Short-ranged interaction effects on $Z_2$ topological phase transitions:
The perturbative mean-field Hartree-Fock method

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Time-reversal symmetric topological insulator is a novel state of matter that a bulk-insulating state carries dissipationless spin transport along the surfaces, embedded by the $Z_2$ topological invariant. In the noninteracting limit, this exotic state has been intensively studied and explored with realistic systems, such as HgTe/(Hg,Cd)Te quantum wells. On the other hand, electronic correlation plays a significant role in many solid-state systems, which further influences topological properties and triggers topological phase transitions. Yet an interacting topological insulator is still an elusive subject, and most related analysis are relied on the Hartree-Fock approximation and numerical simulations. Among the approaches, the Hartree-Fock approximation fails to predict the topological phase transition, in particular at intermediate interaction strength without spontaneously breaking symmetry. In this review, we develop an analytical approach based on a combined perturbative and self-consistent mean-field treatment of interactions that is capable of capturing topological phase transitions beyond either method when used independently. As an illustration of the method, we study the effects of short-ranged interactions on the $Z_2$ topological insulator phase, also known as the quantum spin Hall phase, in three generalized versions of the Kane-Mele model at half-filling on the honeycomb lattice. The results are in excellent agreement with quantum Monte Carlo calculations on the same model, and cannot be reproduced by either a perturbative treatment or a self-consistent mean-field treatment of the interactions. Our analytical approach helps to clarify how the symmetries of the one-body terms of the Hamiltonian determine whether interactions tend to stabilize or destabilize a topological phase. Moreover, our method should be applicable to a wide class of models where topological transitions due to interactions are in principle possible, but are not correctly predicted by either perturbative or self-consistent treatments.

Keywords: Topological Insulator; Topological Invariants; Topological Phase Transition; Quantum Monte Carlo Simulation; Strongly Correlated Electrons.

1. Introduction

The birth of the topological insulators (TI) in recent years has been one of the most exciting events in condensed matter and material science fields due to their novelty and poten-
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tial technological applications\textsuperscript{1,2,3,4,5,6}. Shortly after the theoretical prediction\textsuperscript{7}, the first experimental realization of a time-reversal symmetry (TRS) protected TI was reported in HgTe/(Hg,Cd)Te quantum well\textsuperscript{8,9}. Though in all the accepted experimental examples of TI to date, the presence of the topological state and most of its properties can be well understood within a noninteracting model, it is, however, generally believed that interactions can lead to qualitatively new topological phenomena in both two\textsuperscript{10,11,12,13,14,15,16} and three dimensions\textsuperscript{17,18,19,20,21,22,23}. In two-dimensions, the Kane-Mele (KM) model\textsuperscript{24} has played an especially important role in the study of $Z_2$ TI [also known as quantum spin Hall insulators (QSH)]. The KM model consists of two time-reversed copies of the Haldane model\textsuperscript{25} on a two-dimensional (2D) honeycomb lattice, with real first-neighbor hopping and imaginary second-neighbor hopping arising from spin-orbit coupling (SOC). To study interaction effects, the KM model has been supplemented with an onsite Hubbard $U$-term

$$H_U = U \sum_i n_i \uparrow n_i \downarrow,$$

where $n_{i\sigma}$ is the number of electrons on site $i$ with spin $\sigma$. The so called Kane-Mele-Hubbard (KMH) model is investigated extensively\textsuperscript{26,27,28,29,30,31,32,33,34} particularly with quantum Monte Carlo (QMC) which is free of the fermion sign problem\textsuperscript{28,29,32,34}. Its phase diagram is now well understood. Beyond the critical value of interaction strength $U_c$, there exists a magnetic phase transition which turns a topological state to an easy-plane antiferromagnetic order state.

Recently, several fermion sign-free extensions of the KMH model have been proposed and studied with QMC\textsuperscript{35,36} with the goal of understanding short-ranged interaction effects on the hopping-parameter-driven $Z_2$ topological phase transitions at half-filling and at intermediate interaction, i.e. $U < U_c$. The numerical results concluded that the onsite Hubbard interaction leads either to stabilize the QSH against the parameter that drives the $Z_2$ topological phase transition from a topological insulating phase to a trivial insulating phase or to destabilize it by making it more fragile to the parameter. Though the $Z_2$ topological phase transitions have been examined using QMC, there has been no proposal of an “analytically” physical picture that captures the numerical results. Most important of all, without symmetry breaking, the conventional Hartree-Fock approximation in some cases does not provide any correction to realize the topological boundary shifts observed in QMC.

In this brief review article, we propose an analytical method, dubbed perturbative mean-field Hartree-Fock (PMFHF) method, which combines the perturbative treatment and the mean-field Hartree-Fock treatment. For pedagogy and illustrating the power of a general analytical framework we introduce, we study three variants of KMH–generalized Kane-Mele model (GKM), dimerized Kane-Mele model (DKM), and stagger-potential Kane-Mele model (SKM) described by Eq. (3), Eq. (9) and Eq. (15), supplemented by a Hubbard-$U$ term Eq. (1).

The GKM and DKM models preserve the discrete particle-hole symmetry (PHS) and therefore the stability of the topological phase can be addressed by exact QMC. For interaction strengths below the regime of magnetic instabilities, the QMC results show that the

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Fig. 1. (a) Schematic of the honeycomb lattice with two sublattices labeled $A$ and $B$. The vectors $e_{1/2} = (\pm 1/2, \sqrt{3}/2)$ connect the same sublattice in different unit cells. The lattice constant $a$ is set to 1. (b) Illustration of the Brillouin zone (B.Z.). There are several relevant momenta that are important in the low-energy descriptions of variants of KM models—The usual momenta $K = -K' = (4\pi/3, 0)$ as the locations of the Dirac nodes in the original KM model and the time-reversal-invariant momenta (TRIM) $M_{1,2} \equiv (\pm \pi, \pi/\sqrt{3})$ and $M_3 \equiv (0, 2\pi/\sqrt{3})$. Note that $M_1$ and $M_2$ are related by $C_3$ lattice rotation symmetry. $G_1$ and $G_2$ are the reciprocal lattice vectors.

interactions produce a shift in the location of the phase boundary (opposite directions for the two models). On the other hand, the SKM model breaks PHS and therefore in the positive $U$ side, QMC suffers from the sign problem. Nevertheless, our PMFHF method is general and can be applied to the three different models above regardless of the sign of the interaction. We find that the sign of the shifts and their scaling-law with respect to the interaction strength in the three different models are accurately reproduced by the combination of perturbation theory and a self-consistent mean-field Hartree-Fock calculation, though they are not captured by either one independently. Our results emphasize that short-range interactions can have subtle effects on the stability of topological phases, and may need to be treated by a method analogous to that we use here when other approaches are not available or desirable.

The review article is organized as follows. In Sec. 2 we introduce three variants of the KM models, their low-energy descriptions, and $Z_2$ topological phase transitions in the non-interacting limit. In Sec. 3 we introduce the perturbative mean-field Hartree-Fock method and apply the method to different models followed by self-consistent numerical calculations. In Sec. 4 we present the exactly QMC results and show the consistency between these two approaches. In Sec. 5 we include several relevant discussions, including RG analysis and a more extended $U - V$ interaction effects on the SKM models. In Sec. 6 we conclude with some future perspective of our general analytic method.

2. Variants of the Kane-Mele model and the topological phase transitions in the non-interacting limit

The KM model is one of early proposed models to harbor QSH. In the non-interacting limit, the original KM model consists of real-valued first-neighbor hoppings, $t$, and imaginary second neighbor hoppings, $\lambda_{sa}$. The schematic of the honeycomb lattice with two
sublattices (\(A\) and \(B\)) and the corresponding relevant Brillouin zone (B.Z.) are shown in Fig. 1. Each spin component contributes chirality in the honeycomb lattice, to produce a nontrivial quantum anomalous Hall effect as known in the Haldane model. However, the opposite spin flavor carries opposite chirality, and contributes opposite sign spin Chern number \(C_{\uparrow} = -C_{\downarrow} = 1\). Therefore the system is time-reversal symmetric and total Chern number \(\sum_{\sigma} C_{\sigma} = 0\). The intrinsic topological invariant of topological insulators and QSH is the \(\mathbb{Z}_2\) invariant, \(\nu = 1\) or \(\nu = 0\). With an inversion symmetry, it can be easily evaluated as

\[
(-1)^\nu = \prod_{k \in \text{TRIM}} \prod_n \xi_{2n}(k),
\]

where \(\xi_{2n}(k) = \pm 1\) is the parity of the occupied eigenstates of the noninteracting Hamiltonian at TRIM points. In the KM model, the TRIM points are \(\Gamma = (0, 0)\) and \(M_{1,2,3}\) as shown in Fig. 1(b). Note that due to the presence of time-reversal symmetry, \(\xi_{2n-1}\) and \(\xi_{2n}\) have the same parity. \(\nu = 1\) \((\nu = 0)\) denotes a nontrivial (trivial) state.

In this review article, we will focus on the short-ranged interaction effects on three variants of the KM model at half-filling on the honeycomb lattice. The three variants are what we mentioned in the Introduction section– GKM, DKM, and SKM. The GKM includes real-valued third neighbor hoppings in addition to the original KM model, as illustrated in Fig. 2(a) while the DKM consists of anisotropic hoppings with hopping strength \(t_d\) within a unit cell larger than those between different unit cells, Fig. 3(a). The SKM includes staggered potentials in addition to the Hamiltonian in KM model, Fig. 4(a). From the symmetry perspective, both GKM and DKM conserve the PHS, but DKM explicitly breaks the lattice \(C_3\) rotation symmetry by the center of a honeycomb while GKM still preserve \(C_3\). The SKM, unlike GKM and DKM, explicitly breaks PHS even at half-filling condition due to the presence of the staggered potential. Below we will give the non-interacting description of each model separately.

