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# Majorana fermion representations of magnetic impurity problems

*Author:*
Bingdong Chang

*Supervisor:*
Jens Paaske

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# Chapter 1

# Introduction

In many body physics, we use Green's functions to study the time evolution of an $n$-particle system, which is of great significance in condensed matter theory and particle physics, from which we can construct more convenient diagrammatic techniques. For $n$-particle Green's functions, Wick's theorem could be used to reduce into products of single particle Green's functions.

Sometimes we need to calculate spin correlators, e.g. in spin susceptibility problems or Kondo model, and since spin operators are not bosons nor fermions, we cannot use Wick's theorem to simplify an $n$-spin correlator. Historically there are various attempts to solve this problem [1–3], the method which is most often used is pseudo fermion representation for spin operators, in which spin operator is written as $\vec{S} = \frac{1}{2} c_\sigma \vec{\tau}_{\sigma\sigma'} c^\dagger_{\sigma'}$ and constraints are added to the Hilbert space to remove unphysical states [1].

However, pseudo fermion representation can bring some calculation difficulties sometimes. Consider a simple case of two spin correlator in pseudo fermion language

$$G\left(S_x\left(\tau\right), S_x\left(0\right)\right) = \frac{1}{4}\left\langle T_\tau \left[c^\dagger_{\sigma_1}\left(\tau\right)\tau^x_{\sigma_1\sigma_1'}\left(\tau\right)c_{\sigma_1'}\left(\tau\right)c^\dagger_{\sigma_2}\tau^x_{\sigma_2\sigma_2'}c_{\sigma_2'}\right]\right\rangle \tag{1.1}$$

which is a four fermion correlator, if we draw the Feynman diagram of (1.1) as in FIGURE 1.1, there will be 4 dash lines representing pseudo fermion propagators and two four-leg vertices, thus vertex corrections make the problem complicated.

So we come to ask ourselves if there is a proper representation method for spin operators, by which Wick's theorem still holds and tedious vertex correction could be avoided in spin correlator calculations. It turns out that Majorana representation can solve these two problems, which is the main topic of this thesis.

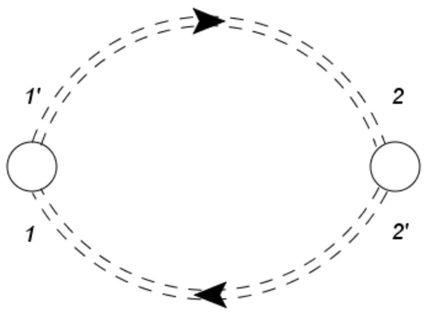


Figure 1.1: Feynman diagram for 2-spin correlator in pseudo fermion representation.

Majorana representation for spin operators was firstly suggested by Martin in 1959 [4] and later rediscovered in high energy physics, recently it was applied to condensed matter physics in various topics [5–8, 13].

In this thesis, spin operators and spin correlators in Majorana language are firstly constructed in chapter 2, then I will follow *A Shnirman, et al (2003)* [5] to show its application in spin boson interaction in Chapter 3. Another application example in Kondo model is given in Chapter 4, which I will follow *M C Cano, et al (2011)* [13]. Finally a brief summary would be given in Chapter 5.

# Chapter 2

# Majorana Representation

## 2.1 Pauli spin matrices and Majorana fermions

For spin $\frac{1}{2}$ systems, we have Pauli spin matrices as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.1}$$

which satisfiy the anticommutation relation and commutation relation for single spin as:

$$\begin{aligned} \{\sigma_a, \sigma_b\} &= 2\delta_{ab}, \\ [\sigma_a,\ \sigma_b] &= 2i\varepsilon_{abc}\sigma_c, \end{aligned} \tag{2.2}$$

in which lower indices $a, b, c$ are $x, y, z$ respectively.

Now introduce Majorana fermions as $\eta_i$ $(i = x, y, z)$, they are real thus $\eta_i^\dagger = \eta_i$, meaning Majorana fermion is its own antiparticle. Majorana fermions are also fermions just as ordinary fermions, thus satisfy anticommutation relation as:

$$\{\eta_\alpha, \eta_\beta\} = 2\delta_{\alpha\beta} \tag{2.3}$$

here $\alpha, \beta, \gamma = x, y, z$. Normal spin matrices can be expressed as cross products of Majorana fermions as $\vec{\sigma} = -\frac{i}{2}\vec{\eta} \times \vec{\eta}$, or more transparently as:

$$\sigma_x = -i\eta_y\eta_z, \quad \sigma_y = -i\eta_z\eta_x, \quad \sigma_z = -i\eta_x\eta_y \tag{2.4}$$

It can be checked easily that the commutation and anticommutation relations of spin matrices can be reproduced by expression (2.4), for example

$$\begin{aligned} &[\sigma_x, \sigma_y] = -[\eta_y\eta_z, \eta_z\eta_x] = -\eta_y\eta_x + \eta_z\eta_x\eta_y\eta_z = 2\eta_x\eta_y = 2i\sigma_z, \\ &\{\sigma_x, \sigma_y\} = 0 \end{aligned} \tag{2.5}$$

here we use the anticommutation relation (2.4).

Now if we introduce another Majorana fermion $\tau_x$ which is in a different Hilbert space (some authors name as "copy-switching" operator, which we shall see),

$$\tau_x = -i\eta_x\eta_y\eta_z \tag{2.6}$$

since $\tau_x$ is also Majorana fermion, $\tau_x^2 = 1$ and $\tau_x = \tau_x^\dagger$ hold which can be checked. Then using anticommutation relations of Majorana fermions, we can decompose spin operator into product of $\tau_x$ and Majorana fermions as,

$$\sigma_\alpha = \tau_x\eta_\alpha \tag{2.7}$$

This is a useful result, since $\tau_x$ commutes with Majorana fermions $\eta_\alpha$, and as we will verify later, $\tau_x$ is free of time evolution, then the spin-spin correlator can be reduced to correlators of two Majorana fermions.

## 2.2 Copy-swithcing operator

Majorana fermions are real, thus we can construct by ordinary fermions as $\eta_\alpha = c_\alpha^\dagger + c_\alpha$. In fact it can be proved that the anticommutation relations of Majorana fermions can be preserved in this bilinear construction:

$$\begin{aligned} &\eta_\alpha\eta_\beta = \left(c_\alpha + c_\alpha^\dagger\right)\left(c_\beta + c_\beta^\dagger\right) = -\left(c_\beta + c_\beta^\dagger\right)\left(c_\alpha + c_\alpha^\dagger\right) = -\eta_\beta\eta_\alpha, (\alpha \neq \beta) \\ &\eta_\alpha^2 = c_\alpha c_\alpha + c_\alpha^\dagger c_\alpha^\dagger + \left\{c_\alpha^\dagger, c_\alpha\right\} = 1 \end{aligned} \tag{2.8}$$

Since each Majorana fermion can be expressed by ordinary fermions with different indices, the whole Hilbert space is then expanded from 2 dimension to $2^3 = 8$ dimension.

However, we could reduce the dimension from 8 to $2^2 = 4$ by define:

$$\begin{aligned} \eta_x &= f^\dagger + f, \\ \eta_y &= i\left(f^\dagger - f\right), \\ \eta_z &= g^\dagger + g \end{aligned} \tag{2.9}$$

here $f, f^\dagger, g, g^\dagger$ are ordinary fermions (these two ordinary fermions can be regarded as two replicas of original spin, which doubles the dimension of the original Hilbert space). According to (2.4), the Majorana fermions can be written as:

$$\begin{aligned} \sigma_x &= \left(f^\dagger - f\right)\left(g^\dagger + g\right); \\ \sigma_y &= -i\left(g^\dagger + g\right)\left(f^\dagger + f\right); \\ \sigma_z &= \left(f^\dagger + f\right)\left(f^\dagger - f\right) = 1 - 2f^\dagger f. \end{aligned} \tag{2.10}$$

or by introducing $\sigma_+ = \frac{1}{2}(\sigma_x + i\sigma_y)$ and $\sigma_- = \frac{1}{2}(\sigma_x - i\sigma_y)$, we have:

$$\sigma_+ = \eta_z f, \quad \sigma_- = f^\dagger \eta_z \tag{2.11}$$

We may also investigate this construction in a more direct way by defining 4 states as:

$$\begin{aligned} |\uparrow_a\rangle &\equiv |00\rangle \\ |\downarrow_a\rangle &\equiv |11\rangle \equiv f^\dagger g^\dagger |00\rangle \\ \\ |\uparrow_b\rangle &\equiv |01\rangle \equiv g^\dagger |00\rangle \\ |\downarrow_b\rangle &\equiv |10\rangle \equiv f^\dagger |00\rangle \end{aligned} \tag{2.12}$$

in this notation, $|s_n\rangle$ represents a single state, $s = \uparrow / \downarrow$ denotes the spin component and $n = a/b$ denotes the spin copies. The states in (2.12) can make up the basis of the 4 dimensional Hilbert space.

Now introduce the "copy-switching" operator $\tau_x$ by defining $\tau_x |s_a\rangle = |s_b\rangle$ and $\tau_x |s_b\rangle = |s_a\rangle$ so that $\tau_x^2 = 1$. Thus we can find following relations:

$$f = \sigma_+ \tau_x, \quad f^\dagger = \sigma_- \tau_x, \quad \eta_z = \sigma_z \tau_x. \tag{2.13}$$

which are proved as below:

$$
\begin{aligned}
&f^{\dagger}\left|\uparrow_a\right\rangle = \left|\downarrow_b\right\rangle = f^{\dagger} g \left|\uparrow_b\right\rangle = f^{\dagger} g \tau_x \left|\uparrow_a\right\rangle = f^{\dagger}\left(g+g^{\dagger}\right)\tau_x\left|\uparrow_a\right\rangle = \sigma_-\tau_x\left|\uparrow_a\right\rangle, \\
&f^{\dagger}\left|\downarrow_a\right\rangle = \sigma_-\tau_x\left|\downarrow_a\right\rangle, \quad f^{\dagger}\left|\uparrow_b\right\rangle = \sigma_-\tau_x\left|\uparrow_b\right\rangle, \quad f^{\dagger}\left|\downarrow_b\right\rangle = \sigma_-\tau_x\left|\downarrow_b\right\rangle
\end{aligned}
\tag{2.14}
$$

thus $f^{\dagger} = \sigma_-\tau_x$.

$$
\begin{aligned}
&f\left|\downarrow_a\right\rangle = \left|\uparrow_b\right\rangle = g^{\dagger} f \left|\downarrow_b\right\rangle = g^{\dagger} f \tau_x \left|\downarrow_a\right\rangle = \left(g+g^{\dagger}\right) f\tau_x\left|\downarrow_a\right\rangle = \sigma_+\tau_x\left|\downarrow_a\right\rangle, \\
&f\left|\uparrow_a\right\rangle = \sigma_+\tau_x\left|\uparrow_a\right\rangle, \quad f\left|\uparrow_b\right\rangle = \sigma_+\tau_x\left|\uparrow_b\right\rangle, \quad f\left|\downarrow_b\right\rangle = \sigma_+\tau_x\left|\downarrow_b\right\rangle
\end{aligned}
\tag{2.15}
$$

thus $f = \sigma_+\tau_x$.

$$
\begin{aligned}
&\eta_z\left|\uparrow_a\right\rangle = \left|\uparrow_b\right\rangle = \tau_x\left|\uparrow_a\right\rangle = \left(1-2f^{\dagger}f\right)\tau_x\left|\uparrow_a\right\rangle, \\
&\eta_z\left|\uparrow_b\right\rangle = \left|\uparrow_a\right\rangle = \tau_x\left|\uparrow_b\right\rangle = \left(1-2f^{\dagger}f\right)\tau_x\left|\uparrow_b\right\rangle, \\
&\eta_z\left|\downarrow_a\right\rangle = \left(g+g^{\dagger}\right) f^{\dagger} g^{\dagger}\left|00\right\rangle = -f^{\dagger}\left(g+g^{\dagger}\right) g^{\dagger}\left|00\right\rangle = -\left|\downarrow_b\right\rangle = \left(1-2f^{\dagger}f\right)\tau_x\left|\downarrow_a\right\rangle, \\
&\eta_z\left|\downarrow_b\right\rangle = \left(g+g^{\dagger}\right) f^{\dagger}\left|00\right\rangle = -f^{\dagger}\left(g+g^{\dagger}\right)\left|00\right\rangle = -\left|\downarrow_a\right\rangle = \left(1-2f^{\dagger}f\right)\tau_x\left|\downarrow_b\right\rangle
\end{aligned}
\tag{2.16}
$$

thus $\eta_z = \sigma_z\tau_x$.

From above relations, we can find that,

$$
\begin{aligned}
\eta_x =& f + f^{\dagger} = \left(\sigma_+ + \sigma_-\right)\tau_x = \sigma_x\tau_x, \\
\eta_y =& i\left(f^{\dagger} - f\right) = i\left(\sigma_+ - \sigma_-\right)\tau_x = \sigma_y\tau_x
\end{aligned}
\tag{2.17}
$$

or write more compactly,

$$
\eta_\alpha = \sigma_\alpha\tau_x, \quad (\alpha = x, y, z) \tag{2.18}
$$

Another important feature is that $\tau_x$ commutes nicely with “all the other” operators: $\eta_{x,y,z}$, $\sigma_{x,y,z}$ and $f$,$f^{\dagger}$ (but doesn't commute with $g$ and $g^{\dagger}$). This conclusion is proved as below:

$$
f^{\dagger}\left|\uparrow_a\right\rangle = \left|\downarrow_b\right\rangle = \tau_x\left|\downarrow_a\right\rangle = \tau_x f^{\dagger} g^{\dagger}\left|\uparrow_a\right\rangle = \tau_x f^{\dagger}\left(g^{\dagger}+g\right)\left|\uparrow_a\right\rangle = \tau_x\sigma_-\left|\uparrow_a\right\rangle \tag{2.19}
$$

it is true for other states, thus $f^{\dagger} = \tau_x\sigma_-$, compare with (2.14), we can get

$$
\left[\tau_x, \sigma_-\right] = 0, \quad \left[\tau_x, f^{\dagger}\right] = \left[\tau_x, \sigma_-\tau_x\right] = 0 \tag{2.20}
$$

similarly,

$$\begin{aligned} &[\tau_x, \sigma_+] = 0, \quad [\tau_x, f] = 0; \\ &[\tau_x, \sigma_z] = \left[\tau_x, 1 - 2f^\dagger f\right] = 0, \quad [\tau_x, \eta_z] = [\tau_x, \sigma_z \tau_x] = 0. \end{aligned} \tag{2.21}$$

and from (2.21), (2.22), it comes naturally that

$$\begin{aligned} &[\tau_x, \sigma_{x,y}] = 0, \\ &[\tau_x, \eta_{x,y}] = 0 \end{aligned} \tag{2.22}$$

From (2.4) and (2.18) it also follows that:

$$\tau_x = \sigma_z \eta_z = -i\eta_x \eta_y \eta_z. \tag{2.23}$$

The procedure above can be reproduced when interchanging $f$ and $g$ fermions and the result is still the same, which suggests that two spin copies in (2.12) construction are equivalent, and $\tau_x$ is the operator that transform one subspace into another, we can restrict the 4 dimensional Hilbert space back to 2 dimension to get original spin.

### 2.2.1 Another access to construct the copy-switching operator

We have seen how copy-switching operator $\tau_x$ is constructed from writing Majorana fermions by ordinary fermions. This result can also be achieved starting from the basis. If we denote the states in (2.12) first, then we can construct spin operators using $f$ and $g$ ordinary fermions as:

$$\begin{aligned} &S_a^+ = gf, \quad S_a^- = f^\dagger g^\dagger, \quad S_a^z = \frac{1}{2}\left[S_a^+, S_a^-\right] = \frac{1}{2}\left(gg^\dagger - f^\dagger f\right); \\ &S_b^+ = g^\dagger f, \quad S_b^- = f^\dagger g, \quad S_b^z = \frac{1}{2}\left[S_b^+, S_b^-\right] = \frac{1}{2}\left(g^\dagger g - f^\dagger f\right). \end{aligned} \tag{2.24}$$

We should always be careful about the order of $f, f^\dagger$ and $g, g^\dagger$, since they are fermionic number operators, obeying $c_i \left|\cdots n_{i-1} n_i n_{i+1} \cdots\right\rangle = (-1)^{\Sigma_i} \left|\cdots n_{i-1} \left(n_i - 1\right) n_{i+1} \cdots\right\rangle$, in which $\Sigma_i = \sum_{j=1}^{i} n_j$. Thus we have

$$\begin{aligned} &\sigma_+ = S_a^+ + S_b^+ = \left(g + g^\dagger\right) f, \\ &\sigma_- = S_a^- + S_b^- = f^\dagger \left(g + g^\dagger\right), \\ &\sigma_z = 2\left(S_a^z + S_b^z\right) = 1 - 2f^\dagger f \end{aligned} \tag{2.25}$$

using relations (2.4),

$$\begin{aligned}
\sigma_x &= \sigma_+ + \sigma_- = \left(g+g^\dagger\right)\left(f-f^\dagger\right) = -i\eta_y\eta_z, \\
\sigma_y &= -i\left(\sigma_+ - \sigma_-\right) = -i\left(g+g^\dagger\right)\left(f+f^\dagger\right) = -i\eta_z\eta_x, \\
\sigma_z &= 1-2f^\dagger f = -i\eta_x\eta_y
\end{aligned} \tag{2.26}$$

thus we can easily solve for $\eta_\alpha$ which has the same result as in (2.9):

$$\eta_x = f+f^\dagger, \quad \eta_y = i\left(f^\dagger - f\right), \quad \eta_z = g+g^\dagger \tag{2.27}$$

In this part we reverse the procedure, but still construct the same Majorana fermions and get the "copy-switching" operator $\tau_x = -i\eta_x\eta_y\eta_z$ similarly. We may also find that even though we change the position of a,b spins in (2.12) and repeat procedure in this part, the result is still the same, which implies again that there is a symmetry on the two spin sites (or $f$ and $g$ ordinary fermions).

## 2.3 Reduction of spin-spin correlators

In this part we shall see how the "copy-switching" operator $\tau_x$ could help in calculating spin correlation functions, but before that we should specify the expectation value of spin operator in Majorana language.

