rangle, \tag{5.19}$$

where A is an arbitrary operator. To prove this, lets $|\gamma\rangle = A^\dagger|\alpha\rangle$, then $\langle\gamma| = \langle\alpha|A$. With that, we can write

$$\langle\alpha|A|\beta\rangle = \langle\gamma|\beta\rangle = \langle\tilde{\beta}|\tilde{\gamma}\rangle = \langle\tilde{\beta}|\Theta|\gamma\rangle = \langle\tilde{\beta}|\Theta A^\dagger|\alpha\rangle = \langle\tilde{\beta}|\Theta A^\dagger\Theta^{-1}\Theta|\alpha\rangle = \langle\tilde{\beta}|\Theta A^\dagger\Theta^{-1}|\tilde{\alpha}\rangle \tag{5.20}$$

Spin-1/2 system

We now want to construct an explicit expression for the time reversal operator for a spin-1/2 system. To do so lets us consider the time reversal symmetry operator on a spin-1/2 system. Analogously to the angular momentum, transformation of the Pauli matrices we should obtain

$$\Theta\sigma_\alpha\Theta^{-1} = -\sigma_\alpha. \tag{5.21}$$

In an attempt to construct a operator that satisfy the relation above, we notice from the definition of the Pauli matrices that $\sigma_y^{-1} = \sigma_y$

$$\sigma_y\sigma_x\sigma_y^{-1} = \sigma_y\sigma_x\sigma_y = -\sigma_x \tag{5.22}$$

$$\sigma_y\sigma_y\sigma_y^{-1} = \sigma_y\sigma_y\sigma_y = +\sigma_y \tag{5.23}$$

$$\sigma_y\sigma_z\sigma_y^{-1} = \sigma_y\sigma_z\sigma_y = -\sigma_z. \tag{5.24}$$

Since σ_y is purely imaginary while σ_x and σ_z are purely real, we have that

$$K\sigma_y = -\sigma_y K \tag{5.25}$$

while

$$K\sigma_{x,z} = \sigma_{x,z}K. \tag{5.26}$$

Notice, however, that

$$(\sigma_y K)i(\sigma_y K)^{-1} = \sigma_y K i\sigma_y K = -i\sigma_y K\sigma_y K = i\sigma_y^2 K^2 = i. \tag{5.27}$$

Therefore $\sigma_y K)$ does not fulfill the requirements for the time reversal operator. Nonetheless,

$$(i\sigma_y K)i(i\sigma_y K)^{-1} = i\sigma_y K i(-i\sigma_y K) = i\sigma_y K\sigma_y K = -i\sigma_y^2 K^2 = -i. \tag{5.28}$$

Then we can define the time reversal operator as

$$\boxed{\Theta = i\sigma_y K.} \tag{5.29}$$

We notice now that

$$\Theta^{-1} = -i(\sigma_y K)^{-1} = -i\sigma_y K = -\Theta. \tag{5.30}$$

From the last equation we have

$$1 = \Theta\Theta^{-1} = -\Theta^2. \tag{5.31}$$

Therefore the operator Θ obeys the following important relation

$$\Theta^2 = -1. \tag{5.32}$$

We can see also that $\langle\psi|\Theta|\phi\rangle = -\langle\phi|\Theta|\psi\rangle$. To show this lets define $|\tilde{\alpha}\rangle = \Theta|\alpha\rangle$ and $|\tilde{\tilde{\alpha}}\rangle = \Theta|\tilde{\alpha}\rangle = \Theta^2|\alpha\rangle = -|\alpha\rangle$, then $\langle\tilde{\tilde{\alpha}}| = -\langle\alpha|$. With that,

$$\langle\psi|\Theta|\phi\rangle = \langle\psi|\tilde{\phi}\rangle = \langle\tilde{\phi}|\psi\rangle^* = \langle\tilde{\tilde{\phi}}|\tilde{\psi}\rangle = \langle\tilde{\tilde{\phi}}|\Theta^{-1}|\tilde{\tilde{\psi}}\rangle = -\langle\phi|\Theta|\psi\rangle. \tag{5.33}$$

It is also useful to calculate the complex conjugate of the matrix element above, which reads

$$\langle\psi|\Theta|\phi\rangle^* = \langle\psi|\tilde{\phi}\rangle^* = \langle\tilde{\phi}|\psi\rangle = \langle\tilde{\psi}|\tilde{\tilde{\phi}}\rangle = \langle\tilde{\psi}|\Theta|\tilde{\phi}\rangle. \tag{5.34}$$

Consider a time reversal invariant system described by the Hamiltonian H. This mean that H commutes with Θ, that is $H\Theta = \Theta H$, or

$$H = H\Theta\Theta^{-1} = \Theta H\Theta^{-1} = H. \tag{5.35}$$

Now if $|\psi\rangle$ is an eigenvector of H with energy E, then $|\psi'\rangle = \Theta|\psi\rangle$ is also an eigenvector of H with the same energy E. The question is whether $|\psi\rangle$ and $|\psi'\rangle$ are equal. If they were equal, then $\Theta^2|\psi\rangle$ then would also be equal to $|\psi\rangle$. However, from Eq. (5.32) $\Theta^2 = -1$, hence $\Theta^2|\psi\rangle = -|\psi\rangle$. Therefore $|\psi\rangle$ and $\Theta|\psi\rangle$ are different. Therefore we conclude that for a spin-1/2 system that is time reversal invariant the eigenenergies are at least double degenerate. This degeneracy guaranteed by the time reversal symmetry are called *Kramer's degeneracy*.

It is interesting to show now that a system of spin-1/2 particles in an external magnetic field is not time reversal invariant. To see this, we can write the full Hamiltonian of the system as

$$H = H_0 + \boldsymbol{S}\cdot\boldsymbol{B} \tag{5.36}$$

where H_0 is supposed to be time reversal invariant, i.e., $\Theta H_0 \Theta^{-1} = H_0$. We see however that, if $\boldsymbol{S} = 1/2$ then $\Theta\boldsymbol{S}\Theta^{-1} = -\boldsymbol{S}$. Therefore,

$$\begin{aligned}\Theta H\Theta^{-1} &= \Theta H_0\Theta^{-1} + \Theta\boldsymbol{S}\cdot\boldsymbol{B}\Theta^{-1} = H_0 + \Theta\boldsymbol{S}\Theta^{-1}\cdot\Theta\boldsymbol{B}\Theta^{-1} = H_0 - \boldsymbol{S}\cdot\boldsymbol{B} \\ &\neq H,\end{aligned} \tag{5.37}$$

where $\boldsymbol{B}$ is regarded as as external[22].

5.0.2 Time reversal symmetry and Bloch Hamiltonian

Consider now a periodic system (a solid for instance) described by the Hamiltonian $\mathcal{H}$, that obey the Schrödinger equation

$$\mathcal{H}|\psi_{n\mathbf{k}}\rangle = E_{n\mathbf{k}}|\psi_{n\mathbf{k}}\rangle. \tag{5.38}$$

From the Bloch theorem $|\psi_{n\mathbf{k}}\rangle$ can be written as

$$|\psi_{n\mathbf{k}}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u_{n\mathbf{k}}\rangle, \tag{5.39}$$

where $|u_{n\mathbf{k}}\rangle$ is a periodic eigenfunction of the cell-periodic Hamiltonian

$$H(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\mathcal{H}e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{5.40}$$

that obey the Shrödinger equation

$$H(\mathbf{k})|u_{n\mathbf{k}}\rangle = E_{n\mathbf{k}}|u_{n\mathbf{k}}\rangle. \tag{5.41}$$

One of the most fundamental physical concept of the topological insulators is the time reversal invariance. The so called protected edge states are indeed guaranteed by time reversal symmetry. Lets then consider a time reversal invariant Hamiltonian $\mathcal{H}$, which then has to satisfy the condition

$$\Theta H(\mathbf{k})\Theta^{-1} = H(-\mathbf{k}). \tag{5.42}$$

This equation tells us that the energy bands comes in pairs, i. e., the eigenstates with vector $+\mathbf{k}$ and $-\mathbf{k}$ have the same energy. They are called *Kramer's pairs.* In general two states composing a Kramer's pair bands denoted by n are related to each other as

$$\Theta|u^{(n)}_{2,\mathbf{k}}\rangle = e^{-i\chi_{n,\mathbf{k}}}|u^{(n)}_{1,-\mathbf{k}}\rangle, \tag{5.43}$$

where $\chi_{n,-\mathbf{k}}$ is an arbitrary phase. We will develop a general theory involving time reversal symmetry operator and Bloch states.

Let $|u_{\alpha,\mathbf{k}}\rangle$ and $|u_{\beta,\mathbf{k}}\rangle$ be arbitrary[1] eigenstates of $H(\mathbf{k})$ where α and β denotes energy bands. The have to satisfy the closure relation

$$\sum_\alpha |u_{\alpha,\mathbf{k}}\rangle\langle u_{\alpha,\mathbf{k}}| = \sum_\beta |u_{\beta,\mathbf{k}}\rangle\langle u_{\beta,\mathbf{k}}| = 1. \tag{5.44}$$

We can find a relation between wave-functions of two distinct bands as,

[1]By arbitrary here means that they are not necessarily Kramer's pairs. Therefore they do not carry Kramer's pair labels.

$$
\begin{aligned}
|u_{\alpha,-\mathbf{k}}\rangle &= \Theta^{-1}|\tilde{u}_{\alpha,-\mathbf{k}}\rangle = -\Theta|\tilde{u}_{\alpha,-\mathbf{k}}\rangle \\
&= -\sum_{\beta}|\tilde{u}_{\beta,\mathbf{k}}\rangle\langle\tilde{u}_{\beta,\mathbf{k}}|\Theta|\tilde{u}_{\alpha,-\mathbf{k}}\rangle = -\sum_{\beta}\langle\tilde{u}_{\beta,\mathbf{k}}|\Theta|\tilde{u}_{\alpha,-\mathbf{k}}\rangle|\tilde{u}_{\beta,\mathbf{k}}\rangle = \sum_{\beta}\langle\tilde{u}_{\alpha,-\mathbf{k}}|\Theta|\tilde{u}_{\beta,\mathbf{k}}\rangle|\tilde{u}_{\beta,\mathbf{k}}\rangle \\
&= \sum_{\beta}\langle\tilde{u}_{\alpha,-\mathbf{k}}|\Theta|\tilde{u}_{\beta,\mathbf{k}}\rangle\Theta|u_{\beta,\mathbf{k}}\rangle = \sum_{\beta}\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle^{*}\Theta|u_{\beta,\mathbf{k}}\rangle = \sum_{\beta}w^{*}_{\alpha\beta}(\mathbf{k})\Theta|u_{\beta,\mathbf{k}}\rangle
\end{aligned}
\tag{5.45}
$$

where we have defined the matrix[23]

$$
w_{\alpha\beta}(\mathbf{k}) = \langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle. \tag{5.46}
$$

We can show that $w(\mathbf{k})$ is unitary. From Eq. (5.46) we can write

$$
\begin{aligned}
\sum_{\alpha}w^{\dagger}_{\gamma\alpha}(\mathbf{k})w_{\alpha\beta}(\mathbf{k}) &= \sum_{\alpha}\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\gamma,\mathbf{k}}\rangle^{*}\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle = \sum_{\alpha}\langle\tilde{u}_{\alpha,-\mathbf{k}}|\Theta|\tilde{u}_{\gamma,\mathbf{k}}\rangle\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle \\
&= -\sum_{\alpha}\langle\tilde{u}_{\gamma,\mathbf{k}}|\Theta|\tilde{u}_{\alpha,-\mathbf{k}}\rangle\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle = \sum_{\alpha}\langle\tilde{u}_{\gamma,\mathbf{k}}|\Theta^{-1}|\tilde{u}_{\alpha,-\mathbf{k}}\rangle\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle \\
&= \sum_{\alpha}\langle\tilde{u}_{\gamma,\mathbf{k}}|u_{\alpha,-\mathbf{k}}\rangle\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle = \langle\tilde{u}_{\gamma,\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle = \langle\tilde{u}_{\gamma,\mathbf{k}}|\tilde{u}_{\beta,\mathbf{k}}\rangle \\
&= \delta_{\gamma\beta}.
\end{aligned}
\tag{5.47}
$$

Another interesting property of $w_{\alpha\beta}$ is

$$
w_{\alpha\beta}(-\mathbf{k}) = \langle u_{\alpha,\mathbf{k}}|\Theta|u_{\beta,-\mathbf{k}}\rangle \Rightarrow w_{\beta\alpha}(-\mathbf{k}) = \langle u_{\beta,\mathbf{k}}|\Theta|u_{\alpha,-\mathbf{k}}\rangle. \tag{5.48}
$$

Therefore, from Eq. (5.33) we obtain

$$
w_{\beta\alpha}(-\mathbf{k}) = -\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\beta,\mathbf{k}}\rangle = -w_{\alpha\beta}(\mathbf{k}). \tag{5.49}
$$

This relation is very interesting and useful, as we will see later. Within a given Kramer's pair bands (n), these states are related to each other by time reversal operator as given in Eq. (5.43),

$$
\Theta|u^{(n)}_{2,\mathbf{k}}\rangle = e^{-i\chi_{n,\mathbf{k}}}|u^{(n)}_{1,-\mathbf{k}}\rangle, \tag{5.50}
$$

or

$$
|u^{(n)}_{1,-\mathbf{k}}\rangle = e^{i\chi_{\alpha,\mathbf{k}}}\Theta|u^{(n)}_{2,\mathbf{k}}\rangle \tag{5.51}
$$

Now

$$
\begin{aligned}
w_{12}(\mathbf{k}) &= \langle u^{(n)}_{1,-\mathbf{k}}|\Theta|u^{(n)}_{2\mathbf{k}}\rangle = e^{-i\chi_{n,\mathbf{k}}}\langle u^{(n)}_{1,-\mathbf{k}}|u^{(n)}_{1,-\mathbf{k}}\rangle \\
&= -e^{-i\chi_{n,\mathbf{k}}}.
\end{aligned}
\tag{5.52}
$$

where we have used Eq. (5.50). From the Eq.(5.52) it becomes clear that the only non-vanishing elements of w are those involving Kramer's pairs. Moreover from Eq. (5.49)

$$w_{21}(-\mathbf{k}) = -w_{12}(\mathbf{k}) \Rightarrow w_{21}(\mathbf{k}) = -w_{12}(-\mathbf{k}). \tag{5.53}$$

Then, from Eq. (5.50) we have

$$w_{21}(\mathbf{k}) \;\; = \;\; -e^{-i\chi_{n,-\mathbf{k}}}. \tag{5.54}$$

We can write the full matrix w as

$$w(\mathbf{k}) = \begin{pmatrix} 0 & e^{-i\chi_{1,\mathbf{k}}} & 0 & 0 & 0 & \cdots \\ -e^{-i\chi_{1,-\mathbf{k}}} & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & e^{-i\chi_{2,\mathbf{k}}} & 0 & \cdots \\ 0 & 0 & -e^{-i\chi_{2,-\mathbf{k}}} & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{5.55}$$

It is also useful to define another matrix associated to the Berry connection, defined in Eq. (4.17),

$$\mathbf{a}_{\alpha\beta}(\mathbf{k}) = i\langle u_{\alpha\mathbf{k}}|\boldsymbol{\nabla}_{\mathbf{k}}|u_{\beta\mathbf{k}}\rangle. \tag{5.56}$$

From Eq. (4.17) we see that the Berry connection can be written as

$$\boldsymbol{A}(\mathbf{k}) = \mathtt{Re}\ \mathbf{a}_{\alpha,\alpha}(\mathbf{k}). \tag{5.57}$$

We know however that $\langle u_\alpha(\mathbf{k})|i\boldsymbol{\nabla}_{\mathbf{k}}|u_\alpha(\mathbf{k})\rangle = \langle u_\alpha(\mathbf{k})|\mathbf{r}|u_\alpha(\mathbf{k})\rangle/\hbar$ is a real quantity, so that $\mathbf{a}_{\alpha,\alpha}(\mathbf{k})$ has to be real. So that we can write simply

$$\boldsymbol{A}(\mathbf{k}) = \ \mathbf{a}_{\alpha,\alpha}(\mathbf{k}). \tag{5.58}$$

We can also write

$$
\begin{aligned}
\mathbf{a}(-\mathbf{k}) &= i\langle u_{\alpha,-\mathbf{k}}|\boldsymbol{\nabla}_{\mathbf{k}}|u_{\beta,-\mathbf{k}}\rangle = i\langle u_{\alpha,-\mathbf{k}}|\boldsymbol{\nabla}_{\mathbf{k}}\sum_{\gamma} w^{*}_{\beta\gamma}(\mathbf{k})\Theta|u_{\gamma\mathbf{k}}\rangle \\
&= \sum_{\gamma} i\langle u_{\alpha,-\mathbf{k}}|\boldsymbol{\nabla}_{\mathbf{k}}\left[w^{*}_{\beta\gamma}(\mathbf{k})\Theta|u_{\gamma\mathbf{k}}\rangle\right] \\
&= \sum_{\gamma} i\langle u_{\alpha,-\mathbf{k}}|\left[\boldsymbol{\nabla}_{\mathbf{k}}w^{*}_{\beta\gamma}(\mathbf{k})\right]\Theta|u_{\gamma\mathbf{k}}\rangle + \sum_{\gamma} i\langle u_{\alpha,-\mathbf{k}}|w^{*}_{\beta\gamma}(\mathbf{k})\Theta\boldsymbol{\nabla}_{\mathbf{k}}|u_{\gamma\mathbf{k}}\rangle \\
&= \sum_{\gamma} i\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\gamma\mathbf{k}}\rangle\boldsymbol{\nabla}_{\mathbf{k}}w^{*}_{\beta\gamma}(\mathbf{k}) + \sum_{\gamma} iw^{*}_{\beta\gamma}(\mathbf{k})\langle u_{\alpha,-\mathbf{k}}|\Theta\boldsymbol{\nabla}_{\mathbf{k}}|u_{\gamma\mathbf{k}}\rangle \\
&= \sum_{\gamma} iw_{\alpha\gamma}(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{*}_{\beta\gamma}(\mathbf{k}) + \sum_{\gamma\delta} iw^{*}_{\beta\gamma}(\mathbf{k})\langle u_{\alpha,-\mathbf{k}}|\Theta|u_{\delta\mathbf{k}}\rangle\langle u_{\delta\mathbf{k}}|\boldsymbol{\nabla}_{\mathbf{k}}|u_{\gamma\mathbf{k}}\rangle \\
&= \sum_{\gamma} iw_{\alpha\gamma}(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}_{\gamma\beta}(\mathbf{k}) + \sum_{\gamma\delta} w^{*}_{\beta\gamma}(\mathbf{k})w_{\alpha\delta}(\mathbf{k})\mathbf{a}_{\delta\gamma}(\mathbf{k}) \\
&= \sum_{\gamma} iw_{\alpha\gamma}(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}_{\gamma\beta}(\mathbf{k}) + \sum_{\gamma\delta} w_{\alpha\delta}(\mathbf{k})\mathbf{a}_{\delta\gamma}(\mathbf{k})w^{*}_{\beta\gamma}(\mathbf{k}) \\
&= \sum_{\gamma} iw_{\alpha\gamma}(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}_{\gamma\beta}(\mathbf{k}) + \sum_{\gamma\delta} w_{\alpha\delta}(\mathbf{k})\mathbf{a}_{\delta\gamma}(\mathbf{k})w^{\dagger}_{\gamma\beta}(\mathbf{k}).
\end{aligned}
\tag{5.59}
$$

Therefore, this equation can be formally written as

$$
\mathbf{a}(-\mathbf{k}) = w(\mathbf{k})\mathbf{a}(\mathbf{k})w^{\dagger}(\mathbf{k}) + iw(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}(\mathbf{k}). \tag{5.60}
$$

Notice that

$$
\mathbf{a}_{\alpha\alpha}(-\mathbf{k}) = \sum_{\gamma} iw_{\alpha\gamma}(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}_{\gamma\alpha}(\mathbf{k}) + \sum_{\gamma\delta} w_{\alpha\delta}(\mathbf{k})\mathbf{a}_{\delta\gamma}(\mathbf{k})w^{\dagger}_{\gamma\alpha}(\mathbf{k}), \tag{5.61}
$$

so that

$$
\begin{aligned}
\mathrm{Tr}[\mathbf{a}(-\mathbf{k})] &= \sum_{\alpha}\mathbf{a}_{\alpha\alpha}(-\mathbf{k}) = \sum_{\alpha\gamma} iw_{\alpha\gamma}(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}_{\gamma\alpha}(\mathbf{k}) + \sum_{\alpha\gamma\delta} w^{\dagger}_{\gamma\alpha}(\mathbf{k})w_{\alpha\delta}(\mathbf{k})\mathbf{a}_{\delta\gamma}(\mathbf{k}) \\
&= \sum_{\gamma\delta}\delta_{\gamma\delta}\mathbf{a}_{\delta\gamma}(\mathbf{k}) + i\mathrm{Tr}[w(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}(\mathbf{k})] = \sum_{\gamma}\mathbf{a}_{\gamma\gamma}(\mathbf{k}) + i\mathrm{Tr}[w(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}(\mathbf{k})] \\
&= \mathrm{Tr}[\mathbf{a}(\mathbf{k})] + i\mathrm{Tr}[w(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}(\mathbf{k})].
\end{aligned}
\tag{5.62}
$$

Replacing $\mathbf{k} \to -\mathbf{k}$ we also obtain

$$
\mathrm{Tr}[\mathbf{a}(\mathbf{k})] = \mathrm{Tr}[\mathbf{a}(-\mathbf{k})] + i\mathrm{Tr}[w(-\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}(-\mathbf{k})]. \tag{5.63}
$$

Since from Eq.(5.49) $w(-\mathbf{k}) = -w(\mathbf{k})$ then o obtain

$$
\mathrm{Tr}[\mathbf{a}(\mathbf{k})] = \mathrm{Tr}[\mathbf{a}(-\mathbf{k})] + i\mathrm{Tr}[w(\mathbf{k})\boldsymbol{\nabla}_{\mathbf{k}}w^{\dagger}(\mathbf{k})]. \tag{5.64}
$$

This relation will be very important for the next section.

