理論磁気応答の基礎とその応用

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PhD Thesis

Theory of magnetic response in nodal semimetals
(ノーダル半金属における磁場応答の理論)

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Chapter 1

Introduction

1.1 Purpose of the study

In the ordinary metal, it is well-known that the magnetic susceptibility consists of Pauli paramagnetism (spin term) and Landau diamagnetism (orbital term). Pauli paramagnetism is positive magnetic susceptibility, while Landau diamagnetism is negative susceptibility. However, it is not always true when we have spin-orbit (SO) interaction in the system. The SO interaction may give rise to a new term of magnetic susceptibility, which is not the spin paramagnetism nor the orbital diamagnetism.

The purpose of study is to understand the magnetic response of various materials with strong spin-orbit coupling (SOC), including two-dimensional (2D) Rashba/Dresselhaus system, the 2D surface state of topological insulator, and three-dimensional (3D) nodal semimetals. We start with the well-known spin-orbit coupled system, i.e. 2D electron gas (2DEG) with Rashba and Dresselhaus SOC. In both cases, the spin-orbit interaction is induced by the inversion symmetry breaking. The Rashba effect occurs when there is structural inversion asymmetry in the junction of semiconductor hetero-structures \[ 1 \], while the Dresselhaus effect occurs when the asymmetry exist in bulk crystal structure.\[ 2 \] Although the energy dispersion at zero magnetic field is essentially equivalent in both Rashba and Dresselhaus systems, but the spin texture on the momentum space is completely different between them. We will show that this leads to a significant difference in the spin-orbit cross term in the magnetic...
susceptibility.

Moreover, there are a variety of novel topological materials in which the spin-orbit coupling is essential, such as topological insulator, the Dirac semimetal, and the Weyl semimetal. They are new, but the magnetic response is not well known. The topological insulator is a bulk insulator with topological surface states.\cite{4, 5, 6, 7, 8} The Weyl and Dirac semimetals are the systems with 3D gapless spectrum where the energy bands touch at isolated points in the momentum space.\cite{9, 61, 62, 63, 64, 10, 14, 16, 18, 19, 23} We expand our standard knowledge of paramagnetism/diamagnetism to those novel materials by calculating the magnetic susceptibility.

This thesis will be organized as follows: In Chapter 2, we calculate the magnetic susceptibility for 2DEG with Rashba SOC and Dresselhaus SOC, and also the 2D Dirac surface states of the topological insulator. In Chapter 3, we present the detailed calculation of the magnetic response for 3D Dirac/Weyl semimetals. Lastly, the conclusion will be presented in Chapter 4.

1.2 Background

1.2.1 Magnetism of metals

In the ordinary metal, it is well-known that the magnetic susceptibility consists of Pauli paramagnetism and Landau diamagnetism. Pauli paramagnetism is caused by the spin magnetic moment, while the Landau diamagnetism originates from the orbital cyclotron motion. In the Pauli paramagnetism, an external magnetic field shifts the energy levels up and down by $\pm \mu_B H$, where $\mu_B$ is Bohr magneton, $H$ is the magnetic field applied. This immediately results in different numbers in the up spins and down spins at the equilibrium and thus the system has a finite magnetization as a whole. In Landau diamagnetism, on the other hand, the electrons makes a circular motion under the Lorentz force, and it gives the magnetization. In the quantum mechanics, the energy spectrum is quantized into the discrete levels $(n+1/2)\hbar \omega_c$ where $n$ is integer and the spacing width is $\hbar \omega_c$ between the levels. $\hbar$ is Planck constant $h$ divided by $2\pi$ and $\omega_c$ is the cyclotron frequency. This is called the Landau quantization and this correctly explains the diamagnetic behavior.\cite{21} For free electron, the magnitude of Landau diamagnetism is 3 times smaller than the Pauli paramagnetism. In total,
therefore, the magnetic susceptibility is paramagnetic.

The above classic argument applies to the spin-independent free electron system with the quadratic dispersion \( E = \frac{p^2}{2m} \). If the system has the spin-orbit interaction, then the spin magnetism and the orbital magnetism cannot be treated independently and we need a different approach to describe the magnetic response. In this thesis, we show that the magnetic susceptibility in SOC is generally composed of three terms; the spin-spin term (\( \chi_{\text{spin}} \)), the orbital-orbital term (\( \chi_{\text{orb}} \)), and also the spin-orbital term (\( \chi_{\text{SO}} \)). We calculate those three terms for different electronic systems introduced in the following, and argue the characteristic property of each term in a systematic manner.

1.2.2 Rashba / Dresselhaus system

As mentioned before, the Pauli paramagnetism comes from the contribution of spins and Landau diamagnetism comes from the orbital contribution. However it’s not always true if we have system having spin-orbit coupling (SOC). The SOC effect may give rise the cross term of spin-orbit contribution. Here we explain the well-known spin-orbit coupled system, i.e. 2DEG with Rashba and Dresselhaus SOC. In both cases, the spin-orbit interaction is induced by the inversion symmetry breaking.

The Rashba effect occurs when there is structural inversion asymmetry in the junction of semiconductor hetero-structures. This effect was proposed by Bychkov-Rashba to explain the splitting phenomena at GaAs – Al\(_x\)Ga\(_{1-x}\)As heterostructures in
CHAPTER 1. INTRODUCTION

Figure 1.2: Side view: (a). Band dispersion of 2DEG without SOC, (b). band dispersion for 2DEG with SOC. Top view: (c). Spin orientation for 2DEG with Rashba SOC, (d). spin orientation for 2DEG with Dresselhaus SOC.

n- and p-type layers. [1, 2] Recently, experimental observations of giant Rashba spin-orbit coupling have been reported. [30, 31, 32, 33, 34] Theoretical research of magnetic response in 2DEG with the contribution of Rashba effect had been recently calculated. [35, 36] The Dresselhaus effect occurs when the asymmetry exist in crystal structure of the bulk material. This theory was proposed by Dresselhaus in 1955 to describe the SOC effect in zinc blende structures material. [3]

In the Rashba / Dresselhaus spin orbit interaction, the electrons feel the effective Zeeman field depending on the electronic momentum, so that the spin direction correlates with the momentum direction. Although the spectrum at zero magnetic field is essentially equivalent in both Rashba and Dresselhaus systems, the spin texture in the momentum space is completely different as illustrated in Fig. 1.2. Specifically, if
Figure 1.3: The cone shaped band dispersion of the surface of topological insulator (left). The view of the Fermi surface from the top (right). The spin’s vector is perpendicular to momentum $k$.

we rotate the equi-energy contour in the momentum space in the clock-wise direction, then the spin also rotates in the clockwise direction in Rashba system, while in the counter-clockwise direction in the Dresselhaus system. In that sense, the two systems have opposite ”chirality” (or ”handedness”) of the spin texture. The similar chiral spin texture is also found in the surface states of the topological insulator. The topological insulators are electronic systems which have a bulk band gap but also have protected conducting states on the surface. The 3D topological insulators such as $\text{Bi}_2\text{Se}_3$ and $\text{Bi}_2\text{Te}_3$, the surface state band is approximates the 2D Dirac cone, where the spin direction correlates with the momentum as in Fig. 1.3.

In this thesis, we calculate the magnetic susceptibility of Rashba /Dresselhaus systems and also 2D Dirac mode for the surface states of the 2D topological insulator. We demonstrate that the spin-momentum relationship makes an essential difference in the spin-orbit cross term, and determines the amplitude and sign of the total susceptibility.

1.2.3 Weyl / Dirac semimetals

In this thesis, we also theoretically investigate the magnetic response of three-dimensional (3D) gapless electron systems. The 3D version of the gapless band structure was the-
CHAPTER 1. INTRODUCTION

Figure 1.4: Three dimensional schematic image of the Weyl semimetal in momentum space. [47]

oretically proposed by 46, 51, 61, 62, 63, 64, 10, 14, 16, 18, 19, 23. In very recent experiments, such 3D gapless electron systems were actually realized in various materials 46, 58, 52, 53, 54, 55.

In 2D, the analogous Hamiltonian is $H(k) = v(k_x \sigma_x + k_y \sigma_y)$ where $\sigma_x, \sigma_y$ are the Pauli matrices and $v$ is the velocity parameter. In 3D, the analogous Hamiltonian is $H(k) = v(k_x \sigma_x + k_y \sigma_y + k_z \sigma_z)$ with all three Pauli matrices, and it is called a Weyl Hamiltonian as it describes a pair of linear bands degenerating at a point. When the two different Weyl points happen to merge at a single momentum, the system is called the Dirac semimetal, since the effective Hamiltonian is given by $4 \times 4$ Dirac Hamiltonian around the four-fold degenerate point.

In 2D gapless electron system (e.g., graphene), the low energy effective theory at point degeneracies between the conduction and valence bands takes the form, $H(k) = v(k_x \sigma_x + k_y \sigma_y)$ where $\sigma_x, \sigma_y$ are the Pauli matrices and $v$ is the velocity parameter. In 3D, the analogous Hamiltonian is $H(k) = v(k_x \sigma_x + k_y \sigma_y + k_z \sigma_z)$ with all three Pauli matrices, and it is called a Weyl Hamiltonian as it describes a pair of linear bands degenerating at a point. When the two different Weyl points happen to merge at a single momentum, the system is called the Dirac semimetal, since the effective Hamiltonian is given by $4 \times 4$ Dirac Hamiltonian around the four-fold degenerate point.

If the Weyl points are isolated in the momentum space, on the contrary, the system is called the Weyl-semimetal, and the effective Hamiltonian at each Weyl point is given by $2 \times 2$ Weyl Hamiltonian. The schematic image of Weyl semimetal is shown in Fig. 1.4 [47].

Therefore, we have three different categories of 3D band structures, the trivial insulator (fully gapped), the Dirac semimetal and the Weyl semimetal. The Dirac
semimetal exists on the phase boundary between the trivial insulator and the Weyl semimetal. The Dirac semimetal can generally occur when the system has both the time-reversal (T) symmetry and the spacial-inversion (I) symmetry and the Weyl semimetal can be obtained by breaking either of T or I symmetries \[9\]. In recent experiments these three-dimensional gapless band structures are actually realized in specific compounds. The Dirac semimetal phase was found in $\beta$-cristobalite BiO$_2$, Cd$_3$As$_2$ and Na$_3$Bi $[16, 58, 52]$, and the experimental realization of a Weyl semimetal state have been recently reported in TaAs and NbAs. $[53, 54, 55, 56]$

The existence of Dirac points near the Fermi level is responsible for various unusual physical properties. One of the most spectacular examples is the magnetic susceptibility, which is quite distinct from the conventional Landau diamagnetism. In two-dimensional graphene, the electronic orbital diamagnetism contains a singularity expressed as a delta function in Fermi energy, which diverges at Dirac point where the two bands stick, and vanishes otherwise. $[41, 42, 43]$ The similar calculation of the orbital magnetism was also done for 3D Dirac Hamiltonian, $[50]$ and it was shown that the susceptibility in the gapless case becomes a logarithmic function in the Fermi energy.

The result seems to directly apply to the Dirac and Weyl semimetals, but there is an important difference between the real relativistic Dirac Hamiltonian and the effective Dirac Hamiltonian in the solid state physics. In the Dirac and Weyl semimetals, the external magnetic field $B$ enters the Hamiltonian in two independent manners, one in the orbital part where $p$ is changed to $p + eA$ with the vector potential $A$, and the other in the spin Zeeman term $g\mu_B B$, where $g$ is the $g$-factor and $\mu_B$ is the Bohr magneton. The two different magnetic field terms give rise to the different terms in the magnetic susceptibility, the spin-spin term, the orbital-orbital term, and the spin-orbital cross term, which are not captured in the previous calculation including only the orbital part. In this thesis, we calculate those components and correctly describe the total magnetic response in the three-dimensional gapless semimetals. First we calculate analytically the Landau level spectrum of $4 \times 4$ linear Hamiltonian which covers Dirac and Weyl semimetal phases. Then we take the derivative of the thermodynamic potential to get the magnetic susceptibility.
Chapter 2

2DEG with Rashba/Dresselhaus SOC and 2D Dirac System

In this chapter, we calculate the magnetic susceptibility of Rashba/Dresselhaus systems and also 2D Dirac mode for the surface states of the 2D topological insulator. We show that the spin-momentum relationship governs the sign the spin-orbit cross term, and that significantly affects the amplitude and sign of the total susceptibility.