Consider a simple case in which a single spin interacts with an external B field, the Hamiltonian is thus,

$$H = -BS_z = -\frac{1}{2}B\sigma_z \tag{2.28}$$

the expectation value $\langle S_z\rangle$ is

$$\begin{aligned}
\langle S_z\rangle =& \frac{1}{2}\langle\sigma_z\rangle = \frac{1}{2Z}Tr\left[\sigma_z e^{\frac{1}{2}\beta B\sigma_z}\right] = \frac{1}{2}\frac{\sum_{i,j}\langle n_i|\,\sigma_z^{ij}e^{-\beta H_{ij}}\,|n_j\rangle}{\sum_{i,j}e^{-\beta H_{ij}}} \\
=& \frac{1}{2}\frac{e^{\frac{\beta B}{2}} - e^{\frac{-\beta B}{2}}}{e^{\frac{\beta B}{2}} + e^{\frac{-\beta B}{2}}} = \frac{1}{2}\tanh\left(\frac{\beta B}{2}\right)
\end{aligned} \tag{2.29}$$

here $|n_i\rangle\,/\,|n_j\rangle = |{\uparrow}\rangle$ or $|{\downarrow}\rangle$. If we write (2.28) in Majorana language, then

$$H = \frac{i}{2}B\eta_x\eta_y = \frac{i}{2}B(f+f^\dagger)(f-f^\dagger) = Bf^\dagger f - \frac{B}{2} \tag{2.30}$$

we can observe the eigenenergies in Majorana language are still $\pm\frac{B}{2}$ not surprisingly, since ordinary fermion $f$ is just a copy of the original spin. Then we can calculate expectation value of $S_z$ as

$$\langle S_z \rangle = \frac{1}{2} \langle \sigma_z \rangle = \frac{1}{2} \frac{e^{\frac{\beta B}{2}} - e^{\frac{-\beta B}{2}}}{e^{\frac{\beta B}{2}} + e^{\frac{-\beta B}{2}}} = \frac{1}{2} \tanh\left(\frac{\beta B}{2}\right) \tag{2.31}$$

which is the same as in (2.30), verifying Majorana representation in another way.

Now consider a general Hamiltonian of a spin system which depends on the spin operators, e.g. a Zeeman Hamiltonian or Kondo Hamiltonian, since $\tau_x$ commutes with them, it is then time independent $d\tau_x/dt = 0$ based on the Heisenberg equation. For a two spin correlator, we can decompose each spin into product of $\tau_x$ and a Majorana fermion and obtain:

$$\left\langle \sigma_\alpha (t) \sigma_\beta \left(t'\right) \right\rangle = \left\langle \eta_\alpha (t) \tau_x (t) \eta_\beta \left(t'\right) \tau_x \left(t'\right) \right\rangle = \left\langle \eta_\alpha (t) \tau_x \eta_\beta \left(t'\right) \tau_x \right\rangle = \left\langle \eta_\alpha (t) \eta_\beta \left(t'\right) \right\rangle \tag{2.32}$$

This is also true in multi-spin situation, for instance, a four spin correlator:

$$\langle \sigma_\alpha (t_1) \sigma_\beta (t_2) \sigma_\gamma (t_3) \sigma_\delta (t_4) \rangle = \langle \eta_\alpha (t_1) \eta_\beta (t_2) \eta_\gamma (t_3) \eta_\delta (t_4) \rangle \tag{2.33}$$

Thus the normal spin-spin correlators transform into the correlators of corresponding Majorana fermions. If we write (2.32) one step further with $\alpha, \beta = x$,

$$\left\langle \sigma_x (t) \sigma_x \left(t'\right) \right\rangle = \left\langle \eta_x (t) \eta_x \left(t'\right) \right\rangle = \left\langle \left(f (t) + f^\dagger (t)\right) \left(f \left(t'\right) + f^\dagger \left(t'\right)\right) \right\rangle \tag{2.34}$$

We can clearly see that instead of 4-fermion correlator in pseudo fermion representation that gives a pair bubble diagram, the spin correlator is now reduced to a 2 fermion correlator, when we draw the Feynman diagram, we just need to calculate self energy in a lower order without vertex correction. Later we will testify the simplicity of this method through calculations.

## 2.4 Gauge-invariance considerations

From relation (2.4), it is clear that the normal spin operators are invariant under a gauge transformation of $\eta_\alpha \to -\eta_\alpha$, in other words, this representation has a discrete $Z_2$ symmetry.

Such gauge transformations can be realized by introducing the fourth Majorana fermion $\tau_y$ as

$$\tau_y = i\left(g^\dagger - g\right) \tag{2.35}$$

then $\eta_z \to \tau_y \eta_z \tau_y^{-1} = -\eta_z$ holds (this is because of the anticommutation relationship of Majorana fermions, $\{\eta_z, \tau_y\} = 0$). From this, it can be seen that when the dimension of Hilbert space reduces from 8 to 4, we actually perform a symmetry transformation,or $2^3 \to 2^2 = 8/2$, which is guaranteed by the fact that Majorana fermion is bilinear combination of ordinary operators.

Using $\tau_x$ and $\tau_y$ obtained above, we can also construct a third $\tau$-operator $\tau_z$ as $i\tau_z = \tau_x \tau_y$, which follows

$$\tau_z = \left(1 - 2f^\dagger f\right)\left(1 - 2g^\dagger g\right) \tag{2.36}$$

we could easily verify that $\tau_z |s_a\rangle = |s_a\rangle$, $\tau_z |s_b\rangle = -|s_b\rangle$, so $\tau_z$ only changes the sign of wavefunction on $b$ site. After some algebra, we have the anticommutation relations as $\{\tau_z, \eta_\alpha\} = 0$ and $\{\tau_z, \tau_{x,y}\} = 0$. So we have a gauge transformation as: $\eta_\alpha \to \tau_z \eta_\alpha {\tau_z}^{-1} = -\eta_\alpha$, and $\tau_x \to \tau_z \tau_x {\tau_z}^{-1} = -\tau_x$. Now consider a time dependent gauge transformation: $|\Psi\rangle \to U|\Psi\rangle$ in which,

$$U = e^{\frac{i}{2}\pi\tau_y\phi(t)}, \quad \phi(t) = 0, 1. \tag{2.37}$$

which we can expand as below,using the fact that $\tau_y^2 = 1$:

$$\begin{aligned}
U =& 1 + \frac{i\pi}{2}\tau_y\phi(t) + \frac{1}{2!}\left(\frac{i\pi}{2}\tau_y\phi(t)\right)^2 + \frac{1}{3!}\left(\frac{i\pi}{2}\tau_y\phi(t)\right)^3 + \dots \\
=& \left(1 - \frac{1}{2!}\left(\frac{\pi}{2}\phi(t)\right)^2 + \frac{1}{4!}\left(\frac{\pi}{2}\phi(t)\right)^4 - \dots\right) + i\left(\frac{\pi}{2}\tau_y\phi(t) - \frac{1}{3!}\left(\frac{\pi}{2}\phi(t)\right)^3) + \dots\right) \\
=& \cos\left(\frac{\pi\phi(t)}{2}\right) + i\tau_y \sin\left(\frac{\pi\phi(t)}{2}\right) \\
=& \begin{cases} 1 & \text{if } \phi(t) = 0 \\ i\tau_y & \text{if } \phi(t) = 1 \end{cases}
\end{aligned} \tag{2.38}$$

then we have the transformed operators as:

$$\begin{aligned}
\eta_\alpha \to U\eta_\alpha U^{-1} &= \begin{Bmatrix} \eta_\alpha & \text{if } \phi(t)=0 \\ \tau_y\eta_\alpha{\tau_y}^{-1} = -\eta_\alpha & \text{if } \phi(t)=1 \end{Bmatrix} = (-1)^{\phi(t)}\eta_\alpha \\
\tau_x \to U\tau_x U^{-1} &= \begin{Bmatrix} \tau_x & \text{if } \phi(t)=0 \\ \tau_y\tau_x{\tau_y}^{-1} = -\tau_x & \text{if } \phi(t)=1 \end{Bmatrix} = (-1)^{\phi(t)}\tau_x
\end{aligned} \tag{2.39}$$

here anticommutation relations $\{\tau_y, \eta_\alpha\} = 0$ and $\{\tau_y, \tau_x\} = 0$ are used. So $\tau_x$ is no longer time-independent under the gauge transformation of $U$.

Or in another way of thinking, the transformed state $\left|\tilde{\Psi}\right\rangle$ is:

$$\left|\tilde{\Psi}\right\rangle = U\left|\Psi\right\rangle = e^{\frac{i}{2}\pi\tau_y\phi(t)}\left|\Psi\right\rangle \tag{2.40}$$

thus the transformed Hamiltonian $\tilde{H}$ can be calculated as below

$$\begin{aligned}
&\tilde{H}\left|\tilde{\Psi}\right\rangle = i\partial_t\left|\tilde{\Psi}\right\rangle = (i\dot{U} + Ui\partial_t)\left|\Psi\right\rangle = (i\dot{U}U^{-1} + UHU^{-1})\left|\tilde{\Psi}\right\rangle \\
&H \to \tilde{H} = i\dot{U}U^{-1} + UHU^{-1} = H - \frac{\pi}{2}\tau_y\dot{\phi}(t)
\end{aligned} \tag{2.41}$$

thus $\dot{\tau}_x = i\left[\tilde{H}, \tau_x\right] \neq 0$ since $[\tau_y, \tau_x] \neq 0$, then the Majorana fermion correlator is no longer gauge invariant according to (2.32):

$$\left\langle \eta_\alpha(t)\,\eta_\alpha(t')\right\rangle \to (-1)^{\phi(t)-\phi(t')}\left\langle \eta_\alpha(t)\,\eta_\alpha(t')\right\rangle \tag{2.42}$$

So in order to make the Majorana spin correlator gauge invariant, we need to add a phase factor of $(-1)^{\phi(t)-\phi(t')}$ to fix the gauge, meanwhile the ordinary spin correlator is still gauge invariant:

$$\left\langle \sigma_\alpha(t)\,\sigma_\beta(t')\right\rangle \to (-1)^{\phi(t)+\phi(t)-\phi(t')-\phi(t')}\left\langle \eta_\alpha(t)\,\tau_x(t)\,\eta_\beta(t')\,\tau_x(t')\right\rangle = \left\langle \sigma_\alpha(t)\,\sigma_\beta(t')\right\rangle \tag{2.43}$$

### 2.4.1 Interpretation of $\tau_\alpha$ operators

The $\tau_\alpha$ operators can be interpreted in another way, which may be more transparent. Consider about the construction in (2.12), the original space is expanded yielding two spin copies f and g as $|fg\rangle = |f\rangle \otimes |g\rangle$, state on each position could be either $|0\rangle$ or $|1\rangle$, then we have $|\uparrow_a\rangle$ as $|0\rangle_f \otimes |0\rangle_g$, and so on. By definition of "copy-switching" operator, we have:

$$\begin{aligned}
&\tau_x: \quad \tau_x|00\rangle = |01\rangle, \quad \tau_x|11\rangle = |10\rangle, \quad \tau_x|01\rangle = |00\rangle, \quad \tau_x|10\rangle = |11\rangle;\\
&\tau_y: \quad \tau_y|00\rangle = i|01\rangle, \quad \tau_y|11\rangle = i|10\rangle, \quad \tau_y|01\rangle = -i|00\rangle, \quad \tau_y|10\rangle = -i|11\rangle;\\
&\tau_z: \quad \tau_z|00\rangle = |00\rangle, \quad \tau_z|11\rangle = |11\rangle, \quad \tau_z|01\rangle = -|01\rangle, \quad \tau_z|10\rangle = -|10\rangle
\end{aligned} \tag{2.44}$$

We could easily find that $\tau_\alpha$ operators can be written as tensorial products of two spin matrices:

$$\tau_x = 1 \otimes \sigma_x, \quad \tau_y = \sigma_z \otimes \sigma_y, \quad \tau_z = \sigma_z \otimes \sigma_z \tag{2.45}$$

giving properties analogous to Majorana fermions, not surprisingly: ${\tau_\alpha}^2 = 1$, $\tau_\alpha \tau_\beta = i\epsilon_{\alpha\beta\gamma}\tau_\gamma$, $\tau_\alpha^\dagger = \tau_\alpha$.

## 2.5 Wick's theorem for spin operators

We have mentioned in chapter 1 that Wick's theorem cannot be applied directly for spin operators, we shall see that with Majorana representation, spin operator correlators can be transformed into familiar ordinary fermion correlators, in which case Wick's theorem still holds. First start with a simple example: an imaginary time Green's function of two spins 1 and 2 both in $x$-direction,

$$G\left(S_{x,1}(\tau_1)\, S_{x,2}(\tau_2), S_{x,1'}(\tau_1')\, S_{x,2'}(\tau_2')\right) = \left\langle T_\tau\left[S_{x,1}(\tau_1)\, S_{x,2}(\tau_2)\, S_{x,2'}(\tau_2')\, S_{x,1'}(\tau_1')\right]\right\rangle \tag{2.46}$$

use Majorana representation for spin operators $S_\alpha = \frac{1}{2}\tau_x\eta_\alpha$, remember $\tau_x$ is time independent, we have

$$\begin{aligned}
\text{Eq(2.46)} &= \left(\frac{1}{2}\right)^4 \left\langle T_\tau\left[\tau_{x,1}\eta_{x,1}(\tau_1)\,\tau_{x,2}\eta_{x,2}(\tau_2)\,\tau_{x,2'}\eta_{x,2'}(\tau_2')\,\tau_{x,1'}\eta_{x,1'}(\tau_1')\right]\right\rangle\\
&= \left(\frac{1}{2}\right)^4 \left\langle T_\tau\left[\eta_{x,1}(\tau_1)\,\eta_{x,2}(\tau_2)\,\eta_{x,2'}(\tau_2')\,\eta_{x,1'}(\tau_1')\right]\right\rangle\\
&= \left(\frac{1}{2}\right)^4 \Big\langle T_\tau\Big[\left(f_1(\tau_1) + f_1^\dagger(\tau_1)\right)\left(f_2(\tau_2) + f_2^\dagger(\tau_2)\right)\\
&\quad \left(f_2'(\tau_2') + f_{2'}^\dagger(\tau_2')\right)\left(f_1'(\tau_1') + f_{1'}^\dagger(\tau_1')\right)\Big]\Big\rangle
\end{aligned} \tag{2.47}$$

now expand the result and write in a compact manner,

$$\begin{aligned}
\text{Eq}(2.47) &= \left(\frac{1}{2}\right)^4 \left(G_0^{(2)}\left(12, 1'2'\right) + G_0^{(2)}\left(1'2, 12'\right) - G_0^{(2)}\left(12', 1'2\right) + G_0^{(2)}\left(1'2', 12\right)\right) \\
&= \left(\frac{1}{2}\right)^4 \left( \begin{vmatrix} G_0\left(1, 1'\right) & G_0\left(1, 2'\right) \\ G_0\left(2, 1'\right) & G_0\left(2, 2'\right) \end{vmatrix} + \begin{vmatrix} G_0\left(1', 1\right) & G_0\left(1', 2'\right) \\ G_0\left(2, 1\right) & G_0\left(2, 2'\right) \end{vmatrix} \right. \\
&\quad \left. - \begin{vmatrix} G_0\left(1, 1'\right) & G_0\left(1, 2\right) \\ G_0\left(2', 1'\right) & G_0\left(2', 2\right) \end{vmatrix} + \begin{vmatrix} G_0\left(1', 1\right) & G_0\left(1', 2\right) \\ G_0\left(2', 1\right) & G_0\left(2', 2\right) \end{vmatrix} \right)
\end{aligned} \tag{2.48}$$

In first line we have used the Wick's theorem for fermions on each of the 2-fermion Green's functions. The results is somehow understandable since Majorana fermion has no "arrow" diagrammatically, meaning the fermions can travel both forwards and backwards. We can imagine that for n-spin situation, we will get $2^n$ Green's function of n-fermions, each of them can be decomposed into single particle Green's functions using Wick's theorem, which will give $(2^n \cdot n!)$ terms in total. Using the above routine, we can thus use Wick's theorem to simplify Green's functions of spin operators.

# Chapter 3

# Application in dissipative spin dynamics

By using Majorana representation, we have realized in chapter 2 that the relation $\langle\sigma_\alpha(t)\,\sigma_\beta(t')\rangle = \langle\eta_\alpha(t)\,\eta_\beta(t')\rangle$ can be used to simplify spin correlation calculation sometimes, since $\langle\sigma_\alpha(t)\,\sigma_\beta(t')\rangle = \left\langle c^\dagger_{1'}(t)\tau^\alpha_{1'1}(t)c_1(t)c^\dagger_{2'}(t')\tau^\beta_{2'2}(t')c_2(t')\right\rangle$ in pseudo fermion language is of higher order and vertex correction is thus necessary (here $c^\dagger_{1'}$,$c_1$,$c^\dagger_{2'}$ and $c_2$ are Dirac fermions, $\tau^\alpha_{1'1}$ and $\tau^\beta_{2'2}$ are spin matrices respectively). While $\langle\eta_\alpha(t)\,\eta_\beta(t')\rangle$ is a single fermion Green function, we need to calculate the self energy only. In this part we shall see how this method works in dissipative spin dynamics.

Spin relaxation in magnetic field can be described macroscopically by Bloch equation,

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{M} = -\vec{B}\times\vec{M} - \frac{1}{T_1}(M_z - M_0)\,\vec{z} - \frac{1}{T_2}(M_x\vec{x} + M_y\vec{y}) \tag{3.1}$$

in which $\vec{M} = (M_x, M_y, M_z) = (\langle S_x\rangle, \langle S_y\rangle, \langle S_z\rangle)$ is the magnetization, $1/T_1$ and $1/T_2$ are relaxation rate and dephasing rate respectively. The three components of Bloch equation are thus:

$$\begin{aligned}\frac{\mathrm{d}M_x}{\mathrm{d}t} &= \gamma(M_yB_z - M_zB_y) - \frac{M_x}{T_2}\\ \frac{\mathrm{d}M_y}{\mathrm{d}t} &= \gamma(M_zB_x - M_xB_z) - \frac{M_y}{T_2}\\ \frac{\mathrm{d}M_z}{\mathrm{d}t} &= \gamma(M_xB_y - M_yB_x) - \frac{M_z - M_0}{T_1}\end{aligned} \tag{3.2}$$

in which $\gamma$ is gyromagnetic ratio for electron, $M_0$ is the magnetization in steady state. Consider an electron interacts with a bosonic bath [5], the Hamiltonian can be written

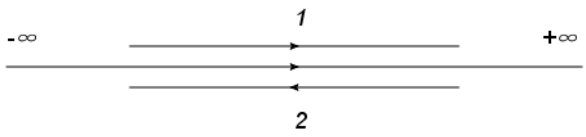


FIGURE 3.1: Keldysh contour $c_K$, two branches represent normal time ordering contour 1 and reversed time ordering contour 2, thus any time point $t_2$ on contour 2 is always larger than $t_1$ on contour 1

as:

$$H = -\frac{1}{2}B\sigma_z - \frac{1}{2}X\sigma_x + H_{bath} \tag{3.3}$$

first term on the right hand side is Zeeman Hamiltonian, $X$ is a fluctuating bosonic observable of the bath coupled to $\sigma_x$, $H_{bath}$ determines the statistics of fluctuation of boson field. We want to perform a calculation with $-\frac{1}{2}X\sigma_x$ as a perturbation using Majorana representation, we shall see that the dissipation process of spin can be described by $T_1$ and $T_2$ just as Bloch equation suggests.

