Spontaneous Time-Reversal Symmetry Breaking in Two Dimensional Electronic Systems

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Spontaneous Time-Reversal Symmetry Breaking in Two-Dimensional Electronic Systems

by

WEI LIU

A dissertation submitted to the Graduate Faculty in Physics in partial fulfillment of the requirements for the degree of Doctor of Philosophy, The City University of New York

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Abstract

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Wei Liu

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The discovery of high temperature superconductivity inspired a number of novel proposals, one of which, put forward by C.M.Varma, involves the breaking of time-reversal symmetry to explain the physics of the underdoped pseudogap phase. It was proposed that time-reversal symmetry is spontaneously broken as a result of strong repulsion between the Cu-O electrons to form loop-currents in the system. In this work, we developed a general theory to study the quantum phase transitions in the 2 dimensional strongly interacting electronic systems in which time-reversal symmetry is spontaneously broken in the ground state. We first applied the theory of magnetic groups to identify electronic current-loop patterns in two physically relevant systems: (i) 2-band model involving spinless electrons on a honeycomb lattice with next-nearest-neighbor (nnn) interactions; (ii) 3-band CuO$_2$ model with and without lattice distortions. Next, by examining the correlation function within the standard ring and ladder Dyson series approximations, we identify the effective Hamiltonian with the relevant interactions responsible for creating low-energy fluctuations near the quantum critical point. The mean-field analysis of this effective Hamiltonian elucidated the fact that time-reversal symmetry breaking in a
2-band model is in the same universality class as the interband particle-hole pair condensation instability which occurs in the semi-conductors under large enough particle-hole attraction. Using Hubbard-Stratonovich transformation and functional integral method, we are able to investigate this instability and the static susceptibility in the condensed phase both in half-filling and doped case. Away from half-filling, because the condensates are metallic and couple to the gapless collective intraband particle-hole excitations, we find that the static susceptibility is generically negative as a result of this coupling, which implies that the condensates are unstable.
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Chapter 1

Introduction

1.1 Quantum Phase Transition

Thermal phase transitions, usually triggered by fluctuations caused by tuning the temperature $T$ close to some special value $T_c$ are widely studied. As the temperature is lowered, thermal fluctuations decrease and eventually will cease as $T \to 0$. However, quantum fluctuations do not stop at zero temperature. These quantum fluctuations can trigger phase transitions known as quantum phase transitions (QPT) which describes an abrupt change in the ground state of a many-body system. For this to happen, the amplitude of these fluctuations needs to be controlled which can be accomplished by tuning a parameter in the Hamiltonian governing the system. Two examples of QPT are demonstrated below.
1.1.1 The Transverse Ising Models

The transverse Ising Hamiltonian was introduced by de Gennes [1] in order to study the order-disorder transition in some double-well ferroelectric system, such as KH$_2$PO$_4$. The mean field phase diagram [2] and the study of susceptibilities gave good qualitative agreement with the experimental results. In the ferroelectric phase of KH$_2$PO$_4$ each proton of the hydrogen bond can occupy one of the two minima of the double-well created by oxygen atoms. In the pseudo-spin picture, we ascribe a fictitious spin $S_i = 1/2$ to the $i$th proton, such that $S^z_i = \pm 1/2$ correspond to two different states respectively [1]. The energy of the proton system will be of the form

$$H = -\Gamma \sum_i S^x_i - \sum_{\langle ij \rangle} J_{ij} S^z_i S^z_j$$  \hspace{1cm} (1.1)$$

where $\Gamma$ is the tunneling integral, and $J_{ij}$ describes an interaction between proton sites.

The ground state of $H$ is easily derived in the semi-classical approximation by putting $S^x_i = 1/2 \cos \theta$ and $S^z_i = 1/2 \sin \theta$, the energy per proton is

$$E = -\frac{1}{2}\Gamma \sin \theta - \frac{1}{4} J_0 \cos^2 \theta$$  \hspace{1cm} (1.2)$$

where $J_0 = \sum_j J_{ij}$, i.e. the uniform system has been assumed. The energy can be minimized for the condition

$$\sin \theta = \frac{\Gamma}{J_0}$$  \hspace{1cm} (1.3)$$
This suggests that if $\Gamma < J_0$, the ground state is partially polarized, $\langle S^x \rangle = \frac{1}{2} \Gamma / J_0$, $\langle S^z \rangle = \frac{1}{2} \sqrt{1 - (\Gamma / J_0)^2}$. Whereas for $\Gamma \geq J_0$, the ground state is polarized in the $x$ direction with $\langle S^x \rangle = \frac{1}{2}$, $\langle S^z \rangle = 0$.

Figure 1.1: The value of $\langle S^x \rangle$ and $\langle S^z \rangle$ as a function of $\Gamma / J_0$ at $T = 0$. The QPT appears when $\Gamma / J_0 = 1$.

The finite-temperature behavior of the above transverse Ising model is obtained by using the mean field theory [2]. Assuming the system to be uniform, we can assign a uniform mean field value $\langle S^z \rangle$ for all $i$ and use $J_0 = \sum_i J_{ij}$. We write the mean field Hamiltonian as

$$H_{mf} = -\Gamma \sum_i S^x_i - 2J_0 \langle S^z \rangle \sum_i S^z_i = \sum_i H_i$$  \hspace{1cm} (1.4)

In the mean field approximation the many body problem is reduced to a one body problem by assuming a effective local magnetic field $\mathbf{h} = \Gamma \hat{x} + 2J_0 \langle S^z \rangle \hat{z}$. The partition function on each site $i$ is given by

$$Z_i = \text{Tr}[e^{-\beta H_i}] = \text{Tr}[e^{\beta (\Gamma S^x_i + 2J_0 \langle S^z \rangle S^z_i)}] = 2 \cosh(\beta h)$$  \hspace{1cm} (1.5)
where \( h = \frac{1}{2} \sqrt{\Gamma^2 + 4J_0^2 \langle S^z \rangle^2} \). Thus

\[
\langle S^z \rangle = \frac{1}{2 \cosh(\beta h)} \text{Tr}[S^z_i e^{\beta(\Gamma S^x_i + 2J_0 \langle S^z \rangle S^z_i)}] = \frac{J_0 \langle S^z \rangle}{h} \tanh(\beta h) \tag{1.6}
\]

\[
\langle S^x \rangle = \frac{\Gamma}{h} \tanh(\beta h) \tag{1.7}
\]

The self-consistent equation is

\[
1 = \frac{J_0}{h} \tanh(\beta h) \tag{1.8}
\]

The transition temperature is given by

\[
1 = \frac{J_0}{\Gamma} \tanh(\beta_c \Gamma) \Rightarrow \frac{\Gamma}{J_0} = \tanh \left( \frac{\Gamma}{J_0 k_B T_c} \right) \tag{1.9}
\]

The line given by this equation separate the ferro-magnetic and para-magnetic phase [3]

![Figure 1.2](image)

Figure 1.2: Inside the line is a ferro-magnetic phase, which \( \langle S^z \rangle \neq 0 \). The para-magnetic phase is where \( \langle S^z \rangle = 0 \).
1.1.2 One-Dimensional Spinless Two-Band Model

The simplest 2-band model involves choosing $s$ and $p_y$ orbitals along a 1D chain in the $\hat{y}$ direction as in Fig.1.3.

\[
\begin{array}{ccc}
- & + & - \\
- & + & - \\
\end{array}
\]

Figure 1.3: Along the $\hat{y}$ direction, there are two atomic orbitals on each lattice point, $s$ orbital and $p_y$ orbital. The lattice spacing is $a$.

The real space tight binding Hamiltonian is easily written

\[
H = \epsilon_s \sum_i s_i^\dagger s_i + \epsilon_{p} \sum_i p_i^\dagger p_i - t_s \sum_i s_i^\dagger s_{i+1} + t_p \sum_i p_i^\dagger p_{i+1} \\
+ t_{ps} \sum_i (s_i^\dagger p_{i+1} - s_{i+1}^\dagger p_i) + h.c. \quad (1.10)
\]

Use the Fourier transform, we express the Hamiltonian in the $k$ space

\[
H(k) = \begin{pmatrix}
\epsilon_s - 2t_s \cos(ka) & 2it_{ps} \sin(ka) \\
-2it_{ps} \sin(ka) & \epsilon_p + 2t_p \cos(ka)
\end{pmatrix} \quad (1.11)
\]

$\epsilon_s$ and $\epsilon_p$ are the local atomic energies of the $s$ and $p$ orbitals in the atom and $t_s$, $t_p$ and $t_{sp}$ are the $s-s$, $p-p$ and $s-p$ hopping energies. Only for demonstration, we assume $t_s = t_p = t$ and write $\epsilon_s = \epsilon_0 + \epsilon$, $\epsilon_p = \epsilon_0 - \epsilon$. Scaling the energy w.r.t. $2t$, we have

\[
H(k) = \epsilon_0 I + \begin{pmatrix}
\tilde{\epsilon} - \cos(ka) & i\tilde{t}_{ps} \sin(ka) \\
-i\tilde{t}_{ps} \sin(ka) & -\tilde{\epsilon} + \cos(ka)
\end{pmatrix} \quad (1.12)
\]
The energy eigenvalues are

$$E_k^\pm = \epsilon_0 \pm \sqrt{(\tilde{\epsilon} - \cos ka)^2 + \tilde{t}_{ps}^2 \sin^2 ka} \quad (1.13)$$

At the center of the Brillouin zone $k = 0$, when $\tilde{\epsilon} = 1$, we have two degenerate levels. By tuning $\tilde{\epsilon}$ across the critical value $\tilde{\epsilon} = 1$, the system experience the level crossing, which is a quantum phase transition. This is actually phase transition to the topological insulator [4]. A qualitative argument can be given here. We fist write the Hamiltonian as

$$H(k) = \left( \epsilon_0 I - \cos(ka)\sigma_z - \tilde{t}_{ps} \sin(ka)\sigma_y \right) + \tilde{\epsilon} \sigma_z \quad (1.14)$$
$$= H_0 + \tilde{\epsilon} H_1 \quad (1.15)$$

When $\tilde{\epsilon}$ is close to zero, we expected the system in the eigenstates of $H_0$ with small fluctuation induced by $H_1$. When $\tilde{\epsilon}$ is very large, the system is in the eigenstates of $H_1$ with $H_0$ treated as a perturbation. So in between, at $\tilde{\epsilon} = 1$ a level crossing is occurred, which is a sign of quantum phase transition.

The quantitive argument need to calculate the Berry phase of each band. We first write the Hamiltonian as (we have discarded the $I$ part because it is irrelevant in the argument)

$$H(k) = E_k \cos \theta_k \sigma_z - E_k \sin \theta_k \sigma_y \quad (1.16)$$
where \( E_k = \sqrt{\tilde{\epsilon} - \cos ka}^2 + \tilde{t}_{ps}^2 \sin^2 ka \) and

\[
\cos \theta_k = \frac{\tilde{\epsilon} - \cos ka}{\sqrt{(\tilde{\epsilon} - \cos ka)^2 + \tilde{t}_{ps}^2 \sin^2 ka}} \quad (1.17)
\]

\[
\sin \theta_k = \frac{\tilde{t}_{ps} \sin ka}{\sqrt{(\tilde{\epsilon} - \cos ka)^2 + \tilde{t}_{ps}^2 \sin^2 ka}} \quad (1.18)
\]

We first rotate the Hamiltonian to the \( \sigma_x \) and \( \sigma_y \) basis by using the unitary transformation \( U^\dagger H_k U \), where

\[
U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad (1.19)
\]

Then we have

\[
H_k = \begin{pmatrix} 0 & -e^{-i\theta_k} \\ -e^{i\theta_k} & 0 \end{pmatrix} \quad (1.20)
\]

This Hamiltonian is written in the new \(|+\rangle = \frac{1}{\sqrt{2}}(|s_k\rangle + |p_k\rangle)\) and \(|-\rangle = \frac{1}{\sqrt{2}}(|s_k\rangle - |p_k\rangle)\) basis.

The eigenstates are (\( \pm \) corresponds to the \( \pm E_k \) eigenvalues respectively)

\[
|\psi_k, \pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm e^{-i\theta_k}|-\rangle) \quad (1.21)
\]

The Berry phase in the tight-binding model is defined as

\[
\gamma_n = \oint \langle \psi_k, n | i \nabla_k | \psi_k, n \rangle \quad (1.22)
\]
where \( n \) is the band index, and \( \mathcal{C}_{BZ} \) means a closed path in the Brillouin zone. In 1-dimension, the closed path is \( (-\frac{\pi}{a}, \frac{\pi}{a}) \).

\[
\gamma_n = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \langle \psi_{k,n} | i \nabla_k | \psi_{k,n} \rangle = \frac{n^2}{2} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \frac{d\theta_k}{dk} \tag{1.23}
\]

\[
= -\frac{1}{2} \int_{-\pi}^{\pi} d(ka) \frac{\tilde{t}_{ps}(1 - \tilde{\epsilon} \cos ka)}{(\tilde{\epsilon} - \cos ka)^2 + \tilde{t}_{ps}^2 \sin^2 ka} \tag{1.24}
\]

Let us set \( \tilde{t}_{ps} = 1 \) only for demonstration. We then have

\[
\gamma_n = -\frac{1}{2} \int_{-\pi}^{\pi} d(ka) \frac{(1 - \tilde{\epsilon} \cos ka)}{(\tilde{\epsilon} - \cos ka)^2 + \tilde{t}_{ps}^2 \sin^2 ka} \tag{1.25}
\]

Define \( z = e^{i(ka)} \), we have

\[
\gamma_n = -\frac{1}{4} \int_{|z|=1} dz \frac{\tilde{\epsilon} z^2 - 2z + \tilde{\epsilon}}{i \tilde{\epsilon} (z - \tilde{\epsilon})(z - \frac{1}{\tilde{\epsilon}})} \tag{1.26}
\]

- \( \tilde{\epsilon} > 1 \): Both \( z = 0 \) and \( z = 1/\tilde{\epsilon} \) are inside the unit circle \( |z| = 1 \). According to the residue theorem, the integral is

\[
\gamma_n = -\frac{\pi}{2} \left(1 - 1 \right) = 0 \tag{1.27}
\]

- \( \tilde{\epsilon} < 1 \): Both \( z = 0 \) and \( z = \tilde{\epsilon} \) are inside the unit circle \( |z| = 1 \). We have

\[
\gamma_n = -\frac{\pi}{2} \left(1 + 1 \right) = -\pi \tag{1.28}
\]
In sum, we have

\[ \gamma_n = -\pi \, \Theta(1 - \tilde{\epsilon}) \]  

(1.29)

Where \( \Theta(x) \) is the step function. From this expression, we see a quantum phase transition from \( \gamma_\pm = 0 \) to \( \gamma_\pm = -\pi \) accompanying with a gap closing.

![Diagram showing the gap in the system closes at \( \tilde{\epsilon} = 1 \) where the quantum phase transition happens.](image)

Figure 1.4: The gap in the system closes at \( \tilde{\epsilon} = 1 \) where the quantum phase transition happens.

### 1.2 Order Parameter and Mean Field Theory

An order parameter is a measure of the degree of order in a system. It is normally zero in the disordered phase and nonzero in the ordered phase, for example, \( \langle S_z^2 \rangle \) in the transverse Ising model studied in the introduction. A nonzero order parameter is a sign of the symmetry breaking in the ordered phase, for example the breaking of the \( Z_2 \) symmetry \( S_i^z \rightarrow -S_i^z \) in the transverse Ising model. The \( \gamma_n \) in the second example is different from the \( \langle S_z^2 \rangle \). It is called a topological order, and the phase transition doesn’t break any symmetry. This type of the system is not our concern in the work.
In the modern classification scheme, phase transitions are divided into two broad categories depending on the continuity of the order parameter:

1. First order phase transitions involve a discontinuous jump of the order parameter. A well known example is the liquid-gas transition, where the density serves as the order parameter.

2. Second order phase transitions are also called continuous phase transitions. The order parameter changes continuously from the disordered phase to the ordered phase, however, the susceptibility of the order parameter is divergent at the quantum critical point. Examples of such quantum phase transitions are ferromagnetic transition and the superconducting transition. Our work focuses on this type of the phase transitions.

A many-body system with interactions is generally very difficult to solve exactly. Such models consider a large number of interacting individuals who interact with each other, for example a coulomb gas. However, after specifying the order parameter during the quantum phase transition, a mean field theory (MFT) can be applied. The idea of MFT is to approximate the effect of all the other individuals on any given individuals by a single averaged effect, and this averaged effect is usually chosen to be the order parameter. Thus we reduce the many-body problem to a one-body problem. Many useful results can be extracted just simply by doing the MFT. Two examples which related to our work will be given.
1.2.1 BCS Theory

The BCS (Bardeen-Cooper-Schrieffer) theory [5] relies on the work of Cooper. In his monumental work, he showed that due to the electron-phonon interaction, at adequately low temperature, a pair state of electrons can occur and has a lower energy than the Fermi energy, which implies that the pair is bound. A paired electron is one with opposite momentum and spin. Based on the work of Cooper, a proposed Hamiltonian is taken to be

\[ H = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,l} V_{kl} c_{k\uparrow}^\dagger c_{-k\downarrow} c_{l\downarrow} c_{l\uparrow} \]  

(1.30)

The first term is the kinetic energy of the electrons with \( \epsilon_k = \frac{k^2}{2m} \). The second term is the translation of the phonon mediated electron-electron interaction.

In the superconducting state, we expect the formation of the Cooper pairs, so the expectation value of the “anomalous” operator \( c_{-k\downarrow} c_{k\uparrow} \) is nonzero. Apply the MFT by defining the order parameter

\[ \Delta_k = -\sum_l V_{kl} \langle c_{-l\downarrow} c_{l\uparrow} \rangle \]  

(1.31)

The mean field Hamiltonian is

\[ H_{mf} = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} - \sum_k \Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow} - \sum_k \Delta_k^* c_{-k\downarrow} c_{k\uparrow} - \text{const}_V \]  

(1.32)

where \( \text{const}_V = -\sum_{k,l} V_{kl} \langle c_{k\uparrow}^\dagger c_{-k\downarrow} \rangle \langle c_{-l\downarrow} c_{l\uparrow} \rangle \). We’ll drop this term from here on, but it is important when comparing the total energy of BCS state with other states.
Next we follow the method of Bogoliubov and define the linear transformation

\[ c_{k\uparrow} = u_k^* \gamma_{k\uparrow} + v_k \gamma_{-k\downarrow} \] (1.33)

\[ c_{-k\downarrow} = -v_k^* \gamma_{k\uparrow} + u_k \gamma_{-k\downarrow} \] (1.34)

Also notice that the $H_{mf}$ doesn’t conserve the number of the electrons. So in order to allow the exchange of the particles, we put a chemical potential term into the free energy $F$. Applying the Bogoliubov transformation, we have the new form of the Hamiltonian as

\[
F = \sum_k \xi_k \left( |u_k|^2 \gamma_{k\uparrow}^\dagger \gamma_{k\uparrow} + |v_k|^2 \gamma_{-k\downarrow}^\dagger \gamma_{-k\downarrow} \right) + \sum_k \xi_k \left( |u_k|^2 \gamma_{-k\uparrow}^\dagger \gamma_{-k\downarrow} + |v_k|^2 \gamma_{k\downarrow}^\dagger \gamma_{k\uparrow} \right) \\
+ \sum_k \left( \Delta_k u_k v_k^* + \Delta_k^* v_k u_k^* \right) \left( \gamma_{k\uparrow}^\dagger \gamma_{-k\downarrow}^\dagger - \gamma_{-k\uparrow} \gamma_{k\downarrow} \right) \\
+ \sum_k \epsilon_k \left( 2u_k v_k^* \gamma_{k\uparrow}^\dagger \gamma_{-k\downarrow}^\dagger \gamma_{-k\downarrow}^\dagger \gamma_{k\uparrow}^\dagger \right) \\
- \sum_k \left( \Delta_k^2 - \Delta_k^* v_k^2 - \Delta_k v_k^* \right) \gamma_{k\uparrow}^\dagger \gamma_{-k\downarrow}^\dagger - \sum_k \left( \Delta_k u_k^* v_k^2 - \Delta_k^* u_k^* v_k^2 \right) \gamma_{-k\uparrow} \gamma_{k\downarrow}^\dagger \] (1.35)

where $\xi_k = \epsilon_k - \mu$, and also the inversion symmetry ( $u_{-k} = u_k$ ) has been used.

We determine the value of $u_k$ and $v_k$ by demanding the off-diagonal terms (terms proportional to $\gamma_{k\uparrow}^\dagger \gamma_{-k\downarrow}^\dagger$ and $\gamma_{-k\uparrow} \gamma_{k\downarrow}^\dagger$) to vanish. We have

\[ 2\xi_k u_k v_k + \Delta_k^* v_k^2 \gamma_{k\uparrow}^\dagger - \Delta_k u_k^2 \gamma_{k\downarrow}^\dagger = 0 \] (1.36)

Times $\Delta_k^* v_k^2$ on both sides,
\[
\left( \frac{\Delta^*_k v_k}{u_k} \right)^2 + 2\xi_k \left( \frac{\Delta^*_k u_k}{u_k} \right) - |\Delta_k|^2 = 0 \tag{1.37}
\]

and then

\[
\frac{\Delta^*_k v_k}{u_k} = \sqrt{\xi_k^2 + |\Delta_k|^2 - \xi_k} = E_k - \xi_k \tag{1.38}
\]

Combine with the normalization condition \(|u_k|^2 + |v_k|^2 = 1\), we have

\[
|u_k|^2 = \frac{1}{2} \left( 1 + \frac{\xi_k}{E_k} \right) \tag{1.39}
\]

\[
|v_k|^2 = \frac{1}{2} \left( 1 - \frac{\xi_k}{E_k} \right) \tag{1.40}
\]

Now, the Hamiltonian can be simplified as (we have used \(\gamma_{k\uparrow}^\dagger \gamma_{k\uparrow} = 1 - \gamma_{k\uparrow}^\dagger \gamma_{k\uparrow}\))

\[
F = \sum_k \xi_k \left( |u_k|^2 - |v_k|^2 \right) \left( \gamma_{k\uparrow}^\dagger \gamma_{k\uparrow} + \gamma_{-k\downarrow}^\dagger \gamma_{-k\downarrow} \right) + 2 \sum_k \xi_k |v_k|^2 \\
+ \sum_k \left( \frac{\Delta^*_k v_k}{u_k} + \frac{\Delta_k u_k^*}{u_k} \right) |u_k|^2 \left( \gamma_{k\uparrow}^\dagger \gamma_{k\uparrow} + \gamma_{-k\downarrow}^\dagger \gamma_{-k\downarrow} - 1 \right) \tag{1.41}
\]

\[
\Rightarrow F = \sum_k E_k \gamma_{k\uparrow}^\dagger \gamma_{k\uparrow} + \sum_k E_k \gamma_{-k\downarrow}^\dagger \gamma_{-k\downarrow} + \sum_k (\xi_k - E_k) \tag{1.42}
\]

where \(E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}\), which is the dispersion of the Bogoliubov quasiparticle \(\gamma_{k\sigma}^\dagger\). If \(|FS\rangle\) is the free electron ground state, the ground state of the supercon-
ducting state is given by (with proper normalization.)

\[ |\text{BCS}\rangle \propto \prod_{k,\sigma} \gamma_{k\sigma} |FS\rangle \] (1.43)

The superconducting excited state is given by

\[ \gamma_{k_1\sigma_1}^{\dagger} \gamma_{k_2\sigma_2}^{\dagger} \cdots \gamma_{k_n\sigma_n}^{\dagger} |\text{BCS}\rangle \] (1.44)

The spectrum of the elementary excitations in the normal and the superconducting state is shown below.

![Energy Spectrum](image)

Figure 1.5: The energies of the elementary excitations in the normal (bottom) and superconducting (top) states as a function of \( \xi_k \).

Because \( \xi_k = \epsilon_k - \mu \), at \( k = k_F \), which \( \xi_{k_F} = \epsilon_{k_F} - \mu = 0 \). So at \( k_F \) the energy gap reaches its maximum \( \Delta_{k_F} \). From this we found that the order parameter we have define earlier in the MFT has the physical meaning of the energy gap in the system.

Using the definition of the order parameter in the MFT, we can evaluate the
transition temperature $T_c$.

$$\Delta_k = - \sum_i V_{kl} \langle c_{-\downarrow l} c_{\uparrow i} \rangle \quad (1.45)$$

$$= - \sum_i V_{kl} u_i^* v_i \left( 1 - \gamma_i \gamma_{i+} - \gamma_i \gamma_{i-} \right) \quad (1.46)$$

$$= - \sum_i V_{kl} u_i^* v_i \left( 1 - 2n_F(E_i) \right) \quad (1.47)$$

$$= - \sum_i V_{kl} \frac{\Delta_i}{2E_i} \tanh \left( \frac{\beta E_i}{2} \right) \quad (1.48)$$

If we adopt the approximation given by Cooper with the Cooper energy $\hbar \omega_c$

$$V_{kl} = \begin{cases} 
- V & \text{for } \epsilon_F < \epsilon_k < \epsilon_F + \hbar \omega_c \\
0 & \text{else}
\end{cases} \quad (1.49)$$

$$\Delta_k = \Delta \quad (1.50)$$

We have

$$\frac{1}{V} = \frac{1}{2} \sum_k' \frac{\tanh \left( \frac{\beta E_k}{2} \right)}{E_k} \quad (1.51)$$

where $\sum_k'$ means the summation is only over $k$ satisfy $\epsilon_F < \epsilon_k < \epsilon_F + \hbar \omega_c$.

- At zero temperature, the gap equation can be easily evaluated for $\Delta = \Delta_0$

$$\frac{1}{V} = \nu_0 \int_0^{\hbar \omega_c} \frac{d\xi}{\sqrt{\xi^2 + \Delta_0}} = \nu_0 \sinh^{-1} \frac{\hbar \omega_c}{\Delta_0} \simeq \ln \frac{2\hbar \omega_c}{\Delta_0} \quad (1.52)$$
where \( \nu_0 \) is the density of the states. So

\[
\Delta_0 \approx 2\hbar\omega_c \exp\left( -\frac{1}{\nu_0 V} \right)
\]  

(1.53)

- At \( T_c \) when the transition occurs, the gap \( \Delta = 0 \). Then

\[
\frac{1}{V} = \nu_0 \int_0^{\hbar\omega_c} d\xi \frac{1}{\xi} \tanh \left( \frac{\xi}{2k_B T_c} \right)
\]

(1.54)

which solved approximately we have

\[
k_B T_c \approx 1.14 \hbar\omega_c \exp\left( -\frac{1}{\nu_0 V} \right)
\]

(1.55)

### 1.2.2 Exciton Condensation in the Semiconductor

G. D. Mahan [6, 7] considered the possible existence of an exciton in the doped direct gap semiconductors. Such exciton corresponds to a bound state of the conduction electron and valence hole created by the optical absorption process. The binding energy of this exciton can be calculated by using MFT on a simplified model Hamiltonian [8].