2.1 Hamiltonian and Landau Levels

2.1.1 2DEG with Rashba and Dresselhaus Spin-Orbit Coupling

We start from the Hamiltonian of 2DEG with mass $m$ without magnetic field written as

$$\mathcal{H}_0 = \frac{\mathbf{p}^2}{2m},$$

(2.1)

From the equation we know the energy band is a parabolic curve in momentum (Fig. 2.1 (a)). Next, we consider the Hamiltonian of 2DEG with Rashba SOC in presence of magnetic field $B$ parallel to $z$ axis,\[2\]

$$\mathcal{H}_R = \frac{\pi^2}{2m} - \frac{\lambda_R}{\hbar} (\pi_x\sigma_y - \pi_y\sigma_x) + b\sigma_z,$$

(2.2)

The Zeeman term is added as the consequence of the magnetic field presence in the system. In the Dresselhaus SOC case, we only consider the linear Dresselhaus SO
The Hamiltonian is written as

\[ H_D = \frac{\pi^2}{2m} + \frac{\lambda_D}{\hbar}(\pi_x \sigma_x - \pi_y \sigma_y) + b \sigma_z. \]  (2.3)

Here \( \sigma_x, \sigma_y, \sigma_z \) is Pauli matrices, \( \lambda_R(\lambda_D) \) is Rashba (Dresselhaus) coefficient, and

\[ \pi = \mathbf{p} + e\mathbf{A}, \]  (2.4)

where \( \mathbf{A} \) is vector potential giving in the magnetic field by \( \mathbf{B} = \nabla \times \mathbf{A} \). Here note that \( b \) is also dependent on the external magnetic field \( B \) as

\[ b = \frac{1}{2} g \mu_B B, \]  (2.5)

where and \( g \) is \( g \)-factor and \( \mu_B = \frac{e \hbar}{2m_0} \) is the Bohr magneton, and \( m_0 \) is the bare electron mass.

When we add Rashba (Dresselhaus) term into the Hamiltonian, the energy band splits into two bands crossing at zero point forming a single Dirac point like state as in graphene and other Dirac materials (see Fig. 2.1 (b)). Where \( \varepsilon_{SO} \) here is spin-orbit energy proportional to Rashba(Dresselhaus) coefficient \( \lambda_R(\lambda_D) \).

Figure 2.1: Energy band of 2DEG (a) without Rashba (Dresselhaus) SOC, and (b) with Rashba(Dresselhaus) SOC.

To calculate the Landau level we define a lower and uppering operators as

\[ a^\dagger = \frac{1}{\sqrt{2e\hbar B}}(\pi_x + i\pi_y) \]  (2.6)

\[ a = \frac{1}{\sqrt{2e\hbar B}}(\pi_x - i\pi_y), \]  (2.7)
2.1. HAMILTONIAN AND LANDAU LEVELS

and we rewrite the Hamiltonian as

$$H_R(n \leq 1) = \begin{bmatrix} \hbar \omega_c (a^\dagger a + \frac{1}{2}) + b & \frac{\sqrt{2} \lambda_R}{l_B} ia \\ -\frac{\sqrt{2} \lambda_R}{l_B} i a^\dagger & \hbar \omega_c (a^\dagger a + \frac{1}{2}) - b \end{bmatrix}. \quad (2.8)$$

These operators operate on the Landau-level wave function $\phi_n$ as $a \phi_n = \sqrt{n} \phi_{n-1}$ and $a^\dagger \phi_n = \sqrt{n+1} \phi_{n+1}$. In Rashba system the eigenfunction can be written as $(c_1 \phi_{n-1}, c_2 \phi_n)$ for $n \geq 1$, the Hamiltonian matrix for the vector $(c_1, c_2)$ then becomes

$$H_R(n \leq 1) = \begin{bmatrix} \hbar \omega_c (n - \frac{1}{2}) + b & i \frac{\sqrt{2} \lambda_R}{l_B} \sqrt{n} \\ -i \frac{\sqrt{2} \lambda_R}{l_B} \sqrt{n} & \hbar \omega_c (n + \frac{1}{2}) - b \end{bmatrix}. \quad (2.9)$$

This gives the two energy levels

$$\varepsilon_{R,n} = n\hbar \omega_c + s \sqrt{\left(\frac{1}{2} \hbar \omega_c - b\right)^2 + \left(\frac{\sqrt{2} n \lambda_R}{l_B}\right)^2} \quad (2.10)$$

where $s = \pm$, $\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency and $l_B = \sqrt{\frac{\hbar}{eB}}$ is the magnetic length. For $n = 0$, the wave function is written as $(0, c_2 \phi_0)$ which gives the only one levels

$$\varepsilon_{R,n=0} = \frac{1}{2} \hbar \omega_c - b. \quad (2.11)$$

The level $\varepsilon_s$ can be viewed as the $n = 0$ part of $\varepsilon_{R,n}$ in Eq. (2.10), but $s = -$ part is missing.

In Dresselhauss system the eigenfunction can be written as $(c_3 \phi_n, c_4 \phi_{n-1})$ for $n \geq 1$, the Hamiltonian matrix for the vector $(c_3, c_4)$ then becomes

$$H_D(n \leq 1) = \begin{bmatrix} \hbar \omega_c (n + \frac{1}{2}) + b & \frac{\sqrt{2} \lambda_D}{l_B} \sqrt{n} \\ \frac{\sqrt{2} \lambda_D}{l_B} \sqrt{n} & \hbar \omega_c (n - \frac{1}{2}) - b \end{bmatrix}. \quad (2.12)$$

This gives the two energy levels

$$\varepsilon_{D,n} = n\hbar \omega_c + s \sqrt{\left(\frac{1}{2} \hbar \omega_c + b\right)^2 + \left(\frac{\sqrt{2} n \lambda_D}{l_B}\right)^2} \quad (2.13)$$

where $s = \pm$. For $n = 0$, the wave function is written as $(c_3 \phi_0, 0)$ which gives the only one levels

$$\varepsilon_{D,n=0} = \frac{1}{2} \hbar \omega_c + b. \quad (2.14)$$

The level $\varepsilon_s$ can be viewed as the $n = 0$ part of $\varepsilon_{D,n}$ in Eq. (2.13), but $s = -$ part is missing. Note that Eqs. (2.9) and (2.12) differ only in the sign in front of of $b$. 

\[ \text{end} \]
Figure 2.2: Landau level spectrum of Rashba system (solid lines) and Dresselhaus (dashed lines) system for $\lambda_R = \lambda_D = 2 \sqrt{\frac{\hbar^2 e B_0}{m^*}}$ and $g_m = m_0/m^*$. Where $B_0$ is unit of magnetic field.

Fig. 2.2 is the plot of Landau level for Rashba system (solid lines) and Dresselhaus system (dashed lines) with $\lambda_R = \lambda_D$ and the same $g$-factor. Their energy levels in $B \to 0$ limit are differ only in $n = 0$, while all other levels are almost degenerate.

### 2.1.2 2D Dirac System

Now we consider the 2D Dirac Hamiltonian which describes the surface state of the 3D topological insulator. It is similar to the Rashba /Dresselhaus system, while the $p^2$ term is absent.

The Hamiltonian is,

$$
\mathcal{H}_{\text{Dirac}}^R = \begin{bmatrix}
0 & v i (p_x - i p_y) \\
- v i (p_x + i p_y) & 0 
\end{bmatrix}
$$

and

$$
\mathcal{H}_{\text{Dirac}}^D = \begin{bmatrix}
0 & v (p_x + i p_y) \\
v (p_x - i p_y) & 0 
\end{bmatrix}
$$
which are analogous to the Rashba and Dresselhaus systems, respectively. It looks similar to graphene, but here the vector components correspond to the real spin degree of freedom. The two Hamiltonians have different spin-texture as a function of momentum. The surface band of the typical topological insulators such as Bi$_2$Se$_3$ corresponds to the case Eq.(2.15). The differences between those Hamiltonians are the imaginary parts in the off diagonal parts and the sign in front of $p_y$. Although the Hamiltonians are different, their energy bands are identical, written as

$$\epsilon_{s,R,D} = s v p$$

where $s = \pm$.

We can see the plot for the energy bands in Fig. 2.3. We have Dirac point at (0,0).

Figure 2.3: Energy bands for 2D Dirac systems [Eqs. (2.15) and (2.16)] at zero magnetic field.

The Hamiltonian in presence of external magnetic field $B$ in $z$ axis is

$$\mathcal{H}^{R}_{\text{Dirac}} = \begin{bmatrix} b & vi(\pi_x - i\pi_y) \\ -vi(\pi_x + i\pi_y) & -b \end{bmatrix}$$

and

$$\mathcal{H}^{D}_{\text{Dirac}} = \begin{bmatrix} b & v(\pi_x + i\pi_y) \\ v(\pi_x - i\pi_y) & -b \end{bmatrix}$$
for Rashba dan Dresselhaus case respectively.

Figure 2.4: Landau levels for 2D Dirac systems. Solid and dashed thick lines are the \( n = 0 \) level for the Rashba type [Eq. (2.15)], and Dresselhaus type [Eq. (2.16)], respectively. Thin curves are \( n \neq 0 \) levels which are shared by the two cases.

The Landau levels for both cases are identical for \( n \neq 0 \)

\[ \varepsilon_{s}^{R,D} = s\sqrt{(b)^2 + v^22heBn}. \]  

(2.20)

For \( n = 0 \) the Landau level is,

\[ \varepsilon_{n=0}^{R,D} = \alpha_{R,D}b \]  

(2.21)

where,

\[ \alpha_{R,D} = \begin{cases} 
\alpha_R = -1 & \text{for Rashba type,} \\
\alpha_D = 1 & \text{for Dresselhaus type.} 
\end{cases} \]

\section{2.2 Magnetic susceptibility}

The magnetic susceptibility can be derived from the thermodynamic potential. The thermodynamic potential of the system at temperature \( T \) is written as

\[ \Omega = -\frac{1}{\beta} \sum_{\alpha} \ln[1 + \exp -\beta(\varepsilon_{\alpha} - \zeta)], \]  

(2.22)
2.2. MAGNETIC SUSCEPTIBILITY

where $\alpha$ is the index labeling the all eigenstates of the system, $\beta = 1/k_B T$, and $\zeta$ is the chemical potential. The magnetization is then given by

$$M = -\frac{\partial \Omega}{\partial B} = -\left(\frac{\partial \Omega}{\partial B_{\text{spin}}} + \frac{\partial \Omega}{\partial B_{\text{orb}}}\right).$$  \hfill (2.23)

The magnetic susceptibility is given by three components

$$\chi = -\left.\frac{\partial M}{\partial B}\right|_{B=0} = \left[\frac{\partial^2 \Omega}{\partial B^2_s} - 2\frac{\partial^2 \Omega}{\partial B_s \partial B_{\text{orb}}} - \frac{\partial^2 \Omega}{\partial B^2_{\text{orb}}}\right]_{B=0} \equiv \chi_{\text{spin}} + \chi_{\text{so}} + \chi_{\text{orb}}.$$  \hfill (2.24)

We analytically derived the magnetic susceptibility using the Landau level spectrum Eq. (2.10) and Eq. (2.11). The thermodynamic potential in Eq. (2.22) per unit volume can be written as,

$$\Omega = -\frac{1}{\beta} \frac{1}{2\pi l_B^2} \sum_{s=\pm} \sum_{n=0}^{\infty} \phi[\varepsilon_{\mu sn}] \left(1 - \delta_{n0} \frac{1 - \tau_s}{2}\right),$$  \hfill (2.25)

where

$$\phi(\varepsilon_{\mu sn}) = \ln[1 + \exp -\beta(\varepsilon_{\mu sn} - \zeta)],$$  \hfill (2.26)

$l_B = \sqrt{\hbar/(eB_{\text{orb}})}$ is the magnetic length, $\zeta$ is the chemical potential.