## 3.1 Majorana representation with Keldysh technique

Now we will use Keldysh technique as introduced in [10]. Consider the Green function of the bosonic bath on a Keldysh contour $c_K$ which is illustrated in FIGURE 3.1, $\hat{G}_X(t,t') \equiv -i\langle T_K X(t) X(t')\rangle$, here $\hat{G}_X$ with a hat represents a matrix in Keldysh space, $T_K$ is time ordering on Keldysh contour. The four components of $G_X$ can be written out as below:

$$\begin{aligned}
\hat{G}_X(t,t') &\equiv \begin{pmatrix} G_{11}(t,t') & G_{12}(t,t') \\ G_{21}(t,t') & G_{22}(t,t') \end{pmatrix} = \begin{pmatrix} -i\langle TX(t)X(t')\rangle & -i\langle X(t')X(t)\rangle \\ -i\langle X(t)X(t')\rangle & -i\left\langle \tilde{T}X(t)X(t')\right\rangle \end{pmatrix} \\
&= \begin{pmatrix} -i\langle TX(t)X(t')\rangle & G_X^{<} \\ G_X^{>} & -i\left\langle \tilde{T}X(t)X(t')\right\rangle \end{pmatrix} \\
&= \theta(t-t')\begin{pmatrix} -i\langle TX(t)X(t')\rangle & G_X^{<} \\ G_X^{>} & -i\left\langle \tilde{T}X(t)X(t')\right\rangle \end{pmatrix} + \theta(t'-t)\begin{pmatrix} -i\langle TX(t)X(t')\rangle & G_X^{<} \\ G_X^{>} & -i\left\langle \tilde{T}X(t)X(t')\right\rangle \end{pmatrix} \\
&= \theta(t-t')\begin{pmatrix} G_X^{>} & G_X^{<} \\ G_X^{>} & G_X^{<} \end{pmatrix} + \theta(t'-t)\begin{pmatrix} G_X^{<} & G_X^{<} \\ G_X^{>} & G_X^{>} \end{pmatrix}
\end{aligned} \tag{3.4}$$

here $G_{ij}$ component represents $t$ and $t'$ on $i,j$ contour respectively as in FIGURE 3.1, thus $G_{12}$ and $G_{21}$ will give lesser and greater Greens function respectively, $T$ is the normal time order and $\tilde{T}$ is like a reversed time order. If we perform a linear transformation on $\hat{G}_X$ with a rotation of $L = I + \frac{1}{2}(-\sigma_x + i\sigma_y)$, then

$$\begin{aligned}
\hat{G}_X(t,t') \to & L^\dagger \hat{G}_X(t,t') L \\
=& \theta(t-t') \begin{pmatrix} 0 & 0 \\ G_X^>(t,t') - G_X^<(t,t') & G_X^<(t,t') \end{pmatrix} + \theta(t'-t) \begin{pmatrix} 0 & G_X^<(t,t') - G_X^>(t,t') \\ 0 & G_X^>(t,t') \end{pmatrix} \\
=& \begin{pmatrix} 0 & \theta(t'-t)\left(G_X^<(t,t') - G_X^>(t,t')\right) \\ \theta(t-t')\left(G_X^>(t,t') - G_X^<(t,t')\right) & G_X^<(t,t') + G_X^>(t,t') \end{pmatrix} \\
=& \begin{pmatrix} 0 & G_X^A(t,t') \\ G_X^R(t,t') & G_X^K(t,t') \end{pmatrix}
\end{aligned} \tag{3.5}$$

here $G_X^A$, $G_X^R$ are advanced and retarded Green's functions that we are familiar with, from which the spectrum of states can be calculated, while Keldysh component $G_X^K$ is a combination of greater and lesser Green's functions, which contain information about occupation of the states. Here different Green's functions for boson are listed below for convenience:

$$\begin{aligned}
G_X^>(t,t') =& -i\left\langle X(t) X(t') \right\rangle, \\
G_X^<(t,t') =& -i\left\langle X(t') X(t) \right\rangle, \\
G_X^A(t,t') =& \theta(t'-t)\left(G_X^<(t,t') - G_X^>(t,t')\right) = i\theta(t'-t)\left\langle \left[X(t), X(t')\right] \right\rangle, \\
G_X^R(t,t') =& \theta(t-t')\left(G_X^>(t,t') - G_X^<(t,t')\right) = -i\theta(t-t')\left\langle \left[X(t), X(t')\right] \right\rangle, \\
G_X^K(t,t') =& G_X^<(t,t') + G_X^>(t,t') = -i\left\langle \left\{X(t), X(t')\right\} \right\rangle
\end{aligned} \tag{3.6}$$

from relations above, it is easy to observe that $G_X^K$ correlation is symmetric for $t \leftrightarrow t'$, while $G_X^> - G_X^<$ is antisymmetric for $t \leftrightarrow t'$. Thus we can write the symmetric and antisymmetric components $S_X$ and $A_X$ using Green's functions in (3.6) as:

$$\begin{aligned}
G_X^K =& G_X^< + G_X^> = -2iS_X \\
G_X^R - G_X^A =& G_X^< - G_X^> = -2iA_X
\end{aligned} \tag{3.7}$$

set $t' = 0$, we can write $S_X$ and $A_X$ as function of time $t$ as:

$$\begin{aligned}
S_X(t) =& \frac{1}{2}\left\langle \{X(t), X(0)\} \right\rangle, \\
A_X(t) =& \frac{1}{2}\left\langle [X(t), X(0)] \right\rangle
\end{aligned} \tag{3.8}$$

from which we can easily observe that $\langle X(t)\,X(0)\rangle = S_X(t) + A_X(t)$, with $S_X(t)$ and $A_X(t)$ as symmetric and antisymmetric functions of time not surprisingly: $S_X(t) = S_X(-t)$, $A_X(t) = -A_X(-t)$.

Now we have constructed Green functions of bosonic environment in Keldysh space above. For the single spin, it can be represented using Majorana fermions which can be further written as bi-combination of Dirac fermions, we will call these Dirac fermions in expanded Hilbert space as $f$ fermions, since Majorana fermions have no direction in Feynman diagram, it would be convenient to use Bogolubov-Nambu spinor notations as $\Psi \equiv \left(f, f^\dagger\right)^T$ and $\Psi^\dagger \equiv \left(f^\dagger, f\right)$. Like we did in the boson part, we can also define Green's function in Keldysh contour for spinor $\Psi$ as $\hat{\hat{G}}_\Psi = -i\left\langle T_K \Psi(t)\,\Psi^\dagger(t')\right\rangle$, here two hats in $\hat{\hat{G}}_\Psi$ is used to indicate this is a $4\times 4$ matrix, which is a tensorial product of Keldysh and Nambu space which would be shown later. Using the definition of $\Psi$ spinor, we have the greater and lesser Green functions as:

$$\begin{aligned}
\hat{G}^>_\Psi(t,t') =& -i\left\langle \begin{pmatrix} f(t)\,f^\dagger(t') & f(t)\,f(t') \\ f^\dagger(t)\,f^\dagger(t') & f^\dagger(t)\,f(t') \end{pmatrix} \right\rangle, \\
\hat{G}^<_\Psi(t,t') =& i\left\langle \begin{pmatrix} f^\dagger(t')\,f(t) & f(t')\,f(t) \\ f^\dagger(t')\,f^\dagger(t) & f(t')\,f^\dagger(t) \end{pmatrix} \right\rangle
\end{aligned} \tag{3.9}$$

which are $2\times 2$ matrices, with these relations we can construct Green's function $\hat{\hat{G}}_\Psi$ in Keldysh space in $4\times 4$ matrix form as below:

$$\begin{aligned}
\hat{\hat{G}}_\Psi(t,t') &= \begin{pmatrix} \hat{G}^{11}_\Psi(t,t') & \hat{G}^<_\Psi(t,t') \\ \hat{G}^>_\Psi(t,t') & \hat{G}^{22}_\Psi(t,t') \end{pmatrix} \\
&= \begin{pmatrix} -i\left\langle T\begin{pmatrix} f(t)\,f^\dagger(t') & f(t)\,f(t') \\ f^\dagger(t)\,f^\dagger(t') & f^\dagger(t)\,f(t') \end{pmatrix}\right\rangle & i\left\langle \begin{pmatrix} f^\dagger(t')\,f(t) & f(t')\,f(t) \\ f^\dagger(t')\,f^\dagger(t) & f(t')\,f^\dagger(t) \end{pmatrix}\right\rangle \\ -i\left\langle \begin{pmatrix} f(t)\,f^\dagger(t') & f(t)\,f(t') \\ f^\dagger(t)\,f^\dagger(t') & f^\dagger(t)\,f(t') \end{pmatrix}\right\rangle & -i\left\langle \tilde{T}\begin{pmatrix} f(t)\,f^\dagger(t') & f(t)\,f(t') \\ f^\dagger(t)\,f^\dagger(t') & f^\dagger(t)\,f(t') \end{pmatrix}\right\rangle \end{pmatrix}
\end{aligned} \tag{3.10}$$

perform a rotation analogously with $\hat{\hat{L}} = \begin{pmatrix} \hat{1} & 0 \\ -\hat{1} & \hat{1} \end{pmatrix}$, which is also a $4\times4$ matrix, we have

$$\hat{\hat{G}}_\Psi(t,t') \to \hat{\hat{L}}^\dagger \hat{\hat{G}}_\Psi(t,t')\hat{\hat{L}} = \begin{pmatrix} \hat{0} & \theta(t'-t)\left(\hat{G}^<_\Psi(t,t') - \hat{G}^>_\Psi(t,t')\right) \\ \theta(t-t')\left(\hat{G}^>_\Psi(t,t') - \hat{G}^<_\Psi(t,t')\right) & \hat{G}^K_\Psi(t,t') \end{pmatrix}$$
$$= \left\langle \begin{pmatrix} \hat{0} & i\theta(t'-t)\begin{pmatrix} \{f(t),f^\dagger(t')\} & \{f(t),f(t')\} \\ \{f^\dagger(t),f^\dagger(t')\} & \{f^\dagger(t),f(t')\} \end{pmatrix} \\ -i\theta(t-t')\begin{pmatrix} \{f(t),f^\dagger(t')\} & \{f(t),f(t')\} \\ \{f^\dagger(t),f^\dagger(t')\} & \{f^\dagger(t),f(t')\} \end{pmatrix} & -i\begin{pmatrix} [f(t),f^\dagger(t')] & [f(t),f(t')] \\ [f^\dagger(t),f^\dagger(t')] & [f^\dagger(t),f(t')] \end{pmatrix} \end{pmatrix} \right\rangle$$
$$= \begin{pmatrix} \hat{0} & \begin{pmatrix} G^A_f(t,t') & 0 \\ 0 & -G^R_f(t',t) \end{pmatrix} \\ \begin{pmatrix} G^R_f(t,t') & 0 \\ 0 & -G^A_f(t',t) \end{pmatrix} & \begin{pmatrix} -G^K_f(t,t') & 0 \\ 0 & G^K_f(t',t) \end{pmatrix} \end{pmatrix} \tag{3.11}$$

Now perform another rotation with $\hat{\hat{L}}_1 = \begin{pmatrix} & \hat{1} \\ \hat{1} & \end{pmatrix}$ on $\hat{\hat{L}}^\dagger \hat{\hat{G}}_\Psi \hat{\hat{L}}$ in last step,

$$\begin{aligned} \hat{\hat{L}}^\dagger \hat{\hat{G}}_\Psi(t,t')\hat{\hat{L}} \to & \underline{\hat{\hat{G}}}_\Psi(t,t') = \hat{\hat{L}}_1 \hat{\hat{L}}^\dagger \hat{\hat{G}}_\Psi(t,t')\hat{\hat{L}} \\ &= \begin{pmatrix} \begin{pmatrix} G^R_f(t,t') & 0 \\ 0 & -G^A_f(t',t) \end{pmatrix} & \begin{pmatrix} -G^K_f(t,t') & 0 \\ 0 & G^K_f(t',t) \end{pmatrix} \\ \hat{0} & \begin{pmatrix} G^A_f(t,t') & 0 \\ 0 & -G^R_f(t',t) \end{pmatrix} \end{pmatrix} \end{aligned} \tag{3.12}$$

we can observe that the diagonal terms in (3.12), which are retarded and advanced Green's functions, characterize the states, while the two off-diagonal terms are Keldysh components containing information about occupation of fermionic states. Since $\underline{\hat{\hat{G}}}_\Psi$ has such good structures, later we will use $\underline{\hat{\hat{G}}}_\Psi$ instead of $\hat{\hat{G}}_\Psi$.

We can construct the right handed and conjugate left handed Dyson equations in Keldysh-Nambu space as below:

$$\begin{aligned} \left(\underline{\hat{\hat{G}}}^{-1}_{\Psi,0}(t,t') - \underline{\hat{\hat{\Sigma}}}_\Psi(t,t')\right) \otimes \underline{\hat{\hat{G}}}_\Psi(t,t') &= \delta\left(t-t'\right)\cdot\hat{\hat{1}} \\ \underline{\hat{\hat{G}}}_\Psi(t,t') \otimes \left(\underline{\hat{\hat{G}}}^{-1}_{\Psi,0}(t,t') - \underline{\hat{\hat{\Sigma}}}_\Psi(t,t')\right) &= \delta\left(t-t'\right)\cdot\hat{\hat{1}} \end{aligned} \tag{3.13}$$

with $\underline{\hat{\hat{G}}}_{\Psi,0}$ and $\underline{\hat{\hat{\Sigma}}}_{\Psi}$ as bare Green's function and self energy, or in another form,

$$\underline{\hat{\hat{G}}}_{\Psi}^{-1} = \underline{\hat{\hat{G}}}_{\Psi,0}^{-1} - \underline{\hat{\hat{\Sigma}}}_{\Psi} \tag{3.14}$$

It should be noticed that we can perform other rotations to get the same $\underline{\hat{\hat{G}}}_{\Psi}$, for example, we can follow the fashion of Keldysh rotation [9], given that $\hat{\hat{G}}_{\psi} = \begin{pmatrix} \hat{G}_{\psi}^{11} & \hat{G}_{\psi}^{12} \\ \hat{G}_{\psi}^{21} & \hat{G}_{\psi}^{22} \end{pmatrix}$, making use of the relations as below, which are easy to proof,

$$\begin{aligned} \hat{G}_{\psi}^{R} &= \hat{G}_{\psi}^{11} - \hat{G}_{\psi}^{12} = \hat{G}_{\psi}^{21} - \hat{G}_{\psi}^{22}, \\ \hat{G}_{\psi}^{A} &= \hat{G}_{\psi}^{11} - \hat{G}_{\psi}^{21} = \hat{G}_{\psi}^{12} - \hat{G}_{\psi}^{22}, \\ \hat{G}_{\psi}^{K} &= \hat{G}_{\psi}^{11} + \hat{G}_{\psi}^{22} = \hat{G}_{\psi}^{21} + \hat{G}_{\psi}^{12}. \end{aligned} \tag{3.15}$$

first we make a transformation from $\hat{\hat{G}}_{\Psi}$ to $\breve{G}_{\Psi}$ as $\breve{G}_{\Psi} = \begin{pmatrix} \hat{1} & \\ & -\hat{1} \end{pmatrix} \hat{\hat{G}}_{\Psi}$, define $\hat{\hat{L}}_2$ as $\hat{\hat{L}}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{1} & -\hat{1} \\ \hat{1} & \hat{1} \end{pmatrix}$, which is like a $4 \times 4$ matrix form of Keldysh rotation, then we apply $\hat{\hat{L}}_2$ on $\breve{G}_{\Psi}$ to get $\underline{\hat{\hat{G}}}_{\Psi}$

$$\breve{G}_{\psi} \to \underline{\hat{\hat{G}}}_{\Psi} = \hat{\hat{L}}_2 \breve{G}_{\psi} \hat{\hat{L}}_2^{\dagger} \tag{3.16}$$

which can be checked is the same as in (3.12).