We consider a simple model semiconductor, with direct gap \( E_G \) and isotropic non degenerate bands. The conduction band is empty and the valence band is fully filled. Then we use some pumping mechanism to create particle-hole pair in the system. Counting the interaction between holes and particles, we have the model
Hamiltonian

\[ H = \sum_k \epsilon_k b_k^\dagger b_k - \sum_k \epsilon_k a_k^\dagger a_k - \frac{V}{L^2} \sum_{k,p,q} u_k u_p b_k^\dagger a_{k+p} a_p b_{p+q} \]  

(1.56)

where \( b_k^\dagger \) and \( a_k^\dagger \) are the creation operators of the conduction and valence electrons and \( \epsilon_k = \frac{E_G}{2} + \frac{k^2}{2m} \), \( E_G \) is the gap energy, and we have also assumed equal mass of the conduction and valence electrons just for simplification. \( u_k \) gives a high energy cut-off in the order of the Fermi energy.

\[ u_k = \begin{cases} 1 & \text{if } |\epsilon_k - \mu| < \xi_0 \\ 0 & \text{if } |\epsilon_k - \mu| > \xi_0 \end{cases} \]  

(1.57)

In the MFT, we define the order

\[ \Delta = \frac{V}{L^2} \sum_k u_k a_k^\dagger b_k \]  

(1.58)

The mean field Hamiltonian is

\[ H_{mf} = \sum_k \epsilon_k b_k^\dagger b_k - \sum_k \epsilon_k a_k^\dagger a_k - \sum_k \Delta u_k b_k^\dagger a_k - \sum_k \Delta^* u_k a_k^\dagger b_k + \frac{L^2}{V} |\Delta|^2 \]  

(1.59)

The particles and holes are pumped into the system, so the number of particles and holes are not conserved. We need to add a chemical potential term \(-\mu \sum_k (b_k^\dagger b_k + a_k^\dagger a_k)\).
\( a_k a_k^{\dagger} \) into the free energy. The free energy reads

\[
F = \sum_k (\epsilon_k - \mu) b_k^{\dagger} b_k - \sum_k (\epsilon_k - \mu) a_k^{\dagger} a_k - \sum_k \Delta u_k b_k^{\dagger} a_k - \sum_k \Delta^* u_k a_k^{\dagger} b_k + \frac{L^2}{V} |\Delta|^2 - \sum_k \mu
\]  

(1.60)

Define a linear transformation

\[
\alpha_k^{\dagger} = \cos \theta_k a_k^{\dagger} + \sin \theta_k b_k^{\dagger} \quad \text{(1.61)}
\]

\[
\beta_k^{\dagger} = -\sin \theta_k a_k^{\dagger} + \cos \theta_k b_k^{\dagger} \quad \text{(1.62)}
\]

where \((E_k = \sqrt{\xi_k^2 + |\Delta|^2} \text{ and } \xi_k = \epsilon_k - \mu)\)

\[
\sin \theta_k = \sqrt{\frac{E_k - \xi_k}{2E_k}} \quad \cos \theta_k = \sqrt{\frac{E_k + \xi_k}{2E_k}}
\]  

(1.63)

The free energy can be written as

\[
F = \sum_k' E_k \beta_k^{\dagger} \beta_k - \sum_k' E_k \alpha_k^{\dagger} a_k - \mu \sum_k' 1 + \frac{L^2}{V} |\Delta|^2
\]  

(1.64)

\(\sum_k'\) is a restricted sum which has a cut-off defined in Eq.(1.57). Minimized the free energy w.r.t. the order parameter \(\Delta\), we have

\[
\frac{1}{L^2} \sum_k' \frac{1}{2E_k} \left( -n_F(E_k) + n_F(-E_k) \right) = \frac{1}{V}
\]  

(1.65)

The chemical potential \(\mu\) is determined by the identity \(\partial F/\partial \mu = -N\), where \(N\) is
the total number of particles and holes which have been pumped into the system.

$$\sum\limits_k^\prime \left[ 1 + \frac{\xi_k}{E_k} \left( n_F(E_k) - n_F(-E_k) \right) \right] = N \quad (1.66)$$

In the zero temperature, $n_F(E_k) = 0$ while $n_F(-E_k) = 1$. Then we have

- Gap equation for determining the order parameter $\Delta$

$$\frac{1}{L^2} \sum_k^\prime \frac{1}{2E_k} = \frac{1}{V} \quad (1.67)$$

- Number equation for determining the chemical potential $\mu$

$$\sum_k^\prime \left[ 1 - \frac{\xi_k}{E_k} \right] = \sum_k^\prime 2\sin^2 \theta_k = N \quad (1.68)$$

The quantum phase transition is shown in the Fig.1.6

---

**Figure 1.6**: Left figure: Particle-hole pairs are created in the original system. Right figure: Because of the condensation of the excitons, an energy gap $2\Delta$ appears at $k = k_0$ for $\epsilon_{k_0} = \mu$. 
Comparing with BCS theory: In the exciton model, if we adopt the substitution $a_k^\dagger \rightarrow c_{-k\downarrow}$, $b_k^\dagger \rightarrow c_{k\uparrow}$ in the mean field Hamiltonian Eq.(1.59), we have

$$H_{mf} \rightarrow \sum_k \epsilon_k c_{k\uparrow}^\dagger c_{k\uparrow} - \sum_k \epsilon_k c_{-k\downarrow}^\dagger c_{-k\downarrow} - \sum_k \Delta u_k c_{k\uparrow}^\dagger c_{-k\downarrow} - \sum_k \Delta^* u_k c_{-k\downarrow} c_{k\uparrow} + \frac{L^2}{V} |\Delta|^2$$

(1.69)

If we think that $u_k$ gives a high energy cut-off as the Cooper energy $\hbar \omega_c$, then this mean field Hamiltonian is the same as the BCS mean field Hamiltonian Eq.(1.32) with the Cooper approximation Eq.(1.50). The ground state of the exciton model $|\Phi_0\rangle$ should have a similar form as the BCS ground state Eq.(1.43):

$$|\Phi_0\rangle \propto \prod_k \beta_k a_k^\dagger |FS\rangle$$

(1.70)

In BCS, $|FS\rangle$ is the ground state of the free electrons. Similarly in the exciton model, $|FS\rangle$ denotes the original ground state which has fully filled lower band $a$ and empty upper band $b$, i.e. $|FS\rangle = \prod_k a_k^\dagger |0\rangle$. With the normalization, we have

$$|\Phi_0\rangle = \prod_k \left( \cos \theta_k + \sin \theta_k b_k^\dagger a_k \right) |FS\rangle$$

(1.71)

### 1.3 High $T_c$ Superconductor

One of the most interesting quantum phase transition phenomenas is the high temperature superconductor (HTS). First discovered in 1986 by IBM researchers Karl Müller and Johannes Bednorz [9], this incredible phenomena has aroused lots of physicists’ interests and many pioneer work and novel proposals have been done
in the past 30 years. Comparing to the conventional or metallic superconductors, whose transition temperatures (predicted by BCS theory) below 30K, HTS have been observed with transition temperatures as high as 138K. HTS are generally considered as compounds of copper and oxygen (the cuprates), however, several iron-based compounds (the iron pnictides) are now know to be superconducting at high temperatures. Our work focuses on the cuprate superconductors. The widely accepted phase diagram of the cuprate superconductor in terms of the temperature and the hole doping is shown in Fig.1.7:

![Phase Diagram](image)

Figure 1.7: A schematic universal phase diagram for the cuprates.

Region I is the strange metal phase which shows a non-Fermi liquid behavior in resistivity $\rho(T) \simeq \rho_0 + \rho_1 T$ and in all the other transport properties. Marginal Fermi liquid theory [10] is phenomenologically successful in this region and a quantum critical point (QCP) at zero temperature and optimal doping is anticipated by the theory. Given a QCP, Region III, the Fermi liquid phase follows at overdoped region. Region II is called pseudogap phase because an anisotropic gap in the one-particle spectra at the chemical potential is observed. Since the broken
symmetry in region II is due to the condensation of the fluctuations in region I, a knowledge of the former specifies the nature of the latter [11].

Many theoretical models have been proposed to explore the pseudogap phase. One of the most promising and interesting proposal is given by C. M. Varma [11–14]. In his proposal, certain current loop patterns are formed in each unit cell of the CuO$_2$ plane, therefore translational symmetry is preserved but time reversal symmetry is spontaneously broken in the pseudogap phase. The model is consistent with many experiments [15–19]. The polarized elastic neutron diffraction experiment [16] demonstrated the emergence of an unusual long-range electronic order in the pseudogap phase of the yttrium-barium family of cuprates. This form of order was independently confirmed in another sample [15] of the yttrium-barium family, and also found in samples of three other cuprate families [17–19].

Varma proposed two possible loop-currents patterns [11–14] in cuprates and are shown in Fig.1.9:

![Figure 1.8: Real space current loops pattern in one unit cell of CuO$_2$. Solid circles (●) correspond to Copper atoms and the open circles (○) are the Oxygen atoms. The net magnetic momentum per unit cell is zero, thus such patterns when extended over the entire lattice will preserve the translational symmetry of the lattice.](image)

The presence of spontaneously generated loop-currents break time-reversal symmetry because the complex expectation value of $\langle c_i c_{i+1} \rangle = \chi e^{i\phi}$ in the groundstate
between two nearest neighbor sites, produces a local “magnetic flux”. Note that the net magnetic moment is zero in each unit cell, thus no global magnetic field is generated, not is a staggered flux phase generated when extended over the entire lattice.

In Fig.1.9, the right pattern is considered to be the suitable candidate of the time reversal violated (TRV) state [11]. Also notice that, there are three other degenerate current loop configuration which can be generated by rotations of $\pi/2$, $\pi$, $3\pi/2$ of the original pattern [20]:

![Figure 1.9: Four degenerate configurations related by rotations of angles $\pi/2$, $\pi$, $3\pi/2$.](image)

A cuprate superconductor in the loop current state will condensate into one of these four possible ground states. Thus collective fluctuations shall take the system to any of the other three configurations. Therefore three modes of the fluctuations are to be expected [20]. One such mode of fluctuations has been observed [21].

### 1.4 Outline

Inspired by Varma’s proposal, our work is aimed to develop a systematic microscopic theory to explain the spontaneous time reversal breaking phase transitions in the two-dimensional system. This dissertation is organized as follows. In Chap-
ter 2, we introduce the magnetic group theory and show its applications to classify
the possible current carrying states in the 2 dimensional electronic systems. Two
specific lattice models are studied: (i) 2-band model involving spinless electrons
on a honeycomb lattice with next-nearest-neighbor (nnn) interactions; (ii) 3-band
CuO$_2$ model with and without lattice distortions. In Chapter 3, we give a general
mean-field treatment for the 2-band model and calculate the collective excitations
in the ordered phase. In Chapter 4, we study the correlation function within the
standard ring and ladder Dyson series approximations, and are able to get the ef-
fective many body Hamiltonian which captures most of the physics at the quantum
critical point (QCP) and map the 2-band problem to XL problem. In Chapter 5
and Chapter 6, By using the functional integral method on the effective Hamil-
tonian, we study the XL phase in two different two-band models: a continuum
degenerate semiconductor model where T symmetry is not broken, and a lattice
model model where the condensate breaks T symmetry. And we show the destabilization
in both cases.
Chapter 2

Magnetic Point Group and Current Loop Patterns

Group theory is one of the most successful mathematical theories applied in the Physics. For example, the Lie groups in the particle physics and the point groups and space groups in the condensed matter physics. Because we are studying the time reversal breaking through the phase transition in the condensed matter physics, the magnetic group becomes the very suitable tool in our research. Apart from the symmetry operations (translations, rotations, inversion etc.) in the ordinary point group and space group, magnetic group involves a new symmetry operation—time reversal operation. It is important then to first figure out the physical meaning of the time reversal operator.

2.1 Time Inversion

Let us denote the time reversal operator by $\Theta$. 
Consider a system represented by state vector $|\alpha, t_0\rangle$; $\Theta|\alpha, t_0\rangle$ is called time reversed state in which all the velocities (including spin of the electrons) have opposite directions to those in $|\alpha, t_0\rangle$. Generally speaking, $|\alpha, t_0\rangle$ is a new state of the same system at time $t_0$, but if we evolve $\Theta|\alpha, t_0\rangle$ in the time under the influence of Hamiltonian, it behaves as the system is going back in time. Remember that the operator $1 - i\frac{\hbar H}{\delta t}$ corresponds to the “evolving” in time by a small amount $\delta t$, where $H$ is the Hamiltonian of the system.

If the system has time reversal symmetry, it has to go back to the original state up to a phase factor after experiencing the following process: prepare the system in the state $|\alpha, t_0\rangle$ at time $t_0$; evolve the system under the system’s Hamiltonian $H$ by time interval $\delta t$; apply time reversal operator $\Theta$, and evolve the resulting system under the same Hamiltonian $H$ by the same amount of time interval $\delta t$; apply the time reversal operator $\Theta$ again. The mathematics expressed this physical process is:

$$\Theta(1 - i\frac{\hbar H}{\delta t})\Theta(1 - i\frac{\hbar H}{\delta t})|\alpha, t_0\rangle = e^{i\varphi}|\alpha, t_0\rangle$$  \hspace{1cm} (2.1)

$$\Rightarrow \langle\alpha, t_0|\Theta(1 - i\frac{\hbar H}{\delta t})\Theta(1 - i\frac{\hbar H}{\delta t})|\alpha, t_0\rangle = e^{i\varphi}\langle\alpha, t_0|\alpha, t_0\rangle$$

$$\Rightarrow \langle\alpha, t_0|\Theta^2|\alpha, t_0\rangle - \langle\alpha, t_0|\Theta(iH\Theta + \Theta iH)|\alpha, t_0\rangle \frac{1}{\hbar}\delta t = e^{i\varphi}$$  \hspace{1cm} (2.2)

Then we have

$$iH\Theta = -\Theta iH$$  \hspace{1cm} (2.3)

$$\langle\alpha, t_0|\Theta^2|\alpha, t_0\rangle = e^{i\varphi}$$  \hspace{1cm} (2.4)
• First, let us look at Eq.(2.3). If we assume $\Theta$ is a linear operator, then $H\Theta = -\Theta H$; Consider $|\psi_n\rangle$ as one of the eigenstate of the system with eigenvalue $E_n$, then $H\Theta|\psi_n\rangle = -\Theta H|\psi_n\rangle = -E_n\Theta|\psi_n\rangle$. This doesn’t make sense even for free particle case, because the equation would lead to a negative energy spectrum for the free particles. So $\Theta$ has to be anti-linear. So,

\[ \Theta c = c^*\Theta \quad \text{c is some number} \quad (2.5) \]

\[ H\Theta = \Theta H \quad (2.6) \]

• Second, Eq.(2.4) tells us that $\Theta^2$ acting on any arbitrary state $\psi\rangle$ will lead to $e^{i\psi}|\psi\rangle$, and the superposition of state $|\psi\rangle$ principle forces the phase factor $e^{i\psi}$ to be independent of state $|\psi\rangle$. (Proof: $\Theta^2|\psi\rangle = e^{i\psi}|\psi\rangle; \Theta^2|\phi\rangle = e^{i\phi}|\phi\rangle; |\gamma\rangle = a|\psi\rangle + b|\phi\rangle; \Theta|\gamma\rangle = e^{i\gamma}|\gamma\rangle = a e^{i\psi}|\psi\rangle + b e^{i\phi}|\phi\rangle; \langle\gamma|e^{-i\gamma}e^{i\gamma}|\gamma\rangle = 1 = |a|^2 + |b|^2 + a^*b e^{-i(\psi-\phi)} + ab^*e^{i(\psi-\phi)}$; so for any $|\psi\rangle, |\phi\rangle, \psi - \phi = 0$).

However,

\[ \Theta^3|\psi\rangle = \Theta e^{i\psi}|\psi\rangle = e^{-i\psi}\Theta|\psi\rangle \quad (2.7) \]

\[ \Theta^3|\psi\rangle = \Theta^2(\Theta|\psi\rangle) = e^{i\psi}\Theta|\psi\rangle \quad (2.8) \]

Compare these two equations, we have $(e^{i\psi})^2 = 1 \Rightarrow e^{i\psi} = \pm 1$. So that

\[ \Theta^2 = \pm 1 \quad (2.9) \]

These three equations, Eq.(2.5) and Eq.(2.9) are the basic properties of the time re-
universal operator \( \Theta \), while Eq.(2.6) is the criteria for the system having time reversal symmetry.

1. Now, starting from Eq.(2.5): \( \Theta c = c^{*} \Theta \), we find “complex conjugate operator” \( K \) do the same thing: \( Kc = c^{*} K \). So it is reasonable to say \( \Theta = VK \) with \( Vc = cV \). We also know \( \Theta |x\rangle = |x\rangle \), where \( |x\rangle \) is the state in the space representation. (This relation is from the definition of the time reversal operator \( \Theta \), and we have chosen the phase to be 1). We have

\[
\Theta |\psi\rangle = \Theta \int dx \ |x\rangle \langle x|\psi\rangle = \int dx \ |x\rangle \langle x|\psi\rangle^{*} \tag{2.10}
\]

Then

\[
\langle \Theta \phi | \Theta \psi \rangle = \int dx \int dx' \langle \phi | x' \rangle^{*} \langle x' | x | \psi \rangle^{*} \tag{2.12}
\]

\[
= \int dx \langle \psi | x \rangle \langle x | \phi \rangle = \langle \psi | \phi \rangle \tag{2.13}
\]

Eq.(2.13) also holds for the complex conjugate operator \( K \).

Put \( \Theta = VK \) into Eq.(2.13), we obtain:

\[
\langle \Theta \phi | \Theta \psi \rangle = \langle \phi | K^{\dagger} V^{\dagger} VK | \psi \rangle \tag{2.14}
\]

\[
= \langle \phi | (V^{\dagger})^{*} K^{\dagger} K (V)^{*} | \psi \rangle \tag{2.15}
\]

\[
= \langle \psi | (V^{\dagger} V)^{*} | \phi \rangle = \langle \psi | \phi \rangle \tag{2.16}
\]

This is true for any \( |\psi\rangle \) and \( |\phi\rangle \). We can conclude that \( V \) is a unitary operator.
and $\Theta$ is an anti-unitary operator.

2. From $\Theta c = c^* \Theta$ and $\Theta x = x \Theta$, we can derive $\Theta p = -p \Theta$.

Proof: Because $p = i \frac{\partial}{\partial x}$, we have $\Theta i \frac{\partial}{\partial x} = -i \frac{\partial}{\partial x} \Theta$.

3. For no-spin case, we have $\Theta \psi(x) = \psi^*(x)$.

Proof:

$$\Theta \psi(x) = \langle x | \Theta | \psi \rangle = \langle x | \Theta \int dx' | x' \rangle \langle x' | \psi \rangle = \langle x | \int dx' | x' \rangle \langle x' | \psi \rangle^* = \psi^*(x)$$

4. For $1/2$ spins case: The spins behaves as angular momenta, so that they anti-commute with $\Theta = VK$. For $1/2$ spin, we choose the standard Pauli matrices as the representation of the $1/2$ spin. We have for $i$th spin:

$$\Theta S_{ix} = VK S_{ix} = VS_{ix}K = -S_{ix} \Theta = -S_{ix} VK$$

$$\Theta S_{iy} = VK S_{iy} = -VS_{iy}K = -S_{iy} \Theta = -S_{iy} VK$$

$$\Theta S_{iz} = VK S_{iz} = VS_{iz}K = -S_{iz} \Theta = -S_{iz} VK$$

Hence: $VS_{ix} = -S_{ix} V; VS_{iy} = S_{iy} V; VS_{iz} = -S_{iz} V$.

The suitable choice for $V$ is $V = S_{iy}$. For a system containing $N$ number of spin $1/2$ particles, we have

$$\Theta = \prod_{i=1}^{N} S_{iy} K$$
Notice that

$$\Theta^2 = \prod_i^N (-S_i y S_i y) K K = (-1)^N$$  \hspace{1cm} (2.23)$$

So for the system containing even number of 1/2 spin particles, $\Theta^2 = 1$, for odd number $\Theta^2 = -1$. This matches the property we have derived for $\Theta$, Eq.(2.9).

### 2.2 Magnetic Point Group

#### 2.2.1 Definition of the Magnetic Point Groups

Regardless of any magnetic moment or loop-current in the system, the system has certain point group symmetry called $G = \{g_1, g_2, \ldots\}$. Now if we put magnetic moment or current loop on the Bravis lattice points, we will possibly reduce the original point group symmetry and also bring in new symmetries. the set of all these symmetry operators will form a magnetic point group, $M = \{g_\alpha, a_\beta\}$. $g_\alpha$ is a unitary operator, while $a_\beta$ is an anti-unitary operator. $a_\beta$ can be written as $a_\beta = \Theta g_\beta$, $\Theta$ is the time-reversal operator.

Three basic properties are listed below,

1. $g_\alpha$ form a point group, i.e. $G_0 = \{g_\alpha\}$.

2. $g_\alpha \neq g_\beta$ if $\Theta$ is not in the $M$.

**proof:** If there is a $g_\gamma$ for which $g_\gamma$ and $\Theta g_\gamma$ are both in the magnetic group $M$. Because $g_\gamma^{-1}$ is also in the $M$, $\Theta g_\gamma g_\gamma^{-1} = \theta$ is in the $M$, which is contradictory.
to the prescription.

3. Number of $g_\alpha$’s is the same as the number of $a_\beta$’s.

   \textit{proof}: First, we choose some $a_\beta$ then multiplied by all $g_\alpha$, this will generate some anti-unitary operators $a_\theta$, due to the reason that the multiplication of one unitary and one anti-unitary operator result in an anti-unitary operator. From the definition of the group, we know that all the $a_\theta$’s are inside the group $M$. So the number of $a_\beta \geq g_\alpha$.

   Second, we choose some $a_\beta$, then multiplied by all $a_\theta$, this will generate some unitary operators $g_\gamma$. Again, all the $g_\gamma$ belong to group $M$. So the number of $a_\beta \leq g_\alpha$.

Magnetic point groups can be classified into three types:

I. $M = G$.

   In type I groups, the magnetic point group $M$ is just one of the ordinary 32 point groups. The $\Theta$ is not presented. We will not discuss these groups here.

II. $M = G + \Theta G$.

   In type II magnetic point groups, the time reversal operator $\Theta$ is explicitly contained, which means the described system is time reversal invariant. If the system is governed by the Hamiltonian $H$, then $\Theta$ is commute with $H$. Type II magnetic point groups are also called \textit{grey} groups. If we think the $\Theta$ operator brings \textit{black} to \textit{white} or \textit{vice versa}, now because system is invariant under $\Theta$ operations, the system takes color \textit{black} and \textit{white} simultaneously, and the term \textit{grey} is used.
III. $M = G_0 + \Theta(G - G_0)$.

In type III magnetic point groups, the time reversal operator $\Theta$ is not alone contained, ($\Theta$ is not a symmetric operator of the system). The system breaks the time reversal symmetry. This type of the groups is also called black and white group, because now we can color the system with black and white with the $\Theta$ changing the black to white or vice versa.

$G_0$ itself forms a group, and number of the elements in $G_0$ is equal to the number of the elements in $\Theta(G - G_0)$. So $G_0$ is the subgroup of $G$ of index 2. Because it may be several different ways to choose a halving subgroup of a given point group $G$, so it could be more than 32 type III magnetic point groups. In fact, there is a total 58 type III magnetic point groups.

The system described by type III magnetic groups breaks time reversal symmetry. So these are the groups we are going to focus on.

We illustrate the derivation of type III magnetic point groups from the ordinary point groups $G$ by considering the example of the black and white point groups that are derived from $C_{4v}$ the point group of they symmetry operations of a square.

![Symmetry operations in the point group $C_{4v}$ of a square.](image)

Figure 2.1: The symmetry operations in the point group $C_{4v}$ of a square.
A square has symmetry operations \( \{E, C_{4z}, C_{4z}^{3}, C_{2z}, \sigma_{x}, \sigma_{y}, \sigma_{da}, \sigma_{db}\} \). These symmetry operations form the point group \( C_{4v} \). From the previous discussion, we know that in order to construct the magnetic group, we need to find the halving subgroup of the \( C_{4v} \). There are two such groups, \( C_{2v} \) and \( C_{4} \).

1. \( C_{4} \) as the subgroup.

   The \( C_{4} \) point group is \( \{E, C_{4z}, C_{4z}^{3}, C_{2z}\} \), exactly half of the \( C_{4v} \). From the definition of the type III magnetic group, \( M = G_{0} + \Theta(G - G_{0}) \), we can construct the corresponding magnetic group, \( 4m'm' \). The primes indicate the symmetry operations now combined with \( \Theta \).

   \[
   \{E, C_{4z}, C_{4z}^{3}, C_{2z}, \Theta\sigma_{x}, \Theta\sigma_{y}, \Theta\sigma_{da}, \Theta\sigma_{db}\} \tag{2.24}
   \]

   The lattice system described by the \( 4m'm' \) magnetic point group can be demonstrated by drawing black and white patches on the original square lattice.

![Figure 2.2: The black and white illustrations of 4m'm'.](image-url)
Under operations \( E, C_{4z}, C_{4z}^3, C_{2z} \) the black or white patches remain the same color. Other operations \( \sigma_x, \sigma_y, \sigma_{da}, \sigma_{db} \) leave the black patches where there were white ones before and vice versa. But combined with \( \Theta \), which turns the white (black) color to black (white), \( \Theta \sigma_x, \Theta \sigma_y, \Theta \sigma_{da}, \Theta \sigma_{db} \) leave the square indistinguishable from its initial state.

2. \( C_{2v} \) as the subgroup.

One possible choice of the \( C_{2v} \) point group is \( \{E, C_{2z}, \sigma_x, \sigma_y\} \). The corresponding magnetic group is called 4\( 'mm' \).

\[
\{E, C_{2z}, \sigma_x, \sigma_y, \Theta C_{4z}, \Theta C_{4z}^3, \Theta \sigma_{da}, \Theta \sigma_{db}\} \tag{2.25}
\]

The black and white illustration is

![Figure 2.3: The black and white illustrations of 4\( 'mm' \)](image)

There is another possible choice of \( C_{2v} \) which is \( \{E, C_{2z}, \sigma_{da}, \sigma_{db}\} \). The corresponding magnetic group is 4\( 'm'm \).

\[
\{E, C_{2z}, \sigma_{da}, \sigma_{db}, \Theta C_{4z}, \Theta C_{4z}^3, \Theta \sigma_x, \Theta \sigma_y\} \tag{2.26}
\]
However, this magnetic point group $4'm'm$ is related to the former $4'mm'$ by a $\pi/4$ rotation of the $x$ and $y$ axes about the $z$ axis. So these two are essentially equivalent. Two patterns are said to be equivalent if they can be transformed into each other by altering the orientation of the axes.

In the above example, we have successfully constructed two magnetic point groups from the original $C_{4v}$ point group. There are totally 58 type III magnetic groups which can be constructed from the 32 point groups.

### 2.2.2 The Corepresentations of Magnetic Groups

After specifying the definition of the magnetic groups, it is naturally to ask what is the irreducible representations of the magnetic groups. In the magnetic groups, it is called corepresentations, and again we only study the type III magnetic groups. We have learned that the type III magnetic groups can be expressed as $M = G_0 + \Theta(G - G_0)$. Let us say $\Gamma$ is an irreducible representation of $G_0 = \{g_\alpha\}$ with basis $\{\psi_\mu\}$. Then from the representation theory, we have

\[ g_\alpha \psi_\mu = \sum_\nu D_{\nu\mu}(g_\alpha) \psi_\mu \]  

(2.27)

which $D_{\nu\mu}$ is the representation matrix of $\Gamma$. And because $g_\alpha$ is the symmetry operator of the system, $\psi_\mu$ has to be the eigenstate of the Hamiltonian $H$ of the system.

\[ H\psi_\mu = E^\Gamma \psi_\mu \]  

(2.28)
Now let us choose any antiunitary operator from $M$, say $a_\kappa$. $a_\kappa$ is a symmetry operator of the system, so we have

$$a_\kappa H \psi_\mu = Ha_\kappa \psi_\mu = E a_\kappa \psi_\mu$$  \hspace{1cm} (2.29)

This tells us that $a_\kappa \{ \psi_\mu \}$ is also the basis functions of the Hamiltonian.

We now show that $\{ \psi_\mu, a_\kappa \psi_\mu \}$ form a complete basis for the magnetic group $M$. Meaning the vector space spanned by $\{ \psi_\mu, a_\kappa \psi_\mu \}$ is invariant under $M$.

- **Unitary operators** $g_\alpha$ acting on $\{ \psi_\mu \}$.

$$g_\alpha \psi_\mu = \sum_\nu D_{\nu \mu}(g_\alpha) \psi_\nu$$  \hspace{1cm} (2.30)

- **Anti-unitary operators** $a_\beta$ acting on $\{ \psi_\mu \}$.

$$a_\beta \psi_\mu = a_\kappa a_\kappa^{-1} a_\beta \psi_\mu = a_\kappa \sum_\nu D_{\nu \mu}(a_\kappa^{-1} a_\beta) \psi_\nu$$

$$= \sum_\nu D_{\nu \mu}^*(a_\kappa^{-1} a_\beta) a_\kappa \psi_\nu$$  \hspace{1cm} (2.31)

- **Unitary operators** $g_\alpha$ acting on $\{ a_\kappa \psi_\mu \}$.

$$g_\alpha a_\kappa \psi_\mu = a_\kappa (a_\kappa^{-1} g_\alpha a_\kappa) \psi_\mu = a_\kappa \sum_\nu D_{\nu \mu}(a_\kappa^{-1} g_\alpha) \psi_\nu$$

$$= \sum_\nu D_{\nu \mu}^*(a_\kappa^{-1} g_\alpha) a_\kappa \psi_\nu$$  \hspace{1cm} (2.32)
Anti-unitary operators $a_\beta$ acting on $\{a_\kappa \psi_\mu\}$.

$$a_\beta a_\kappa \psi_\mu = \sum_\nu D_{\nu\mu}(a_\beta a_\kappa)\psi_\nu$$  \hspace{1cm} (2.33)

From the above relations, we see that $\{g_\alpha\}$ and $\{a_\beta\}$ can be represented as the linear transformations in the vector space spanned by $\{\psi_\mu, a_\kappa \psi_\mu\}$. The corresponding matrix representations are

$$\Delta(g_\alpha) = \begin{pmatrix} D(g_\alpha) & 0 \\ 0 & D^*(a_\kappa^{-1}g_\alpha a_\kappa) \end{pmatrix}$$  \hspace{1cm} (2.34)

$$\Delta(a_\beta) = \begin{pmatrix} 0 & D(a_\beta a_\kappa) \\ D^*(a_\kappa^{-1}a_\beta) & 0 \end{pmatrix}$$  \hspace{1cm} (2.35)

This set of the matrices is called the corepresentations of the magnetic group $M$.

The choice of $a_\kappa$ is arbitrary, any anti-unitary operator in the magnetic group $M$ serves the purpose. It can be shown that the corepresentations $\Delta$ generated by different $a_\kappa$ related by a unitary transformation, so in the representation theory, the two corepresentations are equivalent.

Though the matrices $\Delta$ derived above are the corepresentations of the magnetic group $M$, but the irreducibility is still need to be discussed.

Case A: All $D(g_\alpha)$ are not equivalent to $D^*(a_\kappa^{-1}g_\alpha a_\kappa)$, i.e. there is no unitary matrix $U$ which satisfies $D(g_\alpha) = UD^*(a_\kappa^{-1}g_\alpha a_\kappa)U^{-1}$.