Time reversal symmetry and the topological $\mathbb{Z}_2$ invariant

Let suppose that some parameter of the Hamiltonian varies periodically in the momentum space with periodicity $\boldsymbol{G}$. That is, if at certain momentum $\mathbf{k}$ the system is described by $H(\mathbf{k})$, then at some other momentum $\mathbf{k}+\boldsymbol{G}$ the Hamiltonian returns to its original value $H(\mathbf{k}+\boldsymbol{G})$. Mathematically, this assertion can be written as

$$H(\mathbf{k}+\boldsymbol{G}) = H(\mathbf{k}). \tag{5.65}$$

Under time reversal operation the Hamiltonian transforms as

$$H(-\mathbf{k}) = \Theta H(\mathbf{k})\Theta^{-1}. \tag{5.66}$$

We can find momenta $\boldsymbol{\Lambda}$ such that the Hamiltonian is symmetric under time reversal transformation, i. e, $H(\Lambda) = H(-\Lambda)$. Obviously, $\Lambda = 0$ immediately satisfies this condition. From Eq. (5.65) we find

$$H(-\boldsymbol{\Lambda}) = H(\boldsymbol{\Lambda}) = H(-\boldsymbol{\Lambda}+\boldsymbol{G}). \tag{5.67}$$

The mapping of the reciprocal space to the first Brillouin zone consider vectors separated by one reciprocal lattice vector to be identical[24]. With this, from the last expression we find $-\boldsymbol{\Lambda}+\boldsymbol{G} = \boldsymbol{\Lambda}$ leading to $\boldsymbol{\Lambda} = \boldsymbol{G}/2$. We conclude then that H is time reversal symmetric at $\boldsymbol{\Lambda} = 0$ and $\boldsymbol{\Lambda} = \boldsymbol{G}/2$. At these momenta we have then

$$H(\boldsymbol{\Lambda}) = \Theta H(\boldsymbol{\Lambda})\Theta^{-1}. \tag{5.68}$$

As we have seen earlier at momenta $\boldsymbol{\Lambda}$ the Hamiltonian the system is at least double degenerate. In other words, if the system has $2N$ bands, we will find N double degenerate bands such that $|u^{(n)}_{1\boldsymbol{\Lambda}}\rangle \neq |u^{(n)}_{2,\boldsymbol{\Lambda}}\rangle$ both with energy $E^{(n)}_{1\boldsymbol{\Lambda}} = E^{(n)}_{2\boldsymbol{\Lambda}}$). Since $|u^{(n)}_{1\boldsymbol{\Lambda}}\rangle$ and $|u^{(n)}_{2,\boldsymbol{\Lambda}}\rangle$ are Kramer's pair they are related to each other by Eq. (5.50), giving

$$\Theta|u^{(n)}_{2,\boldsymbol{\Lambda}}\rangle \quad = \quad e^{-i\chi_{n,\boldsymbol{\Lambda}}}|u^{(n)}_{1,-\boldsymbol{\Lambda}}\rangle. \tag{5.69}$$

Then,

$$w^{(n)}_{12}(\boldsymbol{\Lambda}) = \langle u^{(n)}_{1,-\boldsymbol{\Lambda}}|\Theta|u^{(n)}_{2,\boldsymbol{\Lambda}}\rangle = e^{-i\chi_{n,\boldsymbol{\Lambda}}}\langle u^{(n)}_{1,-\boldsymbol{\Lambda}}|u^{(n)}_{1,-\boldsymbol{\Lambda}}\rangle = e^{-i\chi_{n,\boldsymbol{\Lambda}}}. \tag{5.70}$$

and From Eq. (5.49)

$$w^{(n)}_{21}(\boldsymbol{\Lambda}) = -w^{(n)}_{12}(-\boldsymbol{\Lambda}) = -\langle u^{(n)}_{1,\boldsymbol{\Lambda}}|\Theta|u^{(n)}_{2,-\boldsymbol{\Lambda}}\rangle \tag{5.71}$$

Since at momenta $\boldsymbol{\Lambda}$ the Hamiltonian is time reversal invariant, then $|u^{(n)}_{i\boldsymbol{\Lambda}}\rangle = |u^{(n)}_{i,-\boldsymbol{\Lambda}}\rangle$. Therefore

$$w^{(n)}_{21}(\boldsymbol{\Lambda}) = -\langle u^{(n)}_{1,-\boldsymbol{\Lambda}}|\Theta|u^{(n)}_{2,\boldsymbol{\Lambda}}\rangle = -w^{(n)}_{12}(\boldsymbol{\Lambda}) = -e^{-i\chi_{n,\boldsymbol{\Lambda}}} \tag{5.72}$$

Equation (5.72) shows that at the time reversal invariant momenta $\mathbf{\Lambda}$ the matrix w is fully antisymmetric.

$$w(\mathbf{\Lambda}) = \begin{pmatrix} 0 & e^{-i\chi_{1,\mathbf{\Lambda}}} & 0 & 0 & 0 & \cdots \\ -e^{-i\chi_{1,\mathbf{\Lambda}}} & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & e^{-i\chi_{2,\mathbf{\Lambda}}} & 0 & \cdots \\ 0 & 0 & -e^{-i\chi_{2,\mathbf{\Lambda}}} & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{5.73}$$

It is interesting to notice that if M is a $m \times m$ antisymmetric matrix ($M^T = -M$)then

$$\det[M] = \det[M^T] = \det[-M] = (-1)^m \det[M]. \tag{5.74}$$

Notice that if m is odd then $\det[M] = 0$. In our case, if the Hamiltonian has N Kramer's pairs the $w(\mathbf{\Lambda})$ is a even-dimensional $2N \times 2N$ matrix. Therefore, $\det[w(\mathbf{\Lambda})] \neq 0$.

A now well known quantity usually defined for a given antisymmetric matrix M is it Pfaffian, introduced by Johann Friedrich Pfaff, and it is denoted by

$$\mathrm{Pf}[M] = M_{12}. \tag{5.75}$$

Despite the very complicated algebra involved in the theory, the Pfaffian of $w(\mathbf{\Lambda})$ is given by

$$\begin{aligned} \mathrm{Pf}[w(\mathbf{\Lambda})] &= w_{12}(\mathbf{\Lambda}) w_{34}(\mathbf{\Lambda}) \cdots w_{2N-1,2N}(\mathbf{\Lambda}) \\ &= e^{-i\chi_{1,\mathbf{\Lambda}}} e^{-i\chi_{2,\mathbf{\Lambda}}} \ldots e^{-i\chi_{N,\mathbf{\Lambda}}} = e^{-i\sum_{i=1}^{N} \chi_{i\mathbf{\Lambda}}} \end{aligned} \tag{5.76}$$

This quantity is related to the determinant of $w(\mathbf{\Lambda})$ as

$$\mathrm{Pf}[w(\mathbf{\Lambda})]^2 = \det[w(\mathbf{\Lambda})]. \tag{5.77}$$

Equation (5.77) shows that the $\det[w(\mathbf{\Lambda})]$ is always non negative. The topological invariant ν is defined as

$$(-1)^\nu = \prod_i \frac{\mathrm{Pf}[w(\mathbf{\Lambda}_i)]}{\sqrt{\det[w(\mathbf{\Lambda}_i)]}}, \tag{5.78}$$

where $\mathbf{\Lambda}_i$ are the time reversal symmetric momenta o the Brillouin zone.

To get some more clear idea of the meaning of this quantity lets consider as an example a simple two-dimensional model where the Hamiltonian possesses only two bands. In this case the matrix $w(\mathbf{\Lambda})$ is a 2×2 matrix, given by

$$w(\mathbf{\Lambda}) = \begin{bmatrix} 0 & w_{12}(\mathbf{\Lambda}) \\ -w_{12}(\mathbf{\Lambda}) & 0 \end{bmatrix} = \begin{pmatrix} 0 & e^{-i\chi_{\mathbf{\Lambda}}} \\ -e^{-i\chi_{\mathbf{\Lambda}}} & 0 \end{pmatrix}. \tag{5.79}$$

Then $\det[w(\mathbf{\Lambda})] = [w_{12}(\mathbf{\Lambda})]^2 = e^{-2i\chi_{\mathbf{\Lambda}}}$ and $\mathrm{Pf}[w(\mathbf{\Lambda})] = w_{12}(\mathbf{\Lambda}) = e^{-i\chi_{\mathbf{\Lambda}}}$. As we have shown above, there are vectors in the Brillouin zone where the Hamiltonian is time-reversal symmetric, they are $\mathbf{\Lambda}_1 = 0$ and $\mathbf{\Lambda}_2 = \boldsymbol{G}/2$. They corresponds to four point in the first Brillouin zone, namely $\mathbf{\Lambda}_1 = (0, 0)$,$\mathbf{\Lambda}_2 = (0, \pi)$, $\mathbf{\Lambda}_3 = (\pi, 0)$ and $\mathbf{\Lambda}_4 = (\pi, \pi)$. Then

$$(-1)^\nu = \prod_{i=1}^{4} \frac{\mathrm{Pf}[w(\mathbf{\Lambda}_i)]}{|\mathrm{Pf}[w(\mathbf{\Lambda}_i)]|}, \tag{5.80}$$

where we have used the Eq. (5.77). More explicitly, in terms of the matrix elements of w we have

$$(-1)^\nu = \prod_{i=1}^{4} \frac{w_{12}(\mathbf{\Lambda}_i)}{|w_{12}(\mathbf{\Lambda}_i)|} = \prod_{i=1}^{4} \mathrm{sign}[w_{12}(\mathbf{\Lambda}_i)]. \tag{5.81}$$

From Eq. (5.52) we see that $w_{12}(\mathbf{\Lambda}_i)$ is the projection of the time reversed state $\Theta|u_{2,\mathbf{\Lambda}_i}\rangle$ onto the state $|u_{1,\mathbf{\Lambda}_i}\rangle$ (they form a Kramer's pair) and the time reversal symmetric momenta $\mathbf{\Lambda}_i$. We observe then that if $\mathrm{sign}[w_{12}(\mathbf{\Lambda}_i)] = 1$ then the time reversed $\Theta|u_{2,\mathbf{\Lambda}_i}\rangle$ is in a sense "parallel" to $|u_{1,\mathbf{\Lambda}_i}\rangle$, but it is "anti-parallel" if $\mathrm{sign}[w_{12}(\mathbf{\Lambda}_i)] = -1$ or *twisted.* The rhs of the Eq. (5.81) is positive if an *even* number of Kramer's pair are *twisted* and negative otherwise. Therefore, for an *even* number of *twisted* Kramer pairs ν is even while for an *odd* number of *twisted* Kramer pairs ν odd. This shows that ν is defined only modulo 2. We can set the two values of $\nu = 0, 1$ to define two topologically distinct phases that are called *trivial* $(\nu = 0)$ and *non trivial* $(\nu = 1)$. ν is then the $\mathbb{Z}_2$ number that topologically classifies all the time reversal invariant insulators with $2N$ occupied bands.

6

Majorana Fermions in realistic wires

Lets start with the Hamiltonian

$$H = H_{\mathrm{dot}} + H_{\mathrm{lead}} + H_{\mathrm{wire}} + H_{\mathrm{dot-lead}} + H_{\mathrm{dot-wire}}, \tag{6.1}$$

where

$$H_{\mathrm{dot}} = \sum_{s} \varepsilon_{0,s} c_{0,s}^{\dagger} c_{0,s} + U n_{\uparrow} n_{\downarrow}, \tag{6.2}$$

$$H_{\mathrm{lead}} = \sum_{\mathbf{k},s} \varepsilon_{\mathbf{k},s} c_{\mathbf{k},s}^{\dagger} c_{\mathbf{k},s} \tag{6.3}$$

$$H_{\mathrm{dot-lead}} = \sum_{\mathbf{k},s} \left(V_{\mathbf{k}} c_{0,s}^{\dagger} c_{\mathbf{k},s} + V_{\mathbf{k}} c_{\mathbf{k},s}^{\dagger} c_{0,s} \right) \tag{6.4}$$

$$H_{\mathrm{dot-wire}} = -t_0 \sum_{s} \left(c_{0,s}^{\dagger} c_{1,s} + c_{1,s}^{\dagger} c_{0,s} \right). \tag{6.5}$$

Finally we can write

$$H_{\mathrm{wire}} = H_0 + H_R + H_{SC}, \tag{6.6}$$

where

$$H_0 = \sum_{j=1,s}^{N} \left(-\mu + V_Z \sigma_{ss}^{z} \right) c_{js}^{\dagger} c_{js} - t \sum_{j=1,s}^{N-1} \left(c_{j+1,s}^{\dagger} c_{j,s} + c_{j,s}^{\dagger} c_{j+1,s} \right), \tag{6.7}$$

$$H_R = \sum_{j=1}^{N-1} \sum_{ss'} (-i\alpha_R) c^\dagger_{j+1,s} \hat{z} \cdot (\vec{\sigma}_{ss'} \times \hat{x})\, c_{j,s'} + H.c. \tag{6.8}$$

and

$$H_{\rm SC} = \Delta \sum_{j=1}^{N} \left(c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} + c_{j\uparrow} c_{j\downarrow} \right). \tag{6.9}$$

Before calculating the Green's functions, let us first to expand the Hamiltonian (6.8). Note that

$$\vec{\sigma}_{ss'} \times \hat{x} = \sigma^z_{ss'} \hat{y} - \sigma^y_s s' \hat{z}, \tag{6.10}$$

therefore

$$\hat{z} \cdot (\vec{\sigma}_{ss'} \times \hat{x}) = -\sigma^y_{ss'}. \tag{6.11}$$

With this we can write

$$H_{\rm R} = \sum_j \alpha_R \left(c^\dagger_{j+1,\uparrow} c_{j,\downarrow} + c^\dagger_{j,\downarrow} c_{j+1,\uparrow} - c^\dagger_{j,\uparrow} c_{j+1,\downarrow} - c^\dagger_{j+1,\downarrow} c_{j,\uparrow} \right). \tag{6.12}$$

The Hamiltonian for the wire becomes then

$$\begin{aligned} H_{\rm wire} \;\; = \;\; & \sum_{j=1,s}^{N} \varepsilon_{j,s} c^\dagger_{j,s} c_{j,s} - t \sum_{j=1,s}^{N-1} \left(c^\dagger_{j+1,s} c_{j,s} + c^\dagger_{j,s} c_{j+1,s} \right) + \Delta \sum_{j=1}^{N} \left(c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} + c_{j\downarrow} c_{j\uparrow} \right) \\ & + \sum_j \alpha_R \left(c^\dagger_{j+1,\uparrow} c_{j,\downarrow} + c^\dagger_{j,\downarrow} c_{j+1,\uparrow} - c^\dagger_{j,\uparrow} c_{j+1,\downarrow} - c^\dagger_{j+1,\downarrow} c_{j,\uparrow} \right) \end{aligned} \tag{6.13}$$

6.1 Electron Green's function

Let us start by calculating the local Green's function for the wire only. We start by assuming that the chain has N sites and we will calculate the Green's function of the site $N-1$ in the presence of the site N only. We define the local Green's function as

$$G_{js,js'}(\omega) \equiv \langle\langle c_{j,s}; c^\dagger_{j,s'} \rangle\rangle. \tag{6.14}$$

The equation of motion for the Green's function $G_{N-1s,N-1s'}(\omega)$ is

$$\omega \langle\langle c_{N-1,s}; c^\dagger_{N-1,s'} \rangle\rangle = \delta_{ss'} + \langle\langle [c_{N-1,s}, H]; c^\dagger_{N-1,s'} \rangle\rangle. \tag{6.15}$$

Now

$$[c_{N-1,\uparrow}, H] = \varepsilon_{N-1,\uparrow} c_{N-1,\downarrow} + \Delta c^\dagger_{N-1,\downarrow} - t c_{N,\uparrow} - \alpha_R c_{N,\downarrow} \tag{6.16}$$

and

$$[c_{N-1,\downarrow}, H] = \varepsilon_{N-1,\downarrow} c_{N-1,\downarrow} - \Delta c^{\dagger}_{N-1,\uparrow} - t c_{N,\downarrow} + \alpha_R c_{N,\uparrow} \tag{6.17}$$

Then we have

$$\begin{aligned}(\omega - \varepsilon_{N-1,\uparrow})\langle\langle c_{N-1,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle &= \delta_{s'\uparrow} + \Delta\langle\langle c^{\dagger}_{N-1,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle - t\langle\langle c_{N,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle \\ &\quad -\alpha_R\langle\langle c_{N,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle \end{aligned}\tag{6.18}$$

and

$$\begin{aligned}(\omega - \varepsilon_{N-1,\uparrow})\langle\langle c_{N-1,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle &= \delta_{s'\downarrow} - \Delta\langle\langle c^{\dagger}_{N-1,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle - t\langle\langle c_{N,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle \\ &\quad +\alpha_R\langle\langle c_{N,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle. \end{aligned}\tag{6.19}$$

Note that the two new Green's functions $\langle\langle c^{\dagger}_{N-1,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle$ and $\langle\langle c^{\dagger}_{N-1,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle$ appeared. Their equation of motion read

$$\omega\langle\langle c^{\dagger}_{N-1,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle = \langle\langle [c^{\dagger}_{N-1,\downarrow}, H]; c^{\dagger}_{N-1,s'}\rangle\rangle \tag{6.20}$$

and

$$\omega\langle\langle c^{\dagger}_{N-1,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle = \langle\langle [c^{\dagger}_{N-1,\uparrow}, H]; c^{\dagger}_{N-1,s'}\rangle\rangle. \tag{6.21}$$

$$[c^{\dagger}_{N-1,\downarrow}, H] = -\varepsilon_{N-1,\downarrow} c^{\dagger}_{N-1,\downarrow} + \Delta c_{N-1,\uparrow} + t c^{\dagger}_{N,\downarrow} - \alpha_R c^{\dagger}_{N,\uparrow} \tag{6.22}$$

$$[c^{\dagger}_{N-1,\uparrow}, H] = -\varepsilon_{N-1,\uparrow} c^{\dagger}_{N-1,\uparrow} - \Delta c_{N-1,\downarrow} + t c^{\dagger}_{N,\uparrow} + \alpha_R c^{\dagger}_{N,\downarrow}. \tag{6.23}$$

Then we find

$$\begin{aligned}(\omega + \varepsilon_{N-1,\downarrow})\langle\langle c^{\dagger}_{N-1,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle &= \Delta\langle\langle c_{N-1,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle + t\langle\langle c^{\dagger}_{N,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle \\ &\quad -\alpha_R\langle\langle c^{\dagger}_{N,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle \end{aligned}\tag{6.24}$$

and

$$\begin{aligned}(\omega + \varepsilon_{N-1,\uparrow})\langle\langle c^{\dagger}_{N-1,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle &= -\Delta\langle\langle c_{N-1,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle + t\langle\langle c^{\dagger}_{N,\uparrow}; c^{\dagger}_{N-1,s'}\rangle\rangle \\ &\quad +\alpha_R\langle\langle c^{\dagger}_{N,\downarrow}; c^{\dagger}_{N-1,s'}\rangle\rangle. \end{aligned}\tag{6.25}$$

From the above we see that it is useful to define the Green's function matrix

$$\mathbf{G}_{i,j}(\omega) = \begin{pmatrix} \langle\langle c_{i,\uparrow}; c^\dagger_{j,\uparrow}\rangle\rangle & \langle\langle c_{i,\uparrow}; c^\dagger_{j,\downarrow}\rangle\rangle & \langle\langle c_{i,\uparrow}; c_{j,\uparrow}\rangle\rangle & \langle\langle c_{i,\uparrow}; c_{j,\downarrow}\rangle\rangle \\ \langle\langle c_{i,\downarrow}; c^\dagger_{j,\uparrow}\rangle\rangle & \langle\langle c_{i,\downarrow}; c^\dagger_{j,\downarrow}\rangle\rangle & \langle\langle c_{i,\downarrow}; c_{j,\uparrow}\rangle\rangle & \langle\langle c_{i,\downarrow}; c_{j,\downarrow}\rangle\rangle \\ \langle\langle c^\dagger_{i,\uparrow}; c^\dagger_{j,\uparrow}\rangle\rangle & \langle\langle c^\dagger_{i,\uparrow}; c^\dagger_{j,\downarrow}\rangle\rangle & \langle\langle c^\dagger_{i,\uparrow}; c_{j,\uparrow}\rangle\rangle & \langle\langle c^\dagger_{i,\uparrow}; c_{j,\downarrow}\rangle\rangle \\ \langle\langle c^\dagger_{i,\downarrow}; c^\dagger_{j,\uparrow}\rangle\rangle & \langle\langle c^\dagger_{i,\downarrow}; c^\dagger_{j,\downarrow}\rangle\rangle & \langle\langle c^\dagger_{i,\downarrow}; c_{j,\uparrow}\rangle\rangle & \langle\langle c^\dagger_{i,\downarrow}; c_{j,\downarrow}\rangle\rangle \end{pmatrix}, \tag{6.26}$$

and

$$\mathbf{g}_{j,j}(\omega) = \begin{pmatrix} \frac{1}{\omega-\varepsilon_\uparrow} & 0 & 0 & 0 \\ 0 & \frac{1}{\omega-\varepsilon_\downarrow} & 0 & 0 \\ 0 & 0 & \frac{1}{\omega+\varepsilon_\uparrow} & 0 \\ 0 & 0 & 0 & \frac{1}{\omega+\varepsilon_\downarrow} \end{pmatrix}, \tag{6.27}$$

With this we can write the Green's function in the form:

$$\begin{aligned} \mathbf{G}_{N-1,N-1}(\omega) &= \mathbf{g}_{N-1,N-1}(\omega) + \mathbf{g}_{N-1,N-1}(\omega)\mathbf{V}\mathbf{G}_{N-1,N-1}(\omega) \\ &\quad + \mathbf{g}_{N-1,N-1}(\omega)\mathbf{t}\mathbf{G}_{N,N-1}(\omega), \end{aligned} \tag{6.28}$$

where

$$\mathbf{V} = \begin{pmatrix} 0 & 0 & 0 & \Delta \\ 0 & 0 & -\Delta & 0 \\ 0 & -\Delta & 0 & 0 \\ \Delta & 0 & 0 & 0 \end{pmatrix} \tag{6.29}$$

and

$$\mathbf{t} = \begin{pmatrix} -t & -\alpha_R & 0 & 0 \\ -\alpha_R & -t & 0 & 0 \\ 0 & 0 & t & \alpha_R \\ 0 & 0 & -\alpha_R & t \end{pmatrix}, \tag{6.30}$$

We can still write the expression (6.28) as in the more compact form,

$$\mathbf{G}_{N-1,N-1}(\omega) = \tilde{\mathbf{g}}_{N-1,N-1}(\omega) + \tilde{\mathbf{g}}_{N-1,N-1}(\omega)\mathbf{t}\mathbf{G}_{N,N-1}(\omega), \tag{6.31}$$

where we have defined

$$\tilde{\mathbf{g}}_{j,j}(\omega) = (1-\mathbf{V})^{-1}\mathbf{g}_{j,j}(\omega). \tag{6.32}$$

Now we can write

$$\mathbf{G}_{N,N-1}(\omega) = \tilde{\mathbf{g}}_{N,N}(\omega)\hat{\mathbf{t}}^\dagger\mathbf{G}_{N-1,N-1}(\omega) \tag{6.33}$$

Replacing the Eq. (6.33) into (6.28) we obtain

$$\mathbf{G}_{N-1,N-1}(\omega) = \left[1 - \tilde{\mathbf{g}}_{N-1,N-1}(\omega)\mathbf{t}\tilde{\mathbf{g}}_{N,N}(\omega)\mathbf{t}^\dagger\right]^{-1}\tilde{\mathbf{g}}_{N-1,N-1}(\omega) \tag{6.34}$$

6.1.1 The Green's function for the dot

At the dot site we have

$$\langle\langle c_{0,s}; c^\dagger_{0,s'}\rangle\rangle = \delta_{ss'} + \langle\langle [c_{0,s}, H]; c^\dagger_{0,s'}\rangle\rangle. \tag{6.35}$$

Now,

$$[c_{0,s}, H] = \varepsilon_{0,s} c_{0,s} + U n_{0,\bar{s}} c_{0,s} - t_0 c_{1,s} + \sum_{\mathbf{k}} V_{\mathbf{k}} c_{\mathbf{k},s} \tag{6.36}$$

then

$$(\omega - \varepsilon_{0,s})\,\langle\langle c_{0,s}; c^\dagger_{0,s'}\rangle\rangle = \delta_{ss'} + U\langle\langle n_{0,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle - t_0\langle\langle c_{1,s}; c^\dagger_{0,s'}\rangle\rangle + \sum_{\mathbf{k}} V_{\mathbf{k}}\langle\langle c_{\mathbf{k},s}; c^\dagger_{0,s'}\rangle\rangle \tag{6.37}$$

Now we need three other Green's functions of the right side of the equation above. Last focus on the first and last one. Their equation of motion read

$$\begin{aligned}(\omega - \varepsilon_{0,s} - U)\,\langle\langle n_{0,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \;=\;& \langle n_{0,\bar{s}}\rangle\delta_{ss'} + \langle c^\dagger_{0,\bar{s}} c_{0,s}\rangle\delta_{s',\bar{s}} + \sum_{\mathbf{k}} V_{\mathbf{k}}\langle\langle n_{0,\bar{s}} c_{\mathbf{k},s}; c^\dagger_{0,s'}\rangle\rangle \\ &+ \sum_{\mathbf{k}} V_{\mathbf{k}}\langle\langle c^\dagger_{0,\bar{s}} c_{\mathbf{k},\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle - \sum_{\mathbf{k}} V^*_{\mathbf{k}}\langle\langle c^\dagger_{\mathbf{k},\bar{s}} c_{0,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \\ &- t_0\langle\langle n_{0,\bar{s}} c_{1,s}; c^\dagger_{0,s'}\rangle\rangle - t_0\langle\langle c^\dagger_{0,\bar{s}} c_{1,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \\ &+ t_0\langle\langle c^\dagger_{1,\bar{s}} c_{0,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle.\end{aligned} \tag{6.38}$$