2.2.1 2DEG with Rashba and Dresselhaus Spin-Orbit Coupling

The energy defined as,

$$\varepsilon_{\mu sn} = x_n + s \sqrt{(\Delta x/2 + \mu b)^2 + x_n x_{SO}}$$  \hfill (2.27)

with

$$x_n = n\Delta x, \quad \Delta x = 2\hbar eB_{\text{orb}}, \quad x_{SO} = \frac{2m^* \lambda_{SO}^2}{\hbar}.$$  \hfill (2.28)

Here $\lambda_{SO}$ is Rashba(or Dresselhaus) constant, $\lambda_{R(or D)}$. The variable $\mu = \pm 1$ denotes Rashba and Dresselhaus systems as we already know that the difference of their energy
level is the sign in front of \( b \),

\[
\mu = \begin{cases} 
-1 & \text{for Rashba system,} \\
1 & \text{for Dresselhaus system.}
\end{cases}
\]  

(2.29)

We also introduced the variable \( \tau_s = \pm 1 \) as

\[
\tau_s = \begin{cases} 
-1 & \text{when } \varepsilon_{s0} = -\varepsilon_0, \\
1 & \text{when } \varepsilon_{s0} = \varepsilon_0.
\end{cases}
\]  

(2.30)

Equivalently, we have \( \tau_s = +1 \) when the Landau level sequence of \((s)\) start from \( n = 0 \), while \( \tau_s = -1 \) when it start from \( n = 1 \) (i.e., the \( n = 0 \) level is missing).

In small magnetic field, using the Euler-Maclaurin formula, the thermodynamic potential can be expanded in power of \( B_{\text{orb}} \) as

\[
\Omega = \Omega_0 + \alpha_1(B_{\text{orb}}) + \alpha_2(B_{\text{orb}}^2) + \mathcal{O}(B_{\text{orb}}^3)
\]  

(2.31)

where

\[
\Omega_0 = -\frac{1}{\beta} \frac{1}{2\pi l_B^2} \sum_{s=\pm} \int_0^\infty \varphi(x,0) dx,
\]  

(2.32)

\[
\alpha_1 = -\frac{1}{\beta} \frac{1}{2\pi l_B^2} \sum_{s=\pm} \frac{e\hbar}{m^*} \left( \frac{\tau_s}{2} \varphi(0,0) + \int_0^\infty \frac{\partial \varphi(x,\Delta x)}{\partial \Delta x} \bigg|_{\Delta x=0} dx \right)
\]  

(2.33)

Eq. (2.33) expresses the contribution of spin-orbit part. The first term in the bracket tells us that SO term is solely dependent of \( n=0 \) Landau level.

\[
\alpha_2 = -\frac{1}{\beta} \frac{1}{2\pi l_B^2} \sum_{s=\pm} \frac{1}{2} \left( \frac{e\hbar}{m^*} \right)^2 \left( \int_0^\infty \frac{\partial^2 \varphi(x,\Delta x)}{\partial \Delta x^2} \bigg|_{\Delta x=0} dx + \tau_s \frac{\partial \varphi(0,\Delta x)}{\partial \Delta x} \bigg|_{\Delta x=0} - \frac{1}{12} \frac{\partial \varphi(x,0)}{\partial x} \bigg|_{x=0} \right)
\]  

(2.34)

Then we have,

\[
\chi_{\text{orb}} = -2\alpha_2, \quad \chi_{\text{spin}} = -\frac{\partial^2 \Omega_0}{\partial B_{\text{spin}}} \\
\chi_{\text{SO}} = -2 \frac{\partial \alpha_1}{\partial B_{\text{spin}}} \bigg|_{B_{\text{spin}}=0}
\]  

(2.35)
2.2. MAGNETIC SUSCEPTIBILITY

Here we expect that only $\chi_{SO}$ has opposite signs in Rashba and Dresselhaus systems, because it is the first derivative in $b$. While $\chi_{\text{spin}}$ and $\chi_{\text{orb}}$ is even-number (2 or 0) derivative in $b$, so the sign of $b$ doesn’t change the results.

Finally, we get the magnetic susceptibility as

$$\chi_{\text{orb}}^* = \frac{1}{2} \sqrt{1 + \frac{\varepsilon_F}{\varepsilon_{SO}} \theta(-\varepsilon_F) \theta(\varepsilon_F + \varepsilon_{SO})}$$

$$- \frac{1}{6} \theta(\varepsilon_F) - \frac{2}{3} \varepsilon_{SO} \delta(\varepsilon_F),$$

(2.36)

and

$$\chi_{\text{spin}}^* = \frac{1}{2} g_m^2 \sqrt{1 + \frac{\varepsilon_F}{\varepsilon_{SO}} \theta(-\varepsilon_F) \theta(\varepsilon_F + \varepsilon_{SO})}$$

$$+ \frac{1}{2} \theta(\varepsilon_F) g_m^2,$$

(2.37)

where

$$g_m = \frac{g m^*}{2m_0},$$

(2.38)

$$\chi^* = \chi/\chi_0, \text{ and}$$

$$\chi_0 = \frac{e^2}{2\pi m^*}$$

(2.39)

is unit of susceptibility and

$$\varepsilon_{SO} = \frac{m^* \lambda_R^2}{2\hbar^2},$$

(2.40)

$\chi_{\text{spin}}$ and $\chi_{\text{orb}}$ are completely identical for both systems if if they share the equal $\varepsilon_{SO}$. Our stressing point is that $\chi_{SO}$ comes with opposite signs, written as

$$\chi_{SO}^* = \mu g_m \sqrt{1 + \frac{\varepsilon_F}{\varepsilon_{SO}} \theta(-\varepsilon_F) \theta(\varepsilon_F + \varepsilon_{SO})}. $$

(2.41)

The sign of $\mu$ will change as the system changes.

The difference of $\chi_{SO}$ in both systems results the difference of total magnetic susceptibility, expressed as

$$\chi_{\text{Total}}^* = \frac{1}{2} \sqrt{1 + \frac{\varepsilon_F}{\varepsilon_{SO}} (g_m + \mu)^2 \theta(-\varepsilon_F) \theta(\varepsilon_F + \varepsilon_{SO})}$$

$$+ \frac{1}{2} (g_m^2 - \frac{1}{3})^2 \theta(\varepsilon_F) - \frac{2}{3} \varepsilon_{SO} \delta(\varepsilon_F).$$

(2.42)
Figure 2.5: Magnetic Susceptibility for Rashba system ($\chi_R$): (a) $\chi_{R\text{orb}}$ (b) $\chi_{R\text{spin}}$ (c) $\chi_{R\text{SO}}$ (d) $\chi_{R\text{Total}}$. Dashed lines are analytical results and solid lines are numerical results with $k_B T = 0.01\varepsilon_{\text{SO}}$. 
Figure 2.6: Magnetic Susceptibility for Dresselhaus system ($\chi_D$): (a) $\chi_{D_{\text{orb}}}$ (b) $\chi_{D_{\text{spin}}}$ (c) $\chi_{D_{\text{SO}}}$ (d) $\chi_{D_{\text{Total}}}$. Dashed lines are analytical results and solid lines are numerical results with $k_B T = 0.01 \varepsilon_{\text{SO}}$. 
2.2.2 2D Dirac

Now, we focus on The Dirac cone in Rashba and Dresselhaus case.

\[
\chi_{SO}^{2D}(\chi_0) = -\alpha_{R,D} g\mu_B e \pi\hbar 
\left( -\theta(-|\varepsilon_F|) + 2\theta(\varepsilon_F) \right) 
\]

(2.45)

The energy defined as,

\[
\varepsilon_{sn}^{R,D} = s\sqrt{b^2 + x_n} 
\]

(2.43)

with

\[
x_n = n\Delta x, \quad \Delta x = 2v^2\hbar eB_{orb}. 
\]

(2.44)

Figure 2.7: $\chi_{SO}$ for Rashba(solid black line) and Dresselhaus(dashed red lines) 2D Dirac cone.

2.3 Discussion

In Fig. 2.5 and Fig. 2.6, we show the magnetic susceptibility as a function of the Fermi energy $\varepsilon_F$ in 2D Rashba and Dresselhaus systems, respectively. Here (a) the orbital component, (b) the spin component, (c) the spin-orbit component, and (d)
the total susceptibility are plotted in separate panels. We can see that Rashba and Dresselhaus systems have identical orbital and spin susceptibility for $\lambda_R = \lambda_D$. The orbital susceptibility $X_{orb}$ is positive (paramagnetic) in $\varepsilon_F < 0$, and it diverges to the negative infinity at $\varepsilon_F = 0$, and becomes constant in $\varepsilon_F > 0$. The divergence at zero energy is related to the band crossing point in the energy bands of zero magnetic field. This crossing point resembles Dirac point in graphene case. It has been shown that the orbital magnetic susceptibility of graphene diverges at zero energy $^{38}$. The spin magnetic susceptibility $X_{spin}$ is always paramagnetic due to its dependency of $g^2$. In negative Fermi energy it is an increasing function of Fermi energy, and it becomes constant in positive Fermi energy.

The difference of Rashba case and Dresselhaus case comes from the spin-orbit cross susceptibility, $X_{SO}$. The sign of the spin-orbit magnetic susceptibility is completely opposite in Rashba and Dresselhaus systems, as argued in Eq. (2.41) and also seen in panel (c) of Figs. 2.5 and 2.6. $X_{SO}$ is linear in $g_m$, so it is diamagnetic or paramagnetic depending on $g_m$. The $X_{SO}$ is solely determined by $n = 0$ Landau level, while other susceptibility components depend on the whole Landau level spectrum. Indeed, the sign of the energy of $n = 0$ Landau level is opposite in Rashba and Dresselhaus systems, while all other Landau levels are just identical. This fact agrees with that the difference between Rashba and Dresselhaus systems is only found in $X_{SO}$.

The difference in $X_{SO}$ significantly affects the total magnetic susceptibility. We show the total susceptibilities for the Rashba and Dresselhaus systems in (d) of Figs. 2.5 and 2.6. In $\varepsilon_F < 0$, the total magnetic susceptibility is always paramagnetic as is obvious from the first term of Eq. (2.42). In $\varepsilon_F > 0$, the total susceptibility is purely given by the $X_{orb}$ and $X_{spin}$ just as in the conventional metal without SOC, and it can be paramagnetic or diamagnetic depending on $g$-factor. The central delta-function peak is orbital effect, and it always exists independently of $g_m$.

In 2D Dirac case, the Rashba type and Dresselhaus type spin texture results in the opposite sign in $X_{SO}$ as shown in Eq. (2.45), and also plotted in Fig. 2.7. We see the positive step function for the former and the negative step function in the latter. This is essentially the same behavior as the discrete steps found in 2DEG with Rashba and Dresselhaus SOC in Figs. 2.5 and 2.6.

In the material with large $|g|$ factor, i.e. GaAs, with $m/m0 = 0.067, g = -0.44, g_m =$
\[ -0.015 \text{ we will have large value of } \chi_{\text{spin}} \text{ and } \chi_{\text{SO}}. \]

Refer to the results in Fig. 2.5, the magnetic susceptibility will be paramagnetic for negative Fermi energy and diamagnetic for positive Fermi energy.

