Interaction effects on topological phase transitions via numerically exact quantum Monte Carlo calculations

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We theoretically study topological phase transitions in four generalized versions of the Kane-Mele-Hubbard model with up to \(2 \times 18^2\) sites. All models are free of the fermion-sign problem allowing numerically exact quantum Monte Carlo (QMC) calculations to be performed to extremely low temperatures. We numerically compute the \(Z_2\) invariant and spin Chern number \(C_{\sigma}\) directly from the zero-frequency single-particle Green’s functions, and study the topological phase transitions driven by the tight-binding parameters at different on-site interaction strengths. The \(Z_2\) invariant and spin Chern number, which are complementary to each another, characterize the topological phases and identify the critical points of topological phase transitions. Although the numerically determined phase boundaries are nearly identical for different system sizes, we find strong system-size dependence of the spin Chern number, where quantized values are only expected upon approaching the thermodynamic limit. For the Hubbard models we considered, the QMC results show that correlation effects lead to shifts in the phase boundaries relative to those in the non-interacting limit, without any spontaneously symmetry breaking. The interaction-induced shift is non-perturbative in the interactions and cannot be captured within a “simple” self-consistent calculation either, such as Hartree-Fock. Furthermore, our QMC calculations suggest that quantum fluctuations from interactions stabilize topological phases in systems where the one-body terms preserve the \(D_3\) symmetry of the lattice, and destabilize topological phases when the one-body terms break the \(D_3\) symmetry.

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I. INTRODUCTION

Electron interactions in topological insulators¹–²⁰ have been a topic of intense research in recent years.²¹–²⁶ It is crucial to go beyond the mean-field level to capture important fluctuation effects originating in the electronic correlations, as this can be decisive in determining the phase.²⁷–³² Exact diagonalization studies are inhibited by significant finite-size effects,³³ though they are unbiased by any particular ansatz in the way mean-field theories are. In this work, we study correlation effects in topological insulators by considering the Kane-Mele-Hubbard model and several variants with numerically exact projective quantum Monte Carlo (QMC) calculations. Due to their particle-hole symmetry, these models are free of the fermion minus sign problem, and QMC simulations provide a great opportunity to study correlation effects in topological matter with an unbiased theoretical approach. We are able to accurately treat correlations, compute interacting topological invariants such as the \(Z_2\) invariant and spin Chern number, and identify topological phase transitions through the zero-frequency single-particle Green’s function.³⁴,³⁵ We thus avoid complications associated with ground-state evolution under twisted boundary conditions,³⁶ where numerical computations of a manifold ground states is required, and potential subtleties regarding energy gap closures must be addressed.³⁶

Strictly speaking, the ground state is altered when twisted boundary conditions are introduced. The existence of a family of ground states smoothly connected to one and another, and a finite spectral gap are required for the use of twisted boundary conditions. Meeting these conditions can be especially challenging when approaching a phase transition where excitation gaps can become very small. Moreover, the use of the twisted boundary conditions is not practical in large-scale simulations, such as QMC; hence current implementations of twisted boundary conditions in interacting models have mainly focused on small sizes where exact diagonalization techniques have been used.³⁸,³⁹ In addition, the initial use of twisted boundary conditions for defining the spin Chern number introduced edge effects, which initially cast doubt on its robustness as a bulk topological invariant.⁴⁰,⁴¹

Therefore, it is worth revisiting topological phase transitions from the point-of-view of spin Chern numbers, particularly in the context of systems with interactions and finite-size effects present. We observe in our numerical QMC results a dichotomy in the role of on-site Hubbard interactions: Depending on the underlying lattice symmetry, they favor either a topological or trivial phase. Although our results are only limited to the class of models with particle-hole symmetry and \(S^z\) conservation, they could be hints of a more general principle regarding the interplay between point-group symmetry and interactions.

The remainder of this paper is organized as follows. In Section II we introduce the Kane-Mele model and the four variants of it that we study. We compare and contrast the particular spatial symmetries exhibited by these toy models. In Section III we follow up with a discussion.
on the time-reversal invariant topological $Z_2$ index and the spin Chern number with a focus on their numerical implementation in the presence of interactions. Next in Section IV which is the main part of our work, we present computations of topological indices in the presence intermediately strong interactions for the models introduced in Section II. This is followed up with discussions, interpretation, and speculation regarding these results in Section V. Then in Section VI we conclude with a summary and conclusions. Also included in the appendices are details regarding our quantum Monte Carlo methodology and supporting numerical results on the spin Chern number.

II. THE KANE-MELE MODEL AND SEVERAL VARIANTS

The Kane-Mele (KM) model, an early model supporting a $Z_2$ topological insulator (TI) on the honeycomb lattice\cite{47,48} remains central to the study of interaction effects in TI. The honeycomb lattice is a Bravais (triangular) lattice with a two-point basis (labeled as A and B). The vectors connecting two neighboring sites are $\mathbf{a}_{1,2} = \pm \frac{\sqrt{3}}{2} a \hat{x} + \frac{1}{2} a \hat{y}$ and $\mathbf{a}_3 = -a \hat{y}$, where $a$ is the lattice constant between two nearest-neighbor sites as shown in Fig. I (a); we set $a = 1$ hereafter. The Hamiltonian reads as

$$H_{KM} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + i \lambda_{SO} \sum_{\langle \langle i,j \rangle \rangle} \sum_{\sigma} \sigma c_{i\sigma}^\dagger \nu_{ij} c_{j\sigma},$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) a spin $\sigma$ fermion on site $i$ and $\sigma$ runs over $\uparrow$ and $\downarrow$. Here, $\langle \langle \cdots \rangle \rangle$ denotes second-neighbor terms given by vectors $\mathbf{b}_1 = \mathbf{a}_2 - \mathbf{a}_3$, $\mathbf{b}_2 = \mathbf{a}_3 - \mathbf{a}_1$ and $\mathbf{b}_3 = \mathbf{a}_1 - \mathbf{a}_2$ describing the spin-orbit coupling $\lambda_{SO}$. $i = 1, 2, 3$, and $\nu_{ij} = 1$ for counter-clockwise hopping and $\nu_{ij} = 1$ otherwise\cite{47}.

For our numerical study, we consider four time-reversal symmetric model Hamiltonians which are KM model-like: (i) the generalized Kane-Mele (GKM) model, the KM model with a spin-independent real-valued third-neighbor hopping term, (ii) the dimerized Kane-Mele (DKM), the KM model with a biased nearest-neighbor hopping along the $\mathbf{a}_1$ direction, (iii) the $t_L$-KM model, the KM model with 5-th neighbor hopping, and (iv) the $t_{3N}$-dimerized KM model, which is a hybrid of model (i) and (ii).

All of the models are generalized versions of the KM models, and at half-filling, they preserve the particle-hole symmetry. In the non-interacting limit, they host a topological-insulator/trivial insulator phase transition by tuning tight-binding parameters. However, there exists crucial differences among the models. The GKM model (i) and the $t_L$-KM model (iii) preserve the six-fold rotation or $C_6$ symmetry of the honeycomb lattice, whereas the DKM model (ii) and the $t_{3N}$-dimerized model (iv) explicitly break it down to $C_2$ with the bias in the $\mathbf{a}_1$ direction. In the following we will mainly focus on the GKM and DKM models.

The wallpaper or 2D space group of the honeycomb lattice is $p6m$ which is symmorphic and has $D_6$ as its point group. The different models considered are meant to represent different modifications of the bare KM model such that the $D_6$ symmetry is either preserved or broken but which nevertheless exhibits a topological insulator phase transition. However, time-reversal, spin-$S^z$, inversion, and particle hole symmetry are preserved in all these models.

For models (i-iv) that hoppings which are additions to the KM model includes spin-orbit coupling in the form of spin-dependent second nearest neighbor hopping that favors the topological insulator phase. We shall see in models (i-iv) that hoppings which are additions to the KM model will, at sufficient strengths, overcome this tendency of the spin-orbit coupling and stabilize the trivial phase without breaking any symmetries.

Resuming our discussion on symmetry, recall that $D_6 \cong D_3 \times Z_2^{(i)}$, where the (i) superscript in $Z_2^{(i)}$ denotes 2D inversion about the center of the hexagon. Furthermore $D_3 \cong C_3 \times Z_2^{(m)}$ where the (m) denotes reflection about a vertical mirror plane i.e. $Z_2^{(m)} \equiv \sigma_v$ in Schönhflies notation. Moreover, in two dimensions inversion is isomorphic to rotation by $180^\circ$ or $Z_2^{(i)} \cong C_2$. Models (i-iv) are selected to maintain $Z_2^{(i)}$ inversion symmetry but may either preserve or break $D_3$ down to $Z_2^{(m)}$ or completely. A further essential property that is common to these models is the absence of QMC sign problems in their respective Hubbard model incarnations, which are obtained by the inclusion of an on-site Hubbard interaction.