In this case, it is easy to start with the subgroup $G_0 = \{g_\alpha\}$. From the above discussions we know that $\{\psi_\mu, a_\kappa \psi_\mu\}$ are the complete basis of the $G_0$. Define
the inner product of two wave functions as $\langle \psi(r), \phi(r) \rangle = \int dr \, \psi^*(r)\phi(r)$, then we have

$$
\langle \psi_\mu, a_\kappa \psi_\nu \rangle = \frac{1}{h} \sum_\alpha (g_\alpha \psi_\mu, g_\alpha a_\kappa \psi_\nu) = \frac{1}{h} \sum_\alpha \sum_\gamma D^*_{\gamma\mu}(g_\alpha) \sum_\beta D^*_{\beta\nu}(a_\kappa^{-1} g_\alpha a_\kappa)(\psi_\gamma, a_\kappa \psi_\beta) \tag{2.36}
$$

where $h$ is the number of the elements in the group $G_0$. In the last step, we have used previous result $g_\alpha a_\kappa \psi_\nu = \sum_\beta D^*_{\beta\nu}(a_\kappa^{-1} g_\alpha a_\kappa) a_\kappa \psi_\beta$. Because $D(g_\alpha) = UD^*(a_\kappa^{-1} g_\alpha a_\kappa)U^{-1}$, from the great orthogonality theorem, we have

$$
\frac{1}{h} \sum_\alpha D^*_{\gamma\mu}(g_\alpha) D^*_{\beta\nu}(a_\kappa^{-1} g_\alpha a_\kappa) = 0 \tag{2.37}
\Rightarrow \langle \psi_\mu, a_\kappa \psi_\nu \rangle = 0 \tag{2.38}
$$

So basis $\{\psi_\mu\}$ and basis $\{a_\kappa \psi_\nu\}$ are orthogonal to each other, any $a_\kappa \psi_\nu$ can not be expressed as linear combination of $\psi_\mu$. The corepresentations $\Delta(g_\alpha)$ and $\Delta(a_\beta)$ obtained in Eq.(2.34) and Eq.(2.35) are irreducible representations.

**Case B:** $D(g_\alpha)$ are equivalent to $D^*(a_\kappa^{-1} g_\alpha a_\kappa)$, i.e. there is a unitary matrix $U$ which satisfies $D(g_\alpha) = UD^*(a_\kappa^{-1} g_\alpha a_\kappa)U^{-1}$ for all the $g_\alpha$’s.

Put $g_\alpha = a_\kappa^{-1} g_\beta a_\kappa$ into $D(g_\alpha) = UD^*(a_\kappa^{-1} g_\alpha a_\kappa)U^{-1}$ and take the complex conjugate for both sides, we have

$$
D^*(a_\kappa^{-1} g_\alpha a_\kappa) = U^* D[(a_\kappa^{-1})^2 g_\beta(a_\kappa)^2](U^*)^{-1} \tag{2.39}
$$
From $D(g_\beta) = UD^*(a_\kappa^{-1}g_\beta a_\kappa)U^{-1}$, we also have $D^*(a_\kappa^{-1}g_\beta a_\kappa) = U^{-1}D(g_\beta)U$.

Put into Eq.(2.39), we have

$$U^{-1}D(g_\beta)U = U^*D[(a_\kappa^{-1})^2g_\beta(a_\kappa)^2](U^*)^{-1}$$

(2.40)

$$= U^*D[(a_\kappa^{-1})^2D(g_\beta)D(a_\kappa^2)(U^*)^{-1}$$

(2.41)

The last step we have used fact that $(a_\kappa^{-1})^2$, $g_\beta$ and $a_\kappa^2$ are unitary operators.

Then

$$D(g_\beta) = UU^*D^{-1}(a_\kappa^2)D(g_\beta)D(a_\kappa^2)(UU^*)^{-1}$$

(2.42)

$$\Rightarrow D(g_\beta)\{(UU^*)D^{-1}(a_\kappa^2)\} = \{(UU^*)D^{-1}(a_\kappa^2)\}D(g_\beta)$$

(2.43)

which is true for all $g_\beta$. According to Schur’s Lemma, we have

$$UU^*D^{-1}(a_\kappa^2) = \lambda I$$

(2.44)

$$\Rightarrow D(a_\kappa^2) = \frac{UU^*}{\lambda}, \quad D^*(a_\kappa^2) = \frac{U^*U}{\lambda^*}$$

(2.45)

From Eq.(2.39), we find that $D(a_\kappa^2) = UD^*(a_\kappa^{-1}a_\kappa^2a_\kappa)U^{-1} = UD^*(a_\kappa^2)U^{-1} \rightarrow D^*(a_\kappa^2) = \frac{U^{-1}UU^*U}{\lambda} = \frac{U^*U}{\lambda}$. With Eq.(2.45), we see that $\lambda$ is real. Next using the unitary properties of $D(a_\kappa^2)$ and $U$, we have

$$\det\left[D^\dagger(a_\kappa^2)D(a_\kappa^2)\right] = \det\left[D^\dagger(a_\kappa^2)D^*(a_\kappa^2)\right]$$

$$= \det\left[D(a_\kappa^2)\right]\det\left[D^*(a_\kappa^2)\right] = I$$

(2.46)
Same for \( \det[U] \det[U^*] = I \). Then

\[
\det \left[ D(a_\kappa^2) \right] \det \left[ D^*(a_\kappa^2) \right] = \frac{\det[U^*U] \det[UU^*]}{\lambda^2} \quad (2.47)
\]

\[
\Rightarrow \quad \lambda = \pm 1 \quad (2.48)
\]

We reached an important relation

\[
UU^* = \pm D(a_\kappa^2) \quad (2.49)
\]

The straightforward way to specify whether exists an irreducible representation is to see if one can block diagonalize all the matrices for one representation in the same way. To do so in our magnetic group case, we first use a unitary matrix \( N \) defined as

\[
N = \begin{pmatrix}
I & 0 \\
0 & U
\end{pmatrix} \quad (2.50)
\]

to block diagonalize \( \Delta(g_\alpha) \) in a way that it has the same diagonal elements.

\[
N\Delta(g_\alpha)N^{-1} = \begin{pmatrix}
D(g_\alpha) & 0 \\
0 & D(g_\alpha)
\end{pmatrix} \quad (2.51)
\]

Correspondingly, the basis become \( \{ \psi_\mu, U^{-1}a_\kappa \psi_\nu \} \). And \( \Delta(a_\beta) \) becomes

\[
N\Delta(a_\beta)N^{-1} = \begin{pmatrix}
0 & D(a_\beta a_\kappa)(U^*)^{-1} \\
D^*(a_\kappa^{-1}a_\beta) & 0
\end{pmatrix} \quad (2.52)
\]
Define a set of new basis \( \phi^+ = \{ \psi_{\mu} + U^{-1}a_\kappa \psi_{\nu} \} \), \( \phi^- = \{ \psi_{\mu} - U^{-1}a_\kappa \psi_{\nu} \} \), The \( \Delta \)'s under this basis transformation become

\[
\tilde{\Delta}(g_\alpha) = \begin{pmatrix}
D(g_\alpha) & 0 \\
0 & D(g_\alpha)
\end{pmatrix}
\] (2.53)

\[
\tilde{\Delta}(a_{\beta}) = \frac{1}{2} \begin{pmatrix}
D(a_\beta a_\kappa)(U^*)^{-1} + UD^*(a_\kappa^{-1}a_\beta) & -D(a_\beta a_\kappa)(U^*)^{-1} + UD^*(a_\kappa^{-1}a_\beta) \\
D(a_\beta a_\kappa)(U^*)^{-1} - UD^*(a_\kappa^{-1}a_\beta) & -D(a_\beta a_\kappa)(U^*)^{-1} - UD^*(a_\kappa^{-1}a_\beta)
\end{pmatrix}
\] (2.54)

Because \( UU^* = \pm D(a_\kappa^2) \), we have

- If \( D(a_\kappa^2) = UU^* \), then

\[
\tilde{\Delta}(a_{\beta}) = \begin{pmatrix}
D(a_\beta a_\kappa^{-1})U & 0 \\
0 & -D(a_\beta a_\kappa^{-1})U
\end{pmatrix}
\] (2.55)

\( \tilde{\Delta}(a_{\beta}) \) is block diagonalized in the same way as \( \tilde{D}(g_\alpha) \). So in this situation, the \( \tilde{\Delta} \) representation is reducible.

- If \( -D(a_\kappa^2) = UU^* \), then

\[
\tilde{\Delta}(a_{\beta}) = \begin{pmatrix}
0 & D(a_\beta a_\kappa^{-1})U \\
-D(a_\beta a_\kappa^{-1})U & 0
\end{pmatrix}
\] (2.56)

In this situation, the \( \tilde{\Delta} \) representation is irreducible.
Here we list the results in this section. The type III magnetic group $M = G_0 + \Theta(G - G_0)$, where $G_0 = \{g_\alpha\}$ is the subgroup of the point group $G$ of index 2. $g_\alpha$ is the unitary operator. $a_\beta \in \Theta(G - G_0)$ is the anti-unitary operator in $M$ which obeys $a_\beta = \Theta g_\beta$ with $g_\beta \in G$ but $g_\beta \notin G_0$. The corepresentations of $M$ are

1. $D(g_\alpha) = UD^*(a_\kappa^{-1}g_\alpha a_\kappa)U^{-1}$, $U$ is some unitary matrix.

Dimension of the original irreducible representation is doubled

$$
\Delta(g_\alpha) = \begin{pmatrix} D(g_\alpha) & 0 \\ 0 & D^*(a_\kappa^{-1}g_\alpha a_\kappa) \end{pmatrix} \quad (2.57)
$$

$$
\Delta(a_\beta) = \begin{pmatrix} 0 & D(a_\beta a_\kappa) \\ D^*(a_\kappa^{-1}a_\beta) & 0 \end{pmatrix} \quad (2.58)
$$

2. $D(g_\alpha) = UD^*(a_\kappa^{-1}g_\alpha a_\kappa)U^{-1}$ and $D(a_\kappa^2) = UU^*$.

We have two different irreducible representations

$$
\Gamma^{(1)}: \quad \Delta(g_\alpha) = D(g_\alpha); \quad \Delta(a_\beta) = D(a_\beta a_\kappa^{-1})U \quad (2.59)
$$

$$
\Gamma^{(2)}: \quad \Delta(g_\alpha) = D(g_\alpha); \quad \Delta(a_\beta) = -D(a_\beta a_\kappa^{-1})U \quad (2.60)
$$

3. $D(g_\alpha) = UD^*(a_\kappa^{-1}g_\alpha a_\kappa)U^{-1}$ and $-D(a_\kappa^2) = UU^*$. 

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Dimension of the original irreducible representation is doubled

\[
\Delta(g_\alpha) = \begin{pmatrix}
D(g_\alpha) & 0 \\
0 & D^*(a_\kappa^{-1}g_\alpha a_\kappa)
\end{pmatrix}
\]  \hspace{1cm} (2.61)

\[
\Delta(a_\beta) = \begin{pmatrix}
0 & D(a_\beta a_\kappa) \\
D^*(a_\kappa^{-1}a_\beta) & 0
\end{pmatrix}
\]  \hspace{1cm} (2.62)

2.3 Spontaneous Time Reversal Breaking and Current Loops in the 2D Lattice

If during the quantum phase transition, some current loops are induced in the 2D lattice system, the system will obviously break the time reversal symmetry. The system in such phase should be able to be described by the type III magnetic group, because type III magnetic group doesn’t contain the time reversal operator $\Theta$ as the symmetry operations. Because the lattice should always have the symmetry as the identity representation of the corresponding group, the magnetic group analysis should tell us what kinds of the current-loop patterns can be formed during the quantum phase transition.

In this section we will study two models, one is the 2D honeycomb lattice (Graphene), the other one is the 2D copper-oxide plane (CuO$_2$).

2.3.1 Current-Loop Patterns in Graphene

Let us first look at Graphene. Graphene has $C_{6v}(6mm)$ point group symmetry. $6mm$ is the international notation, 6 means there is a 6-fold rotation axis in the
system, and two $m$’s means there are two different kinds of reflection symmetry in the system. The symmetry operations are listed below.

$$C_{6v} = \{E, C_2, 2C_3, 2C_6, 3\sigma_d, 3\sigma_v\}$$

(2.63)

Figure 2.4: Symmetry operations of the Graphene.

From the previous section, we can construct all possible type III magnetic group of the $C_{6v}(6mm)$. There are only two possible type III magnetic groups.

$$6m'm' = \{C_6\} + \{3\Theta\sigma_d, 3\Theta\sigma_v\}$$

(2.64)

$$6'm'm = \{C_{3v}\} + \{\Theta C_2, 2\Theta C_6, 3\Theta\sigma_v\}$$

(2.65)

In $6m'm'$ the 6-fold rotation symmetry is conserved, while in $6'm'm$ only the 3-fold rotation remains. Notice that there is another possible construction $6'm'm' = \{C_{3v}\} + \{\Theta C_2, 2\Theta C_6, 3\Theta\sigma_v\}$. However, it is related to $6'm'm$ by a $\pi/6$ rotation, so they essentially are two identical groups.

Now according to these two magnetic groups, we are going to construct the loop currents in the system. First we want to construct current loops between nearest neighbor (n.n.) sites. We can put a current on one bond (denote as an arrow), and
then apply all the symmetry operations from the magnetic group on this current bond and it will generate the current loop patterns for us. By doing so we have

Figure 2.5: The current-loop pattern generate by the magnetic group $6m'm'$ in one unit cell.

$6'm'm'$ cannot generate current patterns only with the n.n. sites.

However, due to the translational symmetry, we need to pave this unit cell to the entire plane. Then we see each nearest neighbour bond current cancel each other. So such pattern is not possible.

Figure 2.6: Cancelation of the n.n. bond current loop in a translational invariant system.

We resort to the next nearest neighbor (n.n.n.) bond current. The magnetic groups are the same. So in the same spirit, this time we found both of them can generate possible translational invariant current-loop patterns [22].
Figure 2.7: The two current-loop patterns with the n.n.n. bond current.

In the quantum phase transition, the system will condense into the pattern with lower free energy.

2.3.2 Current-Loop Patterns in CuO$_2$

CuO$_2$ plane has $C_{4v}(4mm)$ point group symmetry.

\[ C_{4v} = \{E, C_2, 2C_4, 2\sigma_v, 2\sigma_d\} \]

Figure 2.8: Symmetry operations of the CuO$_2$ plane.

Follow the same procedure as in the Graphene’s analysis, we can construct two
possible type III magnetic point groups.

\[ 4m'm' = \{C_4\} + \{2\Theta\sigma_d, 2\Theta\sigma_v\} \]  \hspace{1cm} (2.66)

\[ 4'm'm = \{C_{2v}\} + \{2\Theta C_4, 2\Theta\sigma_v\} \]  \hspace{1cm} (2.67)

Applying the same method as for the Graphene case, we found the possible patterns are

Figure 2.9: Two possible current loop patterns in the CuO\(_2\) plane. Notice that the second pattern doesn’t involve copper-oxygen bond currents.

If we have some rhombic or orthorhombic distortion at the beginning, which reduces the original \(C_{4v}(4mm)\) symmetry to \(C_{2v}(mm2)\) point group symmetry, we can have two other patterns in the CuO\(_2\) plane which are described by magnetic point group \(mm'2'\) and \(m'm2'\):

Figure 2.10: Two possible current loop patterns in the distorted CuO\(_2\) plane.
These two magnetic groups essentially the same because they related by a $\pi/4$ rotation of the coordinates. Here we wrote as two just for clarification reason. Notice that the first pattern in the graph is the one proposed by C. M. Varma as the candidate for the spontaneous time reversal symmetry breaking in the High-$T_c$ superconductors.
Chapter 3

Mean Field Theory of TRV Phase in Graphene

In this chapter, we will study the possible spontaneous time reversal violation (TRV) in Graphene (honeycomb lattice) just by using mean field method. As mentioned in the introduction, mean field theory alone contains many useful physics about the order parameter, quantum critical point and even low energy collective excitations in the ordered phase. However, the analysis of the basic band structure of Graphene is still the most fundamental of all. We will give the brief derivation of the band structure of the graphene first.


3.1 Band Structure of Graphene

3.1.1 The Tight-Binding Method

Graphene is made out of carbon atoms arranged in hexagonal structure. There are two different carbon atoms (denote as “A” and “B” in the figure) in each unit cell (the hexagon in the graph). The center of each unit cell is sitting on the lattice point of the Bravis lattice. \( t_n \)'s are the lattice vector, and \( a_n \)'s are the lattice replacement from the center of the unit cell to atom A.

In this section, we only discuss the nearest neighbor (n.n.) hopping “t”. Then the tight-binding Hamiltonian of Graphene in the real space can be easily written. We have

\[
H_0 = -t \sum_{\langle i,j \rangle} A_i^\dagger B_j + \text{h.c.} \tag{3.1}
\]

Adopt the Fourier transformation for the second quantization operator in the tight
binding,

\[ A_i^\dagger = \frac{1}{L} \sum_k e^{i_k(R_{n_i}+a_i)} A_k^\dagger \tag{3.2} \]

The Hamiltonian written in the momentum space is

\[ H_0(k) = -\sum_k \epsilon_k e^{-i\theta_k} A_k^\dagger B_k - \sum_k \epsilon_k e^{i\theta_k} B_k^\dagger A_k \tag{3.3} \]

where \((t \text{ is the nearest neighbor hopping energy, and } t > 0.)\)

\[ \epsilon_k e^{i\theta_k} = t \sum_{a_n} e^{i_k a_n} \tag{3.4} \]

In the matrix form, the Hamiltonian is written as

\[ H_0(k) = \begin{pmatrix} 0 & -\epsilon_k e^{i\theta_k} \\ -\epsilon_k e^{-i\theta_k} & 0 \end{pmatrix} \tag{3.5} \]

Notice the basis is \((B_k^\dagger \ A_k^\dagger)\).

The eigenvalues are \(\pm \epsilon_k\), \(\epsilon_k \geq 0\) for any \(k\). Define the eigenstate as \(\psi_\pm(k) = (b_\pm \ a_\pm)^T\), we have

- For \(+\epsilon_k\),

\[ (-\epsilon_k)b_+ - \epsilon_k e^{i\theta_k} a_+ = 0 \quad \Rightarrow \quad \frac{a_+}{b_+} = \frac{1}{-\epsilon_k} \tag{3.6} \]

So \(\psi_+^\dagger(k) = \frac{1}{\sqrt{2}} (A_k^\dagger - e^{i\theta_k} B_k^\dagger)\).
• For $-\epsilon_k$,

$$\epsilon_k \beta_- - \epsilon_k e^{i\theta_k} a_- = 0 \Rightarrow \frac{a_-}{b_-} = \frac{1}{e^{i\theta_k}}$$

(3.7)

So $\psi_-^\dagger(k) = \frac{1}{\sqrt{2}}(A_k^\dagger + e^{i\theta_k} B_k^\dagger)$.

The corresponding reciprocal lattice of Graphene is still hexagonal,

Figure 3.2: The reciprocal lattice of Graphene. The graph shows the first Brillouin zone.

$K$ and $K'$ are two different Dirac points in the reciprocal lattice of Graphene. The typical choice of the Dirac points are

$$K = \left( \frac{4\pi}{3\sqrt{3}a}, 0 \right) \quad K' = \left( -\frac{4\pi}{3\sqrt{3}a}, 0 \right)$$

(3.8)

We can plot the Graphene’s band structure along the line in the momentum space $\Gamma \rightarrow K \rightarrow K' \rightarrow \Gamma$. We see that the energy gap disappears at the Dirac points $K$ and $K'$, Fig.(3.3). Many novel physics involve preserving or breaking the Dirac points. We will see in our time reversal violated phase transition, the degeneracy at the Dirac points is destroyed due to the symmetry breaking.
From the definition of $\theta_k$, Eq. (3.4), we found that at the Dirac point, $\theta_k$ is not defined. So is the wave function $\psi_\pm(k)$. The physics around the Dirac point is usually studied by expanding the Hamiltonian around it. Let us consider the expansion of the Hamiltonian and the eigenstates around the Dirac point $K = \left( \frac{4\pi}{3\sqrt{3}a}, 0 \right)$. We write $k = K + q$. The expansion we first need to show is $\sum_{a_n} \exp(iK \cdot a_n)$. We will use the fact that $\sum_{a_n} \exp(iK \cdot a_n) = 0$.

\[
\sum_{a_n} e^{ik \cdot a_n} = \sum_{a_n} e^{i(K+q) \cdot a_n} = \sum_{a_n} \cos((K+q) \cdot a_n) + i \sum_{a_n} \sin((K+q) \cdot a_n)
\]

\[
= \sum_{a_n} \cos(K \cdot a_n) \cos(q \cdot a_n) - \sum_{a_n} \sin(K \cdot a_n) \sin(q \cdot a_n)
\]

\[
+ i \sum_{a_n} \sin(K \cdot a_n) \cos(q \cdot a_n) + i \sum_{a_n} \cos(K \cdot a_n) \sin(q \cdot a_n)
\]

\[
\sim -\left(-\frac{\sqrt{3}}{2}\right)(q \cdot a_1) - \frac{\sqrt{3}}{2}(q \cdot a_2) + i\left(-\frac{1}{2}\right)(q \cdot a_1) + i\left(-\frac{1}{2}\right)(q \cdot a_2) + i(q \cdot a_3)
\]

\[
= -\frac{3a}{2}(q_x + iq_y)
\]

In the Hamiltonian, we are dealing with $-t \sum_{a_n} e^{ik \cdot a_n}$, then the expansion around
Dirac point $K$ is

$$-t \sum_{a_n} e^{i(K+q) \cdot a_n} = \frac{3at}{2} (q_x + i q_y) = |q| v_F e^{i \theta q}$$  \hspace{1cm} (3.12)$$

The matrix expression of the Hamiltonian around the Dirac point $K$ is

$$H_0(q) = |q| v_F \begin{pmatrix}
0 & e^{i \theta q} \\
e^{-i \theta q} & 0
\end{pmatrix}$$  \hspace{1cm} (3.13)$$

The eigenvalues are $E_{\pm}(q) = \pm v_F |q|$. The corresponding eigenstates are

$$E_+(q) = v_F |q| : \quad \psi_+(q) = \frac{1}{\sqrt{2}} (A_{K+q}^\dagger + e^{i \theta q} B_{K+q}^\dagger)$$  \hspace{1cm} (3.14)$$

$$E_-(q) = -v_F |q| : \quad \psi_-(q) = \frac{1}{\sqrt{2}} (A_{K+q}^\dagger - e^{i \theta q} B_{K+q}^\dagger)$$  \hspace{1cm} (3.15)$$

We see that the energy dispersion around the Dirac point is linear, $E_{\pm}(q) = \pm v_F |q|.$

### 3.1.2 Berry Phase In Graphene

In quantum mechanics, Berry phase is a geometric phase, in addition to the dynamic phase, captured by the wave function after the adiabatic evolution on a closed loop in the parameter space [23]. We now consider its realization in Bloch bands (crystalline solids) [24]. For the periodic potential $V(r + R) = V(R)$, where $R$ is the lattice vector, the single electron's wave function $\psi_{nk}(r)$ ($n$ is the band
index) should obey the Bloch’s theorem:

\[ \psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r}) \]  \hspace{1cm} (3.16)

The single electron Hamiltonian which determines the band structure of the crystal is

\[ H = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}) \]  \hspace{1cm} (3.17)

This Hamiltonian is \( \mathbf{k} \) dependent. In order to comply with the general formalism of the Berry phase [24], we make the following unitary transformation to obtain a \( \mathbf{k} \)-dependent Hamiltonian:

\[ H(\mathbf{k}) = e^{-i\mathbf{k} \cdot \mathbf{r}} H e^{i\mathbf{k} \cdot \mathbf{r}} = \left( \frac{\hat{\mathbf{p}} + \hbar \mathbf{k}}{2m} \right)^2 + V(\mathbf{r}) \]  \hspace{1cm} (3.18)

The transformed eigenstate \( \psi_{n\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k} \cdot \mathbf{r}} \psi_{n\mathbf{k}}(\mathbf{r}) \) is just the cell-periodic part of the Bloch function [25]. And it satisfies the strict periodic boundary condition

\[ \psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \psi_{n\mathbf{k}}(\mathbf{r}) \]  \hspace{1cm} (3.19)

This boundary condition ensures that all the eigenstates live in the same Hilbert space. Thus we can justify the Brillouin zone as the parameter space of the Hamiltonian \( H(\mathbf{k}) \) and \( |\psi_{n\mathbf{k}}\rangle \) as the basis function.

If we force \( \mathbf{k} \) to vary on a closed loop in the momentum space, then the Bloch state
will pick up a Berry phase:

$$\gamma_n = \oint_C d\mathbf{k} \cdot \langle u_{nk} | i\nabla_k | u_{nk} \rangle$$  \hspace{1cm} (3.20)$$

We emphasize that $\gamma_n$ is gauge-invariant as long as the path $C$ is closed.

However in the band structure calculations, we always use tight-binding approximation. So we need to establish the relation between the tight-binding wave function to the $|u_{nk}\rangle$. For a two level system, suppose we have atom $A$ and atom $B$ in one unit cell, and the atomic wave functions are denoted as $\phi_A(r)$ and $\phi_B(r)$. Then for the tight-binding wave function, we have

$$\psi_{nk}(r) = \frac{1}{\sqrt{N}} \sum_l \left( e^{i\mathbf{k} \cdot \mathbf{R}_l^A} a_{nk} \phi_A(r - \mathbf{R}_l^A) + e^{i\mathbf{k} \cdot \mathbf{R}_l^B} b_{nk} \phi_B(r - \mathbf{R}_l^B) \right)$$  \hspace{1cm} (3.21)$$

where $\mathbf{R}_l^A$ or $\mathbf{R}_l^B$ is the position of atom $A$ or atom $B$. This wave function satisfies the Bloch's theorem:

$$\psi_{nk}(r + \mathbf{R}) = \frac{1}{\sqrt{N}} \sum_l \left( e^{i\mathbf{k} \cdot \mathbf{R}_l^A} a_{nk} \phi_A(r + \mathbf{R} - \mathbf{R}_l^A) + e^{i\mathbf{k} \cdot \mathbf{R}_l^B} b_{nk} \phi_B(r + \mathbf{R} - \mathbf{R}_l^B) \right)$$

$$= e^{i\mathbf{k} \cdot \mathbf{R}} \frac{1}{\sqrt{N}} \sum_m \left( e^{i\mathbf{k} \cdot \mathbf{R}_m^A} a_{nk} \phi_A(r - \mathbf{R}_m^A) + e^{i\mathbf{k} \cdot \mathbf{R}_m^B} b_{nk} \phi_B(r - \mathbf{R}_m^B) \right)$$

$$= e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{nk}(r)$$  \hspace{1cm} (3.22)$$
From the previous discussion, we have

\[
\begin{align*}
    u_{nk}(r) &= e^{-ikr} \psi_{nk}(r) \\
    &= e^{-ikr} \frac{1}{\sqrt{N}} \sum_l \left( e^{iR_A^l a_{nk} \phi_A(r - R_A^l)} + e^{iR_B^l b_{nk} \phi_B(r - R_B^l)} \right)
\end{align*}
\]

Put this expression into the definition of the Berry phase Eq.(3.20), we have

\[
\begin{align*}
    \gamma_n &= \oint \mathbf{k} \cdot \left( u_{nk} |i \nabla_k |u_{nk} \right) = \oint \mathbf{k} \cdot \int dr \ u_{nk}^*(r) i \nabla_k u_{nk}(r) \\
    &= \oint \mathbf{k} \cdot \int dr \ u_{nk}^*(r)r u_{nk}(r) - \frac{1}{N} \oint \mathbf{k} \cdot \sum_l \left( |a_{nk}|^2 R_A^l + |b_{nk}|^2 R_B^l \right) \\
    &+ \frac{1}{N} \sum_l i \oint \mathbf{k} \cdot \left( a_{nk}^* \nabla_k a_{nk} + b_{nk}^* \nabla_k b_{nk} \right) \\
\end{align*}
\]

(3.23)

We have used the fact that in the tight-binding \( \int dr \ \phi_A^*(r - R_A^l) \phi_B(r - R_B^l) = 0 \) and \( \int dr \ \phi_A^*(r - R_A^l) \phi_A(r - R_A^m) = \delta_{lm} \). We also have \( \int dr \ u_{nk}^*(r)r u_{nk}(r) = 0 \) because it is an integral of an odd function. \( \frac{1}{N} \sum_l R_A^l = 0 \) because in the Bravis lattice there always exists \(-R_A^l\). Then the Berry phase is just simply

\[
\gamma_n = i \oint \mathbf{k} \cdot \left( a_{nk}^* \nabla_k a_{nk} + b_{nk}^* \nabla_k b_{nk} \right) \\
\]  

(3.24)

With this equation, we can calculate the Berry phase in Graphene.

Let us consider the \( \mathbf{k} \) very close to the Dirac point \( \mathbf{K} = (\frac{4\pi}{3\sqrt{3}}, 0) \), i.e. \( \mathbf{k} = \mathbf{K} + \mathbf{q} \).
The eigenfunctions respect to this expansion are

\[ E_+ (\mathbf{q}) = v_F |\mathbf{q}| : \quad \psi_+ (\mathbf{q}) = \frac{1}{\sqrt{2}} (A^\dagger_{\mathbf{K}+\mathbf{q}} + e^{i\theta_\mathbf{q}} B^\dagger_{\mathbf{K}+\mathbf{q}}) \] (3.25)

\[ E_- (\mathbf{q}) = -v_F |\mathbf{q}| : \quad \psi_- (\mathbf{q}) = \frac{1}{\sqrt{2}} (A^\dagger_{\mathbf{K}+\mathbf{q}} - e^{i\theta_\mathbf{q}} B^\dagger_{\mathbf{K}+\mathbf{q}}) \] (3.26)

where \( \tan \theta_\mathbf{q} = q_y/q_x \). At the Dirac points, we have \( q_x, q_y = 0 \), which means \( \theta_\mathbf{q} \) is not defined at the Dirac points. This is because at the the Dirac points, the energy gap closed and energy states are degenerate. As the result, the eigenstates are not defined at the Dirac points, we cannot define the topological index. But according to the topological phase transition theory, the gap closed state is the quantum critical point separating the topological phase (with nonzero topological number) and trivial insulator phase (zero topological number). So we can calculate the Berry phase in the graphene by reaching from the topological phase. The way to do it is we first adding a gap opening term \( \Delta \sigma_z \) into Graphene’s Hamiltonian Eq.(3.13). This added term \( \Delta \sigma_z \) can be derived from the spin-orbital coupling in Graphene [26] or simply a mass term in Boron Nitride [27]. And then we take the limit \( \Delta \to 0 \) in the Berry phase expression [28]. Follow this procedure, we first have

\[ H(\mathbf{q}) = \begin{pmatrix} \Delta & |\mathbf{q}|v_F e^{i\theta_\mathbf{q}} \\ |\mathbf{q}|v_F e^{-i\theta_\mathbf{q}} & -\Delta \end{pmatrix} \] (3.27)

The eigenvalues are \( E_\pm (\mathbf{q}) = \pm \epsilon = \pm \sqrt{\Delta^2 + (|\mathbf{q}|v_F)^2} \). The corresponding eigen-
states are

\[ \psi_+^\dagger(q) = \frac{\Delta + \epsilon}{\sqrt{2\epsilon(\epsilon + \Delta)}} A_{K+q}^\dagger + \frac{v_F |q| e^{-i\theta_q}}{\sqrt{2\epsilon(\epsilon + \Delta)}} B_{K+q}^\dagger \]  
(3.28)

\[ \psi_-^\dagger(q) = \frac{v_F |q| e^{i\theta_q} \sqrt{2\epsilon(\epsilon + \Delta)}}{\sqrt{2\epsilon(\epsilon + \Delta)}} A_{K+q}^\dagger - \frac{\Delta + \epsilon}{\sqrt{2\epsilon(\epsilon + \Delta)}} B_{K+q}^\dagger \]  
(3.29)

With this choice of the form, the wave functions are well defined at the Dirac point \( K \). This can be seen by putting \( |q| = 0 \), and we have \( \psi_+^\dagger(0) = A_{K+q}^\dagger \) and \( \psi_-^\dagger(0) = -B_{K+q}^\dagger \).