We now use the Hubbard I decoupling procedure,

$$\langle\langle n_{0,\bar{s}} c_{1,s}; c^\dagger_{0,s'}\rangle\rangle \approx \langle n_{0,\bar{s}}\rangle\langle\langle c_{1,s}; c^\dagger_{0,s'}\rangle\rangle \tag{6.39a}$$

$$\sum_{\mathbf{k}} V_{\mathbf{k}}\langle\langle n_{0,\bar{s}} c_{\mathbf{k},s}; c^\dagger_{0,s'}\rangle\rangle \approx \langle n_{0,\bar{s}}\rangle \sum_{\mathbf{k}} V_{\mathbf{k}}\langle\langle n_{0,\bar{s}} c_{\mathbf{k},s}; c^\dagger_{0,s'}\rangle\rangle \tag{6.39b}$$

$$\sum_{\mathbf{k}} V_{\mathbf{k}}\langle\langle c^\dagger_{0,\bar{s}} c_{\mathbf{k},\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \approx \sum_{\mathbf{k}} V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}} c_{\mathbf{k},\bar{s}}\rangle\langle\langle c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \tag{6.39c}$$

$$\sum_{\mathbf{k}} V^*_{\mathbf{k}}\langle\langle c^\dagger_{\mathbf{k},\bar{s}} c_{0,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \approx \sum_{\mathbf{k}} V^*_{\mathbf{k}}\langle c^\dagger_{\mathbf{k},\bar{s}} c_{0,\bar{s}}\rangle\langle\langle c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \tag{6.39d}$$

$$\langle\langle c^\dagger_{0,\bar{s}} c_{1,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \approx \langle c^\dagger_{0,\bar{s}} c_{1,\bar{s}}\rangle\langle\langle c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \tag{6.39e}$$

$$\langle\langle c^\dagger_{1,\bar{s}} c_{0,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \approx \langle c^\dagger_{1,\bar{s}} c_{0,\bar{s}}\rangle\langle\langle c_{0,s}; c^\dagger_{0,s'}\rangle\rangle. \tag{6.39f}$$

Within the Hubbard I decoupling procedure we assume that $\sum_{\mathbf{k}} V^*_{\mathbf{k}}\langle c^\dagger_{\mathbf{k},\bar{s}} c_{0,\bar{s}}\rangle = \sum_{\mathbf{k}} V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}} c_{\mathbf{k},\bar{s}}\rangle$ and that $\langle c^\dagger_{0,\bar{s}} c_{1,\bar{s}}\rangle = \langle c^\dagger_{1,\bar{s}} c_{0,\bar{s}}\rangle$. With these approximations we obtain

$$\begin{aligned}(\omega - \varepsilon_{0,s} - U)\,\langle\langle n_{0,\bar{s}} c_{0,s}; c^\dagger_{0,s'}\rangle\rangle \;=\;& \langle n_{0,\bar{s}}\rangle\delta_{ss'} + \langle c^\dagger_{0,\bar{s}} c_{0,s}\rangle\delta_{s',\bar{s}} + \langle n_{0,\bar{s}}\rangle \sum_{\mathbf{k}} V_{\mathbf{k}}\langle\langle c_{\mathbf{k},s}; c^\dagger_{0,s'}\rangle\rangle \\ &- t_0\langle n_{0,\bar{s}}\rangle\langle\langle c_{1,s}; c^\dagger_{0,s'}\rangle\rangle.\end{aligned} \tag{6.40}$$

Replacing Eq. (6.40) into (6.37) we obtain

$$\begin{aligned}(\omega-\varepsilon_{0,s})\,\langle\langle c_{0,s};c_{0,s'}^{\dagger}\rangle\rangle &= \delta_{ss'}+\frac{U\langle n_{0,\bar{s}}\rangle\delta_{ss'}+U\langle c_{0,\bar{s}}^{\dagger}c_{0,s}\rangle\delta_{\bar{s}s'}}{\omega-\varepsilon_{0,s}-U}-\left(1+\frac{U\langle n_{0,\bar{s}}\rangle}{\omega-\varepsilon_{0,s}-U}\right)\\ &\times\sum_{\mathbf{k}}V_{\mathbf{k}}\langle\langle c_{\mathbf{k},s};c_{0,s'}^{\dagger}\rangle\rangle-\left(1+\frac{U\langle n_{0,\bar{s}}\rangle}{\omega-\varepsilon_{0,s}-U}\right)t_0\langle\langle c_{1,s};c_{0,s'}^{\dagger}\rangle\rangle.\end{aligned} \tag{6.41}$$

Now we can easily obtain an expression for $\langle\langle c_{\mathbf{k},s};c_{0,s'}^{\dagger}\rangle\rangle$,

$$\langle\langle c_{\mathbf{k},s};c_{0,s'}^{\dagger}\rangle\rangle=\frac{V_{\mathbf{k}}^{*}}{\omega-\varepsilon_{\mathbf{k}}}\langle\langle c_{0,s};c_{0,s'}^{\dagger}\rangle\rangle. \tag{6.42}$$

Replacing Eq. (6.42) into Eq. (6.43) we obtain

$$\begin{aligned}(\omega-\varepsilon_{0,s})\,\langle\langle c_{0,s};c_{0,s'}^{\dagger}\rangle\rangle &= \delta_{ss'}+\frac{U\langle n_{0,\bar{s}}\rangle\delta_{\bar{s}s'}+U\langle c_{0,\bar{s}}^{\dagger}c_{0,s}\rangle\delta_{\bar{s}s'}}{\omega-\varepsilon_{0,s}-U}+\left(1+\frac{U\langle n_{0,\bar{s}}\rangle}{\omega-\varepsilon_{0,s}-U}\right)\\ &\times\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k}}}\langle\langle c_{0,s};c_{0,s'}^{\dagger}\rangle\rangle-\left(1+\frac{U\langle n_{0,\bar{s}}\rangle}{\omega-\varepsilon_{0,s}-U}\right)t_0\langle\langle c_{1,s};c_{0,s'}^{\dagger}\rangle\rangle.\end{aligned} \tag{6.43}$$

or

$$\begin{aligned}&\left[\omega-\varepsilon_{0,s}-\left(1+\frac{U\langle n_{0,\bar{s}}\rangle}{\omega-\varepsilon_{0,s}-U}\right)\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k}}}\right]\langle\langle c_{0,s};c_{0,s'}^{\dagger}\rangle\rangle=\delta_{ss'}\\ &+\frac{U\langle n_{0,\bar{s}}\rangle\delta_{ss'}+U\langle c_{0,\bar{s}}^{\dagger}c_{0,s}\rangle\delta_{\bar{s}s'}}{\omega-\varepsilon_{0,s}-U}-\left(1+\frac{U\langle n_{0,\bar{s}}\rangle}{\omega-\varepsilon_{0,s}-U}\right)t_0\langle\langle c_{1,s};c_{0,s'}^{\dagger}\rangle\rangle.\end{aligned} \tag{6.44}$$

To simplify the expression above we will assume the wide band limit, in which take $\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k}}}=-i\Gamma$. With this, we can write

$$\begin{aligned}&\left[1+i\left(\frac{1}{\omega-\varepsilon_{0,s}}+\frac{U\langle n_{0,\bar{s}}\rangle}{(\omega-\varepsilon_{0,s})(\omega-\varepsilon_{0,s}-U)}\right)\Gamma\right]\langle\langle c_{0,s};c_{0,s'}^{\dagger}\rangle\rangle=\frac{\delta_{ss'}}{\omega-\varepsilon_{0,s}}\\ &+\frac{U\langle n_{0,\bar{s}}\rangle\delta_{ss'}+U\langle c_{0,\bar{s}}^{\dagger}c_{0,s}\rangle\delta_{\bar{s}s'}}{(\omega-\varepsilon_{0,s})(\omega-\varepsilon_{0,s}-U)}-\left(\frac{1}{\omega-\varepsilon_{0,s}}+\frac{U\langle n_{0,\bar{s}}\rangle}{(\omega-\varepsilon_{0,s})(\omega-\varepsilon_{0,s}-U)}\right)t_0\langle\langle c_{1,s};c_{0,s'}^{\dagger}\rangle\rangle.\end{aligned} \tag{6.45}$$

Where we have divided both sides of the Eq. (6.50) by $\omega-\varepsilon_{0,s}$. With some algebraic manipulation we can write

$$\begin{aligned}[1+ig_{0s,0s}(\omega)\Gamma]\,\langle\langle c_{0,s};c_{0,s'}^{\dagger}\rangle\rangle &= g_{0s,0s}(\omega)\delta_{ss'}+\frac{U\langle c_{0,\bar{s}}^{\dagger}c_{0,s}\rangle\delta_{\bar{s}s'}}{(\omega-\varepsilon_{0,s})(\omega-\varepsilon_{0,s}-U)}\\ &-g_{0s,0s}(\omega)t_0\langle\langle c_{1,s};c_{0,s'}^{\dagger}\rangle\rangle.\end{aligned} \tag{6.46}$$

where we have defined

$$g_{0s,0s}(\omega) = \frac{1-\langle n_{0,\bar{s}}\rangle}{\omega-\varepsilon_{0,s}} + \frac{\langle n_{0,\bar{s}}\rangle}{\omega-\varepsilon_{0,s}-U}, \tag{6.47}$$

that is the exact Green's function for the dot in the atomic approximation ($V_{\mathbf{k}} = t_0 = 0$).

Our work is not yet done, since we will need the Green's function $\langle\langle c^\dagger_{0,s}; c^\dagger_{0,s'}\rangle\rangle$. This Green's function would be always zero if no superconducting pairing were present in the wire. Proceeding in the same way we have done up to here we obtain

$$\begin{aligned}\left[1+i\left(\frac{1}{\omega+\varepsilon_{0,s}} + \frac{U\langle n_{0,\bar{s}}\rangle}{(\omega-\varepsilon_{0,s})(\omega+\varepsilon_{0,s}+U)}\right)\Gamma\right]\langle\langle c^\dagger_{0,s}; c^\dagger_{0,s'}\rangle\rangle &= \frac{-U\langle c^\dagger_{0,\bar{s}}c_{0,s}\rangle\delta_{s'\bar{s}}}{(\omega+\varepsilon_{0,s})(\omega+\varepsilon_{0,s}+U)} \\ &+\left(\frac{1}{\omega+\varepsilon_{0,s}} + \frac{U\langle n_{0,\bar{s}}\rangle}{(\omega+\varepsilon_{0,s})(\omega+\varepsilon_{0,s}+U)}\right)t_0\langle\langle c^\dagger_{1,s}; c^\dagger_{0,s'}\rangle\rangle.\end{aligned} \tag{6.48}$$

We can also define

$$h_{0s,0s}(\omega) = \frac{1+\langle n_{0,\bar{s}}\rangle}{\omega+\varepsilon_{0,s}} - \frac{\langle n_{0,\bar{s}}\rangle}{\omega+\varepsilon_{0,s}+U}, \tag{6.49}$$

to write

$$[1+ih_{0s,0s}\Gamma]\,\langle\langle c^\dagger_{0,s}; c^\dagger_{0,s'}\rangle\rangle = \frac{-U\langle c^\dagger_{0,\bar{s}}c^\dagger_{0,s}\rangle\delta_{s'\bar{s}}}{(\omega+\varepsilon_{0,s})(\omega+\varepsilon_{0,s}+U)} + h_{0s,0s}t_0\langle\langle c^\dagger_{1,s}; c^\dagger_{0,s'}\rangle\rangle. \tag{6.50}$$

We can now define the undressed Green's function for the dot

$$\mathbf{g}_{0,0}(\omega) = \begin{bmatrix} \tilde{g}_{0\uparrow,0\uparrow}(\omega) & \frac{A_g(\omega)U\langle c^\dagger_{0,\downarrow}c_{0,\uparrow}\rangle}{(\omega-\varepsilon_{0,\uparrow})(\omega-\varepsilon_{0,\uparrow}-U)} & 0 & \frac{A_g(\omega)U\langle c_{0,\downarrow}c_{0,\uparrow}\rangle}{(\omega-\varepsilon_{0,\uparrow})(\omega-\varepsilon_{0,\uparrow}-U)} \\ \frac{A_g(\omega)U\langle c^\dagger_{0,\uparrow}c_{0,\downarrow}\rangle}{(\omega-\varepsilon_{0,\downarrow})(\omega-\varepsilon_{0,\downarrow}-U)} & \tilde{g}_{0\downarrow,0\downarrow}(\omega) & \frac{A_g(\omega)U\langle c_{0,\uparrow}c_{0,\downarrow}\rangle}{(\omega-\varepsilon_{0,\downarrow})(\omega-\varepsilon_{0,\downarrow}-U)} & 0 \\ 0 & \frac{A_h(\omega)U\langle c^\dagger_{0,\uparrow}c^\dagger_{0,\downarrow}\rangle}{(\omega+\varepsilon_{0,\uparrow})(\omega+\varepsilon_{0,\uparrow}+U)} & \tilde{h}_{0\uparrow,0\uparrow}(\omega) & \frac{A_h(\omega)U\langle c_{0,\downarrow}c^\dagger_{0,\uparrow}\rangle}{(\omega+\varepsilon_{0,\uparrow})(\omega+\varepsilon_{0,\uparrow}+U)} \\ \frac{A_h(\omega)U\langle c^\dagger_{0,\downarrow}c^\dagger_{0,\uparrow}\rangle}{(\omega+\varepsilon_{0,\downarrow})(\omega+\varepsilon_{0,\downarrow}+U)} & 0 & \frac{A_h(\omega)U\langle c_{0,\uparrow}c^\dagger_{0,\downarrow}\rangle}{(\omega+\varepsilon_{0,\downarrow})(\omega+\varepsilon_{0,\downarrow}+U)} & \tilde{h}_{0\downarrow,0\downarrow}(\omega) \end{bmatrix}, \tag{6.51}$$

with $A_g(\omega) = [1+i\Gamma g_{0s,0s}(\omega)]^{-1}$, $A_h(\omega) = [1+i\Gamma h_{0s,0s}(\omega)]^{-1}$, $\tilde{g}_{0s,0s}(\omega) = A_g(\omega)g_{0s,0s}(\omega)$ and $\tilde{h}_{0s,0s}(\omega) = A_h(\omega)h_{0s,0s}(\omega)$. The coupling of the quantum dot with the first site of the wire is define as

$$\mathbf{t}_0 = \begin{pmatrix} -t_0 & 0 & 0 & 0 \\ 0 & -t_0 & 0 & 0 \\ 0 & 0 & t_0 & 0 \\ 0 & 0 & 0 & t_0 \end{pmatrix}. \tag{6.52}$$

Note that the Green's function matrix (6.51) depends on various expectation values, namely, the two occupations $\langle n_{0\uparrow}\rangle$ and $\langle n_{0\downarrow}\rangle$, appearing in the diagonal elements of $\mathbf{g}_{0,0}(\omega)$.

These occupations are readily calculated as

$$\langle n_{0\uparrow}\rangle = -\frac{1}{\pi}\int_{\infty}^{\infty} f(\omega)\mathrm{Im}\ [\mathbf{G}_{0,0}(\omega)]_{1,1}d\omega, \tag{6.53}$$

and

$$\langle n_{0\downarrow}\rangle = -\frac{1}{\pi}\int_{\infty}^{\infty} f(\omega)\mathrm{Im}\ [\mathbf{G}_{0,0}(\omega)]_{2,2}d\omega, \tag{6.54}$$

where $f(\omega)$ is the Fermi function. There are other and eight other quantities appearing in the off-diagonal terms of the matrix (6.51). However, we note that, due to the anti-commutation relations between fermionic operators, there are in fact only four independent quantities that are calculated as

$$\langle c^{\dagger}_{0,\downarrow}c_{0,\uparrow}\rangle = -\langle c_{0,\uparrow}c^{\dagger}_{0,\downarrow}\rangle = -\frac{1}{\pi}\int_{\infty}^{\infty} f(\omega)\mathrm{Im}\ [\mathbf{G}_{0,0}(\omega)]_{1,2}d\omega, \tag{6.55a}$$

$$\langle c^{\dagger}_{0,\uparrow}c_{0,\downarrow}\rangle = -\langle c_{0,\downarrow}c^{\dagger}_{0,\uparrow}\rangle = -\frac{1}{\pi}\int_{\infty}^{\infty} f(\omega)\mathrm{Im}\ [\mathbf{G}_{0,0}(\omega)]_{2,1}d\omega, \tag{6.55b}$$

$$\langle c_{0,\downarrow}c_{0,\uparrow}\rangle = -\langle c_{0,\uparrow}c_{0,\downarrow}\rangle = -\frac{1}{\pi}\int_{\infty}^{\infty} f(\omega)\mathrm{Im}\ [\mathbf{G}_{0,0}(\omega)]_{1,4}d\omega. \tag{6.55c}$$

and

$$\langle c^{\dagger}_{0,\uparrow}c^{\dagger}_{0,\downarrow}\rangle = -\langle c^{\dagger}_{0,\downarrow}c^{\dagger}_{0,\uparrow}\rangle = -\frac{1}{\pi}\int_{\infty}^{\infty} f(\omega)\mathrm{Im}\ [\mathbf{G}_{0,0}(\omega)]_{4,1}d\omega, \tag{6.55d}$$

Because all of then are non-diagonal in spin index, they can be neglected in a preliminary calculation, at least for $\varepsilon_{\mathrm{dot}} + g_{\mathrm{dot}}V_Z \gg \varepsilon_F$.

6.2 Beyond the Hubbard I approximation

To go beyond the Hubbard I approximation and access the Kondo physics we will use the effective model, where only the spin up electrons couple with the single Majorana mode in the wire. This is described by the model

$$\begin{aligned} H_{\text{eff}} &= \sum_s \varepsilon_{\text{dot}} c^\dagger_{0,s} c_{0,s} + U n_{0,\uparrow} n_{0,\downarrow} + \lambda \left(c_{0,\downarrow} - c^\dagger_{0,\downarrow} \right) \gamma_1 + \sum_{\mathbf{k},s} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},s} c_{\mathbf{k},s} \\ &\quad + \sum_{\mathbf{k},s} V_{\mathbf{k}} \left(c^\dagger_{0,s} c_{\mathbf{k},s} + c^\dagger_{\mathbf{k},s} c_{0,s} \right). \end{aligned} \tag{6.56}$$

Let us start by calculating the local Green's function for the dot. Since the up and down spin components are now different, we will first calculate ofr spin down. then

$$(\omega - \varepsilon_{0,\downarrow}) \langle\langle c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle = 1 + U \langle\langle n_{0,\uparrow} c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle + \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle c_{\mathbf{k},\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle - \lambda \langle\langle \eta_1 ; c^\dagger_{0,\downarrow} \rangle\rangle. \tag{6.57}$$

Now,

$$(\omega - \varepsilon_{\mathbf{k},\downarrow}) \langle\langle c_{\mathbf{k},\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle = V^*_{\mathbf{k}} \langle\langle c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle, \tag{6.58}$$

therefore we can write

$$\left(\omega - \varepsilon_{0,\downarrow} - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \varepsilon_{\mathbf{k},\downarrow}} \right) \langle\langle c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle = 1 + U \langle\langle n_{0,\uparrow} c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle - \lambda \langle\langle \eta_1 ; c^\dagger_{0,\downarrow} \rangle\rangle. \tag{6.59}$$

$$\begin{aligned} (\omega - \varepsilon_{0,\downarrow} - U) \langle\langle n_{0,\uparrow} c_{0,\uparrow} ; c^\dagger_{0,\downarrow} \rangle\rangle &= \langle n_{0,\uparrow} \rangle + \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle n_{0,\uparrow} c_{\mathbf{k},\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle + \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle c^\dagger_{0,\uparrow} c_{\mathbf{k},\uparrow} c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle \\ &\quad - \sum_{\mathbf{k}} V^*_{\mathbf{k}} \langle\langle c^\dagger_{\mathbf{k},\uparrow} c_{0,\uparrow} c_{0,\downarrow} ; c_{0,\downarrow} \rangle\rangle + \lambda \langle\langle n_{0,\uparrow} \eta_1 ; c^\dagger_{0,\downarrow} \rangle\rangle \end{aligned} \tag{6.60}$$

Now,

$$\begin{aligned} (\omega - \varepsilon_{\mathbf{k},\downarrow}) \langle\langle n_{0,\uparrow} c_{\mathbf{k},\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle &= \sum_{\mathbf{q}} V_{\mathbf{q}} \langle\langle c^\dagger_{0,\uparrow} c_{\mathbf{q},\uparrow} c_{\mathbf{k},\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle - \sum_{\mathbf{q}} V^*_{\mathbf{q}} \langle\langle c^\dagger_{\mathbf{q},\uparrow} c_{0,\uparrow} c_{\mathbf{k},\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle \\ &\quad + V^*_{\mathbf{k}} \langle\langle n_{0,\uparrow} c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle, \end{aligned} \tag{6.61}$$

$$\begin{aligned} (\omega - \varepsilon_{0,\downarrow} + \varepsilon_{0,\uparrow} - \varepsilon_{\mathbf{k},\downarrow}) \langle\langle c^\dagger_{0,\uparrow} c_{\mathbf{k},\uparrow} c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle &= \langle c^\dagger_{0,\uparrow} c_{\mathbf{k},\uparrow} \rangle + \sum_{\mathbf{q}} V_{\mathbf{q}} \langle\langle c^\dagger_{0,\uparrow} c_{\mathbf{k},\uparrow} c_{\mathbf{q},\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle \\ + V_{\mathbf{k}} \langle\langle c^\dagger_{0,\uparrow} c_{0,\uparrow} c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle - \sum_{\mathbf{q}} V^*_{\mathbf{q}} \langle\langle c^\dagger_{\mathbf{q},\uparrow} c_{\mathbf{k},\uparrow} c_{0,\downarrow} ; c^\dagger_{0,\downarrow} \rangle\rangle &- \lambda \langle\langle c^\dagger_{0,\uparrow} c_{\mathbf{k},\uparrow} \eta_1 ; c^\dagger_{0,\downarrow} \rangle\rangle, \end{aligned} \tag{6.62}$$

and

$$(\omega-\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}-U)\,\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle=\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle+\sum_{\mathbf{q}}V_{\mathbf{q}}\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}c_{\mathbf{q},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$+\sum_{\mathbf{q}}V_{\mathbf{q}}\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{q},\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle-V_{\mathbf{k}}\langle\langle c^\dagger_{0,\uparrow}c_{0,\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle-\lambda\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle. \quad (6.63)$$

Here we make the following approximations:

$$(\omega-\varepsilon_{\mathbf{k},\downarrow})\,\langle\langle n_{0,\uparrow}c_{\mathbf{k},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle = \sum_{\mathbf{q}}V_{\mathbf{q}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{q},\uparrow}\rangle\langle\langle c_{\mathbf{k},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle-\sum_{\mathbf{q}}V^*_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\uparrow}c_{0,\uparrow}\rangle\langle\langle c_{\mathbf{k},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$+V^*_{\mathbf{k}}\langle\langle n_{0,\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle, \quad (6.64)$$

$$(\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow})\,\langle\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle=\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle+\sum_{\mathbf{q}}V_{\mathbf{q}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle\langle\langle c_{\mathbf{q},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$+V_{\mathbf{k}}\langle\langle n_{0,\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle-\sum_{\mathbf{q}}V^*_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\uparrow}c_{\mathbf{k},\uparrow}\rangle\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle-\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle\lambda\langle\langle\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle, \quad (6.65)$$

and

$$(\omega-\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}-U)\,\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle=\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle+\sum_{\mathbf{q}}V_{\mathbf{q}}\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle\langle\langle c_{\mathbf{q},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$+\sum_{\mathbf{q}}V_{\mathbf{q}}\langle c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{q},\uparrow}\rangle\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle-V_{\mathbf{k}}\langle n_{0,\uparrow}\rangle\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle-\lambda\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle\langle\langle\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle. \quad (6.66)$$