From the above results, we conclude that the spin texture in the momentum space is crucial for the sign of \( \chi_{\text{SO}} \), and it deeply influences the observed total susceptibility. In the next section, we calculate the magnetic response in the Dirac / Weyl semimetals and also demonstrate that the spin-momentum relationship is important in those systems.
Chapter 3

3D Dirac/Weyl Semimetal

In this chapter, we calculate magnetic susceptibility in 3D Dirac semimetal and Weyl semimetal. We first introduce $4 \times 4$ Hamiltonian which covers the Dirac semimetal, Weyl semimetal as well as the gapped semiconductor. Then we applied the general formulation in the previous section to the Hamiltonian, and analytically obtain the three susceptibility components: spin-spin term, the orbital-orbital term, and the spin-orbital cross term. We also consider the Hamiltonian with the opposite chirality in the spin texture, and argue about how it affects the magnetic susceptibility.

3.1 Electronic Structures of Dirac and Weyl Semimetals

3.1.1 Band dispersion at Zero Magnetic Field

We will introduce $4 \times 4$ Dirac-Weyl Hamiltonian matrix. In the absence of the magnetic field the Hamiltonian is,

$$H = \begin{pmatrix}
  m + b & 0 & v p_z & v (p_x - i p_y) \\
  0 & m - b & v (p_x + i p_y) & -v p_z \\
  v p_z & v (p_x - i p_y) & -m + b & 0 \\
  v (p_x + i p_y) & -v p_z & 0 & -m - b
\end{pmatrix}, \quad (3.1)$$
Figure 3.1: Energy spectrum for Dirac semimetal case. $m$ and $b$ are equal to zero. Where $v$ is taken as 1.

Figure 3.2: Energy spectrum for semiconducting case ($m = 1, b = 0.5$). Where $v$ is taken as 1. The spectrum is fully gapped.
3.1. ELECTRONIC STRUCTURES OF DIRAC AND WEYL SEMIMETALS

Figure 3.3: Energy spectrum for Weyl semimetal case \((m = 0.5, b = 1)\). The two bands are touching in \(p = (0,0,\pm\sqrt{b^2 - m^2}/v)\). Where \(v\) is taken as 1.

where \(m\) is an effective mass, \(v\) is the velocity parameter, and \(b\) is the intrinsics Zeeman-like term coupled to the electronic spin, which may exist in magnetic materials without the time-reversal symmetry. We assume \(m > 0\) and \(b > 0\) in the following.

By diagonalizing the Hamiltonian matrix, we obtain the energy spectrum as,

\[
\varepsilon(p) = \pm\sqrt{m^2 + b^2 + v^2p^2 \pm 2b\sqrt{v^2p_z^2 + m^2}}. \tag{3.2}
\]

For the case of \(p_x = p_y = 0\), we will have the energy spectrum in \(p_z\) direction which is given by

\[
\varepsilon(0,0,p_z) = \pm|b| \pm \sqrt{v^2p_z^2 + m^2}. \tag{3.3}
\]

The energy spectrum \(\varepsilon(0,0,p_z)\) is plotted in Figs. 3.1, 3.2, and 3.3 for three different cases of \(m = b = 0\), \(m > b\) and \(b > m\), respectively. The case of \(m = b = 0\) is the Dirac semimetal, where we have the four-fold degeneracy at the zero energy and the dispersion is completely linear. The second one \(m > b\) describes the semiconducting case where the spectrum is gapped in the energy range between \(E = m - b\) and \(-m + b\). The last one \(b > m\) is the Weyl semimetal case where the the middle two bands touching at the wave points \(p = (0,0,\pm\sqrt{b^2 - m^2}/v)\).
3.1.2 Landau Level Structures

In the case of the presence of magnetic field $B$ perpendicular to $z$ axis, the Hamiltonian (3.1) becomes,

$$H = \begin{bmatrix}
    m + b & 0 & v\pi_z & v(\pi_x - i\pi_y) \\
    0 & m - b & v(\pi_x + i\pi_y) & -v\pi_z \\
    v\pi_z & v(\pi_x - i\pi_y) & -m + b & 0 \\
    v(\pi_x + i\pi_y) & -v\pi_z & 0 & -m - b \\
\end{bmatrix}, \quad (3.4)$$

where

$$\pi = p + eA, \quad (3.5)$$

and $A$ is vector potential giving in the magnetic field by $B = \nabla \times A$. Here note that $b$ is also dependent on the external magnetic field $B$ as

$$b = b_0 + g\mu_B B, \quad (3.6)$$

where $b_0$ is the intrinsic Zeeman term in the absence of $B$, and $g$ is $g$-factor and $\mu_B = e\hbar/(2m_0)$ is the Bohr magneton, and $m_0$ is the bare electron mass. We define a lower and uppering operators,

$$a^\dagger = \frac{1}{\sqrt{2e\hbar B}}(\pi_x + i\pi_y) \quad (3.7)$$

$$a = \frac{1}{\sqrt{2e\hbar B}}(\pi_x - i\pi_y), \quad (3.8)$$

which operate on the Landau-level wave function $\phi_n$ as $a\phi_n = \sqrt{n}\phi_{n-1}$ and $a^\dagger\phi_n = \sqrt{n+1}\phi_{n+1}$. The eigenfunction can be written as $(c_1\phi_{n-1}, c_2\phi_n, c_3\phi_{n-1}, c_4\phi_n)$ for $n \geq 1$, the Hamiltonian matrix for the vector $(c_1, c_2, c_3, c_4)$ then becomes

$$H_{n \leq 1} = \begin{bmatrix}
    m + b & 0 & vp_z & \Delta_B\sqrt{n} \\
    0 & m - b & \Delta_B\sqrt{n} & -vp_z \\
    vp_z & \Delta_B\sqrt{n} & -m + b & 0 \\
    \Delta_B\sqrt{n} & -vp_z & 0 & -m - b \\
\end{bmatrix}, \quad (3.9)$$

where

$$\Delta_B = \sqrt{2\hbar^2eB}. \quad (3.10)$$
This gives the four energy levels

$$\varepsilon_{s\mu p,z n} = s\sqrt{m^2 + b^2 + v^2 p_z^2 + \Delta_B^2 n} + \mu 2b\sqrt{v^2 p_z^2 + m^2}$$

(3.11)

where \(s, \mu = \pm\). For \(n = 0\), the wave function is written as \((0, c_2\phi_0, 0, c_4\phi_0)\) and the Hamiltonian matrix for \((c_2, c_4)\) becomes

$$H_{n=0} = \begin{bmatrix} m + b & vp_z \\ vp_z & -m + b \end{bmatrix},$$

(3.12)

which gives the only two levels

$$\varepsilon_{\mu p,z 0} = b + \mu \sqrt{v^2 p_z^2 + m^2},$$

(3.13)

with \(\mu = \pm\). The level \(\varepsilon_{\mu p,z 0}\) can be viewed as the \(n = 0\) part of \(\varepsilon_{s\mu p,z n}\) in Eq. (3.11), but either of \(s = \pm\) branches is missing.

The Landau level spectrum is plotted against \(p_z\) in Figs. 3.4, 3.5 and 3.6 for \(m = b = 0\), \(m > b\) and \(b > m\), respectively. We note that the Landau levels of \(n \leq 1\) [Eq. (3.11)] is completely electron-hole symmetric with respect to the zero energy because the existence of \(s = \pm\) branches, while that of \(n = 0\) [Eq. (3.13)] is not symmetric except for \(b = 0\). The dashed curves in the figures indicate the energy level \(-\varepsilon_{\mu 0}\) which actually does not exist. As we will see in the following sections, the symmetry breaking of \(n = 0\) level is actually responsible for the electron-hole asymmetric term in the magnetic susceptibility.

### 3.2 Formula to Calculate Magnetic Susceptibility

#### 3.2.1 Decomposition of susceptibility

In the following we will calculate analytically the magnetic susceptibility of the Dirac-Weyl Hamiltonian.

The thermodynamic potential is written as

$$\Omega = -\frac{1}{\beta} \frac{1}{2\pi l_B^2} \int_{-\infty}^{\infty} \frac{dp_z}{2\pi \hbar} \sum_{s=\pm} \sum_{\mu=\pm} \sum_{n=0}^{\infty} \varphi[\varepsilon_{s\mu p,z}(x_n)] \left(1 - \delta_{n0} \frac{1 - \tau_{s\mu p,z}}{2}\right),$$

(3.14)

where

$$\varphi(\varepsilon) = \ln[1 + \exp -\beta(\varepsilon - \zeta)],$$

(3.15)
CHAPTER 3. 3D DIRAC/WEYL SEMIMETAL

Figure 3.4: Landau level energy spectrum for $m = b = 0$.

Figure 3.5: Landau level energy spectrum for $m = 1, b = 0.5$. The dashed line is non exist energy level.
Figure 3.6: Landau level energy spectrum for $m = 0.5, b = 1$. The dashed line is non exist energy level.

$l_B = \sqrt{\hbar/(eB_{\text{orb}})}$ is the magnetic length, $\zeta$ is the chemical potential, and we defined

$$
\varepsilon_{s\mu p_z}(x_n) = \varepsilon_{s\mu p_z,n} = s\sqrt{m^2 + b^2 + v^2p_z^2 + x_n + \mu 2b\sqrt{v^2p_x^2 + m^2}}
$$

(3.16)

with

$$
x_n = n\Delta x, \quad \Delta x \equiv \Delta_B^2 = 2hv^2eB_{\text{orb}}.
$$

(3.17)

We also introduced the variable $\tau_{s\mu p_z} = \pm 1$ as

$$
\tau_{s\mu p_z} = \begin{cases} 
1 & \text{when } \varepsilon_{s\mu p_z,0} = \varepsilon_{\mu p_z,0}, \\
-1 & \text{when } \varepsilon_{s\mu p_z,0} = -\varepsilon_{\mu p_z,0}.
\end{cases}
$$

(3.18)

Equivalently, we have $\tau_{s\mu p_z} = +1$ when the Landau level sequence of $(s, \mu, p_z)$ start from $n = 0$, while $\tau_{s\mu p_z} = -1$ when it start from $n = 1$ (i.e., the $n = 0$ level is missing).

In weak magnetic field, the summation over $n$ in Eq. [3.14] can be written as a continuous integral over variable $x$, and additional terms can be Taylor-expanded in $B_{\text{orb}}$. For convenience, we introduce the notation,

$$
F(x) = \varphi[\varepsilon_{s\mu p_z}(x)].
$$

(3.19)
By using the Euler-Maclaurin formula, we can rewrite the summation over \( n \) in the case of \( \tau_{s\mu p_z} = 1 \) (i.e., \( n \) starts from 0) as,

\[
\sum_{n=0}^{\infty} F(x_n) = \frac{1}{\Delta x} \left[ \int_{0}^{\infty} F(x)dx + F(0) \frac{\Delta x}{2} - F'(0) \frac{\Delta x^2}{12} + \mathcal{O}(\Delta x^3) \right] \quad (3.20)
\]

and in the case of \( \tau_{s\mu p_z} = -1 \) (i.e., \( n \) starts from 1) as,

\[
\sum_{n=1}^{\infty} F(x_n) = \frac{1}{\Delta x} \left[ \int_{0}^{\infty} F(x)dx - F(0) \frac{\Delta x}{2} - F'(0) \frac{\Delta x^2}{12} + \mathcal{O}(\Delta x^3) \right] \quad (3.21)
\]

The two expressions are united into a single equation as

\[
\sum_{n=0}^{\infty} F(x_n) \left( 1 - \delta_{n0} - \frac{\tau_{s\mu p_z}}{2} \right) = \frac{1}{\Delta x} \left[ \int_{0}^{\infty} F(x)dx + \tau_{s\mu p_z} F(0) \frac{\Delta x}{2} - F'(0) \frac{\Delta x^2}{12} + \mathcal{O}(\Delta x^3) \right] \quad (3.22)
\]