Now write Hamiltonian unperturbed from spin-boson interaction in (3.3) with relation (2.10), we have a Hamiltonian that contains a quadratic term of $f$ fermion with free energy of $B$,

$$H = -\frac{1}{2} B \sigma_z + V = -\frac{1}{2} B \left(1 - 2f^{\dagger} f\right) + V = B f^{\dagger} f - \frac{1}{2} B + V \tag{3.17}$$

remember components in (3.12) are:

$$\begin{aligned} G_f^{>}(t,t') &= -i \left\langle f(t) f^{\dagger}(t') \right\rangle \\ G_f^{<}(t,t') &= i \left\langle f^{\dagger}(t') f(t) \right\rangle \\ G_f^{R}(t,t') &= \theta(t-t') \left(G_X^{>}(t,t') - G_X^{<}(t,t')\right) = -i\theta(t-t') \left\langle \left\{ f(t), f^{\dagger}(t') \right\} \right\rangle \\ G_f^{A}(t,t') &= \theta(t'-t) \left(G_X^{<}(t,t') - G_X^{>}(t,t')\right) = i\theta(t'-t) \left\langle \left\{ f(t), f^{\dagger}(t') \right\} \right\rangle \\ G_f^{K}(t,t') &= G_X^{>}(t,t') + G_X^{<}(t,t') = i \left\langle \left[ f(t), f^{\dagger}(t') \right] \right\rangle \end{aligned} \tag{3.18}$$

using the equation of motion theory on $\hat{\underline{\hat{G}}}_\Psi$ in Keldysh space, we can easily get

$$\left(i\partial_t \cdot \hat{\hat{1}} - B\hat{\hat{\sigma}}_z\right)\hat{\underline{\hat{G}}}_{\Psi,0}(t,t') = \delta\left(t-t'\right)\cdot\hat{\hat{1}} \tag{3.19}$$

here we use $(i\partial_t - B)\, G_f^{R/A} = \delta\,(t-t')$, $i\partial_t G_f^K = G_f^K$, and $\hat{\hat{\sigma}}_z = \begin{pmatrix}\sigma_z & \\ & \sigma_z\end{pmatrix}$ to take care of different signs of diagonal terms in (3.12). We can transform (3.19) to frequency domain as,

$$\hat{\underline{\hat{G}}}_{\Psi,0}^{-1} = \omega\cdot\hat{\hat{1}} - B\hat{\hat{\sigma}}_z \tag{3.20}$$

Now we have constructed Green's function of bosonic field and $f$ fermions using Keldysh technique, and we still need to have Majorana fermions in frame. Define $\hat{G}_\eta \equiv -i\,\langle T_K \eta\,(t)\,\eta\,(t')\rangle$ for Majorana fermion $\eta \equiv \eta_z$, and we can write,

$$\underline{\hat{G}}_\eta = \begin{pmatrix} G_\eta^R & G_\eta^K \\ 0 & G_\eta^A\end{pmatrix} = \begin{pmatrix} -i\theta\,(t-t')\,\langle\{\eta\,(t)\,,\eta\,(t')\}\rangle & i\,\langle[\eta\,(t)\,,\eta\,(t')]\rangle \\ 0 & i\theta\,(t'-t)\,\langle\{\eta\,(t)\,,\eta\,(t')\}\rangle\end{pmatrix} \tag{3.21}$$

with Dyson equation as below, in which $\underline{\hat{\Sigma}}_\eta$ is the self energy for Majorana fermions:

$$\underline{\hat{G}}_\eta^{-1} = \underline{\hat{G}}_{\eta,0}^{-1} - \underline{\hat{\Sigma}}_\eta \tag{3.22}$$

since $G_\eta^R\,(t,t') = i\theta\,(t-t')\,\langle\{\eta\,(t)\,,\eta\,(t')\}\rangle$, using equation of motion theory we can easily get,

$$i\partial_t G_{\eta,0}^R\left(t,t'\right) = \delta\left(t,t'\right)\left\langle\left\{\eta\left(t\right),\eta\left(t'\right)\right\}\right\rangle + \theta\left(t-t'\right)\left\langle\left\{\dot{\eta}\left(t\right),\eta\left(t'\right)\right\}\right\rangle = 2\delta\left(t,t'\right) \tag{3.23}$$

similarly for advanced term $G_{\eta,0}^A$, and $i\partial_t G_{\eta,0}^K = 0$, for $\eta\,(t)$ is independent of time according to Heisenberg equation. In the frequency domain, we have

$$\underline{\hat{G}}_{\eta,0}^{-1} = \frac{1}{2}\omega\cdot\hat{1} \tag{3.24}$$

for simplicity we will write (3.20) and (3.24) in the following way without hats and define $\tau_z^{Nambu} = \hat{\hat{\sigma}}_z$, but keep in mind that Green functions in Keldysh space for $\Psi$ spinors and $\eta$ fermions are $4\times4$ and $2\times2$ matrices respectively:

$$G_{\Psi,0}^{-1} = \omega\cdot 1 - B\tau_z^{Nambu}, \quad G_{\eta,0}^{-1} = \frac{1}{2}\omega\cdot 1 \tag{3.25}$$

Next we will evaluate self energy $\Sigma_\Psi$ and $\Sigma_\eta$, the Feynman diagrams are illustrated in FIGURE 3.2. First we can calculate a simple case $\Sigma_f$ in FIGURE 3.3, in which

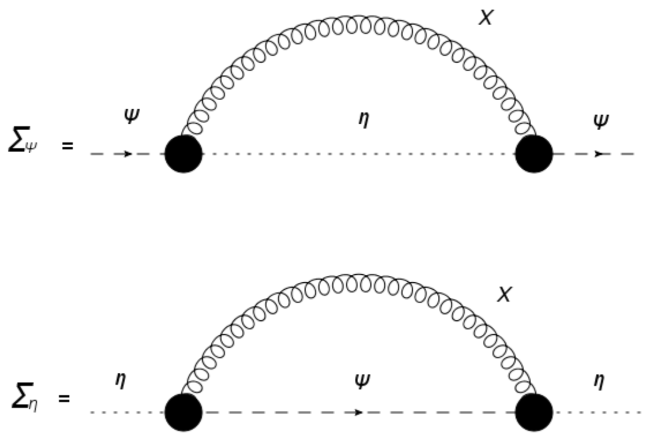


FIGURE 3.2: The lowest order nonvanishing contribution to the self-energy $\hat{\Sigma}_\Psi$ and $\Sigma_\eta$, curly lines for propagator of the bosonic bath $X$, dashed lines for $f\Psi$ spinors, dotted lines for Majorana fermions $\eta$.

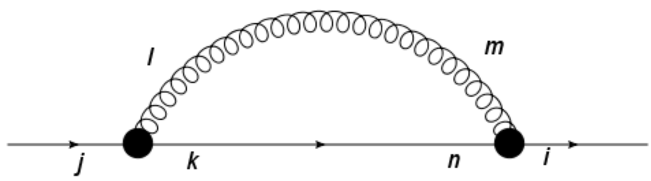


FIGURE 3.3: Self-energy $\Sigma_f$, curly lines for propagator of the bosonic bath $X$, solid lines for the ordinary fermion.

an ordinary fermion $f$ interacts with boson field. Using Feynman rules in Keldysh space [10], the ij component of self energy $\Sigma_f$ can be written as:

$$\Sigma_f^{ij} = \frac{i}{2}\gamma_{im}^n \tilde{\gamma}_{lj}^k G_X^{nk} G_f^{ml} \tag{3.26}$$

in which $\gamma_{im}^n$ and $\tilde{\gamma}_{lj}^k$ represent absorption and emission vertices in FIGURE 3.4, they are third rank tensors, satisfying:

$$\begin{aligned} \gamma_{ij}^1 = \tilde{\gamma}_{ij}^2 = \frac{1}{\sqrt{2}}\delta_{ij}; \\ \gamma_{ij}^2 = \tilde{\gamma}_{ij}^1 = \frac{1}{\sqrt{2}}\sigma_{ij}^1. \end{aligned} \tag{3.27}$$

summing up Keldysh indices in (3.26) we can calculate,

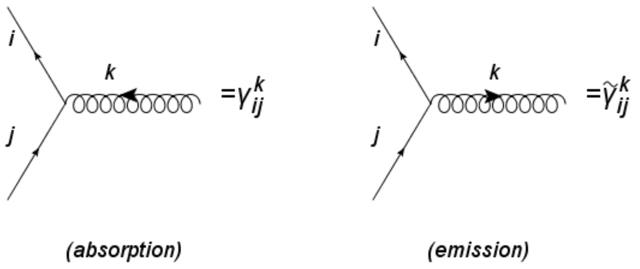


FIGURE 3.4: Feynman rules in Keldysh space for boson fermion interaction vertices.

$$
\begin{aligned}
\Sigma_f^R =&\Sigma_f^{11} = \frac{i}{2}\left(\gamma^1_{11} G_X^{1k} G_f^{1l} \tilde{\gamma}^k_{l1} + \gamma^1_{12} G_X^{2k} G_f^{2l} \tilde{\gamma}^k_{l2}\right) \\
=&\frac{i}{2}\left(\gamma^1_{11} G_X^{11} G_f^{12} \tilde{\gamma}^1_{21} + \gamma^1_{11} G_X^{12} G_f^{11} \tilde{\gamma}^2_{11} + \gamma^1_{11} G_X^{21} G_f^{22} \tilde{\gamma}^1_{21} + \gamma^1_{11} G_X^{22} G_f^{21} \tilde{\gamma}^2_{11}\right) \\
=&\frac{i}{4}\left(G_X^{11} G_f^{12} + G_X^{12} G_f^{11}\right) = \frac{i}{4}\left(G_X^R G_f^K + G_X^K G_f^R\right)
\end{aligned}
\tag{3.28}
$$

here we used the fact that 21 component Green's functions $G_X^{21}$ and $G_f^{21}$ in Keldysh space are zero. By a same procedure, the advanced and Keldysh components of the self energy can also be calculated as below:

$$
\begin{aligned}
\Sigma_f^A =&\Sigma_f^{22} = \frac{i}{2}\left(\gamma^1_{22} G_X^{1k} G_f^{2l} \tilde{\gamma}^k_{l2} + \gamma^2_{21} G_X^{2k} G_f^{1l} \tilde{\gamma}^k_{l2}\right) \\
=&\frac{i}{2}\left(\gamma^1_{22} G_X^{11} G_f^{21} \tilde{\gamma}^1_{12} + \gamma^1_{22} G_X^{12} G_f^{22} \tilde{\gamma}^2_{22} + \gamma^2_{21} G_X^{21} G_f^{11} \tilde{\gamma}^1_{12} + \gamma^2_{21} G_X^{22} G_f^{12} \tilde{\gamma}^2_{22}\right) \\
=&\frac{i}{4}\left(G_X^{12} G_f^{22} + G_X^{22} G_f^{12}\right) = \frac{i}{4}\left(G_X^A G_f^K + G_X^K G_f^A\right)
\end{aligned}
\tag{3.29}
$$

$$
\begin{aligned}
\Sigma_f^K =&\Sigma_f^{12} = \frac{i}{2}\left(\gamma^1_{11} G_X^{1k} G_f^{1l} \tilde{\gamma}^k_{l2} + \gamma^2_{12} G_X^{2k} G_f^{2l} \tilde{\gamma}^k_{l2}\right) \\
=&\frac{i}{2}\left(\gamma^1_{11} G_X^{11} G_f^{11} \tilde{\gamma}^1_{12} + \gamma^1_{11} G_X^{12} G_f^{12} \tilde{\gamma}^2_{22} + \gamma^2_{12} G_X^{21} G_f^{21} \tilde{\gamma}^1_{12} + \gamma^2_{12} G_X^{22} G_f^{22} \tilde{\gamma}^2_{22}\right) \\
=&\frac{i}{4}\left(G_X^{11} G_f^{11} + G_X^{12} G_f^{12} + G_X^{12} G_f^{22}\right) = \frac{i}{4}\left(G_X^R G_f^R + G_X^K G_f^K + G_X^A G_f^A\right)
\end{aligned}
\tag{3.30}
$$

since $\Sigma_f^< = \frac{1}{2}\left(\Sigma_f^K - \Sigma_f^R + \Sigma_f^A\right)$, using results in (3.28), (3.29) and (3.30), we have

$$
\begin{aligned}
\Sigma_f^< =&\frac{i}{4}\left(\left(G_X^R - G_X^R + G_X^A\right) G_f^K + \left(G_X^A - 2G_X^<\right) G_f^R + \left(G_X^R + 2G_X^<\right) G_f^A\right) \\
=&\frac{i}{4}\left(2G_X^< \left(G_f^K - G_f^R + G_f^A\right) + G_X^R G_f^A + G_X^A G_f^R\right) \\
=&\frac{i}{2} G_X^< G_f^<
\end{aligned}
\tag{3.31}
$$

the last two terms $G_X^R G_f^A + G_X^A G_f^R$ in second line of (3.31) vanish when we integrate the energy $\epsilon$ of $G_X^{R/A}(\epsilon)$ and $G_f^{A/R}(\omega - \epsilon)$ on complex plane. Similarly we can derive $\Sigma_f^> = \frac{i}{2} G_X^> G_f^>$. The above analytic continuation results are similar to Langreth theorem [15].

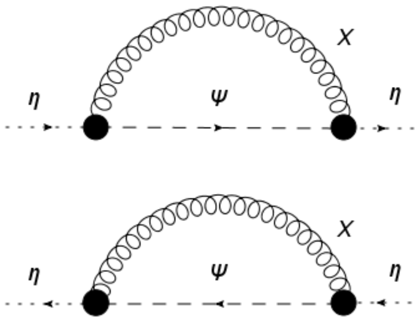


FIGURE 3.5: Two diagrams are equivalent, with $\Psi$ propagator in upper one represent 11 component of $G_\Psi^>$, while the lower one represent 22 component of $G_\Psi^>$.

Now we want to calculate $\Sigma_\eta$ and $\Sigma_\Psi$ in FIGURE 3.2, if we remind ourselves of the form of $G_\Psi$ as in relation (3.9), and notice that two diagrams in FIGURE 3.5 are equivalent,we can write

$$\Sigma_\eta^> = \frac{i}{2} G_X^> \frac{1}{2} \begin{pmatrix} 1 & -1 \end{pmatrix} G_\Psi^> \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{i}{4} G_X^> \begin{pmatrix} 1 & -1 \end{pmatrix} G_\Psi^> \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{3.32}$$

$$\Sigma_\eta^< = \frac{i}{2} G_X^< \frac{1}{2} \begin{pmatrix} 1 & -1 \end{pmatrix} G_\Psi^< \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{i}{4} G_X^< \begin{pmatrix} 1 & -1 \end{pmatrix} G_\Psi^< \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{3.33}$$

while $\Sigma_\Psi$ should be a $2 \times 2$ matrix as:

$$\Sigma_\Psi^> = \frac{i}{4} \hat{\lambda} G_X^> G_\eta^>, \quad \Sigma_\Psi^< = \frac{i}{4} \hat{\lambda} G_X^< G_\eta^< \tag{3.34}$$

in which $\hat{\lambda} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$. Now using relations (3.28), (3.29) and (3.34), we have:

$$\begin{aligned}
\Sigma_\Psi^R(\epsilon) - \Sigma_\Psi^A(\epsilon) =& \frac{i}{4} \hat{\lambda} \int \frac{\mathrm{d}\omega}{2\pi} \left( \left( G_X^R(\epsilon+\omega) - G_X^A(\epsilon+\omega) \right) G_\eta^K(\omega) + G_X^K(\epsilon+\omega) \left( G_\eta^R(\omega) - G_\eta^A(\omega) \right) \right) \\
=& \frac{i}{4} \hat{\lambda} \int \frac{\mathrm{d}\omega}{2\pi} \left( \left( G_X^R(\epsilon+\omega) - G_X^A(\epsilon+\omega) \right) h_\eta(\omega) + G_X^K(\epsilon+\omega) \right) \left( G_\eta^R(\omega) - G_\eta^A(\omega) \right) \\
=& \frac{1}{4} \hat{\lambda} \int \frac{\mathrm{d}\omega}{2\pi} \Gamma_\eta(\omega) \left( \left( G_X^R(\epsilon+\omega) - G_X^A(\epsilon+\omega) \right) h_\eta(\omega) + G_X^K(\epsilon+\omega) \right)
\end{aligned} \tag{3.35}$$

in which $\Gamma_\eta(\omega) = -2\mathrm{Im}G_\eta^R(\omega) = i\left(G_\eta^R(\omega) - G_\eta^A(\omega)\right)$ is the energy spectrum function which is a $\delta$-function. Here we used the relation $G_\eta^K(\omega) = h_\eta(\omega)\left(G_\eta^R(\omega) - G_\eta^A(\omega)\right)$ assuming the system in thermal equilibrium (fluctuation-dissspation theorem [11]), which is easy to derive and $h_\eta(\omega) = \tanh\left(\frac{\beta\omega}{2}\right)$. In this situation, the Keldysh Green's function contains no more information than the retarded ones, thus could be written in a compact manner. Now if we only consider the range near $\omega = 0$, since $h_\eta(\omega) = -h_\eta(-\omega)$, we have $h_\eta(\omega) = 0$, (3.35) becomes:

$$\Sigma_\Psi^R - \Sigma_\Psi^A = \frac{1}{4}\hat{\lambda} G_X^K = -\frac{i}{2}\hat{\lambda} S_X \tag{3.36}$$

similarly we can derive $\Sigma_\Psi^K$ as below,

$$\begin{aligned}
\Sigma_\Psi^K(\epsilon) =& \frac{i}{4}\hat{\lambda}\int\frac{\mathrm{d}\omega}{2\pi}\left(G_X^R(\epsilon+\omega)G_\eta^R(\omega) + G_X^K(\epsilon+\omega)G_\eta^K(\omega) + G_X^R G_\eta^A(\omega)\right) \\
=& \frac{i}{4}\hat{\lambda}\int\frac{\mathrm{d}\omega}{2\pi}\Big(G_X^R(\epsilon+\omega)\left(G_\eta^R(\omega) - G_\eta^A(\omega)\right) + G_X^A(\epsilon+\omega)\left(G_\eta^A(\omega) - G_\eta^R(\omega)\right) \\
& + G_X^K(\epsilon+\omega)G_\eta^K(\omega)\Big) \\
=& \frac{i}{4}\hat{\lambda}\int\frac{\mathrm{d}\omega}{2\pi}2i\mathrm{Im}G_\eta^R(\omega)\left(G_X^R(\epsilon+\omega) - G_X^A(\epsilon+\omega) + G_X^K(\epsilon+\omega)h_\eta(\omega)\right) \\
\to& \frac{1}{4}\hat{\lambda}\left(G_X^R(\epsilon) - G_X^A(\epsilon)\right), \quad (\omega\to 0) \\
=& -\frac{i}{2}A_X(\epsilon)
\end{aligned} \tag{3.37}$$

since we have $\Sigma_\Psi^R$ and $\Sigma_\Psi^A$ analogous to (3.28) and (3.29),

$$\begin{aligned}
\Sigma_\Psi^R =& \frac{i}{4}\hat{\lambda}\left(G_X^R G_\Psi^K + G_X^K G_\Psi^R\right) \\
\Sigma_\Psi^A =& \frac{i}{4}\hat{\lambda}\left(G_X^A G_\Psi^K + G_X^K G_\Psi^A\right)
\end{aligned} \tag{3.38}$$

which will yield opposite sign for $\Sigma_\Psi^R$ and $\Sigma_\Psi^A$, Using relation (3.36), we easily get:

$$\Sigma_\Psi^R = -\frac{i}{4}\hat{\lambda} S_X = -i\lambda\Gamma, \quad \Sigma_\Psi^A = \frac{i}{4}\hat{\lambda} S_X = i\lambda\Gamma \tag{3.39}$$

in which $\Gamma \equiv \frac{1}{4}S_X$. Now we have written self energy components of $\Psi$ spinors $\Sigma_\Psi^R$, $\Sigma_\Psi^A$ and $\Sigma_\Psi^K$ by bosonic Green's functions $A_X$ and $S_X$ only, where $\Sigma_\Psi^{R/A}$ related to the symmetric one $S_X$, while $\Sigma_\Psi^K$ related to antisymmetric $A_X$.

