Coexistence of magnetic and topological phases in the asymmetric Kane-Mele-Hubbard model

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Abstract. Motivated by recent experiments on ultracold atoms trapped in optical lattices, we investigate
the mass imbalance effects on the Kane-Mele-Hubbard model. Using the variational cluster approach,
we show that the mass imbalance introduces the spin anisotropy in the magnetic structure and induces the
topological phase transition between the topological phases with helical edge state and chiral edge state. We
also show that the intermediate state with coexistence of magnetic and topological phases can be realized
as the integer quantum Hall effect.

1. Introduction
Recently, the novel properties resulting from the topological structure of matter have attracted much
attention in condensed matter physics because the topologically nontrivial surface state and specific
magnetoelectric response were detected in real materials such as HgTe-CdTe quantum wells [1, 2] and
some bismuth-based compounds such as Bi$_2$Se$_3$ and Bi$_{1-x}$Se$_x$ [3, 4]. The most significant issues in such
studies are the detection of novel topological features in systems where the interaction, impurities and
crystallographic symmetries are relevant, as well as the elucidation of the origins of these features. In
particular, a large number of calculations have been carried out to show the importance of the interatomic
interaction on topological phases [5, 6, 7, 8, 9, 10, 11, 12], including the phases in real $d$ and $f$ electron
materials [13, 14, 15]; many possibilities of the emergence of novel topological phases due to correlation
effects have in fact been reported [16, 17, 18, 19, 20, 21, 22, 23, 24, 25].

Besides the real materials, ultracold atomic gases trapped in optical lattices have also been developed
in recent years, which enable us to simulate the quantum many-body problems; e.g., in the last decade
the artificial gauge fields have been studied extensively to reproduce the integer and fractional quantum
Hall effects in optical lattices. In particular, the realization of the well-known topological band insulator
in the Haldane and Hofstadter models was reported recently [26, 27, 28, 29].

In our study, motivated by such developments in the field, we consider the topological band-insulator
state with mass imbalance. The “mass imbalance” is a term in ultracold atomic physics and can be
introduced by mixing two species of fermionic atoms such as $^6$Li and $^{40}$K. In previous studies, the mass
imbalanced system has been considered mainly in the following two respects: the symmetry broken
phase driven by the mass imbalance effect [30, 31] and the orbital-selective Mott transition where only
a part of the bands becomes insulating due to correlation effects [32, 33, 34, 35]. In our study of the
mass imbalanced system, we in particular consider the existence of the intermediate state between
the magnetic and topological phases, which we studied in the Bernevig-Hughes-Zhang model [1, 2],
where the conservation of the $z$ component of the total spin quantum number allows the existence of the
intermediate state [24, 25]. However, we note that the mass imbalanced system in general breaks the
time-reversal symmetry, and therefore, the topological phase in our model is protected only by the the conservation of the $z$ component of the total spin quantum number.

In this paper, we will investigate the effects of mass imbalance in the Kane-Mele-Hubbard model [36], where we adopt the variational cluster approach (VCA) based on the self-energy functional theory (SFT) [37, 38, 39]. We will show that the mass imbalance introduces the spin anisotropy and induces the topological phase transition. We will in particular confirm that the intermediate state appears between the magnetic and topological phases as the integer quantum Hall effect.

2. Model and method

We use the extended Kane-Mele-Hubbard model with mass imbalance, where the mass imbalance is introduced as the spin-dependent (or spin asymmetric) hopping $t_{ir} = t (1 + r \delta)$ between the nearest-neighbor sites and spin-dependent imaginary hopping $i \lambda_{ir} = i \lambda (\sigma + \delta)$ between the next-nearest-neighbor sites, which is illustrated in Fig. 1(a). The Hamiltonian reads

\[ H = \sum_{(ij)\sigma} t_{ir} c_{ir}^\dagger c_{jr} + \sum_{\langle(ii)\sigma\rangle} i \lambda_{ir} \Sigma_{i} c_{ir}^\dagger c_{ir} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \]  

(1)

where $(ij)$ indicates the nearest-neighbor bonds and $\langle(ii)\rangle$ indicates the next-nearest-neighbor bonds. $c_{ir}$ is the annihilation operator of a fermionic particle with spin $\sigma$ at site $i$, and $n_{i\sigma} = c_{ir}^\dagger c_{ir}$ is the number operator. It should be noted that the mass imbalance $\delta$ breaks the time-reversal symmetry, and therefore, only the conservation of the $z$ component of the total spin quantum number is significant for the symmetry protection of the topological phase [22, 23, 24, 25]. In our calculation, we assume a value $\lambda/t = 0.2$ for simplicity.

