Magnetic Orders of Correlated Topological Insulators at Finite Temperature

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In this paper, we study the magnetic orders of two dimensional correlated topological insulators including the correlated Chern insulator and the correlated $Z_2$ topological insulator at finite temperature. For the 2D correlated Chern insulator, we found that thermal-fluctuation-induced magnetic order appears in the intermediate interaction region of the correlated Chern insulator. On the contrary, for the correlated $Z_2$ topological insulator there doesn’t exist the thermal-fluctuation-induced magnetic order. In the end, we give an explanation on the difference.

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In recent years, the physics community has witnessed a series of exciting discoveries. Among them, topological insulator (TI) is quite impressive and has become a rapidly-developing field. As the first example, the integer quantum Hall (IQH) effect is a remarkable achievement in condensed matter physics. To describe the IQH effect, the Chern number or so called TKNN number, $C$, is introduced by integrating over the Brillouin zone (BZ) of the Berry field strength. So, this type of topological insulator with IQH effect is called the Chern insulator. Recently, a new class of topological insulator with time-reversal symmetry is discovered with the quantized spin quantum Hall (IQH) effect is a remarkable achievement. For the 2D correlated Chern insulator, of which the Hamiltonian is

$$H = H_H + H' + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{\langle i,\sigma \rangle} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} + h.c. \quad (1)$$

where $H_H$ is the Hamiltonian of the spinful Haldane model on a honeycomb lattice which is given by

$$H_H = -t \sum_{\langle i,j \rangle,\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c.) - t' \sum_{\langle \langle i,j \rangle \rangle,\sigma} e^{i\phi_{ij}} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}. \quad (2)$$

Here $t$ and $t'$ are the nearest neighbor (NN) hopping and the next-nearest neighbor (N NN) hopping, respectively. There exists a complex phase $\phi_{ij}$ into the NNN hopping which is set to be the direction of the positive phase clockwise $|\phi_{ij}| = \frac{\pi}{3}$. $H'$ denotes an on-site staggered energy which is $H' = \varepsilon \sum_{i \in A, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} - \varepsilon \sum_{i \in B, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$. $U$ is the on-site Coulomb repulsion strength. $(i,j)$ and $\langle \langle i,j \rangle \rangle$ denote two sites of the NN and the NNN links, respectively. $\hat{n}_{i\uparrow}$ and $\hat{n}_{i\downarrow}$ are the number operators of electrons with up-spin and down-spin respectively. $\mu$ is the chemical potential and $\mu = U/2$ at half-filling for our concern in this paper.

For free electrons, $U = 0$, we can see that there exist energy gaps $\Delta_{f1}$, $\Delta_{f2}$ near the two Dirac points $k_1 = -\frac{2\pi}{3}(1, 1/\sqrt{3})$ and $k_2 = \frac{2\pi}{3}(1, 1/\sqrt{3})$ as $\Delta_{f1} = |2\varepsilon - 6\sqrt{3}t'|$ and $\Delta_{f2} = 2\varepsilon + 6\sqrt{3}t'$, respectively. There exist two phases separated by the phase boundary $\Delta_{f1} = 0$: the Chern insulator with Chern number $C = 2$ and the normal band insulator (NI) state. In the Chern insulator, due to the quantum anomalous Hall (QAH) effect with a quantized (charge) Hall conductivity $\sigma_H = 2e^2/h$, we denote the Chern insulator by "QAH".

Mean field approach: With the increasing of the interaction, the correlated Chern insulator is unstable against an antiferromagnetic (AF) spin-density-wave (SDW) which is described by $\langle \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \rangle = \frac{1}{2}[1 + (-1)^i \sigma M]$ where the local order parameter $M$ is the staggered magnetization. We set $\sigma = +1$ for spin up and $\sigma = -1$ for spin down.