Noting that \( \Delta x \propto B_{\text{orb}} \), the thermodynamic potential can be expanded within the second order of \( B_{\text{orb}} \) as

\[
\Omega = \Omega_0 + \lambda_1 B_{\text{orb}} + \lambda_2 B_{\text{orb}}^2 + \mathcal{O}(B_{\text{orb}}^3), \quad (3.23)
\]

where

\[
\Omega_0 = -\frac{1}{\beta} \frac{1}{2\pi l_B^2} \frac{1}{\Delta x} \int_{-\infty}^{\infty} \frac{dp_z}{2\pi \hbar} \sum_{s=\pm} \sum_{\mu=\pm} \int_{0}^{\infty} \varphi[\varepsilon_{s\mu p_z}(x)]dx + \tau_{s\mu p_z} \varphi[\varepsilon_{s\mu p_z}(0)] \frac{\Delta x}{2} - \frac{\partial}{\partial x} \varphi[\varepsilon_{s\mu p_z}(x)] \big|_{x=0} \frac{\Delta x^2}{12} + \mathcal{O}(\Delta x^3), \quad (3.24)
\]

\[
\lambda_1 = \frac{1}{\beta} \frac{1}{4\pi l^2 v^2} \int_{-\infty}^{\infty} \frac{dp_z}{2\pi \hbar} \sum_{s=\pm} \sum_{\mu=\pm} \tau_{s\mu p_z} \varphi[\varepsilon_{s\mu p_z}(0)] \frac{2\hbar ev^2}{2}, \quad (3.25)
\]

\[
\lambda_2 = \frac{1}{\beta} \frac{1}{4\pi l^2 v^2} \int_{-\infty}^{\infty} \frac{dp_z}{2\pi \hbar} \sum_{s=\pm} \sum_{\mu=\pm} (-1) \frac{\partial}{\partial x} \varphi[\varepsilon_{s\mu p_z}(x)] \big|_{x=0} \frac{4\hbar^2 e^2 v^4}{12}. \quad (3.26)
\]

Finally, the three susceptibility components are written in terms of \( \Omega_0, \lambda_1, \lambda_2 \) as

\[
\chi_{\text{spin}} = -\frac{\partial^2 \Omega_0}{\partial B_{\text{spin}}^2} \bigg|_{B_{\text{spin}}=0}, \quad \chi_{\text{SO}} = -\frac{\partial \lambda_1}{\partial B_{\text{spin}}} \bigg|_{B_{\text{spin}}=0}, \quad \chi_{\text{orb}} = -2\lambda_2. \quad (3.27)
\]
3.2. FORMULA TO CALCULATE MAGNETIC SUSCEPTIBILITY

3.2.2 Calculation of $\chi_{\text{spin}}$, $\chi_{\text{SO}}$, and $\chi_{\text{orb}}$

3.2.3 $\chi_{\text{spin}}$ term

For zero magnetic field $B_{\text{orb}} = 0$, we have

$$\Omega(B_{\text{orb}} = 0) = -\frac{1}{\beta} \int_{-\infty}^{\infty} \frac{dp_z}{2\pi\hbar} \sum_{s = \pm} \sum_{\mu = \pm} \int_{0}^{\infty} \frac{dp_x dp_y}{4\pi^2\hbar^2} \varphi[\varepsilon_{s\mu p_z}(v^2(p_x^2 + p_y^2))],$$

(3.28)

where

$$\varepsilon_{s\mu p_z}(v^2(p_x^2 + p_y^2)) = s \sqrt{v^2(p_x^2 + p_y^2) + \Delta_B^2},$$

and,

$$\Delta = b + \mu \sqrt{v^2 p_z^2 + m^2};$$

(3.29)

$s = \mu$ is $\pm$.

Denote more simply expression for $p_x$ and $p_y$, we have

$$v^2(p_x^2 + p_y^2) \equiv v^2 p_\perp \equiv x$$

$$\int \int \frac{dp_x dp_y}{(2\pi\hbar)^2} = \int_{0}^{\infty} \frac{2\pi p_\perp dp_\perp}{(2\pi\hbar)^2} = \int_{0}^{\infty} \frac{2\pi dx}{2v^2(2\pi\hbar)^2} = \frac{1}{4\pi\hbar^2 v^2} \int_{0}^{\infty} dx.$$

Then we rewrite $\Omega_0$ as,

$$\Omega(B_{\text{orb}} = 0) = -\frac{1}{\beta} \int_{-\infty}^{\infty} \frac{dp_z}{2\pi\hbar} \sum_{s = \pm} \sum_{\mu = \pm} \int_{0}^{\infty} \frac{dx}{4\pi\hbar^2 v^2} \varphi[\varepsilon_{s\mu p_z}(x))],$$

(3.30)

To calculate $\chi_{\text{spin}}$, we need to take the second derivative of $\Omega_0$. Replace $vp_z$ with $\Pi_z$, $\chi_{\text{spin}}$ can be written as

$$\chi_{\text{spin}} = -\frac{\partial^2 \Omega_0}{\partial B_{\text{spin}}^2};$$

$$= -(g\mu_B)^2 \frac{\partial^2 \Omega_0}{\partial b^2};$$

$$= -\frac{(g\mu_B)^2}{4\pi\hbar^2 v^2} (\frac{1}{\beta} \int_{-\infty}^{\infty} \frac{d\Pi_z}{2\pi\hbar v} \sum_{s = \pm} \sum_{\mu = \pm} \int_{0}^{\infty} dx \frac{\partial^2}{\partial b^2} \varphi[\varepsilon_{s\mu p_z}(x))]);$$

(3.31)
The first derivative is given by,

\[
\frac{\partial}{\partial b} \varphi(\varepsilon) = \frac{e^{-\beta(\varepsilon-\zeta)}}{1 + e^{-\beta(\varepsilon-\zeta)}} (-\beta) \frac{\partial \varepsilon}{\partial b} = (-\beta) f(\varepsilon) \frac{\partial \varepsilon}{\partial b} \tag{3.32}
\]

where

\[
f(\varepsilon) = \frac{1}{1 + e^{\beta(\varepsilon-\zeta)}} \tag{3.33}
\]

and \(\varepsilon = \varepsilon_{sp\mu_s}(x)\)

The second derivative is given by,

\[
\frac{\partial^2}{\partial b^2} \varphi(\varepsilon) = (-\beta) \left(f'(\varepsilon) \left(\frac{\partial \varepsilon}{\partial b}\right)^2 + f(\varepsilon) \frac{\partial^2 \varepsilon}{\partial b^2}\right) \tag{3.34}
\]

Taking the limit of \(T \to 0\) of Eq.(3.34), Eq.(3.31) becomes

\[
\chi_{\text{spin}} = \chi_{\text{spin}}^P + \chi_{\text{spin}}^V, \tag{3.36}
\]

where \(\chi_{\text{spin}}^P\) is a Pauli paramagnetism term, which given by

\[
\chi_{\text{spin}}^P = \frac{(g\mu_B)^2}{4\pi \hbar^2 v^2} \int_{-\infty}^{\infty} \frac{d\Pi_z}{2\pi \hbar v} \sum_{s=\pm} \sum_{\mu=\pm} \int_0^\infty dx \left(-\delta(\varepsilon - \varepsilon_F) \left(\frac{\partial \varepsilon}{\partial b}\right)^2\right) \tag{3.37}
\]

and \(\chi_{\text{spin}}^V\) is a Van-Vleck paramagnetism term given by

\[
\chi_{\text{spin}}^V = \frac{(g\mu_B)^2}{4\pi \hbar^2 v^2} \int_{-\infty}^{\infty} \frac{d\Pi_z}{2\pi \hbar v} \sum_{s=\pm} \sum_{\mu=\pm} \int_0^\infty dx \left(\theta(\varepsilon_F - \varepsilon) \frac{\partial^2 \varepsilon}{\partial b^2}\right) \tag{3.38}
\]
For Dirac semimetal \((b = m = 0)\) case, \(\mu = \pm\) energy levels are degenerated. If we have the Fermi energy less than zero, we will have only \(s = 1\) contribution for our calculation. Therefore, the Eq. (3.37) now is given by

\[
\chi_P^{\text{spin}} = -\frac{(g \mu_B)^2}{4 \pi \hbar^2 v^2} \int_{-\infty}^{\infty} \frac{d\Pi_z}{2 \pi \hbar v} \sum_{\mu=\pm} \int_0^\infty dx \left( -\delta(\varepsilon - \varepsilon_F) \left( \frac{\Pi_z}{\varepsilon} \right)^2 \right)
\]

\[
= \frac{(g \mu_B)^2}{4 \pi \hbar^2 v^2} \int_{-|\varepsilon_F|}^{\varepsilon_F} \frac{d\Pi_z}{2 \pi \hbar v} \sum_{\mu=\pm} \int_0^\infty d\varepsilon 2\varepsilon \left( \delta(\varepsilon - \varepsilon_F) \left( \frac{\Pi_z}{\varepsilon} \right)^2 \right)
\]

\[
= \frac{(g \mu_B)^2}{8 \pi^2 \hbar^3 v^3} \frac{8|\varepsilon_F|^2}{3}
\]

(3.39)

and the Eq. (3.38) now is given by,

\[
\chi_V^{\text{spin}} = \frac{(g \mu_B)^2}{4 \pi \hbar^2 v^2} \int_{-\varepsilon_c}^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \sum_{\mu=\pm} \int_0^{\varepsilon_c} dx \left( \theta(\varepsilon_F - \varepsilon) \frac{x}{\varepsilon^3} \right)
\]

\[
= \frac{4(g \mu_B)^2}{4 \pi \hbar^2 v^2} \int_0^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \int_0^{\varepsilon_c} dx \left( \theta(\varepsilon_F - \varepsilon) \frac{x}{\varepsilon^3} \right)
\]

\[
= \frac{4(g \mu_B)^2}{4 \pi \hbar^2 v^2} \int_0^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \int_0^{\varepsilon_c} d\varepsilon \left( \frac{\varepsilon^2 - \Pi_z^2}{\varepsilon^3} \right)
\]

\[
= \frac{8(g \mu_B)^2}{4 \pi \hbar^2 v^2} \left( \int_0^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \int_{|\varepsilon_F|}^{\varepsilon_c} d\varepsilon \left( 1 - \frac{\Pi_z^2}{\varepsilon^2} \right) + \int_{|\varepsilon_F|}^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \int_{\varepsilon_F}^{\varepsilon_c} d\varepsilon \left( 1 - \frac{\Pi_z^2}{\varepsilon^2} \right) \right)
\]

\[
= \frac{(g \mu_B)^2}{8 \pi^2 \hbar^3 v^3} \left( \frac{8|\varepsilon_c|^2}{3} - \frac{8|\varepsilon_F|^2}{3} \right)
\]

(3.40)

where \(\varepsilon_c = v p_c\). From the above results we know that the one of the term of \(\chi_V^0\) cancels the term of \(\chi_P^0\). The remaining term is only dependent of \(\varepsilon_c\).