\[ J = 4r^2(1 - \delta^2)/U, \quad \gamma = 2\delta^2/(1 - \delta^2) \quad \text{and} \quad J_k = 4\lambda^2(1 - \delta^2)/U. \]

\[ S_i^r = 1/2 \sum_{\alpha\beta} c_{ir}^\dagger \sigma_{r\alpha}^\dagger c_{i\beta}, \]

is the $r$ component of the spin operator at site $i$ and $\sigma^r$ is the $r$ component of the Pauli matrix. Thus, the next-nearest-neighbor imaginary hopping introduces the $xy$-plane ferromagnetic interaction and the

Let us first consider the strong correlation limit $U/t \gg 1$ of our Hamiltonian. The effective spin Hamiltonian in this limit reads

\[ H_{\text{eff}} = J \sum_{(ij)} \left( S_i \cdot S_j + \gamma S_i^z S_j^z \right) + J_k \sum_{\langle(ii)\rangle} \left\{ -(S_i^x S_j^x + S_i^y S_j^y) + (1 + \gamma) S_i^z S_j^z \right\}, \]

(2)

where $J$ and $J_k$ are the hopping integrals between nearest-neighbor and next-nearest-neighbor spins, respectively. The $z$ component of the spin operator at site $i$ is $S_i^z = \sum_{\alpha} c_{ir}^\dagger \sigma_{z\alpha}^\dagger c_{i\alpha}$. The $x$ and $y$ components are given by $S_i^x = \sum_{\alpha} c_{ir}^\dagger \sigma_{x\alpha}^\dagger c_{i\alpha}$ and $S_i^y = \sum_{\alpha} c_{ir}^\dagger \sigma_{y\alpha}^\dagger c_{i\alpha}$.
mass imbalance \(\delta\) introduces the spin anisotropic interaction in the \(z\) direction, i.e., the Ising anisotropy. Therefore, the ratio \(\lambda/(t\delta)\) should be significant for the determination of the magnetic structures between the \(xy\)AF and \(z\)AF phases, which are defined in Figs. 1 (c) and (b), respectively. In the classical spin limit, the critical line of the magnetic transition can be determined as \(\delta = \sqrt{2}\lambda/t\).

For treating the effects of correlations in this model, we then use the method of VCA based on the SFT. The SFT is the thermodynamically consistent theory that can derive the exact grand potential \(\Omega\) in the infinite system as long as the variational problem \(\delta\Omega[\Sigma] = 0\) is solved exactly. In the VCA framework, the grand potential functional \(\Omega[\Sigma]\) can be calculated as the following functional of the reference self-energy \(\Sigma'\):

\[
\Omega[\Sigma'] = \Omega' - \text{Tr} \ln \left( G_{0}^{-1} - \Sigma' \right) + \text{Tr} \ln G'^{-1},
\]

where \(\Omega'\) and \(G'\) are the exact grand potential and exact Green function of the reference Hamiltonian \(H'\), respectively, which are defined on the small clusters (see Fig. 1(a)). We note that the reference Hamiltonian \(H'\) contains the symmetry-breaking Weiss field such as the magnetic and superconducting orders and the symmetry broken phases are realized via the SFT variational problem. In our system, two types of the magnetic phases are considered, which are illustrated in Figs. 1 (b) and (c). Therefore, in our calculation, we use the following reference Hamiltonian \(H' = H_{6\text{site}} + H_{xy\text{AF}} + H_{z\text{AF}}\) with

\[
H_{xy\text{AF}} = -h_x \sum_{i,a} \epsilon_i c_{i\alpha}^\dagger \sigma_{\alpha\beta}^x c_{i\beta}, \quad H_{z\text{AF}} = -h_z \sum_{i,a} \epsilon_i c_{i\alpha}^\dagger \sigma_{\alpha\beta}^z c_{i\beta},
\]

where \(H_{6\text{site}}\) is the reference Hamiltonian in the 6-site clusters, and \(H_{xy\text{AF}}\) and \(H_{z\text{AF}}\) are the Weiss field Hamiltonians characterizing the two magnetic orders of \(xy\)AF and \(z\)AF. Note that \(\epsilon_i = 1\) \((i \in A)\), \(-1\) \((i \in B)\). The details of the VCA and SFT can be found in Refs. [39, 40].