Specializing to two dimensions, the seminal works of Kane and Mele\cite{47,48}, and later Bernevig et. al.\cite{49}, Schwyzer et. al\cite{50}, Kitaev\cite{51}, and Qi et. al\cite{52} showed that with
only time-reversal symmetry the non-interacting topological phases are classified by a \( \mathbb{Z}_2 \) invariant, which is also generalized to three dimensions by Fu and Kane\(^{34} \) and Moore and Balents\(^{34} \). The physical content of this binary topological index is that it enumerates the number parity of Kramers pairs of gapless edge modes at a boundary of the system with the vacuum—−at least for non-interacting gapped band insulators. With the absence of \( S^z \) mixing, the non-interacting occupied bands may be further categorized by their \( S^z \) polarization, and each spin species is topologically non-trivial carrying a non-zero integral Chern number; \( i.e. \) \( C_\sigma \neq 0, \sigma = \uparrow, \downarrow \).\(^{33} \) However, due to time-reversal symmetry, \( C_\uparrow + C_\downarrow = 0 \), and hence we do not expect an Integer Quantum Hall effect. Nevertheless, if the spin Chern numbers\(^{46,50,57} \) are in the non-trivial topological insulator phase or the \( \mathbb{Z}_2 \) odd phase, the non-mixing of \( 2 \) spin sectors, designates this non-trivial phase as being the QSH phase where on the edge, an odd number of helical edge states carry odd phase. The non-mixing of \( 2 \) spin states, the system with the vacuum—at least for non-interacting limits. In this work, we will demonstrate that the classification by \( C_{\text{spin}} \) will not only be applicable in the non-interacting limit, but can also be extended to finite interaction where our main interests lie. It is also clear that under this classification, a topological phase transition between even and odd values of \( C_{\text{spin}} \) must proceed by an odd variation \( \Delta C_{\text{spin}} \in 2\mathbb{Z} + 1 \).

It will be highlighted in the upcoming sections that crystal symmetry will play a crucial role in the nature of such topological transitions.

(i) Generalized Kane-Mele model

We start with the GKM model previously introduced in Ref.\(^{32} \) whose Hamiltonian is given by

\[
H_{\text{GKM}} = -t \sum_{(i,j)} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda_{\text{SO}} \sum_{(i,j)} \sum_{\sigma} \sigma c_{i\sigma}^\dagger \nu_{ij} c_{j\sigma} - t_{3N} \sum_{\langle (i,j) \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma},
\]

where \( \langle (\cdots) \rangle \) third-neighbor terms, and the vectors connecting third-neighbor terms are given by \( c_i = a_i + b_i \).

At \( t_{3N} = 0 \) and finite spin-orbit coupling \( \lambda_{\text{SO}} \), the model Hamiltonian Eq.\(^{2} \) is reduced to the Kane-Mele model\(^{47,48} \) which is a two-dimensional \( \mathbb{Z}_2 \) topological insulator\(^{47,48} \). Like the KM model, the GKM model is invariant under both the time-reversal symmetry and the honeycomb space group \( p6m \) symmetry with its point group \( D_6 \).

In the large \( t_{3N} \) limit of Eq.\(^{2} \), the system is a trivial insulator, implying the GKM model undergoes a symmetry-preserving topological phase transition as a function of \( t_{3N} \). The GKM model can be recast as \( H_{GKM} = \sum_k \Phi_k^\dagger H_{\text{GKM}}^k \Phi_k \), where \( \Phi_k = (c_{A\uparrow}, c_{B\uparrow}, c_{A\downarrow}, c_{B\downarrow}) \) is a 4-component spinor and \( H_k \) reads

\[
H_{\text{GKM}}^k = \begin{pmatrix}
    f(k) & h(k) & -f(k) & h(k) \\
    h^*(k) & -f(k) & h(k) & f(k)
\end{pmatrix},
\]

where \( h(k) = g(k) - t_{3N} \sum_i e^{ik \cdot a_i}, g(k) = -t \sum_i e^{ik \cdot a_i}, \) and \( f(k) = 2\lambda_{\text{SO}} \sum_i \sin(k \cdot b_i) \); note that \( a_i, b_i \) are real-space vectors to describe nearest, second and third-neighbor hoppings. For most \( t_{3N} \) values, the GKM model is gapped. However a simple analysis of the dispersion will show a gap closure at \( t_{3N}^c = \frac{t}{3} \) independent of \( \lambda_{\text{SO}} \), and permits a change in the topological \( \mathbb{Z}_2 \) index. The schematic phase diagram is shown in Fig.\(^{2} \) (a). For \( t_{3N} < t_{3N}^c \), the system is a \( \mathbb{Z}_2 \) TI, whereas for \( t_{3N} > t_{3N}^c \), the system is a trivial insulator. Thus, there exists a topological phase transition at \( t_{3N} = \frac{t}{3} \).

The non-interacting band structure of the GKM model is depicted in Fig.\(^{2} \) (b). The chosen momenta are along the direction depicted as blue arrows in Fig.\(^{1} \) (b). The gap closes at three TRIM points: \( M_{1,2,3} \), instead of the Dirac point \( K_{1,2} \).

FIG. 2. (Color online) (a) Schematic phase diagram of the GKM model. (b) The noninteracting band structure of the GKM model at \( t_{3N}^c = \frac{t}{3} \) (here using \( \lambda_{\text{SO}} = 0.1t \)). The presented momenta are chosen along the path depicted as blue arrows in Fig.\(^{1} \) (b). The gap closes at three TRIM points: \( M_{1,2,3} \), instead of the Dirac point \( K_{1,2} \).
the \( M_{1,2,3} \) points as well as at the \( K_{1,2} \) points, yielding 5 Dirac points.

Displayed in Fig. 3 are results of a band structure computation in a strip geometry of the GKM model demonstrating the existence of edge states with energies that traverses the bulk energy gap. By counting the number of Kramers pairs of edge states per edge\(^{39,48}\) we note that the GKM model undergoes a topological phase transition as a function of \( t_{3N} \), whereby an odd number of Kramers pairs characteristic of a \( \mathbb{Z}_2 \) topological insulator phase turns into an even number characteristic of a topologically trivial phase\(^{39,48}\). Although the two pairs of Kramers helical states in Fig. 3(b) shows that the GKM model at \( t_{3d} \) is a \( \mathbb{Z}_2 \) trivial insulator\(^{48} \) for each spin flavor the spin Chern number, \( C_\sigma \) is even and nonzero. Namely, \( |C_\sigma| = 2 \neq 0 \) implying nontrivial edge states\(^{38} \) albeit ones not protected by time-reversal symmetry. In addition, since the bulk gap of the GKM model closes at the three time-reversal invariant momenta: \( M_1, M_2 \) and \( M_3 \) [in Fig. 2(b)], we expect that the spin Chern number will suffer an odd variation\(^{50} \) \( \Delta C_\sigma = 3 \) signaling a topological transition from the \( C_\sigma = \pm 1 \) state to the \( C_\sigma = \mp 2 \) state for spin-up and spin-down fermions, respectively.

Note that the appearance of these three Dirac cones, each carrying unit Berry monopole charge, is mandated by the \( C_3 \) crystal symmetry, since \( M_1, M_2, M_3 \) transform amongst themselves in a non-trivial irreducible representation of the unbroken \( C_3 \) symmetry. It must be mentioned that a topological transition with \( \Delta C_\sigma \) odd may also involve an even number of Dirac cones as is the case in the KM model where a staggered \( AB \)-site potential competes with spin-orbit coupling. In this instance, however, the inversion symmetry is broken from the pristine graphene band structure allowing the transfer of an odd amount of Chern number. This is because under broken inversion symmetry, the \( K_1 \) and \( K_2 \) are not required to contribute equally in the transfer of Chern number. The GKM model, however, differs by always maintaining inversion symmetry and in fact the \( M \) points are individually inversion symmetric points. Lastly, from the perspective of the spin Chern numbers, both phases are nontrivial—they exhibit edge robust states so long as \( S^z \) symmetry is preserved, and are classified by the spin Chern number\(^{56,57} \).

(ii) Dimerized Kane-Mele model

The second model we consider, the DKM model is expressed by the following Hamiltonian\(^{49} \)

\[
H_{DKM} = - \sum_{\langle i,j \rangle} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda_{SO} \sum_{\langle i,j \rangle} \sum_\sigma \sigma c_{i\sigma}^\dagger \tau_{ij} c_{j\sigma},
\]

where \( t_{ij} = t_d \) when \( r_j = r_i + a_1 \), whereas \( t_{ij} = t \) otherwise. One can recast the Hamiltonian as \( H_{DKM} = \sum_k \Phi_k^\dagger H_{DKM}^D \Phi_k \), where \( H_k \) is

\[
H_{DKM}^D = \begin{pmatrix}
  f(k) & h'(k) \\
  h'(k)^* & -f(k)
\end{pmatrix}
\]

where \( h'(k) = -t_d e^{i k \cdot a_1} - t \sum_{i=2,3} e^{i k \cdot a_i} \). At \( t_d = t \), Eq. 3 is reduced to the KM model. This kinetic Hamiltonian explicitly breaks the \( C_3 \) subgroup of \( D_6 \) resulting in the point group \( Z_2^{(m)} \times Z_2^{(i)} \) which is a mirror reflection perpendicular to \( a_1 \) and inversion or 180° rotation. A schematic of its phase diagram and band structure at the critical point are shown in Fig. 4.