We choose the closed path \( C \) as a small circle around the Dirac point \( K \). Use the Berry phase expression Eq.(3.24), we have

\[ \gamma_\pm = i \oint_C dq \cdot \langle \psi_\pm(q) | \nabla_q | \psi_\pm(q) \rangle \]  
(3.30)

Because the path \( C \) is a circle, so \( dq = |q| d\theta_q \). So we have

\[ \gamma_\pm = i \oint_C d\theta_q \langle \psi_\pm(q) | \nabla_{\theta_q} | \psi_\pm(q) \rangle \]  
(3.31)

\[ = \pm \int_0^{2\pi} d\theta_q \frac{v_F^2 |q|^2}{2\epsilon(\epsilon + \Delta)} \]  
(3.32)

Now we can take the limit \( \Delta \to 0 \) and we have the Berry phase for Graphene calculated on a closed circle around the Dirac point \( K = (\frac{4\pi}{3\sqrt{3}}, 0) \) is \( \gamma_\pm = \pm \pi \) [27,28]. The Berry phase at the other Dirac point \( K' = (-\frac{4\pi}{3\sqrt{3}}, 0) \) is \( \gamma_\pm = \mp \pi \).
3.2 Mean Field Approximation In Real Space

3.2.1 The Real Space Order Parameter

From the previous magnetic group study, we found that the spontaneous time reversal violation (TRV) phase in Graphene is only possible when the n.n.n. interaction is included. One of the current patterns is shown below

![Figure 3.4: One of the possible current patterns in the TRV phase. Two distinguished current loops are formed in Graphene, current loop passing through atoms \( A \) and current loop passing through atoms \( B \). Both of them will generate magnetic flux \( \Phi \) in the system. For this pattern, both magnetic fluxes are going out of the plane.](image)

Closed current loops will generate magnetic flux in the system, and according to the Peierls substitution, such magnetic flux will induce a complex hopping term, and the phase is proportional to \( \int \mathbf{dr} \cdot \mathbf{A} \), where the integral region is along the bond between two sites and \( \mathbf{A} \) is the magnetic vector potential along the bond. In this spirit, we study one of the n.n.n. bond \( A_1A_3 \). The interaction term is \( \sim A_1^\dagger A_3^\dagger A_3 A_1 \). With the knowledge of the mean field theory, if we assign an order \( \chi e^{i\phi} = \langle A_1^\dagger A_3 \rangle \) to the system, we will generate hopping term \( \sim \chi e^{i\phi} A_3^\dagger A_1 \) in the mean field Hamiltonian. If \( \chi e^{i\phi} \) is complex, the mean field Hamiltonian will contain complex hopping terms and as if there exists vector potential along the bond \( A_1A_3 \).
In the figure demonstrated above, we can assign the same mean field order to other n.n.n. bonds, $A_3A_2$ and $A_2A_1$ and join these three bonds to form a closed loop of the vector potential. Because we don’t consider spin or external magnetic field, from the electrodynamics, such vector potential loop is consistent with the current loop shown in Fig.3.4. So in the mean field calculation, we are going to expect a complex order parameter $\chi e^{i\phi}$ which is the expectation value of the hopping between n.n.n. sites.

For completeness, we will also study the possible order formed on the n.n. bonds.

In the last chapter, we have shown that current loop patterns cannot be formed on the n.n. bonds, so we only study the possible charge density order on the n.n. bonds. Such order is governed by the order parameter $\rho = \frac{1}{2}(\langle A_i^\dagger A_i \rangle - \langle B_i^\dagger B_i \rangle)$.

### 3.2.2 Mean Field Approximation

The minimum Hamiltonian we use for studying the TRV phase transition in Graphene is

\[
H = -t \sum_{\langle i,j \rangle} A_i^\dagger B_j + \text{h.c.} + V_1 \sum_{\langle i,j \rangle} A_i^\dagger A_i B_j^\dagger B_j + V_2 \sum_{\langle\langle i,j \rangle\rangle} A_i^\dagger A_i A_j^\dagger A_j + V_2 \sum_{\langle\langle i,j \rangle\rangle} B_i^\dagger B_i B_j^\dagger B_j
\]

(3.33)

$\langle i, j \rangle$ means nearest neighbor sites while $\langle\langle i, j \rangle\rangle$ means next nearest neighbor sites. Spin degrees of freedom are suppressed to avoid any spin-related time reversal breaking [29]. For the current pattern shown in Fig.3.4, we assign the following
orders in the mean field approximation:

\[
\langle A_1^\dagger A_3 \rangle = \langle A_2^\dagger A_1 \rangle = \langle A_3^\dagger A_1 \rangle = \tilde{\chi} e^{i\phi}
\]  
(3.34)

\[
\langle B_1^\dagger B_3 \rangle = \langle B_2^\dagger B_1 \rangle = \langle B_3^\dagger B_1 \rangle = \tilde{\chi} e^{i\phi}
\]  
(3.35)

and for the n.n. bonds

\[
\frac{1}{2}(\langle A_i^\dagger A_i \rangle - \langle B_i^\dagger B_i \rangle) = \rho
\]  
(3.36)

The mean field Hamiltonian reads

\[
H_{MF} = -t \sum_{\langle i,j \rangle} A_i^\dagger B_j + V_1 \rho \sum_{\langle i,j \rangle} \left( B_j^\dagger B_j - A_i^\dagger A_i \right) + 3V_1 N \rho^2 - V_2 \tilde{\chi} e^{i\phi} \sum_n \left( A_1^\dagger A_2 + A_2^\dagger A_3 + A_3^\dagger A_1 \right)_n
\]

\[
-2V_2 \tilde{\chi} e^{i\phi} \sum_n \left( B_1^\dagger B_2 + B_2^\dagger B_3 + B_3^\dagger B_1 \right)_n + 6V_2 N \tilde{\chi}^2 + h.c.
\]  
(3.37)

"\( \sum_n \)" means summation over all the unit cells and \( N \) is the number of the unit cells.

Use the Fourier transform, we can write the above Hamiltonian in the momentum space as

\[
H_{MF}(k) = -\sum_k \epsilon_k e^{-i k \cdot n} A_k^\dagger B_k - \sum_k \epsilon_k e^{i k \cdot n} B_k^\dagger A_k - 3V_1 \rho \sum_k (A_k^\dagger A_k - B_k^\dagger B_k) + 3V_1 N \rho^2
\]

\[
-2V_2 \tilde{\chi} \sum_k \sum_{\mathbf{t}_n} \cos(\mathbf{k} \cdot \mathbf{t}_n - \phi) A_k^\dagger A_k - 2V_2 \tilde{\chi} \sum_k \sum_{\mathbf{t}_n} \cos(\mathbf{k} \cdot \mathbf{t}_n + \phi) B_k^\dagger B_k + 6V_2 N \tilde{\chi}^2
\]
The corresponding matrix form is

\[
H_{MF}(k) = \begin{pmatrix}
3V_1 \rho - 2V_2 \tilde{\chi} \sum_t \cos(k \cdot t + \phi) & -\epsilon_k e^{i\theta} \\
-\epsilon_k e^{-i\theta} & -3V_1 \rho - 2V_2 \tilde{\chi} \sum_t \cos(k \cdot t - \phi)
\end{pmatrix}
\]  

(3.38)

Eigenvalues are

\[
E_{\pm}(k) = -2V_2 \tilde{\chi} \sum_t \cos(k \cdot t) \cos \phi \pm \sqrt{\epsilon_k^2 + \left(3V_1 \rho + 2V_2 \tilde{\chi} \sum_t \sin(k \cdot t) \sin \phi\right)^2}
\]  

(3.39)

At zero temperature and half filling, and use \( \sum_k \cos(k \cdot t) = 0 \) if the band is fully filled, we can write down the free energy as

\[
F = -\sum_k \sqrt{\epsilon_k^2 + \left(3V_1 \rho + 2V_2 \tilde{\chi} \sum_t \sin(k \cdot t) \sin \phi\right)^2} + 3V_1 N \rho^2 + 6V_2 N \tilde{\chi}^2
\]  

(3.40)

We now minimize the free energy with respect to the order parameter.

\[
\frac{\partial F}{\partial \phi} = 0 \quad \Rightarrow \quad -\sum_k \frac{\left(3V_1 \rho + 2V_2 \tilde{\chi} \sum_t \sin(k \cdot t) \sin \phi\right) \cos \phi}{\sqrt{\epsilon_k^2 + \left(3V_1 \rho + 2V_2 \tilde{\chi} \sum_t \sin(k \cdot t) \sin \phi\right)^2}} = 0
\]  

(3.41)

The solution of \( \phi \) is \( \phi = \frac{\pi}{2}, \frac{3\pi}{2} \). Choice of \( \phi \) depends on the direction of the bond current. Let us choose \( \phi = \frac{\pi}{2} \).
Then we have

\[ \frac{\partial F}{\partial \rho} = 0 \Rightarrow \rho = \frac{1}{6N} \sum_k \frac{3(3V_1 \rho + 2V_2 \bar{\chi} \sum t_n \sin(k \cdot t_n))}{\sqrt{\epsilon_k^2 + (3V_1 \rho + 2V_2 \bar{\chi} \sum t_n \sin(k \cdot t_n))^2}} \]  

(3.42)

\[ \frac{\partial F}{\partial \bar{\chi}} = 0 \Rightarrow \bar{\chi} = \frac{1}{6N} \sum_k \frac{(3V_1 \rho + 2V_2 \bar{\chi} \sum t_n \sin(k \cdot t_n)) \sum t_n \sin(k \cdot t_n)}{\sqrt{\epsilon_k^2 + (3V_1 \rho + 2V_2 \bar{\chi} \sum t_n \sin(k \cdot t_n))^2}} \]  

(3.43)

If \( V_2 = 0 \), the critical value for \( V_1 \) is to put \( \rho = 0 \) in Eq. 3.42

\[ \frac{1}{V_{1c}} = \frac{3}{2N} \sum_k \frac{1}{\epsilon_k} \]  

(3.44)

If \( V_1 = 0 \), the critical value for \( V_2 \) is to put \( \bar{\chi} = 0 \) in Eq. 3.43

\[ \frac{1}{V_{2c}} = \frac{1}{3N} \sum_k \frac{(\sum t_n \sin(k \cdot t_n))^2}{\epsilon_k} \]  

(3.45)

The phase diagram of this system is

![Phase Diagram](image)

Figure 3.5: The phase diagram of the system.
In the “time reversal violated phase (TRV)”, $\rho = 0$ but $\tilde{\chi} \neq 0$. So if we want to study the properties of time reversal breaking, we can focus on this phase region and ignore the $V_1$ part. Then the minimum model to study the TRV phase transition in Graphene is only to include the n.n.n. interaction:

$$H = -t \sum_{(i,j)} A_i^\dagger B_j + \text{h.c.} + V \sum_{\langle i,j \rangle} A_i^\dagger A_i A_j^\dagger A_j + V \sum_{\langle i,j \rangle} B_i^\dagger B_i B_j$$

(3.46)

The self consistent equation is

$$\frac{1}{V} = \frac{1}{3N} \sum_k \frac{(\sum_{t_n} \sin(k \cdot t_n))^2}{\sqrt{\epsilon_k^2 + (2V\tilde{\chi}\sum_{t_n} \sin(k \cdot t_n))^2}}$$

(3.47)

The critical $V_c$ is by putting $\tilde{\chi} = 0$ in the self-consistent equation, and we have

$$V_c = 1.18t$$

(3.48)

where $t$ is the hopping energy. The energy dispersions are

$$E_{\pm}(k) = \pm \sqrt{\epsilon_k^2 + \left(2V\tilde{\chi}\sum_{t_n} \sin(k \cdot t_n)\right)^2}$$

(3.49)

We can see that in contrast to the Graphene situation where the gap closed at the Dirac point $K$ due to $\epsilon_K = 0$, now a finite gap $E_G$ is opened at the Dirac point with the magnitude $E_G = 4V\tilde{\chi} \left|\sum_{t_n} \sin(K \cdot t_n)\right| = 6\sqrt{3}V\tilde{\chi}$. This is so called “Topological Mott Insulator” at half filling [30]. The energy dispersion can be plotted by using one of the self-consistent solution $V = 2t, \tilde{\chi} = 0.067$. 

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Figure 3.6: The band structure of Graphene in the TRV phase. Notice that there are gaps opened at the Dirac points.

3.3 Mean Field Approximation in the Momentum Space

The main problem of doing mean field with order parameter $\langle A_2^\dagger A_1 \rangle = i\chi$ is that the operator doesn’t commute with the operator on the adjacent unit cell. Then it is ambiguous to give a mean value to two non-commuting operator. Also using this mean field Hamiltonian, it is very hard to study the collective mode and also the fluctuations in the problem. So we resort to some new way of doing the mean field approximation.
3.3.1 Effective Model in the Momentum Space

Let us see how this can be done in the Graphene. Graphene’s Hamiltonian with only next nearest neighbour interaction is

$$H = -t \sum_{\langle i,j \rangle} A_i^\dagger B_j + \text{h.c.} + V \sum_{\langle i,j \rangle} A_i^\dagger A_i A_j^\dagger A_j + V \sum_{\langle i,j \rangle} B_i^\dagger B_i B_j^\dagger B_j$$

(3.50)

The pattern we study is still

We first Fourier transform the Hamiltonian into the momentum space,

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{a}_n} A_\mathbf{k}^\dagger B_\mathbf{k} - \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{a}_n} B_\mathbf{k}^\dagger A_\mathbf{k} - \frac{V}{N} \sum_{\mathbf{k},p,q} g(\mathbf{k} - \mathbf{p}) A_{\mathbf{k} + \frac{q}{2}}^\dagger A_{\mathbf{k} - \frac{q}{2}} A_{\mathbf{p} - \frac{q}{2}}^\dagger A_{\mathbf{p} + \frac{q}{2}}$$

$$- \frac{V}{N} \sum_{\mathbf{k},p,q} g(\mathbf{k} - \mathbf{p}) B_{\mathbf{k} + \frac{q}{2}}^\dagger B_{\mathbf{k} - \frac{q}{2}} B_{\mathbf{p} - \frac{q}{2}}^\dagger B_{\mathbf{p} + \frac{q}{2}}$$

(3.51)

Here $\epsilon_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{a}_n} = \sum_{n=1}^{3} \exp(i\mathbf{k} \cdot \mathbf{a}_n)$ and $g(\mathbf{k} - \mathbf{p}) = \sum_{n=1}^{3} \cos[(\mathbf{k} - \mathbf{p}) \cdot \mathbf{t}_n]$. $N$ is the number of unit cells. Because we only interested in the mean field approximation.
right now, only $q = 0$ terms is needed in the interaction. We have

$$H = - \sum_k \epsilon_k e^{-i\hat{\theta}_k} A_k^\dagger B_k - \sum_k \epsilon_k e^{i\hat{\theta}_k} B_k^\dagger A_k - \frac{V}{N} \sum_{k,p} g(k-p) A_k^\dagger A_k A_p^\dagger A_p$$

$$- \frac{V}{N} \sum_{k,p} g(k-p) B_k^\dagger B_k B_p^\dagger B_p$$

(3.52)

Here we are going to introduce the pseudo-spin language [31,32]. We can construct pseudo-spins by using basis $|A_k\rangle$ and $|B_k\rangle$.

$$\sigma^3_k = A_k^\dagger A_k - B_k^\dagger B_k$$

(3.53)

$$\sigma^1_k = e^{-i\hat{\theta}_k} A_k^\dagger B_k + e^{i\hat{\theta}_k} B_k^\dagger A_k$$

(3.54)

$$\sigma^2_k = (-i) \left( e^{-i\hat{\theta}_k} A_k^\dagger B_k - e^{i\hat{\theta}_k} B_k^\dagger A_k \right)$$

(3.55)

$$\sigma^0_k = A_k^\dagger A_k + B_k^\dagger B_k$$

(3.56)

And they satisfy the commutation relations:

$$[\sigma^1_k, \sigma^2_p] = 2i\sigma^3_k \delta_{kp}$$

(3.57)

$$[\sigma^2_k, \sigma^3_p] = 2i\sigma^1_k \delta_{kp}$$

(3.58)

$$[\sigma^3_k, \sigma^1_p] = 2i\sigma^2_k \delta_{kp}$$

(3.59)

Using identities

$$\sigma^3_k \sigma^3_p = A_k^\dagger A_k A_p^\dagger A_p + B_k^\dagger B_k B_p^\dagger B_p - A_k^\dagger A_k B_p^\dagger B_p - B_k^\dagger B_k A_p^\dagger A_p$$

(3.60)

$$\sigma^0_k \sigma^0_p = A_k^\dagger A_k A_p^\dagger A_p + B_k^\dagger B_k B_p^\dagger B_p + A_k^\dagger A_k B_p^\dagger B_p + B_k^\dagger B_k A_p^\dagger A_p$$

(3.61)
We have

\[ H = -\sum_k \epsilon_k \sigma_k^1 - \frac{V}{2N} \sum_{k,p} g(k-p) \sigma_k^3 \sigma_p^3 - \frac{V}{2N} \sum_{k,p} g(k-p) \sigma_k^0 \sigma_p^0 \] (3.62)

where \( \sigma_k^0 \) is a number operator for the state \( k \). As we can see in the mean field approximation, the number of electrons per \( k \) state is fixed, because \( q = 0 \), so this term is not going to contribute in the mean field approximation. So the effective Hamiltonian we have is

\[ H = -\sum_k \epsilon_k \sigma_k^1 - \frac{V}{2N} \sum_{k,p} g(k-p) \sigma_k^3 \sigma_p^3 \] (3.63)

This is similar to the transverse Ising model with long range interaction.

### 3.3.2 Mean Field Approximation in the Momentum Space

In the last section, we have obtained an effective Hamiltonian ready for the mean field approximation. This effective Hamiltonian is in the same class as the transverse Ising model introduced earlier. Following the same procedure as in the mean field calculation in the transverse Ising model, we first assign the order parameter

\[ \left\langle \sigma_k^3 \right\rangle = \cos \phi_k \] (3.64)

Notice that \( \cos \phi_k \) is real because \( (\sigma_k^3)^\dagger = \sigma_k^3 \). Then we have

\[ H_{MF} = -\sum_k \epsilon_k \sigma_k^1 - \frac{V}{N} \sum_{k,p} g(k-p) \cos \phi_p \sigma_k^3 + \frac{V}{2N} \sum_{k,p} g(k-p) \cos \phi_k \cos \phi_p \] (3.65)
Define a real function $\chi_k$

$$\chi_k = \frac{V}{N} \sum_p g(k - p) \cos \phi_p$$  \hspace{1cm} (3.66)

The mean field Hamiltonian is

$$H_{MF} = -\sum_k \epsilon_k \sigma_k^1 - \sum_k \chi_k \sigma_k^3 + \frac{1}{2} \sum_k \chi_k \cos \phi_k$$ \hspace{1cm} (3.67)

Matrix form is (basis are $(B_k^\dagger \ A_k^\dagger)$)

$$H_{MF} = \begin{pmatrix} \chi_k & -\epsilon_k \\ -\epsilon_k & -\chi_k \end{pmatrix}$$ \hspace{1cm} (3.68)

Energy eigenvalues are

$$E_\pm(k) = \pm \sqrt{\chi_k^2 + \epsilon_k^2}$$ \hspace{1cm} (3.69)

At zero temperature and half filling, the free energy is

$$F = -\sum_k \sqrt{\chi_k^2 + \epsilon_k^2} + \frac{1}{2} \sum_k \chi_k \cos \phi_k$$ \hspace{1cm} (3.70)

Minimize the free energy with respect to the order parameter $\cos \phi_p$, we have

$$\frac{\partial F}{\partial (\cos \phi_p)} = -\frac{V}{N} \sum_k \chi_k \frac{g(k - p)}{\sqrt{\chi_k^2 + \epsilon_k^2}} + \frac{1}{2} \chi_p + \frac{V}{2N} \sum_k g(k - p) \cos \phi_k = 0$$

$$\Rightarrow \chi_p = \frac{V}{N} \sum_k \frac{\chi_k g(p - k)}{\sqrt{\chi_k^2 + \epsilon_k^2}}$$ \hspace{1cm} (3.71)
After changing the index, we have

\[ \chi_k = \frac{V}{N} \sum_p \frac{\chi_p \, g(k - p)}{\sqrt{\lambda_p^2 + \epsilon_p^2}} \]  

(3.72)

And with another equation Eq.(3.66) for \( \chi_k \)

\[ \chi_k = \frac{V}{N} \sum_p g(k - p) \cos \phi_p \]  

(3.73)

We can say

\[ \cos \phi_p = \frac{\chi_p}{\sqrt{\lambda_p^2 + \epsilon_p^2}} \]  

(3.74)

Let us look at function \( g(k - p) \) more carefully.

\[ g(k - p) = \sum_{t_n} \left( \cos(k \cdot t_n) \cos(k \cdot t_n) + \sin(k \cdot t_n) \sin(p \cdot t_n) \right) \]  

(3.75)

The self consistent equation for \( \chi_k \) is Eq.(3.72)

\[ \chi_k = \frac{V}{N} \sum_p \frac{\chi_p \, g(k - p)}{\sqrt{\lambda_p^2 + \epsilon_p^2}} \]  

(3.76)

The right hand side after summing over \( p \), left with \( \cos(k \cdot t_n) \) or \( \sin(k \cdot t_n) \) depending on the even or odd property of \( \chi_k \) with respect to \( k \). The left hand side is \( \chi_k \), so \( \chi_k \) should be in the form of \( \cos(k \cdot t_n) \) or \( \sin(k \cdot t_n) \). Furthermore, the order parameter should have at least \( C_3 \) symmetry, so \( \chi_k \) is in the form of \( \sum_{t_n} \cos(k \cdot t_n) \) or \( \sum_{t_n} \sin(k \cdot t_n) \).

Also from observation of the pattern, we found \( H_{MF} \) Eq.(3.68) should have Inver-
sion symmetry $I$ as $IH_{MF}I^{-1} = H_{MF}$. Notice that the Inversion operation here not only changed $\mathbf{k} \rightarrow -\mathbf{k}$, but also swap the $A_k$ and $B_k$. So Inversion symmetry tells us: ($\epsilon_k$ is an even function of $\mathbf{k}$)

\[
IH_{MF}(\mathbf{k})I^{-1} = \sigma_z H_{MF}(-\mathbf{k})\sigma_x \]

\[
= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \chi_{-\mathbf{k}} & -\epsilon_{-\mathbf{k}} \\ -\epsilon_{-\mathbf{k}} & -\chi_{-\mathbf{k}} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

\[
= \begin{pmatrix} -\chi_{-\mathbf{k}} & -\epsilon_k \\ -\epsilon_k & \chi_{-\mathbf{k}} \end{pmatrix} = H_{MF} = \begin{pmatrix} \chi_k & -\epsilon_k \\ -\epsilon_k & -\chi_k \end{pmatrix}
\]

(3.77)

Then $\chi_k$ has to be an odd function.

We can treat $\chi_k$ as odd function in the $H_{MF}(\mathbf{k})$ and check the time-reversal property. Under Time-Reversal operator $\Theta$, the $k$-space Hamiltonian transform as

\[
\Theta H_{MF}(\mathbf{k})\Theta^{-1} = H_{MF}^*(-\mathbf{k}) \]

\[
= \begin{pmatrix} \chi_{-\mathbf{k}} & -\epsilon_k \\ -\epsilon_k & -\chi_{-\mathbf{k}} \end{pmatrix}^* \]

\[
= \begin{pmatrix} -\chi_k & -\epsilon_k \\ -\epsilon_k & \chi_k \end{pmatrix}
\]

\ne H_{MF}(\mathbf{k})
\]

(3.78)

Time-Reversal symmetry is broken with this order parameter.

In summary, $\chi_k$ embodied our choice of the current pattern can only be in the
form of

$$\chi_k = \chi \sum_{t_n} \sin(k \cdot t_n) \tag{3.79}$$

Notice that comparing to the real space mean field, $\chi = 2V \bar{\chi}$. If we put this $\chi_k$ into the self-consistent equation Eq.(3.72), we have

$$\chi_k = \frac{V}{N} \sum_{p} \frac{\chi_p g(k - p)}{\sqrt{\chi_p^2 + \epsilon_p^2}}$$

$$\Rightarrow \chi \sum_{t_n} \sin(k \cdot t_n) = \frac{V}{N} \sum_{p} \frac{\chi \sum_{t_n} \sin(p \cdot t_n) g(k - p)}{\sqrt{\chi^2 \left(\sum_{t_n} \sin(p \cdot t_n)\right)^2 + \epsilon_p^2}} \tag{3.80}$$

This expression involves the summation

$$\sum_{p} \frac{\sum_{t_n} \sin(p \cdot t_n) g(k - p)}{\sqrt{\chi^2 \left(\sum_{t_n} \sin(p \cdot t_n)\right)^2 + \epsilon_p^2}} \tag{3.81}$$

Because $\sum_{t_n} \sin(p \cdot t_n)$ is an odd function, and $\sum_{p}$ go over the entire Brillouin Zone, only odd part from $g(k - p)$ will contribute. So the summation reduces to

$$\sum_{p} \frac{\sum_{t_n} \sin(p \cdot t_n) \sum_{t_m} \sin(k \cdot t_m) \sin(p \cdot t_m)}{\sqrt{\chi^2 \left(\sum_{t_n} \sin(p \cdot t_n)\right)^2 + \epsilon_p^2}}$$

$$= \sum_{t_m} \sin(k \cdot t_m) \sum_{p} \frac{\sin(p \cdot t_m) \sum_{t_n} \sin(p \cdot t_n)}{\sqrt{\chi^2 \left(\sum_{t_n} \sin(p \cdot t_n)\right)^2 + \epsilon_p^2}} \tag{3.82}$$
Due to the $C_3$ symmetry, we have

\[
\sum_{\mathbf{p}} \frac{\sin(\mathbf{p} \cdot \mathbf{t}_1) \sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n)}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}} = \sum_{\mathbf{p}} \frac{\sin(\mathbf{p} \cdot \mathbf{t}_2) \sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n)}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}}
\]

\[
= \sum_{\mathbf{p}} \frac{\sin(\mathbf{p} \cdot \mathbf{t}_3) \sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n)}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}} = \frac{1}{3} \sum_{\mathbf{p}} \frac{(\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}}
\]

Then the $\mathbf{p}$ summation Eq. 3.82 becomes

\[
\sum_{\mathbf{p}} \frac{\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n) \sum_{\mathbf{t}_m} \sin(\mathbf{k} \cdot \mathbf{t}_m) \sin(\mathbf{p} \cdot \mathbf{t}_m)}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}} = \sum_{\mathbf{p}} \frac{\sum_{\mathbf{t}_n} \sin(\mathbf{k} \cdot \mathbf{t}_m) \frac{1}{3} \sum_{\mathbf{p}} \frac{(\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}}}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}}
\]

(3.83)

Now we put this relation back to Eq. 3.80, we have

\[
\chi \sum_{\mathbf{t}_n} \sin(\mathbf{k} \cdot \mathbf{t}_n) = \frac{V}{N} \sum_{\mathbf{p}} \frac{\chi \sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n) g(\mathbf{k} - \mathbf{p})}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}}
\]

\[
\Rightarrow \chi \sum_{\mathbf{t}_n} \sin(\mathbf{k} \cdot \mathbf{t}_n) = \sum_{\mathbf{t}_n} \sin(\mathbf{k} \cdot \mathbf{t}_m) \frac{V}{3N} \sum_{\mathbf{p}} \frac{\chi (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}}
\]

\[
\Rightarrow \frac{1}{V} = \frac{1}{3N} \sum_{\mathbf{p}} \frac{(\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2}{\sqrt{\chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{p} \cdot \mathbf{t}_n))^2 + \epsilon_p^2}}
\]

(3.84)

Which is exactly the same as the mean field result in the real space order parameter Eq.(3.47). This finite $\chi$ breaks the time reversal symmetry [33].
3.3.3 Universality of the Phase Transition

The self consistent equation for $\chi$ is

$$\frac{1}{V} = \frac{1}{3N} \sum_k \frac{(\sum_{t_n} \sin(k \cdot t_n))^2}{\sqrt{\epsilon_k^2 + \chi^2 (\sum_{t_n} \sin(k \cdot t_n))^2}} \quad (3.85)$$

And from that we can obtain the expression for the critical value for $\tilde{V}$, which is

$$\frac{1}{V_c} = \frac{1}{3N} \sum_k \frac{(\sum_{t_n} \sin(k \cdot t_n))^2}{\epsilon_k} \quad (3.86)$$

We have $V_c = 1.183t$.