### 2.1. Generalized Kane-Mele Model

The GKM Hamiltonian is

\[
H_G = -\sum_{jk} \sum_{\sigma} t_{jk} c_{j\sigma}^\dagger c_{k\sigma} + i\lambda_{so} \sum_{\langle\langle\langle jk \rangle\rangle\rangle} \sum_{\sigma} \sigma c_{j\sigma}^\dagger \nu_{jk} c_{k\sigma},
\]

with \(t_{jk} = t\) for \(j, k \in \langle jk \rangle\), \(t_{jk} = t_3\) for \(j, k \in \langle\langle jk \rangle\rangle\), and zero else, where \(\langle\langle\langle\rangle\rangle\rangle\) represent the nearest neighbors, the second neighbors, and the third neighbors. \(\nu_{jk} = +1(-1)\) for (counter-)clockwise second-neighbor hopping and without lack of generality, we choose \(t, \lambda_{so}, t_3 > 0\). \(\sigma = \uparrow(\downarrow) = +(-)\). The operator \(c_{i\sigma}^\dagger (c_{i\sigma})\) creates (annihilates) an electron on site \(i\) with spin \(\sigma\). The schematic is shown in Fig. 2(a).

For clarity, from here forward we replace the site labeling \(j\) with \(j = \{r, a\}\), where \(r\) runs over the Bravais lattice of unit cells of the honeycomb network and \(a\) runs over the two sites \((A\) and \(B)\) in the unit cell shown in Fig. 1(a). The GKM can be expressed in momentum
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Fig. 2. (a) Schematic of the GKM model and (b) the band spectrums at the topological phase transition (gap closing). The blue dashed lines represent the imaginary second neighbor hoppings and the arrow directions represent their signs. The red lines represent the $t_3$ hoppings. At the phase transition point, the bands gaps close at three TRIM $M_a = 1, 2, 3$, unlike the usual KM model.

space as

$$H_G = \sum_{k \in B.Z.} \Psi_k^\dagger \cdot h_G \cdot \Psi_k = \sum_{k \in B.Z.} \Psi_k^\dagger \begin{pmatrix} 0 & -tf(k) - t_3 f_3(k) \\ -t^* f^*(k) & 0 \end{pmatrix} \otimes I_{2 \times 2} + \begin{pmatrix} 2\lambda_{so}g(k) & 0 \\ 0 & -2\lambda_{so}g(k) \end{pmatrix} \otimes \sigma_z \Psi_k \equiv \sum_{k \in B.Z.} \Psi_k^\dagger [M_G(k) \otimes I_{2 \times 2} + 2\lambda_{so}g(k) \tau_x \otimes \sigma_z] \Psi_k,$$

where $\Psi_k^T \equiv (\Psi_k^T \Psi_k^T) = (c_k(A) c_k(B) c_k(A) c_k(B))$. $\sigma_z$ and $\tau_x$ are Pauli matrices for spin and sublattice degrees of freedom. $g(k) \equiv - \sin(k \cdot e_1) + \sin(k \cdot e_2) + \sin(k \cdot (e_1 - e_2)), f(k) = 1 + e^{i k \cdot e_1} + e^{i k \cdot e_2}, f_3(k) = e^{i k \cdot (e_1 + e_2)} + 2 \cos[k \cdot (e_1 - e_2)].$

The B.Z. is shown in Fig. 1(b). In the KM-type models that we consider, only a few momentum points that are relevant for the low-energy descriptions. Besides the usual wavevectors $K = -K' = (4\pi/3, 0)$ in the original KM model, the TRIM points located at $M_{1,2} \equiv (\pm \pi, \pi/\sqrt{3})$ and $M_3 \equiv (0, 2\pi/\sqrt{3})$ also need to be considered. In GKM, when we vary the third neighbor hopping strength $t_3$, we find that the band gaps close at all TRIM points, $M_a = 1, 2, 3$ as shown in Fig. 2(b) At the TRIM, the diagonal elements of the Hamiltonian matrices vanish, $g(M_a) = 0$, and the band gaps in GKM are controlled by the off-diagonal elements, which are related to real-valued first and third neighbor hoppings. Focusing on the gap closing points (TRIM), we can write down the low-energy description of GKM,

$$\mathcal{H}_G^\sigma = \Delta t_G \Psi^\sigma_{M_a} \tau_x \Psi^\sigma_{M_a}.$$
where we introduce $\Delta t_G = t - 3t_3$. The band gap of GKM is
\[ \Delta E_G = 2 |\Delta t_G|, \]  
which vanishes at $t_3^c = \frac{1}{3} t_{36}^{39,36}$. At $t_3^c$, a topological phase transition takes place, from the nontrivial QSH state with $|C_\sigma| = 1$, $\nu = 1$, to the trivial insulating state $|C_\sigma| = 2$, $\nu = 0^{39,36}$. Note that although the $|C_\sigma| = 2$ state is trivial in the $Z_2$ aspect, the state belongs to the classification of a two-dimensional topological crystalline insulator with mirror Chern number $C_m = 2$. Under such meaning, it is still topologically nontrivial\(^{39}\).

2.2. Dimerized Kane-Mele Model

Second variant of the KM model is the DKM. The model is given "dimerizing" one of nearest neighbor hoppings, and the Hamiltonian $H_D$ reads as
\[ H_D = - \sum_{(jk)} \sum_{\sigma} t_{jk} c^\dagger_{j\sigma} c_{k\sigma} + i\lambda_{so} \sum_{\langle(jk)\rangle} \sum_{\sigma} \sigma c^\dagger_{j\sigma} t_{jk} c_{k\sigma}, \]  
where $t_{ij} = t_d (t)$ if the two sites $\langle jk \rangle$ belong to the same (different) unit cell(s), and we choose $t_d (t) > 0$. The schematic of the DKM is illustrated in Fig. 3(a). Similarly, we replace the site labeling $j$ with $j = \{ r, a \}$ and the DKM can be expressed in momentum space as
\[ H_D = \sum_{\mathbf{k} \in B.Z.} \Psi^\dagger_{\mathbf{k}} \cdot h_D \cdot \Psi_{\mathbf{k}}, \]  
where $f_d(k) = e^{i\mathbf{k} \cdot \mathbf{e}_1} + e^{i\mathbf{k} \cdot \mathbf{e}_2}$. When we vary the dimerized hopping amplitude $t_d$ while fixing $t$, we find the band gap only closes at $M_3$ due to the breakdown of $C_3$ rotation as shown in Fig. 3(b). Similar to GKM, the band gap at TRIM ($M_3$) is also controlled by the off-diagonal terms since $g(M_3) = 0$. Focusing on the $M_3$, we can write down the low-energy descriptions of DKM,
\[ \mathcal{H}^\sigma_D = \Delta t_D \Psi^\dagger_{\mathbf{M}_3} \tau_x \Psi_{\mathbf{M}_3}, \]  
where $\Delta t_D = 2t - t_d$. The band gap is
\[ \Delta E_D = 2 |\Delta t_D|, \]  
which vanishes at $t_d^c = 2t$ as the critical point. Upon increasing $t_d$, the topological phase transition turns the $C_\sigma = \pm 1$ QSH state to the $C_\sigma = 0$ trivial insulating state\(^{39,36}\).
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2.3. Stagger-potential Kane-Mele Model

So far, the GKM and DKM that we have discussed both conserve the inversion symmetry as well as PHS. Now we shift our focus on the SKM which breaks inversion symmetry due to the presence of staggered potentials. The SKM Hamiltonian, $H_S$, is

$$H_S = -t \sum_{\langle jk \rangle} \sum_{\sigma} c_{j\sigma}^\dagger c_{k\sigma} + i\lambda_{so} \sum_{\langle jk \rangle} \sum_{\sigma} \sigma c_{j\sigma}^\dagger \nu_{jk} c_{k\sigma} + M \sum_j \sum_{\sigma} \epsilon_j c_{j\sigma}^\dagger c_{j\sigma},$$

with $\epsilon_j = \pm 1$ for sublattice $j \in \{A, B\}$. The schematic of SKM is shown in Fig. 4(a). We note that due to the presence of the staggered potentials, the PHS is explicitly broken. The SKM Hamiltonian can be expressed in the momentum space as

$$H_S = \sum_{\mathbf{k} \in B.Z.} \Psi_\mathbf{k}^\dagger \cdot h_S \cdot \Psi_\mathbf{k}$$

$$= \sum_{\mathbf{k} \in B.Z.} \Psi_\mathbf{k}^\dagger \left[ \begin{array}{cc} M & -tf(\mathbf{k}) \\ -tf^*(\mathbf{k}) & -M \end{array} \right] \otimes \mathbb{I}_{2 \times 2} +$$

$$\quad \quad \quad \quad + \left[ \begin{array}{cc} 2\lambda_{so}g(\mathbf{k}) & 0 \\ 0 & -2\lambda_{so}g(\mathbf{k}) \end{array} \right] \otimes \sigma_z \Psi_\mathbf{k}$$

$$\equiv \sum_{\mathbf{k} \in B.Z.} \Psi_\mathbf{k}^\dagger \left[ M_S(\mathbf{k}) \otimes \mathbb{I}_{2 \times 2} + 2\lambda_{so}g(\mathbf{k})\tau_z \otimes \sigma_z \right] \Psi_\mathbf{k},$$

where $f(\mathbf{k})$ and $g(\mathbf{k})$ are defined in GKM. While varying the strength of the staggered potentials, we find that the band gaps close at the usual locations of two independent Dirac nodes ($\mathbf{K} = -\mathbf{K}' = (4\pi/3, 0)$), Fig. 4(b). Focusing on the gap closing points, we know there are only two gapless bands (2 gapless spin-$\downarrow$ bands at $\mathbf{K}$ and 2 gapless spin-$\uparrow$ bands at $\mathbf{K}'$). Since these two bands are related by the TRS, $T : \Psi_\mathbf{k}^\sigma \rightarrow e^{i\pi \sigma} \Psi_{-\mathbf{k}}^\sigma$ with $\sigma = \uparrow (\downarrow) = 1 (2)$, we can simply focus on one spin species of fermions at one Dirac node, say $\mathbf{K}$. Fig. 3. (a) Schematic of the DKM model and (b) the band spectrum at the topological phase transition. The blue dashed lines represent the imaginary second neighbor hoppings and the arrow directions represent their signs. The red lines represent the anisotropic $t_d$ hoppings with $t_d > t$, which breaks $C_3$ rotation. At the phase transition, the band gaps only close at TRIM $M_3$ due to the breaking of $C_3$ symmetry.
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Fig. 4. (a) Schematic of the SKM model and (b) the band spectrum at the topological phase transition. (a) The red (green) dots at sublattice \( A(B) \) represent the staggered potential strength \( M(-M) \). The blue dashed lines represent the imaginary second neighbor hoppings and the arrow directions represent their signs. (b) At the phase transition point, the bands gaps close at the usual locations of Dirac nodes, \( (\mathbf{K} = -\mathbf{K}' = (4\pi/3, 0)) \). The rest of the Dirac cones are related by \( C_3 \) rotation.