A topological phase transition will occur by tuning \( t_d \) to twice the nearest-neighbor hopping. In this instance
the conduction and valence bands touch at a single Dirac cone at the $M_1$ point when $t_d^c = 2t$ (again independent of the value of $\lambda_{SO}$). This critical point separates a trivial and the topological insulator phase, as shown in Fig. 4(b). Thus, the trivial insulator phase $(t_d > t_d^c)$ has zero spin Chern number and its variation is $|\Delta C_\sigma| = 1$ during the topological phase transition.

From the symmetry perspective, the transition in the DKM model greatly differs from the GKM model since $C_3$ is completely broken leaving only mirror and inversion $Z_2^{(m)} \times Z_2^{(i)}$ symmetries of the original $D_6$ point group. Besides the trivial $\Gamma$ point, the $M_1$ point – where the single critical Dirac cone appears – is the only inversion symmetric point which also respects the residual mirror symmetry. Thus, the topological phase transition proceeds as a unit change of spin Chern number and hence the topological $Z_2$ index. In summary, we see that at least in the non-interacting limit, point group symmetry can greatly influence the form of the electronic structure of the critical point straddling a QSH phase and trivial phase.

(iii) $t_L$ Kane-Mele model

The next model on our list is the $t_L$-KM model which supplements the KM model with a four-lattice-constant-range hopping of strength $t_L$. Similar to the $t_{3N}$ term in the GKM model, the tight-binding parameter, $t_L$, in the $t_L$-KM model preserves the $D_6$ point group symmetry of the honeycomb lattice. The model Hamiltonian reads as

$$H_{t_L} = -t \sum_{\langle i,j \rangle} \sigma c_{i\sigma}^\dagger c_{j\sigma} + i\lambda_{SO} \sum_{\langle i,j \rangle} \sigma c_{i\sigma}^\dagger \nu_{ij} c_{j\sigma}$$

where the first two terms describe the KM model, and in the third term $\nu_{ij}$ denotes the real-valued hopping with the distance of $4a$. The lattice structure is shown in Fig. 6(a). Similar to the GKM model, in the non-interacting limit, there exists a topological phase transition from the $Z_2$ topological insulator to the trivial insulator state. In this instance, the boundary is located at $t_L = \frac{1}{4}t$ with three $M_1$, $M_2$, $M_3$ Dirac cones. For simplicity, we do not discuss the properties of the edge dispersion as they are qualitatively similar to the GKM model.

(iv) $t_{3N}$-Dimerized Kane-Mele model

The final model we consider is the $t_{3N}$-dimerized KM model which is constructed by the combination of one third-neighbor hopping (instead of three) and the bond dimerization in the KM model. As shown in Fig. 6(b), the solid blue lines denote the dimerized bonds with $t_d$ strength and the purple dotted lines denote the diagonal $t_{3N}$ hopping. The Hamiltonian reads as

$$H_{t_{3N}} = -t \sum_{\langle i,j \rangle} \sigma c_{i\sigma}^\dagger c_{j\sigma} + i\lambda_{SO} \sum_{\langle i,j \rangle} \sigma c_{i\sigma}^\dagger \nu_{ij} c_{j\sigma}$$

where $t_{ij} = t$ if $r_j = r_i + a_3$; otherwise $t_{ij} = t$. The first two terms give the DKM model. The real-valued diagonal $t_{3N}$ hopping is selected along $c_3 = \sqrt{3}a x - a y$.

The simultaneous presence of the dimerized bonds and $t_{3N}$ bonds breaks the $Z_2^{(m)}$ mirror reflection and $C_3$ rotational symmetry of $D_6 \cong (C_3 \times Z_2^{(m)}) \times Z_2^{(i)}$. Thus the $D_3$ subgroup is completely broken, however the $Z_2^{(i)}$ inversion symmetry is still respected. There also exists a topological phase transition between the $Z_2$ topological insulator...
III. NUMERICAL EVALUATION OF TOPOLOGICAL INDICES

For each generalization or variant of the Kane-Mele model, an on-site Hubbard interaction will be added, and interacting phase diagrams containing the trivial and topological phases are obtained via QMC simulations. But first we review and discuss the quality of numerically computed topological indices of the finite clusters in the non-interacting limit.

The first and most important topological index is the Z$_2$ invariant of a two-dimensional non-interacting topological insulator. When inversion symmetry is present, the noninteracting Z$_2$ invariant is determined as

$$ (-1)^{\nu} = \prod_{k \in \text{TRIM}} \prod_{m} \xi_{2m}(k_i), $$

where $\xi_{2m}(k_i)$ is the parity of 2$m$-th occupied Hamiltonian eigenstate at the time reversal invariant momentum (TRIM); in the KM models, they are $\Gamma$ and $M_{1,2,3}$ as depicted in Fig. 1(b). (2$m$ – 1)-th and 2$m$-th states share the same parity and are a Kramers pair, and therefore should only be counted once in the determination of the topological invariant. The time-reversal invariant topological insulator phase is stable in the weakly interacting limit and the Z$_2$ index is also well defined in the case of weak-interactions. It may be obtained conveniently from the zero-frequency single-particle Green’s function. Specialized to the presence of inversion symmetry, the Fu-Kane expression Eq. (6) with interactions generalizes to

$$ (-1)^{\nu} = \prod_{k_i \in \text{TRIM}} \tilde{\eta}(k_i), $$

where $\tilde{\eta}(k_i)$ are the parity eigenvalues (one per Kramer’s pair) of the R-zero states of the zero-frequency Green’s functions at TRIM. R- and L-zeros are terms used to refer to eigenfunctions of the zero-frequency single particle Green’s function $G_\sigma(i\omega_n,0,k)$. Eigenvectors $|v_{n k \sigma}\rangle$ with band index $n$, spin $\sigma$, crystal momentum $k$ and eigenvalue such that

$$ G_\sigma(i\omega_n,0,k)|v_{n k \sigma}\rangle = \lambda_{n k \sigma}|v_{n k \sigma}\rangle $$

are called R-zeros when $\lambda_{n k \sigma} > 0$, and L-zeros when $\lambda_{n k \sigma} < 0$. In the non-interacting limit, R-zeros correspond to occupied states below the Fermi-energy. (Note that Eq. (8) is often expressed in terms of the inverse Green’s function. Since our system consists of 2 x 2 matrices for each spin value, we can equivalently express the formula directly in terms of the Green’s function. One need only exercise care in the meaning of L-zeros, R-zeros, and singularities of the Greens functions.) The singular case $G_\sigma(i\omega_n,0,k) \sim 1/\omega$ as $\omega \to 0$ corresponds to the presence of gapless quasiparticles where a gapped topological insulating phase is not well-defined. The interesting case of $G_\sigma(i\omega_n,0,k) = 0$ or $\lambda_{n k \sigma} = 0$ is an indication of the onset of an interaction driven metal-insulator transition in the Brinkman-Rice sense. Either a pole singularity or zero of $G_\sigma(i\omega_n,0,k)$ may induce a change in the topological index. This expression for the $(-1)^{\nu}$ index is immensely useful and convenient in determining the topological phase of an interacting time-reversal invariant system, but is however limited to the inversion symmetric situations.

The second topological index that will concern us is the spin Chern number defined by Eq. (1) in the QSH context. The Chern numbers $C_{\sigma}$ of the $S^z$ projected bands are expressed in terms of one particle spectral projectors as

$$ C_{\sigma} = \frac{i}{2\pi} \int d^2k \epsilon^{\nu\mu} \text{Tr} [P_\sigma(k) \partial_\mu P_\sigma(k) \partial_\nu P_\sigma(k)], $$

where $P_\sigma(k) = \sum_n |v_{n k \sigma}\rangle \langle v_{n k \sigma}|$ is the single particle spectral projector onto R-zero states. Here we have used the Berry curvature in $k$-space interpretation of the spin-Chern number as opposed to the original formulation in terms of twisted boundary conditions. We will often refer to $C_{\sigma}$ as the spin Chern number as well, since in the case of $S^z$ conservation—which applies to all cases considered in this work—the spin Chern number is proportional to $C_{\sigma}$, up to a sign determined by convention. More importantly, it is the parity–even or oddness–of $C_{\sigma}$, not its sign, that determines the time-reversal topological Z$_2$ index. When $S^z$ is not a good quantum number, the expression Eq. (11) for the spin Chern number defined in the thermodynamic limit—that is without twisted boundary conditions—may be generalized to the case without $S^z$ conservation rigorously. Even though we will not consider these situations in this work, we would like to point out that it is certainly possible to generalize our numerical methods for the computation of the spin Chern number and hence the Z$_2$ index for interacting systems where $S^z$ is not conserved.