We need to do some suitable approximation to get the universality. We first plot the function $\frac{(\sum_{t_n} \sin(k \cdot t_n))^2}{\epsilon_k}$.

![Figure 3.7: Function $\frac{(\sum_{t_n} \sin(k \cdot t_n))^2}{\epsilon_k}$ in the $k$-space. The main contributions of this function to the "$\sum_{k}$" are around the Dirac points.](image)

We can see that the main contributions to the integral are from the function value at the Dirac points. So we can draw two circles around the Dirac points and the inside areas are the main region contributed to the integral. From this approximation we can obtain a cut-off for our problem when $V - V_c$ is small.
We use the following approximations at Dirac Points \((\mathbf{k} = \mathbf{K} + \mathbf{q})\):

\[
\left( \sum_{\mathbf{t}_n} \sin(\mathbf{k} \cdot \mathbf{t}_n) \right)^2 = \frac{27}{4} \quad \sum_{\mathbf{t}_n} \cos(\mathbf{k} \cdot \mathbf{t}_n) = \frac{9}{4} a^2 |\mathbf{q}|^2
\]  

(3.87)

Then Eq.(3.86) becomes (factor “2” is due to two circles around Dirac Points)

\[
\frac{1}{V_c} = 2 \times \frac{1}{3N} \frac{L^2}{4\pi^2} \int_{0}^{k_A} dq \frac{2\pi q}{4\sqrt{\frac{a^2}{4} t^2 a^2 q^2}}
\]

\[
\Rightarrow k_A = \frac{2\pi t N a}{3V_c L^2}
\]  

(3.88)

Now we study the self-consistent equation for \(\chi\), Eq.(3.85). Also remember that \(\chi\) is very small when \(V\) is very close to \(V_c\).

\[
\frac{1}{V} = \frac{1}{3N} \sum_{\mathbf{k}} \frac{(\sum_{\mathbf{t}_n} \sin(\mathbf{k} \cdot \mathbf{t}_n))^2}{\sqrt{\epsilon_k^2 + \chi^2 (\sum_{\mathbf{t}_n} \sin(\mathbf{k} \cdot \mathbf{t}_n))^2}}
\]

\[
\Rightarrow \frac{1}{V} = \frac{3L^2}{2\pi N} \int_{0}^{k_A} dq \frac{1}{\sqrt{t^2 a^2 q^2 + 3\chi^2}}
\]

\[
\Rightarrow \frac{2\pi t^2 N a^2}{3L^2 V} = \sqrt{3V^2 \chi^2 + t^2 a^2 k_A^2} - \sqrt{3\chi} \approx t k_A - \sqrt{3\chi}
\]

(3.89)

\[
\Rightarrow \chi \approx \frac{4\pi t^2 (V - V_c)}{27V_c^2}
\]  

(3.90)

\[
\frac{L^2}{N a^2}
\]

is the area of one unit cell, which is \(\frac{3\sqrt{3}}{2}\). \(\chi\) is linearly proportional to \(V - V_c\).
3.3.4 Low Energy Collective Mode in the TRV Phase

In the above section, we have cast the problem into a minimum model, the transverse Ising problem with Hamiltonian Eq.(3.63),

$$H = -\sum_k \epsilon_k \sigma^1_k - \frac{V}{2N} \sum_{k,p} g(k-p) \sigma^3_k \sigma^3_p$$  \hspace{1cm} (3.91)

And we have also shown the possible TRV phase transition in this model. Now in the TRV phase, we are going to find the low energy excitations i.e. the low energy collective mode in the system. It is straight forward to be done in the pseudo-spin language. Use equation of motion \( \frac{d}{dt} \sigma^j_k = i[H, \sigma^j_k] \), we have

\[
\begin{align*}
\frac{d\sigma^1_k}{dt} &= \Delta_k \sigma^2_k \\
\frac{d\sigma^2_k}{dt} &= -\Delta_k \sigma^1_k + 2 \sin \alpha_k \frac{V}{N} \sum_p g(k-p)(\sin \alpha_p \sigma^1_p - \cos \alpha_p \sigma^3_p) \\
\frac{d\sigma^3_k}{dt} &= 0
\end{align*}
\]  \hspace{1cm} (3.92)
Where

\[
\sin \alpha_k = \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \chi^2 \left( \sum_{t_n} \sin(k \cdot t_n) \right)^2}}
\]

\[
\Delta_k = 2 \sqrt{\epsilon_k^2 + \chi^2 \left( \sum_{t_n} \sin(k \cdot t_n) \right)^2}
\]  

Second derivative of $\sigma_k^2$ is

\[
\ddot{\sigma}_k^2 = -\Delta_k^2 \sigma_k^2 + 2 \sin \alpha_k \frac{V}{N} \sum_p g(k - p) \sin \alpha_p \Delta_p \sigma_p^2
\]

$\sigma_k^2$ can be expressed as

\[
\sigma_k^2 = u_k(t) \sigma^1 + v_k(t) \sigma^2
\]

Put this expression into the Eq.(3.96), we have the expression for $v_k(t)$ as (same equation for $u_k(t)$)

\[
\ddot{v}_k(t) = -\Delta_k^2 v_k(t) + \sin \alpha_k \frac{4V}{N} \sum_p g(k - p) \epsilon_p v_p(t)
\]

Now if we use Fourier transform

\[
v_k(t) = \int d\omega e^{-i\omega t} v_k(\omega)
\]
We have

\[(\Delta_k^2 - \omega^2) v_k(\omega) = \sin \alpha_k \frac{4V}{N} \sum_p g(k - p) \epsilon_p v_p(\omega)\]  

(3.99)

One of the possible solutions is

\[v_k(\omega) = \frac{\sin \alpha_k \sum t_n \sin (k \cdot t_n)}{\Delta_k^2 - \omega^2}\]  

(3.100)

The reason we chose this solution is as follows. Put this expression into Eq.(3.99), we have

\[\frac{4V}{3N} \sum_p \epsilon_p \frac{\sin \alpha_p (\sum t_n \sin (p \cdot t_n))^2}{\Delta_p^2 - \omega^2} = 1\]  

(3.101)

\[\omega, \text{ the energy of the low lying excitation mode can be obtained by solving this self-consistent equation.}\]

This mode doesn’t exist in the disordered phase (normal phase). So at the quantum critical point where \(\chi = 0\), we expect \(\omega \to 0\) in the ordered phase region. Then we have

\[\frac{1}{3N} \sum_p \left(\frac{(\sum t_n \sin (p \cdot t_n))^2}{\epsilon_p}\right) = \frac{1}{V_c}\]  

(3.102)

which is the self-consistent equation for the critical \(V\).
3.4 Berry Phase in the TRV phase

We have discussed the Berry phase in Graphene in the previous section. In Graphene, if we choose the closed path $C$ around the Dirac points $K = (\frac{4\pi}{3\sqrt{3}}, 0)$ and $K' = (-\frac{4\pi}{3\sqrt{3}}, 0)$, the corresponding Berry phases are $\gamma_\pm = \pm\pi$ and $\gamma'_\pm = \mp\pi$ where $\gamma_\pm$ is for the upper band and $\gamma_\mp$ is for the lower band. The total berry phase is 0 if we add $\gamma_\pm$ and $\gamma'_\pm$.

For studying the Berry phase in the TRV phase of Graphene, we still use the mean field approximation. The mean field Hamiltonian is

$$H_{MF} = \begin{pmatrix} \chi \epsilon_k - \epsilon_k \\ -\epsilon_k & -\chi \epsilon_k \end{pmatrix}$$

$$= \begin{pmatrix} \chi \sum_{t_n} \sin(k \cdot t_n) & -\epsilon_k \\ -\epsilon_k & -\chi \sum_{t_n} \sin(k \cdot t_n) \end{pmatrix}$$ 

We examine two closed circles around the two different Dirac points. We first look at the path around $K = (\frac{4\pi}{3\sqrt{3}}, 0)$. Put momentum $k = K + q$, and for small $|q|$, we can do the expansion and we have

$$H_{MF}(K + q) = \begin{pmatrix} \frac{3\sqrt{3}}{2} \chi \left(1 - \frac{3}{4} |q|^2 a^2\right) & |q|v_F e^{i\theta_q} \\ |q|v_F e^{-i\theta_q} & -\frac{3\sqrt{3}}{2} \chi \left(1 - \frac{3}{4} |q|^2 a^2\right) \end{pmatrix}$$ 

From this expansion, we see that all $H_{MF}$ is invariant on the closed circle path around the Dirac point $K$. Because of this, we can directly apply Eq. (3.32),

$$\gamma_\pm = \pm\pi \left(1 - \frac{3\sqrt{3}}{2} \chi \left(1 - \frac{3}{4} |q_0|^2 a^2\right) \right) \sqrt{\frac{27}{4} \chi^2 \left(1 - \frac{3}{4} |q_0|^2 a^2\right)^2 + |q_0|^2 v_F^2}$$ 

where $|q_0|$ is the radius of the closed circle path. In the above expression, when
\( \chi \to 0 \), we reached the case in Graphene with \( \gamma_\pm = \pm \pi \).

The Berry phase around the \( K' \) point is different. Write \( k = K' + q \), the mean field Hamiltonian becomes

\[
H_{MF}(K' + q) = \begin{pmatrix}
\frac{-3\sqrt{3}}{2} \chi \left(1 - \frac{3}{4} |q|^2 a^2\right) & |q| v_F e^{-i\theta_q} \\
|q| v_F e^{i\theta_q} & \frac{3\sqrt{3}}{2} \chi \left(1 - \frac{3}{4} |q|^2 a^2\right)
\end{pmatrix}
\]

(3.106)

We see that \( H_{MF}(K + q) \neq H_{MF}^*(K' - q) \) due to the time reversal symmetry broken. Now apply the same calculation for the Berry phase, we have

\[
\gamma'_\pm = \mp \pi \left(1 + \frac{\frac{3\sqrt{3}}{2} \chi \left(1 - \frac{3}{4} |q|^2 a^2\right)}{\sqrt{\frac{27}{4} \chi^2 \left(1 - \frac{3}{4} |q_0|^2 a^2\right)^2 + |q_0|^2 v_F^2}}\right)
\]

(3.107)

We see that \( \gamma_{\text{tot}} = \gamma_\pm + \gamma'_\pm \neq 0 \) which is different from the case of Graphene in the normal state. Furthermore, we can also show that if we only break the inversion symmetry but preserve the time reversal symmetry (Boron Nitride crystal), the summation of two Berry phases are zero. So the total Berry phase \( \gamma_{\text{tot}} \neq 0 \) is a unique topological property of the TRV phase in Graphene [34].
Chapter 4

RPA and Exciton Sector

Mean field theory has played a very important role in the condensed matter physics. It made important contributions to the explanation of the electronic structure in solids. The theory approximates the many body Hamiltonian to a single particle Hamiltonian. However, the effects of the correlated motions of many particles cannot be described in this way. In order to go beyond the mean field theory, we will use the quantum field theory in condensed matter physics.

4.1 Stationary Approximation

Quantum field theory in statistical mechanics is a very powerful tool in dealing with the many body problems. After writing down the partition function, we introduce an auxiliary field which couples to the quadratic order parameter term. Then we can eliminate the quartic terms in the partition function by doing Hubbard-Stratonovich transformation. Functional integral method and the stationary approximation can be applied to the newly transformed partition function expression,
and it shall match the mean field result.

### 4.1.1 Order Parameter in the Momentum Space

![Diagram](image)

Remember in the mean field theory, we have defined the order parameter \( \langle A_1^+ A_3 \rangle = \chi e^{i\phi} \) and showed that the time reversal broken required that the imaginary part of \( \langle A_1^+ A_3 \rangle \) to be non-zero, i.e. \( \phi \neq 0 \). So it is naturally to define a new operator \( \hat{\Phi}_n^A = \frac{1}{2i}(A_1^+ A_m - A_m^+ A_n) \). Because \( \hat{\Phi}_n^A = -\hat{\Phi}_m^A \), the sequence of the \( n, m \) need to be restricted. When \( n = 1, 2, 3 \), correspondingly \( m = 3, 1, 2 \). Same definition to \( \hat{\Phi}_n^B \). The Fourier transform of \( \hat{\Phi}_n^A \) is defined as

\[
\hat{\Phi}_n^A(q) = \sum_{R_l} \hat{\Phi}_n^A e^{-i q R_l - i \frac{1}{2} (a_n + a_m)}
\]

(4.1)

Do the same Fourier transform for \( A_1^+ \), we have

\[
\hat{\Phi}_n^A(q) = \frac{1}{2iN} \sum_{k_1, k_2} \sum_{R_l} e^{i(q - k_1 - k_2) R_l - i \frac{1}{2} (a_n + a_m)} \left( e^{i k_1 a_n - i k_2 a_m} - e^{i k_1 a_m - i k_2 a_n} \right) A_1^+ A_{k_2}
\]

(4.2)

The \( R_l \) summation gives us the momentum conservation. We write \( k_1 = k + \frac{1}{2} q \)
and \( k_2 = k - \frac{1}{2}q \), and we have

\[
\hat{\Phi}^A_{nm}(q) = \sum_k \sin[k \cdot (a_n - a_m)] A^\dagger_{k + \frac{q}{2}} A_{k - \frac{q}{2}}
\]  

(4.3)

\( \hat{\Phi}^A(q) \) is defined as the summation of all three \( \hat{\Phi}^A_{nm} \), so we have

\[
\hat{\Phi}^A(q) = \sum_k \sum_{t_n} \sin(k \cdot t_n) A^\dagger_{k + \frac{q}{2}} A_{k - \frac{q}{2}}
\]  

(4.4)

The same definition for \( \hat{\Phi}^B(q) \).

\[
\hat{\Phi}^B(q) = -\sum_k \sum_{t_n} \sin(k \cdot t_n) B^\dagger_{k + \frac{q}{2}} B_{k - \frac{q}{2}}
\]  

(4.5)

According to the pattern we have chosen, we can define a physical quantity \( \hat{\Phi} = \frac{1}{\sqrt{3}} (\hat{\Phi}^A + \hat{\Phi}^B) \). So we have

\[
\hat{\Phi}(q) = \sum_k \frac{1}{\sqrt{3}} \sum_{t_n} \sin(k \cdot t_n) \left( A^\dagger_{k + \frac{q}{2}} A_{k - \frac{q}{2}} - B^\dagger_{k + \frac{q}{2}} B_{k - \frac{q}{2}} \right)
\]  

(4.6)

\[
= \sum_k S_k \left( A^\dagger_{k + \frac{q}{2}} A_{k - \frac{q}{2}} - B^\dagger_{k + \frac{q}{2}} B_{k - \frac{q}{2}} \right)
\]  

(4.7)

where \( S_k = \frac{1}{\sqrt{3}} \sum_{t_n} \sin(k \cdot t_n) \). In the TRV state, we have \( \langle \hat{\Phi}(q) \rangle \neq 0 \). Since we have specify the order operator in our model, we can try to derive an effective Hamiltonian for our model.
4.1.2 The Effective Hamiltonian Under Symmetry Consideration

We start with the Hamiltonian

\[
H = -\sum_{k} \epsilon_k e^{-i\theta_k} A_k^\dagger B_k - \sum_{k} \epsilon_k e^{i\theta_k} B_k^\dagger A_k - \frac{V}{N} \sum_{k,p,q} g(k-p) A_{k+q}^\dagger A_{k-q} A_{p+q}^\dagger A_{p-q}
\]

\[
-\frac{V}{N} \sum_{k,p,q} g(k-p) B_{k+q}^\dagger B_{k-q} B_{p+q}^\dagger B_{p-q} \tag{4.8}
\]

Here \( \epsilon_k e^{i\theta_k} = \sum_{n=1}^3 \exp(i k \cdot a_n) \) and \( g(k-p) = \sum_{n=1}^3 \cos[(k-p) \cdot t_n] \). \( N \) is the number of unit cells. The hopping part of the above Hamiltonian is just the Graphene Hamiltonian. We first diagonalize this part and have two new creation operators \( b_k^\dagger \) and \( a_k^\dagger \) which satisfy

\[
b_k^\dagger = \frac{1}{\sqrt{2}} \left( e^{-i\theta_k/2} A_k^\dagger - e^{i\theta_k/2} B_k^\dagger \right) \tag{4.9}
\]

\[
a_k^\dagger = \frac{1}{\sqrt{2}} \left( e^{-i\theta_k/2} A_k^\dagger + e^{i\theta_k/2} B_k^\dagger \right) \tag{4.10}
\]

Written in the diagonal basis of the hopping part, we have

\[
H = \sum_k \epsilon_k \psi_k^\dagger \tau_3 \psi_k - \frac{V}{2N} \sum_{k,p,q} g(k-p) \left[ \psi_{k+q}^\dagger \tau_1 e^{i \delta_{k,q} \tau_1} \psi_{k-q}^\dagger \right] \left[ \psi_{p+q}^\dagger \tau_1 e^{-i \delta_{p,q} \tau_1} \psi_{p-q}^\dagger \right]
\]

\[
-\frac{V}{2N} \sum_{k,p,q} g(k-p) \left[ \psi_{k+q}^\dagger \tau_1 e^{i \delta_{k,q} \tau_1} \psi_{k-q}^\dagger \right] \left[ \psi_{p+q}^\dagger \tau_1 e^{-i \delta_{p,q} \tau_1} \psi_{p-q}^\dagger \right] \tag{4.11}
\]

Here \( \delta_{k,q} = \theta_{k+q/2} - \theta_{k-q/2} \) and \( \psi_k^\dagger = (b_k^\dagger a_k^\dagger) \) diagonalized the hopping part of the Hamiltonian.
Graphene has $C_{6v}$ symmetry, and $g(\mathbf{k} - \mathbf{p})$ is the structure function. We can decompose $g(\mathbf{k} - \mathbf{p})$ with the guide of the group theory. We first list the character table of $C_{6v}$ here (see, for example, Ref. [35] for notation use)

\[\begin{array}{c|cccccc}
E & 2C_6 & 2C_3 & C_2 & 3\sigma_v & 3\sigma_d \\
\hline
A_1 & 1 & 1 & 1 & 1 & 1 & 1 \\
A_2 & 1 & 1 & 1 & 1 & -1 & -1 \\
B_1 & 1 & -1 & 1 & -1 & 1 & -1 \\
B_2 & 1 & -1 & 1 & -1 & -1 & 1 \\
E_1 & 2 & 1 & -1 & -2 & 0 & 0 \\
E_2 & 2 & -1 & -1 & 2 & 0 & 0 \\
\end{array}\]

We decomposed $g(\mathbf{k} - \mathbf{p})$ as

\[g(\mathbf{k} - \mathbf{p}) = S_k S_p + S_k^1 S_p^2 + S_k^2 S_p^1 + C_k C_p + C_k^1 C_p^2 + C_k^2 C_p^1\] (4.13)
where

\[ S_k = \frac{1}{\sqrt{3}} \left( \sin(k \cdot t_1) + \sin(k \cdot t_2) + \sin(k \cdot t_3) \right) \tag{4.14} \]

\[ S_{k}^1 = \frac{1}{\sqrt{3}} \left( \sin(k \cdot t_1) + e^{i\frac{2\pi}{3}} \sin(k \cdot t_2) + e^{i\frac{4\pi}{3}} \sin(k \cdot t_3) \right) \tag{4.15} \]

\[ S_{k}^2 = \frac{1}{\sqrt{3}} \left( \sin(k \cdot t_1) + e^{i\frac{4\pi}{3}} \sin(k \cdot t_2) + e^{i\frac{2\pi}{3}} \sin(k \cdot t_3) \right) \tag{4.16} \]

\[ C_k = \frac{1}{\sqrt{3}} \left( \cos(k \cdot t_1) + \cos(k \cdot t_2) + \cos(k \cdot t_3) \right) \tag{4.17} \]

\[ C_{k}^1 = \frac{1}{\sqrt{3}} \left( \cos(k \cdot t_1) + e^{i\frac{2\pi}{3}} \cos(k \cdot t_2) + e^{i\frac{4\pi}{3}} \cos(k \cdot t_3) \right) \tag{4.18} \]

\[ C_{k}^2 = \frac{1}{\sqrt{3}} \left( \cos(k \cdot t_1) + e^{i\frac{4\pi}{3}} \cos(k \cdot t_2) + e^{i\frac{2\pi}{3}} \cos(k \cdot t_3) \right) \tag{4.19} \]

These six functions are the basis of the certain irreducible representations of \( C_{6v} \) group. We have

<table>
<thead>
<tr>
<th>( B_1 )</th>
<th>( S_k )</th>
<th>( A_1 )</th>
<th>( C_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_1 )</td>
<td>( { S_{k}^1, S_{k}^2 } )</td>
<td>( E_2 )</td>
<td>( { C_{k}^1, C_{k}^2 } )</td>
</tr>
</tbody>
</table>

(4.20)

So in the symmetry language, the decomposition of \( g(k - p) \) is

\[ g(k - p) = B_1 \cdot B_1 + 2E_1 \cdot E_1 + A_1 \cdot A_1 + 2E_2 \cdot E_2 \tag{4.21} \]

We have learned that the second order phase transition accompanied by the breaking of the symmetry of the system. With the decomposition of \( g(k - p) \), Eq.(4.61), we have decomposed the Hamiltonian into different symmetry channels. During the phase transition, the system will condensate into one of the symmetry channels. And in our case, it favors the \( B_1 \) symmetry channel with interaction vertex.
τ₁. This can be seen from Eq.(4.7), the order parameter operator in the momentum space. So we expect that the minimum effective model to study TRV phase transition is only to keep the $B_1$ symmetry channel with interaction vertex $τ_1$. We have

$$H = \sum_k \epsilon_k \psi_k^\dagger \tau_3 \psi_k - \frac{V}{2N} \sum_{k,p,q} S_k \left[ \psi_{k+q}^\dagger \tau_1 e^{i\delta_{k,q}\tau_1} \psi_{k+q} \right] S_p \left[ \psi_{p+q}^\dagger \tau_1 e^{-i\delta_{p,q}\tau_1} \psi_{p+q} \right]$$

$$= \sum_k \epsilon_k \psi_k^\dagger \tau_3 \psi_k - \frac{V}{2N} \sum_q \hat{\Phi}^\dagger(q) \hat{\Phi}(q)$$

where $\hat{\Phi}^\dagger(q) = \sum_k S_k \left[ \psi_{k+q/2}^\dagger \tau_1 e^{i\delta_{k,q}\tau_1} \psi_{k+q/2} \right]$.

### 4.1.3 Hubbard Stratonovich Transformation and Stationary Approximation

We use the effective Hamiltonian derived in the last section

$$H = \sum_k \epsilon_k \psi_k^\dagger \tau_3 \psi_k - \frac{V}{2N} \sum_q \hat{\Phi}^\dagger(q) \hat{\Phi}(q)$$

and going to write down the partition function of the system. First we write down the action $S$. The action is $S = \int_0^\beta d\tau \mathcal{L}$, with Lagrangian $\mathcal{L}$ defined as

$$\mathcal{L} = \sum_k \psi_k(\tau)(\partial_\tau - \mu + \epsilon_k \tau_3) \psi_k(\tau) - \frac{V}{2N} \sum_q \hat{\Phi}^\dagger(q, \tau) \hat{\Phi}(q, \tau)$$

Introducing the auxiliary field $\phi(q, \tau)$ which couples to $\hat{\Phi}^\dagger(q, \tau)$ and by applying
the Hubbard-Stratonovich we have

$$L = \frac{N}{2V} \sum_q |\phi(q, \tau)|^2 + \sum_k \psi^\dagger_k(\tau)(\partial_\tau - \mu + \epsilon_k \tau_3)\psi_k(\tau) - \frac{1}{2} \phi(q, \tau) \hat{\Phi}^\dagger(q, \tau) - \frac{1}{2} \phi^*(q, \tau) \hat{\Phi}(q, \tau)$$

(4.25)

Put $q \to -q$ in the $\frac{1}{2} \phi^*(q, \tau) \hat{\Phi}(q, \tau)$, we have

$$L = \sum_k \psi^\dagger_{k+q}(\tau) \left[ (\partial_\tau - \mu + \epsilon_k \tau_3)\delta_{q,0} - \frac{1}{2} \left( \phi(q, \tau) + \phi^*(-q, \tau) \right) S_k e^{i\delta\theta_k q \tau_1} \right] \psi^\dagger_{k-q}(\tau)$$

$$+ \frac{N}{2V} \sum_q |\phi(q, \tau)|^2$$

(4.26)

Because $\hat{\Phi}(q, \tau) = \sum_k S_k [\psi^\dagger_{k-q}(\tau) e^{-i\delta\theta_k q \tau_1} \psi_{k+q}(\tau)]$, and $\delta\theta_{k,q} = \theta_{k+q} - \theta_{k-q}$ is odd under $q \to -q$. We have the relation $\hat{\Phi}^\dagger(-q, \tau) = \hat{\Phi}(q, \tau)$. This indicates that the auxiliary field $\phi^*(-q, \tau) = \phi(q, \tau)$. Also for $q = 0$ we have $\phi^*(0, \tau) = \phi(0, \tau)$.

Write the action $S = \int_0^\beta d\tau L$ in the frequency space, we have

$$S = \frac{N}{2\beta V} \sum_q |\phi_q|^2 + \sum_{k,k'} \psi^\dagger_k \left[ (-i\epsilon_n - \mu + \epsilon_k \tau_3) \delta_{k,k'} - \frac{1}{\beta} \phi(k - k') \right] S_{\frac{1}{2}(|k+k'|)} e^{i\delta\theta_{k,k'} \tau_1} \psi^\dagger_{k'}$$

(4.27)

where $k = (k, i\epsilon_n)$.

In the stationary approximation, we first put $\phi(q, \tau) = \phi_0 \delta_{q,0}$ in Eq.(4.26). According to the Fourier transform, this is equivalent to put $\frac{1}{\beta} \phi(k - k') = \phi_0 \delta_{k,k'}$ in
Eq. (4.27). Then we have the action under stationary approximation as

\[ S_{\text{stat}} = \frac{N\beta}{2V} \phi_0^2 + \sum_k \bar{\psi}_k (-i\epsilon_n - \mu + \epsilon_k \tau_3 - \phi_0 S_k \tau_1) \psi_k \]  

(4.28)

The partition function is

\[ Z_{\text{stat}} = \int \mathcal{D}[\psi^\dagger] \mathcal{D}[\psi] e^{-S_{\text{stat}}} \]  

(4.29)

Integrating out the fermionic field, we have

\[ Z_{\text{stat}} = \exp(-\mathcal{A}[\phi_0]) \]  

(4.30)

where

\[ \mathcal{A}[\phi_0] = -\sum_k \ln \left[ \left( 1 + e^{\beta(-E_k - \mu)} \right) \left( 1 + e^{\beta(\mu + E_k)} \right) \right] + \frac{N\beta}{2V} \phi_0^2 \]  

(4.31)

with \( E_k = \sqrt{\epsilon_k^2 + \phi_0^2 S_k^2} \). The stationary approximation is done by minimizing \( \mathcal{A}[\phi_0] \) with respect to \( \phi_0 \), i.e. \( \frac{\partial}{\partial \phi_0} \mathcal{A}[\phi_0] = 0 \). We then have

\[ \sum_k \frac{1}{e^{\beta(E_k - \mu)} + 1} (-\beta) \frac{\phi_0 S_k^2}{E_k} + \sum_k \frac{1}{e^{\beta(-E_k - \mu)} + 1} \beta \frac{\phi_0 S_k^2}{E_k} = \frac{N\beta}{V} \phi_0 \]  

\[ \Rightarrow \quad \frac{1}{V} = \frac{1}{N} \sum_k \frac{S_k^2}{E_k} \frac{f(\xi_k^-) - f(\xi_k^+)}{E_k} \]  

(4.32)

where \( \xi_k^\pm = \pm E_k - \mu \), and \( f(x) \) is the Fermi-Dirac distribution function. At zero
temperature and half-filling, we have

\[ \frac{1}{V} = \frac{1}{N} \sum_k \frac{S_k^2}{E_k} = \frac{1}{3N} \sum_k \frac{(\sum_{t_n} \sin(p \cdot t_n))^2}{\sqrt{\epsilon_k^2 + \frac{1}{3} \phi_0^2 (\sum_{t_n} \sin(p \cdot t_n))^2}} \]  \hspace{1cm} (4.33)

which is exactly the same as the self-consistent equation we have obtained in the mean field approximation, Eq.(3.84) with \( \phi_0 = \sqrt{3} \chi \).

### 4.2 RPA and the Effective Hamiltonian

In the last section, we have used the effective Hamiltonian Eq.(4.23) to study the TRV phase transition in Graphene. The derivation of the Hamiltonian is based on the mean field result and the symmetry properties of the system. In this section, we will give a more rigorous proof.