Focusing on \( \mathbf{K} \), we can write down the effective low-energy description as

\[
\mathcal{H}_{\text{SKM}}^\uparrow(\mathbf{K}) = \psi_{\mathbf{K}}^\dagger \begin{pmatrix} M - 2\lambda_{so}(\mathbf{K}) & 0 \\ 0 & -M + 2\lambda_{so}(\mathbf{K}) \end{pmatrix} \psi_{\mathbf{K}}^\dagger. \tag{18}
\]

Therefore, the band gap of SKM is

\[
\Delta E_{\text{SKM}} = 2|M - 2\lambda_{so}(\mathbf{K})|. \tag{19}
\]

We know \( \lambda_{so}(\pm\mathbf{K}) = \frac{3\sqrt{3}}{2}t \) and the gap closes at \( M' = \sqrt{3}\lambda_{so} \) in the non-interacting limit. Similar to the DKM variant, the topological phase transition turns the QSH state to a topologically trivial state with \( |C_\sigma| = 0 \).

3. \( U/t \) expansion and mean-field Hartree-Fock decouplings

Next we start the discussions of correlation effects on the QSH state. The simplest correlation effect is considered by studying the variants of KMH Hamiltonian \( H = H_{G,D,S} + H_U \), where \( H_U \) represents the short-ranged Hubbard interaction, Eq. (1). According to the low-energy descriptions for the three variants of KM models, Eqs. (7) and (13) for GKM and DKM, and Eq. (18) for SKM, first we notice that the gaps for GKM and DKM vanish at the TRIM, unlike the usual KM model, and are controlled by the off-diagonal elements describing the hoppings between different sublattices. On the other hand, the gaps for SKM vanish at the usual momenta \( \mathbf{K} \) and \( \mathbf{K}' \), and are controlled by the diagonal elements describing the more ordinary mass terms consisting of staggered potentials and the second-order hoppings (SOC). As far as the mechanism for the topological phase boundary shifts due to the presence of the short-range Hubbard interaction is concerned, we should distinguish the SKM from GKM and DKM. From the symmetry perspective, GKM and DKM both satisfy PHS while SKM breaks PHS. We will discuss these two different cases separately in the following two subsections.
The conventional Hartree-Fock approximation performs the series expansion in $U/t$ up to first-order,
\[ O(U/t) \]
\[ U \sum_{\text{all site}} n_{i\uparrow} n_{i\downarrow} \simeq \frac{U}{2} \sum_{\text{r},a=A,B} \left( \langle n(\text{r}, a) \rangle n(\text{r}, a) + \langle s_z(\text{r}, a) \rangle s_z(\text{r}, a) \right), \tag{20} \]
where $n \equiv n_{\uparrow} + n_{\downarrow}$, and $s_z \equiv n_{\uparrow} - n_{\downarrow}$. $\langle n \rangle$ and $\langle s_z \rangle$ are the order parameters to describe the charge-density-wave and spin-density wave orders. We have explicitly neglected the constant $\langle n_j \rangle^2$ appearing in the Hartree-Fock Hamiltonian since it only shifts the total energy.

The Hartree-Fock decoupled Hamiltonian only gives an overall density correction which renormalizes the chemical potential without renormalizing the bare hopping amplitudes. In order to generate terms that renormalize the hopping amplitudes from a "local" interaction $U$, a perturbation up to second order of $O(U/t)^2$ is needed, which contains eight-fermion terms consisting of fermions at two different sublattices $A$ and $B$. For combining the two approaches of perturbation and mean-field Hartree-Fock treatment, we explicitly borrow the concepts from the Renormalization Group (RG)\(^3\). Schematically, we start from a partition function of the full interacting Hamiltonian $H = H_0 + H_U$ and expand the interacting term. After the expansion, we mean-field decouple the interacting term to generate bilinear terms which consist of two-point correlation functions between sites $i$ and $j$, $\chi_{ij}^* \equiv \langle c_i^\dagger c_j \rangle$. We then re-exponentiate the terms to be combined with the original bare Hamiltonian $H_0$ and examine how the bare Hamiltonian gets renormalized. We call this method the perturbative mean-field Hartree-Fock method (PMFHF). The schematic mathematical expression is
\[ Z = \int \mathcal{D}[\psi^\dagger, \psi] e^{-H} = \int \mathcal{D}[\psi^\dagger, \psi] e^{-H_0} \left( 1 - \langle H_U \rangle_{MF} + \frac{1}{2} \langle H_U^2 \rangle_{MF} - \cdots \right) \]
\[ \simeq \int \mathcal{D}[\psi^\dagger, \psi] e^{-H_0} \left( 1 - \langle H_U \rangle_{MF} + \frac{1}{2} \langle H_U^2 \rangle_{MF} - \cdots \right) \]
\[ \simeq \int \mathcal{D}[\psi^\dagger, \psi] e^{-\left[ H_0 + \langle H_U \rangle_{MF} + \frac{1}{2} \langle H_U^2 \rangle_{MF} + \cdots \right]}, \tag{21} \]
where we can see the first order correction $\delta H_1$ to the bare Hamiltonian is $\langle H_U \rangle_{MF}$, which is simply the Hartree-Fock term, and the second order correction is $\delta H_2 = -\frac{1}{2} \langle H_U^2 \rangle_{MF}$. After the mean-field treatment, the correction terms $\delta H_{1/2}$ are functions of variables $\chi_{ij}$ which need to be determined self-consistently. We will use the PMFHF method to examine the three different variants of KM models.

### 3.1. Perturbative mean-field Hartree-Fock decoupling for GKM and DKM

In the GKM and DKM, the feature that the band gaps are controlled by the off-diagonal terms describing the hoppings hints that we need to perform the perturbation up to second order. Performing the expansion in $U/t$ up to second order, we obtain the contributions to the bare Hamiltonians as $\delta H = \delta H_1 + \delta H_2$, where the $\delta H_{1(2)}$ represent the first (second) order corrections. The $\delta H_1$ term is just the first-order mean-field decouplings given
by Eq. (20). As suggested by the QMC results, no charge density wave orders and magnetic instability are found at intermediate interaction strengths. Thus, we preserve the translational symmetry, and set ⟨s_±(r, a)⟩ = 0 as well as ⟨n(r, a)⟩ = ⟨n⟩. In momentum space, δH_1(k) = \sum_{k \in B.Z.} \Psi_k^\dagger h_1(k) \Psi_k, with

\[ h_1(k) = \frac{U}{2} \left( \langle n_A \rangle \right) \otimes \mathbb{1}_{2 \times 2} = \frac{U}{2} \langle n \rangle \mathbb{1}_{4 \times 4}, \]  

(22)

where we explicitly used the fact that ⟨n_A⟩ = ⟨n_B⟩ = ⟨n⟩ above.

The second-order correction δH_2 consists of two terms, δH_2 = δH_2^{(1)} + δH_2^{(2)}:

\[ δH_2^{(1)} = -\frac{U^2}{2} \sum_{r, r', a} n_\uparrow(r, a) n_\uparrow(r', a) n_\downarrow(r, a) n_\downarrow(r', a), \]  

(23)

and

\[ δH_2^{(2)} = -U^2 \sum_{r, r'} n_\uparrow(r, A) n_\uparrow(r', B) n_\downarrow(r, A) n_\downarrow(r', B). \]  

(24)

For simplicity in performing PMFHF for δH_2^{(1)}, we assume r' = r + \vec{E}_\mu, where \vec{E}_\mu runs over the Bravais lattice of the unit cell that is connected to r. The PMFHF gives

\[ δH_2^{(1)} = \frac{U^2}{2} \sum_{k, \vec{E}_\mu, \sigma, a} \left( \langle n_\sigma(a) \rangle \chi_{l\sigma}(\vec{E}_\mu, a) \right) \times \left( e^{-ik \cdot \vec{E}_\mu} \chi_{l\sigma}(\vec{E}_\mu, a) \right) \times \left[ (\chi_{l\sigma}(\vec{E}_\mu, a))^\dagger c_{k\sigma}^\dagger (a) c_{k\sigma} (a) + H.c. \right], \]  

(25)

where we define the ℓ-neighbor hopping correlation [\chi_{l\sigma}(\vec{E}_\mu, a)]^\dagger (r + \vec{E}_\mu, a) c_{\sigma}(r, a), with ℓ being the number of sites covered by \vec{E}_\mu. For correlations between the same sublattices, ℓ is always even. \( \uparrow = \downarrow \) and vice versa. For the GKM and DKM models, we restrict ℓ = 2 for second neighbor hopping (SOC) renormalization and \vec{E}_\mu = \{\vec{e}_1, \vec{e}_2, \vec{e}_3 \equiv \vec{e}_1 - \vec{e}_2\}, which is enough to capture the essential physics of the QMC results. Under PMFHF, δH_2^{(1)} only renormalizes the diagonal terms of the Hamiltonian matrices.