Substitute (3.39) into Dyson's equation (3.25), we get

$$\begin{aligned}
G_\Psi^{-1} =& \omega\cdot 1 - B\tau_z^{Nambu} - \Sigma_\Psi \\
=& \begin{pmatrix}
\omega - B + i\Gamma & -i\Gamma & \frac{i}{2}A_X & -\frac{i}{2}A_X \\
-i\Gamma & \omega + B + i\Gamma & -\frac{i}{2}A_X & \frac{i}{2}A_X \\
0 & 0 & \omega - B - i\Gamma & i\Gamma \\
0 & 0 & i\Gamma & \omega + B - i\Gamma
\end{pmatrix}
\end{aligned} \tag{3.40}$$

from which we have $\left|G_\Psi^{-1}\right| = \left(\omega^2 - B^2\right)^2 + 4\omega^2\Gamma^2$, some simple algebra will give the components of $G_\Psi$ as

$$\begin{aligned}
G_\Psi^K =& \frac{1}{\left|G_\Psi^{-1}\right|}\begin{pmatrix} -\frac{i}{2}A_X\left(\omega+B\right)^2 & \frac{i}{2}A_X\left(\omega^2-B^2\right) \\ \frac{i}{2}A_X\left(\omega^2-B^2\right) & -\frac{i}{2}A_X\left(\omega-B\right)^2 \end{pmatrix} \\
=& \frac{iA_X\begin{pmatrix} -\left(\omega+B\right)^2 & \omega^2-B^2 \\ \omega^2-B^2 & -\left(\omega-B\right)^2 \end{pmatrix}}{2\left(\left(\omega^2-B^2\right)^2+4\omega^2\Gamma^2\right)} \\
G_\Psi^R =& \frac{1}{\left|G_\Psi^{-1}\right|}\begin{pmatrix} \left(\omega+B+i\Gamma\right)\left(\omega^2-B^2-2i\omega\Gamma\right) & i\Gamma\left(\omega^2-B^2-2i\omega\Gamma\right) \\ i\Gamma\left(\omega^2-B^2-2i\omega\Gamma\right) & \left(\omega-B+i\Gamma\right)\left(\omega^2-B^2-2i\omega\Gamma\right) \end{pmatrix} \\
=& \frac{1}{\omega^2-B^2+2i\omega\Gamma}\begin{pmatrix} \omega+B+i\Gamma & i\Gamma \\ i\Gamma & \omega-B+i\Gamma \end{pmatrix}
\end{aligned} \tag{3.41}$$

similarly for $G_\Psi^A$, and in total we have:

$$\begin{aligned}
G_\Psi^{R/A} &= \frac{\begin{pmatrix} \omega+B\pm i\Gamma & \pm i\Gamma \\ \pm i\Gamma & \omega-B\pm i\Gamma \end{pmatrix}}{\omega^2-B^2\pm 2i\omega\Gamma} \\
G_\Psi^K &= \frac{iA_X\begin{pmatrix} -\left(\omega+B\right)^2 & \omega^2-B^2 \\ \omega^2-B^2 & -\left(\omega-B\right)^2 \end{pmatrix}}{2\left(\left(\omega^2-B^2\right)^2+4\omega^2\Gamma^2\right)}
\end{aligned} \tag{3.42}$$

substitute (3.42) into the thermal equilibrium equation $G_\Psi^K\left(\omega\right) = h_\Psi\left(\omega\right)\left(G_\Psi^R\left(\omega\right) - G_\Psi^A\left(\omega\right)\right)$, we have

$$h_\Psi\left(\omega\right) = \frac{iA_X}{2}\cdot\frac{1}{2i\Gamma} = \frac{A_X\left(\omega\right)}{S_X\left(\omega\right)} = \frac{\Sigma_\Psi^K\left(\omega\right)}{\Sigma_\Psi^R\left(\omega\right) - \Sigma_\Psi^A\left(\omega\right)} \tag{3.43}$$

Using these results we are thus able to find $\Sigma_\eta$ in FIGURE 3.2. Since

$$\begin{aligned}
\Sigma_\eta^K(\epsilon) &= \frac{1}{4}\left(G_X^R(\epsilon+\omega) - G_X^A(\epsilon+\omega) + h_\Psi\left(\omega\right)G_X^K(\epsilon+\omega)\right) \\
\Sigma_\eta^R(\epsilon) - \Sigma_\eta^A(\epsilon) &= \frac{1}{4}\left(G_X^K(\epsilon+\omega) + h_\Psi\left(\omega\right)\left(G_X^R(\epsilon+\omega) - G_X^A(\epsilon+\omega)\right)\right)
\end{aligned} \tag{3.44}$$

which are analogous to (3.35) and (3.37). Consider a narrow range near $\omega = 0$, for short-correlated noise $\Sigma_\eta^K = 0$, using $h_\Psi\left(\omega\right)$ obtained in (3.43),

$$\Sigma_\eta^R - \Sigma_\eta^A = \frac{1}{4}\left(-2iS_X + \frac{A_X}{S_X}\left(-2iA_X\right)\right) = -2i\cdot\frac{S_X}{4}\left(1+\frac{A_X^2}{S_X^2}\right) = -2i\tilde{\Gamma} \tag{3.45}$$

$\tilde{\Gamma}$ depends on $B$ when $\omega$ in narrow range near 0, which is defined as

$$\tilde{\Gamma} \equiv \frac{S_X(B)}{4}\left(1+\frac{A_X^2(B)}{S_X^2(B)}\right) \tag{3.46}$$

similarly, we can solve Green's functions of Majorana fermion $\eta$ in Keldysh space. Firstly from (3.44) we have

$$\Sigma_\eta^K = 0, \quad \Sigma_\eta^R = -i\tilde{\Gamma}, \quad \Sigma_\eta^A = i\tilde{\Gamma} \tag{3.47}$$

substitute into Dyson's equation (3.25),

$$G_\eta^{-1} = \frac{1}{2}\omega \cdot 1 - \Sigma_\eta = \begin{pmatrix} \frac{1}{2}\omega + i\tilde{\Gamma} & 0 \\ 0 & \frac{1}{2}\omega - i\tilde{\Gamma} \end{pmatrix} \tag{3.48}$$

it's easy to derive,

$$G_\eta^{R/A} = \frac{2}{\omega \pm 2i\tilde{\Gamma}}, \quad G_\eta^K = 0 \tag{3.49}$$

thus by performing Keldysh technique, using thermal equilibrium equation, we can calculate the components of self energy $\Sigma_\Psi$ and $\Sigma_f$ (FIGURE 3.2) in Keldysh space, which are functions of symmetric and antisymmetric components of bosonic field $S_X$ and $A_X$. Then by kinetic equations, Green's functions for $\Psi$ spinor and $\eta$ fermion in Keldysh space can be derived, we will see in section 3.2 that transversal and longitudinal spin susceptibilities can be calculated using above results.

## 3.2 spin-spin correlators

Now we can evaluate spin-spin correlators with knowledge of single-fermion Green's functions obtained in section 3.1. First consider a two fermion correlator in Keldysh contour: $\Pi_{xx} \equiv -i\langle T_K \sigma_x(t)\sigma_x(t')\rangle$. We know from (2.32) that it can be reduced to Majorana fermion correlators, for example, the greater one $\Pi_{xx}^>$ as:

$$\begin{aligned} \Pi_{xx}^> &= -i\left\langle \sigma_x(t)\sigma_x(t')\right\rangle = -i\left\langle \eta_x(t)\eta_x(t')\right\rangle \\ &= -i\left\langle f^\dagger(t) f(t') + f(t) f(t') + f^\dagger(t) f^\dagger(t') + f(t) f(t')\right\rangle \\ &= (1 \quad 1)\, G_\Psi^> \begin{pmatrix} 1 \\ 1 \end{pmatrix} \end{aligned} \tag{3.50}$$

since $G_\Psi^> = \frac{1}{2}\left(G_\Psi^K + G_\Psi^R - G_\Psi^A\right)$, use $G_\Psi^{R/A}$ and $G_\Psi^K$ from (3.42),

$$\begin{aligned}\Pi_{xx}^> =& \frac{i}{4}\frac{A_X + S_X}{\left(\omega^2 - B^2\right)^2 + 4\omega^2\Gamma^2}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}-\left(\omega + B\right)^2 & \omega^2 - B^2 \\ \omega^2 - B^2 & -\left(\omega - B\right)^2\end{pmatrix}\begin{pmatrix}1 \\ 1\end{pmatrix} \\ =& \frac{-iB^2\left(S_X + A_X\right)}{\left(\omega^2 - B^2\right)^2 + 4\omega^2\Gamma^2}\end{aligned} \tag{3.51}$$

similarly we can derive $\Pi_{xx}^<$ as

$$\Pi_{xx}^< = \frac{-iB^2\left(A_X - S_X\right)}{\left(\omega^2 - B^2\right)^2 + 4\omega^2\Gamma^2} \tag{3.52}$$

Now consider $i\Pi_{xx}^>$,
(1) In the limit of weak noise or magnetic field dominates: $\Gamma\left(B\right) \ll B$, there are two peaks $\omega = \pm B$ in the spectrum, with dephasing rate as $T_2^{-1} = \Gamma\left(B\right) = \frac{S_X(B)}{4} \propto \left\langle X^2\left(\omega = \pm B\right)\right\rangle$, which is equivalent to the dephasing rate described in Bloch equation in (3.1);
(2) In the opposite limit $\Gamma\left(\omega\right) \gg B$ in which bosonic bath dominates,

$$i\Pi_{xx}^> \rightarrow \frac{B^2\left(A_X + 4\Gamma\right)}{\omega^2\left(\omega^2 + 4\Gamma^2\right)} = \frac{B^2\left(A_X + 2\Gamma_Z\right)}{\omega^2\left(\omega^2 + 2\Gamma_Z^2\right)} \tag{3.53}$$

here $\Gamma_Z = 2\Gamma$, near $\omega = 0$ the antisymmetric component $A_X \rightarrow 0$, thus develops a single peak at $2\Gamma_Z B^2/\left(\omega^2 + \Gamma_Z^2\right)$, the width of this peak as $2B^2/\Gamma_Z = B^2/\Gamma\left(0\right)$.

Similarly, using results in (3.49) the longitudinal spin-spin correlator $\Pi_{zz}$ is directly

$$\begin{aligned}\Pi_{zz}^> =& - i\left\langle\sigma_z\left(t\right)\sigma_z\left(t'\right)\right\rangle = -i\left\langle\eta_z\left(t\right)\eta_z\left(t'\right)\right\rangle = G_\eta^> \\ =& \frac{1}{2}\left(G_\eta^K + G_\eta^R - G_\eta^A\right) = \frac{-4i\tilde{\Gamma}}{\omega^2 + 4\tilde{\Gamma}^2}\end{aligned} \tag{3.54}$$

consider expectation value of $\sigma_z$

$$\begin{aligned}&\left\langle\sigma_z\right\rangle = \left\langle 1 - 2f^\dagger f\right\rangle = 1 - 2n_F\left(\omega\right) = \frac{e^{\beta\omega} - 1}{e^{\beta\omega} + 1} = \tanh\left(\frac{\beta\omega}{2}\right) = h_\eta\left(\omega\right) \\ &h_\eta\left(\omega\right) = \frac{A_X\left(\omega\right)}{S_X\left(\omega\right)}\end{aligned} \tag{3.55}$$

then we can write $\tilde{\Gamma}$ as

$$\tilde{\Gamma} \equiv \frac{S_X\left(B\right)}{4}\left(1 - \frac{A_X^2\left(B\right)}{S_X^2\left(B\right)}\right) = T_2^{-1}\left(1 - \left\langle\sigma_z\right\rangle^2\right) \tag{3.56}$$

from (3.54), (3.56), we have:

$$i\Pi_{zz}^{>} = \frac{4T_2^{-1}\left(1-\langle\sigma_z\rangle^2\right)}{\omega^2+4T_2^{-2}\left(1-\langle\sigma_z\rangle^2\right)} \tag{3.57}$$

introduce $T_1^{-1} = 2T_2^{-1}$, which is like the relaxation rate in Bloch equation. Consider a narrow range near $\omega = 0$, notice that when $\omega = 0$, $\langle\sigma_z\rangle = 1$, (3.57) could be rewritten as below:

$$i\Pi_{zz}^{>} = \langle\sigma_z\rangle^2 2\pi\delta(\omega) + \left(1-\langle\sigma_z\rangle^2\right)\frac{2T_1^{-1}}{\omega^2+T_1^{-2}} \tag{3.58}$$

It should be noticed that in the article [5], they have the form in (3.58), which seems right in physical intuition, since the integral over energy $\omega$ will give an identity. However, in my calculation, the (3.56) should be

$$\tilde{\Gamma} \equiv \frac{S_X(B)}{4}\left(1+\frac{A_X^2(B)}{S_X^2(B)}\right) = T_2^{-1}\left(1+\langle\sigma_z\rangle^2\right) \tag{3.59}$$

which results in

$$i\Pi_{zz}^{>} = \langle\sigma_z\rangle^2 2\pi\delta(\omega) + \left(1+\langle\sigma_z\rangle^2\right)\frac{2T_1^{-1}}{\omega^2+T_1^{-2}} \tag{3.60}$$

which is apparently different from the authors' result (3.58), thus a clear explanation still needs further investigation.

Now we are able to see that in a spin-boson perturbative regime, by using Majorana representation, we can evaluate the dissipation of spin dynamics, which is characterized by dephasing rate $T_2^{-1}$ and relaxation rate $T_1^{-a}$ just as Bloch equation. In this process, only first-order self energy are calculated diagrammatically without higher order terms and vertex corrections [12], which simplifies calculation to a large extent.

# Chapter 4

# Application in Kondo effect in quantum dots

In previous chapter, we have seen how Majorana representation could bring calculation simplicity for spin-spin correlators, it's natural to apply this method to Kondo model as well, in which spin correlators are involved [13].

Kondo effect is a temperature dependent conductance phenomena in which a novel electron scattering mechanism is involved - a spin flip interaction between the impurity spin and conduction electrons.

Kondo effect is characterized with Kondo temperature $T_K$, in which a divergence happens and Kondo effect dominates. In low temperature limit $T < T_K$ (strong coupling regime), the conductance is temperature scaling by renormalization group theory, when two leads are symmetric, it reads,

$$G\left(T\right) = G_0 \left(1 - c_1 \left(\frac{T}{T_K}\right)^2\right) \tag{4.1}$$

in which $c_1$ is a constant, $G_0 = 2e^2/\hbar$ is conductance unit. When $T > T_K$ (weak coupling regime), the conductance is

$$G\left(T\right) = G_0 \frac{c_2}{\log^2\left(\frac{T}{T_K}\right)} \tag{4.2}$$

The total Hamiltonian in Kondo model is $H = H_0 + H_K$, with

$$H_0 = \sum_{k,\sigma,\alpha} \epsilon_k c^\dagger_{\alpha,k,\sigma} c_{\alpha,k,\sigma} \tag{4.3}$$

is free Hamiltonian for electrons in the lead, $\alpha$ = left/right represents leads on different side, thus it is symmetric with the same free energy $\epsilon_k$ on either side of the dot. The Kondo Hamiltonian, which describes interaction of conduction electrons with magnetic impurity in the dot, can be written as below:

$$H_K = \frac{1}{4} J \sum_{\alpha} \sum_{\sigma,\sigma',\sigma_1,\sigma_2} \sum_{k_1,k_2} (\vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1\sigma_2}) \left( c^\dagger_{d\sigma} c_{d\sigma'} c^\dagger_{\alpha k_1 \sigma_1} c_{\alpha k_2 \sigma_2} \right) \tag{4.4}$$

in which $\sigma_d$ and $\sigma_{\sigma_1\sigma_2}$ are spin operators for impurity and electron respectively. J is the exchange interaction, in ferromagnetic case $J < 0$, the conductance will keep on increasing when temperature decreases, while $J > 0$ for antiferromagnetic in which conductance decreases when temperature $T \to 0$. We will consider about antiferromagnetic situation. For simplicity, define $c_{0\sigma} = \sum_{k,\alpha} c_{\alpha k \sigma}/\sqrt{2}$ summing over leads and momentum, and we can rewrite (4.4) as:

$$H_K = \frac{1}{4} J \sum_{\sigma,\sigma'} \sum_{\sigma_1,\sigma_2} (\vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1\sigma_2}) \left( c^\dagger_{d\sigma} c_{d\sigma'} c^\dagger_{0\sigma_1} c_{0\sigma_2} \right) \tag{4.5}$$

in order to calculate the conductance we need to calculate T-matrix, which can be derived using equation of motion theory, and gives

$$T(\tau) = -\frac{J}{2} \langle S_z \rangle - \frac{J^2}{4} \sum_{\sigma_1,\sigma_2} \left\langle T_\tau \left( c_{0\sigma_1}(\tau) \vec{\sigma}_{\sigma\sigma_1} \cdot \vec{S}(\tau) c_{0\sigma_2}(\tau)^\dagger \vec{\sigma}_{\sigma_2\sigma} \cdot \vec{S}(0) \right) \right\rangle \tag{4.6}$$

in which second term describes the spin flip process.

In this chapter, we shall see how Majorana representation could be used in Kondo model, both in $B = 0$ and a finite Zeeman field.