#### 4.2.1 Functional Integral and RPA

In the last section, we started with the effective Hamiltonian Eq.(4.23),

\[ H = \sum_k \epsilon_k \tau_3 \psi_k - \frac{V}{2N} \sum_q \hat{\Phi}(q) \hat{\Phi}(q) \]  \hspace{1cm} (4.34)

and have written down the action \( S \) in the momentum-frequency space,

\[ S = \frac{N}{2\beta V} \sum_q |\phi_q|^2 + \sum_{k,k'} \psi_k^\dagger \left[ (-i\epsilon_n - \mu + \epsilon_k \tau_3) \delta_{k,k'} - \frac{1}{\beta} \hat{\Phi}(k-k') S_{\frac{1}{2}(k+k')} e^{\frac{i}{2} \tau_1 \cdot 1} \right] \psi_{k'} \]  \hspace{1cm} (4.35)

In stead of doing the stationary approximation, we are going to do the functional
The partition function is
\[ Z = \int \mathcal{D}[\phi^*] \mathcal{D}[\phi] \mathcal{D}[\psi^\dagger] \mathcal{D}[\psi] e^{-S} \] (4.36)

Integrating out the fermionic fields \( \psi \), we have
\[ Z = \int \mathcal{D}[\phi^*] \mathcal{D}[\phi] \exp(-S_{\text{eff}}[\phi^*, \phi]) \] (4.37)

where
\[ S_{\text{eff}}[\phi^*, \phi] = -\text{Tr} \ln G^{-1} + \frac{N}{2\beta V} \sum_q |\phi_q|^2 \] (4.38)
\[ G^{-1}(k, k') = (-i\epsilon_n - \mu + \epsilon_k \tau_3) \delta_{k,k'} - \frac{1}{\beta} \phi(k - k') S_{\frac{1}{2}(k+k')} e^{\frac{1}{2}(\theta_k - \theta_{k'}) \tau_1 \tau_1} \] (4.39)

Notice that \( G^{-1} \) is a \( 2 \times 2 \) matrix. We write \( \text{Tr} \ln G^{-1} = \text{Tr} \ln G_0^{-1} - \sum_n \frac{1}{n} \text{Tr}(G_0 \Sigma)^n \).

The question now is what is \( G_0^{-1} \)? If we approach the QCP from the disordered phase (normal state of Graphene), we would use
\[ G_0^{-1}(k, k') = (-i\epsilon_n - \mu + \epsilon_k \tau_3) \delta_{k,k'} \] (4.40)
\[ \Sigma(k, k') = -\frac{1}{\beta} \phi(k - k') S_{\frac{1}{2}(k+k')} e^{\frac{1}{2}(\theta_k - \theta_{k'}) \tau_1 \tau_1} \] (4.41)

and we also expect that for \( k - k' = 0 \), \( \phi(0) \) should be 0 because there is no order
in the normal state of the system. Define $Z_0 = \exp(\text{Tr} \ln G_0^{-1})$, we have

$$
\frac{Z}{Z_0} = \int \mathcal{D}[\phi^*] \mathcal{D}[\phi] \exp \left[ - \sum_n \frac{1}{n} \text{Tr}(G_0 \Sigma)^n - \frac{N}{2 \beta V} \sum_q |\phi_q|^2 \right] \tag{4.42}
$$

Inverse the Eq.(4.40), we have

$$
G_0(k) = \frac{(i\epsilon_n + \mu)\tau_0 + \epsilon_k \tau_3}{(i\epsilon_n - \mu - \epsilon_k)(i\epsilon_n - \mu + \epsilon_k)} \tag{4.43}
$$

We first look at the lowest order $n = 1$ expansion in $Z/Z_0$.

$$
-\text{Tr}(G_0 \Sigma) = \frac{1}{\beta} \sum_k \text{Tr}[G_0(k)\tau_1 S_k \phi(0)] = 0 \tag{4.44}
$$

Because in the disordered phase, $\phi(0) = 0$.

Now the lowest order is $n = 2$. We first have

$$
-\frac{1}{2} \text{Tr}(G_0 \Sigma)^2 = -\frac{1}{2} \text{Tr}\left[ G_0(k)\Sigma(k, k')G_0(k')\Sigma(k', k) \right] \tag{4.45}
$$

Define $k = (k - \frac{q}{2}, i\epsilon_n)$, $k' = (k + \frac{q}{2}, i\epsilon_n + iq_m)$, $q = k - k' = (q, iq_m)$, $\delta \theta_{k, q} = \theta_{k+\frac{q}{2}} - \theta_{k-\frac{q}{2}}$. The above expression becomes

$$
-\frac{1}{2\beta^2} \sum_{k, i\epsilon_n} S_k^2 \text{Tr}\left[ G_0(k - \frac{q}{2}, i\epsilon_n)e^{-\frac{i}{2} \delta \theta_{k, q} \tau_1} \tau_1 G_0(k + \frac{q}{2}, i\epsilon_n + iq_m)e^{\frac{i}{2} \delta \theta_{k, q} \tau_1} \tau_1 \right] |\phi(q)|^2 \tag{4.46}
$$
Define the polarization \( \chi(q) \) as

\[
\chi_0(q) = -\frac{1}{\beta N} \sum_{k, \epsilon_n} S_k^2 \text{Tr} \left[ G_0(k - \frac{q}{2}, i\epsilon_n) e^{-\frac{i}{2} \delta \theta_{k,q} \tau_1} \tau_1 G_0(k + \frac{q}{2}, i\epsilon_n + i\eta_m) e^{\frac{i}{2} \delta \theta_{k,q} \tau_1} \tau_1 \right]
\]

(4.47)

Ignoring the higher order of \( \phi(q), \phi^*(q) \), the \( S_{\text{eff}}[\phi^*, \phi] \) can be written as in the quadratic form

\[
S_{\text{eff}}[\phi^*, \phi] = \sum_q \left( \frac{N}{2\beta} - \frac{N}{2\beta} \chi_0(q) \right) |\phi(q)|^2
\]

(4.48)

This is the so-called RPA approximation. The coefficient \( |\phi(q)|^2 \) is (half) of the inverse of the propagator of the auxiliary field \( \phi(q) \),

\[
D(q) = \frac{V}{1 - V\chi_0(q)}
\]

(4.49)

We define

\[
\Gamma(q) = \frac{1}{1 - V\chi_0(q)}
\]

(4.50)

It can be shown that \( \Gamma(q) \) is the summation of the Dyson series of the ladder diagrams. This can be seen by write \( \Gamma(q) \) as

\[
\Gamma(q) = 1 + V\chi_0(q)\Gamma(q) = 1 + V\chi_0(q) + V\chi_0(q)V\chi_0(q) + ...
\]

\[
= 1 + V \left( \chi_0(q) + \chi_0(q)V\chi_0(q) + ... \right)
\]

(4.51)
The series inside the parenthesis can be demonstrated diagrammatically as

\[
\begin{align*}
\chi_0 & \quad + \quad \chi_0(-V)\chi_0
\end{align*}
\]

We proceed by calculating \( \chi_0(q) \). From Eq.(4.47), we have

\[
\chi_0(q) = -\frac{1}{\beta N} \sum_{k,\epsilon_n} S_k^2 \text{Tr} \left[ G_0(k + \frac{q}{2}, i\epsilon_n) e^{-\frac{i}{2} \delta \theta_{k,q}\tau_1} G_0(k + \frac{q}{2}, i\epsilon_n + iq_m) e^{\frac{i}{2} \delta \theta_{k,q}\tau_1} \right]
\]

\[
= -\frac{2}{\beta N} \sum_{k,\epsilon_n} S_k^2 \frac{(i\epsilon_n + \mu)(i\epsilon_n + iq_m + \mu) - \epsilon_{k+\frac{q}{2}} \epsilon_{k-\frac{q}{2}} \cos \delta \theta_{k,q}}{(i\epsilon_n - \epsilon_{k-\frac{q}{2}})(i\epsilon_n - \epsilon_{k+\frac{q}{2}})(i\epsilon_n + iq_m - \epsilon_{k+\frac{q}{2}})(i\epsilon_n + iq_m - \epsilon_{k-\frac{q}{2}})}
\]

After doing the \( i\epsilon_n \) summation, we found that the contribution to \( \chi_0(q) \) is from two parts, namely \( \chi_{0\perp}(q) \) for the inter-band contribution and \( \chi_{0\parallel}(q) \) from the intra-band contribution.

- **Inter-Band**

\[
\chi_{0\perp}(q) = \frac{1}{2N} \sum_k S_k^2 \left( 1 + \cos \delta \theta_{k,q} \right) \left[ \frac{f(\epsilon_{k+\frac{q}{2}}) - f(\epsilon_{k-\frac{q}{2}})}{iq_m - (\epsilon_{k+\frac{q}{2}} - \epsilon_{k-\frac{q}{2}})} + \frac{f(\epsilon_{k+\frac{q}{2}}) - f(\epsilon_{k-\frac{q}{2}})}{iq_m - (\epsilon_{k+\frac{q}{2}} - \epsilon_{k-\frac{q}{2}})} \right]
\]

\[
= \frac{1}{2N} \sum_k S_k^2 \left( 1 + \cos \delta \theta_{k,q} \right) \left[ \Pi_{+-}(k, q) + \Pi_{--}(k, q) \right]
\]
\( \chi_0(q) \) contains a standard Linhard-type function, \( \Pi_{++} \) and \( \Pi_{--} \). It has a well-known FL singularity with different limiting values [38], i.e. dynamical limit which take \( q \to 0 \) first and the static limit which take \( iq_m \to 0 \) first. The QCP is studied from the function \( \Gamma(q) \) under the static limit. From the expression of 
\[
\Gamma(q) = \frac{1}{1 - V \chi_0(q)}
\]
we see that in the static limit, \( \Gamma(0) \) diverges at a critical value \( V_c \) satisfying \( 1 - V_c \chi(0) = 0 \). The \( V_c \) determines the QCP equals
\[
\frac{1}{V_c} = \chi_0(0) = \frac{1}{N} \sum_k S^2_k \frac{f(\epsilon_k^+) - f(\epsilon_k^-)}{\epsilon_k} \]
(4.57)

For half-filling we have
\[
\frac{1}{V_c} = \frac{1}{N} \sum_k \frac{S^2_k}{\epsilon_k}
\]
(4.58)

This is the same expression for \( V_c \) as we have obtained before Eq.(3.86). But the difference is this time we obtained the expression from the disordered side \( \phi_0 = 0 \), before we were reaching QCP from the ordered side \( \phi_0 \to 0 \).
4.2.2 Orthogonality between Different Symmetry Channels in the Ladder Diagrams

In the last section, we have successfully use the effective Hamiltonian to find the same QCP as in the mean field calculation. The effective Hamiltonian is

\[ H = \sum_k \epsilon_k \psi_k^\dagger \tau_3 \psi_k - \frac{V}{2N} \sum_q \hat{\Phi}^\dagger(q) \hat{\Phi}(q) \]  
(4.59)

where \( \hat{\Phi}^\dagger(q) = \sum_k S_k \left[ \psi_{k+\frac{q}{2}}^\dagger \tau_1 e^{i \frac{\delta_{k,q}}{2} \tau_1} \psi_{k+\frac{q}{2}} \right] \). The RPA corresponds to a Dyson series of the ladder diagrams. However, as we can see the full Hamiltonian contains more terms than the effective Hamiltonian. Whether these extra terms contribute to the RPA is what we are going to find out in this section.

The full Hamiltonian is

\[ H = \sum_k \epsilon_k \psi_k^\dagger \tau_3 \psi_k - \frac{V}{2N} \sum_{k,p,q} g(k-p) \left[ \psi_{k+\frac{q}{2}}^\dagger \tau_1 e^{i \frac{\delta_{k,q}}{2} \tau_1} \psi_{k-\frac{q}{2}} \right] \left[ \psi_{p+\frac{q}{2}}^\dagger \tau_0 e^{i \frac{\delta_{p,q}}{2} \tau_1} \psi_{p-\frac{q}{2}} \right] 
- \frac{V}{2N} \sum_{k,p,q} g(k-p) \left[ \psi_{k+\frac{q}{2}}^\dagger \tau_1 e^{i \frac{\delta_{k,q}}{2} \tau_1} \psi_{k-\frac{q}{2}} \right] \left[ \psi_{p+\frac{q}{2}}^\dagger \tau_1 e^{-i \frac{\delta_{p,q}}{2} \tau_1} \psi_{p+\frac{q}{2}} \right] \]  
(4.60)

Here \( \delta_{k,q} = \theta_{k+\frac{q}{2}} - \theta_{k-\frac{q}{2}} \) and \( \psi_k^\dagger = (b_k^\dagger a_k^\dagger) \) diagonalized the hopping part of the Hamiltonian.

From the symmetry arguments, we decomposed \( g(k-p) \) as

\[ g(k-p) = S_k S_p + S_k^l S_p^l + S_k S_p^2 + S_k^l S_p^1 + C_k C_p + C_k^l C_p + C_k^2 C_p^1 \]  
(4.61)
where

\[
S_k = \frac{1}{\sqrt{3}} \left( \sin(k \cdot t_1) + \sin(k \cdot t_2) + \sin(k \cdot t_3) \right) \quad (4.62)
\]

\[
S_k^1 = \frac{1}{\sqrt{3}} \left( \sin(k \cdot t_1) + e^{i \frac{2\pi}{3}} \sin(k \cdot t_2) + e^{i \frac{4\pi}{3}} \sin(k \cdot t_3) \right) \quad (4.63)
\]

\[
S_k^2 = \frac{1}{\sqrt{3}} \left( \sin(k \cdot t_1) + e^{i \frac{4\pi}{3}} \sin(k \cdot t_2) + e^{i \frac{2\pi}{3}} \sin(k \cdot t_3) \right) \quad (4.64)
\]

\[
C_k = \frac{1}{\sqrt{3}} \left( \cos(k \cdot t_1) + \cos(k \cdot t_2) + \cos(k \cdot t_3) \right) \quad (4.65)
\]

\[
C_k^1 = \frac{1}{\sqrt{3}} \left( \cos(k \cdot t_1) + e^{i \frac{2\pi}{3}} \cos(k \cdot t_2) + e^{i \frac{4\pi}{3}} \cos(k \cdot t_3) \right) \quad (4.66)
\]

\[
C_k^2 = \frac{1}{\sqrt{3}} \left( \cos(k \cdot t_1) + e^{i \frac{4\pi}{3}} \cos(k \cdot t_2) + e^{i \frac{2\pi}{3}} \cos(k \cdot t_3) \right) \quad (4.67)
\]

These six functions are the basis of the certain irreducible representations of $C_{6v}$ group. We have

<table>
<thead>
<tr>
<th>$B_1$</th>
<th>$S_k$</th>
<th>$A_1$</th>
<th>$C_k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$ :</td>
<td>${S_k^1, S_k^2}$</td>
<td>$E_2$ :</td>
<td>${C_k^1, C_k^2}$</td>
</tr>
</tbody>
</table>

For the further discussion, we write the decomposition of $g(k - p)$ as

\[
g(k - p) = \sum_{\alpha = s, c} \sum_{\nu = 0}^2 \mathcal{A}_\nu^\alpha(k) \mathcal{A}_\nu^\alpha(p) \quad (4.69)
\]

Where $\mathcal{A}_0^{s/c}(k) = S_k/C_k$, while $\{\mathcal{A}_1^{s/c}, \mathcal{A}_2^{s/c}\}$ are the basis for the two dimensional irreducible representations $E_1/E_2$. Now according to the ladder diagram calculation, each block of the ladder diagram including all the symmetry channels can be
written as

\[ \mathcal{L}_{ij}^{\alpha \nu, \beta \mu} (q) = \frac{-1}{\beta N} \sum_{k, i \epsilon_n} \mathcal{A}^{\alpha}_\nu(k) \mathcal{A}^{\beta}_\mu(k) \text{ Tr} \left[ G_0(k - \frac{q}{2}, i \epsilon_n)e^{-\frac{i}{2} \delta q \cdot \tau_1 \tau_i} G_0(k + \frac{q}{2}, i \epsilon_n + i q_m)e^{\frac{i}{2} \delta q \cdot \tau_1 \tau_j} \right] \]

(4.70)

\[ i, j = 0, 1. \text{ } \mathcal{L}_{11}^{s_1, s_1}(q) \text{ is the } \chi_0(q) \text{ we have defined earlier. According to the ladder series, the first diagram in the series is} \]

\[ \text{This is } \mathcal{L}_{11}^{s_1, s_1}(q), \text{ which is } \chi_0(q) \text{ evaluated earlier.} \]

The second one is

In this diagram the wiggly line divide the diagram into two blocks (see Appendix). Now the wiggly line represents one of the symmetry channels in the interaction instead of only $S_k$ symmetry channel in the effective Hamiltonian. The block on the left is $\mathcal{L}_{1j}^{s_1, \beta \mu}(q)$ while the right one is $\mathcal{L}_{i1}^{\alpha \nu, s_1}(q)$. For $j = 0$ or 1, the expressions
of $\mathcal{L}^{s_1, \beta \mu}_{ij}$ are

$$
\mathcal{L}^{s_1, \beta \mu}_{11}(q) = \frac{-2}{\beta N} \sum_{k, \epsilon_n} S_k A^\beta_\mu(k) \frac{(i \epsilon_n + \mu)(i \epsilon_n + i q_m + \mu) - \epsilon_{k-\frac{q}{2}} \epsilon_{k+\frac{q}{2}} \cos \delta \theta_{k,q}}{(i \epsilon_n - \epsilon_{k-\frac{q}{2}})(i \epsilon_n - \epsilon_{k-\frac{q}{2}})(i \epsilon_n + i q_m - \epsilon_{k+\frac{q}{2}})(i \epsilon_n + i q_m - \epsilon_{k+\frac{q}{2}})}
$$

(4.71)

$$
\mathcal{L}^{s_1, \beta \mu}_{10}(q) = \frac{-2}{\beta N} \sum_{k, \epsilon_n} S_k A^\beta_\mu(k) \frac{i \epsilon_{k+\frac{q}{2}} \epsilon_{k-\frac{q}{2}} \sin \delta \theta_{k,q}}{(i \epsilon_n - \epsilon_{k-\frac{q}{2}})(i \epsilon_n - \epsilon_{k-\frac{q}{2}})(i \epsilon_n + i q_m - \epsilon_{k+\frac{q}{2}})(i \epsilon_n + i q_m - \epsilon_{k+\frac{q}{2}})}
$$

(4.72)

The frequency $i \epsilon_n$ summation can be done, and we have

$$
\mathcal{L}^{s_1, \beta \mu}_{11}(q) = \frac{1}{2 N} \sum_k S_k A^\beta_\mu(k) \left( 1 + \cos \delta \theta_{k,q} \right) \left[ \Pi_{-+}(k, q) + \Pi_{+-}(k, q) \right]
$$

$$
+ \frac{1}{2 N} \sum_k S_k A^\beta_\mu(k) \left( 1 - \cos \delta \theta_{k,q} \right) \left[ \Pi_{++}(k, q) + \Pi_{--}(k, q) \right]
$$

(4.73)

$$
\mathcal{L}^{s_1, \beta \mu}_{10}(q) = \frac{1}{2 N} \sum_k S_k A^\beta_\mu(k) \sin \delta \theta_{k,q} \left[ \Pi_{--}(k, q) + \Pi_{++}(k, q) - \Pi_{+-}(k, q) - \Pi_{-+}(k, q) \right]
$$

(4.74)

where

$$
\Pi_{ss'}(k, q) = \frac{f(\epsilon_{k+\frac{q}{2}}) - f(\epsilon_{k-\frac{q}{2}})}{iq_m - (\epsilon_{k+\frac{q}{2}} - \epsilon_{k-\frac{q}{2}})}
$$

(4.75)

QCP is found by looking at the divergence of the Dyson series of the ladder diagrams in the static limit. The static limit is obtained by taking $iq_m \to 0$ first, and
then $q \rightarrow 0$. Then in the static limit, we have

$$\mathcal{L}_{11}^{s1,\beta\mu}(0) = \frac{1}{N} \sum_{k} S_{k} A_{\mu}^{\beta}(k) \frac{f(\epsilon_{k}^{-}) - f(\epsilon_{k}^{+})}{\epsilon_{k}}$$

(4.76)

$$\mathcal{L}_{10}^{s1,\beta\mu}(0) = 0$$

(4.77)

We found that $\mathcal{L}_{10}^{s1,\beta\mu}(0)$ had no contribution to the QCP. For $\mathcal{L}_{11}^{s1,\beta\mu}(0)$ more symmetry arguments are required. From the group theory, we know that every $A_{\mu}^{\beta}$ function belongs to certain irreducible representation of the $C_{6v}$ point group.

<table>
<thead>
<tr>
<th>$B_1$ : $S_k$</th>
<th>$A_1$ : $C_k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1 : {S_k^1, S_k^2}$</td>
<td>$E_2 : {C_k^1, C_k^2}$</td>
</tr>
</tbody>
</table>

(4.78)

$\epsilon_{k}$ is the energy function of the normal state in Graphene. It belongs to $A_1$, the identity representation of the $C_{6v}$ point group, same irreducible representation as function $C_k$. The summation of the momentum $k$ is over the first Brillouine zone of Graphene. The region has the full $C_{6v}$ symmetry even in the doped case. Then from the group theory argument, $\mathcal{L}_{10}^{s1,\beta\mu}(0)$ is non-zero only if the combination $S_{k} A_{\mu}^{\beta}(k)$ belongs to the identity irreducible representation $A_1$. The only solution is $A_{\mu}^{\beta}(k) = S_{k}$. This can easily be seen from the multiplication of the characters.

Above arguments applied to the other block $\mathcal{L}_{11}^{\alpha\nu,s1}(q)$. The $n$th order ladder diagram can be divided into $n + 1$ blocks. We can start from either side of the block and applied the above result to any block. We found that all the blocks have to
be $L_{11,11}^{sl}(q)$ in order to survive in the static limit. So we reach the conclusion that the effective Hamiltonian is enough in the static limit.

### 4.3 Exciton Sector in RPA

In the previous section, we have defined $\Gamma(q) = \frac{1}{1-V\chi_0(q)}$ with $\chi_0(q) = \chi_{0\perp}(q) + \chi_{0\parallel}(q)$. And

\[
\chi_{0\perp}(q) = \frac{1}{2N} \sum_k S_k^2 \left( 1 + \cos \delta \theta_{k,q} \right) \left[ \Pi_{-+}(k,q) + \Pi_{+-}(k,q) \right] \tag{4.79}
\]

\[
\chi_{0\parallel}(q) = \frac{1}{2N} \sum_k S_k^2 \left( 1 - \cos \delta \theta_{k,q} \right) \left[ \Pi_{++}(k,q) + \Pi_{--}(k,q) \right] \tag{4.80}
\]

It is very insightful to write $\cos \delta \theta_{k,q} = 1 - (1 - \cos \delta \theta_{k,q})$, then we have for $\chi_0(q)$,

\[
\chi_0(q) = \frac{1}{2N} \sum_k S_k^2 \left( 1 - \cos \delta \theta_{k,q} \right) \left[ \Pi_{++}(k,q) + \Pi_{--}(k,q) - \Pi_{-+}(k,q) - \Pi_{+-}(k,q) \right] \\
+ \frac{1}{N} \sum_k S_k^2 \left[ \Pi_{-+}(k,q) + \Pi_{+-}(k,q) \right] \tag{4.81}
\]

\[
= \chi_0'(q) + \chi_0^{ex}(q) \tag{4.82}
\]

Then the $\Gamma(q)$ is

\[
\Gamma(q) = \frac{1}{1-V\chi_0^{ex}(q) - V\chi_0'(q)} \tag{4.83}
\]

$\chi_0^{ex}(q)$ is an excitonic term except an extra $S_k^2$ factor coming from the interaction. This form gives us the hint that the problem could possibly be understood in the exciton language. This is what we are going to do in the next chapter.
Chapter 5

Theory of the Excitonic Liquid State in Semiconductor

In the two band system, an exciton (particle-hole pair) can be formed by exciting an electron from the valence band to the conduction band. If the binding energy $E_B$ of the exciton is tuned to be larger than the direct excitation threshold energy $E_D$, the virtual excitons form spontaneously in the groundstate and destabilize the formal Fermi liquid (FL) state [39]. As a result a new ground state can be formed by hybridizing the two bands [40]. A new uniform order is formed in such state, $\langle a_k^\dagger b_k \rangle \neq 0$, where $a_k^\dagger/a_k$ and $b_k^\dagger/b_k$ are the electron creation/annihilation operators in the relevant bands. We call this state “excitonic liquid” (XL) state.

As we have seen, the TRV state in Graphene can be understood from this excitonic instability. Furthermore in our model, the excitons (particle-hole pairs) are spontaneously formed and the direct gap $E_G$ is 0 in Graphene. This is different from the much studied excitonic insulator state formed when the number of free conduction
Figure 5.1: A two band model is shown. Both quadratic bands have the same mass and the valence band is partially filled (chemical potential $\mu$ is located in the valence band. $\mu$ is measured from the center of the gap). $E_G$ is the minimum gap in the system. $E_D$ is the direct excitation threshold. The location of the exciton is given by $E = E_D - E_B$. When $E_D = E_B$, there is no energy cost to form an exciton.

electrons and valence holes are finite. The latter can occur either naturally when the bands cross at the Fermi level (semimetal with bandgap $E_G < 0$) or can be created artificially by optically pumping a semiconductor ($E_G > 0$) [41, 42]. The excitonic insulator problem has been shown to be mathematically equivalent to the BCS model with electron-hole pairs instead of electron-electron pairs [41, 43–46]. For generality, we will first develop the XL theory in semiconductors. The TRV phase transition can be described by the XL theory and will be shown later.
5.1 The Model Hamiltonian

We considered the well studied, two quadratic bands with equal mass, spinless fermion model with a direct bandgap $E_G > 0$, Fig.5.1. This model has been widely used in the study of the Mahan exciton problem [8,41,47]. The Hamiltonian with the chemical potential term is

$$K = \sum_k \epsilon_k (b_k^\dagger b_k - a_k^\dagger a_k) - \frac{V}{L^2} \sum_{k,p,q} \mathcal{A}(k) \mathcal{A}(p) a_{k+q}^\dagger b_k b_p a_{p+q} - \mu \sum_k (b_k^\dagger b_k + a_k^\dagger a_k)$$

(5.1)

where $b_k^\dagger$ and $a_k^\dagger$ are the creation operators of the conduction and valence electrons and $\epsilon_k = E_G/2 + k^2/2m$, $E_G$ is the gap energy. $\mathcal{A}(k)$ gives a high energy cut-off in the order of the Fermi energy.

$$\mathcal{A}(k) = \begin{cases} 
1 & \text{if } | - \epsilon_k - \mu | < \Lambda \\
0 & \text{if } | - \epsilon_k - \mu | > \Lambda 
\end{cases}$$

(5.2)

Hole doping is assumed throughout, so our $\mu = -E_G - k_F^2/2m$ at zero temperature. The cutoff energy $\Lambda \sim \mathcal{O}(E_G)$. Use the notation $\psi_k^\dagger = (b_k^\dagger, a_k^\dagger)$ and with the cutoff simplification, we can write the interaction as a product of bilinear operators. The Hamiltonian becomes

$$K = \sum_k \psi_k^\dagger (\epsilon_k \tau_3 - \mu) \psi_k - \frac{V}{L^2} \sum_q \hat{\Phi}^\dagger(q) \hat{\Phi}(q)$$

(5.3)

where, $\hat{\Phi}(q) = \sum_k \psi_k^\dagger \tau^+ \psi_{k+q}$ = $\sum_k b_k^\dagger a_{k+q}$, and $\tau^+$ is the band index raising operator. The prime on the $k$-sum explicitly enforces the restriction on $\mathcal{A}(k)$. 

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We explore the possibility of a uniform XL state with the order $V\langle \Phi(q) \rangle / L^2 = \phi_0 \delta_{q,0}$. Because the similarity between our model Hamiltonian Eq.(5.3) and the effective Hamiltonian Eq.(6.1), we expect the XL phase transition can be again anticipated from the behavior of the renormalized interaction $VT(q)$. In the ladder approximation, the $\Gamma(q)$ has the general form

$$\Gamma(q) = \frac{1}{1 - V\chi_0(q)} \quad (5.4)$$

$\chi_0(q)$ in the disordered phase can be calculated by using the functional integral method with the ladder approximation,

$$\chi_0(q) = \frac{1}{L^2} \sum_k' \frac{f(\epsilon_{k+q}^+) - f(\epsilon_k^-)}{i\epsilon_m - (\epsilon_{k+q}^+ - \epsilon_k^-)} \quad (5.5)$$

The energies $\epsilon_k^\pm = \pm \epsilon_k - \mu_0$ are the band energies measured from the chemical potential $\mu_0$ in the noninteracting system. Since we have assumed hole doping, at zero temperature $f(\epsilon_{k+q}^+) = 0$ and $f(\epsilon_k^-) = 1$ for $|k| > k_F$. $k_F$ is the noninteracting Fermi wavevector that fixes the filling. In the static limit $q \to 0, iq_m \to 0$, we have

$$\chi_0(0) = \frac{1}{L^2} \sum_{|k| > k_F} \frac{1}{2\epsilon_k} = \sum_k'' \frac{1}{2\epsilon_k} \quad (5.6)$$

with $\sum_{k}'' = 1/L^2 \sum_{|k| > k_F}$. Hence $\Gamma(0)$ diverges at a critical $V_c$ satisfying $1 - V_c\chi_0(0) = 0$ indicating the phase transition into the XL phase. The critical $V_c$
determines the QCP equals

\[
\frac{1}{V_c} = \sum_\mathbf{k}'' \frac{1}{2\epsilon_\mathbf{k}}
\]  

(5.7)

5.2 Binding Energy of a Single Exciton

In this section, we explore the XL phase transition in the exciton language. We show below that the above instability is related to the formation of Cooper-like pairs of interband particle-hole (\(p-h\)) pairs with zero energy. The analysis is the same as the theory of Cooper pair formation in the background of a “rigid” Fermi sea of particles. We look for the ground state energy and wave function of a single particle-hole (\(p-h\)) pair. The \(p-h\) pair wave function is formed as a linear combination of pair wave functions, \(\varphi_\mathbf{k}\), of single \(p-h\) pairs created by annihilating an electron from inside of the Fermi surface, \(|FS\rangle\), of the partially filled valence band and recreating it at the same \(k\) value in the empty conduction band:

\[
|\phi_0\rangle = \sum_\mathbf{k}'' \varphi_\mathbf{k} b_\mathbf{k}^\dagger a_\mathbf{k} |FS\rangle
\]  

(5.8)

The summation extends from \(k_F\) to cutoff. The energy of the pair can be found from the time evolution of the pair wave function

\[
-i \sum_\mathbf{k}'' \varphi_\mathbf{k} \frac{d(b_\mathbf{k}^\dagger a_\mathbf{k})}{dt} = \sum_\mathbf{k}'' \varphi_\mathbf{k} [K, b_\mathbf{k}^\dagger a_\mathbf{k}]
\]  

(5.9)
The stationary solution to this Schrödinger equation is

\[ E \sum_k \varphi_k b_k^\dagger a_k = \sum_k \varphi_k \left[ K, b_k^\dagger a_k \right] \]
\[ = \sum_k \left[ 2\epsilon_k \varphi_k - \frac{V}{L^2} \sum_p \varphi_p \left( a_p^\dagger a_p - b_p^\dagger b_p \right) \right] b_k^\dagger a_k \]  

(5.10)

(5.11)

The Cooper model assumes a rigid Fermi sea, which is equivalent to decoupling the interaction terms by averaging over the Fermi sea \( \langle a_p^\dagger a_p - b_p^\dagger b_p \rangle = f(\epsilon_p^-) - f(\epsilon_p^+) \).