For the PMFHF of the δH_2^{(2)}, we introduce (r', a) = (r + \vec{E}_\nu, a), with \vec{E}_\nu being the vectors connected to r. Note that \vec{E}_\nu contain \vec{e}_0 \equiv \vec{0}, which means the two sites are in the same unit cell. We obtain

\[ δH_2^{(2)} = U^2 \sum_{k, \vec{E}_\nu, \sigma} \left[ e^{-ik \cdot \vec{E}_\nu} \chi_{m\sigma}(\vec{E}_\nu, AB) \left( \chi_{m\sigma}(\vec{E}_\nu, AB) \right)^\dagger c_{k\sigma}^\dagger (B) c_{k\sigma} (A) + H.c. \right], \]  

(26)

where \[ \chi_{m\sigma}(\vec{E}_\nu, AB) \] \equiv \langle c_{\sigma}^\dagger (r + \vec{E}_\nu, B) c_{\sigma}(r, A) \rangle, with m being the number of sites covered by \vec{E}_\nu. Since \vec{E}_\nu connects two different sublattices, m is always odd. For simplicity, we restrict m = 1, 3 for the GKM to capture the renormalizations of the first and third neighbor hoppings and m = 1 for the DKM. For more efficient numerical calculations, we can utilize symmetries [C_2, Inversion + complex conjugation (T^*), TRS, PHS for
both GKM and DKM while there is an additional $C_3$ for GKM] to reduce the number of
variables in each model.

Above in Eqs. (25), (26), and (27), we performed the perturbation up to $O(U^2/t^2)$
and utilized symmetry arguments to simplify the expressions of the corrections to the bare
Hamiltonians as functions of hopping correlations $\chi - s$. For determining the shift of the
phase transition location, we will rely on the low-energy descriptions around the gap closing
points, located at TRIM for GKM/DKM and $\pm K$ for SKM. Focusing on the gap closing
points, we will define the renormalized gap equations for three variants of KM models be-
low and later we will numerically solve for the parameters $\chi$-s to determine how the bands
gaps get renormalized.

3.1.1. **PMFHF for the GKM model and the gap equation**

For the hoppings between different sublattices, we choose $\tilde{E}_m = \{\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2\}$ for $m = 1$ and $\tilde{E}_m = \{\pm(\mathbf{e}_1 - \mathbf{e}_2), \mathbf{e}_1 + \mathbf{e}_2\}$ for $m = 3$. We can simplify Eqs. (25)–(26) by identifying
$\chi_{m\sigma}(\tilde{E}_m, AB) = \chi_{m\sigma} = \chi_m$, $\chi_{2\sigma}(\mathbf{e}_1, a) = -\chi_{2\sigma}(\mathbf{e}_2, a) = -\chi_{2\sigma}(\mathbf{e}_1 - \mathbf{e}_2, a)$, and
$\chi_{2\sigma}(\mathbf{e}_\mu, a) = \chi_{2\sigma}(\mathbf{e}_\mu, a) = -\chi_{2\sigma}(\mathbf{e}_\mu, a)$, where we use the fact that $\chi_{2\sigma}(\mathbf{e}_\mu, a) \in \mathbb{P}$. For
clarity, we introduce $\chi_{2\sigma}(\mathbf{e}_1, a) = i\chi_{2\sigma}(a)$ and $\chi_{2\sigma}(A) = -\chi_{2\sigma}(B) \equiv \chi_2 \in \mathbb{R}$.

\[
\delta H_2^{(1)} = U^2 \sum_{\mathbf{k}, \sigma, a} \left[ \frac{3}{2} \frac{(n_{\sigma}(a))}{\chi_2} - (-1)^{\sigma+a} g(\mathbf{k}) \chi_3^3 \right] c^\dagger_\sigma(\mathbf{k}, a) c_\sigma(\mathbf{k}, a). \tag{27}
\]

\[
\delta H_2^{(2)} = -U^2 \sum_{\mathbf{k}, \sigma} \left[ f(\mathbf{k}) \chi_1^3 + f_3(\mathbf{k}) \chi_3^3 \right] c^\dagger_\sigma(\mathbf{k}, a) c_\sigma(\mathbf{k}, B) + \text{H.c.}. \tag{28}
\]

At $\pm K$, $g(\pm K)$ vanishes. Eq. (27) simply renormalizes the chemical potential and Eq. (28)
renormalizes the off-diagonal elements (renormalize the hopping amplitudes).

After we add the corrections due to the interaction into the bare Hamiltonian, we focus
on the low-energy descriptions near the gap closing momenta TRIM: $M_{a=1,2,3}$. At $M_3$,
we find $g(M_3) = 0$, $f(M_3) = -1$, and $f_3(M_3) = 3$. We then define the gap equation
near the TRIM as

\[
\Delta_G = t - 3t_3 + U^2 \left( \chi_1^3 - 3\chi_3^3 \right). \tag{29}
\]

For the noninteracting critical point, $t_3 = \frac{1}{3} t$. At weak-coupling, $U/t \ll 1$, we can ap-
proximate $\chi_1$ and $\chi_3$ to be the noninteracting values. We find that $\chi_1 \simeq 0.20705$ and
$\chi_3 \simeq 0.03064$ and the $U^2$ correction is roughly $0.00879 U^2$. We conclude that in the weak-
coupling limit, the topological phase is more stable against the third neighbor hoppings
since we need larger $t_3$ to close the gap, coinciding with the QMC result [35,36].

3.1.2. **PMFHF for the DKM model and the gap equation**

For the hoppings between different sublattices we only need to consider the renormaliza-
tions of the first neighbor hoppings $t$ and $t_d$ with $m = 1$. Since the $C_3$ rotation is broken,
the hopping amplitudes within a unit cell are no longer equivalent to those between different unit cells. Utilizing symmetry considerations, we can identify the hopping amplitudes within the same unit cell $\chi_1(e_0, AB) = \chi_1^d(e_0, AB) \equiv \chi_1^d$. For the hopping between different unit cells $\chi_1^d(e_1, AB) = \chi_1^d(e_2, AB) \equiv \chi_1$. For the second neighbor hopping, we have $\chi_2(e_1, a) = -\chi_2(e_2, a) \equiv \chi_2^d(e_1, a, a), \chi_2(e_{\mu=1,2,3}, a) = -\chi_2^d(e_{\mu}, a)$, and $\chi_2(e_\mu, A) = -\chi_2(e_\mu, B)$. For clarity, we define $\chi_2^d(e_1, a) = -\chi_2^d(e_2, a) \equiv i\chi_2^d(a)$, $\chi_2^d(e_1, A) \equiv i\chi_2^d(a)$. We further introduce $\chi_2^d(a) \equiv (-1)^{\sigma+1}\chi_2$ and $\chi_2^d(a) \equiv (-1)^{\sigma+1}\chi_2$, with $a = A (B) = 1 (2)$. The second-order corrections to the bare Hamiltonian are

\[ \delta H_2^{(1)} = U^2 \sum_{\mathbf{k}, \sigma, \alpha} \left\{ (n_\sigma(a)) \left( 2 \chi_2^d(\mathbf{k}) + (\chi_2^d(\mathbf{k}))^2 \right) - (-1)^{\sigma+\alpha} \left[ -\sin(\mathbf{k} \cdot e_1) + \sin(\mathbf{k} \cdot e_2) \right] \times \chi_2^d + \sin(\mathbf{k} \cdot (e_1 - e_2))(\chi_2^d)^2 \right\} c_\sigma^d(\mathbf{k}, a) c_\sigma^d(\mathbf{k}, a) \]  

\[ \delta H_2^{(2)} = -U^2 \sum_{\mathbf{k}, \sigma} \left[ (\chi_1^d)^3 + e^{i\mathbf{k} \cdot e_1} + e^{i\mathbf{k} \cdot e_2} \right] (\chi_1^d)^3 c_\sigma^d(\mathbf{k}, A) c_\sigma(\mathbf{k}, B) + \text{H.c.,} \]  

where $\sigma = \uparrow (\downarrow) = 1 (2)$. For the DKM model, the gaps close at $M_3$ only. We focus on the gap closing momentum $M_3$ and we can define the corresponding gap equation as

\[ \Delta_D = 2t - t_d - U^2 \left( (\chi_1^d)^3 - 2(\chi_1^d)^2 \right). \]  

Focusing on the critical point, $t_d = 2t$, at the $U/t \ll 1$, we find that $\chi_1 \simeq 0.15770$ and $\chi_1^d \simeq 0.36627$. The $U^2$ correction to the gap equation is $-0.04189U^2 < 0$. We conclude that in the weak-coupling regime the topological phase is more fragile to the dimerization. This is also consistent with the observation from the QMC study.\[3,34,36\]

### 3.2. Perturbative mean-field Hartree-Fock decoupling for SKM

For SKM, since the bands gaps are controlled by the usual diagonal elements of the Hamiltonian, it is sufficient to perform the perturbation to first-order ($O(U/t)$) and then apply usual mean-field decoupling, which is already given in Eqs. (20) and (22). We find the $O(U/t)$ term can give corrections to the diagonal terms leading to a shift of the $Z_2$ topological phase transition in the SKM.