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2}
\caption{Calculated grand potential functional \(\Omega - \Omega_{h_x = 0}\) as a function of the Weiss fields \(h_x\) and \(h_y\) at \(\delta = 0.2\) [in (a) and (b)] and 0.8 [in (d) and (e)]. Also shown are the calculated local magnetic moments \(m_x\) and \(m_z\) as a function of the Hubbard interaction \(U/t\) at \(\delta = 0.2\) [in (c)] and \(\delta = 0.8\) [in (f)].}
\end{figure}
3. Results and discussion

First, let us discuss the effects of mass imbalance on the magnetic phases in the Kane-Mele-Hubbard model. In Figs. 2 (a) and (b), we show the results for the ground potential $\Omega - \Omega_{h=0}$ as a function of the Weiss fields $h_x$ and $h_z$ at $\delta = 0.2$, where $\Omega_0$ is the grand potential at zero Weiss fields. We find that the grand potentials of both the $xy$AF and $z$AF phase have the single stationary point at some value of $h_x$ and $h_z$. This result indicates that both of the magnetic transitions are of the second order and the $z$AF ($xy$AF) phase is favored at $U/t \geq 5.50$ ($U/t \geq 3.37$). Moreover, from the view point of the energy gain, we find that the $xy$AF phase is realized at $U/t \geq 5.50$. These results are similar to the results of the original Kane-Mele-Hubbard model without mass imbalance, and therefore, the present $xy$AF phase without time-reversal symmetry corresponds to the $xy$AF phase in the original model [6, 7, 8, 9, 10].

On the other hand, the results in Figs. 2 (d) and (e) show the ground potential at a larger value of $\delta = 0.8$. Here, we confirm the absence of the stationary points in the grand potential for the $xy$AF phase, corresponding to the absence of the $xy$AF phase. The $z$AF phase is instead favored in this region with the large mass imbalanced $\delta = 0.8$. Therefore, as we mentioned for the strong-coupling limit, the mass imbalance introduces the Ising anisotropy and the $z$AF phase is realized as a result of the mass imbalance effect. Moreover, in the case of $\delta = 1.0$ (or $t_\parallel = 0$), the instability towards the $z$AF phase should be increased due to the nearly flat-band structure of the down-spin fermion. As a result of this instability, the magnetic transition occurs at $U = 0$, and therefore, the Haldane-model–like single-spin integer quantum Hall phase cannot be detected in the symmetry unbroken phase, as in the TBI($c$) phase shown in Fig. 3 (d). In Figs. 2 (c) and (f), we show the results for the local magnetic moment $m_\sigma$ ($\sigma = z, x$) at $\delta = 0.2$ and 0.8 as the function of the Hubbard interaction $U/t$, which is defined as

$$m_\sigma = \frac{2}{L} \sum_i \epsilon_i \langle S_i^\sigma \rangle = \frac{1}{L} \sum_p \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \text{Tr}[\sigma^\sigma G(p, i\omega)],$$

(5)

where $G$ is the single-particle Green function $G = (G_0 - \Sigma')^{-1}$ calculated in VCA and $L$ is the total number of lattice sites.

Next, let us consider the topological properties in our model based on the calculated topological numbers [41, 42]. In our calculation, we use the Chern number $N_{\text{ChN}} = N_\uparrow + N_\downarrow$ and spin Chern number $N_{\text{SchN}} = (N_\uparrow - N_\downarrow)/2$, where $N_\sigma$ ($\sigma = \uparrow, \downarrow$) can be obtained as

$$N_\sigma = \frac{\epsilon_{\mu\nu}}{24\pi^2} \int d^3 p \text{tr} [P_\sigma G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\nu G^{-1}]$$

$$= \frac{\epsilon_{\mu\nu}}{6V} \sum_p \int_{-\infty}^{\infty} d\omega \text{tr} [P_\sigma G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\nu G^{-1}],$$

(6)

where $P_\sigma$ is the projection operator for spin $\sigma$ that satisfies $P_\uparrow + P_\downarrow = 1$ and $P_\uparrow - P_\downarrow = \sigma_z$, and we use the notations $\partial_\mu = \partial/\partial p^\mu, p^\mu = (p, i\omega)$, Levi-Civita symbol $\epsilon_{\mu\nu}$, and $V = (3\sqrt{3}/4)L$. We should note that the topological invariants such as the Chern number and spin Chern number given above are quantized as long as the particle number and $z$-component of the total spin are conserved, respectively. Therefore, if the system does not have the spin rotational symmetry that conserves the $z$-component of the total spin, the spin Chern number has an ill-defined value as shown in Fig. 3 (a). Moreover, from the view point of the topological invariants given above, it is shown that some topological phase transitions are realized in the fermionic system, which correspond to zeros and poles of the Green function. The latter can in particular be understood as the bulk-gap closing. The former-type topological phase transition has recently been reported in the DMRG study of the one-dimensional fermionic system [43].