One then obtains the Bethe-Goldstone equation:

\[ E \varphi_k = 2\epsilon_k \varphi_k - V \sum_p \varphi_p \]  

(5.12)

Substituting \( \phi_0 = \sum_p \varphi_p \) and do the restricted summation \( \sum''_k \) on both sides of the above equation, we have

\[ \frac{1}{V} = -\sum_k \frac{1}{E - 2\epsilon_k} \]  

(5.13)

Set \( E = 0 \) gives Eq.(5.7) for the critical \( V_c \) at QCP. Since \( E \) is measured from the chemical potential Fig.5.1, when \( V > V_c \), it becomes favorable to create particle-hole pairs out of the Fermi sea thus destabilizing the normal groundstate.

A possible cure for this instability is to assume a new Hatree-Fock solution built of virtual excitons. This is equivalent to assigning a non-zero expectation value to \( V \langle \hat{\phi}(q) \rangle / L^2 = \phi_0 \delta_{q,0} \). Notice that the order parameter is not invariant under a
global $U(1)$ rotation, $e^{i\frac{\theta}{2} \tau_3} \psi_k$ of the relative phase between the two bands,

$$e^{i\frac{\theta}{2} \tau_3} \Phi(q)e^{-i\frac{\theta}{2} \tau_3} = e^{-i\theta} \sum_k b_{k+q}^+ a_{k+q} = e^{-i\theta} \Phi(q)$$ (5.14)

However the Hamiltonian is invariant under this $U(1)$ rotation because the interaction part is $\Phi(q)\Phi(q)$. Hence the condensation spontaneously breaks the $U(1)$ symmetry. The associated Goldstone mode is easily identified with the phase of the XL order parameter. We note, however, that the enhanced $U(1)$ symmetry of $H$ exists because terms such as $a^\dagger a^\dagger b b$ and $a^\dagger a^\dagger a b$ that do not conserve the particle number in each band are omitted in our model. It is therefore only an approximate symmetry in general and when spontaneously broken will give rise to a massive pseudo-Goldstone mode [48,49]. For the sake of generality, we suppress the gapless phase fluctuations in our simplified model by assuming $\phi_0$ to be real.

We proceed to look for a mean field solution by assigning the order parameter $V\langle \Phi(q)\rangle/L^2 = \phi_0 \delta_{q,0}$ in the Hamiltonian Eq.(5.3). Remember that $\phi_0$ is assumed real. The mean field Hamiltonian is

$$K_{MF} = \sum_k \psi_k^\dagger (\epsilon_k \tau_3 - \phi_0 \tau_1 - \mu) \psi_k - \frac{L^2}{V} \phi_0^2$$ (5.15)

Diagonalizing $K_{MF}$, we obtain $\xi_k^\pm = \pm E_k - \mu$ as the eigen energy, where $E_k = \sqrt{\epsilon_k^2 + \phi_0^2}$.

Here we need to mention a very important point. As we have seen in the introduction, under a suitable particle-hole transformation $a_k \rightarrow c_{-k}^\dagger$ and $b_k \rightarrow c_{k}^\dagger$,
the Mahan exciton Hamiltonian mapped to the continuum fermion model with attractive interactions [50, 51], whose mean field solution corresponds exactly to the BCS Hamiltonian. But in Mahan’s problem, because the particle-hole pairs are pumped into the system optically, the number operator is \( \hat{n}_k = b_k^\dagger b_k + a_k a_k^\dagger \) in contrast to the number operator in our problem \( \hat{n}_k = a_k^\dagger a_k + b_k^\dagger b_k \).

In our case, if we do the same particle-hole transformation in the mean field expression of the model Hamiltonian, Eq.(5.15), we will see that it is mapped to a BCS mean field solution in the Zeeman field only when \( E_G < 0 \). This corresponds to the semi-metal case studied in the excitonic insulator [52, 53]. In the excitonic insulator, the chemical potential \( \mu \) maps to the magnetic field \( h \) in the BCS, and the gap \( E_G \) maps to the fixed BCS chemical potential \( \mu_{\text{BCS}} = -E_G/2 \). (\( \mu_{\text{BCS}} > 0 \), so it could only maps to \( E_G < 0 \), the semimetal situation.)

However, in our case, \( E_G > 0 \). When \( E_G > 0 \), the levels never cross and all states up to the non-interacting Fermi wavevector \( k_F \) are filled. Because \( K_{\text{MF}} \) commutes with the individual number operator per \( k \) state \( \hat{n}_k = a_k^\dagger a_k + b_k^\dagger b_k \), every \( k \)-state up to the non-interacting \( k_F \) remains occupied as \( V \) is tuned through the QCP. It implies the Fermi wavevector \( k_F \) is not renormalized and a sharp Fermi surface exists in the condensed phase.

The two new hybridized states denoted as \( c_{k\pm} \) corresponding to \( \pm E_k \) respectively
are

\[ c_{k+} = u_k b_k - v_k a_k \]  \hspace{1cm} (5.16)

\[ c_{k-} = u_k a_k + v_k b_k \]  \hspace{1cm} (5.17)

with

\[ u_k^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_k}{E_k} \right) \quad \text{and} \quad v_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k}{E_k} \right) \]  \hspace{1cm} (5.18)

For hole doped case, the ground state of the XL phase is

\[ |XL\rangle = \prod_{|k|>k_F} \prime \ c_{k-}^\dagger |0\rangle \]  \hspace{1cm} (5.19)

where \( |0\rangle \) is the vacuum. However, it is more intuitive to use a new “vacuum” \( |FS\rangle = \prod_{|k|>k_F} \prime a_k^\dagger |0\rangle \) which is the noninteracting Fermi surface corresponding to the partially filled valence band. Then the \( |XL\rangle \) is

\[ |XL\rangle = \prod_{|k|>k_F} \prime (u_k + v_k b_k^\dagger a_k) |FS\rangle \]  \hspace{1cm} (5.20)
5.3 Order Parameter Fluctuations

The existence of a sharp Fermi surface in the XL phase implies that gapless particle-hole excitations exists at the Fermi surface, which can couple to the fluctuations of the order-parameter of the XL. The fluctuations about the mean-field solution are most easily calculated using the standard functional integral method. The partition function will be expanded around the stationary solution (which is consistent with the mean field solution), and the amplitude fluctuations of the order parameter will be studied in the static limit.

5.3.1 Action in the XL phase

The Hamiltonian is

$$H = \sum_k \psi_k^\dagger [\epsilon_k \tau_3 - \mu] \psi_k - \frac{V}{L^2} \sum_q \hat{\Phi}^\dagger(q) \hat{\Phi}(q)$$  \hspace{1cm} (5.21)

where

$$\hat{\Phi}(q) = \sum_k' \psi_k^\dagger \tau^+_q \psi_{k+q}$$  \hspace{1cm} (5.22)

The action is $S = \int_0^\beta d\tau \mathcal{L}$, and the Lagrangian is

$$\mathcal{L} = \sum_k \psi_k^\dagger(\tau) (\partial_\tau - \mu + \epsilon_k \tau_3) \psi_k(\tau) - \frac{V}{L^2} \sum_q \hat{\Phi}^\dagger(q, \tau) \hat{\Phi}(q, \tau)$$  \hspace{1cm} (5.23)
where

\[ \hat{\Phi}(q, \tau) = \sum_k' \psi_k^\dagger(\tau) \tau^+ \psi_{k+q}(\tau) \] (5.24)

Use the Hubbard-Stratonovich transformation, and define the auxiliary fields as

\[ \phi(q, \tau) = \frac{V}{L^2} \hat{\Phi}(q, \tau) \quad \text{and} \quad \phi^*(q, \tau) = \frac{V}{L^2} \hat{\Phi}^\dagger(q, \tau) \]

we have the Lagrangian in terms of the \( \psi \) and \( \varphi \) fields as

\[ L[\varphi, \psi] = \sum_k \psi_k^\dagger(\tau)(\partial_\tau - \mu + \epsilon_k \tau_3) \psi_k(\tau) + \sum_q \left( \frac{L^2}{V} \phi^*(q, \tau) \phi(q, \tau) - \phi(q, \tau) \hat{\Phi}^\dagger(q, \tau) - \phi^*(q, \tau) \hat{\Phi}(q, \tau) \right) \] (5.25)

In the \( \phi(q, \tau) \hat{\Phi}^\dagger(q, \tau) \), we first put \( q \to -q \), and then shift the \( k \) sum inside \( \hat{\Phi}^\dagger(q, \tau) \), we have

\[ \phi(q, \tau) \hat{\Phi}^\dagger(q, \tau) = \phi(-q, \tau) \sum_k' \psi_k^\dagger(\tau) \tau^- \psi_{k+q}(\tau) \] (5.26)

The Lagrangian can be simplified as

\[ L[\phi, \psi] = \sum_{k,q} \psi_k^\dagger(\tau) \left[ (\partial_\tau - \mu + \epsilon_k \tau_3) \delta_{q,0} - \phi^*(q, \tau) \tau^+ - \phi(-q, \tau) \tau^- \right] \psi_{k+q}(\tau) \]

\[ + \frac{L^2}{V} \sum_q \phi^*(q, \tau) \phi(q, \tau) \] (5.27)

We define

\[ \delta \phi(q, \tau) = \phi(q, \tau) - \phi_0 \delta_{q,0} \quad \text{and} \quad \delta \phi^*(q, \tau) = \phi^*(q, \tau) - \phi_0 \delta_{q,0} \] (5.28)
Remember that the order parameter $\phi_0$ is real.

The quadratic field part in the Lagrangian can be written as

$$\sum_{q} \phi^*(q, \tau)\phi(q, \tau) = \sum_{q \neq 0} \phi^*(q, \tau)\phi(q, \tau) + \left( \phi^*(0, \tau) - \phi_0 + \phi_0 \right) \left( \phi(0, \tau) - \phi_0 + \phi_0 \right)$$

$$= \left[ \sum_{q \neq 0} \phi^*(q, \tau)\phi(q, \tau) + \left( \phi^*(0, \tau) - \phi_0 \right) \left( \phi(0, \tau) - \phi_0 \right) \right]$$

$$+ \phi_0 \left( \phi^*(0, \tau) - \phi_0 \right) + \phi_0 \left( \phi(0, \tau) - \phi_0 \right) + |\phi_0|^2 \quad (5.29)$$

$$= \phi_0^2 + \phi_0\delta\phi^*(0, \tau) + \phi_0\delta\phi(0, \tau) + \sum_{q} \delta\phi^*(q, \tau)\delta\phi(q, \tau) \quad (5.30)$$

The Lagrangian can be rewritten as

$$\mathcal{L}[\phi, \psi] = \frac{L^2}{V} \phi_0^2 + \frac{L^2}{V} \phi_0\delta\phi^*(0, \tau) + \frac{L^2}{V} \phi_0\delta\phi(0, \tau) + \frac{L^2}{V} \sum_{q} \delta\phi^*(q, \tau)\delta\phi(q, \tau)$$

$$+ \sum_{k,q} \psi_k^\dagger(\tau) \left[ \delta\phi^*(q, \tau)\delta\phi(q, \tau) \right] \psi_{k+q}(\tau) \quad (5.31)$$

The action $S$ is defined as $S = \int^\beta_0 d\tau \mathcal{L}$.

$$S = \sum_{k,q} \int^\beta_0 d\tau \psi_k^\dagger(\tau) \left[ \delta\phi^*(q, \tau)\delta\phi(q, \tau) \right] \psi_{k+q}(\tau)$$

$$+ \frac{L^2}{V} \int^\beta_0 d\tau \sum_{q} \delta\phi^*(q, \tau)\delta\phi(q, \tau) \quad (5.32)$$

Use the Fourier transform, we can write the action in the momentum and frequency space.
Define the 4-momentum $k = (k, i\epsilon_n)$, we have

$$ S = \sum'_{k,k'} \psi^+_k \left[ (-i\epsilon_n - \mu + \epsilon_k \tau_3 - \phi_0 \tau_1) \delta_{kk'} - \frac{1}{\beta} \delta \phi^*_k \tau^+ - \frac{1}{\beta} \delta \phi_{k'} \tau^- \right] \psi_{k'} + \frac{L^2}{V} \int_0^\beta d\tau \sum_q \phi^*(q, \tau) \phi(q, \tau) $$

(5.33)

Write the Action in a more compact form, we have

$$ S = \sum'_{k,k'} \psi^+_k G^{-1}_{kk'} \psi_{k'} + \frac{L^2}{V} \int_0^\beta d\tau \sum_q \phi^*(q, \tau) \phi(q, \tau) $$

(5.34)

The fermionic field integral in the partition function will give us the desired form of the action $S_{\text{eff}}$ as

$$ S_{\text{eff}} = -\text{Tr} \ln G^{-1} + \frac{L^2}{V} \int_0^\beta d\tau \sum_q \phi^*(q, \tau) \phi(q, \tau) $$

(5.35)

Write $G^{-1} = G_0^{-1}(1 - G_0 \Sigma)$, we have

$$ \text{Tr} \ln G^{-1} = \text{Tr} \ln G_0^{-1} + \text{Tr} \ln (1 - G_0 \Sigma) $$

(5.36)

$$ = \text{Tr} \ln G_0^{-1} - \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr}(G_0 \Sigma)^n $$

(5.37)

As $k$ stands for 4-momentum $(k, i\epsilon_n)$, the first term in the “Tr ln” expansion is

$$ \text{Tr} \ln G_0^{-1} = \sum'_{k} \ln G_0^{-1}(k) $$

(5.38)

This choice of $G_0^{-1}(k)$ is different from the case we have studied before. Because this time we are working in the ordered phase, $G_0^{-1}(k)$ is chosen to be $-i\epsilon_n - \mu + \ldots$
\[ \epsilon_k \tau_3 - \phi_0 \tau_1 \]. So we have

\[
G_0(k, i\epsilon_n) = -\frac{(i\epsilon_n + \mu)\tau_0 + \epsilon_k \tau_3 - \phi_0 \tau_1}{(i\epsilon_n - \xi_k^+)(i\epsilon_n - \xi_k^-)}, \quad \xi_k^\pm = \pm \sqrt{\epsilon_k^2 + \phi_0^2} - \mu = \pm E_k - \mu
\]  

(5.39)

And

\[
\Sigma_{kk'} = \frac{1}{\beta} \delta \phi_{k'}^{*} \tau^+ + \frac{1}{\beta} \delta \phi_{k'-\kappa} \tau^-
\]  

(5.40)

We write \( S_{\text{eff}} \) up to the quadratic order as

\[
S_{\text{eff}} = S_{\text{eff}}^{(0)} + S_{\text{eff}}^{(1)} + S_{\text{eff}}^{(2)}
\]  

(5.41)

The first order in the expansion is zero because the expansion is around the stationary solution. This will also be shown later.

1. 0th order, \( S_{\text{eff}}^{(0)} \):

\[
S_{\text{eff}}^{(0)} = -\text{Tr} \ln G_0^{-1} + \frac{\beta L^2}{V} \phi_0^2
\]  

(5.42)

\[
= \beta \sum_k' \xi_k^- f(\xi_k^-) + \frac{\beta L^2}{V} \phi_0^2
\]  

(5.43)

This expression is the same as if we have done the stationary approximation.

Minimize w.r.t. \( \phi_0 \) will give the self-consistent equation for \( \phi_0 \),

\[
-\frac{1}{2L^2} \sum_k' \frac{f(\xi_k^-)}{E_k} + \frac{1}{V} = 0
\]  

(5.44)
2. 1st order, $S_{\text{eff}}^{(1)}$:

\[
S_{\text{eff}}^{(1)} = \text{Tr}(G_0 \Sigma) + \frac{L^2}{V} \phi_0 \int_0^\beta d\tau \, \delta \phi(0, \tau) + \frac{L^2}{V} \phi_0 \int_0^\beta d\tau \, \delta \phi^*(0, \tau) \\
= \sum' \text{Tr}\left[(G_0)_{kk'} \Sigma_{kk'}\right] + \frac{L^2}{V} \phi_0 \delta \phi_0 + \frac{L^2}{V} \phi_0 \delta \phi^*_0 \\
= \delta \phi_0 \left(\frac{L^2}{V} \phi_0 + \frac{1}{\beta} \sum_{k,i\epsilon_n} \text{Tr}\left[G_0(k, i\epsilon_n)\right]\right) + \delta \phi^*_0 \left(\frac{L^2}{V} \phi_0 + \frac{1}{\beta} \sum' \text{Tr}\left[G_0(k, i\epsilon_n)\right]\right) \\
= \delta \phi_0 \left(\frac{L^2}{V} \phi_0 - \phi_0 \sum_k \frac{f(\xi_k)}{2E_k}\right) + \delta \phi^*_0 \left(\frac{L^2}{V} \phi_0 - \phi_0 \sum_k \frac{f(\xi_k)}{2E_k}\right) = 0
\]

We have use the fact that $\phi_0$ is determined by the stationary approximation.

3. 2nd order, $S_{\text{eff}}^{(2)}$:

\[
S_{\text{eff}}^{(2)} = \frac{1}{2} \text{Tr}(G_0 \Sigma G_0 \Sigma) + \frac{L^2}{V} \int_0^\beta d\tau \sum_q \delta \phi^*(q, \tau) \delta \phi(q, \tau) \\
= \sum' \frac{1}{2} \text{Tr}\left[(G_0)_{kk1} \Sigma_{k1k2} (G_0)_{k2k3} \Sigma_{k3k}\right] + \frac{L^2}{V} \int_0^\beta d\tau \sum_q \delta \phi^*(q, \tau) \delta \phi(q, \tau) \\
= \sum' \frac{1}{2} \text{Tr}\left[(G_0)_{kk'} \Sigma_{kk'} (G_0)_{kk'} \Sigma_{kk'}\right] + \frac{L^2}{V} \int_0^\beta d\tau \sum_q \delta \phi^*(q, \tau) \delta \phi(q, \tau)
\]

where $\Sigma_{kk'} = \frac{1}{\beta} \delta \phi_{k'-k}^+ + \frac{1}{\beta} \delta \phi_{k-k'}^-$. Define 4-momentum $q = (q, i\omega_m) = (k', i\epsilon_{n'} - i\epsilon_n)$. We have

\[
S_{\text{eff}}^{(2)} = \frac{L^2}{\beta V} \sum_q |\delta \phi_q|^2 + \frac{1}{\beta^2} \sum_{k,q} \left\{ \delta \phi_q^* \delta \phi_{-q}^* \frac{1}{2} \text{Tr}\left[G_0(k)\tau^+ G_0(k + q)\tau^+\right] \\
+ \delta \phi_q^* \delta \phi_{-q} \frac{1}{2} \text{Tr}\left[G_0(k)\tau^+ G_0(k + q)\tau^-\right] + \delta \phi_{-q}^* \delta \phi_q \frac{1}{2} \text{Tr}\left[G_0(k)\tau^- G_0(k + q)\tau^+\right] \\
+ \delta \phi_{-q} \delta \phi_q \frac{1}{2} \text{Tr}\left[G_0(k)\tau^- G_0(k + q)\tau^-\right] \right\}
\]

(5.47)
If we define \( \eta_q^\dagger = (\delta \phi_q^*, \delta \phi_{-q}) \), we can write \( S_{\text{eff}}^{(2)} \) as

\[
S_{\text{eff}}^{(2)} = \frac{L^2}{\beta V} \sum_q |\delta \phi_q|^2 + \frac{1}{\beta} \sum_q \frac{1}{2} \eta_q^\dagger M \eta_q 
\]

(5.48)

\( M \) is a \( 2 \times 2 \) matrix defined as

\[
M = \frac{1}{\beta} \sum_k' \begin{pmatrix}
\text{Tr} \left[ G_0(k) \tau^+ G_0(k + q) \tau^- \right] & \text{Tr} \left[ G_0(k) \tau^+ G_0(k + q) \tau^- \right] \\
\text{Tr} \left[ G_0(k) \tau^- G_0(k + q) \tau^- \right] & \text{Tr} \left[ G_0(k) \tau^- G_0(k + q) \tau^- \right]
\end{pmatrix}
\]

(5.49)

If we define \( u_k^2 = \frac{1}{2} \left( 1 + \epsilon_k / E_k \right) \) and \( v_k^2 = \frac{1}{2} \left( 1 - \epsilon_k / E_k \right) \) (these relations have been obtained from the mean field calculation Eq.5.18), we have

\[
M_{11} = \sum_k' \left\{ \frac{u_k^2}{\omega_m - \xi_k^+} \frac{f(\xi_k^+)}{\xi_k^+ - \xi_k^-} + \frac{v_k^2}{\omega_m - \xi_k^-} \frac{f(\xi_k^-)}{\xi_k^- - \xi_k^+} \right\} \\
+ u_k^2 \psi_k^+ \frac{f(\xi_k^+)}{\omega_m - \xi_k^+} \frac{f(\xi_k^-)}{\xi_k^-} + v_k^2 \psi_k^- \frac{f(\xi_k^-)}{\omega_m - \xi_k^-} \frac{f(\xi_k^+)}{\xi_k^+}
\]

(5.50)

\[
M_{12} = \sum_k' u_k v_k u_{k+q} v_{k+q} \left\{ \frac{f(\xi_{k+q}^+)}{\omega_m - \xi_{k+q}^+} \frac{f(\xi_{k+q}^-)}{\xi_{k+q}^-} + \frac{f(\xi_k^+)}{\omega_m - \xi_k^+} \frac{f(\xi_k^-)}{\xi_k^-} \right\} \\
- \frac{f(\xi_k^+)}{\omega_m - \xi_k^-} \frac{f(\xi_{k+q}^-)}{\xi_{k+q}^-} + \frac{f(\xi_k^-)}{\omega_m - \xi_k^+} \frac{f(\xi_{k+q}^+)}{\xi_{k+q}^+}
\]

(5.51)
\[ M_{22} = \sum_k \left\{ v_k u_{k+q} \frac{f(\xi_k^+)}{\omega_m} - \frac{f(\xi_{k+q}^-)}{\xi_k^+ + \xi_{k+q}^-} + u_k v_{k+q} \frac{f(\xi_k^-)}{\omega_m - \xi_{k+q}^+ + \xi_k^-} \right\} \]

\[ M_{21} = M_{12} \] (5.53)

If we only study the amplitude fluctuation of the order parameter, i.e. the order parameter including the fluctuations is real in the real space. So we have \( \delta \phi_q^* = \delta \phi_{-q} \), then

\[ S^{(2)}_{\text{eff}} = \frac{L^2}{\beta V} \sum_q |\delta \phi_q|^2 + \frac{1}{\beta} \sum_q \frac{1}{2} \eta_q^* M \eta_q \]

\[ = \frac{L^2}{\beta} \sum_q |\delta \phi_q|^2 \left( \frac{1}{V} + \frac{1}{2L^2} \left( M_{11} + M_{22} + M_{12} + M_{21} \right) \right) \] (5.54)

Write \( S^{(2)}_{\text{eff}} \) as

\[ S^{(2)}_{\text{eff}} = \frac{L^2}{\beta} \sum_q [V \Gamma(q)]^{-1} |\delta \phi_q|^2 \] (5.55)

And \( [\Gamma(q)]^{-1} = 1 - V \chi(q) \) which is the generalization of Eq.(4.50) in the ordered phase.
Then we can obtain the relation

\[
\chi(q) = \frac{1}{2L^2} \sum_k \left( u_k v_{k+q} + v_k u_{k+q} \right) \left( f(\xi^+_{k+q}) - f(\xi^+_{k}) \right) \left( \frac{i\omega_m - \xi^+_{k+q} + \xi^+_{k}}{i\omega_m - \xi^+_{k+q} + \xi^+_{k}} \right) \\
+ \frac{1}{2L^2} \sum_k' \left( u_k v_{k+q} - v_k u_{k+q} \right) \left( f(\xi^-_{k+q}) - f(\xi^-_{k}) \right) \left( \frac{i\omega_m - \xi^-_{k+q} + \xi^-_{k}}{i\omega_m - \xi^-_{k+q} + \xi^-_{k}} \right)
\]

(5.56)

The above \( \chi(q) \) can be separated into two parts, contribution from the inter-band \( \chi_\perp(q) \) and the contribution from the intra-band \( \chi_\parallel(q) \). We then have

\[
\chi_\perp(q) = \frac{1}{2L^2} \sum_k' \left( u_k v_{k+q} - v_k u_{k+q} \right) \left( f(\xi^+_{k+q}) - f(\xi^+_{k}) \right) \left( \frac{i\omega_m - \xi^+_{k+q} + \xi^+_{k}}{i\omega_m - \xi^+_{k+q} + \xi^+_{k}} \right)
\]

(5.57)

\[
\chi_\parallel(q) = \frac{1}{2L^2} \sum_k \left( u_k v_{k+q} + v_k u_{k+q} \right) \left( f(\xi^+_{k+q}) - f(\xi^+_{k}) \right) \left( \frac{i\omega_m - \xi^+_{k+q} + \xi^+_{k}}{i\omega_m - \xi^+_{k+q} + \xi^+_{k}} \right)
\]

(5.58)

### 5.3.2 Order Parameter Fluctuations

The hybridization of the bands in the XL phase couples the order parameter to the gapless fermions at the Fermi surface. The intraband polarization \( \chi_\parallel(q) \) represents this coupling. Physically it generates an additional “mass” for the bosonic propagator. Depending on the sign of the mass, the condensate may or may not be stable. To determine the sign, we will take the static limit of \( \chi(q) \). The limit
can be studied by first putting $i\omega_m = 0$ and then taking $\mathbf{q} \to 0$. Remember that

$$u^2_k = \frac{1}{2} \left( 1 + \epsilon_k / E_k \right) \text{ and } v^2_k = \frac{1}{2} \left( 1 - \epsilon_k / E_k \right)$$

- Inter-Band $\chi(\mathbf{q} \to 0, i q_m = 0)$.

We have

$$\chi(\mathbf{q} \to 0, i q_m = 0) = \frac{1}{2L^2} \sum_k' \left( u^2_k - v^2_k \right) \left( \frac{f(\xi^+_k)}{-\xi^+_k + \xi^+_k} - \frac{f(\xi^-_k)}{-\xi^-_k + \xi^-_k} \right)$$

$$= \frac{1}{2L^2} \sum_k' f(\xi^-_k) \frac{\epsilon_k}{E^3_k}$$

$$= \frac{1}{2L^2} \sum_k' \frac{f(\xi^-_k)}{E_k} - \frac{1}{2L^2} \sum_k f(\xi^-_k) \frac{\phi^2_0}{E^3_k} \tag{5.59}$$

The density of states is

$$\nu(\epsilon) = \nu_0 \frac{\epsilon}{\sqrt{\epsilon^2 - \phi^2_0}} \Theta \left( \epsilon - \sqrt{\epsilon^2 + \phi^2_0} \right) \tag{5.60}$$

$\nu_0$ is the density of the states of Graphene. Then

$$\frac{1}{2L^2} \sum_k' f(\xi^-_k) \frac{\phi^2_0}{E^3_k} = \nu_0 \int_{|\mu|}^{\Lambda} \frac{d\epsilon}{2\sqrt{\epsilon^2 - \phi^2_0}} = \nu_0 \frac{1}{2} \log \left( \frac{\Lambda + \sqrt{\Lambda^2 - \phi^2_0}}{|\mu|} \right)$$

$$= \frac{1}{2L^2} \sum_k' f(\xi^-_k) \frac{\phi^2_0}{E^3_k} \tag{5.61}$$

and

$$-\frac{1}{2L^2} \sum_k' f(\xi^-_k) \frac{\phi^2_0}{E^3_k} = -\nu_0 \frac{1}{2} \int_{|\mu|}^{\Lambda} \frac{\phi^2_0 d\epsilon}{\sqrt{\epsilon^2 - \phi^2_0}} = -\nu_0 \frac{1}{2} \left( \frac{\sqrt{\Lambda^2 - \phi^2_0}}{\Lambda} - \frac{\sqrt{|\mu|^2 - \phi^2_0}}{|\mu|} \right)$$

$$\sim -\nu_0 \frac{\phi^2_0}{2|\mu| |\mu| + \sqrt{|\mu|^2 - \phi^2_0}} \tag{5.62}$$

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Last step if \( \Lambda >> |\mu| \), we can ignore the \( \phi_0^2/\Lambda^2 \) term.

- Intra-Band \( \chi_\parallel(q \to 0, iq_m = 0) \).