For the next case, we put \(m \neq 0\) where \(b\) is still equal to zero. The Dirac point in the previous case is not exist because of the appearance of the effective mass here. If we assume the Fermi energy negative and lies inside the gap, the susceptibility will be a constant. Now, if the Fermi energy lies below the gap \((\varepsilon_F < -|m|)\) the Eq. (3.37) is given by

\[
\chi_P^{\text{spin}} = 8 \frac{(g \mu_B)^2}{4 \pi \hbar^2 v^2} \int_0^{\sqrt{\varepsilon_F^2 - m^2}} \frac{d\Pi_z}{2 \pi \hbar v} \sqrt{\Pi_z^2 + m^2} \frac{1}{|\varepsilon_F|}
\]

(3.41)
and the Van Vleck term now is given by

\[ \chi_{\text{spin}}^V = 8 \left( \frac{g \mu_B}{2 \pi \hbar v} \right)^2 \left( \int_{0}^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \int_{|\varepsilon_F|}^{\varepsilon_c} d\varepsilon \left( 1 - \frac{(\Pi_z^2 + m^2)}{\varepsilon^2} \right) \right) \]

\[ = 8 \left( \frac{g \mu_B}{2 \pi \hbar^2 v^2} \right)^2 \left( \int_{0}^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \int_{(\Pi_z^2 + m^2)}^{\varepsilon_c} d\varepsilon \left( 1 - \frac{(\Pi_z^2 + m^2)}{\varepsilon^2} \right) \right) \]

\[ + \int_{0}^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \left( \left( \varepsilon_c + \frac{(\Pi_z^2 + m^2)}{\varepsilon_c} \right) - \left( \frac{2 \sqrt{\Pi_z^2 + m^2}}{\varepsilon_c} \right) \right) \]  \hspace{1cm} (3.42)

As well as \( b = m = 0 \) case, Pauli term is canceled by one of Van Vleck terms, and the remaining terms are

\[ \chi_{\text{spin}} = 8 \left( \frac{g \mu_B}{8 \pi^2 \hbar^2 v^3} \right)^2 m^2 \ln \frac{\varepsilon_F^2 - m^2 + |\varepsilon_F|}{m} + \chi_{\text{spin}}(0) \]  \hspace{1cm} (3.43)

where \( \chi_{\text{spin}}(0) \) is the constant corresponds to the susceptibility for zero Fermi energy. Here is given by

\[ \chi_{\text{spin}}(0) = 8 \left( \frac{g \mu_B}{8 \pi^2 \hbar^2 v^3} \right)^2 \int_{0}^{\varepsilon_c} \frac{d\Pi_z}{2 \pi \hbar v} \left( \frac{\varepsilon_c + \Pi_z^2 + m^2}{\varepsilon_c} - 2 \sqrt{\Pi_z^2 + m^2} \right). \]  \hspace{1cm} (3.44)

### 3.2.4 \( \chi_{\text{SO}} \) term

To obtain \( \chi_{\text{SO}} \), we have to take the first derivative of \( \lambda_1 \) on \( B_{\text{spin}} \). We will start from the energy spectrum for \( x = 0 \), which is given by

\[ \varepsilon_{s\mu p_z}(0) = s \left| b + \mu \sqrt{v^2 p_z^2 + m^2} \right|. \]  \hspace{1cm} (3.45)

For more simply calculation, we can convert the above equation to

\[ \varepsilon_{s\mu p_z}'(0) = \mu' b + s' \sqrt{v^2 p_z^2 + m^2} \]  \hspace{1cm} (3.46)

where,

\[ \chi_{\text{SO}} = - \left. \frac{\partial \lambda_1}{\partial B_{\text{spin}}} \right|_{B_{\text{spin}}=0} \]  \hspace{1cm} (3.47)

For \( T \to 0 (B \to \infty) \), we have

\[ \varphi(\varepsilon) = \ln(1 + \exp \beta(\varepsilon - \varepsilon_F)) \]

\[ \approx - \beta(\varepsilon - \varepsilon_F) \theta(\varepsilon_F - \varepsilon) \]  \hspace{1cm} (3.48)
3.2. FORMULA TO CALCULATE MAGNETIC SUSCEPTIBILITY

or,

\[-\frac{1}{\beta} \varphi(\varepsilon) = (\varepsilon - \varepsilon_F)\theta(\varepsilon_F - \varepsilon)\]  

(3.49)

For \(\varepsilon_F = 0\),

\[\lambda_1 = \frac{1}{4\pi\hbar^2v^2} \int_{-\infty}^{\infty} \frac{dp_z}{2\pi\hbar} \sum_{s',\mu'} (\varepsilon_{s'\mu'p_z} - \varepsilon_F)\theta(\varepsilon_F - \varepsilon_{s'\mu'p_z}) \frac{2\hbar ev^2}{2}\]

(3.50)

For \(0 < \varepsilon_F < (b - m)\)

Define,

\[|p_+| = \sqrt{(\varepsilon + b)^2 - m^2/v}\]

\[|p_-| = \sqrt{(\varepsilon - b)^2 - m^2/v}\]  

(3.51)

Then,

\[\lambda_1 = \frac{1}{4\pi\hbar^2v^2} \int_{-p_c}^{p_c} \frac{dp_z}{2\pi\hbar} \Lambda(p_z) \frac{2\hbar ev^2}{2}\]  

(3.52)

For \(p_+ < |p_z|\),

\[\Lambda(p_z) = \sum_{s',\mu'} \mu' (\mu'b + s'\sqrt{v^2p_z^2 + m^2 - \varepsilon_F})\]

\[= (b - \sqrt{v^2p_z^2 + m^2 - \varepsilon_F}) - (-b - \sqrt{v^2p_z^2 + m^2 - \varepsilon_F})\]

\[= 2b\]  

(3.53)

For \(p_- < |p_z| < p_+\)

\[\Lambda(p_z) = (b - \sqrt{v^2p_z^2 + m^2 - \varepsilon_F}) - (-b + \sqrt{v^2p_z^2 + m^2 - \varepsilon_F})\]

\[= 3b - \sqrt{v^2p_z^2 + m^2 + \varepsilon_F}\]  

(3.54)

For \(|p_z| < p_-\)

\[\Lambda(p_z) = -(b + \sqrt{v^2p_z^2 + m^2 - \varepsilon_F}) - (-b - \sqrt{v^2p_z^2 + m^2 - \varepsilon_F})\]

\[= 2b + 2\varepsilon_F\]  

(3.55)
Then we have,

\[
\lambda_1 = \frac{1}{4\pi\hbar^2v^2} \int_{-p_c}^{p_c} \frac{dp_z}{2\pi \hbar} \Lambda(p_z) \frac{2\hbar ev^2}{2}
\]

\[
= \frac{1}{4\pi\hbar^2v^2} \int_{0}^{p_c} \frac{dp_z}{2\pi \hbar} \Lambda(p_z) \frac{2\hbar ev^2}{2}
\]

\[
= \frac{1}{4\pi\hbar^2v^2} \int_{0}^{p_c} \frac{1}{2\pi \hbar} (2) \left[ \int_{0}^{p_-} dp_z (2b + 2\varepsilon_F) + \int_{p_-}^{p_+} dp_z (3b - \sqrt{v^2p_z^2 + m^2} + \varepsilon_F)\right]
\]

\[
+ \int_{p_+}^{p_-} dp_z 2b \right] \frac{2\hbar ev^2}{2}
\]

\[
= \frac{1}{4\pi\hbar^2v^2} \int_{0}^{p_c} \frac{1}{2\pi \hbar} (2) \left[ (2b + 2\varepsilon_F)p_- + (3b + \varepsilon_F)(p_+ - p_-) + 2b(p_c - p_+)ight]
\]

\[
- \left[ \int_{p_-}^{p_+} dp_z \sqrt{v^2p_z^2 + m^2} \right] \frac{2\hbar ev^2}{2}
\]

(3.56)

For \((b - m) < \varepsilon_F < (b + m)\)

Define,

\[|p_+| = \sqrt{(\varepsilon + b)^2 - m^2/v}\]

For \(p_+ < |p_z|\),

\[\Lambda(p_z) = (b - \sqrt{v^2p_z^2 + m^2} - \varepsilon_F) - (b - \sqrt{v^2p_z^2 + m^2} - \varepsilon_F)\]

\[= 2b\] (3.57)

For \(|p_z| < p_+\)

\[\Lambda(p_z) = (b - \sqrt{v^2p_z^2 + m^2} - \varepsilon_F) - (b + \sqrt{v^2p_z^2 + m^2} - \varepsilon_F)\]

\[-(b - \sqrt{v^2p_z^2 + m^2} - \varepsilon_F)\]

\[= 3b - \sqrt{v^2p_z^2 + m^2} + \varepsilon_F\] (3.58)

Then we have,

\[
\lambda_1 = \frac{1}{4\pi\hbar^2v^2} \int_{0}^{p_c} \frac{1}{2\pi \hbar} (2) \left[ \int_{0}^{p_+} dp_z (3b - \sqrt{v^2p_z^2 + m^2} + \varepsilon_F) + \int_{p_+}^{p_-} dp_z 2b \right] \frac{2\hbar ev^2}{2}
\]

\[
= \frac{1}{4\pi\hbar^2v^2} \int_{0}^{p_c} \frac{1}{2\pi \hbar} (2) \left[ (3b + \varepsilon_F)p_+ + 2b(p_c - p_+) - \int_{0}^{p_+} dp_z \sqrt{v^2p_z^2 + m^2} \right] \frac{2\hbar ev^2}{2}
\]

(3.59)

For \(\varepsilon_F > (b + m)\)
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Define,

\[
\begin{align*}
|p_+| &= \sqrt{(\varepsilon + b)^2 - m^2}/v \\
|p_-| &= \sqrt{(\varepsilon - b)^2 - m^2}/v
\end{align*}
\]  

(3.60)

For \(p_+ < |p_z|\),

\[
\Lambda(p_z) = (b - \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F) - (-b - \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F)
\]

\[= 2b
\]

(3.61)

For \(p_- < |p_z| < p_+\),

\[
\Lambda(p_z) = (b - \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F) - (-b + \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F) \\
-(-b - \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F)
\]

\[= 3b - \sqrt{v^2 p_z^2 + m^2} + \varepsilon_F
\]

(3.62)

For \(|p_z| < p_-\),

\[
\Lambda(p_z) = (b + \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F) - (-b + \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F) \\
+(b - \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F) - (-b - \sqrt{v^2 p_z^2 + m^2} - \varepsilon_F)
\]

\[= 4b
\]

(3.63)

Then we have,

\[
\lambda_1 = \frac{1}{4\pi\hbar^2v^2} \frac{1}{2\pi\hbar}(2)[(4b)p_+ + (3b + \varepsilon_F)(p_+ - p_-) + 2b(p_c - p_+)] \\
- \int_{p_+}^{p_-} dp_z \sqrt{v^2 p_z^2 + m^2} \left[ \frac{2\hbar v^2}{2} \right]
\]

(3.64)

For semiconducting case \(\chi_{SO}\) is given by,

\[
\chi_{SO} = -\frac{eg\mu_B}{2\pi^2\hbar^2v} \left( \sqrt{(\varepsilon_F + b)^2 - m^2} + 2\varepsilon_c \right)
\]

(3.65)

for \(|b - m| < \varepsilon_F < |b + m|\) and,

\[
\chi_{SO} = -\frac{eg\mu_B}{2\pi^2\hbar^2v} \left( \sqrt{(\varepsilon_F + b)^2 - m^2} + \sqrt{(\varepsilon_F - b)^2 - m^2} + 2\varepsilon_c \right)
\]

(3.66)

for \((b + m) < \varepsilon_F\).