The inversion symmetric invariant of Eq. (7) and the $S^z$ conserving spin Chern number of Eq. (11) exhibit a complementary relationship. The former is only applicable to inversion symmetric Hamiltonians, but does not require the $S^z$ conservation. The latter, however, does not require inversion symmetry but is nevertheless conveniently computed only for $S^z$ conserving Hamiltonians. Moreover, the spin Chern number, which may be any integer value in the thermodynamic limit, carries more information and thus a finer topological classification than the Z$_2$ index, and can remain quantized even when time-reversal symmetry is broken. However there is an obvious bias towards...
favoring Eq. (7) because by construction it is always integrable in finite sized systems. Whilst Eq. (9) will in general yield non-integral values in finite-size systems where the Berry curvature over the BZ is no longer smooth. The practicalities of numerically computing the spin Chern number and its sensitivities to finite system size will be the subject of our next discussion.

For an interacting system, we compute the zero-frequency single-particle Green’s function with QMC and then determine its eigenvectors and eigenvalues. The determination of the topological response of a system by the zero-frequency Green’s function has been demonstrated in both the non-interacting and interacting limit in Ref. [41]. Both expressions (7) and (9) sidestep difficulties associated with using twisted boundary conditions [42], which requires multiple numerically expensive calculations of a non-degenerate ground state. It is also inapplicable when artificial edge degeneracies are encountered and is usually only practical with exact diagonalization [39].

The fact that both of the expressions and their interacting generalizations [41] only rely on the zero-frequency single-particle Green’s functions, is very convenient since more sophisticated numerical simulation methods like QMC and Dynamical Mean-field Theory [43] (which cannot provide ground state wave functions) can be implemented in determining the topological phases with interactions. The zero-frequency property also implies that numerical analytical continuation does not need to be employed. The computation of Eq. (7) for finite-size interacting systems has been previously performed in Refs. [32,33], and is straightforward. There is, however, a requirement that only cluster shapes with BZs containing a TRIM points may be studied with this method.

By contrast computing, Eq. (9) for interacting systems is a relatively new enterprise and we describe our numerical method for its computation in finite sizes in Appendix B. Our results for the non-interacting GKM model are shown in Fig. 7. It is evident that, even in the non-interacting limit, this method of evaluating the topological response of a system that we will turn to shortly. However, the source of the “non-integerness” of the Chern number is associated with the need to approximate the k-space gradients of projector $P_{\sigma}$ from a finite set of points in the BZ, cf Eq. (10). This also implies that – rigorously speaking – an exact integer value is only ever attainable in the thermodynamic limit. This is an important implication since it means that topological classification as captured by the Chern number and its myriad generalization is an effect that is only rigorously stably protected in the thermodynamic limit. This is intuitively clear since, only in the thermodynamic limit do the energy gaps between smoothly connected Bloch states collapse. The remaining finite energy gaps are the band gaps that are the source of the topological protection of a ground state.

The finite-size computations of Eq. (9) shown in Fig. 7 with non-integral results are an honest reflection of the limitation of working with finite-size clusters. We note that an alternative method by Fukui et al. [44] sidesteps this with a construction which always yields an integer result. However this can be misleading since the accuracy of the results requires a critical mesh size, which Fukui et al. have estimated. Moreover, the integer-valued results obtained by their method excludes the possibility of using a finite-size scaling analysis to judge the convergence of their results and is a weakness in their method. These considerations also apply to the integral inversion $Z_2$ invariant $(-1)^\nu$ which should and does fluctuate with cluster size: There is a shift in boundaries based on this invariant with changing cluster size and shape.

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The need for large cluster sizes, however, is compensated by the QMC method which provides access to ground state correlators of cluster sizes significantly larger than those manageable by exact diagonalization. Furthermore, it is not necessary to have a manifold of ground states (which also has to be of a sufficient density) as is required with the twisted boundary conditions.
method. Another important point to note from Fig. 4 is that at a fixed cluster size, the tendency to an integer value improves, the further away the tuning parameter is from the critical point. Furthermore the many-body excitation gap remains open through that portion of parameter space and the single particle Green’s function at zero frequency develops no poles or singularities, permitting us to invoke the principle of adiabatic continuity and infer the thermodynamic value of the spin-Chern number of the entire portion of phase space from the finite-size scaling in the large $t_{3N}$ limit and when $t_{3N} = 0$.

With this information the sudden discontinuity in the numerical Chern number can then be used to pinpoint the critical point. This is the general strategy that we employ in mapping out a phase diagram of both non-interacting and interacting models. In the case of an interacting model phase diagram, we have one more tuning parameter which is the interaction strength itself. The free model can then be trivially classified and when robust excitation gaps persists above the numerical ground state, the principle of adiabatic continuity can be used to reliably map out a phase diagram from sudden jumps in the numerical Chern number. As a consistency check, we also compare the spin Chern number with the $Z_2$ invariant using Eq. (7) at various tight-binding parameters and interaction strength, as shown in Fig. 8.

IV. EFFECTS OF INTERACTIONS IN HUBBARD MODEL EXTENSIONS OF THE KANE-MELE VARIANTS

We now come to the main part of the paper where we discuss the effects of the Hubbard interaction on interacting topological insulator models. To obtain ground state correlators and capture correlation effects, we use projective quantum Monte Carlo to study interacting variants of the KM model, Eq. (2)-(5) to which an on-site Hubbard term is added, $H \rightarrow H + \frac{U}{2} \sum_i (n_i - 1)^2$ where $U > 0$ is the strength of the repulsive on-site Hubbard interaction and $n_i$ is the number operator on site $i$. In our QMC calculations, the number of sites is $N = 2 \times L^2$, where $L$ takes the values 6, 12 and 18. The largest system sizes are far beyond current capabilities for exact diagonalization studies, rendering our “unbiased” calculations on interaction effects in topological systems important for going beyond mean-field approaches and the severe finite-size limitations of exact diagonalization studies. The QMC methodology is described in detail in Appendix A.

(i) Generalized Kane-Mele Hubbard model

We first turn our attention to interaction effects in the GKM-Hubbard model, i.e. $H_{GKM} + U$. Previously in Ref. [33], the correlation effects were discovered to result in a shift of the phase boundary that can be accurately computed with QMC simulations: with increasing $U$, $t_{3N}$ shifts to larger values (compared to the vertical blue line in Fig. 8). This behavior was identified by evaluating the $Z_2$ invariant from exploiting the inversion symmetry of the single-particle Green’s function and using Eq. (7). The QMC results showed that at $U = 4t$ the topological phase transition boundary moves into the trivial insulator phase by roughly 10%. Thus, correlation stabilizes the topological phase in the GKM-Hubbard model.

Here we demonstrate that the topological phase transition can also be clearly identified by computing the spin Chern numbers as shown in the lower panels of Fig. 8. We chose intermediate interaction strengths $U = 3t$ and $U = 4t$, which are below the threshold required to induce magnetic ordering or any other symmetry breaking. For comparison, we also depict the $Z_2$ invariant vs $t_{3N}$ for the 12 $\times$ 12 cluster. For both $U$ values, Figs 8(a) and (b) show marked changes in the spin Chern number at the same locations, as the $Z_2$ invariant varies for the 12 $\times$ 12 cluster (guided by the dotted lines).

We observe that in the GKM-Hubbard model the QMC sampling still maintains the time-reversal symmetric relation $C_\uparrow = -C_\downarrow$ within tiny error bars, so long as $t_{3N}$ is far from the phase boundary. When the value of $t_{3N}$ is close to the topological phase transition, one needs to
increase the sampling to recover the relation. Similar to the non-interacting limit, the spin Chern numbers in Figs. 9 converge to integers only as $t_{3N}$ is far away from the critical point. The spin-up Chern numbers in the $Z_2$ regime is $C_\uparrow \simeq +1$ ($t_{3N} = 0.2t$) and turns to $C_\uparrow \simeq -2$ after the topological phase transitions ($t_{3N} = 0.5t$), indicated in the $12 \times 12$ and $18 \times 18$ clusters. The significant variation in $C_\sigma$, $|\Delta C_\sigma| \simeq 3$, can be used to identify the parameter-driven topological phase transition at finite $U$ in the finite-size clusters. Moreover, by adiabatic continuity to the non-interacting limit, we can also confidently identify the two phases between the topological phase transition.