We have

\[
\chi_\parallel(q \to 0, iq_m = 0) = \frac{1}{2L^2} \sum_k' 4u_k^2v_k \lim_{q \to 0} \frac{f(\xi_k+q) - f(\xi_k^-)}{-\xi_k+q + \xi_k^-} \\
= \frac{1}{L^2} \sum_k' \frac{\phi_0^2}{2E_k^2} \frac{\partial f(\xi_k^-)}{\partial \xi_k^-} \left( q \cdot \nabla_k \xi_k^- \right) \\
= \frac{\nu_0}{2} \int |\mu| \frac{\phi_0^2}{\epsilon \sqrt{\epsilon^2 - \phi_0^2}} \delta(-\epsilon + |\mu|) \\
= \frac{\nu_0}{2|\mu| \sqrt{\mu^2 - \phi_0^2}} 
\]

(5.63)

In sum, in the static limit, we have

\[
\lim_{q \to 0, iq_m = 0} \chi(q) = \chi_\perp(0) + \chi_\parallel(0) \\
= \frac{1}{2L^2} \sum_k' \frac{f(\xi_k^-)}{E_k} + \frac{\nu_0 \phi_0^2}{2|\mu|} \left( -\frac{1}{|\mu| + \sqrt{\mu^2 - \phi_0^2}} + \frac{1}{\sqrt{\mu^2 - \phi_0^2}} \right) 
\]

(5.64)

In the static limit, the bosonic propagator equals

\[
[V\Gamma(0)]^{-1} = 1 - V\chi(0) = 1 - \frac{V}{2L^2} \sum_k' \frac{f(\xi_k^-)}{E_k} - \frac{\nu_0 V \phi_0^2}{2|\mu|} \left( -\frac{1}{|\mu| + \sqrt{\mu^2 - \phi_0^2}} + \frac{1}{\sqrt{\mu^2 - \phi_0^2}} \right) \\
\approx 1 - \frac{V}{2L^2} \sum_k' \frac{f(\xi_k^-)}{E_k} - \frac{\nu_0 V \phi_0^2}{4\epsilon^2_F} 
\]

(5.65)
From the self-consistent equation Eq.(5.44), we finally reach the expression for the
bosonic propagator in the static limit

\[ [\Gamma(0)]^{-1} = -\frac{\nu_0 V \phi_0^2}{4\epsilon_F^2} < 0 \]  

(5.66)

The mass term in the bosonic propagator (the correlation function of the order
parameter) in the ordered phase is negative. This implies an instability of the XL
phase.

5.3.3 The \( q^2 \) Dependence in \([\Gamma(q)]^{-1}\)

For completeness, we will show the \( q^2 \) dependence in the bosonic propagator
\([\Gamma(q)]^{-1}\). We assume zero temperature and hole doping. We first put \( iq_m = 0 \).

**Inter-Band** \( \chi_{\perp}(q, 0) \)

\[
\chi_{\perp}(q, 0) = \frac{1}{2L^2} \sum_{k} \left( u_k u_{k+q} - v_k v_{k+q} \right)^2 \left( \frac{f(\xi_{k+q})}{-\xi_{k+q} + \xi_k^+} + \frac{-f(\xi_k)}{-\xi_{k+q} + \xi_k^-} \right) 
\]  

(5.67)
In order to calculate $q^2$ terms, we put $\phi_0 = 0$ in the $\chi_\perp(q, 0)$, and we have

$$
\frac{1}{2L^2} \sum_k' \left( \frac{f(\epsilon_{k+q})}{\epsilon_{k+q} + \epsilon_k} + \frac{f(\epsilon_k)}{\epsilon_k + \epsilon_{k-q}} \right) = \frac{1}{2L^2} \sum_k' \left( \frac{f(\epsilon_k)}{\epsilon_{k+q} + \epsilon_k} + \frac{f(\epsilon_k)}{\epsilon_k + \epsilon_{k-q}} \right)
$$

$$
= \frac{1}{2L^2} \sum_k' f(\epsilon_k) \left( \frac{1}{2\epsilon_k - (q \cdot k)/m + q^2/2m} + \frac{1}{2\epsilon_k + (q \cdot k)/m + q^2/2m} \right)
$$

$$
= \frac{1}{8\pi^2} \int_{k_F}^{k_A} k \, dk \int_0^{2\pi} d\theta \left( \frac{1}{2\epsilon_k - kq \cos \theta/m + q^2/2m} + \frac{1}{2\epsilon_k + kq \cos \theta/m + q^2/2m} \right)
$$

(5.68)

Because of the symmetry in the $\theta$, the two terms yield the same result after the $\theta$ integral. We only need to calculate one of them. We do the substitution $z = \exp(i\theta)$, and $\cos \theta = \frac{1}{2}(z + 1/z)$.

$$
\int_0^{2\pi} d\theta \frac{1}{2\epsilon_k - kq \cos \theta/m + q^2/2m} = -\frac{2m}{kq} \int_{|z|=1} \frac{dz}{iz} \frac{1}{(z + 1/z) - 4m\epsilon_k - q^2}
$$

$$
= -\frac{2m}{kq} \frac{1}{iz} \int_{|z|=1} \frac{dz}{(z - z_-)(z - z_+)}
$$

(5.69)

where

$$
z_{\pm} = \frac{1}{2kq} \left( 4m\epsilon_k + q^2 \pm \sqrt{(4m\epsilon_k + q^2)^2 - 4k^2q^2} \right)
$$

(5.70)

The piece under the square root is always greater than 0, and the $z_-$ is always inside the unit circle $|z| = 1$. So we have for the integral

$$
-\frac{4m\pi}{kq} z_- - z_+ = \frac{4m\pi}{\sqrt{16m^2\epsilon_k^2 + (8m\epsilon_k - 4k^2)q^2 + q^4}}
$$

(5.71)

Remember that $\epsilon_k = k^2/2m + E_G/2$, and put back the $k$ integral, we have (ignore
the $q^4$ term, and 2 is because of the other $\theta$ integral term)

$$2 \times \frac{1}{8\pi^2} \int_{k_F}^{k_F} kdk \frac{4m\pi}{\sqrt{16m^2\epsilon_k^2 + 4mE_Gq^2}} = \frac{\nu_0}{2} \int_{\epsilon_F}^{\epsilon_F} d\epsilon_k \frac{1}{\sqrt{\epsilon_k^2 + \frac{E_Gq^2}{2m}}}$$

$$= \frac{\nu_0}{2} \int_{\epsilon_F}^{\epsilon_F} d\epsilon_k \frac{1}{\epsilon_k} - \frac{\nu_0}{8} \int_{\epsilon_F}^{\epsilon_F} d\epsilon_k \frac{E_G}{\epsilon_k^3} \frac{q^2}{2m}$$

(5.72)

The first term is a constant, which is the same as put in $\phi_0 = 0$ in $\chi_{\perp}(0,0)$. The second term is a $q^2$ term which is

$$\frac{\nu_0 E_G q^2}{16\epsilon_F^2 2m}$$

(5.73)

**Intra-Band $\chi_{\parallel}(q,0)$**

$$\chi_{\parallel}(q,0) = \frac{1}{2L^2} \sum'_{k} \left( u_k v_{k+q} + v_k u_{k+q} \right)^2 \frac{f(\xi_{k+q}^-) - f(\xi_k^-)}{-\xi_{k+q}^- + \xi_k^-}$$

(5.74)

The structure factor $\left( u_k v_{k+q} + v_k u_{k+q} \right)^2$ is zero when $\phi_0 = 0$, so we can first expand it to the $\phi_0^2$ order. We have

$$\chi_{\parallel}(q,0) = \frac{1}{8L^2} \sum'_{k} \frac{\phi_0^2}{E_k + E_{k+q}} \left( \frac{\epsilon_{k+q}}{\epsilon_k} + \frac{\epsilon_k}{\epsilon_{k+q}} + 2 \right) \frac{f(\xi_{k+q}^-) - f(\xi_k^-)}{-\xi_{k+q}^- + \xi_k^-}$$

(5.75)

Now the $q^2$ can come from the structure factor or the Lindhard like function. But either way, the $q^2$ correction in the $\chi_{\parallel}(q,0)$ is proportional to $\phi_0^2 q^2$.

- $q^2$ from the structure factor. In this situation, we can put $q \to 0$ limit in the
other part, and have

\[
\frac{1}{8L^2} \sum_k' \frac{\phi_0^2}{E_k + E_{k+q}} \left( \frac{\epsilon_{k+q}}{\epsilon_k} + \frac{\epsilon_k}{\epsilon_{k+q}} + 2 \right) \delta(\xi_k^-) = \frac{\phi_0^2}{8} \sum_k' \frac{(\epsilon_{k+q} + \epsilon_k)^2}{\epsilon_k \epsilon_{k+q} (E_k + E_{k+q})} \delta(\xi_k^-) \tag{5.76}
\]

In sum, we see that except the first case, all the other $q^2$ terms are proportional to $q^2 \phi_0^2 / |\mu_0|^3$, while in the first case it is proportional to $q^2 e_g / \epsilon_F^2$. So in the semiconductor and close to the quantum critical point, $q^2 E_G / \epsilon_F^2$ will dominate and gives us a $\gamma q^2$, $\gamma > 0$ correction in the $1 - V \chi(q)$.

**The Static Screening**

Put the above result together, we have the $[VT(q)]^{-1}$ in the static screening limit ($iq_m = 0$) as

\[
[VT(q,0)]^{-1} = \nu_0 \phi_0^2 \frac{1}{2|\mu|} \left( \frac{1}{|\mu| + \sqrt{\mu^2 - \phi_0^2}} - \frac{1}{\sqrt{\mu^2 - \phi_0^2}} \right) + \gamma q^2, \quad \gamma > 0 \tag{5.77}
\]
Chapter 6

Theory of the Excitonic Liquid State in Graphene

In this chapter, we will apply the theory to Graphene to study the possible XL phase transition in the honeycomb lattice.

6.1 The Model Hamiltonian

The effective Hamiltonian with the chemical potential is

\[ K = \sum_k \psi_k^\dagger (\epsilon_k \tau_3 - \mu) \psi_k - \frac{V}{2N} \sum_q \hat{\Phi}^\dagger(q) \hat{\Phi}(q) \]  

(6.1)

where \( \hat{\Phi}^\dagger(q) = \sum_k S_k \left[ \psi_k^\dagger \tau_1 e^{i \delta_{k,q} a \tau_3} \psi_{k+q}^\dagger \right] \). The divergence of \( \Gamma(q) = \frac{1}{1 - V \chi_0(q)} \) appeared at a critical \( V_c \) in the static limit. In the hole doping case, the \( V_c \) deter-
mines the QCP equals

\[ \frac{1}{V_c} = \chi_0(0) = \frac{1}{N} \sum_k S_k^2 \frac{f(\epsilon_k)}{\epsilon_k} \] (6.2)

### 6.2 Binding Energy of a Single Exciton

We look for the wave function of a single particle-hole (p-h) pair. The p-h pair wave function is formed as a linear combination:

\[ |\phi_0\rangle = \sum_k \varphi_k b_k^\dagger a_k |FS\rangle \] (6.3)

Here the prime summation denotes the lower \( k_F \) cutoff which is different from the prime sum in the semiconductor situation. The energy of the pair can be found from the time evolution of the pair wave function

\[ -i \sum_k \varphi_k \frac{d(b_k^\dagger a_k)}{dt} = \sum_k \varphi_k \left[ K, b_k^\dagger a_k \right] \] (6.4)

Assuming that a well defined pair state exists with energy \( E \), a stationary solution
is assumed

\[
E \sum' \varphi_k b_k^\dagger a_k = \sum' \varphi_k \left[K, b_k^\dagger a_k\right] \nonumber
\]

\[
= 2 \sum' \epsilon_k \varphi_k b_k^\dagger a_k + \frac{V}{2} \sum' S_k(b_k^\dagger a_k + a_k^\dagger b_k) \left[\frac{1}{N} \sum' \varphi_p S_p(b_p^\dagger b_p - a_p^\dagger a_p)\right] \nonumber
\]

\[
+ \frac{V}{2} \left[\frac{1}{N} \sum_p \varphi_p S_p(b_p^\dagger b_p - a_p^\dagger a_p)\right] \sum_k S_k(b_k^\dagger a_k + a_k^\dagger b_k) \quad (6.5)
\]

Because the appearance of the operator \(a_k^\dagger b_k\), we need another equation for it.

This can be done by applying the Hermitian conjugate on both sides of the above equation and assuming \(\varphi_k\) is real, which will be shown later. We have

\[
E \sum' \varphi_k a_k^\dagger b_k = 2 \sum' \epsilon_k \varphi_k a_k^\dagger b_k + \frac{V}{2} \sum' S_k(b_k^\dagger a_k + a_k^\dagger b_k) \left[\frac{1}{N} \sum' \varphi_p S_p(b_p^\dagger b_p - a_p^\dagger a_p)\right] \nonumber
\]

\[
+ \frac{V}{2} \left[\frac{1}{N} \sum_p \varphi_p S_p(b_p^\dagger b_p - a_p^\dagger a_p)\right] \sum_k S_k(b_k^\dagger a_k + a_k^\dagger b_k) \quad (6.6)
\]

Adopt the rigid FS approximation and hence the interaction of the pair with the FS is replaced by the average \(\langle a_p^\dagger a_p - b_p^\dagger b_p \rangle = f(\epsilon_p^-) - f(\epsilon_p^+)\). Also combining these two equations, we have

\[
E \sum' \varphi_k (b_k^\dagger a_k + a_k^\dagger b_k) = 2 \sum' \epsilon_k \varphi_k (b_k^\dagger a_k + a_k^\dagger b_k) - 2V \left[\frac{1}{N} \sum' \varphi_p S_p\right] \sum_k S_k(b_k^\dagger a_k + a_k^\dagger b_k) \quad (6.7)
\]
We then obtain the equation

\[ E\varphi_k = 2\epsilon_k \varphi_k - 2V \left[ \frac{1}{N} \sum_p' \varphi_p S_p \right] S_k \]  

(6.8)

When \( V = 0 \), we have the bare p-h energy, \( E = 2\epsilon_k \). The attraction \( V \) lowers the bare energy. To make further progress, the range of \( \varphi_k \) has to be defined. Clearly, \( \varphi_k = 0 \) for \( k \notin FS \). The high energy cutoff is not necessary here, because as we can see later on the high energy cutoff can be pushed to \( \infty \) without causing any divergence in the problem. Then we have the equation for \( \varphi_k \) as

\[ \varphi_k = -\frac{2VS_k \left( \frac{1}{N} \sum_p' \varphi_p S_p \right)}{E - 2\epsilon_k} \]  

(6.9)

Multiply \( S_k \) on both sides and then sum over the restricted \( k \) we get the equation,

\[ 1 = -\frac{2V}{N} \sum_k' \frac{S_k^2}{E - 2\epsilon_k} \]  

(6.10)

At \( V_c \), a zero energy bound state is found. Setting \( E = 0 \), we have

\[ \frac{1}{V_c} = \frac{1}{N} \sum_k' \frac{S_k^2}{\epsilon_k} \]  

(6.11)

When \( V > V_c \), it becomes favorable to create particle-hole pairs out of the fermi-sea, thus destabilizing the FS. We proceed to look for a mean field solution by assigning the order parameter \( V\langle \Phi(q) \rangle/L^2 = \phi_0 \delta_{q,0} \) in the Hamiltonian Eq.(6.1).
Remember that $\phi_0$ is assumed real. The mean field Hamiltonian is

$$K_{\text{MF}} = \sum_k \psi_k^\dagger (\epsilon_k \tau_3 - \phi_0 S_k \tau_1 - \mu) \psi_k - \frac{N}{V} \phi_0^2$$  \hspace{1cm} (6.12)$$

Diagonalizing $K_{\text{MF}}$, we obtain $\xi_k^{\pm} = \pm E_k - \mu$ as the eigen energy, where $E_k = \sqrt{\epsilon_k^2 + \phi_0^2 S_k^2}$. A gap opened at the Dirac points as have mentioned before. Because $K_{\text{MF}}$ commutes with the individual number operator per k state $\hat{n}_k = a_k^\dagger a_k + b_k^\dagger b_k$, every k-state up to the non-interacting $k_F$ remains occupied as $V$ is tuned through the QCP. It implies the Fermi wavevector $k_F$ is not renormalized and a sharp Fermi surface exists in the condensed phase.

The two new hybridized states denoted as $c_{k\pm}$ corresponding to $\pm E_k$ respectively are

$$c_{k+} = u_k b_k - v_k a_k \hspace{1cm} (6.13)$$

$$c_{k-} = u_k a_k + v_k b_k \hspace{1cm} (6.14)$$

with

$$|u_k|^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_k}{E_k} \right) \quad |v_k|^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k}{E_k} \right) \hspace{1cm} (6.15)$$

For hole doped case, the ground state of the XL phase is

$$|XL\rangle = \prod_{|k|>k_F} c_{k-}^\dagger |0\rangle \hspace{1cm} (6.16)$$
where $|0\rangle$ is the vacuum. However, it is more intuitive to use a new “vacuum” $|FS\rangle = \prod_k a_k^\dagger |0\rangle$ which is the noninteracting Fermi surface corresponding to the partially filled valence band. Then the $|XL\rangle$ is

$$|XL\rangle = \prod_{|k| > k_F} (u_k + v_k b_k^\dagger a_k) |FS\rangle$$

(6.17)

Here $u_k = \sqrt{\frac{E_k + \epsilon_k}{2E_k}} e^{\frac{i\theta_k}{2}}$, $v_k = \sqrt{\frac{E_k - \epsilon_k}{2E_k}} \frac{\phi_0 S_k}{|\phi_0 S_k|} e^{\frac{i\theta_k}{2}}$. Here the extra $e^{\frac{i\theta_k}{2}}$ is to make the wave function single valued around the Dirac points. However, this extra phase is not going to effect the stability calculations.

### 6.3 Order Parameter Fluctuations

In order to study the fluctuations, we introduce the Hubbard-Stratonovich fields $\phi(q, \tau)$ that couple to $\Phi^\dagger(q)$. Integrating out the fermions, we get $Z = \int D[\phi^*] D[\phi] e^{-S_{\text{eff}}[\phi^*, \phi]}$, where

$$S_{\text{eff}} = -\text{Tr} \ln G^{-1} + \frac{N}{2\beta V} \sum_q |\phi_q|^2$$

(6.18)

$$G^{-1}(k, k') = (-i\epsilon_n - \mu + \epsilon_k \tau_3) \delta_{k,k'} - \frac{1}{\beta} \phi(k - k') S_{\frac{1}{2}}(k + k') e^{\frac{i}{2}(\theta_k - \theta_{k'})\tau_3 \tau_1}$$

(6.19)

The mean-field theory results correspond to the uniform saddle-point solution $\phi(q, iq_m) = \beta \phi_0 \delta_{m,0} \delta_{q,0}$. The trace can be evaluated by writing $\text{Tr} \ln G^{-1} =$
\[ \text{Tr ln } G_0^{-1} - \sum_n \frac{1}{n} \text{Tr}(G_0 \Sigma)^n \text{ with} \]

\[ G_0(k, k') = \frac{(i\epsilon_n + \mu)\tau_0 + \epsilon_k \tau_3 - \phi_0 S_k \tau_1}{(i\epsilon_n - \xi^+_k)(i\epsilon_n - \xi^-_k)} \delta_{k,k'}, \quad \xi^\pm_k = \pm \sqrt{\epsilon^2_k + \phi_0^2 S_k^2 - \mu} \]

\[ \Sigma(k, k') = \frac{1}{\beta} \delta \phi(k - k') S_{\frac{1}{2}(k+k')} \epsilon^\pm_{\frac{1}{2}(\theta_k - \theta_{k'})} \tau_1 \tau_1 \] (6.20)

We can study the \( S \) order by order.

**0th Order**

\[ S^{(0)}_{\text{eff}} = -\text{Tr ln } G_0^{-1} + \frac{\beta N}{2V} \phi_0^2 \]

\[ = \beta \sum_k \xi^- k f(\xi^-_k) + \frac{\beta N}{2V} \phi_0^2 \] (6.22)

Minimize w.r.t. \( \phi_0 \), we will have the self-consistent equation

\[ \frac{1}{V} = \frac{1}{\beta \sum_k f(\xi^-_k) S_k^2}{\sqrt{\epsilon^2_k + S_k^2 \phi_0^2}} \] (6.23)

The critical value \( V_c \) can be found by putting \( \phi_0 = 0 \),

\[ \frac{1}{V_c} = \frac{1}{\beta \sum_k f(\xi^-_k) S_k^2}{\epsilon_k} \] (6.24)
1st Order

\[ S_{\text{eff}}^{(1)} = \text{Tr}(G_0 \Sigma) + \frac{N}{2V} \phi_0 \delta \phi_0 + \frac{N}{2V} \phi_0 \delta \phi^*_0 \]  
\[ = \sum_{k,k'} \text{Tr}[(G_0)_{kk'} \Sigma_{k'k}] + \frac{N}{V} \phi_0 \delta \phi_0 \]  
\[ = \delta \phi_0 \left( \frac{N \phi_0}{V} + \frac{1}{\beta} \sum_{k,i \epsilon_n} \text{Tr} \left[ G_0(k,i \epsilon_n) \tau_1 S_k \right] \right) \]  
\[ = \delta \phi_0 \left( \frac{N \phi_0}{V} - \sum_k f(\xi_0) \frac{\phi_0 S_k^2}{E_k} \right) \]  
\[ = 0 \]  

2nd Order

\[ S_{\text{eff}}^{(2)} = \frac{1}{2} \text{Tr}(G_0 \Sigma G_0 \Sigma) + \frac{N}{\beta V} \sum_q |\delta \phi_q|^2 \]  
\[ = \sum_{k,k_1,k_2,k_3} \frac{1}{2} \text{Tr}[(G_0)_{kk_1} \Sigma_{k_1k_2}(G_0)_{k_2k_3} \Sigma_{k_3k}] + \frac{N}{\beta V} \sum_q |\delta \phi_q|^2 \]  
\[ = \sum_{k,k'} \frac{1}{2} \text{Tr}[(G_0)_{kk} \Sigma_{kk'}(G_0)_{k'k'} \Sigma_{k'k}] + \frac{N}{\beta V} \sum_q |\delta \phi_q|^2 \]  

We have

\[ S_{\text{eff}}^{(2)} = \frac{1}{\beta^2} \sum_q |\delta \phi_q|^2 \sum_k \sum_{i \epsilon_n} S_k^2 \left( i \epsilon_n + \mu \right) \left( i \epsilon_n + i q_m + \mu \right) - \epsilon_{k+\frac{1}{2}} \epsilon_{k-\frac{1}{2}} \cos \theta_{k,q} + \phi_{0}^2 S_{k+\frac{1}{2}} S_{k-\frac{1}{2}} \]  
\[ + \frac{N}{2\beta V} \sum_q |\delta \phi_q|^2 \]  
\[ = \frac{N}{2\beta V} \sum_q |\delta \phi_q|^2 (1 - V \chi(q)) \]  

\( \chi(q) = \chi_{\perp}(q) + \chi_{\parallel}(q) \) can be separated into inter and intra band contribution.
• Inter-Band

\[
\chi_\perp(q) = \frac{1}{2N} \sum_k S_k^2 \left(1 + \frac{\epsilon_k + \frac{q}{2}\epsilon_k - \frac{q}{2}}{E_{k+\frac{q}{2}}E_{k-\frac{q}{2}}} \cos \delta \theta_{k,q} - \frac{\phi_0 S_{k+\frac{q}{2}}S_{k-\frac{q}{2}}}{E_{k+\frac{q}{2}}E_{k-\frac{q}{2}}} \right) \times \\
\frac{\left[f(\xi_{k-\frac{q}{2}}^+) - f(\xi_{k+\frac{q}{2}}^+)\right] - \left[f(\xi_{k-\frac{q}{2}}^-) - f(\xi_{k+\frac{q}{2}}^-)\right]}{i q_m - \xi_{k+\frac{q}{2}}^+ + \xi_{k-\frac{q}{2}}^-}
\]  

(6.34)

• Intra-Band

\[
\chi_\parallel(q) = -\frac{1}{2N} \sum_k S_k^2 \left(1 - \frac{\epsilon_k + \frac{q}{2}\epsilon_k - \frac{q}{2}}{E_{k+\frac{q}{2}}E_{k-\frac{q}{2}}} \cos \delta \theta_{k,q} + \frac{\phi_0 S_{k+\frac{q}{2}}S_{k-\frac{q}{2}}}{E_{k+\frac{q}{2}}E_{k-\frac{q}{2}}} \right) \times \\
\frac{\left[f(\xi_{k-\frac{q}{2}}^+) - f(\xi_{k+\frac{q}{2}}^+)\right] - \left[f(\xi_{k-\frac{q}{2}}^-) - f(\xi_{k+\frac{q}{2}}^-)\right]}{i q_m - \xi_{k+\frac{q}{2}}^+ + \xi_{k-\frac{q}{2}}^-}
\]  

(6.35)

With the definition \( u_k = \sqrt{\frac{E_k + \epsilon_k}{2E_k}} e^{i\theta_k}, \ v_k = \sqrt{\frac{E_k - \epsilon_k}{2E_k}} h_0 S_k e^{i\theta_k} \) and \( \Pi_{ss'} = (f(\xi_{k-\frac{q}{2}}^+) - f(\xi_{k+\frac{q}{2}}^+))/(i q_m + \xi_{k-\frac{q}{2}}^+ - \xi_{k+\frac{q}{2}}^+). \) We have

• Inter-Band

\[
\chi_\perp(q) = -\frac{1}{N} \sum_k S_k^2 \left[ u_{k-\frac{q}{2}} u_{k+\frac{q}{2}} - v_{k-\frac{q}{2}} v_{k+\frac{q}{2}} \right]^2 \cos^2 \frac{\delta \theta_{k,q}}{2} \\
+ \left[ u_{k-\frac{q}{2}} v_{k+\frac{q}{2}} - v_{k-\frac{q}{2}} u_{k+\frac{q}{2}} \right]^2 \sin^2 \frac{\delta \theta_{k,q}}{2} \left( \Pi_{++} + \Pi_{--} \right) \]  

(6.36)
• Intra-Band

\[
\chi\parallel(q) = -\frac{1}{N} \sum_k S_k^2 \left[ \left| u_{k-\frac{q}{2}} u_{k+\frac{q}{2}} + v_{k-\frac{q}{2}} v_{k+\frac{q}{2}} \right|^2 \sin^2 \frac{\delta_{k,q}}{2} + \left| u_{k-\frac{q}{2}} v_{k+\frac{q}{2}} + v_{k-\frac{q}{2}} u_{k+\frac{q}{2}} \right|^2 \cos^2 \frac{\delta_{k,q}}{2} \right] \left( \Pi_{++} + \Pi_{--} \right) \tag{6.37}
\]

**Static Limit**

In the static limit, we take \(iq_m = 0\) first and then \(q \to 0\). Notice that \(\sin^2(\delta_{k,q}/2) = 0\) in this limit so we have

• Intra-Band

\[
\chi\parallel(0) = \frac{1}{N} \sum_k \frac{\phi_{0,k}^2 S_k^4}{E_k^2} \delta(\xi_k) \tag{6.38}
\]

\[
= \nu_0 \int_{\epsilon_F}^{\Lambda} \epsilon \, d\epsilon \, \frac{\phi_{0,k}^2 S_k^4}{\epsilon^2 + \phi_{0,k}^2 S_k^2} \delta(\epsilon - \epsilon_F) \tag{6.39}
\]

\[
\approx \frac{\nu_0 \phi_{0,k}^2 S_k^4}{\epsilon_F} \tag{6.40}
\]

• Inter-Band

\[
\chi\perp(0) = \frac{1}{N} \sum_k f(\xi_k^-) \frac{S_k^2}{E_k} \frac{\epsilon_k^2}{E_k^3} \tag{6.41}
\]

\[
= \frac{1}{N} \sum_k f(\xi_k^-) \frac{S_k^2}{E_k} - \frac{1}{N} \sum_k f(\xi_k^-) \frac{\phi_{0,k}^2 S_k^4}{E_k^3} \tag{6.42}
\]

\[
= \frac{1}{N} \sum_k f(\xi_k^-) \frac{S_k^2}{E_k} - \nu_0 \phi_{0,k}^2 \int_{\epsilon_F}^{\Lambda} \epsilon \, d\epsilon \, \frac{S_k^4}{(\epsilon^2 + \phi_{0,k}^2 S_k^2)^2} \tag{6.43}
\]

The first piece is \(1/V\) from the self-consistent equation. For the second piece,
we have \((\Lambda \to \infty)\)

\[
\nu_0 \phi_0^2 \int_{\epsilon_F}^{\Lambda} \frac{\epsilon \, d\epsilon}{(\epsilon_0^2 + \phi_0^2 S_k^2)^{3/2}} < \nu_0 \phi_0^2 S_k^d \int_{\epsilon_F}^{\infty} \frac{1}{\epsilon^3} = \frac{\nu_0 \phi_0^2 S_k^d}{\epsilon_F} \quad (6.44)
\]

So again, we have for \([VT(q)]^{-1} = 1 - V\chi(q)\) in the static limit

\[
[VT(0)]^{-1} < 0 \quad (6.45)
\]

The XL phase is unstable.
Chapter 7

Conclusions

We have shown that the mean-field solution for the interband particle-hole condensate with a sharp Fermi surface, which we call an excitonic liquid (XL) is unstable in the presence of the gapless fermions at the Fermi surface. We demonstrate this destabilization in two models, both of which stabilize an uniform XL phae at the mean-field level. Our results therefore suggest that a uniform condensate of virtual excitons, with or without spontaneous time reversal symmetry breaking, is an unstable phase at $T = 0$. In particular, we show that the static limit of the effective interaction in the particle-hole channel is negative, thus a Ginzburg-Landau type description of the ordered phase is in general not possible.

A possible cure for this instability might be to assume a non-uniform ($q \neq 0$) mean-field state. However, our results suggest that condensates with a sharp Fermi surface will always tend to be unstable as a result of the collective FL excitations. A mechanism to open a gap to stabilize such a phase is unclear at the moment.
Bibliography