In SKM, we focus at the gap closing momenta $\pm \mathbf{K}$. Focusing on $\mathbf{K}$, we know that the off-diagonal elements in the Hamiltonian, Eq. (17), become linear in $\mathbf{k}$ and vanish exactly at $\mathbf{K}$. We find that two of the four bands with eigenvalues $E_1 = M - 2\lambda_{so}g(\mathbf{K}) + U \langle n_A \rangle / 2$ and $E_2 = -M + 2\lambda_{so}g(\mathbf{K}) + U \langle n_B \rangle / 2$ get inverted by tuning the mass $m$ and $\lambda_{so}$. We can define the gap function $\Delta_S(\mathbf{K}) \equiv \Delta_S$ as

\[ \Delta_S(\mathbf{K}) = 2M - 4\lambda_{so}g(\mathbf{K}) - \frac{U}{2} \left( \langle n_B \rangle - \langle n_A \rangle \right). \]  

For a constant staggered potential $M$ and SOC $\lambda_{SO}$, the sign of the $U$ correction term is determined by the sign of $U$ (with $\langle n_B \rangle > \langle n_A \rangle$ assumed). As a consequence, a repulsive
Short-ranged interaction effects on the $\mathbb{Z}_2$ topological phase transition

3.3. Self-consistent perturbative mean-field Hartree-Fock calculations

In the self-consistent numerical calculations, we set the honeycomb lattice consist of 400 × 400 unit cells and set $t = 1$ and $\lambda_{so} = 0.4$. The results at finite $U/t > 0$ for the GKM and DKM are shown in Figs. 5(a) and 5(b). The x-axis is the square of the interaction strength and the y-axis is the boundary shift amount, $\Delta t_{c3} = t_{c3}(U, \chi) - t_{c3}(0, \chi)$ and $\Delta t_{cd} = t_{cd}(U, \chi) - t_{cd}(0, \chi)$, where we introduced the renormalized hopping amplitudes. Both cases show that the amount of the boundary shifts are linearly proportional to $U^2/t^2$. In (a), the inset is the illustration of GKM model on the honeycomb lattice. The red lines represent the $t_{c3}$ hoppings. In (b), the inset represent the DKM model on the honeycomb lattice with anisotropic hopping $t_{cd}$ that breaks $C_3$ rotation, and the red lines represent the $t_{cd}$ hoppings with $t_{cd} > t$. A positive shift (open red squares) indicates that the topological phase is stabilized; a negative shift (open blue diamonds) it is destabilized.

interaction will stabilize the QSH phase, whereas an attractive interaction destabilizes in the SKM model. This feature is significantly different from the GKM and DKM models, where the gap equations have corrections proportional to $U^2$, cf Eqs. (29) and (32). In addition, unlike the case here, due to the PHS in the half-filled GKM and DKM models, the topological phase boundary shifts in GKM and DKM are independent of the sign of interactions.

In addition, within PMFHF, we find that the hopping amplitudes are almost independent of

-0.7 -0.5 -0.3 -0.1
0 4 8 12 16

$U^2/t^2$

Fig. 5. Self-consistent PMFHF data for QSH boundary shifts for (a) $\Delta t_{c3} = t_{c3}(U, \chi) - 1/3t$ in the GKM model and (b) $\Delta t_{cd} = t_{cd}(U, \chi) - 2t$ in the DKM model, where $t_{c3}(U, \chi), t_{cd}(U, \chi)$ are the renormalized hopping amplitudes which are functions of $U$ and the two-point correlation functions $\chi_{ij}$ between sites $i$ and $j$. Both cases show that the amount of the boundary shifts are linearly proportional to $U^2/t^2$. In (a), the inset is the illustration of GKM model on the honeycomb lattice. The red lines represent the $t_{c3}$ hoppings. In (b), the inset represent the DKM model on the honeycomb lattice with anisotropic hoppings that breaks $C_3$ rotation, and the red lines represent the $t_{cd}$ hoppings with $t_{cd} > t$. A positive shift (open red squares) indicates that the topological phase is stabilized; a negative shift (open blue diamonds) it is destabilized.
$U/t$ and, hence, the amount of boundary shift is linearly proportional to the $(U/t)^2$.  

Fig. 6. Self-consistent PMFHF data for QSH boundary shift $\Delta M_c = M_c(U) - \sqrt{3} \lambda_{SO}$ in the SKM models with (a) $U/t > 0$ and (b) $U/t = -|U|/t < 0$. Note that in both cases, the amounts of the boundary shift, red open squares, are linearly proportional to $U/t$.

On the other hand, the SKM model breaks PHS and the results at positive $U/t > 0$ cannot be directly compared with those obtained in QMC since QMC has the sign problem. We therefore consider the both positive $U/t > 0$ and negative $U/t < 0$ cases in the SKM model. The self-consistent PMFHF results in $U/t < 0$ case can be compared with the results in QMC, while the results for $U/t > 0$, though can not directly be compared with QMC results, are presented for completeness. The results at finite $U/t$ are shown in Fig. 6. For $U/t > 0$, Fig. 6(a) shows that under PMFHF the topological phase is more stabilized against the staggered potential strength and the shift of the topological phase boundary is linearly proportional to $U/t$. On the other hand, for $U/t = -|U|/t < 0$, the topological phase is more fragile to the staggered potential strength.

4. Sign-free determinant projector QMC

To further verify the PMFHF theory, we perform sign-free projective QMC simulations for the variants of the KM models with onsite interactions, and then compare with the PMFHF results. In the projector algorithm, an observable $O$ is measured as

$$
\langle O \rangle = \lim_{\Theta \to \infty} \frac{\langle \Psi_T | e^{-\frac{\Theta}{2} H} O e^{-\frac{\Theta}{2} H} | \Psi_T \rangle}{\langle \Psi_T | e^{-\Theta H} | \Psi_T \rangle},
$$

where $|\Psi_T\rangle$ is a trial wave function. The ground state wave function $|\Psi_0\rangle$ are filtered out through applying the projection operator $e^{-\frac{\Theta}{2} H}$ onto $|\Psi_T\rangle$; thus we require $\langle \Psi_T | \Psi_0 \rangle \neq 0$. For the variants of the KM model, the lowest single-particle states of $H_G$, $H_D$ and $H_S$ are good candidates for $|\Psi_T\rangle$ in the simulations. $\Theta$ is the projective parameter and plays the role as the imaginary time axes in the QMC algorithm. In practice, we discretize $\Theta$ into $M$ tiny slices with $\Delta\tau$ to rewrite the projection operator as $e^{-\Theta H} = [e^{-\Delta\tau H}]^M$, where
where $\alpha$ is a two-component HS transformation $e^{-\Delta \tau H}$ involves non-bilinear fermionic operators, i.e. $H_U \sim c_i^\dagger c_j^\dagger c_j c_i$. We need to resort to discrete Hubbard-Stratonovich (HS) transformations$^{15,16,17}$ to transform $e^{-\Delta \tau H_U}$ into a bilinear form by introducing auxiliary fields. For $U > 0$, we can have a two-component HS transformation$^{15}$

$$e^{-\Delta \tau H_U (n-1)^2} = \frac{1}{2} \sum_{s=\pm 1} e^{i \alpha s(n-1)},$$  \hspace{1cm} (36)$$

where $\alpha = \cos^{-1} (e^{-\Delta \tau U}).$ We can also use the four-component counterpart$^{19}$

$$e^{-\Delta \tau \frac{U}{2} (n-1)^2} = \frac{1}{4} \sum_{s=\pm 1, \pm 2} \gamma(s) e^{i \sqrt{\Delta \tau U} \eta(s) (n-1)} + O(\Delta \tau^4),$$  \hspace{1cm} (37)$$

where

$$\gamma(\pm 1) = (1 + \sqrt{6}/3), \quad \eta(\pm 1) = \pm \sqrt{2(3 - \sqrt{6})},$$

$$\gamma(\pm 2) = (1 - \sqrt{6}/3), \quad \eta(\pm 2) = \pm \sqrt{2(3 + \sqrt{6})}.$$  \hspace{1cm} (38)$$

For the latter one, the systematic error of the HS transformation of order can be controlled by selecting appropriately small values for $\Delta \tau$. For $U < 0$, we resort to the other two-component HS transformation$^{15}$

$$e^{\Delta \tau \frac{U}{2} (n-1)^2} = \frac{1}{2} \sum_{s=\pm 1} e^{\alpha' s(n-1)},$$  \hspace{1cm} (39)$$

where $\alpha' = \cosh^{-1} (e^{\Delta \tau |\frac{U}{2}|}).$ In most cases, $\Delta \tau t = 0.1$ and $\Delta \tau t = 0.05$ are chosen in QMC simulation.

For a $N$-site system, the cost of the two-component HS transformation is to introduce $2^{N M}$ auxiliary fields. For the four-component counterpart, the cost is about having $4^{N M}$ auxiliary fields. The integration over all auxiliary field configurations $\{s_{i,\tau}\}$ is performed using stochastic Monte Carlo sampling. In Eq. (34) with the two-component HS transformations, the partition function $\langle \Psi_0 | \Psi_0 \rangle$ is evaluated as

$$\langle \Psi_0 | \Psi_0 \rangle = \langle \Psi_T | e^{-\Theta H} | \Psi_T \rangle = \langle \Psi_T | \prod_{\tau=1}^{M} e^{-\Delta \tau H_{G,D,S}} e^{-\Delta \tau H_U} | \Psi_T \rangle$$

$$= \lim_{\Theta \to \infty} \sum_{\{s_{i,\tau}\}} \prod_i \prod_{\sigma} w_{\sigma} (s_{i,\tau}).$$  \hspace{1cm} (40)$$