## 4.1 Apply Majorana representation in B=0 field

When there is no external magnetic field, the total Hamiltonian is still $H = H_0 + H_K$. From chapter 2 we know that spin operator can be written out by Majorna fermions as $\vec{\sigma} = -\frac{i}{2} \vec{\eta} \times \vec{\eta}$, as we shall see later that in Kondo model, a Majorna fermion cannot scatter into itself, thus we choose to use the identity as $\eta^2 = \frac{1}{2}$, thus we have relations as,

$$\begin{aligned} \vec{S} &= -\frac{i}{2} \vec{\eta} \times \vec{\eta} \\ \vec{S} &= \tau_x \eta, \quad \text{with} \quad \tau_x = -2i\eta_1\eta_2\eta_3 \end{aligned} \tag{4.7}$$

substitute into Kondo Hamiltonian, we have,

$$
\begin{aligned}
H_K =& J\vec{S}_d \sum_{\sigma_1,\sigma_2} c^{\dagger}_{0\sigma_1} \frac{\vec{\sigma}_{\sigma_1\sigma_2}}{2} c_{0\sigma_2} \\
=& -\frac{iJ}{2}\eta_1\eta_2 \left(c^{\dagger}_{0\uparrow}c_{0\uparrow} - c^{\dagger}_{0\downarrow}c_{0\downarrow}\right) - \frac{iJ}{2}\eta_2\eta_3 \left(c^{\dagger}_{0\uparrow}c_{0\downarrow} + c^{\dagger}_{0\downarrow}c_{0\uparrow}\right) + \frac{iJ}{2}\eta_3\eta_1 \left(c^{\dagger}_{0\uparrow}c_{0\downarrow} - c^{\dagger}_{0\downarrow}c_{0\uparrow}\right) \\
=& -\frac{iJ_0}{2} \left(c^{\dagger}_{0\uparrow}c_{0\uparrow} - c^{\dagger}_{0\downarrow}c_{0\downarrow}\right)\eta_1^{\dagger}\eta_2 - \frac{iJ}{2} \left(c^{\dagger}_{0\uparrow}c_{0\downarrow} + c^{\dagger}_{0\downarrow}c_{0\uparrow}\right)\eta_2^{\dagger}\eta_3 - \frac{iJ}{2} \left(c^{\dagger}_{0\uparrow}c_{0\downarrow} - c^{\dagger}_{0\downarrow}c_{0\uparrow}\right)\eta_1^{\dagger}\eta_3
\end{aligned}
\tag{4.8}
$$

in the last step, we make use of the property of $\eta_\alpha = \eta_\alpha^{\dagger}$. We may see that the interaction of conduction electron and impurity is rewritten as electron-Majoarana fermion interactions, this will give a four-leg vertex diagrammatically as in FIGURE 4.1, instead of 2 vertices by pseudo fermion representation, which is of a simpler form.

Now consider the T matrix in (4.6), which is a six fermion correlator in pseudo fermion representation, we shall see in Majorana language it can be written as a four fermion correlator. First remember that spin operators can be decomposed into products of Majorana fermions and a "copy-switching" operator $\tau_x$ as $\sigma_\alpha = \tau_x\eta_\alpha$, with $\tau_x = -i\eta_1\eta_2\eta_3$. Thus we can write spin correlation function as,

$$
\begin{aligned}
\chi\left(\vec{S}(\tau), \vec{S}(0)\right) =& -\left\langle T_\tau\left(\vec{S}(\tau)\vec{S}(0)\right)\right\rangle = -\left\langle T_\tau\left(\tau_x(\tau)\vec{\eta}(\tau)\tau_x(0)\vec{\eta}(0)\right)\right\rangle \\
=& G_{\tau_x}(\tau)G_{\vec{\eta}}(\tau)
\end{aligned}
\tag{4.9}
$$

now the 4 fermion correlator $\chi\left(\vec{S}(\tau), \vec{S}(0)\right)$ is written as product of a 2 fermion correlator $G_{\vec{\eta}}(\tau) = -\left\langle T_\tau\vec{\eta}(\tau)\vec{\eta}(0)\right\rangle$ and $G_{\tau_x}$, which is a sign function as

$$
G_{\tau_x} = -\left\langle T_\tau\tau_x(\tau)\tau_x(0)\right\rangle = -\frac{1}{2}\mathrm{sgn}(\tau) \tag{4.10}
$$

where we used the identity $\tau_x^2 = \frac{1}{2}$ and anticommutation relation of $\tau_x$ as a Majorana fermion. Then we could write the second order spin flip term in T-matrix (4.6) as:

$$
\begin{aligned}
T^{(2)}(\tau) =& -\frac{J^2}{4}\sum_{\sigma_1,\sigma_2}\left\langle T_\tau\left(c_{0\sigma_1}(\tau)\vec{\sigma}_{\sigma\sigma_1}\cdot\vec{S}(\tau)c_{0\sigma_2}(\tau)^{\dagger}\vec{\sigma}_{\sigma_2\sigma}\cdot\vec{S}(0)\right)\right\rangle \\
=& -\frac{J^2}{4}G_{\tau_x}(\tau)\sum_{\sigma_1\sigma_2}\sum_{a,b}\left\langle T_\tau\left(c_{0\sigma_1}(\tau)\sigma^a_{\sigma\sigma_1}\eta_a(\tau)c^{\dagger}_{0\sigma_2}(0)\sigma^b_{\sigma_2\sigma}\eta_b(0)\right)\right\rangle
\end{aligned}
\tag{4.11}
$$

from the second line in (4.11) we can easily see the spin flip term is now a 4 fermion correlator. To be more specific, consider the second order component for spin up $T^{(2)}_{\uparrow}(\tau)$,

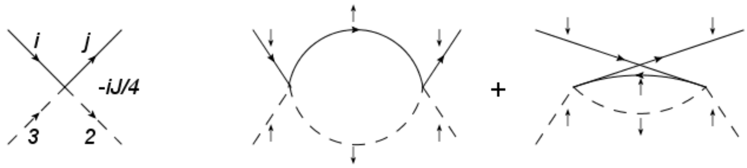


FIGURE 4.1: (*left*) Interaction vertex of Kondo Hamiltonian by Majorana representation as in (4.8), dashed lines for Majorana fermions and solid lines for conduction electrons. (*right*) Kondo Hamiltonian in pseudo fermion representation, dash lines represent pseudo fermions for impurity spin and solid lines for conduction electrons.

which can be written as below

$$\begin{aligned} T_{\uparrow}^{(2)}(\tau) &= -\frac{J^2}{4} G_{\tau_x}(\tau) \left\langle T_\tau \left[ \left( c_\downarrow \eta_1 - i c_\downarrow \eta_2 + c_\uparrow \eta_3 \right)(\tau) \left( c_\downarrow^\dagger \eta_1 + i c_\downarrow^\dagger \eta_2 + c_\uparrow^\dagger \eta_3 \right)(0) \right] \right\rangle \\ &= -\frac{J^2}{4} G_{\tau_x}(\tau) \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} M(\tau) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \end{aligned} \tag{4.12}$$

the first line in (4.12) is because

$$\begin{aligned} &\langle 0 | \sum_{a,\sigma_1} c_{0\sigma_1}(\tau) \sigma^a_{\sigma_1\uparrow} \eta_a(\tau) = \langle 0 | \left( c_\downarrow \eta_1 - i c_\downarrow \eta_2 + c_\uparrow \eta_3 \right)(\tau) \\ &\sum_{b,\sigma_2} c^\dagger_{0\sigma_2}(0) \sigma^b_{\sigma_2\uparrow} \eta_b(0) |0\rangle = \sum_{a,\sigma_2} \left( \sigma^b_{\sigma_2\uparrow} \right)^T \eta_b(0) c^\dagger_{0\sigma_2}(0) |0\rangle = \left( c_\downarrow^\dagger \eta_1 + i c_\downarrow^\dagger \eta_2 + c_\uparrow^\dagger \eta_3 \right)(0) |0\rangle \end{aligned} \tag{4.13}$$

$M(\tau)$ is a matrix with 9 four-fermion correlator elements

$$M(\tau) = \begin{pmatrix} \left\langle c_\downarrow \eta_1 c_\downarrow^\dagger \eta_1 \right\rangle & i \left\langle c_\downarrow \eta_1 c_\downarrow^\dagger \eta_2 \right\rangle & \left\langle c_\downarrow \eta_1 c_\uparrow^\dagger \eta_3 \right\rangle \\ -i \left\langle c_\downarrow \eta_2 c_\downarrow^\dagger \eta_1 \right\rangle & \left\langle c_\downarrow \eta_2 c_\downarrow^\dagger \eta_2 \right\rangle & -i \left\langle c_\downarrow \eta_2 c_\uparrow^\dagger \eta_3 \right\rangle \\ \left\langle c_\uparrow \eta_3 c_\downarrow^\dagger \eta_1 \right\rangle & i \left\langle c_\uparrow \eta_3 c_\downarrow^\dagger \eta_2 \right\rangle & \left\langle c_\uparrow \eta_3 c_\uparrow^\dagger \eta_3 \right\rangle \end{pmatrix} \tag{4.14}$$

from which we can see the second order spin flip term can be written in terms of interaction between impurity Majorana fermions and conduction electrons, if we draw Feynman diagram as in FIGURE 4.2, the shaded box represents interaction part, e.g.the lowest order contribution of perturbation would be a single bubble $\langle \sigma_1 \eta_i \sigma_2 \eta_j \rangle \delta_{12} \delta_{ij}$ (first term on right hand side in FIGURE 4.2). If we take ramdom phase approximation (RPA), total correlator can be expanded as a series of bubbles of all orders. For each bubble it reads,

$$\Pi_{0\eta}(\tau) = G_{0c}(\tau) G_{0\eta}(\tau) \tag{4.15}$$

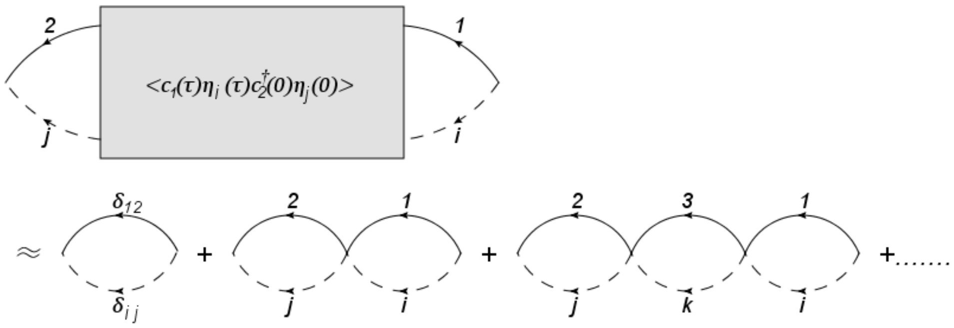


FIGURE 4.2: Second order spin flip term $T_{\uparrow}^{(2)}$ can be written as interaction of conduction electrons (solid lines) and impurity Majorana fermions (dashed lines), which in RPA is expanded as series of polarized bubbles.

since Majorana fermions are of zero free energy, while conduction electrons with $\epsilon_k$ free energy, the propagators for conduction electron and Majorana fermion can be written as below,

$$G_{0c}\left(i\omega\right) = \frac{1}{i\omega}, \quad G_{0\eta}\left(i\omega\right) = \frac{1}{i\omega + \epsilon_k} \tag{4.16}$$

taking Matsubara sum of $\Pi_{0\eta}(\tau)$, we can calculate,

$$\begin{aligned}
\Pi_{0\eta}(i\omega_n) =& \sum_k \sum_{ik_n} G_{0\eta}(i\omega_n - ik_n) G_{0c}(ik_n - \epsilon_k) \\
=& \sum_k \sum_{ik_n} \left[ n_F(\epsilon_k) G_{o\eta}(i\omega_n - \epsilon_k) - n_F(i\omega_n) G_{0c}(i\omega_n - \epsilon_k) \right] \\
=& -\frac{1}{2} \sum_k \frac{1 - 2n_F(\epsilon_k)}{i\omega_n - \epsilon_k} \\
=& -\frac{1}{2} \sum_k \frac{\tanh(\frac{\epsilon_k}{2T})}{i\omega_n - \epsilon_k} \rightarrow -\frac{1}{2} \sum_k \frac{\mathrm{sgn}(\epsilon_k)}{i\omega_n - \epsilon_k}
\end{aligned} \tag{4.17}$$

here we used the fact that $\omega_n$ is bosonic Matsubara frequency, in the last line $\tanh(\frac{\epsilon_k}{2T})$ tends to a sign function in low temperature limit. Consider a conduction band with half bandwidth=D and density of states $\nu_F = 1/2D$, we can write retarded part of (4.17) in real and imaginary parts as below,

$$\begin{aligned}
\Pi^R_{0\eta}(\omega) =& -\frac{1}{2}\int_{-D}^{+D} \mathrm{d}\epsilon_k \nu_F(\epsilon_k)\Theta(D^2-\omega^2)\mathrm{sgn}(\epsilon_k)(\frac{1}{\omega-\epsilon_k} - i\pi\delta(\omega-\epsilon_k)) \\
=& -\frac{\nu_F}{2}\int_{-D}^{+D} \mathrm{d}\epsilon_k \Theta(D^2-\epsilon_k^2)\frac{\mathrm{sgn}(\epsilon_k)}{\omega-\epsilon_k} + \frac{i\pi\nu_F}{2}\int_{-D}^{+D}\mathrm{d}\epsilon_k\Theta(D^2-\epsilon_k^2)\delta(\omega-\epsilon_k) \\
=& -\frac{\nu_F}{2}(\int_{-D}^{0} + \int_{0}^{\omega-\eta} + \int_{\omega+\eta}^{D})\mathrm{d}\epsilon_k\frac{\mathrm{sgn}(\epsilon_k)}{\omega-\epsilon_k} + \frac{i\pi\nu_F}{2}\int_{-D}^{+D}\mathrm{d}\epsilon_k\Theta(D^2-\epsilon_k^2)\mathrm{sgn}(\epsilon_k)\delta(\omega-\epsilon_k) \\
=& \frac{\nu_F}{2}\log\left|\frac{\omega^2-D^2}{\omega^2}\right| + \frac{i\pi\nu_F}{2}\mathrm{sgn}(\omega)\Theta(D^2-\omega^2)
\end{aligned} \tag{4.18}$$

By observation from FIGURE 4.2 and equation (4.14), we may find 3 diagonal terms in $M(\tau)$ are just single bubbles which can be expressed as $\Pi_{0\eta}$, while 6 off-diagonal terms are two bubbles connected by a four leg vertex with vertex strength as $J/2$.

$$J\left[\Pi_{0\eta} * \Pi_{0\eta}\right](\tau) = J\int_0^\beta d\tau_1 \Pi_{0\eta}(\tau-\tau_1)\Pi_{0\eta}(\tau_1) \tag{4.19}$$

thus first two terms of RPA series for $T^{(2)}_\uparrow(\tau)$ would be

$$T^{(2)}_\uparrow(\tau) = -\frac{J^2}{4}G_{\tau_x}(\tau)\left(3\Pi_{0\eta} + 6\frac{J}{2}\Pi_{0\eta} * \Pi_{0\eta}\right)(\tau) \tag{4.20}$$

Now we need to calculate the perturbation of all orders in RPA series. Since interaction process in off-diagonal terms has a coefficient 2 times larger than diagonal ones. We may characterize $n$-th order interaction into 2 categories, in first kind of process, Majorana fermions with same indices go in and out with a coefficient of $a_n$, while $b_n$ for Majorana fermion changes its indice, as shown in FIGURE 4.3, from which we can find the recursion rule as:

$$a_n = 2b_{n-1}, \quad b_n = a_{n-1} + b_{n-1} \tag{4.21}$$

with initial value as $a_0 = 1$, $a_1 = 0$ and $b_0 = 0$, $b_1 = 1$, it's not difficult to find $a_n + b_n = 2^n$. Now T-matrix $T^{(2)}_\uparrow$ can be written as below,

$$\begin{aligned}
T^{(2)}_\uparrow(\tau) =& -\frac{J^2}{4}G_{\tau_x}(\tau)\left(3\Pi_{0\eta} + \frac{J}{4}6\Pi_{0\eta} * \Pi_{0\eta} + \cdots\right)(\tau) \\
=& -\frac{3J^2}{4}G_{\tau_x}(\tau)\sum_{n=0}(a_n + 2b_n)\left(\frac{J}{2}\right)^n \underbrace{\left[\Pi_{0\eta} * \cdots * \Pi_{0\eta}\right]}_{(n+1)\text{terms}}(\tau) \\
=& -\frac{3J^2}{4}G_{\tau_x}(\tau)\Pi_\eta(\tau)
\end{aligned} \tag{4.22}$$

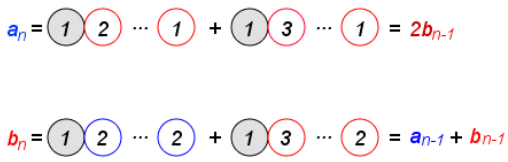


FIGURE 4.3: Two different $n$-th order interaction processes with coefficient $a_n$ and $b_n$, $\alpha = 1, 2, 3$ stand for Majorana fermion indice $\eta_\alpha$. Blue color stands for Majorana fermion with same index coming in and going out, red color means Majorana fermions change index after the process.

in which $\Pi_\eta(\tau)$ is derived by the recursion relation as,

$$\Pi_\eta(\tau) = \frac{\Pi_{0\eta}}{1 - J\Pi_{0\eta}} \tag{4.23}$$

Now we can summing up Matsubara frequencies for fermions to calculate second order component of T matrix as below,

$$\begin{aligned}
T_\uparrow^{(2)}(i\omega_n) =& -\frac{3J^2}{16}\frac{1}{\beta}\sum_{i\nu_1} G_{\tau_x}(i\nu_1)\,\Pi_\eta(i\omega_n - i\nu_1)\,e^{i\nu_1\tau} \\
=& -\frac{3J^2}{4}\frac{1}{2\pi i}\int d\tau \oint_{C_1+C_2} dz \Pi_\eta(i\omega_n - z)\, n_F(z)\, e^{z\tau} \\
=& -\frac{3J^2}{8}\frac{1}{2\pi i}\int d\tau \int_{-\infty}^{\infty} d\epsilon\,(\Pi_\eta(i\omega_n - \epsilon + i\eta) - \Pi_\eta(i\omega_n - \epsilon - i\eta))\,e^{\epsilon\tau} \\
=& -\frac{3J^2}{8\pi}\int d\tau \int_{-\infty}^{\infty} d\epsilon 2\Pi''_\eta(i\omega_n - \epsilon)\, n_F(\epsilon)\, e^{\epsilon\tau} \\
=& -\frac{3J^2}{8\pi}\int d\tau \int_{-\infty}^{\infty} d\omega_2\Pi''_\eta(\omega_2)\, n_F(-\omega_2 + i\omega_n)\, e^{(\omega_2 - i\omega_n)\tau} \\
=& \frac{3J^2}{8\pi}\int d\tau \int_{-\infty}^{\infty} d\omega_2\Pi''_\eta(\omega_2)\, n_B(-\omega_2)\, e^{(\omega_2 - i\omega_n)\tau} \\
=& \frac{3J^2}{8\pi}\int_{-\infty}^{\infty} d\omega_2\Pi''_\eta(\omega_2)\int d\tau n_B(-\omega_2)\, e^{(\omega_2 - i\omega_n)\tau} \\
=& \frac{3J^2}{8\pi}\int_{-\infty}^{\infty} d\omega_2\Pi''_\eta(\omega_2)\,\frac{1 + 2n_B(-\omega_2)}{\omega_2 - i\omega_n}
\end{aligned} \tag{4.24}$$

in which $\omega_n$ and $\nu_n$ are both fermionic Matsubara frequencies, $\Pi''_\eta(\omega_2)$ stands for the imaginary part of $\Pi_\eta(\omega_2)$. And it is easy to get the imaginary part of T-matrix $T_\uparrow^{(2)''}(\omega)$ from (4.24) as below

$$\begin{aligned}
T_\uparrow^{(2)''}(\omega) =& \frac{3J^2}{8\pi}\int_{-\infty}^{\infty} d\omega_2\Pi''_\eta(\omega_2)\,(-\coth(\frac{\beta\omega}{2}))\pi\delta(\omega) \\
=& -\frac{3J^2}{8}\Pi''_\eta(\omega)\coth\left(\frac{\beta\omega}{2}\right)
\end{aligned} \tag{4.25}$$