For simplify we now will take the limit o infinite U. To do so we have to go back to Eq. (6.60) and take the limit

$$\lim_{U\to\infty}U\langle\langle n_{0,\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle = \lim_{U\to\infty}\frac{U}{\omega-\varepsilon_{0,s}-U}[\cdots]=\lim_{U\to\infty}\frac{1}{\frac{\omega-\varepsilon_{0,s}}{U}-1}[\cdots]$$
$$=-\lim_{U\to\infty}[\cdots], \quad (6.67)$$

in which the $\cdots$ in the brackets represents the Green's function (6.64)-(6.66). We note that the Green's function (6.66) is proportional to U^{-1}, therefore, upon making $U\to\infty$ it will vanish. Moreover, we will assume $\sum_{\mathbf{q}}V_{\mathbf{q}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{q},\uparrow}\rangle=\sum_{\mathbf{q}}V^*_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\uparrow}c_{0,\uparrow}\rangle$ so that the first two terms of Eq. (6.64) cancel out. The remaining therm of this equation will vanish because it is proportional to U^{-1}. Then we obtain

$$\lim_{U\to\infty}U\langle\langle n_{0,\uparrow}c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle=-\langle n_{0,\uparrow}\rangle-\sum_{\mathbf{k}}\frac{V^*_{\mathbf{k}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}$$
$$-\sum_{\mathbf{k}}\frac{V^*_{\mathbf{k}}}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}\sum_{\mathbf{q}}V_{\mathbf{q}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle\langle\langle c_{\mathbf{q},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle+\sum_{\mathbf{kq}}\frac{V_{\mathbf{k}}V^*_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$+\sum_{\mathbf{k}}\frac{\lambda V^*_{\mathbf{k}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}\langle\langle\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle. \quad (6.68)$$

From Eq. (6.58) we can write

$$\lim_{U\to\infty} U\langle\langle n_{0,\uparrow}c_{0,\downarrow}; c^\dagger_{0,\downarrow}\rangle\rangle = -\langle n_{0,\uparrow}\rangle - \sum_{\mathbf{k}} \frac{V^*_{\mathbf{k}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}$$
$$-\sum_{\mathbf{k}} \frac{V^*_{\mathbf{k}}}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}} \sum_{\mathbf{q}} |V_{\mathbf{q}}|^2 \frac{\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{\mathbf{q},\downarrow}}\langle\langle c_{0,\downarrow}; c^\dagger_{0,\downarrow}\rangle\rangle + \sum_{\mathbf{kq}} \frac{V_{\mathbf{k}}V^*_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$+\sum_{\mathbf{k}} \frac{\lambda V^*_{\mathbf{k}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}\langle\langle \eta_1;c^\dagger_{0,\downarrow}\rangle\rangle \tag{6.69}$$

Replacing this expression into Eq. (6.57) we obtain

$$\left[\omega-\varepsilon_{0,\downarrow}-\sum_{\mathbf{k}}\left(\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k},\downarrow}}+\frac{V_{\mathbf{k}}\sum_{\mathbf{q}}V^*_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}\right)+\sum_{\mathbf{k}}\frac{V^*_{\mathbf{k}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}\sum_{\mathbf{q}}\frac{|V_{\mathbf{q}}|^2}{\omega-\varepsilon_{\mathbf{q},\downarrow}}\right]\times$$
$$\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle = 1-\langle n_{0,\uparrow}\rangle-\sum_{\mathbf{k}}\frac{V^*_{\mathbf{k}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}-\lambda\left(1-\sum_{\mathbf{k}}\frac{V^*_{\mathbf{k}}\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\rangle}{\omega-\varepsilon_{0,\downarrow}+\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\downarrow}}\right)$$
$$\times\langle\langle\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle \tag{6.70}$$

We now need to take care of the Green's function $\langle\langle\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle$, which can be written as

$$\omega\langle\langle\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle = -2\lambda\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle + 2\lambda\langle\langle c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle \tag{6.71}$$

Now,

$$\left(\omega+\varepsilon_{0,\downarrow}-\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{\omega+\varepsilon_{\mathbf{k},\uparrow}}\right)\langle\langle c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle = -U\langle\langle n_{0,\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle + \lambda\langle\langle\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle. \tag{6.72}$$

$$(\omega+\varepsilon_{0,\downarrow}+U)\langle\langle n_{0,\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle = \langle n_{0,\uparrow}\rangle + \sum_{\mathbf{k}}V_{\mathbf{k}}\langle\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$-\sum_{\mathbf{k}}V^*_{\mathbf{k}}\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle - \sum_{\mathbf{k}}V^*_{\mathbf{k}}\langle\langle n_{0,\uparrow}c^\dagger_{\mathbf{k},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle + \lambda\langle\langle n_{0,\uparrow}\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle. \tag{6.73}$$

$$(\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}-\varepsilon_{\mathbf{k},\uparrow}+U)\langle\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle = -\sum_{\mathbf{q}}V^*_{\mathbf{q}}\langle\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}c^\dagger_{\mathbf{q},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$\sum_{\mathbf{q}}V_{\mathbf{q}}\langle\langle c^\dagger_{\mathbf{q},\uparrow}c_{\mathbf{k},\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle + V_{\mathbf{k}}\langle\langle c^\dagger_{0,\uparrow}c_{0,\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle + \lambda\langle\langle c^\dagger_{0,\uparrow}c_{\mathbf{k},\uparrow}\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle \tag{6.74}$$

$$(\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow})\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle = -\sum_{\mathbf{q}}V^*_{\mathbf{q}}\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}c^\dagger_{\mathbf{q},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle$$
$$+\sum_{\mathbf{q}}V_{\mathbf{q}}\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{q},\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle + V_{\mathbf{k}}\langle\langle n_{0,\uparrow}c^\dagger_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle + \lambda\langle\langle c^\dagger_{\mathbf{k},\uparrow}c_{0,\uparrow}\eta_1;c^\dagger_{0,\downarrow}\rangle\rangle \tag{6.75}$$

$$(\omega+\varepsilon_{\mathbf{k},\uparrow})\,\langle\langle n_{0,\uparrow}c^{\dagger}_{\mathbf{k},\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle = -V_{\mathbf{k}}\langle\langle n_{0,\uparrow}c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + \sum_{\mathbf{q}} V_{\mathbf{q}}\langle\langle c_{0,\uparrow}c_{\mathbf{q},\downarrow}c^{\dagger}_{\mathbf{k},\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle - \sum_{\mathbf{q}} V^{*}_{\mathbf{q}}\langle\langle c^{\dagger}_{\mathbf{q},\uparrow}c_{0,\uparrow}c^{\dagger}_{\mathbf{k},\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle. \quad (6.76)$$

We see that upon making similar decoupling as before and taking the limit $U\to\infty$, only Eq. (6.75) will contribute. Its approximated expression is

$$(\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow})\,\langle\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle = -\sum_{\mathbf{q}} V^{*}_{\mathbf{q}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle\langle\langle c^{\dagger}_{\mathbf{q},\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + \sum_{\mathbf{q}} V_{\mathbf{q}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{\mathbf{q},\uparrow}\rangle\langle\langle c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + V_{\mathbf{k}}\langle\langle n_{0,\uparrow}c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + \lambda\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle\langle\langle \eta_1;c^{\dagger}_{0,\downarrow}\rangle\rangle. \quad (6.77)$$

Since

$$\langle\langle c^{\dagger}_{\mathbf{q},\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle = \frac{V_{\mathbf{q}}}{\omega+\varepsilon_{\mathbf{q},\downarrow}}\langle\langle c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle \quad (6.78)$$

then,

$$(\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow})\,\langle\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle = -\sum_{\mathbf{q}} \frac{|V_{\mathbf{q}}|^2}{\omega+\varepsilon_{\mathbf{q},\downarrow}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle\langle\langle c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + \sum_{\mathbf{q}} V_{\mathbf{q}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{\mathbf{q},\uparrow}\rangle\langle\langle c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + V_{\mathbf{k}}\langle\langle n_{0,\uparrow}c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + \lambda\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle\langle\langle \eta_1;c^{\dagger}_{0,\downarrow}\rangle\rangle. \quad (6.79)$$

Then,

$$\lim_{U\to\infty} U\langle\langle n_{0,\uparrow}c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle = -\sum_{\mathbf{k}} \frac{V^{*}_{\mathbf{k}}}{\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\sum_{\mathbf{q}} \frac{|V_{\mathbf{q}}|^2}{\omega+\varepsilon_{\mathbf{q},\downarrow}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle\langle\langle c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + \sum_{\mathbf{k}} \frac{V^{*}_{\mathbf{k}}V_{\mathbf{q}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{\mathbf{q},\uparrow}\rangle}{\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\langle\langle c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle + \sum_{\mathbf{k}} \frac{\lambda V^{*}_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle}{(\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\langle\langle \eta_1;c^{\dagger}_{0,\downarrow}\rangle\rangle \quad (6.80)$$

Replacing this expression into Eq. (6.72) we obtain

$$\left[\omega+\varepsilon_{0,\downarrow}-\sum_{\mathbf{k}}\left(\frac{|V_{\mathbf{k}}|^2}{\omega+\varepsilon_{\mathbf{k},\uparrow}}-\frac{V^{*}_{\mathbf{k}}\sum_{\mathbf{q}}V_{\mathbf{q}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{\mathbf{q},\uparrow}\rangle}{\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\right)-\sum_{\mathbf{k}}\frac{V^{*}_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle}{\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\sum_{\mathbf{q}}\frac{|V_{\mathbf{q}}|^2}{\omega+\varepsilon_{\mathbf{q},\downarrow}}\right] \times\langle\langle c^{\dagger}_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle = \lambda\left(1-\sum_{\mathbf{k}}\frac{V^{*}_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle}{(\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\right)\langle\langle \eta_1;c^{\dagger}_{0,\downarrow}\rangle\rangle \quad (6.81)$$

Now, replacing this expression into Eq. (6.71) we obtain

$$\left[\omega-\frac{2\lambda^2\left(1-\sum_{\mathbf{k}}\frac{V^{*}_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle}{(\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\right)}{\omega+\varepsilon_{0,\downarrow}-\sum_{\mathbf{k}}\left(\frac{|V_{\mathbf{k}}|^2}{\omega+\varepsilon_{\mathbf{k},\uparrow}}-\frac{V^{*}_{\mathbf{k}}\sum_{\mathbf{q}}V_{\mathbf{q}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{\mathbf{q},\uparrow}\rangle}{\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\right)-\sum_{\mathbf{k}}\frac{V^{*}_{\mathbf{k}}\langle c^{\dagger}_{\mathbf{k},\uparrow}c_{0,\uparrow}\rangle}{\omega+\varepsilon_{0,\downarrow}-\varepsilon_{0,\uparrow}+\varepsilon_{\mathbf{k},\uparrow}}\sum_{\mathbf{q}}\frac{|V_{\mathbf{q}}|^2}{\omega+\varepsilon_{\mathbf{q},\downarrow}}}\right]\langle\langle \eta_1;c^{\dagger}_{0,\downarrow}\rangle\rangle = -2\lambda\langle\langle c_{0,\downarrow};c^{\dagger}_{0,\downarrow}\rangle\rangle. \quad (6.82)$$

Replacing this expression into Eq. (6.70) we will write

$$
\left[\omega - \varepsilon_{0,\downarrow} - \sum_{\mathbf{k}} \left(\frac{|V_{\mathbf{k}}|^2}{\omega - \varepsilon_{\mathbf{k},\downarrow}} + \frac{V_{\mathbf{k}} \sum_{\mathbf{q}} V_{\mathbf{q}}^* \langle c_{\mathbf{q},\uparrow}^\dagger c_{\mathbf{k},\uparrow} \rangle}{\omega - \varepsilon_{0,\downarrow} + \varepsilon_{0,\uparrow} - \varepsilon_{\mathbf{k},\downarrow}} \right) + \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^* \langle c_{0,\uparrow}^\dagger c_{\mathbf{k},\uparrow} \rangle}{\omega - \varepsilon_{0,\downarrow} + \varepsilon_{0,\uparrow} - \varepsilon_{\mathbf{k},\downarrow}} \sum_{\mathbf{q}} \frac{|V_{\mathbf{q}}|^2}{\omega - \varepsilon_{\mathbf{q},\downarrow}} \right.
$$

$$
\left. - \frac{2\lambda^2 \left(1 - \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^* \langle c_{0,\uparrow}^\dagger c_{\mathbf{k},\uparrow} \rangle}{\omega - \varepsilon_{0,\downarrow} + \varepsilon_{0,\uparrow} - \varepsilon_{\mathbf{k},\downarrow}}\right)}{\omega - \frac{2\lambda^2 \left(1 - \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^* \langle c_{\mathbf{k},\uparrow}^\dagger c_{0,\uparrow} \rangle}{(\omega + \varepsilon_{0,\downarrow} - \varepsilon_{0,\uparrow} + \varepsilon_{\mathbf{k},\uparrow}}\right)}{\omega + \varepsilon_{0,\downarrow} - \sum_{\mathbf{k}} \left(\frac{|V_{\mathbf{k}}|^2}{\omega + \varepsilon_{\mathbf{k},\uparrow}} - \frac{V_{\mathbf{k}}^* \sum_{\mathbf{q}} V_{\mathbf{q}} \langle c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{q},\uparrow} \rangle}{\omega + \varepsilon_{0,\downarrow} - \varepsilon_{0,\uparrow} + \varepsilon_{\mathbf{k},\uparrow}} \right) - \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^* \langle c_{\mathbf{k},\uparrow}^\dagger c_{0,\uparrow} \rangle}{\omega + \varepsilon_{0,\downarrow} - \varepsilon_{0,\uparrow} + \varepsilon_{\mathbf{k},\uparrow}} \sum_{\mathbf{q}} \frac{|V_{\mathbf{q}}|^2}{\omega + \varepsilon_{\mathbf{q},\downarrow}}}} \right] \langle\langle c_{0,\downarrow}; c_{0,\downarrow}^\dagger \rangle\rangle =
$$

$$
1 - \langle n_{0,\uparrow} \rangle - \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^* \langle c_{0,\uparrow}^\dagger c_{\mathbf{k},\uparrow} \rangle}{\omega - \varepsilon_{0,\downarrow} + \varepsilon_{0,\uparrow} - \varepsilon_{\mathbf{k},\downarrow}} \tag{6.83}
$$

Now we need to calculate the Green's function for spin up, whose expression is given by

$$
\left(\omega - \varepsilon_{0,\uparrow} - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \varepsilon_{\mathbf{k},\uparrow}} \right) \langle\langle c_{0,\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle = 1 + U \langle\langle n_{0,\downarrow} c_{0,\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle. \tag{6.84}
$$

$$
\begin{aligned}
(\omega - \varepsilon_{0,\uparrow} - U) \langle\langle n_{0,\downarrow} c_{0,\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle &= \langle n_{0,\downarrow} \rangle + \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle n_{0,\downarrow} c_{\mathbf{k},\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle + \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle c_{0,\downarrow}^\dagger c_{\mathbf{k},\downarrow} c_{0,\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle \\
&- \sum_{\mathbf{k}} V_{\mathbf{k}}^* \langle\langle c_{\mathbf{k},\downarrow}^\dagger c_{0,\downarrow} c_{0,\uparrow}; c_{0,\uparrow} \rangle\rangle - \lambda \langle\langle c_{0,\downarrow} \eta_1 c_{0.\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle + \lambda \langle\langle c_{0,\downarrow}^\dagger \eta_1 c_{0\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle.
\end{aligned} \tag{6.85}
$$

Note that the terms proportional to $V_{\mathbf{k}}$ are similar to those previously calculated and we know how to deal with then. We need to take care of the last two Green's functions, which are given by

$$
\begin{aligned}
(\omega - 2\varepsilon_{0,\uparrow} - U) \langle\langle c_{0,\downarrow} \eta_1 c_{0\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle &= \langle c_{0,\uparrow} \eta_1 \rangle + \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle c_{\mathbf{k},\downarrow} \eta_1 c_{0,\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle \\
&+ \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle c_{0,\downarrow} \eta_1 c_{\mathbf{k},\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle + 2\lambda \langle\langle c_{0,\downarrow} c_{0,\downarrow}^\dagger c_{0,\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle - \lambda \langle\langle c_{0,\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle
\end{aligned} \tag{6.86}
$$

and

$$
\begin{aligned}
(\omega - \varepsilon_{0,\uparrow} + \varepsilon_{0,\downarrow}) \langle\langle c_{0,\downarrow}^\dagger \eta_1 c_{0\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle &= \langle c_{0,\downarrow}^\dagger \eta_1 \rangle + \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle c_{0,\downarrow}^\dagger \eta_1 c_{\mathbf{k},\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle \\
&- \sum_{\mathbf{k}} V_{\mathbf{k}}^* \langle\langle c_{\mathbf{k},\downarrow}^\dagger \eta_1 c_{0\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle - 2\lambda \langle\langle n_{0,\downarrow} c_{0\uparrow}; c_{0,\uparrow}^\dagger \rangle\rangle.
\end{aligned} \tag{6.87}
$$

Since the the Green's function (6.86) is proportional to U^{-1} it vanish upon taking $U \to \infty$.

With similar approximation as we did before we can write

$$
\begin{aligned}
(\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow})\,\langle\langle c_{0,\downarrow}^{\dagger}\eta_1 c_{0\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle &= \langle c_{0,\downarrow}^{\dagger}\eta_1\rangle+\langle c_{0,\downarrow}^{\dagger}\eta_1\rangle\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k},\uparrow}}\langle\langle c_{0,\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle \\
&\quad -\sum_{\mathbf{k}}V_{\mathbf{k}}^{*}\langle c_{\mathbf{k},\downarrow}^{\dagger}\eta_1\rangle\langle\langle c_{0\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle-2\lambda\langle\langle n_{0,\downarrow}c_{0\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle. \qquad (6.88)
\end{aligned}
$$

With these we can write

$$
\begin{aligned}
\lim_{U\to\infty}U\langle\langle n_{0,\downarrow}c_{0,\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle &= -\langle n_{0,\downarrow}\rangle-\sum_{\mathbf{k}}\frac{V_{\mathbf{k}}^{*}\langle c_{0,\downarrow}^{\dagger}c_{\mathbf{k},\downarrow}\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}-\varepsilon_{\mathbf{k},\uparrow}} \\
-\sum_{\mathbf{k}}\frac{V_{\mathbf{k}}^{*}}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}-\varepsilon_{\mathbf{k},\uparrow}}\sum_{\mathbf{q}}|V_{\mathbf{q}}|^2\frac{\langle c_{0,\downarrow}^{\dagger}c_{\mathbf{k},\downarrow}\rangle}{\omega-\varepsilon_{\mathbf{q},\uparrow}}\langle\langle c_{0,\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle &+\sum_{\mathbf{kq}}\frac{V_{\mathbf{k}}V_{\mathbf{q}}^{*}\langle c_{\mathbf{q},\downarrow}^{\dagger}c_{\mathbf{k},\downarrow}\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}-\varepsilon_{\mathbf{k},\uparrow}}\langle\langle c_{0,\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle \\
-\frac{\langle c_{0,\downarrow}^{\dagger}\eta_1\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}}-\frac{\langle c_{0,\downarrow}^{\dagger}\eta_1\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}}\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k},\uparrow}}\langle\langle c_{0,\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle &+\frac{\sum_{\mathbf{k}}V_{\mathbf{k}}^{*}\langle c_{\mathbf{k},\downarrow}^{\dagger}\eta_1\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}}\langle\langle c_{0\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle \quad (6.89)
\end{aligned}
$$

Finally, replacing the last expression into Eq. (6.84) obtain

$$
\begin{aligned}
&\Bigg[\omega-\varepsilon_{0,\uparrow}-\sum_{\mathbf{k}}\left(\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k},\uparrow}}+\frac{V_{\mathbf{k}}\sum_{\mathbf{q}}V_{\mathbf{q}}^{*}\langle c_{\mathbf{q},\downarrow}^{\dagger}c_{\mathbf{k},\downarrow}\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}-\varepsilon_{\mathbf{k},\uparrow}}\right)+\sum_{\mathbf{k}}\frac{V_{\mathbf{k}}^{*}\langle c_{0,\downarrow}^{\dagger}c_{\mathbf{k},\downarrow}\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}-\varepsilon_{\mathbf{k},\uparrow}}\sum_{\mathbf{q}}\frac{|V_{\mathbf{q}}|^2}{\omega-\varepsilon_{\mathbf{q},\uparrow}} \\
&\qquad -\frac{\lambda\sum_{\mathbf{k}}V_{\mathbf{k}}^{*}\langle c_{\mathbf{k},\downarrow}^{\dagger}\eta_1\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}}+\frac{\lambda\langle c_{0,\downarrow}^{\dagger}\eta_1\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}}\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k},\uparrow}}\Bigg]\langle\langle c_{0,\uparrow};c_{0,\uparrow}^{\dagger}\rangle\rangle = \\
&\qquad 1-\langle n_{0,\downarrow}\rangle-\sum_{\mathbf{k}}\frac{V_{\mathbf{k}}^{*}\langle c_{0,\downarrow}^{\dagger}c_{\mathbf{k},\downarrow}\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}-\varepsilon_{\mathbf{k},\uparrow}}-\frac{\lambda\langle c_{0,\downarrow}^{\dagger}\eta_1\rangle}{\omega-\varepsilon_{0,\uparrow}+\varepsilon_{0,\downarrow}}. \quad (6.90)
\end{aligned}
$$

Let us assume now the there is no Zeeman splitting in the dot nor in the leas, then $\varepsilon_{\mathbf{k},\uparrow}=\varepsilon_{\mathbf{k},\uparrow}\equiv\varepsilon_{\mathbf{k}}$ and $\varepsilon_{0,\uparrow}=\varepsilon_{0,\uparrow}\equiv\varepsilon_d$. Moreover, for a flat density of states for the conduction electrons, $\rho_c(\omega)=(1/2D)\Theta(D-|\omega|)$, we have

$$
\begin{aligned}
\sum_{\mathbf{k}}\frac{1}{\omega+i\eta-\varepsilon_{\mathbf{k}}} &= \int_{-\infty}^{\infty}\frac{\Theta(D-|\varepsilon|)}{2D}(-i\pi)\delta(\omega-\varepsilon)d\varepsilon+\int_{-\infty}^{\infty}\frac{\Theta(D-|\varepsilon|)}{2D}\frac{\omega-\varepsilon}{(\omega-\varepsilon)^2+\eta^2}d\varepsilon \\
&= -i\pi\rho_0\Theta(D-|\omega|)-\frac{1}{2D}\ln\Big|\frac{(\omega-D)^2+\eta^2}{(\omega+D)^2+\eta^2}\Big| \\
&= -i\pi\rho_c(\omega)-\frac{1}{2D}\ln\Big|\frac{(\omega-D)^2+\eta^2}{(\omega+D)^2+\eta^2}\Big|, \qquad (6.91)
\end{aligned}
$$

In the wide band limit the logarithm vanishes.

$$
\langle c_{\mathbf{q},\downarrow}^{\dagger}c_{\mathbf{k},\downarrow}\rangle=-\frac{1}{\pi}\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{\mathbf{k},\downarrow};c_{\mathbf{q},\downarrow}^{\dagger}\rangle\rangle_{\omega'}, \qquad (6.92)
$$

where

$$\langle\langle c_{\mathbf{k},\downarrow};c^\dagger_{\mathbf{q},\downarrow}\rangle\rangle = \frac{\delta_{\mathbf{kq}}}{\omega-\varepsilon_{\mathbf{k}}} + \frac{V^2}{(\omega'-\varepsilon_{\mathbf{k}})(\omega'-\varepsilon_{\mathbf{q}})}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \tag{6.93}$$

$$\sum_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\downarrow}c_{\mathbf{k}}\rangle = -\frac{1}{\pi}\int d\omega' f(\omega')\mathrm{Im}\sum_{\mathbf{q}}\frac{\delta_{\mathbf{kq}}}{\omega'-\varepsilon_{\mathbf{k}}} - \frac{V^2}{\pi}\int d\omega' f(\omega')\mathrm{Im}\sum_{\mathbf{q}}\left[\frac{\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{(\omega'-\varepsilon_{\mathbf{k}})(\omega'-\varepsilon_{\mathbf{q}})}\right] \tag{6.94}$$

Now,

$$\sum_{\mathbf{q}}\left[\frac{\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{(\omega'-\varepsilon_{\mathbf{k}})(\omega'-\varepsilon_{\mathbf{q}})}\right] = \left[\frac{\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{\omega'-\varepsilon_{\mathbf{k}}}\sum_{\mathbf{q}}\frac{1}{\omega'-\varepsilon_{\mathbf{q}}}\right] = -i\pi\rho_c(\omega')\frac{\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{\omega'-\varepsilon_{\mathbf{k}}}. \tag{6.95}$$

$$\sum_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\downarrow}c_{\mathbf{k},\downarrow}\rangle = -\frac{1}{\pi}\int d\omega' f(\omega')\mathrm{Im}\frac{1}{\omega'-\varepsilon_{\mathbf{k}}} + V^2\int d\omega' f(\omega')\rho_c(\omega')\mathrm{Im}\left[\frac{i\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{\omega'-\varepsilon_{\mathbf{k}}}\right]. \tag{6.96}$$