Next we present the finite-size analysis for the spin Chern number in the GKM-Hubbard model, shown in Fig. 9. Since only three different sizes, $6 \times 6$, $12 \times 12$ and $18 \times 18$ are available, we are unable to fully capture the scaling behavior. However, the trends are sufficient to infer the value of the thermodynamic spin Chern number. On the other hand, the judgement can be also arrived at by the principle of adiabatic continuity to the non-interacting limit of the GKM model. We tentatively consider the Chern number scaling as $1/L^2$ in Fig. 9 (or $1/L$, not shown here): showing that as the value of $t_{3N}$ is far away from the critical point, the spin Chern numbers extrapolate well to whole integers, $C_\uparrow = 1$ or $C_\uparrow = -2$ in the thermodynamic limit. Thus, these scaling curves are still helpful in distinguishing the topological states with $C_\sigma = 1$ and $C_\sigma = -2$.

Note that near the transition (about $t_{3N} = 0.33t$ and $0.34t$), the scaling analysis is less reliable and one needs bigger sizes to determine the behavior. However, it is still helpful in determining the location of the topological phase transition. In Fig. 9 (a), we can recognize that at $t_{3N} = 0.34t$ the spin Chern number shows a drop with increasing system size; thus it is a trivial state. By contrast, Fig. 9 (b) shows that the spin Chern number at $t_{3N} = 0.34$ does not show a clear drop, suggesting that it is still in the topological insulator regime. Thus, interactions stabilize the topological phase in the GKM-Hubbard model. Note that for $t_{3N}$ values away from the critical value, the finite size scaling behavior is much clearer in terms of how the thermodynamic limit is approached.

Although the values of the spin Chern numbers suffer from strong finite-size effects, the topological phase transition boundary determined by the topological invariant in the GKM-Hubbard model has weak finite-size dependence. For $U = 3t$, on the $6 \times 6$, $12 \times 12$, and $18 \times 18$ clusters, $t_{3N}^c = 0.341t$, $0.337t$ and $0.353t$, respectively. For $U = 4t$, $t_{3N}^c$ are $0.394t$, $0.347t$ and $0.345t$, respectively, suggesting the spin Chern number is a reliable means to detect topological phase transitions in interacting systems.

These interaction effects that cause the critical boundary in phase space to shift must originate from the dynamical quantum fluctuations, since the Hartree-Fock mean-field theory is unable to capture any phase boundary shift (for the $U$ values we consider below the magnetic phase transition)\textsuperscript{73}. We were not able to develop a perturbative argument for this shift, either.

(ii) Dimerized Kane-Mele Hubbard model

We next turn to the DKM-Hubbard model,\textsuperscript{10} $H = H_{DKM} + U$. Recall that at $U = 0$, the critical point occurs at $t_d^c = 2t$ and is independent of value of $\lambda_{SO}$. Similar to the GKM-Hubbard model, correlation effects induce a shift of the phase boundary, but the critical value of $t_d$ moves towards (into) the topological phase. In other words, correlation destabilizes the topological insulator phase—a behavior opposite to the GKM-Hubbard model. With finite interactions at $U = 2t$ and $\lambda_{SO} = 0.2t$, $t_d^c$ is determined within 1.94 and 1.96 by observing the Green’s function behavior and the $Z_2$ topological invariant$\textsuperscript{78}$.

Here we also employ the QMC combined with the computation of the spin Chern number using Eq. (9) and the $Z_2$ index using Eq. (7). Likewise, the values of $U$ we considered were below the magnetic transition. Figs. 11 (a) and (b) show $C_\uparrow$ and the $Z_2$ index vs $t_d$ for $U = 2t$ and $4t$, respectively. In the $12 \times 12$ cluster (red circles), we can see that the spin Chern number jumps at $t_d = 1.97t$ for $U = 2t$ and $t_d = 1.76t$ for $U = 4t$, and, simultaneously, the value of the $Z_2$ index turns from $(-1)^\nu = -1$ to 1 (guided by the dot lines). More strongly in the $12 \times 12$ cluster, one sees that the topological phase transition occurs between the $|C_\sigma| = 1$ state to the $|C_\sigma| = 0$ state and a variation $|\Delta C_\sigma| \approx 1$.

Surprisingly, compared to the GKM-Hubbard model, the interaction in the DKM model brings about a more significant shift in the location of the topological phase transition. In the $L = 12$ cluster, $t_d^c$ at $U = 2t$ is estimated to be $1.97t - 1.98t$, whereas at $U = 4t$ it lies within $1.76t - 1.77t$. The critical point has shifted by roughly 25%. The DKM-Hubbard model also has weaker finite-size effects on the topological phase boundaries. For the $L = 6$ cluster, $t_d^c$ are estimated around $1.95t - 1.96t$ and $1.75t - 1.76t$ for $U = 2t$ and $4t$, respectively. The compar-
FIG. 10. (Color online) The $Z_2$ invariant $(-1)^n$ (upper panels, for $L = 12$ only) and $C_d$ (lower panels) for the DKM-Hubbard model as a function of $t_d/t$ at (a) $U = 2t$ and (b) $U = 4t$. $\lambda_{SO} = 0.2t$ and the systems sizes are chosen as $6 \times 6$ (black squares) and $12 \times 12$ (red circles). At $t_d = t$, the system reduces to the standard KM model and $t_d = 2t$ (vertical blue line) is the critical point for the non-interacting limit. For the sake of clarity, only the data for $C_d$, $n = 1$ is presented here.

FIG. 11. (Color online) The $Z_2$ invariants for interacting and noninteracting cases in the (a) $t_L$-KM model and (b) $t_{3N}$-dimerized KM model at $t_d = 1.8t$. For reference purposes, the non-interacting $Z_2$ invariant were computed and presented as the blue lines using $L \times L = 1200 \times 1200$ clusters. The symbols depict the interacting $Z_2$ invariant by the QMC for $U = 4t$ on $6 \times 6$ (black squares) and $12 \times 12$ (red circles). All calculations are preformed with $\lambda_{SO} = 0.4t$.

theory – such as deciding the number of Dirac cones – between the topological insulator phase and the normal insulator phase, it is reasonable to expect that crystal symmetry will have a significant role to play in shifting phase boundaries.

The QMC results of the correlation effects on these two models are displayed in Fig. 11 where we still used $\lambda_{SO} = 0.4t$ and $U = 4$ to compare with Fig. 9 and Fig. 10. For simplicity, we only show the $Z_2$ invariants as a function of the tight-binding parameters: $t_L$ and $t_{3N}$ in Eq. 1 and Eq. 5, respectively. Note that, near the critical point, $(-1)^n$ shows a poor approximation to an integer value (not $\pm 1$ or $\mp 1$), meaning that more QMC samplings are required. However, we still can distinguish the locations of the correlated topological phase boundaries. From Fig. 11(a), it is clear that with finite interaction, the topological phase transition shifts towards (into) the trivial insulator regime; the topological phase is enlarged and thus correlation stabilizes the topological insulator state in the $t_L$-KM model. For the $6 \times 6$ cluster, $t_L^* = 0.352t - 0.354t$, and for the $12 \times 12$ cluster, $t_L^* = 0.352t - 0.355t$. Like the GKM model, the $t_L^*$ has weak finite-size effect on the phase boundaries.

In the next panel, Fig. 11(b) exhibits the interacting $Z_2$ invariant against the $t_{3N}$ parameter for the $t_{3N}$-dimerized KM model at $t_d = 1.8t$. The non-interacting limit, $t_{3N}^* = 0.2t$, is indicated by the blue line. Turning (iii) $t_L$- and $t_{3N}$-Dimerized Kane-Mele Hubbard models

Lastly, we present QMC results for the on-site Hubbard models of the $t_L$-Kane-Mele model Eq. 1 and the $t_{3N}$-dimerized KM model Eq. 5. These two models represent polar opposites with regard to their non-interacting hopping Hamiltonians. The former like the GKM model preserves the full $D_6$ point group, whilst the latter breaks it down almost completely to just the inversion subgroup $Z_2^{(t)}$. Thus, the $t_{3N}$-dimerized KM model is even less symmetric than the DDM model. The motivation for considering these other variants is to demonstrate more examples of interacting TI phases and the role crystal symmetry or lack thereof might play and help contrast the different outcomes of explicitly breaking or preserving the crystal symmetry of the underlying KM model. Given that for the hopping Hamiltonians that we have set out to study, the crystal symmetry already greatly influences the low-energy character of the critical
on interaction, the phase boundary moves towards (into) the topological state regime; thus correlation destabilizes the topological insulator phase. We have numerically examined that with finite bond dimerization, the topological critical points are always pushed towards the topological insulator regime under correlation.