Still consider a conductance band with density of states (DOS) $\nu_F = 1/2D$ and half-bandwidth as D, using (4.18) and (4.25), we can solve the final result for imaginary part of second-order T-matrix as:

$$\begin{aligned}-\pi\nu_F T_{\uparrow}^{(2)\prime\prime}(\omega) =& -\frac{3\pi\nu_F J^2}{8}\Pi_\eta''(\omega)\coth(\frac{\beta\omega}{2})\\ =&\frac{3\pi^2\nu_F^2 J^2}{8}\frac{\tanh(\frac{\beta\omega}{2})\Theta(D^2-\omega^2)/2}{(1-\frac{\nu_F J}{2}\log(\left|\frac{\omega^2-D^2}{\omega^2}\right|))^2+\frac{\pi^2\rho_0^2 J^2}{4}\left[\tanh(\frac{\beta\omega}{2})\Theta(D^2-\omega^2)\right]^2}\coth(\frac{\beta\omega}{2})\\ =&\frac{3\pi^2\nu_F^2 J^2}{16}\frac{\Theta(D^2-\omega^2)}{(1-\frac{\nu_F J}{2}\log(\left|\frac{\omega^2-D^2}{\omega^2}\right|))^2+\left[\frac{\pi\nu_F J}{2}\tanh(\frac{\beta\omega}{2})\right]^2}\end{aligned} \tag{4.26}$$

if we consider a high cut-off $\omega \ll D$, than the pole of equation (4.26) would be,

$$1-\frac{\nu_F J}{2}\log\frac{D^2}{\omega^2} = 0 \Longrightarrow \omega = De^{-\frac{1}{\nu_F J}} \equiv T_K \tag{4.27}$$

in which $T_K$ is Kondo temperature, which is a scaling invariant for specified $D$ and $J$ (in other words, the system posses universality). We can also write scaling equation in order $J^2$ as,

$$\frac{\mathrm{d}(\nu_F J)}{\mathrm{d}(\log D)} = -\nu_F^2 J^2 \tag{4.28}$$

which is the same as the result by Anderson's poor man's approach [16]. Now consider a situation when $T_K \ll \omega, T \ll D$, in this case, the energy spectrum in (4.26) can be written as

$$\begin{aligned}-\pi\rho_0 T_{\uparrow}^{(2)\prime\prime}(\omega) =&\frac{3\pi^2\nu_F^2 J^2}{16}\frac{1}{(1-\frac{\nu_F J}{2}\log\frac{D^2}{\omega^2})^2}\\ =&\frac{3\pi^2}{16}\frac{1}{(\log\frac{D}{T_K}-\log\frac{D}{\sqrt{\omega^2+T^2}})^2} = \frac{3\pi^2}{16}\frac{1}{(\log\frac{\sqrt{\omega^2+T^2}}{T_K})^2}\end{aligned} \tag{4.29}$$

in which we used the relation $\nu_F J = 1/\log\frac{D}{T_K}$, we may find result in (4.29) leads to the well known perturbative result for conductance $G$ in (4.2).

The result for T-matrix when $\omega > T_K$ is shown in FIGURE 4.4, when $T$ is small, there is a divergence point at $\omega/T_K = 1$. However, when $T$ increases, the second term on denominator of (4.26) starts to dominate and the divergence point moves left, as shown in FIGURE 4.5, when $T$ is finite, the divergence point will disappear finally.

We can also compare the above results with Numerical Renormalization Group method and lowest order Renormalization Group method, as shown in FIGURE 4.6 [13]. we can

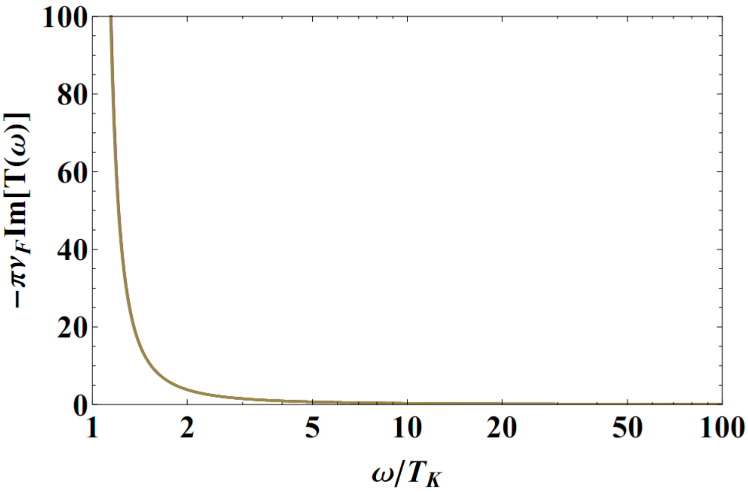


FIGURE 4.4: T-matrix $-\pi\nu_F T_{\uparrow}^{(2)\prime\prime}(\omega)$ for $\omega > T_K$ in low temperature, there is a divergence point at $\omega = T_K$.

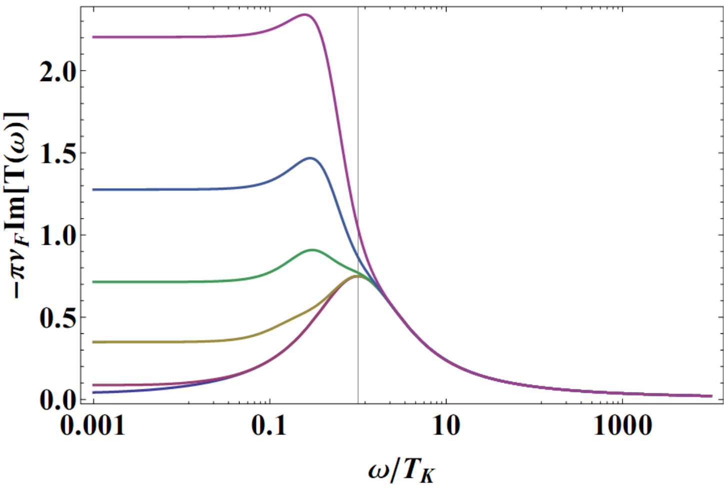


FIGURE 4.5: T-matrix $-\pi\nu_F T_{\uparrow}^{(2)\prime\prime}(\omega)$ in finite temperature, when $T$ increases, the left part when $\omega < T_K$ is lifted and divergence point disappears eventually.

observe that when $T > T_K$, Majorana representation technique has a better fit with NRG result compared to lowest order renormalization group method.

## 4.2 Apply Majorana representation in finite magnetic field

In previous section we have discussed Kondo model without external magnetic field, when a finite B field is present, we can study its effect on Kondo resonance. Introducing Zeeman Hamiltonian $H_Z$, remember that we can write Majorana fermions as $\eta_1 =$

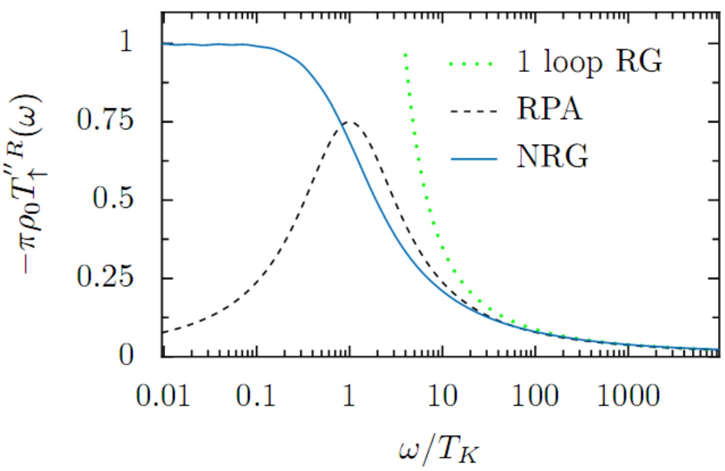


FIGURE 4.6: T-matrix $-\pi\rho_0 T^{(2)''}_{\uparrow}(\omega)$ with different calculation methods, blue line for numerical renormalization group (NRG), green dotted line for one loop renormalization group, and black dashed line for RPA series using Majorna representation.

$\frac{1}{\sqrt{2}}(f+f^\dagger)$ and $\eta_2 = \frac{i}{\sqrt{2}}\left(f-f^\dagger\right)$, then $H_Z$ is

$$H_Z = BS_z = -iB\eta_1\eta_2 = -\frac{i}{2}B\left(f+f^\dagger\right)i\left(f-f^\dagger\right) = Bf^\dagger f - \frac{B}{2} \tag{4.30}$$

we can see Zeeman Hamiltonian is now related to the ordinary fermion $f$. Using same method, Kondo Hamiltonian $H_K$ in (4.5) is now,

$$\begin{aligned} H_K =& \frac{J}{4}\left(c^\dagger_{0\uparrow}c_{0\uparrow} - c^\dagger_{0\downarrow}c_{0\downarrow}\right)\left(2f^\dagger f - 1\right) + \frac{J}{4}\left(c^\dagger_{0\uparrow}c_{0\downarrow} + c^\dagger_{0\downarrow}c_{0\uparrow}\right)\left(f-f^\dagger\right)\eta_3 \\ &- \frac{J}{4}\left(c^\dagger_{0\uparrow}c_{0\downarrow} - c^\dagger_{0\downarrow}c_{0\uparrow}\right)\left(f+f^\dagger\right)\eta_3 \\ =& -\frac{J}{2}\left(c^\dagger_{0\uparrow}c_{0\downarrow}f^\dagger\eta_3 - c^\dagger_{0\downarrow}c_{0\uparrow}f\eta_3\right) + \frac{J}{2}\left(c^\dagger_{0\uparrow}c_{0\uparrow} - c^\dagger_{0\downarrow}c_{0\downarrow}\right)f^\dagger f - \frac{J}{4}\left(c^\dagger_{0\uparrow}c_{0\uparrow} - c^\dagger_{0\downarrow}c_{0\downarrow}\right) \end{aligned} \tag{4.31}$$

in which the last term describes the effect of magnetic field. We can also write second order T matrix for spin up $T^{(2)}_{\uparrow}$ in Majorana language, first consider $M(\tau)$ is now

$$M(\tau) = \begin{pmatrix} \frac{1}{2}\left\langle c_\downarrow(f+f^\dagger)c^\dagger_\downarrow(f+f^\dagger)\right\rangle & \frac{1}{2}\left\langle c_\downarrow(f+f^\dagger)c^\dagger_\downarrow(f^\dagger-f)\right\rangle & \frac{1}{\sqrt{2}}\left\langle c_\downarrow(f+f^\dagger)c^\dagger_\uparrow\eta_3\right\rangle \\ \frac{1}{2}\left\langle c_\downarrow(f-f^\dagger)c^\dagger_\downarrow(f+f^\dagger)\right\rangle & -\frac{1}{2}\left\langle c_\downarrow(f-f^\dagger)c^\dagger_\downarrow(f-f^\dagger)\right\rangle & \frac{1}{\sqrt{2}}\left\langle c_\downarrow(f-f^\dagger)c^\dagger_\uparrow\eta_3\right\rangle \\ \frac{1}{\sqrt{2}}\left\langle c_\uparrow\eta_3 c^\dagger_\downarrow(f+f^\dagger)\right\rangle & \frac{1}{\sqrt{2}}\left\langle c_\uparrow\eta_3 c^\dagger_\downarrow(f^\dagger-f)\right\rangle & \left\langle c_\uparrow\eta_3 c^\dagger_\uparrow\eta_3\right\rangle \end{pmatrix} \tag{4.32}$$

substitute (4.32) into (4.12) and sum up nine elements in $M(\tau)$, we have

$$T^{(2)}_{\uparrow}(\tau) = -\frac{J^2}{4} G_{\tau_x}(\tau)\,(2\left\langle c_{\downarrow} f c^{\dagger}_{\downarrow} f^{\dagger}\right\rangle + \sqrt{2}\left\langle c_{\downarrow} f c^{\dagger}_{\uparrow}\eta_3\right\rangle + \sqrt{2}\left\langle c_{\downarrow}\eta_3 c^{\dagger}_{\uparrow} f^{\dagger}\right\rangle + \left\langle c_{\uparrow}\eta_3 c^{\dagger}_{\uparrow}\eta_3\right\rangle) \tag{4.33}$$

from which we can find there are 4 interaction mechanism, each can be expanded as series of polarized bubble in RPA as in FIGURE 4.7, which is composed of two type of pair bubbles, $\Pi_{0\eta}(\omega)$ and $\Pi_{0f}(\omega)$, since we have,

$$G_{0f}(i\omega_n) = \frac{1}{i\omega_n - B}, \quad G_{0c}(i\omega_n) = \frac{1}{i\omega_n - \epsilon_k} \tag{4.34}$$

taking Matsubara sum, just as in (4.17),

$$\begin{aligned}
\Pi_{0f}(i\omega_n) =& \sum_k \sum_{ip_n} \frac{1}{ip_n - \epsilon_k} \frac{1}{i\omega_n - ip_n - B} = -\sum_k (-\frac{n_F(\epsilon_k)}{i\omega_n - B - \epsilon_k} + \frac{n_F(i\omega_n - B)}{i\omega_n - B - \epsilon_k}) \\
=& -\sum_k \frac{1 - n_F(B) - n_F(\epsilon_k)}{i\omega_n - B - \epsilon_k} = -\frac{1}{2}\sum_k \frac{\tanh\frac{\beta B}{2} + \tanh\frac{\beta\epsilon_k}{2}}{i\omega_n - B - \epsilon_k} \\
\to& \sum_k \frac{1}{i\omega_n - B - \epsilon_k}(\mathrm{sgn}(B) + \mathrm{sgn}(\epsilon_k)) \quad (T \to 0)
\end{aligned} \tag{4.35}$$

in low temperature and finite magnetic field limit ($\omega, B \ll D$), we can calculate the real and imaginary parts of $\Pi^R_{0f}(\omega)$ as in (4.18),

$$\begin{aligned}
\Pi^R_{0f}(\omega) =& -\frac{1}{2}\int_D^D \mathrm{d}\epsilon_k \nu_F \Theta(D^2 - \omega^2)(\mathrm{sgn}(B) + \mathrm{sgn}(\epsilon_k))(\frac{1}{\omega - B - \epsilon_k} - i\pi\delta(\omega - B - \epsilon_k)) \\
=& -\frac{\nu_F}{2}(\int_{-D}^{0} + \int_0^{\omega - B - \eta} + \int_{\omega - B + \eta}^{D})\mathrm{d}\epsilon_k(\frac{\mathrm{sgn}(B)}{\omega - B - \epsilon_k} + \frac{\mathrm{sgn}(\epsilon_k)}{\omega - B - \epsilon_k}) \\
&+ \frac{\pi\nu_F}{2}(\mathrm{sgn}(B) + \mathrm{sgn}(\epsilon_k))\delta(\omega - B - \epsilon_k) \\
=& -\nu_F(\log|\omega - B| - \log|\omega - B - D|) + \frac{i\pi\nu_F}{2}(\mathrm{sgn}(B) + \mathrm{sgn}(\omega - B)) \\
=& \nu_F \log\left|\frac{\omega - D - B}{\omega - B}\right| + i\pi\nu_F\Theta(\omega - B)\Theta(B)
\end{aligned} \tag{4.36}$$

Now denoting the process when $f$ fermion (or $\eta$ fermion) coming in and going out with a coefficient $A_n$, the process when $f$ fermion and $\eta$ fermion on two ends with a coefficient $B_n$, keep in mind that $\eta$ cannot scatter into itself, we can write following

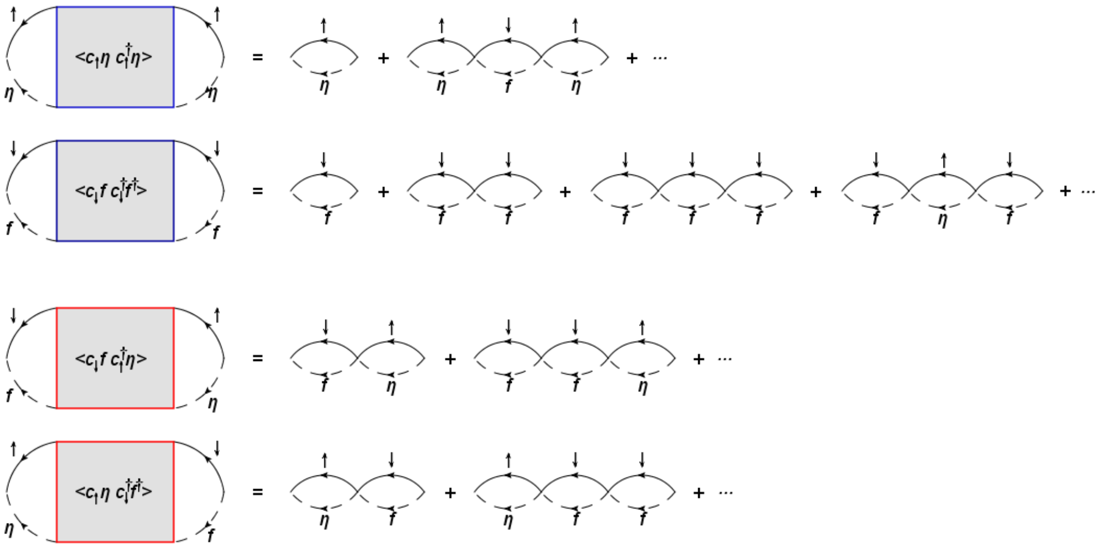


FIGURE 4.7: RPA for different interaction processes in Majorana representation (4.31) under a finite B field, dashed line for Majorana fermion $\eta_3$ and ordinary fermion $f$, solid line for conduction electrons. Blue bordered box stands for same kind of fermion on both sides, red bordered box stands for $\eta$ and $f$ fermion on each side.