The summation $\sum_{\{s_{i,\tau}\}}$ runs over possible auxiliary configurations $s_{i,\tau}$, where $i = 1 \sim N$, $\tau = 1 \sim M$. The probability weight for spin-$\sigma$ reads as

$$w_{\sigma} = \text{Tr} \left[ \prod_{\tau=1}^{M} \exp \left\{ -\Delta \tau \sum_{i,j} c_{i,\sigma}^\dagger H_{G,D,S}^\tau |i,j;\sigma,\sigma \rangle \exp \left\{ \alpha \sum_{i=1}^{N} s_{i,\tau} \left( n_{i,\sigma} - \frac{1}{2} \right) \right\} \right] \right],$$  \hspace{1cm} (41)$$

where $\Theta = \Delta \tau M$ and $\Delta \tau \ll 1$. Further by the first-order Suzuki-Trotter decomposition, $e^{-\Delta \tau H}$ can be decomposed as

$$e^{-\Delta \tau H} \approx e^{-\Delta \tau H_{G,D,S}} e^{-\Delta \tau H_U}. \hspace{1cm} (35)$$
Fig. 7. QMC data for QSH boundary shift (a) \( \Delta t_3^c = t_3^c(U) - \frac{1}{2} t \) in the GKM-Hubbard model, and (b) \( \Delta t_d^c = t_d^c(U) - 2t \) in the DKM-Hubbard model. In (a), the shift is positive, which means QSH is more stable against \( t_3 \) hoppings. More interestingly, the shift amount is linearly proportional to \( (U/t)^2 \), consistent with our mean-field picture. In (b), the shift is negative and linearly proportional to \( (U/t)^2 \). The short-range interaction makes the QSH phase more destabilized by the dimerization \( t_d \). Statistical errors are denoted by the error bars.

with \( \tilde{\alpha} = i\alpha \) for \( U > 0 \) and \( \tilde{\alpha} = \alpha' \) for \( U < 0 \). Note that, in Eq. (41) the notion \( \sigma \) is introduced in \( H_{G,D,S}^{\sigma} \). Without Rashba spin-orbit coupling, the variants of the KM models still preserve \( s_z \), such that \( H_{G,D,S}^{\sigma} \) are decoupled for different spin flavors. For the \( U > 0 \) case, it is easy to show that at half-filling, PHS in the variants of the KM model renders \( w_\uparrow w_\downarrow = |w_\uparrow|^2 > 0 \), such that the Monte Carlo simulations always have positive-definitive sampling. For the \( U < 0 \) case, the time-reversal symmetry guarantees \( w_\uparrow = w_\downarrow^* \), so \( w_\uparrow w_\downarrow \) is the positiveness of \( \xi_1 \). Therefore, we can have sign-free simulations and numerically exact solutions for the repulsive GKM, DKM-Hubbard model and attractive SKM-Hubbard model.

It has been pointed out by a QMC study that it is not easy to get access to the interacting topological phase transition by identifying a gap closing, due to strong finite-size effect in single-particle gaps. The straightforward approach to determine locations of the topological phase transition boundaries is to evaluate the \( Z_2 \) topological index and spin Chern number, in terms of zero-frequency Green’s functions. With the inversion symmetry, the interacting \( Z_2 \) invariant \( \Delta \) is evaluated as

\[
(-1)^\Delta = \prod_{\text{R-zeros}} \xi^{1/2}(\Gamma_i),
\]

where \( \xi(\Gamma_i) \) denotes the parity eigenvalue of the "R-zeros" eigenstates of interacting zero-frequency Green’s function at TRIM points \( \Gamma_i \) [here in the KM model, the TRIM are \( \Gamma = (0,0) \) and \( \Gamma_1,2,3 \) as shown in Fig. 1(b)]. More explicitly,

\[
G(i\omega = 0, \Gamma_i)|\mu\rangle = \mu|\mu\rangle,
\]

with \( \mu > 0 \) and \( P|\mu\rangle = \xi(\Gamma_i)|\mu\rangle \), where \( P \) is the parity operator. The zero-frequency Green’s functions are obtained through time-displaced Green’s functions in the QMC simulations and with Fourier transformation. More detailed procedures has been indicated in the review article.
The numerical results are shown in Fig. 7. The closed (open) red squares and blue diamonds represent the boundary shifts $\Delta t_3^c = t_3^c(U) - \frac{1}{t}t$ and $\Delta t_d^c = t_d^c(U) - 2t$ obtained in the GKM-Hubbard and DKM-Hubbard modes on $6 \times 6$ ($12 \times 12$) clusters, respectively. Here we consider the discretized time step $\Delta \tau = 0.05$. In both models, we sweep the critical points $t_3^c$ and $t_d^c$ at a variety of $U$ (the strength of $U$ is below the critical value to magnetic instability). The topological phase transitions appear when the interacting $Z_2$ invariant has changes $\Delta = -1 \leftrightarrow 1$. In both models, the QMC results show that appropriate sign and amounts of the boundary shift are linearly proportional to $(U/t)^2$ to high accuracy, as the PMFHF theory predicted. This means that the PMFHF can properly capture the correlation effect at the intermediate interaction realm. Note that the linear relations to $(U/t)^2$ are universal and size-independent in the QMC results. Compared with Figs. 5, one can see that the PMFHF theory has captured and interpreted the behavior.

Next we move to the SKM-Hubbard model. Due to the absence of PHS, the QMC simulation on the repulsive SKM-Hubbard model has minus sign problems. Instead, we turn to study the attractive staggered Kane-Mele-Hubbard model ($U = -|U| < 0$ and $\lambda_{so} = 0.2t$) on $6 \times 6$ and $12 \times 12$ sites, and depict the topological boundary shift under correlation in Fig. 8. The QMC results also explicitly support the PMFHF’s prediction, that the topological phase boundary is linearly proportional to the first-order $U/t$, and the negative slope of the $M^c - U$ curve, indicating that the attractive interaction destabilizes the topological phase. For other KM-type models, we believe our approach in this work, $U/t$ expansion + mean-field Hartree-Fock + low-energy gap equation $\Delta(k)$, can essentially capture the interactions effects on the $Z_2$ topological phase transitions, and possibly in more general models as well.

Fig. 8. QMC data for QSH boundary shift in the attractive Kane-Mele-Hubbard model in the presence of staggered potential $M$. The shift amount of the critical $M$, $\Delta M^c = M^c(U) - \sqrt{3}l_{SO}$ is negative and linearly proportional to $U/t$. Note that we chose $\lambda_{so} = 0.2t$ and $U < 0$. PHS is explicitly broken due to the staggered potentials. QMC is only fermion-sign free in the attractive $U < 0$ case.
5. Discussion

Readers may be confused about why the boundary shifts due to the presence of the onsite interaction can not be studied by perturbative methods such as weak-coupling RG analysis at the critical phase in which the gaps close to form Dirac points. We note that such RG analysis can not predict any phase boundary shift. For simplicity and illustration, we focus on the critical phase (semi-metal phase) at the phase transition in SKM below in Sec. 5.1, where the number of relevant degrees of freedom is smaller compared with those in GKM and DKM due to the presence of more number of Dirac nodes at the critical phase. The straightforward thought is that even though the local four-fermion interactions are irrelevant in the critical phase, before they flow to negligible values under RG they can still generate a finite bilinear mass term, which can possibly shift the phase boundary. However, below we will explicitly perform tree-level RG analysis and show that the tree-level RG corrections completely cancel each other, which gives no generation of a bilinear mass term. Hence we conclude that the boundary shift can only be captured by the physics of the lattice model and can not be captured by the coarse-grained continuum theory around $K$ and $K'$. In Sec. 5.2, we will consider a more extended interaction including both Hubbard $U$ and nearest neighbor interaction $V$ in the SKM within the self-consistent PMFHF. The inclusion of the nearest-neighbor $V$ complicates the analysis. We find that whether or not the topological phase is stabilized due to the short-ranged interactions depends on the details of the competition between the onsite $U$ and the nearest-neighbor $V$. From the low energy analysis focusing on $K$ point in the B.Z., we conclude that within the Hartree-Fock picture if $U$ is dominant over $V$ ($U > 6V$) the qualitative result obtained from the case with only onsite $U$, repulsive (attractive) interactions stabilize (destabilize) the topological phase, is still correct in the $U$-$V$ model. However, from the studies of the Kane-Mele-$U$-$V$ model, it may suggest a long-ranged repulsive interaction such as Coulomb interaction may completely destabilize the QSH phase, which is, however, contrary to the recent QMC studies\textsuperscript{51}. The contradiction is due to the underestimation of the effects of the “long-ranged tail” of the Coulomb interaction.

5.1. RG analysis of the critical phase in the SKM model with weak interaction $U$

In this model, since $S^z$ is still conserved, the spin-up and spin-down Hamiltonian can be treated separately. For each spin species, we can diagonalize the Hamiltonian matrix for spectra. There are 2 bands for each spin species. The bands can be characterized by the eigenvector-eigenenergy pairs $\{\hat{c}_b^\alpha(k), c_b^\alpha(k)\}$, where $b = 1, 2$ are band indices. The Hamiltonian can be diagonalized by rewriting the original fermion fields in terms of the complex fermion fields $d_b^\alpha(k)$ in the diagonal basis,

$$c_b^\alpha (r,a) = \sqrt{\frac{1}{N_{uc}} \sum_{b=1,2} \sum_{k \in B.Z.} \hat{c}_b^\alpha(k,a) d_b^\alpha(k) e^{ik\cdot r}}, \quad (44)$$

where $N_{uc}$ is the number of unit cells and the complex fermion field $f$ satisfies the usual anticommutation relation $\{d_b^{\alpha \dagger}(k), d_{b'}^{\alpha'}(k')\} = \delta_{\alpha \alpha'} \delta_{bb'} \delta_{kk'}$. In terms of the new complex
fermion fields, the Hamiltonian becomes
\[
H_{KMs} = \sum_{b=1,2} \sum_{\alpha=\uparrow,\downarrow} \sum_{\mathbf{k} \in \mathbb{B}} \epsilon_b^\alpha(\mathbf{k}) d_b^{\alpha \dagger}(\mathbf{k}) d_b^\alpha(\mathbf{k}).
\]  
(45)

At the critical phase \((\lambda_m^c = 3\sqrt{3}\lambda_m)\), the gaps close at momentums \(\mathbf{K}\) and \(\mathbf{K}' = -\mathbf{K}\). Around these points, only the spin-down fermions are gapless at \(\mathbf{K}\) and spin-up fermions are gapless at \(\mathbf{K}'\). As far as the long-wavelength (low-energy) description is concerned, we can focus on the \(\mathbf{K}\) and \(\mathbf{K}'\) points and perform expansion around these points by introducing a small momentum shift \(\delta \mathbf{k}\).