Our observations of the effects of Hubbard-type interactions on these KM model variants show a systematic pattern: The stability of the topological insulator phase as measured by its occupied volume in the phase diagram is diminished when more of the symmetries of the $D_6$ point group of the lattice are explicitly broken by the Hamiltonian. A posteriori, we elevate our observations to a speculative conjecture of a principle: in the absence of any spontaneous symmetry breaking, the Hubbard interaction will displace the critical line of the interacting topological quantum phase transition in favor of the normal insulator phase if fewer crystal point group symmetries – but which must include inversion – are present in the non-interacting portion of the tight-binding Hamiltonian. The condition regarding spontaneous symmetry breaking excludes competition with magnetic and density-waves phases. This is important to state since at very strong coupling either phase gives way to the Néel ordered phase. It is worth reiterating that due to the special form of these Hamiltonians at half-filling, the QMC methodology employed is free of sign-problems and is essentially an exact method for finite clusters up to statistical noise; which can always be systematically improved with greater sampling. In a related study of the plaquette KM model, which is not too dissimilar from the ones we have considered, qualitatively consistent results are obtained.

V. DISCUSSIONS

We make a few remarks regarding low energy effective theories and present some related speculations. As was previously mentioned, mean-field calculations at the level of the Hartree-Fock approximation in the KM model[17] and also our own computations[23] for models Eqs. (2)-(4) are unable to demonstrate a continuous shift in the topological quantum phase transition boundaries at weak coupling, although a transition to a magnetic state does occur at strong coupling. We rationalize this by noting that the Hubbard $U$ in two dimensions for a low energy effective critical field theory of gapless linearly dispersing Dirac fermions is irrelevant under scaling. In fact, as is well known[22] even in the case of long-range Coulomb interactions in graphene, which is a archetype for this variety of field theory, a Renormalization Group (RG) analysis also produces the conclusion that the Dirac nodes are perturbatively stable, albeit with anomalous scaling dimensions due to quantum fluctuations. Thus the phase boundary shifts – significantly observable only at relatively large $U \sim 3 t$ – that we have observed in our QMC exact computations are effects at intermediately strong interactions, which is beyond the weak-coupling low energy-effective theory description. The implications are that the standard field theoretic RG computations at one loop order would be unreliable in capturing the intermediate strong coupling physics of interest.

Nevertheless, we speculate that an explanation of the dichotomous behavior of the phase boundary shifts must involve the fact that there are a different number of Dirac cones present at the critical topological transition point (three in the GKM and $t_L$-KM models but one in the DKM and $t_{3N}$-dimerized KM models) and that this is the main influence of point group symmetry to the low energy physics. It is tempting to relate our observations to a large-$N$ study[29] of graphene with Hubbard interactions, but we are cautious and reluctant to since $N = 1, 3$ is a very small value of $N$. In spite of this, Functional Renormalization Group (fRG) computations or more recent dimensional regularization studies[30,31] applied to the Hubbard graphene system have been encouraging in describing physics near strong coupling. We will leave these very interesting lines of investigations for future work, as these computations are by no means trivial undertakings.

VI. SUMMARY AND CONCLUSIONS

In this work we have analyzed variants of the archetypical model of a time-reversal symmetric topological insulator, the Kane-Mele model. These generalized models Eqs. (2)-(5) exhibit various space group symmetries of the honeycomb lattice on which they are formulated. In the non-interacting limit, all of the models exhibit a topological phase transitions between a $\mathbb{Z}_2$ topological insulator phase and a normal insulating phase. By means of the unbiased QMC method, we further study the interacting variants of these model systems by including on-site Hubbard interactions. The determinant QMC method that we employ is free of sign problems (at half-filling which is the only filling considered) and is essentially exact up to statistical sampling noise. The regime that interests us most is the intermediate strong $U$ regime before magnetic order sets in. We demonstrate that the topological phase of our numerically exact interacting ground states can be ascertained by computing either the $\mathbb{Z}_2$ invariant or the spin Chern number $C_\sigma$ via the zero-frequency single-particle Green's function. Thus our work is a numerical implementation of the theoretical proposal of Refs. [11] and [12] for finite-size clusters using reliably accurate QMC. The spin Chern number had not been previously computed with QMC, and we argue on technical grounds that it is complementary to the inversion symmetry based expression for the $\mathbb{Z}_2$ invariant.

Accompanied with finite-size scaling analyses and adiabatic continuity to non-interacting limits, – which we numerically observe – we argue that the spin Chern number is a robust classification method of interacting TT’s. Moreover the spin Chern number may be utilized in cir-
cumber of circumstances where inversion and even time-reversal symmetry are absent, and may be generalized to the case where $S^z$ conservation is absent.\footnote{M. W. Young, S.-S. Lee, and C. Kallin, Phys. Rev. B 78, 125316 (2008)} Our numerically exact QMC results suggest that quantum fluctuations from intermediate strong interactions can act to either stabilize or destabilize the topological phase, depending on whether the hopping terms preserve or break lattice symmetries when the lattice point group $D_6$ is explicitly broken down to a subgroup containing $Z_2^{(i)}$ inversion by the tight-binding Hamiltonian, and stabilized when the full $D_6$ symmetry is preserved. We speculate that the mechanism by which this acts is through influencing the form of low energy theory at the quantum critical point - which needs to be handled beyond perturbatively weak coupling - and suggest further avenues of investigation. We hope our work will help stimulate further studies in this direction and provide a baseline for the general expectations for unbiased calculations of correlation effects on topological phase transitions.

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\begin{thebibliography}{99}
\bibitem{Young2008} M. W. Young, S.-S. Lee, and C. Kallin, Phys. Rev. B 78, 125316 (2008).
\bibitem{Pesin2010} D. Pesin and L. Balents, Nat. Phys. 6, 376 (2010).
\bibitem{Kargarian2010} M. Kargarian and G. A. Fiete, Phys. Rev. B 82, 085106 (2010).
\bibitem{Li2010} R. Li, J. Wang, X.-L. Qi, and S.-C. Zhang, Nat. Phys. 6, 284 (2010).
\bibitem{Hohenadler2011} M. Hohenadler, T. C. Lang, and F. F. Assaad, Phys. Rev. Lett. 106, 100403 (2011).
\bibitem{Hohenadler2012} M. Hohenadler, Z. Y. Meng, T. C. Lang, S. Wessel, A. Muramatsu, and F. F. Assaad, Phys. Rev. B 85, 115132 (2012).
\bibitem{Zheng2011} D. Zheng, G.-M. Zhang, and C. Wu, Phys. Rev. B 84, 205121 (2011).
\bibitem{Swingle2011} B. Swingle, M. Barkeshli, J. McGreevy, and T. Senthil, Phys. Rev. B 83, 195139 (2011).
\bibitem{Maciejko2010} J. Maciejko, X.-L. Qi, A. Karch, and S.-C. Zhang, Phys. Rev. Lett. 105, 246809 (2010).
\bibitem{Kargarian2013} M. Kargarian and G. A. Fiete, Phys. Rev. Lett. 110, 156403 (2013).
\bibitem{Levin2012} M. Levin and A. Stern, Phys. Rev. B 86, 115131 (2012).
\bibitem{Levin2009} M. Levin and A. Stern, Phys. Rev. Lett. 103, 196803 (2009).
\bibitem{Moore2008} J. E. Moore, Y. Ran, and X.-G. Wen, Phys. Rev. Lett. 101, 186805 (2008).
\bibitem{Neupert2011} T. Neupert, L. Santos, S. Ryu, C. Chamon, and C. Mudry, Phys. Rev. B 84, 165107 (2011).
\bibitem{Ruegg2012} A. Ruegg and G. A. Fiete, Phys. Rev. Lett. 108, 046401 (2012).
\bibitem{Wan2011} X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).
\bibitem{Hohenadler2013} M. Hohenadler and F. F. Assaad, J. Phys. Cond. Matt. 25, 143201 (2013).
\bibitem{Fiete2012} G. A. Fiete, V. Chua, M. Kargarian, R. Lundgren, A. Ruegg, J. Wen, and V. Zvyuzin, PHYSICA E 44, 845 (2012).
\bibitem{Maciejko2013} J. Maciejko, V. Chua, and G. A. Fiete, Phys. Rev. Lett. 112, 016404 (2014).
\bibitem{Maciejko2013a} J. Maciejko and A. Ruegg, Phys. Rev. B 88, 241101 (2013).
\bibitem{Moore2010} J. E. Moore, Nature 464, 194 (2010).
\bibitem{Hasan2010} M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
\bibitem{Qi2011} X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
\bibitem{Koenig2008} M. König, S. Wiedmann, C. Brune, A. Roth, H. Buhmann, L. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science 318, 766 (2007).
\bibitem{Roth2009} A. Roth, C. Brune, H. Buhmann, L. W. Molenkamp, J. Maciejko, X.-L. Qi, and S.-C. Zhang, Science 325, 294 (2009).
\bibitem{Hsieh2010} D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. Hor, R. J. Cava, and M. Z. Hasan, Nature 452, 970 (2008).
\bibitem{Raghu2009} S. Raghu, X.-L. Qi, C. Honerkamp, and S.-C. Zhang, Phys. Rev. Lett. 100, 046401 (2008).
\bibitem{Zhang2009} Y. Zhang, Y. Ran, and A. Vishwanath, Phys. Rev. B 79, 245331 (2009).
\bibitem{Wen2010} J. Wen, A. Ruegg, C.-C. J. Wang, and G. A. Fiete, Phys. Rev. B 82, 075125 (2010).
\bibitem{Liu2010} Q. Liu, H. Yao, and T. Ma, Phys. Rev. B 82, 045102 (2010).
\bibitem{Ruegg2011} A. Ruegg and G. A. Fiete, Phys. Rev. B 84, 201103 (2011).
\bibitem{Go2010} A. Go, W. Witczak-Krempa, G. S. Jeon, K. Park, and Y. B. Kim, Phys. Rev. Lett. 109, 066401 (2012).
\bibitem{Hung2013} H.-H. Hung, L. Wang, Z.-C. Gu, and G. A. Fiete, Phys. Rev. B 87, 121113 (2013).
\bibitem{Budich2012} J. C. Budich, R. Thomale, G. Li, M. Laubach, and S.-C. Zhang, Phys. Rev. B 86, 201407 (2012).
\bibitem{Budich2012a} J. C. Budich, B. Trauzettel, and G. Sangiovanni, Phys. Rev. B 87, 235104 (2013).
\bibitem{Wang2012} L. Wang, X. Dai, and X. C. Xie, Euro. Phys. Lett.. 98, 57001 (2012).
\bibitem{Yoshida2013} T. Yoshida, R. Peters, S. Fujimoto, and N. Kawakami, Phys. Rev. B 87, 085134 (2013).
\bibitem{Varney2010} C. N. Varney, K. Sun, M. Rigol, and V. Galitski, Phys. Rev. B 82, 115125 (2010).
\bibitem{Varney2011} C. N. Varney, K. Sun, M. Rigol, and V. Galitski, Phys. Rev. B 84, 241105 (2011).
\bibitem{Lang2011} T. C. Lang, A. M. Essin, V. Gurarie, and S. Wessel, Phys.
\end{thebibliography}
Appendix A: Quantum Monte Carlo