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Using the mean-field approach, we can obtain the self-consistent equation for \( M \) by minimizing the free energy at finite temperature in the reduced Brillouin Zone (BZ):

\[
1 = \frac{1}{N_s M} \sum_k \frac{\xi_k + \varepsilon + \Delta_M}{2E_{1,k}} \tanh(\beta E_{1,k}/2) - \frac{\xi_k + \varepsilon - \Delta_M}{2E_{2,k}} \tanh(\beta E_{2,k}/2))
\]

where \( N_s \) is the number of unit cells, \( \beta = 1/k_B T \) and \( \Delta_M = UM/2 \). Then the energy spectrums of electrons are \( E_{1,k} = \sqrt{(\xi_k + \varepsilon + \Delta_M)^2 + |\xi_k|^2} \) and \( E_{2,k} = \sqrt{(\xi_k + \varepsilon - \Delta_M)^2 + |\xi_k|^2} \) where

\[
\xi_k = t \sqrt{3 + 2 \cos(\sqrt{3}k_y) + 4 \cos(3k_x/2) \cos(\sqrt{3}k_y/2)}
\]

\[
\xi_k' = 2t' (\sin(\sqrt{3}k_y) - 4 \cos(3k_x/2) \sin(\sqrt{3}k_y/2)).
\]

**Phase diagram at finite temperature:** To determine the phase diagram at finite temperature, there exist two types of phase transitions: one is the "magnetic" phase transition that separates the magnetic order state with \( M \neq 0 \) and the nonmagnetic state with \( M = 0 \) (solving the Eq. (3)), the other one is the "topological" phase transition that is characterized by the condition of zero fermion-energy gaps, \( \Delta_f = | -6\sqrt{3}t' + 2\varepsilon \pm 2\Delta_M | = 0 \) (see the black lines in Fig. 1). In Fig. 1, the colors show the energy gap of the electrons. After determining the phase boundaries, we get the phase diagram at finite temperature in Fig. 1 for the parameters of \( t'/t = 0.15, \varepsilon = 0.15t \).

From Fig. 1, we can see that for the 2D correlated Chern insulator there exist four phases: Chern insulator (QAH), A-TSDW (TSDW with Chern number \( C = 2 \)), B-TSDW (TSDW with Chern number \( C = 1 \)) and trivial AF-SDW. The Chern insulator exists in the weak-interaction region. With the increasing of \( U/t \), the system turns into A-TSDW state. After the electron’s energy gap is closed at one Dirac point, the system turns into B-TSDW state. With the interaction strength further increasing, the electron’s energy gap is closed at another Dirac point and the system turns into a trivial AF-SDW state.

In the phase diagram, we find an interesting phenomenon: the thermal-fluctuation-induced magnetic order. From Fig. 1, there exists a magnetic order at finite temperature for about \( U/t = 3.5 \) during the temperature \( T/t = 0.1 \sim 0.5 \) [19]. In Fig. 2, we plot the staggered magnetization \( M \) with the increasing of temperature via the interaction strengths \( U \) for the case of \( t'/t = 0.15, \varepsilon = 0.15t \). From Fig. 2, we can see that at \( U/t = 3.5 \) (the black line), the staggered magnetization \( M \) is zero at low temperature. But at higher temperature, the staggered magnetization \( M \) becomes nonzero and has the maximum value at \( T/t \approx 0.25 \) and then with the further increasing of temperature the staggered magnetization \( M \) becomes smaller and smaller down zero. Thus, this magnetic order at finite temperature is assisted by the thermal fluctuations.

Let’s give a brief explanation on the existence of the thermal-fluctuation-induced magnetic order. At zero temperature, the density of state (DOS) inside the energy gap vanishes. At finite temperature, due to the thermal fluctuations, the density of state (DOS) inside the energy gap increases that may help the establish the magnetic
In Fig. 3, we plot the DOS at different temperatures for the case of $U/t = 3.5$, $t'/t = 0.15$, $\varepsilon = 0.15$.

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From Fig. 3, we can see that with the increasing of the temperature, at first the magnetization increase, then the gap of the system becomes bigger again. This result is confirmed by the results of the energy gap in Fig. 4(a) at $U/t = 3.5$. In Fig. 4(b) and (c), we also give the energy gap for $U/t = 3.65$ and 4.0 for different temperatures for the case of $t'/t = 0.15$, $\varepsilon = 0.15t$.

The "topological" phase transition at finite temperature: A related issue is about "topological" phase transition at finite temperature. To check whether there exists true topological phase transition at finite temperature, we calculate the Hall conductivity and the special heat.