For the low-energy description at momentum \(\mathbf{K}\), we find that only the spin-down fermions are gapless and the expansion around \(\mathbf{K}\) by introducing \(\mathbf{k} = \mathbf{K} + \delta \mathbf{k}\), with \(|\delta \mathbf{k}| < \Lambda\), \(\Lambda \ll |\mathbf{K}|\), gives
\[
H_{\mathbf{K}} \simeq \sum_{|\delta \mathbf{k}| < \Lambda} v_F|\delta \mathbf{k}| \left[ \psi_{1R}^\dagger(\delta \mathbf{k}) \psi_{1R}(\delta \mathbf{k}) - \psi_{2R}^\dagger(\delta \mathbf{k}) \psi_{2R}(\delta \mathbf{k}) \right],
\]  
(46)

where we introduced \(d_{\mathbf{k}}^\alpha(\mathbf{K} + \delta \mathbf{k}) = \psi_{bR}^\dagger(\delta \mathbf{k})\) with \(R\) labeling the valley at \(\mathbf{K}\) and \(v_F \equiv \sqrt{3}t/2\) is the Fermi velocity of each band at \(\mathbf{K}\). It is more convenient to transform the continuum fields defined above to real space, defining
\[
\psi_{bR}^\dagger(\mathbf{r}) = \sqrt{\frac{1}{N_{uc}}} \sum_{|\delta \mathbf{k}| < \Lambda} e^{i\delta \mathbf{k} \cdot \mathbf{r}} \psi_{bR}^\dagger(\delta \mathbf{k}).
\]  
(47)

Therefore, in the low-energy description, we can re-express the spin-down fermion field as
\[
c_{\mathbf{k}}(\mathbf{r},a) \simeq \sum_{b=1,2} v_{bR}^\dagger(a) \psi_{bR}^\dagger(\mathbf{r}) e^{i\mathbf{K}_b \cdot \mathbf{r}},
\]  
(48)

where we defined \(v_{bR}^\dagger(\mathbf{K} + \delta \mathbf{k},a) \equiv v_{bR}(a)\).

Similarly, we can also obtain the low-energy description at \(\mathbf{K}'\). At \(\mathbf{K}'\), only the spin-up fermions are gapless and expansion around \(\mathbf{K}'\) with small momentum shift \(\delta \mathbf{k}\) gives
\[
H_{\mathbf{K}'} \simeq \sum_{|\delta \mathbf{k}| < \Lambda} v_F|\delta \mathbf{k}| \left[ \psi_{1L}^\dagger(\delta \mathbf{k}) \psi_{1L}(\delta \mathbf{k}) - \psi_{2L}^\dagger(\delta \mathbf{k}) \psi_{2L}(\delta \mathbf{k}) \right],
\]  
(49)

where similarly we defined \(d_{\mathbf{k}}^\alpha(\mathbf{K}' + \delta \mathbf{k}) = \psi_{bL}^\dagger(\delta \mathbf{k})\). We can define a similar transformation to the real space as above, and the spin-down fermion field can be effectively expressed as
\[
c_{\mathbf{k}}(\mathbf{r},a) \simeq \sum_{b=1,2} v_{bL}^\dagger(a) \psi_{bL}^\dagger(\mathbf{r}) e^{i\mathbf{K}_b' \cdot \mathbf{r}},
\]  
(50)

with \(v_{bL}^\dagger(\mathbf{K}' + \delta \mathbf{k},a) \equiv v_{bL}(a)\), \(L\) labeling the valley at \(\mathbf{K}'\), and remember \(\mathbf{K}' = -\mathbf{K}\). The action for the low-energy description is
\[
S_{0,P} = \int \frac{d^2q dq \omega}{(2\pi)^3} \left[ \psi_{bPa}^\dagger(q)(-i\omega)\psi_{bPa}(q) + H_P \right],
\]  
(51)
with $P = R/L = K/K'$ and $\alpha_{R/L} = \downarrow / \uparrow$ and we use $2 + 1$ dimensional vector $q$ representing frequency and momentum $(\omega, \mathbf{q})$. We can also define the Green’s functions as

$$
\langle \psi_{bL}^\dagger(q)\psi_{bL}(q') \rangle = \langle \psi_{bR}^\dagger(q)\psi_{bR}(q') \rangle = \frac{i\omega - (-1)^b v_F|\mathbf{q}|}{(i\omega)^2 - (v_F|\mathbf{q}|)^2} \delta^{(3)}_{qq'},
$$

and we introduce the abbreviation $\delta^{(3)}_{qq'} = (2\pi)^3\delta(\omega - \omega')\delta^2(\mathbf{q} - \mathbf{q}')$.

In order to write down the general expression of the four-fermion interactions, we need first to obtain the symmetry transformation of the fields defined above. There are $S^z$-conservation, $U(1)$-charge, TRS, and $C_5$ in this system. Except TRS, the other three symmetry transformations are quite transparent. Let’s focus on the symmetry transformation under TRS ($T$), and we find

$$
\begin{align*}
\psi_{bL}^\dagger(a) T \psi_{bL} T^{-1} &= -\psi_{bR}^\dagger(a) \psi_{bR}, \\
\psi_{bR}^\dagger(a) T \psi_{bR} T^{-1} &= \psi_{bL}^\dagger(a) \psi_{bL}.
\end{align*}
\tag{53, 54}
$$

With TRS, the eigenvector-eigenvalue pairs have the property, $\tilde{v}_b^\dagger(k) = [\tilde{v}_b^\dagger(-k)]^*$ and $\tilde{\epsilon}_b^\dagger(k) = \tilde{\epsilon}_b^\dagger(-k)$, which gives $\psi_{bL}^\dagger(a) = \psi_{bR}^\dagger(a)$. We can use the properties above to simplify the TRS transformation in (53) and (54), but as far as the RG analysis presented below is concerned, we don’t need to do that.

The general expressions of the local four-fermion interactions in terms of the continuum fields defined above are shown below. For simplicity in the expression, we define below $f_{b\rho\alpha}(a) \equiv v_{b\rho}^\dagger(a)\psi_{\rho \alpha}^\dagger(r)$, and the local four-fermion action can be written as (repeated $a$ means summation over the eigenvector elements)

$$
S_{\text{int}} = \omega_{11}^2 f_{1L1L}^\dagger(a) f_{1L1L}^\dagger(a) f_{1R1R}^\dagger(a) f_{1R1R}^\dagger(a) + \omega_{12}^2 f_{12L1}^\dagger(a) f_{12L1}^\dagger(a) f_{2R1R}^\dagger(a) f_{2R1R}^\dagger(a) + \\
+ \omega_{22}^2 \left( f_{12L1}^\dagger(a) f_{2R1R}^\dagger(a) f_{2R1R}^\dagger(a) f_{1R1R}^\dagger(a) f_{1L1L}^\dagger(a) f_{2L1L}^\dagger(a) f_{2L1L}^\dagger(a) f_{1R1R}^\dagger(a) f_{1L1L}^\dagger(a) f_{2L1L}^\dagger(a) + \text{H.c.} \right) + \\
+ \lambda_{12}^2 \left( f_{12L1}^\dagger(a) f_{1L1L}^\dagger(a) f_{1R1R}^\dagger(a) f_{1R1R}^\dagger(a) f_{1L1L}^\dagger(a) f_{2L1L}^\dagger(a) f_{2L1L}^\dagger(a) f_{1R1R}^\dagger(a) f_{1L1L}^\dagger(a) f_{2L1L}^\dagger(a) + \text{H.c.} \right) + \\
+ \lambda_{21}^2 \left( f_{2R1R}^\dagger(a) f_{2L1T}^\dagger(a) f_{2R1R}^\dagger(a) f_{2R1R}^\dagger(a) f_{2L1T}^\dagger(a) f_{1R1R}^\dagger(a) f_{1R1R}^\dagger(a) f_{2L1T}^\dagger(a) f_{2R1R}^\dagger(a) f_{2L1T}^\dagger(a) + \text{H.c.} \right) + \\
+ \lambda_{21}^2 \left( f_{2R1R}^\dagger(a) f_{2L1T}^\dagger(a) f_{2R1R}^\dagger(a) f_{2R1R}^\dagger(a) f_{2L1T}^\dagger(a) f_{2L1T}^\dagger(a) f_{2R1R}^\dagger(a) f_{2R1R}^\dagger(a) f_{2L1T}^\dagger(a) + \text{H.c.} \right) + \\
+ \lambda_{12}^2 \left( f_{12L1}^\dagger(a) f_{1L1L}^\dagger(a) f_{1R1R}^\dagger(a) f_{1R1R}^\dagger(a) f_{1L1L}^\dagger(a) f_{2L1L}^\dagger(a) f_{2L1L}^\dagger(a) f_{1R1R}^\dagger(a) f_{1L1L}^\dagger(a) f_{2L1L}^\dagger(a) + \text{H.c.} \right),
\tag{55}
$$

and we remark that in the presence of the onsite interaction $U$, all the bare couplings above are simply equal to $U$.

The RG analysis in a nutshell is first to integrate out the fast-momentum modes defined within a momentum shell between $[\Lambda/b, \Lambda]$, with $b \equiv e^{d\ell} \simeq 1 + d\ell$ slightly bigger than one. Then we rescale the (fermion or boson) fields and the momentum to recast the action back to the original form. After the elimination of the fast-momentum modes and rescaling process, we can examine how the couplings of the interactions change. The mathematical form at the tree-level is

$$
S_{\text{eff,} <} = \langle S_{\text{int}} \rangle,
$$

(56)
where the subscript $>$ means momentum shell integral of the fast-momentum modes.