For Weyl semimetal case \(\chi_{SO}\) is given by,

\[
\chi_{SO} = -\frac{eg\mu_B}{2\pi^2\hbar^2v} \left( \sqrt{(\varepsilon_F + b)^2 - m^2} + \sqrt{(\varepsilon_F - b)^2 - m^2} + 2vp_c \right)
\]

(3.67)
for \((b + m) < \varepsilon_F\).

\[
\chi_{SO} = -\frac{eg\mu_B}{2\pi^2\hbar^2v} \left( \sqrt{(\varepsilon_F + b)^2 - m^2} + 2vp_c \right)
\] (3.68)

for \((b - m) < \varepsilon_F < (b + m)\).

\[
\chi_{SO} = -\frac{eg\mu_B}{2\pi^2\hbar^2v} \left( \sqrt{(\varepsilon_F + b)^2 - m^2} - \sqrt{(\varepsilon_F - b)^2 - m^2} + 2vp_c \right)
\] (3.69)

for \(0 < \varepsilon_F < (b - m)\)

### 3.2.5 \(\chi_{orb}\) term

\[
\lambda_2 = -\frac{1}{\beta} \frac{1}{4\pi^2\hbar^2v^2} \int_{-\infty}^{\infty} dp_z \sum_{s'\mu'} \frac{\partial}{\partial x} \varphi[\varepsilon_{s'\mu'p_z}(x)] \left[ \frac{\theta(\varepsilon_F - \varepsilon_{s'\mu'p_z}(0))}{2\varepsilon_{s'\mu'p_z}(0)} \right]
\] (3.70)

For \(T \rightarrow 0(B \rightarrow \infty)\), we have

\[
-\frac{1}{\beta} \frac{\partial}{\partial x} \varphi[\varepsilon_{s'\mu'p_z}(x)] \bigg|_{x=0} = \frac{\theta(\varepsilon_F - \varepsilon_{s'\mu'p_z}(0))}{2\varepsilon_{s'\mu'p_z}(0)}
\] (3.71)

where,

\[
\varepsilon_{s'\mu'p_z}(0) = s'b + \mu'\sqrt{v^2p_z^2 + m^2}
\]

or,

\[
\varepsilon'_{s'\mu'p_z}(0) = \mu'b + s'\sqrt{v^2p_z^2 + m^2}
\]

and we have,

\[
\lambda_2 = -\frac{1}{\beta} \frac{1}{4\pi^2\hbar^2v^2} \int_{-\infty}^{\infty} dp_z \sum_{s'\mu'} \frac{\theta(\varepsilon_F - \varepsilon'_{s'\mu'p_z}(0))}{2\varepsilon'_{s'\mu'p_z}(0)} \left[ \frac{2\hbar v^2}{(2\hbar v^2)^2} \right]
\] (3.72)

For \(\varepsilon_F = 0\),

\[
\int_{-\infty}^{\infty} dp_z \sum_{s'\mu'} \frac{\theta(\varepsilon_F - \varepsilon'_{s'\mu'p_z}(0))}{2\varepsilon'_{s'\mu'p_z}(0)} = 2 \int_{0}^{p_c} dp_z \Lambda(p_z)
\] (3.73)

Introducing

\[
|p_0| = \frac{1}{v} \sqrt{b^2 - m^2}
\] (3.74)

For \(|p_z| < p_0\),

\[
\Lambda(p_z) = \frac{1}{-b + \sqrt{v^2p_z^2 + m^2}} + \frac{1}{-b - \sqrt{v^2p_z^2 + m^2}}
\] (3.75)
3.2. FORMULA TO CALCULATE MAGNETIC SUSCEPTIBILITY

For $|p_z| > p_0$,

$$\Lambda(p_z) = \frac{1}{-b - \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}}$$  \hspace{1cm} (3.76)$$

Then, Eq. (3.73) becomes,

$$\int_{-\infty}^{\infty} dp_z \sum_{s'\mu'} \frac{\theta(\varepsilon_F - \varepsilon'_{s'\mu'p_z}(0))}{2\varepsilon'_{s'\mu'p_z}(0)} = 2 \left[ \int_0^{p_0} dp_z \left( \frac{1}{-b + \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} \right) 
+ \int_{p_0}^{p} dp_z \left( \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{-b - \sqrt{v^2 p_z^2 + m^2}} \right) \right]$$ \hspace{1cm} (3.77)$$

For $0 < \varepsilon_F < (b - m)$

Define,

$$|p_+| = \sqrt{(\varepsilon + b)^2 - m^2}/v$$
$$|p_-| = \sqrt{(\varepsilon - b)^2 - m^2}/v$$ \hspace{1cm} (3.78)$$

For $p_+ < |p_z|$, 

$$\Lambda(p_z) = \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{-b - \sqrt{v^2 p_z^2 + m^2}}$$ \hspace{1cm} (3.79)$$

For $p_- < |p_z| < p_+$

$$\Lambda(p_z) = \frac{1}{-b + \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{-b - \sqrt{v^2 p_z^2 + m^2}}$$ \hspace{1cm} (3.80)$$

For $|p_z| < p_-$

$$\Lambda(p_z) = \frac{1}{-b + \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{-b - \sqrt{v^2 p_z^2 + m^2}}$$ \hspace{1cm} (3.81)$$

Then we have,

$$\int_{-\infty}^{\infty} dp_z \sum_{s'\mu'} \frac{\theta(\varepsilon_F - \varepsilon'_{s'\mu'p_z}(0))}{2\varepsilon'_{s'\mu'p_z}(0)} = 2 \left[ \int_0^{p_-} dp_z \left( \frac{1}{-b + \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} \right) 
+ \int_{p_-}^{p} dp_z \left( \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{-b - \sqrt{v^2 p_z^2 + m^2}} \right) 
+ \int_{p_0}^{p} dp_z \left( \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} + \frac{1}{-b - \sqrt{v^2 p_z^2 + m^2}} \right) \right]$$ \hspace{1cm} (3.82)$$
For $(b - m) < \varepsilon_F < (b + m)$

Define,

$$|p_+| = \sqrt{(\varepsilon + b)^2 - m^2}/v$$

Then we have,

$$\int_{-\infty}^{\infty} dp_z \sum_{s', \mu'} \frac{\theta(\varepsilon_F - \varepsilon_{s', \mu'}^p(0))}{2\varepsilon_{s', \mu'}^p(0)} = 2 \left[ \int_{p_+}^{p_c} dp_z \left( \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} \right) + \int_{p_+}^{p_c} dp_z \left( \frac{1}{-b - \sqrt{v^2 p_z^2 + m^2}} \right) \right] (3.83)$$

For $\varepsilon_F > (b + m)$

$$\int_{-\infty}^{\infty} dp_z \sum_{s', \mu'} \frac{\theta(\varepsilon_F - \varepsilon_{s', \mu'}^p(0))}{2\varepsilon_{s', \mu'}^p(0)} = 2 \left[ \int_{p_-}^{p_c} dp_z \left( \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} \right) + \int_{p_+}^{p_c} dp_z \left( \frac{1}{b - \sqrt{v^2 p_z^2 + m^2}} \right) \right] (3.84)$$

Finally, we have the final expression of $\chi_{\text{orb}}$ in semiconducting case given by

$$\chi_{\text{orb}} = \frac{e}{24\pi^2 \hbar^2 v} \frac{1}{\sqrt{|m^2 - b^2|}} \left( -2b \arctan\left( \frac{b \varepsilon_c}{\sqrt{|m^2 - b^2|} (\varepsilon_c^2 + m^2)} \right) + 2\sqrt{|m^2 - b^2|} \log(v(\varepsilon_c + \sqrt{\varepsilon_c^2 + m^2}) + b(\arctan\left( \frac{\sqrt{\varepsilon_F + b^2} - m}{\sqrt{|m^2 - b^2|}} \right) + \arctan\left( \frac{b \sqrt{\varepsilon_F + b^2} - m}{\sqrt{|m^2 - b^2|} (\varepsilon_F + b)^2} \right)) + \sqrt{|m^2 - b^2|} \log(v(\sqrt{\varepsilon_F + b^2} - m^2 + (\varepsilon_F + b))) \right) (3.85)$$

for $|b - m| < \varepsilon_F < |b + m|$ and,

$$\chi_{\text{orb}} = \frac{e}{24\pi^2 \hbar^2 v} \frac{1}{\sqrt{|m^2 - b^2|}} \left( -2b \arctan\left( \frac{b \varepsilon_c}{\sqrt{|m^2 - b^2|} (\varepsilon_c^2 + m^2)} \right) + 2\sqrt{|m^2 - b^2|} \log(v(\varepsilon_c + \sqrt{\varepsilon_c^2 + m^2}) + b(\arctan\left( \frac{\sqrt{\varepsilon_F + b^2} - m}{\sqrt{|m^2 - b^2|}} \right) + \arctan\left( \frac{b \sqrt{\varepsilon_F + b^2} - m}{\sqrt{|m^2 - b^2|} (\varepsilon_F + b)^2} \right)) + \sqrt{|m^2 - b^2|} \log(v(\sqrt{\varepsilon_F + b^2} - m^2 + (\varepsilon_F + b))) + b(- \arctan\left( \frac{\sqrt{\varepsilon_F - b^2} - m}{\sqrt{|m^2 - b^2|}} \right) + \arctan\left( \frac{b \sqrt{\varepsilon_F - b^2} - m}{\sqrt{|m^2 - b^2|} (\varepsilon_F - b)^2} \right)) - \sqrt{|m^2 - b^2|} \log(v(\sqrt{\varepsilon_F - b^2} - m^2 + (\varepsilon_F - b))) \right) (3.86)$$

for $(b + m) < \varepsilon_F$. 
3.3 Magnetic susceptibility of Dirac-Weyl semimetals

3.3.1 Time-reversal symmetric case \((b = 0)\)

In this chapter, we argue about the basic properties of the magnetic susceptibility of Dirac-Weyl semimetal in various choices of \((m, b)\). We first consider the case of \(b = 0\), i.e., in the absence of the intrinsic Zeeman term. The susceptibility components at \(T = 0\) are expressed as functions of the Fermi energy \(\varepsilon_F\) as

\[
\chi_{\text{spin}}(\varepsilon_F) = +\frac{e^2 v}{4\pi^2 \hbar} \left( \frac{g}{m_0 v^2} \right)^2 m^2 \theta(|\varepsilon_F| - m) \ln \frac{\sqrt{\varepsilon_F^2 - m^2} + |\varepsilon_F|}{m} + \chi_{\text{spin}}(0),
\]

\[
\chi_{\text{SO}}(\varepsilon_F) = -\frac{e^2 v}{2\pi^2 \hbar} \left( \frac{g}{m_0 v^2} \right) \text{sgn}(\varepsilon_F) \theta(|\varepsilon_F| - m) \sqrt{\varepsilon_F^2 - m^2} + \chi_{\text{SO}}(0),
\]

\[
\chi_{\text{orb}}(\varepsilon_F) = -\frac{e^2 v}{12\pi^2 \hbar} \times \left\{ \begin{array}{ll}
\ln \frac{2\varepsilon_c}{m} & |\varepsilon_F| < m, \\
\ln \frac{2\varepsilon_c}{\sqrt{\varepsilon_F^2 - m^2} + |\varepsilon_F|} & |\varepsilon_F| > m.
\end{array} \right.
\]

Here \(\chi_{\text{spin}}(0)\) and \(\chi_{\text{SO}}(0)\) are constants which solely depend on the energy cut off \(\varepsilon_c\). We should note that these terms may not be physically meaningful because in the real material, the susceptibility generally have some offset which is determined by the whole band structure beyond the present description. In the following, therefore, we argue about relative susceptibility with \(\chi_{\text{spin}}(0)\) and \(\chi_{\text{SO}}(0)\) substracted.

The three susceptibility components in Eq. (3.87) are separately plotted as solid curves in Fig. 3.7 together with the \((90^\circ\)-rotated) band structure in the top panel. The orbital-orbital term \(\chi_{\text{orb}}\) is negative and logarithmically decays in higher \(|\varepsilon_F|\). It actually corresponds to the orbital diamagnetism in 2D graphene, and equivalent to the previous calculation in 3D [50]. The spin-spin term \(\chi_{\text{spin}}\) corresponds to the summation of the Pauli and the van Vleck paramagnetism, and it is positive and increases as \(|\varepsilon_F|\) becomes larger. Interestingly, the spin-orbital term \(\chi_{\text{SO}}\) is an odd function of \(\varepsilon_F\) unlike other two components being even functions, and it monotonically decreases in increasing \(\varepsilon_F\). It is because \(\chi_{\text{SO}}\) is solely contributed by the \(n = 0\) Landau level, which is responsible for breaking the electron-hole symmetry as we argued in Chapter 2.