Now,

$$\left[\frac{i\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{\omega'-\varepsilon_{\mathbf{k}}}\right] = \left[i\mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} - \mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\right]\left[\wp\frac{1}{\omega'-\varepsilon_{\mathbf{k}}} - i\pi\delta(\omega'-\varepsilon_{\mathbf{k}})\right] \tag{6.97}$$

$$\mathrm{Im}\left[\frac{i\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{\omega'-\varepsilon_{\mathbf{k}}}\right] = \left[\mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\wp\frac{1}{\omega'-\varepsilon_{\mathbf{k}}} + \pi\mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\delta(\omega'-\varepsilon_{\mathbf{k}})\right] \tag{6.98}$$

$$\begin{aligned}\sum_{\mathbf{q}}\langle c^\dagger_{\mathbf{q},\downarrow}c_{\mathbf{k},\downarrow}\rangle &= -\frac{1}{\pi}\int d\omega' f(\omega')\mathrm{Im}\frac{1}{\omega'-\varepsilon_{\mathbf{k}}}\\ &+V^2\int d\omega' f(\omega')\rho_c(\omega')\left[\mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\wp\frac{1}{\omega'-\varepsilon_{\mathbf{k}}} + \pi\mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\delta(\omega'-\varepsilon_{\mathbf{k}})\right]\end{aligned} \tag{6.99}$$

$$\begin{aligned}\sum_{\mathbf{kq}}\frac{\langle c^\dagger_{\mathbf{q},\downarrow}c_{\mathbf{k},\downarrow}\rangle}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} &= -\frac{1}{\pi}\int d\omega' f(\omega')\sum_{\mathbf{k}}\frac{-\pi\delta(\omega'-\varepsilon_{\mathbf{k}})}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}}\\ &+V^2\int d\omega' f(\omega')\rho_c(\omega')\left[\mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\sum_{\mathbf{k}}\frac{1}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}}\wp\frac{1}{\omega'-\varepsilon_{\mathbf{k}}}\right.\\ &\left.+\pi\mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\sum_{\mathbf{k}}\frac{\delta(\omega'-\varepsilon_{\mathbf{k}})}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}}\right].\end{aligned} \tag{6.100}$$

$$
\begin{aligned}
\sum_{\mathbf{kq}} \frac{\langle c^\dagger_{\mathbf{q},\downarrow} c_{\mathbf{k},\downarrow}\rangle}{\omega - \Delta\varepsilon - \varepsilon_{\mathbf{k}}} &= \int d\omega' f(\omega') \int d\varepsilon \rho_c(\varepsilon) \frac{\delta(\omega'-\varepsilon)}{\omega - \Delta\varepsilon - \varepsilon} \\
&+ V^2 \int d\omega' f(\omega') \rho_c(\omega') \Big[\mathrm{Re}\langle\langle c_{0,\downarrow}; c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \int d\varepsilon \frac{\rho_c(\varepsilon)}{\omega - \Delta\varepsilon - \varepsilon} \wp \frac{1}{\omega' - \varepsilon} \\
&+ \pi \mathrm{Im}\langle\langle c_{0,\downarrow}; c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \int d\varepsilon \rho_c(\varepsilon) \frac{\delta(\omega'-\varepsilon)}{\omega - \Delta\varepsilon - \varepsilon} \Big] \\
&= \rho_0 \int d\omega' f(\omega') \int_{-D}^{D} d\varepsilon \frac{\delta(\omega'-\varepsilon)}{\omega - \Delta\varepsilon - \varepsilon} \\
&+ V^2 \rho_0 \int d\omega' f(\omega') \rho_c(\omega') \Big[\mathrm{Re}\langle\langle c_{0,\downarrow}; c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \int_{-D}^{D} d\varepsilon \frac{1}{\omega - \Delta\varepsilon - \varepsilon} \wp \frac{1}{\omega' - \varepsilon} \\
&+ \pi \mathrm{Im}\langle\langle c_{0,\downarrow}; c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \int_{-D}^{D} d\varepsilon \frac{\delta(\omega'-\varepsilon)}{\omega - \Delta\varepsilon - \varepsilon} \Big]. \qquad (6.101)
\end{aligned}
$$

We note that

$$
\int_{-D}^{D} d\varepsilon \frac{\delta(\omega'-\varepsilon)}{\omega - \Delta\varepsilon - \varepsilon} = \frac{\Theta(D - |\omega'|)}{\omega - \Delta\varepsilon - \omega'} \qquad (6.102)
$$

and

$$
\begin{aligned}
\int_{-D}^{D} d\varepsilon \frac{1}{\omega - \Delta\varepsilon - \varepsilon} \wp \frac{1}{\omega' - \varepsilon} &= \int_{-D}^{D} d\varepsilon \wp \frac{1}{\omega - \Delta\varepsilon - \varepsilon} \wp \frac{1}{\omega' - \varepsilon} \\
&+ i\pi \int_{-D}^{D} d\varepsilon \delta(\omega - \Delta\varepsilon - \varepsilon) \wp \frac{1}{\omega' - \varepsilon} \\
&= \int_{-D}^{D} d\varepsilon \wp \frac{1}{\omega - \Delta\varepsilon - \varepsilon} \wp \frac{1}{\omega' - \varepsilon} \\
&+ i\pi \int_{-D}^{D} d\varepsilon \delta(\omega - \Delta\varepsilon - \varepsilon) \wp \frac{1}{\omega' - \varepsilon} \\
&= \int_{-D}^{D} d\varepsilon \wp \frac{1}{\omega - \Delta\varepsilon - \varepsilon} \wp \frac{1}{\omega' - \varepsilon} + i\pi \wp \frac{\Theta(D - |\omega - \Delta\varepsilon|)}{\omega' - \omega + \Delta\varepsilon} \\
&= \int_{-D}^{D} d\varepsilon \wp \frac{1}{\omega - \Delta\varepsilon - \varepsilon} \wp \frac{1}{\omega' - \varepsilon} - i\pi \wp \frac{\Theta(D - |\omega - \Delta\varepsilon|)}{\omega - \Delta\varepsilon - \omega'} \qquad (6.103)
\end{aligned}
$$

Then

$$
\begin{aligned}
\sum_{\mathbf{kq}} \frac{\langle c^\dagger_{\mathbf{q},\downarrow} c_{\mathbf{k},\downarrow}\rangle}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} &= \rho_0 \int d\omega' f(\omega') \frac{\Theta(D-|\omega'|)}{\omega-\Delta\varepsilon-\omega'} \\
&+V^2\rho_0 \int d\omega' f(\omega')\rho_c(\omega') \Bigg[\mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \int_{-D}^{D} d\varepsilon \wp\frac{1}{\omega-\Delta\varepsilon-\varepsilon}\wp\frac{1}{\omega'-\varepsilon} \\
&-i\pi \mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \wp\frac{\Theta(D-|\omega-\Delta\varepsilon|)}{\omega-\Delta\varepsilon-\omega'} + \pi \mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \frac{\Theta(D-|\omega'|)}{\omega-\Delta\varepsilon-\omega'}\Bigg]. \\
&= \rho_0 \int_{-D}^{D} d\omega' f(\omega') \wp\frac{1}{\omega-\Delta\varepsilon-\omega'} + i\pi\rho_0 \int_{-D}^{D} d\omega' f(\omega')\delta(\omega-\Delta\varepsilon-\omega') \\
&-i\pi V^2\rho_0^2 \int_{-D}^{D} d\omega' f(\omega') \mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \wp\frac{\Theta(D-|\omega-\Delta\varepsilon|)}{\omega-\Delta\varepsilon-\omega'} \\
&+\pi V^2\rho_0^2 \int_{-D}^{D} d\omega' f(\omega') \frac{\mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{\omega-\Delta\varepsilon-\omega'} \\
&+V^2\rho_0^2 \int_{-D}^{D} d\omega' f(\omega') \mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \int_{-D}^{D} d\varepsilon \wp\frac{1}{\omega-\Delta\varepsilon-\varepsilon}\wp\frac{1}{\omega'-\varepsilon}. \quad (6.104)
\end{aligned}
$$

We can easily show that the las integral of the expression above vanishes in the wide band limit. Then, we finally obtain

$$
\begin{aligned}
\sum_{\mathbf{kq}} \frac{\langle c^\dagger_{\mathbf{q},\downarrow} c_{\mathbf{k},\downarrow}\rangle}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} = \rho_0 \int_{-D}^{D} d\omega' f(\omega') \wp\frac{1}{\omega-\Delta\varepsilon-\omega'} + i\pi\rho_0 f(\omega-\Delta\varepsilon)\Theta(D-|\omega-\Delta\varepsilon|) \\
-i\pi V^2\rho_0^2 \int_{-D}^{D} d\omega' f(\omega') \left[\mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} \wp\frac{\Theta(D-|\omega-\Delta\varepsilon|)}{\omega-\Delta\varepsilon-\omega'} + \frac{i\mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}}{\omega-\Delta\varepsilon-\omega'}\right] (6.105)
\end{aligned}
$$

HERE!

Another quantity that needs to be calculated is

$$
\langle c^\dagger_{0,\downarrow} c_{\mathbf{k},\downarrow}\rangle = -\frac{1}{\pi}\int d\omega' f(\omega') \mathrm{Im}\langle\langle c_{\mathbf{k},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}. \tag{6.106}
$$

With

$$
\langle\langle c_{\mathbf{k},\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} = \frac{V_{\mathbf{k}}}{\omega'-\varepsilon_{\mathbf{k}}}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}. \tag{6.107}
$$

$$
\mathrm{Im}\frac{1}{\omega'-\varepsilon_{\mathbf{k}}}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} = \wp\frac{1}{\omega'-\varepsilon_{\mathbf{k}}}\mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} - i\pi \mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\delta(\omega'-\varepsilon_{\mathbf{k}}) \tag{6.108}
$$

$$
\langle c^\dagger_{0,\downarrow} c_{\mathbf{k},\downarrow}\rangle = -\frac{V}{\pi}\int d\omega' f(\omega')\wp\frac{1}{\omega'-\varepsilon_{\mathbf{k}}}\mathrm{Im}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'} + iV\int d\omega' f(\omega')\mathrm{Re}\langle\langle c_{0,\downarrow};c^\dagger_{0,\downarrow}\rangle\rangle_{\omega'}\delta(\omega'-\varepsilon_{\mathbf{k}}) \tag{6.109}
$$

$$
\begin{aligned}
\sum_{\mathbf{k}} \frac{\langle c_{0,\downarrow}^{\dagger} c_{\mathbf{k},\downarrow}\rangle}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} &= -\frac{V}{\pi}\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \sum_{\mathbf{k}} \frac{1}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} \wp \frac{1}{\omega'-\varepsilon_{\mathbf{k}}} \\
&\quad +iV\int d\omega' f(\omega')\mathrm{Re}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \sum_{\mathbf{k}} \frac{\delta(\omega'-\varepsilon_{\mathbf{k}})}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} \\
&= -\frac{V\rho_0}{\pi}\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \int_{-D}^{D} d\varepsilon \wp \frac{1}{\omega-\Delta\varepsilon-\varepsilon} \wp \frac{1}{\omega'-\varepsilon} \\
&\quad +iV\rho_0\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \int_{-D}^{D} d\varepsilon \delta(\omega-\Delta\varepsilon-\varepsilon) \wp \frac{1}{\omega'-\varepsilon} \\
&\quad +iV\rho_0\int d\omega' f(\omega')\mathrm{Re}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \int_{-D}^{D} d\varepsilon \frac{\delta(\omega'-\varepsilon)}{\omega-\Delta\varepsilon-\varepsilon} \\
&= -\frac{V\rho_0}{\pi}\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \int_{-D}^{D} d\varepsilon \wp \frac{1}{\omega-\Delta\varepsilon-\varepsilon} \wp \frac{1}{\omega'-\varepsilon} \\
&\quad -iV\rho_0\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \wp \frac{\Theta(D-|\omega-\Delta\varepsilon|)}{\omega'-\omega+\Delta\varepsilon} \\
&\quad -iV\rho_0\int d\omega' f(\omega')\mathrm{Re}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \frac{\Theta(D-|\omega'|)}{\omega-\Delta\varepsilon-\omega'}. \qquad (6.110)
\end{aligned}
$$

Finally, in the wide band limit we obtain

$$
\begin{aligned}
\sum_{\mathbf{k}} \frac{\langle c_{0,\downarrow}^{\dagger} c_{\mathbf{k},\downarrow}\rangle}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} &= iV\rho_0\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \wp \frac{\Theta(D-|\omega-\Delta\varepsilon|)}{\omega-\Delta\varepsilon-\omega'} \\
&\quad -iV\rho_0\int_{-D}^{D} d\omega' f(\omega') \frac{\mathrm{Re}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'}}{\omega-\Delta\varepsilon-\omega'}. \qquad (6.111)
\end{aligned}
$$

We can still write

$$
\sum_{\mathbf{k}} \frac{\langle c_{0,\downarrow}^{\dagger} c_{\mathbf{k},\downarrow}\rangle}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} = iV\rho_0\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \wp \frac{\Theta(D-|\omega-\Delta\varepsilon|)}{\omega-\Delta\varepsilon-\omega'}
$$

$$
-iV\rho_0\int_{-D}^{D} d\omega' f(\omega') \wp \frac{\mathrm{Re}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'}}{\omega-\Delta\varepsilon-\omega'} - \pi V\rho_0 \int_{-D}^{D} d\omega' f(\omega')\mathrm{Re}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \delta(\omega-\Delta\varepsilon-\omega'). \qquad (6.112)
$$

$$
\sum_{\mathbf{k}} \frac{\langle c_{0,\downarrow}^{\dagger} c_{\mathbf{k},\downarrow}\rangle}{\omega-\Delta\varepsilon-\varepsilon_{\mathbf{k}}} = iV\rho_0\int d\omega' f(\omega')\mathrm{Im}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'} \wp \frac{\Theta(D-|\omega-\Delta\varepsilon|)}{\omega-\Delta\varepsilon-\omega'}
$$

$$
-iV\rho_0\int_{-D}^{D} d\omega' f(\omega') \wp \frac{\mathrm{Re}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega'}}{\omega-\Delta\varepsilon-\omega'} - \pi V\rho_0 f(\omega-\Delta\varepsilon)\mathrm{Re}\langle\langle c_{0,\downarrow};c_{0,\downarrow}^{\dagger}\rangle\rangle_{\omega-\Delta\varepsilon} \Theta(D-|\omega-\Delta\varepsilon|). \qquad (6.113)
$$

6.3 Beyond the Hubbard I approximation

$$\omega\langle\langle n_{0,\bar{s}}c_{\mathbf{k},s};c^{\dagger}_{0,s'}\rangle\rangle = \langle\langle[n_{0,\bar{s}}c_{\mathbf{k},s},H];c^{\dagger}_{0,s'}\rangle\rangle, \tag{6.114}$$

$$[n_{0,\bar{s}}c_{\mathbf{k},s},H] = [n_{0,\bar{s}},H]c_{\mathbf{k},s} + n_{0,\bar{s}}[c_{\mathbf{k},s},H], \tag{6.115}$$

$$[c_{\mathbf{k},s},H] = \varepsilon_{\mathbf{k},s}c_{\mathbf{k},s} + V^{*}_{\mathbf{k}}c_{0,s} \tag{6.116}$$

$$[n_{0,\bar{s}},H] = -t_0c^{\dagger}_{0,\bar{s}}c_{1,\bar{s}} + t_0c^{\dagger}_{1,\bar{s}}c_{0,\bar{s}} + \sum_{\mathbf{k}}V_{\mathbf{k}}c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}} - \sum_{\mathbf{k}}V^{*}_{\mathbf{k}}c^{\dagger}_{0,\bar{s}}c_{0,\bar{s}} \tag{6.117}$$

then

$$\begin{aligned}(\omega-\varepsilon_{\mathbf{k},s})\,\langle\langle n_{0,\bar{s}}c_{\mathbf{k},s};c^{\dagger}_{0,s'}\rangle\rangle &= -t_0\langle\langle c^{\dagger}_{0,\bar{s}}c_{1,\bar{s}}c_{\mathbf{k},s};c^{\dagger}_{0,s'}\rangle\rangle + t_0\langle\langle c^{\dagger}_{1,\bar{s}}c_{0,\bar{s}}c_{\mathbf{k},s};c^{\dagger}_{0,s'}\rangle\rangle \\ &+\sum_{\mathbf{k}'}V_{\mathbf{k}'}\langle\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k}',\bar{s}}c_{\mathbf{k},s};c^{\dagger}_{0,s'}\rangle\rangle - \sum_{\mathbf{k}'}V^{*}_{\mathbf{k}'}\langle\langle c^{\dagger}_{\mathbf{k}',\bar{s}}c_{0,\bar{s}}c_{\mathbf{k},s};c^{\dagger}_{0,s'}\rangle\rangle + V^{*}_{\mathbf{k}}\langle\langle n_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle\end{aligned} \tag{6.118}$$

$$\omega\langle\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle = \langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle + \langle\langle[c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s},H];c^{\dagger}_{0,s'}\rangle\rangle. \tag{6.119}$$

$$[c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s},H] = c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}[c_{0,s},H] + c^{\dagger}_{0,\bar{s}}[c_{\mathbf{k},\bar{s}},H]c_{0,s} + [c^{\dagger}_{0,\bar{s}},H]c_{\mathbf{k},\bar{s}}c_{0,s} \tag{6.120}$$

$$[c^{\dagger}_{0,\bar{s}},H] = -\varepsilon_{0,\bar{s}}c^{\dagger}_{0,\bar{s}} - Un_{0,s}c^{\dagger}_{0,\bar{s}} + t_0c^{\dagger}_{1,\bar{s}} - \sum_{\mathbf{k}}V^{*}_{\mathbf{k}}c^{\dagger}_{\mathbf{k},\bar{s}} \tag{6.121}$$

then

$$\begin{aligned}[c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s},H] &= \varepsilon_{0,s}c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s} + U\cancelto{0}{c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}n_{0,\bar{s}}c_{0,s}} - t_0c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{1,s} + \sum_{\mathbf{k}'}V_{\mathbf{k}'}c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{\mathbf{k}',s} \\ &\varepsilon_{\mathbf{k},\bar{s}}c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s} + V_{\mathbf{k}}c^{\dagger}_{0,\bar{s}}c_{0,\bar{s}}c_{0,s} - \varepsilon_{\mathbf{k},\bar{s}}c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s} - U\cancelto{0}{n_{0,s}c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s}} + t_0c^{\dagger}_{1,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s} \\ &- \sum_{\mathbf{k}'}V^{*}_{\mathbf{k}'}c^{\dagger}_{\mathbf{k}',\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s}.\end{aligned} \tag{6.122}$$

$$\begin{aligned}(\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s})\,\langle\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle &= \langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle - t_0\langle\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{1,s};c^{\dagger}_{0,s'}\rangle\rangle \\ +\sum_{\mathbf{k}'}V_{\mathbf{k}'}\langle\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{\mathbf{k}',s};c^{\dagger}_{0,s'}\rangle\rangle &+ V_{\mathbf{k}}\langle\langle c^{\dagger}_{0,\bar{s}}c_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle + t_0\langle\langle c^{\dagger}_{1,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle \\ &- \sum_{\mathbf{k}'}V^{*}_{\mathbf{k}'}\langle\langle c^{\dagger}_{\mathbf{k}',\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle.\end{aligned} \tag{6.123}$$

$$\omega\langle\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle = \langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}\rangle + \langle\langle [c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{0,s},H];c^{\dagger}_{0,s'}\rangle\rangle. \tag{6.124}$$

$$[c^{\dagger}_{\mathbf{k},\bar{s}},H] = -\varepsilon_{\mathbf{k},\bar{s}}c^{\dagger}_{\mathbf{k},\bar{s}} - V_{\mathbf{k}}c_{0,\bar{s}} \tag{6.125}$$

$$\begin{aligned}[c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{0,s},H] &= \varepsilon_{0,s}c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{0,s} + Uc^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}n_{0,\bar{s}}c_{0,s} - t_0c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{1,s} + \sum_{\mathbf{k}'}V_{\mathbf{k}'}c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{\mathbf{k}',s}\\ &+\varepsilon_{0,\bar{s}}c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{0,s} + U\cancelto{0}{c^{\dagger}_{\mathbf{k},\bar{s}}n_{0,\bar{s}}c_{0,\bar{s}}c_{0,s}} - t_0c^{\dagger}_{\mathbf{k},\bar{s}}c_{1,\bar{s}}c_{0,s} + \sum_{\mathbf{k}'}V_{\mathbf{k}'}c^{\dagger}_{\mathbf{k},\bar{s}}c_{\mathbf{k}',\bar{s}}c_{0,s} - \varepsilon_{\mathbf{k},\bar{s}}c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{0,s}\\ &-V_{\mathbf{k}}c^{\dagger}_{0,\bar{s}}c_{0,\bar{s}}c_{0,s}\end{aligned} \tag{6.126}$$

then

$$\begin{aligned}(\omega-\varepsilon_{0,s}-\varepsilon_{0,\bar{s}}-U)\langle\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle &= -t_0\langle\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{1,s};c^{\dagger}_{0,s'}\rangle\rangle\\ +\sum_{\mathbf{k}'}V_{\mathbf{k}'}\langle\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{\mathbf{k}',s};c^{\dagger}_{0,s'}\rangle\rangle - t_0\langle\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{1,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle &+ \sum_{\mathbf{k}'}V_{\mathbf{k}'}\langle\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{\mathbf{k}',\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle\\ &-V_{\mathbf{k}}\langle\langle c^{\dagger}_{0,\bar{s}}c_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle.\end{aligned} \tag{6.127}$$

Now in Eqs. (6.118), (6.123) and (6.127) we make the similar approximations as for the Hubbard I level we obtain

$$(\omega-\varepsilon_{\mathbf{k},s})\langle\langle n_{0,\bar{s}}c_{\mathbf{k},s};c^{\dagger}_{0,s'}\rangle\rangle = -\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{\bar{s}s'} + V^{*}_{\mathbf{k}}\langle\langle n_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle, \tag{6.128}$$

$$\begin{aligned}(\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s})\langle\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle &= \langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{ss'} - t_0\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\langle\langle c_{1,s};c^{\dagger}_{0,s'}\rangle\rangle\\ +\sum_{\mathbf{k}'}V_{\mathbf{k}'}\langle c^{\dagger}_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\langle\langle c_{\mathbf{k}',s};c^{\dagger}_{0,s'}\rangle\rangle &+ V_{\mathbf{k}}\langle\langle n_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle + t_0\langle c^{\dagger}_{1,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\langle\langle c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle\\ &-\sum_{\mathbf{k}'}V^{*}_{\mathbf{k}'}\langle c^{\dagger}_{\mathbf{k}',\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\langle\langle c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle.\end{aligned} \tag{6.129}$$

and

$$\begin{aligned}(\omega-\varepsilon_{0,s}-\varepsilon_{0,\bar{s}}-U)\langle\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle &= \langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}\rangle\delta_{ss'} + \langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,s}\rangle\delta_{\bar{s}s'}\\ -t_0\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}\rangle\langle\langle c_{1,s};c^{\dagger}_{0,s'}\rangle\rangle + \sum_{\mathbf{k}'}V_{\mathbf{k}'}\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{0,\bar{s}}\rangle\langle\langle c_{\mathbf{k}',s};c^{\dagger}_{0,s'}\rangle\rangle &- t_0\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{1,\bar{s}}\rangle\langle\langle c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle\\ +\sum_{\mathbf{k}'}V_{\mathbf{k}'}\langle c^{\dagger}_{\mathbf{k},\bar{s}}c_{\mathbf{k}',\bar{s}}\rangle\langle\langle c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle &- V_{\mathbf{k}}\langle\langle n_{0,\bar{s}}c_{0,s};c^{\dagger}_{0,s'}\rangle\rangle.\end{aligned} \tag{6.130}$$