We use the Kubo formula to derive the Hall conductivity $\sigma_H = \lim_{\omega \to 0} \frac{i\omega}{\omega} Q_{xy}(\omega + i\delta)$ where

$$Q_{xy}(i\nu_m) = \frac{1}{N_s\beta} \sum_{k,n} \text{tr}[J_x(k)G(k,i(\omega_n + \nu_m))]$$

with the current operator $J_{x/y}(k) = \frac{\partial H(k)}{\partial k_{x/y}}$ and $G(k,i\omega_n)$ is the Matsubara Green function, $\sigma$ is the spin index. In Fig. 5, we show the Hall conductivity $\sigma_H$ via the interaction for the case of $t'/t = 0.15$, $\varepsilon = 0.15t$. At zero temperature, we can use the Hall conductivity to characterize the topological properties of the system. There exist three plateaus of the Hall conductivity: $\sigma_H = 2e^2/h$ in the Chern insulator (QAH) and A-TSDW, $\sigma_H = e^2/h$ in B-TSDW, $\sigma_H = 0$ in trivial AF-SDW. At finite temperature, the situation changes. From Fig. 5, we can see that at finite temperature, the Hall conductivity $\sigma_H$ smoothly changes with the interaction and the temperature and the plateaus of the Hall conductivity are smeared out. That means there is no true "topological" phase transition at finite temperature.

In addition we calculate the special heat at finite temperature and also don’t find the true "topological" phase transition.

The correlated Kane-Mele model at finite temperature: Next we study the 2D correlated Z_2 topological insulator. Our start point is the correlated Kane-Mele (KM) model which is described by [11,17]

$$H = H_{KM} + H' + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i$$

where $H_{KM}$ is the Hamiltonian of the KM model which
is given by

$$H_{KM} = -t \sum_{\langle i,j \rangle} \left( \hat{c}_i^\dagger \hat{c}_j + \text{h.c.} \right) - t' \sum_{\langle i,j \rangle} \epsilon^{i\phi_{ij}} \hat{c}_i^\dagger \hat{c}_j, \tag{7}$$

and $H'$ denotes an on-site staggered energy which is

$$H' = \varepsilon \sum_{i \in A, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} - \varepsilon \sum_{i \in B, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}. \tag{7}$$

Here we set the on-site staggered energy $\varepsilon$ to be 0.15t.

Without the spin rotation symmetry, the staggered magnetic order is along XY-plane. In this paper we take a staggered magnetic order along X-direction as an example. Now we get the self-consistency equation for $M$ by minimizing the free energy at temperature $T$ in the reduced Brillouin zone as

$$1 = \frac{1}{2N_{\text{s}}} \sum_k \frac{U}{2} \left\{ \frac{1 + \varepsilon (\Delta^2_m + \xi_k^2)^{-\frac{1}{2}}}{-E_{1,k}} \tanh \left( \frac{\beta E_{1,k}}{2} \right) + \frac{1 - \varepsilon (\Delta^2_m + \xi_k^2)^{-\frac{1}{2}}}{-E_{2,k}} \tanh \left( \frac{\beta E_{2,k}}{2} \right) \right\}, \tag{8}$$

where $E_{1,k} = -\sqrt{(\Delta^2_m + \xi_k^2 + \varepsilon)^2 + |\xi_k|^2}$, $E_{2,k} = -\sqrt{(\Delta^2_m + \xi_k^2 - \varepsilon)^2 + |\xi_k|^2}$ and $\Delta_M = UM/2$.

In the phase diagram of correlated KM model, there only exists one phase transition: the magnetic phase transition between a magnetic order state with $M \neq 0$ and a nonmagnetic state with $M = 0$ (solving the Eq. (8)). In Fig. 6, we plot the phase diagram for the case of $t'/t = 0.15$, $\varepsilon = 0.15t$. From the phase diagram, we can see that there exist two phases: the $Z_2$ topological insulator with $M = 0$ and trivial AF-SDW state with $M \neq 0$. In the $Z_2$ topological insulator, due to the nonzero $Z_2$ topological invariant, there exists the quantum spin Hall (QSH) effect. In this paper we denote the $Z_2$ topological insulator by "QSH". From Fig. 6, we can see that the energy gap will be never closed. And there doesn’t exist the thermal-fluctuation-induced magnetic order.

**Discussion and conclusions:** Finally, we discuss why the properties of the correlated Chern insulator are much difference from those of the correlated $Z_2$ topological insulator.

