Phase diagrams of the Kane-Mele-Hubbard model in the presence of an external magnetic field

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Abstract. We studied the Kane-Mele-Hubbard model at half filling with Zeeman magnetic field using rotationally invariant slave boson method. The competition between external magnetic field and spin orbital coupling at large Hubbard $U$ is explored. It is found that different canted antiferromagnetic phases exist in the presence of longitudinal and transverse magnetic fields. With longitudinal external magnetic field and strong electron correlation, the $z$ component of the local moment is preferred by the finite spin-orbital coupling.

1. Introduction

The transition metal oxides such as Iridates have been investigated extensively due to the various physical phenomena driven by the interplay of strong spin-orbital coupling (SOC) and electronic correlations, such as Na$_2$IrO$_3$ etc. Recently, several authors have studied the phase diagram of the Kane-Mele-Hubbard (KMH) model[1, 2], which is used to describe the SOC and topological characters in these correlated systems. Generally, the semimetal is replaced by the $Z_2$ topological band insulator at finite SOC. At large electron correlation, long-range magnetic order breaks time-reversal invariance. The antiferromagnetic (AFM) Mott insulator phase exists and magnetic order is restricted to the xy plane in the presence of SOC.

The application of a magnetic field is a powerful approach to reveal hidden magnetic properties and their relationship with other order parameters. Some novel magnetic field may also exist with an external magnetic field. An external magnetic field breaks time reversal symmetry and it may lead to a Zeeman split to the spin motion. The interplay between the SOC and the Zeeman coupling may break the topological character. and it can also induce a nonlinear magnetic phase with electron Coulomb correlation. In the transition metal oxides such as Iridates system, the interplay between SOC and magnetic field with strong Coulomb correlation is an interesting topic.

In the present study, we investigate the KMH model under the Zeeman magnetic field. The phase diagrams with transverse and longitudinal magnetic fields are studied and the effects of competition between the magnetic field and SOC on local moments are discussed. This paper is organized as follows: we firstly describe the model Hamiltonian and theoretical approach, then the effects of external magnetic fields on the phase diagrams are discussed. The final section is devoted to the conclusion remarks.
2. Model Hamiltonian and Methods

The Kane-Mele model is proposed by Kane and Mele to describe the quantum spin Hall effect in graphene [1, 2]. To investigate the competition between the SOC and magnetic field, we employ the KMH model with external magnetic field, which can be written as follows:

\[ H = \sum_{(ij)\sigma} (t_{ij}c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow}n_{i\downarrow} - \frac{1}{2} \sum_i \mathbf{h} \cdot \mathbf{S}_i + i\lambda_{SO} \sum_{(ij)} v_{ij} c_{i\sigma}^\dagger \sigma^z c_j \]  \hspace{1cm} (1)

where \( c_{i\sigma}^\dagger \) and \( c_{i\sigma} \) are the creation and annihilation operators for an electron of spin \( \sigma \) at site \( i \). \( n_{i\sigma} \) is the corresponding occupation number operator. \( \sigma^z \) is a Pauli matrix. Here \( v_{ij} \) equals \( \pm 1 \) for sublattices A and B. \( \lambda_{SO} \) is the second-neighbor SOC strength. \( U \) is the Coulomb repulsion and \( \mathbf{h} \) is an external magnetic field.

To treat the Coulomb interaction with arbitrary external field and spin-orbital coupling, the rotationally invariant slave boson (RISB) method is adopted[3, 4]. We introduce six slave bosons \( e, p_x, p_z, p_y \) and \( b \) for empty, singly and double occupations, respectively. The enlarged local Hilbert space in the RISB representation is expressed by using these slave bosons and quasiparticle fermions \( f_{\sigma} \). To focus the solution in the physical subspace, four constraints (including normalization, particle and spin constraints) given by Wölfle et al.[3] are introduced. Projecting the KMH model into the RISB representation, the Hamiltonian thus becomes

\[ H = \frac{1}{N} \sum_{aa'\sigma\sigma'} \gamma_{aa'\sigma\sigma'}(k)R_{aa'\sigma\sigma'} + (\varepsilon_0 - \mu)\delta_{\sigma\sigma'} \langle f_{a\sigma}^\dagger f_{a'\sigma'} \rangle + Ub^2 \]  \hspace{1cm} (2)

where \( \varepsilon_0 \) and \( \mu \) are the energy level and chemical potential. \( R_{aa'\sigma\sigma'} \) and \( \gamma_{aa'\sigma\sigma'} \) are the elements of the renormalization matrix[3]. The dispersion \( \gamma_{aa'\sigma'\sigma''}(k) \) is written as