For simplify we now will take the limit o infinite U. To do so we have to go back to Eq. (6.37) and take the limit

$$\lim_{U\to\infty} U\langle\langle n_{0,\bar{s}}c_{0,s};c^\dagger_{0,s'}\rangle\rangle = \lim_{U\to\infty}\frac{U}{\omega-\varepsilon_{0,s}-U}[\cdots] = \lim_{U\to\infty}\frac{1}{\frac{\omega-\varepsilon_{0,s}}{U}-1}[\cdots] = -\lim_{U\to\infty}[\cdots] \tag{6.131}$$

where the $\cdots$ in the brackets represents all the Green's function of the rhs of Eq. 6.38. Note that any of those Green's function that at this stage presents U in its denominator will vanish when the $\lim_{U\to\infty}$ is taken. This is the case of the Green's function (6.130) and, therefore, it can be disregarded. For $t_0 = 0$ we will have then

$$\begin{aligned}\lim_{U\to\infty} U\langle\langle n_{0,\bar{s}}c_{0,s};c^\dagger_{0,s'}\rangle\rangle &= -\langle n_{0,\bar{s}}\rangle\delta_{ss'} - \langle c^\dagger_{0,\bar{s}}c_{0,s}\rangle\delta_{\bar{s}s'} + \sum_{\mathbf{k}}\frac{V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{\bar{s}s'}}{\omega-\varepsilon_{\mathbf{k},s}} \\ &-\sum_{\mathbf{k}}\frac{V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{ss'}}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}} - \sum_{\mathbf{k}\mathbf{k}'}\frac{V_{\mathbf{k}}V_{\mathbf{k}'}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\langle\langle c_{\mathbf{k}',s};c^\dagger_{0,s'}\rangle\rangle}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}} \\ &+\sum_{\mathbf{k}\mathbf{k}'}\frac{V_{\mathbf{k}}V^*_{\mathbf{k}'}\langle c^\dagger_{\mathbf{k}',\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\langle\langle c_{0,s};c^\dagger_{0,s'}\rangle\rangle}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}}\end{aligned} \tag{6.132}$$

Using Eq. (6.42) we obtain

$$\begin{aligned}\lim_{U\to\infty} U\langle\langle n_{0,\bar{s}}c_{0,s};c^\dagger_{0,s'}\rangle\rangle &= -\langle n_{0,\bar{s}}\rangle\delta_{ss'} - \langle c^\dagger_{0,\bar{s}}c_{0,s}\rangle\delta_{\bar{s}s'} + \sum_{\mathbf{k}}\frac{V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{\bar{s}s'}}{\omega-\varepsilon_{\mathbf{k},s}} \\ &-\sum_{\mathbf{k}}\frac{V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{ss'}}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}} + \sum_{\mathbf{k}\mathbf{k}'}\frac{V_{\mathbf{k}}V^*_{\mathbf{k}'}\langle c^\dagger_{\mathbf{k}',\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\langle\langle c_{0,s};c^\dagger_{0,s'}\rangle\rangle}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}} \\ &-\sum_{\mathbf{k}}\frac{V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}}\sum_{\mathbf{k}'}\frac{|V_{\mathbf{k}'}|^2}{\omega-\varepsilon_{\mathbf{k}',s}}\langle\langle c_{0,s};c^\dagger_{0,s'}\rangle\rangle\end{aligned} \tag{6.133}$$

We still make the additional approximation, $\langle c^\dagger_{\mathbf{k}',\bar{s}}c_{\mathbf{k},\bar{s}}\rangle \approx \langle c^\dagger_{\mathbf{k},\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{\mathbf{k}'\mathbf{k}}$. With this, replacing Eq. (6.133) it into (6.37) we obtain

$$\langle\langle c_{0,s};c^\dagger_{0,s'}\rangle\rangle = \frac{(1-\langle n_{0,\bar{s}}\rangle)\delta_{ss'} - \langle c^\dagger_{0,\bar{s}}c_{0,s}\rangle\delta_{\bar{s}s'} - \sum_{\mathbf{k}}\frac{V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{ss'}}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}} + \sum_{\mathbf{k}}\frac{V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle\delta_{\bar{s}s'}}{\omega-\varepsilon_{\mathbf{k},s}}}{\omega-\varepsilon_{0,s}-\sum_{\mathbf{k}}\left(\frac{|V_{\mathbf{k}}|^2}{\omega-\varepsilon_{\mathbf{k},s}}+\frac{|V_{\mathbf{k}}|^2 f_{\mathbf{k}}}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}}\right)+\sum_{\mathbf{k}}\frac{V_{\mathbf{k}}\langle c^\dagger_{0,\bar{s}}c_{\mathbf{k},\bar{s}}\rangle}{\omega-\varepsilon_{0,s}+\varepsilon_{0,\bar{s}}-\varepsilon_{\mathbf{k},s}}\sum_{\mathbf{k}'}\frac{|V_{\mathbf{k}'}|^2}{\omega-\varepsilon_{\mathbf{k}',s}}}. \tag{6.134}$$

Here $f_{\mathbf{k}}$ is the Fermi function.

$$\begin{aligned}
\sum_{\mathbf{k}} \frac{1}{\omega + i\eta - \varepsilon_{\mathbf{k}}} &= \int_{-\infty}^{\infty} \frac{\Theta(D-|\varepsilon|)}{2D}(-i\pi)\delta(\omega-\varepsilon)d\varepsilon + \int_{-\infty}^{\infty} \frac{\Theta(D-|\varepsilon|)}{2D}\frac{\omega-\varepsilon}{(\omega-\varepsilon)^2+\eta^2}d\varepsilon \\
&= -i\pi\rho_0\Theta(D-|\omega|) - \frac{1}{2D}\ln\Big|\frac{(\omega-D)^2+\eta^2}{(\omega+D)^2+\eta^2}\Big| \\
&= -i\pi\rho_c(\omega) - \frac{1}{2D}\ln\Big|\frac{(\omega-D)^2+\eta^2}{(\omega+D)^2+\eta^2}\Big|, \qquad (6.135)
\end{aligned}$$

where $\rho_0 = 1/2D$. For $T = 0$, $f(\varepsilon) = \Theta(\varepsilon_F - \varepsilon)$. Then

$$\begin{aligned}
\sum_{\mathbf{k}} \frac{f_{\mathbf{k}}}{\omega - \varepsilon_{\mathbf{k}}} &= \int_{-\infty}^{\infty} \frac{\Theta(D-|\varepsilon|)}{2D}\Theta(\varepsilon_F-\varepsilon)(-i\pi)\delta(\omega-\varepsilon)d\varepsilon \\
&\quad + \int_{-\infty}^{\infty} \frac{\Theta(D-|\varepsilon|)}{2D}\frac{\Theta(\varepsilon_F-\varepsilon)(\omega-\varepsilon)}{(\omega-\varepsilon)^2+\eta^2}d\varepsilon \\
&= -i\pi\rho_0\Theta(D-|\omega|)\Theta(\varepsilon_F-\omega) - \frac{1}{2D}\ln\Big|\frac{(\varepsilon_F-\omega)^2+\eta^2}{(\omega+D)^2+\eta^2}\Big| \\
&= -i\pi\rho_c(\omega)\Theta(\varepsilon_F-\omega) - \frac{1}{2D}\ln\Big|\frac{(\varepsilon_F-\omega)^2+\eta^2}{(\omega+D)^2+\eta^2}\Big|. \qquad (6.136)
\end{aligned}$$

Similarly,

$$\begin{aligned}
\sum_{\mathbf{k}} \frac{1}{\omega + i\eta + \varepsilon_{\mathbf{k}}} &= \int_{-\infty}^{\infty} \frac{\Theta(D-|\varepsilon|)}{2D}(-i\pi)\delta(\omega+\varepsilon)d\varepsilon + \int_{-\infty}^{\infty} \frac{\Theta(D-|\varepsilon|)}{2D}\frac{\omega+\varepsilon}{(\omega+\varepsilon)^2+\eta^2}d\varepsilon \\
&= -i\pi\rho_0\Theta(D-|\omega|) + \frac{1}{2D}\ln\Big|\frac{(\omega+D)^2+\eta^2}{(\omega-D)^2+\eta^2}\Big| \\
&= -i\pi\rho_c(\omega) - \frac{1}{2D}\ln\Big|\frac{(\omega-D)^2+\eta^2}{(\omega+D)^2+\eta^2}\Big|, \qquad (6.137)
\end{aligned}$$

and

$$\begin{aligned}
\sum_{\mathbf{k}} \frac{f_{\mathbf{k}}}{\omega + \varepsilon_{\mathbf{k}}} &= \int_{-\infty}^{\infty} \frac{\Theta(D-|\varepsilon|)}{2D}\Theta(\varepsilon_F-\varepsilon)(-i\pi)\delta(\omega+\varepsilon)d\varepsilon \\
&\quad + \int_{-\infty}^{\infty} \frac{\Theta(D-|\varepsilon|)}{2D}\frac{\Theta(\varepsilon_F-\varepsilon)(\omega+\varepsilon)}{(\omega+\varepsilon)^2+\eta^2}d\varepsilon \\
&= -i\pi\rho_0\Theta(D-|\omega|)\Theta(\varepsilon_F-\omega) - \frac{1}{2D}\ln\Big|\frac{(\varepsilon_F-\omega)^2+\eta^2}{(\omega+D)^2+\eta^2}\Big| \\
&= -i\pi\rho_c(\omega)\Theta(\varepsilon_F-\omega) + \frac{1}{2D}\ln\Big|\frac{(\omega+\varepsilon_F)^2+\eta^2}{(\omega-D)^2+\eta^2}\Big|. \qquad (6.138)
\end{aligned}$$

Now, if we assume $V_{\mathbf{k}} \equiv V$ we obtain in the wide band limit

$$\langle\langle c_{0,\downarrow}; c^{\dagger}_{0,\downarrow}\rangle\rangle =$$
$$\frac{1-\langle n_{0,\uparrow}\rangle}{\omega-\varepsilon_d+\frac{V^2}{2D}\ln\left|\frac{(\omega-\varepsilon_F)^2+\eta^2}{(\omega+D)^2+\eta^2}\right|+i\Gamma\left[1+\Theta(\omega-\varepsilon_F)\right]-\frac{2\lambda^2}{\omega-\frac{2\lambda^2}{\omega+\varepsilon_d+\frac{V^2}{2D}\ln\left|\frac{(\omega+\varepsilon_F)^2+\eta^2}{(\omega-D)^2+\eta^2}\right|+i\Gamma\left[1+\Theta(\omega-\varepsilon_F)\right]}}}. \tag{6.139}$$

and

$$\langle\langle c_{0,\downarrow}; c^{\dagger}_{0,\downarrow}\rangle\rangle = \frac{1-\langle n_{0,\downarrow}\rangle}{\omega-\varepsilon_d+\frac{V^2}{2D}\ln\left|\frac{(\omega-\varepsilon_F)^2+\eta^2}{(\omega+D)^2+\eta^2}\right|+i\Gamma\left[1+\Theta(\omega-\varepsilon_F)\right]}. \tag{6.140}$$

6.4 Kondo-like Hamiltonian

$$H = \sum_s \varepsilon_{\mathrm{d}} d_s^\dagger d_s + U n_{d\uparrow} n_{d\downarrow} + \lambda \left(d_\downarrow - d_\downarrow^\dagger \right) \gamma_1 + \sum_{\mathbf{k},s} \varepsilon_{\mathbf{k}} c_{\mathbf{k},s}^\dagger c_{\mathbf{k},s} + \sum_{\mathbf{k},s} V_{\mathbf{k}} \left(d_s^\dagger c_{\mathbf{k},s} + c_{\mathbf{k},s}^\dagger d_s \right). \tag{6.141}$$

$$P_0 = (1 - n_{d\uparrow})(1 - n_{d\downarrow}) \tag{6.142a}$$

$$P_1 = n_{d\uparrow}(1 - n_{d\downarrow}) + n_{d\downarrow}(1 - n{+}_{d\uparrow}) \tag{6.142b}$$

$$P_2 = n_{d\uparrow} n_{d\downarrow} \tag{6.142c}$$

Now we can write the effective Hamiltonian in the single occupied subspace as

$$\tilde{H} = H_{11} + H_{10}(E - H_{22})^{-1} H_{01} + H_{12}(1 - H_{22})^{-1} H_{21} \tag{6.143}$$

in which

$$H_{ij} = P_i H P_j. \tag{6.144}$$

Explicitly we have

$$H_{00} = \sum_{\mathbf{k}s} \varepsilon_{\mathbf{k}} c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s} (1 - n_{d\uparrow})(1 - n_{d\downarrow}) = H_0 (1 - n_{d\uparrow})(1 - n_{d\downarrow}) \tag{6.145}$$

$$H_{22} = (2\varepsilon_d + U + H_0) n_{d\uparrow} n_{d\downarrow} \tag{6.146}$$

and

$$H_{11} = (\varepsilon_d + H_0) \sum_s n_{ds}(1 - n_{d\bar{s}}). \tag{6.147}$$

$$H_{01} = \sum_{\mathbf{k}s} V_{\mathbf{k}}^* (1 - n_{d\bar{s}}) c_{\mathbf{k}s}^\dagger d_s + \lambda (1 - n_{d\uparrow}) d_\downarrow \gamma_1 \tag{6.148}$$

$$H_{10} = \sum_{\mathbf{k}s} V_{\mathbf{k}} (1 - n_{d\bar{s}}) d_s^\dagger c_{\mathbf{k}s} + \lambda (1 - n_{d\uparrow}) \gamma_1 d_\downarrow^\dagger \tag{6.149}$$

$$H_{21} = \sum_{\mathbf{k}s} V_{\mathbf{k}} n_{d\bar{s}} d_s^\dagger c_{\mathbf{k}s} + \lambda n_{d\uparrow} \gamma_1 d_\downarrow^\dagger \tag{6.150}$$

$$H_{12} = \sum_{\mathbf{k}s} V_{\mathbf{k}}^* n_{d\bar{s}} c_{\mathbf{k}s}^\dagger d_s + \lambda n_{d\uparrow} d_\downarrow \gamma_1 \tag{6.151}$$

The first term refers to the usual Anderson Hamiltonian. For $H_{10}(E-H_{00})^{-1}H_{01}$ we have

$$\begin{aligned}
H_{10}(E-H_{00})^{-1}H_{01} &= \left(\sum_{\mathbf{k}s} V_{\mathbf{k}}(1-n_{d\bar{s}})d_s^\dagger c_{\mathbf{k}s} + \lambda(1-n_{d\uparrow})\gamma_1 d_\downarrow^\dagger\right)(E-H_{00})^{-1} \\
&\quad \times \left(\sum_{\mathbf{k}s} V_{\mathbf{k}}^*(1-n_{d\bar{s}})c_{\mathbf{k}s}^\dagger d_s + \lambda(1-n_{d\uparrow})d_\downarrow\gamma_1\right) \\
&= \sum_{\substack{\mathbf{k}\mathbf{k}' \\ ss'}} V_{\mathbf{k}}V_{\mathbf{k}'}^*(1-n_{d\bar{s}})d_s^\dagger c_{\mathbf{k}s}(E-H_{00})^{-1}(1-n_{d\bar{s}'})c_{\mathbf{k}'s'}^\dagger d_{s'} \\
&\quad + \sum_{\mathbf{k}s} \lambda V_{\mathbf{k}}(1-n_{d\bar{s}})d_s^\dagger c_{\mathbf{k}s}(E-H_{00})^{-1}(1-n_{d\uparrow})d_\downarrow\gamma_1 \\
&\quad + \sum_{\mathbf{k}s} \lambda V_{\mathbf{k}}^*(1-n_{d\uparrow})\gamma_1 d_\downarrow^\dagger(E-H_{00})^{-1}(1-n_{d\bar{s}})c_{\mathbf{k}s}^\dagger d_s \\
&\quad + \lambda^2(1-n_{d\uparrow})\gamma_1 d_\downarrow^\dagger(E-H_{00})^{-1}(1-n_{d\uparrow})d_\downarrow\gamma_1
\end{aligned} \tag{6.152}$$

Note that

$$c_{\mathbf{k}s}(E-H_{00})^{-1} = \frac{1}{E}c_{\mathbf{k}s}\left(1-\frac{H_{00}}{E}\right)^{-1} = \frac{1}{E}c_{\mathbf{k}s}\sum_n\left(\frac{H_{00}}{E}\right)^n = \frac{1}{E}\sum_n\frac{1}{E^n}c_{\mathbf{k}s}\left(H_{00}\right)^n \tag{6.153}$$

Noting that

$$\begin{aligned}
c_{\mathbf{k}s}H_{00} &= \sum_{\mathbf{k}''s''}\varepsilon_{\mathbf{k}''}c_{\mathbf{k}s}, c_{\mathbf{k}''s''}^\dagger c_{\mathbf{k}''s''} \\
&= \sum_{\mathbf{k}''s''}\varepsilon_{\mathbf{k}''}\delta_{\mathbf{k}''\mathbf{k}}\delta_{s''s}c_{\mathbf{k}s} + \sum_{\substack{\mathbf{k}''\neq\mathbf{k} \\ s''}}\varepsilon_{\mathbf{k}''}c_{\mathbf{k}''s''}^\dagger c_{\mathbf{k}''s''}c_{\mathbf{k}s} \\
&= \varepsilon_{\mathbf{k}}c_{\mathbf{k}s} + \sum_{\substack{\mathbf{k}''\neq\mathbf{k} \\ s''}}\varepsilon_{\mathbf{k}''}c_{\mathbf{k}''s''}^\dagger c_{\mathbf{k}''s''}c_{\mathbf{k}s} \\
&= \left(\varepsilon_{\mathbf{k}} + \sum_{\mathbf{k}''s''}\varepsilon_{\mathbf{k}''}c_{\mathbf{k}''s''}^\dagger c_{\mathbf{k}''s''}\right)c_{\mathbf{k}s} \\
&= \left(\varepsilon_{\mathbf{k}} + H_0\right)c_{\mathbf{k}s}.
\end{aligned} \tag{6.154}$$

Now,

$$c_{\mathbf{k}s}(H_{00})^n = \left(\varepsilon_{\mathbf{k}}+H_0\right)c_{\mathbf{k}s}H_{00}^{n-1} = \left(\varepsilon_{\mathbf{k}}+H_0\right)^2 c_{\mathbf{k}s}H_{00}^{n-2} = \cdots = \left(\varepsilon_{\mathbf{k}}+H_0\right)^n c_{\mathbf{k}s}. \tag{6.155}$$

Therefore,

$$\begin{aligned}
c_{\mathbf{k}s}(E-H_{00})^{-1} &= \frac{1}{E}\sum_n\left(\frac{\varepsilon_{\mathbf{k}}+H_0}{E}\right)^n c_{\mathbf{k}s} = \frac{1}{E}\left(1-\frac{\varepsilon_{\mathbf{k}}+H_0}{E}\right)^{-1}c_{\mathbf{k}s} \\
&= \left(E-\varepsilon_{\mathbf{k}}-H_0\right)^{-1}c_{\mathbf{k}s}.
\end{aligned} \tag{6.156}$$

we use this expression to write

$$(E-H_{00})^{-1}c^{\dagger}_{\mathbf{k}s}=\left[c_{\mathbf{k}s}(E-H_{00})^{-1}\right]^{\dagger}=\left[(E-\varepsilon_{\mathbf{k}}-H_0)^{-1}\,c_{\mathbf{k}s}\right]^{\dagger}=c^{\dagger}_{\mathbf{k}s}\,(E-\varepsilon_{\mathbf{k}}-H_0)^{-1} \tag{6.157}$$

$$\begin{aligned}H_{10}(E-H_{00})^{-1}H_{01} \;=\;& \sum_{\substack{\mathbf{kk'}\\ ss'}} V_{\mathbf{k}}V^*_{\mathbf{k'}}\,(E-\varepsilon_{\mathbf{k}}-H_0)^{-1}\,(1-n_{d\bar{s}})d^{\dagger}_s c_{\mathbf{k}s}(1-n_{d\bar{s}'})c^{\dagger}_{\mathbf{k'}s'}d_{s'}\\ &+\sum_{\mathbf{k}s}\lambda V_{\mathbf{k}}\,(E-\varepsilon_{\mathbf{k}}-H_0)^{-1}\,(1-n_{d\bar{s}})d^{\dagger}_s c_{\mathbf{k}s}(1-n_{d\uparrow})d_{\downarrow}\gamma_1\\ &+\sum_{\mathbf{k}s}\lambda V^*_{\mathbf{k}}(1-n_{d\uparrow})\gamma_1 d^{\dagger}_{\downarrow}c^{\dagger}_{\mathbf{k}s}(1-n_{d\bar{s}})d_s\,(E-\varepsilon_{\mathbf{k}}-H_0)^{-1}\\ &+\lambda^2(E-H_0)^{-1}(1-n_{d\uparrow})\gamma_1 d^{\dagger}_{\downarrow}(1-n_{d\uparrow})d_{\downarrow}\gamma_1\end{aligned} \tag{6.158}$$

Now we will make the approximations by writing

$$(E-\varepsilon_{\mathbf{k}}-H_0)^{-1}=(E-\varepsilon_{\mathbf{k}}-H_0+\varepsilon_d-\varepsilon_d)^{-1}=\frac{1}{\varepsilon_d-\varepsilon_{\mathbf{k}}}\left[1-\frac{E-H_0-\varepsilon_d}{\varepsilon_{\mathbf{k}}-\varepsilon_d}\right]^{-1}. \tag{6.159}$$

In the same way we can write

$$(E-H_0)^{-1}=(E-H_0+\varepsilon_d-\varepsilon_d)^{-1}=\frac{1}{\varepsilon_d}\left(1+\frac{E-H_0-\varepsilon_d}{\varepsilon_d}\right)^{-1}. \tag{6.160}$$

Since we are restricted to the singly occupied subspace, apart from correction quadratic in the coupling, $E-H_0\approx\varepsilon_d$. Also because we are interested in excitation close to the Fermi energy, $\varepsilon_{\mathbf{k}}\ll\varepsilon_d$. Then we can neglect the second term inside the brackets of Eqs. 6.159 and 6.160, since $E-H_0-\varepsilon_d\ll\varepsilon_d,\varepsilon_d-\varepsilon_{\mathbf{k}}$. Therefore we can write

$$(E-\varepsilon_{\mathbf{k}}-H_0)^{-1}\approx\frac{1}{\varepsilon_d-\varepsilon_{\mathbf{k}}} \tag{6.161}$$

and

$$(E-H_0)^{-1}=\frac{1}{\varepsilon_d}. \tag{6.162}$$

Replacing Eqs. 6.161 and 6.162 into Eq. 6.158 we obtain

$$\begin{aligned} H_{10}(E-H_{00})^{-1}H_{01} &= \sum_{\substack{\mathbf{k}\mathbf{k}'\\ ss'}} \frac{V_{\mathbf{k}}V_{\mathbf{k}'}^*}{\varepsilon_d-\varepsilon_{\mathbf{k}}}(1-n_{d\bar{s}})d_s^\dagger c_{\mathbf{k}s}(1-n_{d\bar{s}'})c_{\mathbf{k}'s'}^\dagger d_{s'} \\ &+\sum_{\mathbf{k}s} \frac{\lambda V_{\mathbf{k}}}{\varepsilon_d-\varepsilon_{\mathbf{k}}}(1-n_{d\bar{s}})d_s^\dagger c_{\mathbf{k}s}(1-n_{d\uparrow})d_\downarrow\gamma_1 \\ &+\sum_{\mathbf{k}s} \frac{\lambda V_{\mathbf{k}}^*}{\varepsilon_d-\varepsilon_{\mathbf{k}}}(1-n_{d\uparrow})\gamma_1 d_\downarrow^\dagger c_{\mathbf{k}s}^\dagger(1-n_{d\bar{s}})d_s \\ &+\frac{\lambda^2}{\varepsilon_d}(1-n_{d\uparrow})\gamma_1 d_\downarrow^\dagger(1-n_{d\uparrow})d_\downarrow\gamma_1 \end{aligned} \tag{6.163}$$