It is also important to note that the three susceptibility components have different
magnitudes. The relative magnitudes are roughly estimated as
\[ \frac{\chi_{\text{spin}}}{\chi_{\text{orb}}} \sim \left( \frac{gE}{m_0 v^2} \right)^2, \quad \frac{\chi_{\text{SO}}}{\chi_{\text{orb}}} \sim \frac{gE}{m_0 v^2}, \]
where \( E \) is the energy scale corresponding to \( \varepsilon_F \) and \( m \). Here \( m_0 \) is the bare electron mass which originates from \( \mu_B \) in the Zeeman term. The typical velocity operator is of the order of \( 10^5 \) m/s (e.g., \( 3 \times 10^5 \) m/s for TaAs\(^{[54]} \)), and then \( m_0 v^2 \) becomes the order of 100 meV. In the case of moderate \( \varepsilon_F \) and \( m \) much smaller than 100 meV, therefore, we expect \( \chi_{\text{orb}} \) is dominant so that the system becomes diamagnetic in total.

Finally it is worth to argue the Dirac semimetal case \( m = b = 0 \). Eq. (3.87) except for the constant terms becomes,
\[ \chi_{\text{spin}}(\varepsilon_F) = 0, \]
\[ \chi_{\text{SO}}(\varepsilon_F) = -\frac{e^2 v}{2\pi^2 \hbar} \left( \frac{g}{m_0 v^2} \right) \varepsilon_F, \]
\[ \chi_{\text{orb}}(\varepsilon_F) = -\frac{e^2 v}{12\pi^2 \hbar} \ln \frac{\varepsilon_c}{|\varepsilon_F|} \]
which are plotted in Fig.3.7 as dashed curves. There \( \chi_{\text{spin}} \) completely vanishes, \( \chi_{\text{SO}} \) becomes a simple linear function, and \( \chi_{\text{orb}} \) gives a negative logarithmic peaks which diverges at zero Fermi energy.

### 3.3.2 General cases \((b > 0)\)

We plot the result of semiconducting case \((m > b)\) in Fig.3.8 where the band structure and the plot of \( \chi_{\text{spin}}, \chi_{\text{SO}}, \) and \( \chi_{\text{orb}} \) is shown respectively. Unlike \( b = 0 \) case, we have kink-like structures in all three terms at \( \varepsilon_F = \pm (m+b) \) and \( \pm (m-b) \) corresponding to the specific band structure such as band edges, while the overall behavior is similar to \((m = 1, b = 0)\) case in the previous section: The relative \( \chi_{\text{spin}} \) is paramagnetic inside the energy bands. The spin-orbital term susceptibility is again an odd function unlike other two, but not a simple linear function anymore and it is constant inside the gap. \( \chi_{\text{orb}} \) is diamagnetic and logarithmically decays while it is constant inside the gap.

Lastly, we show the plot of Weyl semimetal case in Fig.3.9. We observe in all three terms the kinks corresponding to the band edges as in the previous gapped case, while the property is now significantly different. Importantly, the diamagnetism \( \chi_{\text{orb}} \) logarithmically diverges at \( \varepsilon_F = 0 \) similarly to the Dirac semimetal case \((m = b = 0)\),
Figure 3.7: Dirac semimetal case \((m = b = 0;\) dashed line) and semiconducting case \((m = 1, b = 0;\) solid line). (a) Band structure. (b) Spin-spin term susceptibility \(\chi_{\text{spin}} - \chi_{\text{spin}}(\varepsilon_F = 0)\). (c) Spin-orbital term susceptibility \(\chi_{\text{SO}} - \chi_{\text{SO}}(\varepsilon_F = 0)\). (d) Orbital-orbital term susceptibility \(\chi_{\text{orb}}\).
and this actually reflects the existence of the linear dispersion around the Weyl nodes at zero energy. In the same region, $\chi_{\text{spin}} - \chi_{\text{spin}}(\varepsilon_F = 0)$ vanishes and this is also similar to the Dirac semimetal case. Outside the linear band region, $\chi_{\text{spin}} - \chi_{\text{spin}}(\varepsilon_F = 0)$ becomes negative near the second band edges $\varepsilon_F = \pm (m + b)$, and it increases again outside. $\chi_{\text{SO}}$ is rather featureless and monotonically decreases in increasing of Fermi energy.

### 3.3.3 Chirality Dependence

Similar to the Rashba/Dresselhaus case in the previous section, the sign of the spin-orbit cross susceptibility $\chi_{\text{SO}}$ depends on the spin-texture in the momentum space. Here we consider the Hamiltonian,

$$
\mathcal{H} = \begin{bmatrix}
    m + b & 0 & vp_z & v(p_x + ip_y) \\
    0 & m - b & v(p_x - ip_y) & -vp_z \\
    vp_z & v(p_x + ip_y) & -m + b & 0 \\
    v(p_x - ip_y) & -vp_z & 0 & -m - b
\end{bmatrix}
$$

(3.90)

where $p_x \pm ip_y$ in Eq. (3.1) is inverted to $p_x \mp ip_y$. The difference between Eq. (3.1) and Eq. (3.90) can be understood as the handedness of the spin texture. Specifically, when we go clockwise around the equienergy contour on $p_x, p_y$ plane (i.e., fix $p_z$), the spin $xy$ component rotates clockwise in Eq. (3.1), while counter-clockwise in Eq. (3.90).

We can calculate the Landau level structures for Eq. (3.90) in the exactly same manner as in Eq. (3.1), then we immediately find that the sign $\tau_{\mu p_z}$ is inverted: namely, the existing level and non-existing level of $n=0$ sector are interchanged. All other Landau levels $n \neq 0$ are identical in Eqs. (3.1) and (3.90). As a result, only the spin-orbit cross susceptibility $\chi_{\text{SO}}$ inverts its sign from Eq. (3.1), while $\chi_{\text{orb}}$ and $\chi_{\text{spin}}$ remains unchanged. Only the $\chi_{\text{SO}}$ is sensitive to the "handedness" of the spin texture, and it affects the total susceptibility.

In Fig. 3.10, we plot $\chi_{\text{SO}}$ for the Dirac semimetals (with $m = b = 0$) with opposite chiralities, i.e., Eqs. (3.1) and (3.90).
Figure 3.8: General semiconducting case \( (m = 1, b = 0.5) \). (a) Band structure. (b) Spin-spin term susceptibility \( \chi_{\text{spin}} - \chi_{\text{spin}} (\epsilon_F = 0) \). (c) Spin-orbital term susceptibility \( \chi_{\text{SO}} - \chi_{\text{SO}} (\epsilon_F = 0) \). (d) Orbital-orbital term susceptibility \( \chi_{\text{orb}} \).
Figure 3.9: Weyl Semimetal Case. \((m = 0.5, b = 1)\). (a) Band structure. (b) Spin-spin term susceptibility \(\chi_{\text{spin}} - \chi_{\text{spin}}(\varepsilon_F = 0)\). (c) Spin-orbital term susceptibility \(\chi_{\text{SO}} - \chi_{\text{SO}}(\varepsilon_F = 0)\). (d) Orbital-orbital term susceptibility \(\chi_{\text{orb}}\).
Figure 3.10: $\chi_{SO}$ for 3D Dirac semimetal case with opposite chirality. Dashed line for Eq. (3.1) and Solid line for Eq. (3.90).
Chapter 4

Conclusion

In this thesis, we calculated the magnetic susceptibility in various types of materials with spin-orbit coupling, including 2DEG with Rashba / Dresselhaus spin-orbit coupling, 2D Dirac model to describe the surface state of 3D topological insulator, and 3D Dirac / Weyl semimetals. The new findings in the thesis are summarized as follows.

(1) General formulation of the spin-orbit cross susceptibility $\chi_{SO}$.

The conventional knowledge tells us that the magnetic susceptibility is composed of the spin part and orbital part. Here we provided a generic formulation to calculate the magnetic susceptibility from the Landau levels, and found that the materials with spin-orbit coupling generally has the spin-orbit cross susceptibility $\chi_{SO}$ on top of the spin susceptibility $\chi_{\text{spin}}$ and orbital susceptibility $\chi_{\text{orb}}$. The important point here is that the Hamiltonian depends on the external magnetic field in two different ways, via the orbital term and the spin Zeeman term, and therefore we have three susceptibility components.

(2) Chirality dependence of $\chi_{SO}$.

The Rashba SOC and Dresselhaus SOC have essentially the same energy dispersions, while the spin-texture on the momentum space is different. Specifically, if we rotate the equi-energy contour in the momentum space, then the spin rotates in the opposite directions in Rashba and Dresselhaus systems. One may naively think that the magnetic susceptibility is insensitive to such the chirality (or handedness) of the spin texture, but here we found it is not the case. Namely, the $\chi_{SO}$ is found to have
opposite signs in Rashba and Dresselhaus case, while \( \chi_{\text{orb}} \) and \( \chi_{\text{spin}} \) are just identical. We also found that the sign of \( \chi_{\text{SO}} \) is closely related to the \( n = 0 \) Landau level, which is also chirality dependent. We applied the same method to the 2D Dirac system and 3D Dirac / Weyl system, and found that the dependence of \( \chi_{\text{SO}} \) on the chirality of the spin texture is quite general.

(3) Magnetic susceptibility of 3D Dirac / Weyl semimetals.

The Dirac / Weyl semimetals are novel materials attracting much interest in the recent years, while very little was known about the magnetic susceptibility. Here we provided systematic calculations of the magnetic susceptibility for generic \( 4 \times 4 \) Hamiltonian, which covers the Dirac semimetal, the Weyl semimetal, and the gapped semiconductor. We calculate the Landau levels and and analytically derive the expression of the magnetic susceptibility. Using the formula, we actually calculated the susceptibility in various different cases.

We found that that \( \chi_{\text{orb}} \) and \( \chi_{\text{spin}} \) are even functions of the Fermi energy i.e., electron hole symmetric with respect to zero energy, while only the \( \chi_{\text{SO}} \) is found to be an odd function of Fermi energy unlike the other two. This makes sense since \( \chi_{\text{SO}} \) is solely determined by the \( n = 0 \) Landau level and it breaks the electron hole symmetry. In the Dirac and Weyl semimetal case, in particular, we showed that \( \chi_{\text{SO}} \) is a monotonically increasing or decreasing function in the Fermi energy, while \( \chi_{\text{orb}} \) is a logarithmic function which diverges at zero energy. The log divergence is reflects the formation of the band touching points. Using the parameters in experimentally-realized Dirac or Weyl semimetals, we showed that \( \chi_{\text{orb}} \) is the largest while other terms also have the significant contributions.

We also investigated the susceptibility of the Hamiltonian with opposite chirality in the spin texture, and confirmed that the sign of \( \chi_{\text{SO}} \) becomes opposite by inverting the chirality, while \( \chi_{\text{orb}} \) and \( \chi_{\text{spin}} \) remain unchanged.

Lastly, let us argue about how one can experimentally observe the effects predicted in this thesis. For Rashba / Dresselhaus system, \( \chi_{\text{SO}} \) governs the total susceptibility in \( \varepsilon_F < 0 \) (below the Dirac point). If one can measure of the magnetic susceptibility in Rashba / Dresselhaus system in \( \varepsilon_F < 0 \), it should be the direct measurement of the chirality dependent part of the magnetic susceptibility. For the surface states of the topological insulator, we predicted the \( \chi_{\text{SO}} \) jumps at the Dirac point, and its the
direction (negative / positive) depends on the chirality of the spin texture. It should be observed as the jump of the total susceptibility in changing the Fermi energy.

For Weyl / Dirac semimetals, our calculation predicts the strong diamagnetism at the band touching point of Weyl and Dirac semimetal, where the $\chi_{\text{orb}}$ logarithmically diverges. This should be observed as the dominant part of the magnetism. On the other hand, $\chi_{\text{SO}}$ is the only term which has different sign in the electron side and the hole side. The present result suggests that the electron side is more paramagnetic or diamagnetic than the hole side, depending on the chirality of the spin texture. So in principle, we can directly detect the chirality by measuring the dependence of the susceptibility on the Fermi energy near the Dirac point. Of course the electron-hole symmetry is generally broken in the real material, and it may also contribute to the electron-hole asymmetry in the susceptibility. The detailed study on this is left for the future work.
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