\[ \gamma_{aa'\sigma'\sigma''}(k) = \begin{cases} -4v_{aa'}\lambda_{SO}\gamma_{SO}(k) + (\varepsilon_0 - \mu) - \frac{1}{2}\sigma^z & \text{if } a = a' \text{ and } \sigma = \sigma'' \\ t\gamma_0(k)(1 - \delta_{aa'}) + \frac{1}{2}(h_x + ih_y)\delta_{aa'} & \text{if } a \neq a' \text{ or } \sigma \neq \sigma'' \\ t\gamma_0(k)(1 - \delta_{aa'}) + \frac{1}{2}(h_x - ih_y)\delta_{aa'} & \text{if } a \neq a' \text{ or } \sigma \neq \sigma'' \end{cases} \]  \hspace{1cm} (3)

where

\[ \gamma_{SO}(k) = 4\cos\left(\frac{\sqrt{3}}{2}k_y\right)\sin\left(\frac{1}{2}k_x\right) + 2\sin(k_x) \]  \hspace{1cm} (4)

\[ \gamma_0(k) = 1 + 2\cos\left(\frac{1}{2}k_x\right)\cos\left(\frac{\sqrt{3}}{2}k_y\right) - 2\cos\left(\frac{1}{2}k_x\right)\sin\left(\frac{\sqrt{3}}{2}k_y\right) \]  \hspace{1cm} (5)

We solve the self-consistency equations that minimize the Eq. 2 by using optimization method[5].

3. Numerical Results

Generically, the full \( SU(2) \) symmetry is broken by SOC terms. Thus the interaction between the SOC and electron Coulomb correlation exhibits rich phases [6, 7, 8, 9, 10, 11]. The existing results show that the topological band insulator (TBI) phase is stabilized by finite SOC. At the critical electron correlation, a transition from TBI phase to in-plane Néel AFM phase occurs[8]. At intermediate electron correlation, a quantum spin liquid phase is also proposed[12]. However, some subsequent results show the direct phase transition from simple metallic phase to the AFM insulator phase[13, 14]. Thus we neglect the spin liquid phase in our work since it can be destroyed by external magnetic field.

We have studied the phase diagram and get the similar results as that given by M. Hohenadler et al.[8] except that the spin liquid phase is excluded. Here we first plot the magnetic phase
increasing SOC due to the competition between the external magnetic field and SOC. A finite SOC induces an in-plane AFM phase due to the spin arrangement in the system. With further increasing SOC, a XYAFMI-TBI phase occurs, which has been proposed by many works[8, 15, 16]. With coupling between the next nearest neighbors[8]. With increasing SOC, we find that the paramagnetic insulator phase appears with $h_z > 0$, the system translates into ferromagnetic insulator phase with the spin arrangements in $x$ direction (XFMI). The phase diagram with finite $h_z$ is also plotted in Fig.1(b). In the canted insulator phase XAFMZFI, the spin arrangements AFM in $x$ direction and ferromagnetic in $z$ direction. We find that the paramagnetic insulator phase appears with increasing SOC due to the competition between the external magnetic field and SOC.

The corresponding magnetic moments at $U/t = 8$ are plotted in Fig. 2. The total magnetic moments are nearly independent on the external field since the local spin has polarized absolutely.
due to the strong electron Coulomb correlation. But the component of the local magnetic moment along the external magnetic field increases considerably with increasing magnetic field. Due to the exchange interaction between next-nearest neighbours [8], the total magnetic moments and components along the external magnetic fields decrease with increasing SOC. As expected, the $x$ component of the local magnetic moment is finite with the $λ_{SO}$ large than critical value as shown in Fig. 2(a). From Fig. 2(b), we find that there is a peak of the $z$ components of the local moments with increasing $λ_{SO}$, which only exists with longitudinal external magnetic field and strong electron correlation. The reason is that the in-plane AFM component is depressed by the finite $λ_{SO}$.

4. Summary
In summary, we have studied the effects of external magnetic field on the magnetic phase diagrams of KMH model. Our results show that the system translates into canted AFM state under external magnetic field, which is destroyed by large SOC. The effects of longitudinal and transverse external magnetic fields on the ground states are very different. Although the magnetism can be suppressed by large SOC under longitudinal magnetic field, a finite SOC favors the longitudinal component of the local magnetic moment.

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6. References
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