Now we need to take care of the doubly occupied subspace. It is eliminated by

$$\begin{aligned} H_{12}(E-H_{22})^{-1}H_{21} &= \left[\sum_{\mathbf{k}s} V_{\mathbf{k}}^* n_{d\bar{s}} c_{\mathbf{k}s}^\dagger d_s + \lambda n_{d\uparrow} d_\downarrow \gamma_1\right](E-H_{22})^{-1} \\ &\times \left[\sum_{\mathbf{k}s} V_{\mathbf{k}} n_{d\bar{s}} d_s^\dagger c_{\mathbf{k}s} + \lambda n_{d\uparrow}\gamma_1 d_\downarrow^\dagger\right] \\ &= \sum_{\substack{\mathbf{k}\mathbf{k}'\\ ss'}} V_{\mathbf{k}'}^* V_{\mathbf{k}} n_{d\bar{s}'} c_{\mathbf{k}'s'}^\dagger d_{s'}(E-H_{22})^{-1} n_{d\bar{s}} d_s^\dagger c_{\mathbf{k}s} \\ &+\sum_{\mathbf{k}s} \lambda V_{\mathbf{k}}^* n_{d\bar{s}} c_{\mathbf{k}s}^\dagger d_s (E-H_{22})^{-1} n_{d\uparrow}\gamma_1 d_\downarrow^\dagger \\ &+\sum_{\mathbf{k}s} \lambda V_{\mathbf{k}} n_{d\uparrow}\gamma_1 d_\downarrow^\dagger (E-H_{22})^{-1} n_{d\bar{s}} d_s^\dagger c_{\mathbf{k}s} \\ &+\lambda^2 n_{d\uparrow} d_\downarrow \gamma_1 (E-H_{22})^{-1} n_{d\uparrow}\gamma_1 d_\downarrow^\dagger. \end{aligned} \tag{6.164}$$

Now,

$$\begin{aligned} (E-H_{22})^{-1}c_{\mathbf{k}s} &= (E-2\varepsilon_d-U-H_0)^{-1}c_{\mathbf{k}s} = (E'-H_0)^{-1}c_{\mathbf{k}s} = \frac{1}{E'}\left(1-\frac{H_0}{E'}\right)^{-1} c_{\mathbf{k}s} \\ &= \frac{1}{E'}\sum_n \frac{1}{(E')^n}(H_0)^n c_{\mathbf{k}s}. \end{aligned} \tag{6.165}$$

$$\begin{aligned} H_0 c_{\mathbf{k}s} &= \sum_{\mathbf{k}''s''} \varepsilon_{\mathbf{k}''} c_{\mathbf{k}''s''}^\dagger c_{\mathbf{k}''s''} c_{\mathbf{k}s} = c_{\mathbf{k}s} \sum_{\substack{\mathbf{k}''\neq\mathbf{k}\\ s''\neq s}} \varepsilon_{\mathbf{k}''} c_{\mathbf{k}''s''}^\dagger c_{\mathbf{k}''s''} \\ &= c_{\mathbf{k}s}\left(\sum_{\mathbf{k}''s''} \varepsilon_{\mathbf{k}''} c_{\mathbf{k}''s''}^\dagger c_{\mathbf{k}''s''} - \varepsilon_{\mathbf{k}} c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s}\right) = \left(c_{\mathbf{k}s}H_0 - \varepsilon_{\mathbf{k}} c_{\mathbf{k}s} c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s}\right) \\ &= c_{\mathbf{k}s}\left(H_0-\varepsilon_{\mathbf{k}}\right). \end{aligned} \tag{6.166}$$

Then,

$$(H_0)^n c_{\mathbf{k}s} = c_{\mathbf{k}s}\left(H_0-\varepsilon_{\mathbf{k}}\right)^n \tag{6.167}$$

$$
\begin{aligned}
(E-H_{22})^{-1}c_{\mathbf{k}s} &= c_{\mathbf{k}s}\frac{1}{E'}\sum_n \frac{(H_0-\varepsilon_{\mathbf{k}})^n}{(E')^n} = c_{\mathbf{k}s}\frac{1}{E'}\left(1-\frac{H_0-\varepsilon_{\mathbf{k}}}{E'}\right)^{-1} \\
&= c_{\mathbf{k}s}\left(E'-H_0+\varepsilon_{\mathbf{k}}\right)^{-1} = c_{\mathbf{k}s}\left(E-2\varepsilon_d-U-H_0+\varepsilon_{\mathbf{k}}\right)^{-1}. \qquad (6.168)
\end{aligned}
$$

Also,

$$
\begin{aligned}
c^{\dagger}_{\mathbf{k}s}(E-H_{22})^{-1} &= \left[(E-H_{22})^{-1}c_{\mathbf{k}s}\right]^{\dagger} = \left[c_{\mathbf{k}s}\left(E'-H_0+\varepsilon_{\mathbf{k}}\right)^{-1}\right]^{\dagger} \\
&= \left(E-2\varepsilon_d-U-H_0+\varepsilon_{\mathbf{k}}\right)^{-1}c^{\dagger}_{\mathbf{k}s}. \qquad (6.169)
\end{aligned}
$$

$$
\begin{aligned}
H_{12}(E-H_{22})^{-1}H_{21} &= \sum_{\substack{\mathbf{k}\mathbf{k}'\\ ss'}} V^*_{\mathbf{k}'}V_{\mathbf{k}}n_{d\bar{s}'}c^{\dagger}_{\mathbf{k}'s'}d_{s'}n_{d\bar{s}}d^{\dagger}_s c_{\mathbf{k}s}\left(E-2\varepsilon_d-U-H_0+\varepsilon_{\mathbf{k}}\right)^{-1} \\
&+\sum_{\mathbf{k}s}\lambda V^*_{\mathbf{k}}\left(E-2\varepsilon_d-U-H_0+\varepsilon_{\mathbf{k}}\right)^{-1}n_{d\bar{s}}c^{\dagger}_{\mathbf{k}s}d_s n_{d\uparrow}\gamma_1 d^{\dagger}_{\downarrow} \\
&+\sum_{\mathbf{k}s}\lambda V_{\mathbf{k}}n_{d\uparrow}\gamma_1 d^{\dagger}_{\downarrow}n_{d\bar{s}}d^{\dagger}_s c_{\mathbf{k}s}\left(E-2\varepsilon_d-U-H_0+\varepsilon_{\mathbf{k}}\right)^{-1} \\
&+\lambda^2(E-H_0-2\varepsilon_d-U)^{-1}n_{d\uparrow}d_{\downarrow}\gamma_1 n_{d\uparrow}\gamma_1 d^{\dagger}_{\downarrow}. \qquad (6.170)
\end{aligned}
$$

Now,

$$
\begin{aligned}
\left(E-2\varepsilon_d-U-H_0+\varepsilon_{\mathbf{k}}\right)^{-1} &= \left[(\varepsilon_{\mathbf{k}}-\varepsilon_d-U)\left(1-\frac{E-\varepsilon_d-H_0}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}\right)\right]^{-1} \\
&= \frac{-1}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}\left(1-\frac{E-\varepsilon_d-H_0}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}\right)^{-1} \\
&\approx \frac{-1}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}. \qquad (6.171)
\end{aligned}
$$

and

$$
\begin{aligned}
(E-H_0-2\varepsilon_d-U)^{-1} &= \left[(\varepsilon_d+U)\left(-1+\frac{E-H_0-\varepsilon_d}{\varepsilon_d+U}\right)\right]^{-1} \\
&= \frac{-1}{\varepsilon_d+U}\left(1-\frac{E-H_0-\varepsilon_d}{\varepsilon_d+U}\right)^{-1} \\
&\approx \frac{-1}{\varepsilon_d+U}. \qquad (6.172)
\end{aligned}
$$

$$
\begin{aligned}
H_{12}(E-H_{22})^{-1}H_{21} &= -\sum_{\substack{\mathbf{k}\mathbf{k}'\\ ss'}}\frac{V^*_{\mathbf{k}'}V_{\mathbf{k}}}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}n_{d\bar{s}'}c^{\dagger}_{\mathbf{k}'s'}d_{s'}n_{d\bar{s}}d^{\dagger}_s c_{\mathbf{k}s} \\
&-\sum_{\mathbf{k}s}\frac{\lambda V^*_{\mathbf{k}}}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}n_{d\bar{s}}c^{\dagger}_{\mathbf{k}s}d_s n_{d\uparrow}\gamma_1 d^{\dagger}_{\downarrow} \\
&-\sum_{\mathbf{k}s}\frac{\lambda V_{\mathbf{k}}}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}n_{d\uparrow}\gamma_1 d^{\dagger}_{\downarrow}n_{d\bar{s}}d^{\dagger}_s c_{\mathbf{k}s} \\
&-\frac{\lambda^2}{\varepsilon_d+U}n_{d\uparrow}d_{\downarrow}\gamma_1 n_{d\uparrow}\gamma_1 d^{\dagger}_{\downarrow}. \qquad (6.173)
\end{aligned}
$$

In order to see how the Kondo-like Hamiltonian appears we will explicitly perform the spin summations of Eqs. 6.163 and 6.173. We will do each term of these expression separately. The first term of the rhs of Eqs. 6.163

$$
\begin{aligned}
H_{10}(E-H_{00})^{-1}H_{01} \;=\; & \sum_{\mathbf{k}\mathbf{k}'} \frac{V_{\mathbf{k}'}^{*}V_{\mathbf{k}}}{\varepsilon_d-\varepsilon_{\mathbf{k}}}\left[n_{d\uparrow}c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow}^{\dagger}+n_{d\downarrow}c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow}^{\dagger}\right] \\
& +\sum_{\mathbf{k}\mathbf{k}'} \frac{V_{\mathbf{k}'}^{*}V_{\mathbf{k}}}{\varepsilon_d-\varepsilon_{\mathbf{k}}}\left[d_{\uparrow}^{\dagger}d_{\downarrow}c_{\mathbf{k}'\downarrow}^{\dagger}c_{\mathbf{k}\uparrow}+c_{\mathbf{k}'\uparrow}^{\dagger}c_{\mathbf{k}\downarrow}\right] \\
& +\sum_{\mathbf{k}} \frac{\lambda V_{\mathbf{k}}}{\varepsilon_d-\varepsilon_{\mathbf{k}}}\left[d_{\uparrow}^{\dagger}d_{\downarrow}c_{\mathbf{k}\uparrow}\gamma_1+n_{d\downarrow}\gamma_1 c_{\mathbf{k}\downarrow}\right] \\
& +\sum_{\mathbf{k}} \frac{\lambda V_{\mathbf{k}}^{*}}{\varepsilon_d-\varepsilon_{\mathbf{k}}}\left[d_{\downarrow}^{\dagger}d_{\uparrow}c_{\mathbf{k}\uparrow}^{\dagger}\gamma_1+n_{d\downarrow}\gamma_1 c_{\mathbf{k}\downarrow}\right] \\
& +\frac{\lambda^2}{\varepsilon_d}n_{d\downarrow} \qquad (6.174)
\end{aligned}
$$

and

$$
\begin{aligned}
H_{12}(E-H_{22})^{-1}H_{21} \;=\; & -\sum_{\mathbf{k}\mathbf{k}'} \frac{V_{\mathbf{k}'}^{*}V_{\mathbf{k}}}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}\left[n_{d\downarrow}c_{\mathbf{k}'\uparrow}^{\dagger}c_{\mathbf{k}\uparrow}+n_{d\uparrow}c_{\mathbf{k}'\downarrow}^{\dagger}c_{\mathbf{k}\downarrow}\right] \\
& -\sum_{\mathbf{k}'\mathbf{k}} \frac{V_{\mathbf{k}'}^{*}V_{\mathbf{k}}}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}\left[c_{\mathbf{k}'\uparrow}^{\dagger}c_{\mathbf{k}\downarrow}d_{\downarrow}d_{\uparrow}^{\dagger}+c_{\mathbf{k}'\downarrow}^{\dagger}c_{\mathbf{k}\uparrow}d_{\uparrow}d_{\downarrow}^{\dagger}\right] \\
& -\sum_{\mathbf{k}} \frac{\lambda V_{\mathbf{k}}^{*}}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}\left[c_{\mathbf{k}\uparrow}^{\dagger}d_{\downarrow}^{\dagger}d_{\uparrow}\gamma_1-c_{\mathbf{k}\downarrow}^{\dagger}(1-n_{d\downarrow})\gamma_1\right] \\
& -\sum_{\mathbf{k}} \frac{\lambda V_{\mathbf{k}}}{\varepsilon_d+U-\varepsilon_{\mathbf{k}}}\left[d_{\downarrow}^{\dagger}d_{\uparrow}\gamma_1 c_{\mathbf{k}\uparrow}-(1-n_{d\downarrow})\gamma_1 c_{\mathbf{k}\downarrow}\right] \\
& -\frac{\lambda^2}{\varepsilon_d+U}n_{d\uparrow}. \qquad (6.175)
\end{aligned}
$$

Note that

$$
\begin{aligned}
n_{d\uparrow}c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow}^{\dagger}+n_{d\downarrow}c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow}^{\dagger} &= \frac{1}{2}(n_{d\uparrow}-n_{d\downarrow})\left(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow}^{\dagger}-c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow}^{\dagger}\right)+\frac{1}{2}(n_{d\uparrow}+n_{d\downarrow})\left(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow}^{\dagger}+c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow}^{\dagger}\right) \\
&= S^z\left(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow}^{\dagger}-c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow}^{\dagger}\right)+\frac{n_d}{2}\left(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow}^{\dagger}+c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow}^{\dagger}\right). \qquad (6.176)
\end{aligned}
$$

and

$$
\begin{aligned}
n_{d\uparrow}c_{\mathbf{k}'\uparrow}^{\dagger}c_{\mathbf{k}\uparrow}+n_{d\downarrow}c_{\mathbf{k}'\downarrow}^{\dagger}c_{\mathbf{k}\downarrow} &= \frac{1}{2}(n_{d\uparrow}-n_{d\downarrow})\left(c_{\mathbf{k}'\uparrow}^{\dagger}c_{\mathbf{k}\uparrow}-c_{\mathbf{k}'\downarrow}^{\dagger}c_{\mathbf{k}\downarrow}\right)+\frac{1}{2}(n_{d\uparrow}+n_{d\downarrow})\left(c_{\mathbf{k}'\uparrow}^{\dagger}c_{\mathbf{k}\uparrow}+c_{\mathbf{k}'\downarrow}^{\dagger}c_{\mathbf{k}\downarrow}\right) \\
&= S^z\left(c_{\mathbf{k}'\uparrow}^{\dagger}c_{\mathbf{k}\uparrow}-c_{\mathbf{k}'\downarrow}^{\dagger}c_{\mathbf{k}\downarrow}\right)+\frac{n_d}{2}\left(c_{\mathbf{k}'\uparrow}^{\dagger}c_{\mathbf{k}\uparrow}+c_{\mathbf{k}'\downarrow}^{\dagger}c_{\mathbf{k}\downarrow}\right), \qquad (6.177)
\end{aligned}
$$

where $S^z = (d_{d\uparrow}-n_{d\downarrow})/2$. Replacing the identities 6.176 and 6.177 into Eqs. 6.174 and Eqs. 6.175, upon some manipulations we replace into Eq. 6.143 to obtain the effective Hamiltonian within the singly occupied subspace:

$$\begin{aligned}\tilde{H} &= \sum_{\mathbf{k}s} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}s} c_{\mathbf{k}s} + \sum_{\mathbf{k}\mathbf{k}'} J_{\mathbf{k}\mathbf{k}'} \left[S^z \left(c^{\dagger}_{\mathbf{k}'\uparrow} c_{\mathbf{k}\uparrow} - c^{\dagger}_{\mathbf{k}'\downarrow} c_{\mathbf{k}\downarrow} \right) + S^+ c^{\dagger}_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} + S^- c^{\dagger}_{\mathbf{k}'\uparrow} c_{\mathbf{k}\downarrow} \right] \\ &+ \sum_{\mathbf{k}\mathbf{k}'} K_{\mathbf{k}\mathbf{k}'} c^{\dagger}_{\mathbf{k}'s} c_{\mathbf{k}s} - \sum_{\mathbf{k}} \left(\Upsilon_{\mathbf{k}} S^+ \gamma_1 c_{\mathbf{k}\uparrow} + \Upsilon^*_{\mathbf{k}} S^- c^{\dagger}_{\mathbf{k}\uparrow} \gamma_1 \right) + \sum_{\mathbf{k}} \left(\hat{T}_{\mathbf{k}} \gamma_1 c_{\mathbf{k}\downarrow} + \hat{T}^*_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\downarrow} \gamma_1 \right) \\ &+ \lambda^2 \left(\frac{n_{d\downarrow}}{\varepsilon_d} - \frac{n_{d\uparrow}}{\varepsilon_d + U} \right). \end{aligned} \tag{6.178}$$

We have introduced the usual s-d coupling

$$J_{\mathbf{k}\mathbf{k}'} = V^*_{\mathbf{k}'} V_{\mathbf{k}} \left(\frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_d} + \frac{1}{\varepsilon_d + U - \varepsilon_{\mathbf{k}'}} \right), \tag{6.179}$$

and the scattering potential

$$K_{\mathbf{k}\mathbf{k}'} = \frac{V^*_{\mathbf{k}'} V_{\mathbf{k}}}{2} \left(\frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_d} - \frac{1}{\varepsilon_d + U - \varepsilon_{\mathbf{k}'}} \right) \tag{6.180}$$

together with

$$\Upsilon_{\mathbf{k}} = \lambda V_{\mathbf{k}} \left(\frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_d} + \frac{1}{\varepsilon_d + U - \varepsilon_{\mathbf{k}}} \right) \tag{6.181}$$

and

$$\hat{T}_{\mathbf{k}} = \lambda V_{\mathbf{k}} \left(\frac{n_{d\downarrow}}{\varepsilon_d - \varepsilon_{\mathbf{k}}} + \frac{n_{d\uparrow}}{\varepsilon_d + U - \varepsilon_{\mathbf{k}}} \right). \tag{6.182}$$

To obtain the Eq. 6.178 we have dropped the c-number

$$\varepsilon_d + \frac{1}{2} \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\varepsilon_{\mathbf{k}} - \varepsilon_d} \tag{6.183}$$

and used the fact that within the singly occupied subspace we have $n_d = 1$, $S^+ = d^{\dagger}_{\uparrow} d_{\downarrow}$, $S^- = d^{\dagger}_{\downarrow} d_{\uparrow}$ and $\gamma_1^2 = 1$.

In the very low-energy regime in which $\varepsilon_{\mathbf{k}} \ll |\varepsilon_d|, |\varepsilon_d + U|$ we can neglect $\varepsilon_{\mathbf{k}}$ in the expressions above. Moreover, assuming $V_{\mathbf{k}} = V$ ($\mathbf{k}$-independent) we can write ($\varepsilon_d < 0$)

$$J_{\mathbf{k}\mathbf{k}'} = |V|^2 \left(\frac{1}{|\varepsilon_d|} + \frac{1}{|\varepsilon_d + U|} \right) \equiv J, \tag{6.184}$$

$$\Upsilon_{\mathbf{k}} = \Upsilon^*_{\mathbf{k}} = \lambda V \left(\frac{1}{|\varepsilon_d|} + \frac{1}{U - |\varepsilon_d|} \right) \equiv \Upsilon \tag{6.185}$$

and

$$\hat{T}_{\mathbf{k}} = \lambda V_{\mathbf{k}} \left(-\frac{n_{d\downarrow}}{|\varepsilon_d|} + \frac{n_{d\uparrow}}{U - |\varepsilon_d|} \right) \equiv \hat{T}. \tag{6.186}$$

In trying to interpret the terms of the Hamiltonian 6.178 we note that, away from the particle-hole symmetry of the dot, the last term act as an effective Zeeman splitting at the impurity. To see this, lets suppose that $\varepsilon_d = -U/2 + \delta\varepsilon$, where $\delta\varepsilon \ll U/2$. Then we can write

$$\frac{1}{\varepsilon_d} = \frac{1}{\delta\varepsilon - U/2} = -\left(\frac{U}{2} - \delta\varepsilon\right)^{-1} = -\frac{2}{U}\left(1 - \frac{2\delta\varepsilon}{U}\right)^{-1} \approx -\frac{2}{U} - \frac{4\delta\varepsilon}{U^2} \tag{6.187}$$

$$\frac{1}{\varepsilon_d + U} = \frac{1}{\delta\varepsilon + U/2} = \left(\frac{U}{2} + \delta\varepsilon\right)^{-1} = \frac{2}{U}\left(1 + \frac{2\delta\varepsilon}{U}\right)^{-1} \approx \frac{2}{U} - \frac{4\delta\varepsilon}{U^2} \tag{6.188}$$

Then,

$$\frac{n_{d\downarrow}}{\varepsilon_d} - \frac{n_{d\uparrow}}{\varepsilon_d + U} = -\frac{2}{U}(n_{d\uparrow} + n_{\downarrow}) + \frac{4\delta\varepsilon}{U^2}(n_{d\uparrow} - n_{\downarrow}) = -\frac{2}{U} + \frac{8\delta\varepsilon}{U^2}S^z. \tag{6.189}$$

We see then that the effective Zeeman field is $B_{\text{eff}} = 8\lambda^2\delta\varepsilon/U^2$, which is quadratic in λ and linear in $\delta\varepsilon$.

7

Topological insulators

7.1 The BHZ model

The basis for the BHZ model is $\{|E_1,+\rangle, |H_1+\rangle, |E_1,-\rangle, |H_1,-\rangle\}$, where in the notation $|\Gamma, m_j\rangle$ we have

$$|E_1,+\rangle = f_{E+,1}(z)|\Gamma_6^-, 1/2\rangle + f_{E+,4}(z)|\Gamma_8^+, 1/2\rangle \equiv |\Gamma_6, +1/2\rangle \tag{7.1a}$$

$$|H_1,+\rangle = f_{H+,3}(z)|\Gamma_8^+, 3/2\rangle \equiv |\Gamma_8, +3/2\rangle \tag{7.1b}$$

$$|E_1,-\rangle = f_{E-,2}(z)|\Gamma_6^-, -1/2\rangle + f_{E-,5}(z)|\Gamma_8^+, -1/2\rangle \equiv |\Gamma_6, -1/2\rangle \tag{7.1c}$$

$$|H_1,-\rangle = f_{H-,6}(z)|\Gamma_8^+, -3/2\rangle \equiv |\Gamma_8, -3/2\rangle. \tag{7.1d}$$

The effective Hamiltonians on this basis are

$$\mathcal{H}_0(\mathbf{k}) = \tilde{\varepsilon}(k)\mathbb{I}_{4\times 4} + \begin{pmatrix} \mathcal{M}(k) + B_E & A(k_x + ik_y) & -iR_0(k_x + ik_y) & -h(\theta) \\ A(k_x - ik_y) & -\mathcal{M}(k) + B_H & h(\theta) & 0 \\ iR_0(k_x - ik_y) & h^*(\theta) & \mathcal{M}(k) - B_E & -A(k_x + ik_y) \\ -h^*(\theta) & 0 & -A(k_x - ik_y) & -\mathcal{M}(k) - B_H \end{pmatrix}, \tag{7.2}$$

where $\mathcal{M}(k) = M - Bk^2$ and $\tilde{\varepsilon}(k) = C - Dk^2$, in which A, B, C and D are the known parameters that depend on the QW geometry and R_0 is related to the linear Rashba SOC due to an electric field applied along the z-direction (perpendicularly to the plane of the QW). In the above we also introduce B_E and B_H as the mass term due to a Zeeman effect resulting from an external magnetic field along the z-axis and $h(\theta) = h_0[\cos(2\theta) + i\sin(2\theta)]$.