The projective quantum Monte Carlo method (QMC) is given by projecting an arbitrary trivial wave function $|\psi_T\rangle$ (requiring $\langle\psi_T|\psi_0\rangle \neq 0$) onto the ground state wave function $|\psi_0\rangle$. The expectation value of an observable $A$ is obtained by

$$
\langle A \rangle = \lim_{\Theta \to \infty} \frac{\langle \psi_T | e^{-\Theta H} A e^{-\Theta H} | \psi_T \rangle}{\langle \psi_T | e^{-\Theta H} | \psi_T \rangle},
$$

where $\Theta$ is the projective parameter. To carry out the procedures numerically, we need to discretize the projection operator $e^{-\Theta H}$ into tiny time propagators $e^{-\Delta \tau H}$ with $\Theta = \Delta \tau M$. $e^{-\Theta H} = (e^{-\Delta \tau H})^M$ where $M$ is the number of time slices and $\Delta \tau$ is chosen as a small number. The first-order Suzuki-Trotter decomposition can further decompose $e^{-\Delta \tau H}$ as

$$
e^{-\Delta \tau H} \simeq e^{-\Delta \tau H_0} e^{-\Delta \tau H_U},
$$

where $H_0$ is the tight-binding Hamiltonian, which could be equation (2) and equation (4), for the GKM model and the DKM model, respectively: $H_U = \frac{U}{2} \sum_i (n_i - 1)^2$ is the repulsive Hubbard on-site interaction; $n_i = \sum_c c_i^c \sigma c_i \sigma$. To represent $e^{-\Delta \tau H_U}$ in terms of the single-particle basis, we need to implement the $SU(2)$-invariant Hubbard-Stratonovich transformation:

$$
e^{-\Delta \tau H_U(n_i - 1)^2} = \frac{1}{4} \sum_{l = \pm 1, \pm 2} \gamma(l) e^{i l \sqrt{\Delta \tau U} \eta(l)(n_i - 1)} + O(\Delta \tau)^3
$$

75. F. F. Assaad, Quantum Monte Carlo methods on lattices: The determinantal approach in Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms, Lecture Notes (NIC Series Vol. 10, 2002).
76. F. F. Assaad, AIP Conf. Proc. 678, 117 (2003).
77. S. Rachel and K. Le Hur, Phys. Rev. B 82, 075106 (2010).
78. W. Wu, S. Rachel, W.-M. Liu, and K. Le Hur, Phys. Rev. B 85, 205102 (2012).
79. J. González, F. Guinea, and M. Vozmediano, Nuclear Physics B 424, 595 (1994).
80. I. F. Herbut, Physical review letters 97, 146401 (2006).
81. L. Janssen and I. F. Herbut, ArXiv e-prints (2014), arXiv:1402.6277 [cond-mat.str-el].
82. I. F. Herbut, V. Juričić, and O. Vafek, Physical Review B 80, 075432 (2009).
83. F. F. Assaad and I. F. Herbut, Physical Review X 3, 031010 (2013).
84. Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad, and A. Muramatsu, Nature 464, 847 (2010).
85. H.-H. Hung, Exotic quantum magnetism and superfluidity in optical lattices (PhD thesis, University of California, San Diego, 2011).
86. N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).
87. J. E. Hirsch, Phys. Rev. B 31, 4403 (1985).
88. F. F. Assaad and M. Imada, J. Phys. Soc. Jpn. 65, 189 (1996).
where $\gamma(\pm 1) = 1 + \sqrt{6}/3$, $\gamma(\pm 2) = 1 - \sqrt{6}/3$; 
$\eta(\pm 1) = \pm \sqrt{2(3 - \sqrt{6})}$ and $\eta(\pm 2) = \pm \sqrt{2(3 + \sqrt{6})}$ are 
4-component auxiliary fields. In the current literature, 
$\Delta \tau t = 0.05$ and $\Theta t = 40$ are used through the content.

Implementing equation $\text{(A2)}$ and $\text{(A3)}$, $H$ turns out to be $\tau$-dependent since $H_U$ is associated with the auxiliary 
field configuration $\eta(l_{i,\tau})$; then $e^{-\Theta H} = \prod_{\tau=1}^M e^{-\Delta \tau H_U}$. 
The denominator of equation $\text{(A1)}$ (named the projector partition function) $\mathcal{Z}$ is evaluated as follows.$^{6,7,75}$

$$
\langle \psi_T | e^{-\Theta H} | \psi_T \rangle = \langle \psi_T | \prod_{\tau=1}^M e^{-\Delta \tau H_U} | \psi_T \rangle \equiv \langle \psi_T | \prod_{\tau=1}^M e^{-\Delta \tau H_U} e^{-\Delta \tau H_F} | \psi_T \rangle
$$

$$
= \left( \frac{1}{4} \right)^{MN} \sum_{\{l_{i,\tau}\}} \left\{ \left( \prod_{i,\tau} \gamma(l_{i,\tau}) \right) \prod_{\sigma} \text{Tr} \left( \prod_{\tau=1}^M e^{-\Delta \tau \sum_i c_{i,\sigma}^\dagger c_{i,\sigma}} e^{i \sqrt{\Delta \tau/2} \eta(l_{i,\tau})(n_{i,\sigma} - \frac{1}{2})} \right) \right\}
$$

$$
= \left( \frac{1}{4} \right)^{MN} \sum_{\{l_{i,\tau}\}} \left\{ \left( \prod_{i,\tau} \gamma(l_{i,\tau}) \right) \det \left( O_\tau[\eta(l_{i,\tau})] \right) \right\},
$$

where $\sum_{l_{i,\tau}}$ runs over possible auxiliary configurations 
$\eta(l_{i,\tau})$, where $i = 1 \sim N$ are site indices and $\tau = 1 \sim M$ 
are imaginary time indices; $H_0$ is the matrix kernel of $H_0$ with spin $\sigma$. Each time propagator 
e^{-\Delta \tau H_U} e^{-\Delta \tau H_F}$ is a $N \times N$ matrix and $\text{Tr}(\prod_{\tau} e^{-\tau}) = \det(O_\sigma)$ represents 
the trace over fermion degrees of freedom.

Given such a $N$-site and $M$-time slice system, the 
summation in the above equation has a degree of $4^NM$, 
and generally, it is impossible to consider all configurations. 
The auxiliary field configuration, $\{ \cdots \eta(l_{i,\tau}) \cdots \}$, however, 
can be determined by Monte Carlo importance samplings.$^{75,76,85}$ For simplicity, we used the Metropolis 
algorithm in this paper.$^{38}$ The physical meaning of 
$\prod_{i,\tau} \gamma(l_{i,\tau}) \prod_{\sigma} \det \left( O_\tau[\eta(l_{i,\tau})] \right)$ is the 
probability weight at the given auxiliary field configuration 
$\{\eta(l_{i,\tau})\}$. When this term is proven positive-
definitive, QMC simulations are free-sign and the rejection 
procedure equation (A7) is well-defined. In the cases 
without Rashba spin-orbital coupling, however, the $G_{\sigma^\prime}$ are non-zero for $\sigma \neq \sigma'$. Therefore, for the 
simplified Kane-Mele-type model, the Green’s functions 
reduce to $2 \times 2$ matrix for each spin. In the main 
text, we implement the QMC and projection operator 
procedures equation (9) on the GKM and DKM model 
to study the parameter-induced topological phase transition.