Figures 3 (a) and (b) show the results for the Chern number $N_{\text{ChN}}$ and spin Chern number $N_{\text{SchN}}$ calculated at $\delta = 0.2$ and 0.8. Note that the values of the Weiss fields optimized by VCA are used in this calculation. In Fig. 3(a), we confirm that the spin Chern number changes from one to zero with the topologically trivial values at $U/t > 3.37$, which corresponds to the magnetic transition point of the $xy$AF.
Calculated spin Chern number $N_{\text{SCN}}$ and Chern number $N_{\text{ChN}}$ as a function of $U/t$ at (a) $\delta = 0.2$ and (b) 0.8. The Weiss-field $h_x$ dependences of $N_{\text{SCN}}$ and $N_{\text{ChN}}$ at $\delta = 0.55$ and $U/t = 3.97$ are also shown in (c). The calculated ground-state phase diagram of our model on the $U/t - \delta$ plane is shown in (d), where the abbreviations are $xy\text{AF}$ ($xy$-plane antiferromagnetic phase), $z\text{AF}$ ($z$-axis antiferromagnetic phase), TBI($h$) (topological band insulator with helical edge states), TBI($c$) (topological band insulator with chiral edge states) and AFTI (antiferromagnetic topological insulator).

This change in the spin Chern number corresponds to the topological phase transition due to the symmetry breaking in the conservation of the $z$ component of the total spin, and therefore, the topologically nontrivial phase becomes topologically trivial at $U/t = 3.37$. This result is similar to the result of the original Kane-Mele-Hubbard model without mass imbalance. In particular, it is also suggested in Ref. [44] that the topologically nontrivial phase in the original model is destroyed by the breaking of both the time-reversal symmetry and total-spin conservation. In other words, if the system does not have the time-reversal symmetry, the topologically nontrivial spin Chern insulator phase and trivial band insulator phase are connected with each other without the gap closing in the presence of the spin-rotational symmetry-breaking term such as the Rashba interaction $\sum_i c_i^\dagger e_z \cdot (\sigma_{\alpha\beta} \times D)c_{i\beta}$. In Fig. 3(b), on the other hand, we confirm the presence of two topological phase transitions at $U/t = 2.55$ and 4.22. The transition at $U/t = 2.55$ demonstrates the existence of the topological phase transition between the two topologically nontrivial phases, i.e., the topological band insulator state with the helical edge states (TBI($h$)) and the topological band insulator state with the chiral edge states (TBI($c$)), which occurs due to the “spin-selective Mott transition” driven by the mass imbalance [32, 33, 34, 35]. The transition at $U/t = 4.22$ is between the antiferromagnetic topological insulator (AFTI) state and topologically trivial antiferromagnetic ($z\text{AF}$) state, where we find that the topological phase transition is absent at the magnetic transition point of the $z\text{AF}$ phase. Thus, at $\delta = 0.8$, the topological phase has the intermediate state where the topological phase coexists with the magnetic order. Such a large difference between the cases at $\delta = 0.2$ and 0.8 is due to the result of the symmetry protection of the topological phases.

To see the character of the intermediate phase, we show in Fig. 3(c) the results for the spin Chern number and Chern number as a function of the spin-rotational symmetry-breaking Weiss field $h_x$.\[\text{Figure 3.}\]
calculated for the TBI($c$) phase ($\delta = 0.55$). Here, we find that the Chern number has the topologically nontrivial value whereas the spin Chern number has the topologically trivial value. Therefore, we can confirm that the TBI($c$) phase is a topological phase that is realized regardless of the absence of the total-spin conservation, and therefore that the intermediate state in Fig. 3(b) is realized as the integer quantum Hall effect.

Finally, let us present the calculated ground-state phase diagram of the asymmetric Kane-Mele-Hubbard model, which is illustrated in Fig. 3(d). We find that the phase diagram consists of five phases, which can be classified by the Landau’s symmetry breaking phases (xyAF and zAF), topologically nontrivial phases (TBI($c$), TBI($h$)) and intermediate state (AFTI). We should note here that the intermediate state between the TBI($c$) and xyAF phase cannot appear in our model due to the first-order transition [see the solid line in Fig. 3(d)] even though the xyAF phase does not destroy the topological phase.

4. Summary
We have employed the method of VCA to investigate the effects of the mass imbalance on the Kane-Mele-Hubbard model. By calculating the local magnetic moment and topological quantum numbers, we have elucidated the fact that the mass imbalance introduces the spin anisotropy in the magnetic structure and induces the topological phase transition as a result of the spin-selective Mott transition. We have furthermore demonstrated that the intermediate phase between the topological band insulator phase with the chiral edge state TBI($c$) and the intermediate state between the TBI($c$) and xyAF phase is realized as the integer quantum Hall effect.

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