Theory of magnetic response in nodal semimetals

著者	HIZBULLAH Intan Fatimah
number	82
学位授与機関	Tohoku University
学位授与番号	理博第3151号
URL	http://hdl.handle.net/10097/00123954

（別紙様式５）

論文内容要旨

(NO. 1)

氏名	Intan Fatimah Hizbullah	提出年	平成　　年
学位論文の 題目	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 ）		

論文目次

Abstract

In ordinary metal, it is well-known that the magnetic susceptibility consists of Pauli paramagnetism (spin effect) and Landau diamagnetism (orbital effect). 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.

A well-known example of spin-orbit coupled system is the 2D electron gas (2DEG) with Rashba and Dresselhaus SOC. The Rashba effect occurs when there is structural inversion asymmetry in the junction of semi-conductor hetero-structures, and the Dresselhaus effect occurs when the asymmetry exist in bulk crystal structure. 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. Specifically, if 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" of the spin texture. This may lead to a significant difference in the magnetic susceptibility, but the detailed study on the chirality effect on the magnetic response has not been carried out.

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. The topological insulator is a bulk insulator with topological surface states. The Weyl and Dirac semimetals are the systems with 3D gapless spectrum where the energy bands touch at isolated points in the momentum space. The magnetic response in those new system is also not well known and a systematic study is needed.

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 consider the Hamiltonian of 2D Rashba /Dresselhaus system, the 2D surface state of topological insulator, and 3D nodal semimetals. We calculate the Landau level spectrum and the thermodynamic potential, and derive the analytical expression of the magnetic susceptibility.
Using the formula, we actually calculate the susceptibility in those systems and argue about the characteristic properties. The magnetic susceptibility in those systems can be formally decomposed into three different contributions: spin-spin term, orbital-orbital term, and spin-orbital cross term.

The results in the thesis are summarized as follows.

1. General formulation of the spin-orbit cross susceptibility

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 on top of the spin susceptibility and orbital susceptibility. 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 spin-orbit cross susceptibility.

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 of the spin texture, but here we found it is not the case. Namely, the spin-orbit cross susceptibility is found to have opposite signs in Rashba and Dresselhaus case, while orbital susceptibility and spin susceptibility are just identical. We also found that the sign of spin-orbit cross susceptibility 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 spin-orbit cross susceptibility 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 4×4 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. As a typical example, we show orbital susceptibility, spin-orbit cross susceptibility and spin susceptibility calculated for the Weyl semimetal phase . We have the strong diamagnetism at the band touching point of Weyl and Dirac semimetal, where the orbital susceptibility logarithmically diverges. This should be observed as the dominant part of the magnetism. On the other hand, spin-orbit cross susceptibility is the only term which has different sign in the electron side and the hole side, where the electron side is more paramagnetic or diamagnetic than the hole side, depending on the chirality of the spin texture.

別　紙

論文審査の結果の要旨

HIZBULLAH 氏提出の博士論文は、スピン軌道相互作用のある物質系における帯磁率に関する理論的研究に関するものである。通常の電子系の帯磁率は、電子の軌道運動に由来する軌道帯磁率と、スピン磁気モーメントに由来するスピン帯磁率からなり、それぞれがランダウ反磁性とパウリ反磁性として知られる。一方で、スピン軌道相互作用が大きな物質では、スピンと軌道の絡み合いが帯磁率にどのような影響を与えるのかは系統的に調べられていなかった。近年トポロジカル絶縁体やワイル半金属など、スピン軌道相互作用が電子構造に重要な役割を持つ物質が広く研究されるようになっており、スピン軌道相互作用を取りいれた帯磁率の理論的理解は重要な問題である。

本博士論文では、スピン軌道相互作用のある電子系の帯磁率を一般的に定式化し、かつ様々な電子系（Rashba 相互作用、Dresselhaus 相互作用、トポロジカル絶縁体表面状態、ディラック半金属、ワイル半金属）に関して実際に帯磁率を計算した。主要な結果は３つからなる。第一に、スピン軌道相互作用がある場合、帯磁率は軌道帯磁率とスピン帯磁率に加え、第３の項「スピン・軌道交差帯磁率」が存在することを一般的な議論より示した。第２に、スピン軌道相互作用にはスピンと運動量の関係性によって「時計回り型」と「反時計回り型」に分類されるが、「スピン・軌道交差帯磁率」だけはこの時計/反時計回りによって符号を変えることを明らかにした。例えばこれによって、古くから知られる Rashba 系と Dresselhaus 系が、よく似たバンド構造を持つにもかかわらず、非常に異なる帯磁率を持つことが示された。第３に、３次元のギャップレス電子系として近年注目を集めるワイル・ディラック電子系の帯磁率を初めて系統的に計算したことである。

この研究で得られた理論の枠組みは、スピン軌道相互作用のあるあらゆる電子系に拡張することできるものであり、汎用性が高く学術的にも価値の高い研究である。以上のことより、本研究は固体電子の物性に対して新しい知見をもたらし，申請者の自立した研究活動を行うに足る高度の研究能力と学識を有することを示した。よってこの論文は博士（理学）の学位論文として合格と認める。