At the tree-level, we find the corrections are

$$
\langle S_{\text{int}} \rangle = -\frac{\Lambda^2}{4\pi} \mathrm{d}\ell \left[ \omega_{11}^a |v_{1R_L}(a)|^2 - \omega_{12}^a |v_{2R_L}(a)|^2 \right] f_{1L_L}(a) f_{1L_L}(a) +
\frac{\Lambda^2}{4\pi} \mathrm{d}\ell \left[ \omega_{22}^a |v_{2R_L}(a)|^2 - \omega_{12}^a |v_{1R_L}(a)|^2 \right] f_{2L_L}(a) f_{2L_L}(a) -
\frac{\Lambda^2}{4\pi} \mathrm{d}\ell \left[ \omega_{11}^a |v_{1L_L}(a)|^2 - \omega_{21}^a |v_{2L_L}(a)|^2 \right] f_{1R_R}(a) f_{1R_R}(a) +
\frac{\Lambda^2}{4\pi} \mathrm{d}\ell \left[ \omega_{22}^a |v_{2L_L}(a)|^2 - \omega_{21}^a |v_{2L_L}(a)|^2 \right] f_{2R_R}(a) f_{2R_R}(a) -
\frac{\Lambda^2}{4\pi} \mathrm{d}\ell \left[ \lambda_{12}^a |v_{1L_L}(a)|^2 - \lambda_{21}^a |v_{2L_L}(a)|^2 \right] \left( f_{1R_R}(a) f_{2R_L}(a) + \text{H.c.} \right) -
\frac{\Lambda^2}{4\pi} \mathrm{d}\ell \left[ \lambda_{12}^a |v_{1R_L}(a)|^2 - \lambda_{21}^a |v_{2R_L}(a)|^2 \right] \left( f_{1L_L}(a) f_{2L_L}(a) + \text{H.c.} \right),
$$

and all the four-fermion couplings are irrelevant,

$$
\frac{dg}{d\ell} = -g,
$$

with $g = \omega^a$-s, $\lambda^a$-s, $u^a$-s introduced above and $\ell$ is the logarithm of the length scale in RG analysis.

The bare couplings of $\omega_{11}^a(\ell = 0) = \omega_{22}^a(0) = \omega_{12}^a(0) = U$, and we numerically check that $|v_{1R_L}(a)|^2 = |v_{2R_L}(a)|^2$, $|v_{1L_L}(a)|^2 = |v_{2L_L}(a)|^2$. At the tree-level RG analysis, all the couplings decays at the same rate under RG flow. Before all the four-fermion couplings flow to negligible values, at some small $\ell_c$, we have $\omega_{11}^a(\ell_c) = \omega_{22}^a(\ell_c) = \omega_{12}^a(\ell_c) = \lambda_{12}^a(\ell_c) = \lambda_{21}^a(\ell_c)$, and hence the bilinear corrections generated by these irrelevant four-fermion interactions completely cancel each other, which leaves no corrections at the tree-level RG analysis. Therefore, we conclude such long-wavelength analysis can not capture the shift of the boundary between the topologically trivial and nontrivial phases. The boundary shift can only be captured, at least in this model, by the lattice Hamiltonian which is not coarse-grained.

### 5.2. SKM-U-V model

We will consider a more extended interaction which includes both the Hubbard $U$ and the nearest-neighbor $V$. The presence of the nearest-neighbor $V$ within Hartree-Fock contribute both the diagonal terms and the off-diagonal terms to the original Hamiltonian. The diagonal terms obviously renormalize the mass terms and the off-diagonal terms renormalize the nearest-neighbor hopping amplitude $t$, resulting in renormalizing the velocity of the Dirac fermions in the critical phase. Within the Hartree-Fock picture, besides the expecta-
The results in this case are qualitatively opposite to those in the repulsive case. When $V > 0$, we can see that in this case. If the nearest-neighbor $V$ is much smaller than $U, V = U/10$, the interactions still tend to stabilize the topological phase. But due to the competition between $U$ and $V$ the topological window is less widened by the interactions. If $V$ is more comparable to $U,V = U/2$ in this case, the effects of $V$ will be dominant over $U$ and will tend to destabilize the topological phase. According to the gap function defined around momentum $K$ point, Eq. (62), the transition point is at $U = 6V$. (b) The attractive interaction case, $U, V < 0$. The results in this case are qualitatively opposite to those in the repulsive case. When $V$ is more comparable to the $U$, the interactions tend to stabilize the topological phase.

Fig. 9. Illustration of the phase boundary shift in the present of both $U$ and $V$ repulsion. We take $t = 1, \lambda_{so} = 0.4, and choose V = U/2$ and $V = U/10$. The blue open dot squares represent the boundary in the case of $V = U/10$ and the open red diamonds line represents the boundary in the case of $V = U/10$. The black line represents the boundary in the present of onsite Hubbard $U$. (a) The repulsive interaction case, $U, V > 0$. We can see that in this case. If the nearest-neighbor $V$ is much smaller than $U, V = U/10$, the interactions still tend to stabilize the topological phase. But due to the competition between $U$ and $V$ the topological window is less widened by the interactions. If $V$ is more comparable to $U,V = U/2$ in this case, the effects of $V$ will be dominant over $U$ and will tend to destabilize the topological phase. According to the gap function defined around momentum $K$ point, Eq. (62), the transition point is at $U = 6V$. (b) The attractive interaction case, $U, V < 0$. The results in this case are qualitatively opposite to those in the repulsive case. When $V$ is more comparable to the $U$, the interactions tend to stabilize the topological phase.

Focusing on momentum $K$, we can see that the two of the four bands with the eigenvalues $E_{1/2} = \pm M \mp 2\lambda_{so}g(K) + \frac{U}{2}\langle n_{A/B} \rangle + 3V\langle n_{B/A} \rangle$ can be inverted due to the tuning of the ratio of $M$ and $\lambda_{so}$. Therefore, we define the gap function as

$$
\Delta(K) = E_1 - E_2 \\
= 2M - 4\lambda_{so}g(K) + \left(\frac{U}{2} - 3V\right)\left[\langle n_A \rangle - \langle n_B \rangle\right].
$$

The nearest-neighbor $V$ contributes additional terms to the full Hamiltonian. In the matrix form, the additional terms can be expressed as

$$
\hat{h}_V(k) = V \begin{pmatrix}
3\langle n_B \rangle & -f_{\uparrow}(k) & 0 & 0 \\
-(f_{\uparrow}(k))^* & 3\langle n_A \rangle & 0 & 0 \\
0 & 0 & 3\langle n_B \rangle & -f_{\downarrow}(k) \\
0 & 0 & -(f_{\downarrow}(k))^* & 3\langle n_A \rangle
\end{pmatrix},
$$

where $f_{\sigma}(k) \equiv (\chi_{\sigma})^* + e^{ik\cdot e_1}(\chi_{\sigma}(e_1))^* + e^{ik\cdot e_2}(\chi_{\sigma}(e_2))^*$. By $C_3$ symmetry, we can simplify the result by identifying $\chi_{\sigma} = \chi_{\sigma}(e_1) = \chi_{\sigma}(e_2)$. We can see that $f_{\sigma}(k)$ is proportional to $f(k)$ defined in Eq. (17) and therefore vanish at momentums $K$ and $K'$.
Due to the presence of the staggered potentials, the density at B is larger than that at A, $\langle n_B \rangle > \langle n_A \rangle$, and the sign of the correction of the last term in the gap function depends on the competition between $U$ and $V$. For repulsive $U, V > 0$, if $U > 6V$, the last term is negative and the repulsive interactions stabilizes the topological phase. However, if $U < 6V$, the last term is positive and then the interactions destabilizes the topological phase. On the other hand, the attractive $U, V < 0$ would give the opposite results to the repulsive case.

For illustration, we numerically check the cases with $t = 1, \lambda_{so} = 0.4$, and choose $V = U/10$ and $V = U/2$ on a honeycomb lattice consisting of $200 \times 200$ unit cells. The results are shown in Fig. 9. The blue open dot squares represent the topological phase boundary shift in the case of $V = U/10$ and the open red diamonds line represents the boundary shift in the case of $V = U/10$. The black dashed line represents the boundary shift in the present of only onsite Hubbard $U$ shown in Fig. 6. Qualitatively, the results between the repulsive and the attractive case are opposite. In the repulsive interaction case, the more short-ranged the repulsive interactions are, the more stable the topological is. On the other hand, in the attractive interaction case, the more extended the attractive interactions are, the more stable the topological phase is. In the end, we remark that the extended repulsion/attraction also enhance the fluctuations of charge/spin which lead to the magnetic phase transition. The extended part of the interaction tends to "decrease" the onsite repulsive interaction. The results will lead to the modification of the familiar two spin exchanges in the large $U$ limit, $J_{rr'} = 4t_{rr'}^2 / U \rightarrow 4t_{rr'}^2 / (V_0 - V_{r-r'})$, where we define $V_0$ corresponds to onsite Hubbard repulsion and $V_{r-r'}$ corresponds to the extend part. Similarly, all the higher order multispin exchange amplitudes are modified and may in fact be relatively more important in systems with extended interactions. Therefore, the magnetic phase transition may occur in a larger value of the onsite interaction strength, which will make the topological phase boundary shifts more obvious.

6. Conclusion

In this review article, we pedagogically introduce a new analytical method combining perturbation and self-consistent mean-field Hartree-Fock treatments. We illustrate our method on three different variants of the Kane-Mele-Hubbard models and find the signs of the shifts and scalings of topological phase boundary are in excellent agreement with quantum Monte-Carlo simulations. We conclude that the shift amounts of the QSH boundary in the generalized Kane-Mele and dimerized Kane-Mele models are proportional to $(U/t)^2$, while that in the stagger-potential Kane-Mele model is linearly proportional to $U/t$. We believe this approach has general applicability, especially in certain three-dimensional topological phase transitions such as the three-dimensional model on the diamond lattice proposed by Fu, Kane, and Mele, where the exact QMC simulations suffer from the sign problem and the system size limitation.
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