For the SDW order in the correlated Chern insulator, the effective Hamiltonian becomes

$$H_0 = v_F p \cdot \alpha + (m_T + m_M + \varepsilon) \beta \tag{9}$$

where $p_i = -i\hbar \nabla_i$ is the momentum operator ($i \in \{x, y\}$), $p_i^2 = p_x^2 + p_y^2$, $v_F$ is the Fermi-velocity. There exist two mass matrices: the mass matrix of the parent topological insulator $m_T = 3\sqrt{3}/2 \eta_2 \otimes I_2$ and the mass matrix from the SDW order $m_M = \Delta_M (I_2 \otimes \sigma_1)$, respectively. Here $\tau$, $\sigma$, and $\eta$ are Pauli matrices that denote the indices of the sublattice, spin, node, respectively. $I_2$ is the 2 x 2 unit matrix, and $\otimes$ represents the Kronecker product. The Dirac matrices can be expressed as a set of 4 x 4 matrices $\alpha_i = \tau_i \otimes I_2$, $\beta = \tau_3 \otimes I_2$. Here we set the on-site staggered energy $\varepsilon$ to be 0.15t. Due to $[m_T, m_M] = 0$, we have the energy gap of the electrons to be $\Delta_f = 2 |\pm m_T + m_M - 2\varepsilon| = |\pm 6\sqrt{3} + 2\Delta_M - 2\varepsilon|$. Thus, the energy gap from the magnetic order $m_M$ competes with that from the parent topological insulator $m_T$. Therefore, we call this system the mass-gap-competition. When we have a small staggered magnetization (or a small $\Delta_M$), the energy gap of the electrons shrinks. With increasing the staggered magnetization, the energy gap will eventually close at the critical point $\Delta_f = 0$. At finite temperature, the thermal fluctuations will excite the quasiparticle and may also smear out the energy gap. Thus, due to the suppression of the energy gap of the parent topological insulator, the magnetic order may be assisted by thermal fluctuations.

For the SDW order in the correlated KM model, the effective Hamiltonian becomes

$$H_0 = v_F p \cdot \alpha + (m_T + m_M + \varepsilon) \beta \tag{10}$$

where the mass term of the parent topological insulator is $m_T = -3\sqrt{3}/2 \eta_3 \otimes \sigma_3$ and the mass term from the SDW order is $m_M = \Delta_M (I_2 \otimes \sigma_1)$, respectively. Due to $\{m_T, m_M\} = 0$, we have the energy gap of the electrons to be $\Delta_f = |\pm 2\sqrt{[m_T]^2 + [m_M]^2 - 2\varepsilon}| = |\pm 2\sqrt{(6\sqrt{3})^2 + |\Delta_M|^2 - 2\varepsilon}|$. From the $Z_2$ topological insulator state of the correlated KM model ($(6\sqrt{3}) - 2\varepsilon > 0$), there exists the magnetic order along XY plane, the energy gap of the electrons will definitely...
increase. Therefore, the energy gap will never close in the magnetic order. Therefore, we call this system the mass-gap-coexistence. The suppression of the energy gap of the parent topological insulator will not help the formation of the magnetic order. Thus, there is no thermal-fluctuation-induced magnetic order in the $Z_2$ topological insulator of the correlated KM model.

At the end of the paper, we generalize the results in the correlated topological insulators to a long range order developed in an insulator. For the long range orders developed in an insulator, there are two different cases: case I, the mass-gap-competition; case II, the mass-gap-coexistence. For case I, the mass gap induced by a long range order $m_O$ competes with the mass gap in the parent insulator $m_T$. Now we have $[m_T, m_M] = 0$ and the energy gap of the system is $\Delta_f = 2|m_T \pm m_M|$. For this case, there may exist the thermal-fluctuation-induced order.

For case II, the mass gap induced by a long range order $m_O$ coexists with the mass gap in the parent insulator $m_T$. Now we have $\{m_T, m_M\} = 0$ and the energy gap of the system is $\Delta_f = 2\sqrt{|m_T|^2 + |m_M|^2}$. For this case, there doesn’t exist the thermal-fluctuation-induced order.

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[19] For the 2D correlated topological insulator with spin rotation symmetry, there is no true long range SDW order at finite temperature. Here, A-TSDW, B-TSDW, trivial AF-SDW orders at finite temperature are all short range magnetic orders. If we consider a quasi-2D system with weakly interlayer coupling, the short range magnetic order may turn into true long range order.
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