A compact form of the Hamiltonian (7.2) is

$$\begin{aligned} H &= \varepsilon(k)\sigma_0 \otimes s_0 + \tilde{M}(k)\sigma_0 \otimes s_z + Ak_x\sigma_z \otimes s_x - Ak_y\sigma_0 \otimes s_y + R_0k_x\sigma_y \otimes \frac{s_z+1}{2} \\ &\quad -R_0k_x\sigma_y \otimes \frac{s_z+1}{2} + B_+\sigma_z \otimes s_0 + B_-\sigma_z \otimes s_0 + h_0\cos(2\theta)\sigma_y \otimes s_y + h_0\sin(2\theta)\sigma_x \otimes s_y. \end{aligned} \tag{7.3}$$

7.1.1 Tight binding model

To derive a discretized version of the Hamiltonian above, we first recall that

$$k_x = -i\frac{\partial}{\partial x} \Rightarrow k_x^2 = -\frac{\partial^2}{\partial x^2} \tag{7.4}$$

and

$$k_y = -i\frac{\partial}{\partial y} \Rightarrow k_y^2 = -\frac{\partial^2}{\partial y^2}. \tag{7.5}$$

Let us now assume that the operators act on a arbitrary wavefunction $F(x, y)$. The discrete version of this function is

$$F(x, y) = F(x = ja, y = \ell a) \equiv F_{j,\ell}, \text{where } j, \ell \text{ are integers.} \tag{7.6}$$

With that, the first and second derivatives become

$$\frac{\partial}{\partial x} \to \frac{1}{2a}\left[F_{j+1,\ell} - F_{j-1,\ell}\right] \tag{7.7}$$

$$\frac{\partial}{\partial y} \to \frac{1}{2a}\left[F_{j,\ell+1} - F_{j,\ell-1}\right] \tag{7.8}$$

$$\frac{\partial^2}{\partial x^2} \to \frac{1}{a^2}\left[F_{j+1,\ell} + F_{j-1,\ell} - 2F_{j,\ell}\right] \tag{7.9}$$

and

$$\frac{\partial^2}{\partial y^2} \to \frac{1}{a^2}\left[F_{j,\ell+1} + F_{j,\ell-1} - 2F_{j,\ell}\right] \tag{7.10}$$

The Hamiltonian becomes:

$$
\begin{aligned}
H \quad = \quad & \sum_{j,\ell} \tilde{\mu} c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_0\right) c_{j,\ell} + t_D \sum_{j,\ell} \Big[c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_0\right) c_{j+1,\ell} + c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_0\right) c_{j-1,\ell} \\
& + c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_0\right) c_{j,\ell+1} + c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_0\right) c_{j,\ell-1} \Big] + \sum_{j,\ell} \left(M + \frac{4B}{a^2} \right) c^{\dagger}_{j,\ell} \left(\sigma_z \otimes s_0\right) c_{j,\ell} \\
& + t_B \sum_{j,\ell} \Big[c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_z\right) c_{j+1,\ell} + c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_z\right) c_{j-1,\ell} + c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_z\right) c_{j,\ell+1} \\
& + c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_z\right) c_{j,\ell-1} \Big] + \frac{iA}{2a} \sum_{j,\ell} \Big[c^{\dagger}_{j,\ell} \left(\sigma_z \otimes s_x\right) c_{j-1,\ell} - c^{\dagger}_{j,\ell} \left(\sigma_z \otimes s_x\right) c_{j+1,\ell} \\
& - c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_y\right) c_{j,\ell-1} + c^{\dagger}_{j,\ell} \left(\sigma_0 \otimes s_y\right) c_{j,\ell+1} \Big] + \frac{iR_0}{2a} \sum_{j,\ell} \Big[- c^{\dagger}_{j,\ell} \left(\sigma_y \otimes \frac{s_z + 1}{2} \right) c_{j+1,\ell} \\
& + c^{\dagger}_{j,\ell} \left(\sigma_y \otimes \frac{s_z + 1}{2} \right) c_{j-1,\ell} + c^{\dagger}_{j,\ell} \left(\sigma_x \otimes \frac{s_z + 1}{2} \right) c_{j,\ell+1} - c^{\dagger}_{j,\ell} \left(\sigma_x \otimes \frac{s_z + 1}{2} \right) c_{j,\ell-1} \Big] \\
& + \sum_{j,\ell} c^{\dagger}_{j,\ell} \left(B_+ \sigma_z \otimes s_0 + B_- \sigma_z \otimes s_z \right) c_{j,\ell}
\end{aligned}
\tag{7.11}
$$

where

$$\mu_D = C + \frac{4D}{a^2}, \tag{7.12}$$

$$\mu_B = C + \frac{4B}{a^2}, \tag{7.13}$$

$$t_D = -\frac{D}{a^2} \tag{7.14}$$

$$t_B - \frac{B}{a^2} \tag{7.15}$$

Since the summation is carried out for all j, ℓ integers we can write:

$$\begin{aligned}
H \quad = \quad & \sum_{j,\ell} \mu_A c^\dagger_{j,\ell} \left(\sigma_0 \otimes s_0\right) c_{j,\ell} + t_D \sum_{j,\ell} \Big[c^\dagger_{j,\ell} \left(\sigma_0 \otimes s_0\right) c_{j+1,\ell} + c^\dagger_{j+1,\ell} \left(\sigma_0 \otimes s_0\right) c_{j,\ell} \\
& + c^\dagger_{j,\ell} \left(\sigma_0 \otimes s_0\right) c_{j,\ell+1} + c^\dagger_{j,\ell+1} \left(\sigma_0 \otimes s_0\right) c_{j,\ell} \Big] + \sum_{j,\ell} \mu_B c^\dagger_{j,\ell} \left(\sigma_z \otimes s_0\right) c_{j,\ell} \\
& + t_B \sum_{j,\ell} \Big[c^\dagger_{j,\ell} \left(\sigma_0 \otimes s_z\right) c_{j+1,\ell} + c^\dagger_{j,\ell+1} \left(\sigma_0 \otimes s_z\right) c_{j,\ell} + c^\dagger_{j,\ell} \left(\sigma_0 \otimes s_z\right) c_{j,\ell+1} \\
& + c^\dagger_{j,\ell+1} \left(\sigma_0 \otimes s_z\right) c_{j,\ell} \Big] + \frac{iA}{2a} \sum_{j,\ell} \Big[c^\dagger_{j+1,\ell} \left(\sigma_z \otimes s_x\right) c_{j,\ell} - c^\dagger_{j,\ell} \left(\sigma_z \otimes s_x\right) c_{j+1,\ell} \\
& - c^\dagger_{j,\ell+1} \left(\sigma_0 \otimes s_y\right) c_{j,\ell} + c^\dagger_{j,\ell} \left(\sigma_0 \otimes s_y\right) c_{j,\ell+1} \Big] + \frac{iR_0}{2a} \sum_{j,\ell} \Big[-c^\dagger_{j,\ell} \left(\sigma_y \otimes \frac{s_z + 1}{2}\right) c_{j+1,\ell} \\
& + c^\dagger_{j+1,\ell} \left(\sigma_y \otimes \frac{s_z + 1}{2}\right) c_{j,\ell} + c^\dagger_{j,\ell} \left(\sigma_x \otimes \frac{s_z + 1}{2}\right) c_{j,\ell+1} - c^\dagger_{j,\ell+1} \left(\sigma_x \otimes \frac{s_z + 1}{2}\right) c_{j,\ell} \Big] \\
& + \sum_{j,\ell} c^\dagger_{j,\ell} \left(B_+ \sigma_z \otimes s_0 + B_- \sigma_z \otimes s_z\right) c_{j,\ell}
\end{aligned} \tag{7.16}$$

Collecting all common terms we obtain

$$\begin{aligned}
H \quad = \quad & \sum_{j,\ell} c^\dagger_{j,\ell} \left(\mu_A \sigma_0 \otimes s_0 + \mu_B \sigma_z \otimes s_0\right) c_{j,\ell} + \sum_{j,\ell} \Big[c^\dagger_{j,\ell} \left(t_D \sigma_0 \otimes s_0 + t_B \sigma_0 \otimes s_z\right) c_{j+1,\ell} \\
& + c^\dagger_{j+1,\ell} \left(t_D \sigma_0 \otimes s_0 + t_B \sigma_0 \otimes s_z\right) c_{j,\ell} + c^\dagger_{j,\ell} \left(t_D \sigma_0 \otimes s_0 + t_B \sigma_0 \otimes s_z\right) c_{j,\ell+1} \\
& + c^\dagger_{j,\ell+1} \left(t_D \sigma_0 \otimes s_0 + t_B \sigma_0 \otimes s_z\right) c_{j,\ell} \Big] + \sum_{j,\ell} \Big\{ c^\dagger_{j+1,\ell} \left[t_A \sigma_z \otimes s_x + t_R \sigma_y \otimes \left(s_z + 1\right)/2\right] c_{j,\ell} \\
& + c^\dagger_{j,\ell} \left[t^*_A \sigma_z \otimes s_x + t^*_R \sigma_y \otimes \left(s_z + 1\right)/2\right] c_{j+1,\ell} + c^\dagger_{j,\ell+1} \left[t^*_A \sigma_0 \otimes s_y + t^*_R \sigma_x \otimes \left(s_z + 1\right)/2\right] c_{j,\ell} \\
& + c^\dagger_{j,\ell} \left[t_A \sigma_0 \otimes s_y t_R \sigma_x \otimes \left(s_z + 1\right)/2\right] c_{j,\ell+1} \Big\} + \sum_{j,\ell} c^\dagger_{j,\ell} \left(B_+ \sigma_z \otimes s_0 + B_- \sigma_z \otimes s_z\right) c_{j,\ell}
\end{aligned} \tag{7.17}$$

where

$$t_A = \frac{iA}{2a} \tag{7.18}$$

$$t_R = \frac{iR_0}{2a} \tag{7.19}$$

$$
\begin{aligned}
H &= \sum_{j,\ell} c_{j,\ell}^\dagger \left[\mu_A \sigma_0 \otimes s_0 + \mu_B \sigma_z \otimes s_0 + B_+ \sigma_z \otimes s_0 + B_- \sigma_z \otimes s_z\right] c_{j,\ell} \\
&\quad + \sum_{j,\ell} \Big\{ c_{j,\ell}^\dagger \left[t_D \sigma_0 \otimes s_0 + t_B \sigma_0 \otimes s_z + t_A^* \sigma_z \otimes s_x + t_R^* \sigma_y \otimes (s_z + 1)/2\right] c_{j+1,\ell} \\
&\quad + c_{j+1,\ell}^\dagger \left[t_D \sigma_0 \otimes s_0 + t_B \sigma_0 \otimes s_z + t_A \sigma_z \otimes s_x + t_R \sigma_y \otimes (s_z + 1)/2\right] c_{j,\ell} \\
&\quad + c_{j,\ell}^\dagger \left[t_D \sigma_0 \otimes s_0 + t_B \sigma_0 \otimes s_z + t_A \sigma_0 \otimes s_y + t_R \sigma_x \otimes (s_z + 1)/2\right] c_{j,\ell+1} \\
&\quad + c_{j,\ell+1}^\dagger \left[t_D \sigma_0 \otimes s_0 + t_B \sigma_0 \otimes s_z + t_A^* \sigma_0 \otimes s_y + t_R^* \sigma_x \otimes (s_z + 1)/2\right] c_{j,\ell} \Big\} \qquad (7.20)
\end{aligned}
$$

$$
\begin{aligned}
H &= \sum_{j,\ell} c_{j,\ell}^\dagger \mu_{j,\ell} c_{j,\ell} + \sum_{j,\ell} \Big(c_{j,\ell}^\dagger t_{x;j,\ell} c_{j+1,\ell} + c_{j+1,\ell}^\dagger t_{x;j,\ell}^\dagger c_{j,\ell} + c_{j,\ell}^\dagger t_{y;j,\ell} c_{j,\ell+1} \\
&\quad + c_{j,\ell+1}^\dagger t_{y;j,\ell}^\dagger c_{j,\ell} \Big). \qquad (7.21)
\end{aligned}
$$

We now see that the operators $t_{x;j,\ell}$ and $t_{y;j,\ell}$ describes a hooping along the x and y direction, respectively. We should recall that $c_{j,\ell}$ is a four component spinor while the coupling is to be represented by a 4×4 matrix. Having this in mind, we can make it explicitly by rewriting the Hamiltonian as

$$
\begin{aligned}
H &= \sum_{\substack{j,\ell \\ \alpha,\beta}} (c_{j,\ell}^\dagger)^\alpha \mu_{j,\ell}^{\alpha,\beta} c_{j,\ell}^\beta + \sum_{\substack{j,\ell \\ \alpha,\beta}} \Big[(c_{j,\ell}^\dagger)^\alpha t_{x;j,\ell}^{\alpha,\beta} c_{j+1,\ell}^\beta + (c_{j+1,\ell}^\dagger)^\alpha (t_{x;j,\ell}^{\beta,\alpha})^* c_{j,\ell}^\beta + (c_{j,\ell}^\dagger)^\alpha t_{y;j,\ell}^{\alpha,\beta} c_{j,\ell+1}^\beta \\
&\quad + (c_{j,\ell+1}^\dagger)^\alpha (t_{y;j,\ell}^{\beta,\alpha})^* c_{j,\ell}^\beta \Big]. \qquad (7.22)
\end{aligned}
$$

In the above we have defined

$$
\mu_{j,\ell} = \begin{pmatrix} \mu_E + \mu_B + B_E & 0 & 0 & 0 \\ 0 & \mu_H - \mu_B + B_H & 0 & 0 \\ 0 & 0 & \mu_E + \mu_B - B_E & 0 \\ 0 & 0 & 0 & \mu_H - \mu_B - B_H \end{pmatrix}, \qquad (7.23)
$$

$$
t_{x;j,\ell} = \begin{pmatrix} t_D + t_B & t_A^* & -it_R^* & 0 \\ t_A^* & t_D - t_B & 0 & 0 \\ it_R^* & 0 & t_D + t_B & t_A^* \\ 0 & 0 & t_A^* & t_D - t_B \end{pmatrix}, \qquad (7.24)
$$

and

$$
t_{y;j,\ell} = \begin{pmatrix} t_D + t_B & -it_A & t_R & 0 \\ it_A & t_D - t_B & 0 & 0 \\ t_R & 0 & t_D + t_B & it_A \\ 0 & 0 & it_A & t_D - t_B \end{pmatrix}, \qquad (7.25)
$$

where

$$\mu_E = C + M \tag{7.26}$$

and

$$\mu_H = C - M \tag{7.27}$$

We are now in position to introduce the p-wave superconductor pairing Hamiltonian

$$H_\Delta = \sum_{j,\ell} \left[\Delta^E_{j,\ell} (c^{E+}_{j,\ell})^\dagger (c^{E-}_{j,\ell})^\dagger + (\Delta^E_{j,\ell})^* c^{E-}_{j,\ell} c^{E+}_{j,\ell} + \Delta^H_{j,\ell} (c^{H+}_{j,\ell})^\dagger (c^{H-}_{j,\ell})^\dagger + (\Delta^H_{j,\ell})^* c^{H-}_{j,\ell} c^{H+}_{j,\ell} \right] \tag{7.28}$$

$$H_\Delta = \sum_{\substack{j,\ell \\ \alpha,\beta}} \left[(c^\dagger_{j,\ell})^\alpha \Delta^{\alpha,\beta}_{j,\ell} (c^\dagger_{j,\ell})^\beta + c^\beta_{j,\ell} (\Delta^{\beta,\alpha}_{j,\ell})^* c^\alpha_{j,\ell} \right], \tag{7.29}$$

where

$$\Delta_{j,\ell} = \begin{pmatrix} 0 & 0 & \Delta^E_{j,\ell} & 0 \\ 0 & 0 & 0 & \Delta^H_{j,\ell} \\ \Delta^E_{j,\ell} & 0 & 0 & 0 \\ 0 & \Delta^H_{j,\ell} & 0 & 0 \end{pmatrix}, \tag{7.30}$$

$$\mathbf{G}_{1,1} = \left[\begin{array}{cccc|cccc}
\langle\langle E+_{1,1}; E+^{\dagger}_{1,1}\rangle\rangle & \langle\langle E+_{1,1}; H+^{\dagger}_{1,1}\rangle\rangle & \langle\langle E+_{1,1}; E-^{\dagger}_{1,1}\rangle\rangle & \langle\langle E+_{1,1}; H-^{\dagger}_{1,1}\rangle\rangle & \langle\langle E+_{1,1}; E+^{\dagger}_{1,2}\rangle\rangle & \langle\langle E+_{1,1}; H+^{\dagger}_{1,2}\rangle\rangle & \langle\langle E+_{1,1}; E-^{\dagger}_{1,2}\rangle\rangle & \langle\langle E+_{1,1}; H-^{\dagger}_{1,2}\rangle\rangle \\
\langle\langle H+_{1,1}; E+^{\dagger}_{1,1}\rangle\rangle & \langle\langle H+_{1,1}; H+^{\dagger}_{1,1}\rangle\rangle & \langle\langle H+_{1,1}; E-^{\dagger}_{1,1}\rangle\rangle & \langle\langle H+_{1,1}; H-^{\dagger}_{1,1}\rangle\rangle & \langle\langle H+_{1,1}; E+^{\dagger}_{1,2}\rangle\rangle & \langle\langle H+_{1,1}; H+^{\dagger}_{1,2}\rangle\rangle & \langle\langle H+_{1,1}; E-^{\dagger}_{1,2}\rangle\rangle & \langle\langle H+_{1,1}; H-^{\dagger}_{1,2}\rangle\rangle \\
\langle\langle E-_{1,1}; E+^{\dagger}_{1,1}\rangle\rangle & \langle\langle E-_{1,1}; H+^{\dagger}_{1,1}\rangle\rangle & \langle\langle E-_{1,1}; E-^{\dagger}_{1,1}\rangle\rangle & \langle\langle E-_{1,1}; H-^{\dagger}_{1,1}\rangle\rangle & \langle\langle E-_{1,1}; E+^{\dagger}_{1,2}\rangle\rangle & \langle\langle E-_{1,1}; H+^{\dagger}_{1,2}\rangle\rangle & \langle\langle E-_{1,1}; E-^{\dagger}_{1,2}\rangle\rangle & \langle\langle E-_{1,1}; H-^{\dagger}_{1,2}\rangle\rangle \\
\langle\langle H-_{1,1}; E+^{\dagger}_{1,1}\rangle\rangle & \langle\langle H-_{1,1}; H+^{\dagger}_{1,1}\rangle\rangle & \langle\langle H-_{1,1}; E-^{\dagger}_{1,1}\rangle\rangle & \langle\langle H-_{1,1}; H-^{\dagger}_{1,1}\rangle\rangle & \langle\langle H-_{1,1}; E+^{\dagger}_{1,2}\rangle\rangle & \langle\langle H-_{1,1}; H+^{\dagger}_{1,2}\rangle\rangle & \langle\langle H-_{1,1}; E-^{\dagger}_{1,2}\rangle\rangle & \langle\langle H-_{1,1}; H-^{\dagger}_{1,2}\rangle\rangle \\
\hline
\langle\langle E+_{1,2}; E+^{\dagger}_{1,1}\rangle\rangle & \langle\langle E+_{1,2}; H+^{\dagger}_{1,1}\rangle\rangle & \langle\langle E+_{1,2}; E-^{\dagger}_{1,1}\rangle\rangle & \langle\langle E+_{1,2}; H-^{\dagger}_{1,1}\rangle\rangle & \langle\langle E+_{1,2}; E+^{\dagger}_{1,2}\rangle\rangle & \langle\langle E+_{1,2}; H+^{\dagger}_{1,2}\rangle\rangle & \langle\langle E+_{1,2}; E-^{\dagger}_{1,2}\rangle\rangle & \langle\langle E+_{1,2}; H-^{\dagger}_{1,2}\rangle\rangle \\
\langle\langle H+_{1,2}; E+^{\dagger}_{1,1}\rangle\rangle & \langle\langle H+_{1,2}; H+^{\dagger}_{1,1}\rangle\rangle & \langle\langle H+_{1,2}; E-^{\dagger}_{1,1}\rangle\rangle & \langle\langle H+_{1,2}; H-^{\dagger}_{1,1}\rangle\rangle & \langle\langle H+_{1,2}; E+^{\dagger}_{1,2}\rangle\rangle & \langle\langle H+_{1,2}; H+^{\dagger}_{1,2}\rangle\rangle & \langle\langle H+_{1,2}; E-^{\dagger}_{1,2}\rangle\rangle & \langle\langle H+_{1,2}; H-^{\dagger}_{1,2}\rangle\rangle \\
\langle\langle E-_{1,2}; E+^{\dagger}_{1,1}\rangle\rangle & \langle\langle E-_{1,2}; H+^{\dagger}_{1,1}\rangle\rangle & \langle\langle E-_{1,2}; E-^{\dagger}_{1,1}\rangle\rangle & \langle\langle E-_{1,2}; H-^{\dagger}_{1,1}\rangle\rangle & \langle\langle E-_{1,2}; E+^{\dagger}_{1,2}\rangle\rangle & \langle\langle E-_{1,2}; H+^{\dagger}_{1,2}\rangle\rangle & \langle\langle E-_{1,2}; E-^{\dagger}_{1,2}\rangle\rangle & \langle\langle E-_{1,2}; H-^{\dagger}_{1,2}\rangle\rangle \\
\langle\langle H-_{1,2}; E+^{\dagger}_{1,1}\rangle\rangle & \langle\langle H-_{1,2}; H+^{\dagger}_{1,1}\rangle\rangle & \langle\langle H-_{1,2}; E-^{\dagger}_{1,1}\rangle\rangle & \langle\langle H-_{1,2}; H-^{\dagger}_{1,1}\rangle\rangle & \langle\langle H-_{1,2}; E+^{\dagger}_{1,2}\rangle\rangle & \langle\langle H-_{1,2}; H+^{\dagger}_{1,2}\rangle\rangle & \langle\langle H-_{1,2}; E-^{\dagger}_{1,2}\rangle\rangle & \langle\langle H-_{1,2}; H-^{\dagger}_{1,2}\rangle\rangle
\end{array}\right], \tag{7.31}$$

$$\mathbf{g}_{1,1} = \left[\begin{array}{cccc|cccc}
\frac{1}{\omega-\tilde{\mu}_{E+}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\omega-\tilde{\mu}_{H+}} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{\omega-\tilde{\mu}_{E-}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{\omega-\tilde{\mu}_{H-}} & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & \frac{1}{\omega-\tilde{\mu}_{E+}} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\omega-\tilde{\mu}_{H+}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\omega-\tilde{\mu}_{E-}} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\omega-\tilde{\mu}_{H-}}
\end{array}\right], \tag{7.32}$$

$$\mathbf{G}_{1,1} = \mathbf{g}_{1,1} + \mathbf{g}_{1,1}\mathbf{V}\mathbf{G}_{1,1} + \mathbf{g}_{1,1}\mathbf{W}\mathbf{G}_{\mathbf{2,1}}, \tag{7.33}$$

where

$$\mathbf{V}_{1,1} = \left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & t_D + t_B & -it_A & t_R & 0 \\ 0 & 0 & 0 & 0 & it_A & t_D - t_B & 0 & 0 \\ 0 & 0 & 0 & 0 & t_R & 0 & t_D + t_B & -it_A \\ 0 & 0 & 0 & 0 & 0 & 0 & -it_A & t_D - t_B \\ \hline t_D + t_B & -it_A^* & t_R^* & 0 & 0 & 0 & 0 & 0 \\ it_A^* & t_D - t_B & 0 & 0 & 0 & 0 & 0 & 0 \\ t_R^* & 0 & t_D + t_B & it_A^* & 0 & 0 & 0 & 0 \\ 0 & 0 & it_A^* & t_D - t_B & 0 & 0 & 0 & 0 \end{array}\right], \tag{7.34}$$

and

$$\mathbf{W}_{1,1} = \left[\begin{array}{cccc|cccc} t_D + t_B & t_A^* & -it_R^* & 0 & 0 & 0 & 0 & 0 \\ t_A & t_D - t_B & 0 & 0 & 0 & 0 & 0 & 0 \\ it_R & 0 & t_D + t_B & t_A^* & 0 & 0 & 0 & 0 \\ 0 & 0 & t_A & t_D - t_B & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & t_D + t_B & t_A^* & -it_R^* & 0 \\ 0 & 0 & 0 & 0 & t_A & t_D - t_B & 0 & 0 \\ 0 & 0 & 0 & 0 & it_R & 0 & t_D + t_B & t_A^* \\ 0 & 0 & 0 & 0 & 0 & 0 & t_A & t_D - t_B \end{array}\right], \tag{7.35}$$

We can still write:

$$\mathbf{G}_{1,1} = [1 - \mathbf{g}_{1,1}\mathbf{V}]^{-1}\mathbf{g}_{1,1} + [1 - \mathbf{g}_{1,1}\mathbf{V}]^{-1}\mathbf{g}_{1,1}\mathbf{W}\mathbf{G}_{\mathbf{2},\mathbf{1}} = \tilde{\mathbf{g}}_{1,1} + \tilde{\mathbf{g}}_{1,1}\mathbf{W}\mathbf{G}_{\mathbf{2},\mathbf{1}} \tag{7.36}$$

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