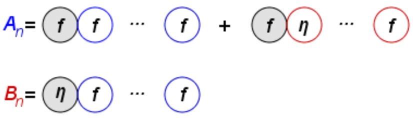


FIGURE 4.8: Different combination choices in four processes of RPA series in FIGURE 4.7. Blue color stands for same kind of fermion on both sides, while red color stands for $\eta$ and $f$ fermion on each side.

relations by observing RPA series in FIGURE 4.7.

$$\begin{aligned}
\left\langle c_\uparrow \eta c_\uparrow^\dagger \eta \right\rangle &= \Pi_{0\eta} + 2(\frac{J\Pi_{0\eta}}{2}) \sum_{n=0}^{+\infty} A_n (\frac{J}{2})^n \\
\left\langle c_\uparrow \eta c_\downarrow^\dagger f^\dagger \right\rangle &= \sum_{n=0}^{\infty} B_n (\frac{J}{2})^n \\
\left\langle c_\downarrow f c_\uparrow^\dagger \eta \right\rangle &= \sum_{n=0}^{\infty} B_n (\frac{J}{2})^n \\
\left\langle c_\downarrow f c_\downarrow^\dagger f^\dagger \right\rangle &= \sum_{n=0}^{\infty} A_n (\frac{J}{2})^n
\end{aligned} \tag{4.37}$$

now we need to calculate the coefficient $A_n$ and $B_n$, from FIGURE 4.8 we have the recursion rule as,

$$\begin{aligned}
A_n &= \Pi_{0f}(A_{n-1} + \sqrt{2} B_{n-1}) \\
B_n &= \sqrt{2}\Pi_{0\eta} A_{n-1}
\end{aligned} \tag{4.38}$$

with $A_0 = \Pi_{0f}$ and $B_0 = 0$, write in a compact form as below

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \begin{pmatrix} \Pi_{0f} & \sqrt{2}\Pi_{0f} \\ \sqrt{2}\Pi_{0\eta} & 0 \end{pmatrix} \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} = \begin{pmatrix} \Pi_{0f} & \sqrt{2}\Pi_{0f} \\ \sqrt{2}\Pi_{0\eta} & 0 \end{pmatrix}^n \begin{pmatrix} \Pi_{0f} \\ 0 \end{pmatrix} \tag{4.39}$$

from which we can solve for $A_n$ and $B_n$ as,

$$\begin{aligned} A_n =& \frac{2^{-1-n}\Pi_{0f}\left(-\sqrt{\Pi_{0f}} + \sqrt{\Pi_{0f} + 8\Pi_{0\eta}}\right)\left(\Pi_{0f} - \sqrt{\Pi_{0f}}\sqrt{\Pi_{0f} + 8\Pi_{0\eta}}\right)^n}{\sqrt{\Pi_{0f} + 8\Pi_{0\eta}}} \\ &+ \frac{2^{-1-n}\Pi_{0f}\left(\sqrt{\Pi_{0f}} + \sqrt{\Pi_{0f} + 8\Pi_{0\eta}}\right)\left(\Pi_{0f} + \sqrt{\Pi_{0f}}\sqrt{\Pi_{0f} + 8\Pi_{0\eta}}\right)^n}{\sqrt{\Pi_{0f} + 8\Pi_{0\eta}}} \\ B_n =& - \frac{2^{\frac{1}{2}-n}\sqrt{\Pi_{0f}}\Pi_{0\eta}\left(\left(\Pi_{0f} - \sqrt{\Pi_{0f}}\sqrt{\Pi_{0f} + 8\Pi_{0\eta}}\right)^n - \left(\Pi_{0f} + \sqrt{\Pi_{0f}}\sqrt{\Pi_{0f} + 8\Pi_{0\eta}}\right)^n\right)}{\sqrt{\Pi_{0f} + 8\Pi_{0\eta}}} \end{aligned} \tag{4.40}$$

Although the results seem annoying, it turns out that when summing up contributions of four processes in (4.37), the total perturbed bubble $\Pi(\omega)$, which is what we want to investigate, has a relatively simple form as

$$\begin{aligned} \Pi(\omega) =& \Pi_{0\eta} + 2\sum_{n=0}^{\infty}(\frac{J}{2})^n \left[\left(1 + (\frac{J\Pi_{0\eta}(\omega)}{2})^2\right) A_n + \sqrt{2}B_n\right] \\ =& \frac{\Pi_{0\eta} + 2\Pi_{0f} + \frac{3}{2}J\Pi_{0f}\Pi_{0\eta}}{1 - \frac{J}{2}\Pi_{0f} - \frac{J^2}{2}\Pi_{0f}\Pi 0\eta} \end{aligned} \tag{4.41}$$

we should notice that from (4.18) and (4.36), when magnetic field goes to zero, with low temperature and high bandwidth, $\Pi_{0\eta} \approx \Pi_{0f}$, and (4.41) will be,

$$\Pi(\omega) = \frac{3\Pi_{0\eta} + \frac{3}{2}J\Pi_{0\eta}^2}{1 - \frac{J}{2}\Pi_{0\eta} - \frac{J^2}{2}\Pi_{\eta}^2} = \frac{3\Pi_{0\eta}}{1 - J\Pi_{0\eta}} \tag{4.42}$$

which is exactly the same as (4.23) that we have already calculated in zero magnetic field case. Substitute (4.41) into (4.33), we finally have the second order T-matrix as,

$$-\pi\nu_F T_{\uparrow}^{(2)\prime\prime}(\omega) = \frac{\pi\nu_F J^2}{8}\mathrm{sgn}(\omega)\mathrm{Im}\left(\frac{\Pi_{0\eta} + 2\Pi_{0f} + \frac{3}{2}J\Pi_{0f}\Pi_{0\eta}}{1 - \frac{J}{2}\Pi_{0f} - \frac{J^2}{2}\Pi_{0f}\Pi 0\eta}\right) \tag{4.43}$$

from which we can plot the spectrum when $B = 5000T_K$ as in FIGURE 4.9. When frequency $\omega$ goes to infinity, it was suggested in [17] that such asymptotes exist:

$$-\pi\nu_F T_{\uparrow}^{(2)\prime\prime}(\omega) \approx \pi^2 \frac{3 \mp 2\sigma M}{16\log^2\left|\frac{\omega}{T_K}\right|}, \quad \omega \to \pm\infty \tag{4.44}$$

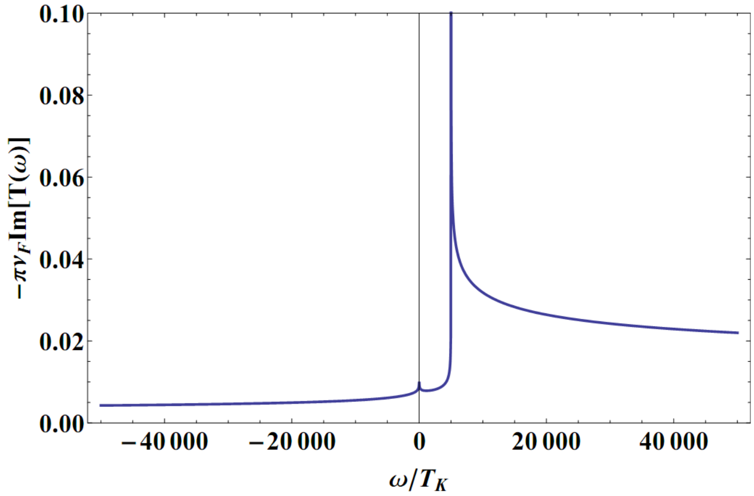


FIGURE 4.9: Second order T-matrix $-\pi\nu_F T_\uparrow^{(2)\prime\prime}(\omega)$ calculated by RPA in Majorana representation,with a finite magnetic field $B = 5000T_K$. Kondo peak at $\omega = B$ and asymptote at $\omega \to \pm\infty$ (4.45) can be observed.

in which $M = 2\langle S_z \rangle$ is the magnetization of impurity spin renormalized to 1. From (4.44) we could easily get following limits:

$$\begin{aligned} -\pi\nu_F T_\uparrow^{(2)\prime\prime}(\omega) &\approx \pi^2 \frac{5}{16\log^2\left|\frac{\omega}{T_K}\right|}, \quad \omega \to +\infty \\ -\pi\nu_F T_\uparrow^{(2)\prime\prime}(\omega) &\approx \pi^2 \frac{1}{16\log^2\left|\frac{\omega}{T_K}\right|}, \quad \omega \to -\infty \end{aligned} \tag{4.45}$$

these asymptotes can be easily verified in FIGURE 4.9. However we may also find a peak when $\omega \to 0$, this divergence point is given by $\Pi_{0\eta}(\omega)$ in (4.18), which is spurious since when $\omega \approx 0$, there should be an asymptote [17] as,

$$-\pi\nu_F T_\uparrow^{(2)\prime\prime}(\omega = 0) \approx \pi^2 \frac{1}{16\log^2\left|\frac{\omega}{T_K}\right|} \tag{4.46}$$

this spurious peak can be flattened when $B$ increases, which is shown in FIGURE 4.10.

We may also compare the above spectral function with the result by perturbative renormalization group scheme [17], in the limit of $\omega \to \pm\infty$, two curves agree with each other perfectly according to the asymptotes (4.45), in low temperature limit, the RPA result is not fully equivalent to perturbative RG scheme, which may be a consequence of non-RPA contributions in the renormalization group method.

In this chapter, we followed the track of [13] and applied Majorana representation in Kondel model. In the limit of $|\omega| \ll D$, when magnetic field is zero, we could reproduce pool man's scaling result successfully. In finite magnetic field, the spectral function calculated agrees with the result by perturbative renormalization group method in the

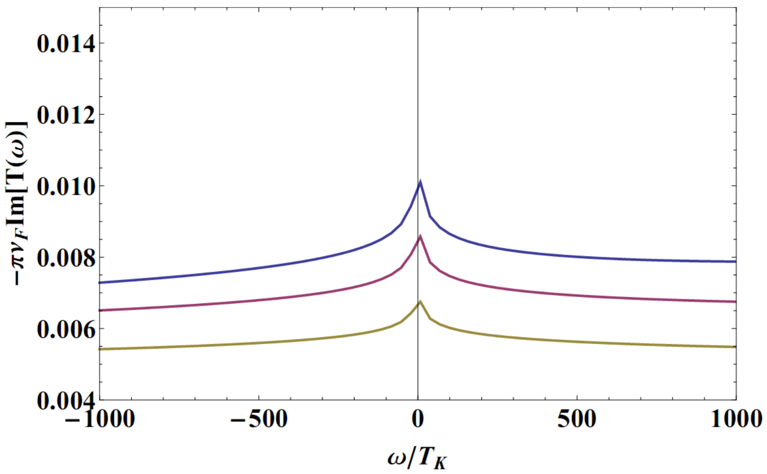


FIGURE 4.10: When B increases, $B = 5000T_K$, $10000T_K$ and $30000T_K$, the spurious peak of $-\pi\nu_F T_{\uparrow}^{(2)\prime\prime}(\omega = 0)$ in FIGURE 4.9 is flattened.

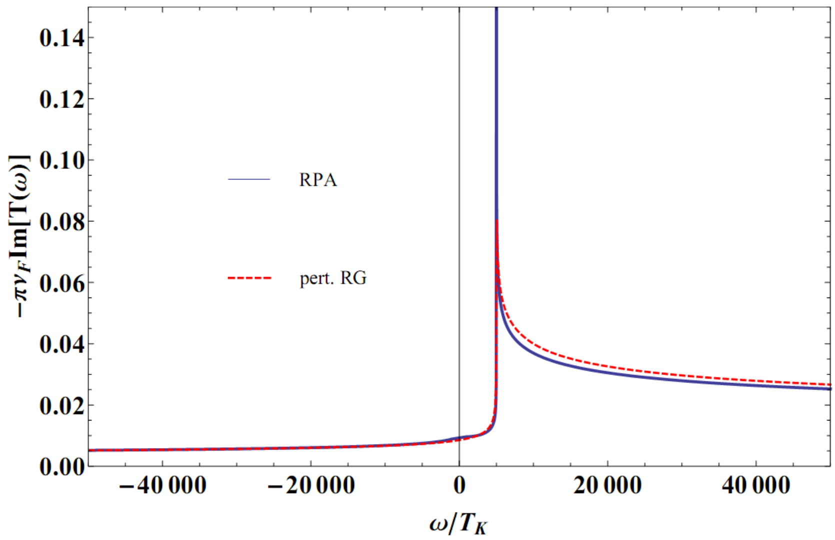


FIGURE 4.11: Solid blue line is for spectrum calculated by RPA in Majorana language, dashed red line is the result by perturbative renormalization group method [17]. Two curves agree with each other in large frequencies.

limit of $B \ll \omega \ll D$ and $-D \ll \omega \ll -B$, however a spurious peak would occur on $\omega \to 0$ limit.

It should be noticed that there are a few places of typos in the original article [13]. The last factor in (36) should be $\mathrm{Im}\frac{\Pi^R_{0\eta}(\omega)}{1-J\Pi^R_{0\eta}(\omega)}$; the second term in (37) should be $i\pi\frac{\rho_0}{2}\mathrm{Sign}(\omega)\Theta(D^2-\omega^2)$, which follows a $(\rho_0 J)^2\Theta(D^2-\omega^2)$ term on the nominator in (38). In (41), the third line should come with a minus sign. The final results are not effected.

# Chapter 5

# Summary

In this thesis we discussed about Majorana representation for spin operators and its application in spin correlator calculations.

Since there exist some difficulties in pseudo fermion representation, e.g. vertex correction and unavailability of Wick's theorem, Majorana representation was constructed for spin operators. By introducing a new "copy-switching" operator $\tau_x$, we found that the order of spin correlator can be lowered by a factor of 2 compared to pseudo fermion representation, which can avoid cumbersome vertex corrections. It was also shown that by writing correlator of spin operator in Majorana language, Wick's theorem can still be used.

Next we gave an example of how this technique can be used in spin-boson interaction model. With Keldysh technique and thermal equilibrium condition, spin susceptibilities $\Pi_{xx}$ and $\Pi_{zz}$ were calculated, which are just self energies in Majorana language instead of pair bubbles, and the results suggested relaxation rate and dephasing rate as described by classic Bloch equation.

Another example was given about Majorana representation in Kondo model. By rewriting the Kondo Hamiltonian $H_K$ and spin flip T-matrix $T_\sigma^{(2)}(\tau)$, series of polarized pair bubbles are drawn diagrammatically for $T_\sigma^{(2)}(\tau)$. The energy spectrum for conduction electrons was thus obtained by RPA both in zero magnetic field and a finite B field. When B=0 and $\omega \ll D$, we could reproduce pool man's scaling result. When $B \neq 0$, a Kondo peak appears at $\omega = B$, and we have the asymptotes in large frequency limit, which agrees with perturbative renormalization group method, however, in the limit of $\omega \to 0$, a spurious point occurs which is related to RPA and needs further correction.

We have examined Majorana representation is a useful tool to simplify our calculations, however, whether this technique can be successfully used in other perturbation regimes and more complex spin systems still requires further investigations.

# Chapter 6

# Acknowledgement

I would like to thank my supervisor, Prof.Jens Paaske for leading me into the wonderful world of condensed matter theory, he is always available for my questions and the discussions were quite beneficial and inspiring. I would like to thank Marius Simonsen for his help during my master's program.

# Bibliography


[1] A A Abrikosov. Electron scattering on magnetic impurities in metals and anomalous resistivity effects. *Physics*, **2**, 5-20 (1965).

[2] Y L Wang, S Shtrikman, H Callen. Wick's theorem for spin-1/2 operators, with an application to spin waves in antiferromagnets. *Physical Review*, **148**, 419 (1966).

[3] R Frésard, J Kroha, P Wölfle. The pseudoparticle approach to strongly correlated electron systems. In *"Strongly Correlated Systems", A. Avella and F. Mancini Eds., Springer Series in Solid-State Sciences*, **171**, 65-101 (2012).

[4] J L Martin. Generalized classical dynamics, and the'classical analogue'of a fermi oscillator. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences*, **251**, 536–542 (1959).

[5] A Shnirman, Y Makhlin. Spin-spin correlators in the majorana representation. *Physical Review Letters*, **91**, 207204 (2003).

[6] W Mao, P Coleman, C Hooley, D Langreth. Spin dynamics from majorana fermions. *Physical Review Letters*, **91**, 207203 (2003).

[7] A M Tsvelik. New fermionic description of quantum spin liquid state. *Physical Review Letters*, **69**, 2142 (1992).

[8] P Coleman, E Miranda, A Tsvelik. Three-body bound states and the development of odd-frequency pairing. *Physical Review Letters*, **74**, 1653 (1995).

[9] L V Keldysh. Diagram technique for nonequilibrium processes. *Sov. Phys. JETP*, **20**, 1018-1026 (1965).

[10] J Rammer. Quantum field-theoretical methods in transport theory of metals. *Reviews of Modern Physics*, **58**, 323-359 (1986).

[11] A Kamenev, A Levchenko. Keldysh technique and non-linear $\sigma$-model: basic principles and applications. *Advances in Physics*, **58**, 197-319 (2009).

[12] J Paaske, A Rosch, J Kroha, P Wölfle. Nonequilibrium transport through a Kondo dot: Decoherence effects. *Physical Review B*, **70**, 155301 (2004).

[13] M C Cano, S Florens. Magnetotransport in the kondo model with ferromagnetic exchange interaction. *arXiv preprint arXiv:1112.0925* (2011).

[14] R D Mattuck. *A guide to Feynman diagrams in the many-body problem.* (Courier Dover Publications, 2004).

[15] H Haug, A Jauho. *Quantum kinetics in transport and optics of semiconductors.* (Springer, 2008).

[16] A C Hewson. *The Kondo Problem to Heavy Fermions.* (Cambridge University Press, 1997).

[17] A Rosch, T A Costi, J Paaske, P Wölfle. Spectral function of the Kondo model in high magnetic fields. *Physical Review B*, **68**, 014430 (2003).