To evaluate the time-displaced Green’s function $G(r, \tau)$. 
The unequal-time Green’s function is defined as$^{38}$

$$
G_{\sigma}(r, r_i, r_j) = \langle \psi_0 | c_{\sigma}(r, r_i) c_{\sigma}^\dagger(r_j) | \psi_0 \rangle
$$

$$
= \langle \psi_0 | e^{i \tau H} c_{\sigma}(r, r_i) e^{-i \tau H} c_{\sigma}^\dagger(r_j) | \psi_0 \rangle.
$$

Then we perform the Fourier transform from real space 
to momentum space $r \rightarrow k$, and imaginary time to the 
Matsubara frequency $\tau \rightarrow i \omega$,

$$
G_{\sigma}(i \omega, k) = \frac{1}{\beta} \int_0^\beta d\tau e^{i \omega \tau} \frac{1}{N} \sum_{r_i, r_j} e^{i k (r_i - r_j)} G_{\sigma}(r, r_i, r_j).
$$

The zero-frequency is given setting $i \omega = 0$. To calculate 
the spin Chern number $C_{\sigma}$, however, we need the single-
particle Green’s functions for all momentum points and 
implement equation (9). This procedure is slightly 
different from the approach to evaluate the $\mathbb{Z}_2$ index, for

which only time-reversal invariant momentum points are 
required. For sign-freeness QMC simulations, one can accurately 
calculate the zero-frequency Green’s functions 
in system sizes which are larger than the small clusters 
in an exact diagonalization and then evaluate the spin 
Chern numbers using the projection operators equation (9).

This approach is useful to identify different topological 
phases in the interacting system without using twisted 
boundary conditions.

Note that for more generic cases, the Green’s functions 
are a $4 \times 4$ matrix,$^{5,6}$ i.e.,

$$
G = \begin{pmatrix}
G_{\uparrow\uparrow} & G_{\uparrow\downarrow}
\end{pmatrix}
\begin{pmatrix}
G_{\downarrow\uparrow} & G_{\downarrow\downarrow}
\end{pmatrix},
$$

where $G_{\uparrow\uparrow} = G_{\uparrow\downarrow}$, $G_{\downarrow\uparrow} = G_{\downarrow\downarrow}$ as defined in equation (A5), and $G_{\uparrow\downarrow} = \langle c_{\uparrow}(\tau) c_{\downarrow}^\dagger \rangle$. Without Rashba spin-orbital 
coupling, however, the $G_{\sigma^\prime}$ are non-zero for $\sigma \neq \sigma'$. Therefore, for the 
simplified Kane-Mele-type model, the Green’s functions 
reduce to $2 \times 2$ matrix for each spin. In the main 
text, we implement the QMC and projection operator 
procedures equation (9) on the GKM and DKM model 
to study the parameter-induced topological phase transition.

In the noninteracting KM models, due to the inversion 
symmetry, the $2 \times 2$ Green’s functions at the time-reversal 
invariant momentum points (TRIM) can be simply expressed as

$$
G_{\uparrow\uparrow}(i \omega = 0, k_i) = \alpha_{k_i} \sigma^x, \quad k_i \in \text{TRIM},
$$

where some coefficients multiply the $\sigma^x$ Pauli matrix, and 
in equation (7), $\tilde{\eta}(k_i)$ is well-defined. In the cases 
of finite $U$, $\tilde{\eta}(k_i) = \pm 1$ and the relation equation (A7) 
are not guaranteed in a single measurement in the QMC 
simulations, however. Instead, they should be obtained 
by sufficiently large number of QMC simulations.

To interpret this, we present two benchmark results for 
the matrix elements of the zero-frequency Green’s functions 
at $k_i = M_1$, $y_{ij} = |G(i \omega = 0, M_1)|_{ij}$, vs the number
of measurements \((m)\) in Figs. 12 \(\lambda_{SO} = 0.4t\) and \(U = 4t\) are used. The test system size is \(2 \times 6^2\). To recover equation (A7), one should expect that \(\text{Re}[g_{12}] \simeq \text{Re}[g_{21}]\), and \(\text{Im}[g_{12}] = \text{Im}[g_{21}] = ||g_{11}(22)|| \simeq 0\). It has been demonstrated that the values of \(\text{Re}[g_{12}] = \alpha_k\), can be used to identify the topological property.

Fig. 12 (a) shows \(t_{3N} = 0.32t\) in the \(Z_2\) topological insulator phase and (b) for \(t_{3N} = 0.37t\). \(\lambda_{SO} = 0.4t\) and \(U = 4t\). \(\text{Re}[g_{ij}]\) and \(\text{Im}[g_{ij}]\) denote the real part and imaginary part of \(\langle G(0,M_\mu)\rangle\), respectively; \(||g_{ii}\rangle\) denotes the diagonal component of \(G(0,M_\mu)\) in magnitudes.

For other \(k\) and interacting case, equation (A7) does not hold. However, for the non-interacting case we found that the value of resulting spin Chern number \(C_\sigma\) is not sensitive to the number of samplings provided they are large enough in number. Throughout our paper, we choose the number of measurements large enough (mostly over several thousands) to determine the \(2 \times 2\) single-particle Green’s function, and then calculate the spin Chern numbers.

### Appendix B: Projection operator expression of the Spin-Chern number

In this section we provide a description of the projection operator expression used to evaluate the spin Chern number for finite lattices and its practical numerical implementation. The expression for the Chern numbers using the projection operators onto the occupied bands is

\[
C_\sigma = \frac{1}{2\pi i} \int_{\text{B.Z.}} \text{Tr} \left( P_\sigma dP_\sigma \wedge dP_\sigma \right) \\
= \frac{1}{2\pi i} \int_{\text{B.Z.}} \text{Tr} \left\{ P_\sigma(k) \left[ \partial_{k_x} P_\sigma(k) \partial_{k_y} P_\sigma(k) - \partial_{k_y} P_\sigma(k) \partial_{k_x} P_\sigma(k) \right] \right\} dk_x dk_y, \tag{B1}
\]

where \(P_\sigma(k)\) is the spectral projector operator constructed using the Bloch eigenvectors (eigenspace) at \(k\) with energies below the Fermi energy \(\epsilon_F\), i.e., \(E_\sigma(k) < \epsilon_F\) and for spin sector-\(\sigma\). A merit of this formulation of the Chern number is the manifest independence of the \(U(1)\) phases of the Bloch states. The Bloch eigenstates themselves are obtained from diagonalizing the interacting zero-frequency Green’s functions

\[
G_\sigma(k,0)|\mu_i\rangle = \mu_i |\mu_i\rangle, \tag{B2}
\]

and then

\[
P_\sigma(k) = \sum_{\mu_i \geq 0} |\mu_i\rangle \langle \mu_i|, \tag{B3}
\]

where choosing \(\mu_i > 0\) corresponds to selecting occupied bands \(E_\mu \leq \epsilon_F\), i.e. \(P_\sigma(0,0)\). The projection operator formula above is manifestly \(U(1)\) gauge invariant. The integral is over the Brillouin zone (BZ), and, in practical numerical application, the region of integration over the BZ does not need to be a Wigner-Seitz unit cell in reciprocal lattice space, as long as the entire reciprocal lattice unit cell is covered.

In a finite-size system, the set of \(k\)-vectors is discretized, so we will need to replace the integral with the summation over finite momentum points. For convenience we can map the momentum points as a \(N = L_x \times L_y\) square grid of spacing \(h\) and label each \(k\) with discrete coordinate indices \(\{m,n\}\). Then we can approximate the partial derivatives \(\partial_{k_x} P_\sigma(k)\) and \(\partial_{k_y} P_\sigma(k)\) using the symmetric finite difference as

\[
\partial_{k_x} P_\sigma(k) \approx \frac{P_{\sigma,i+1,j} - P_{\sigma,i-1,j}}{2h}, \\
\partial_{k_y} P_\sigma(k) \approx \frac{P_{\sigma,i,j+1} - P_{\sigma,i,j-1}}{2h}.
\]

Thus, in equation (B1) we simplify

\[
P_\sigma(k) \left[ \partial_{k_x} P_\sigma(k), \partial_{k_y} P_\sigma(k) \right] \approx \frac{P_{\sigma,i,j}}{4h^2} \left( \left[P_{\sigma,i+1,j}, P_{\sigma,i,j+1}\right] + \left[P_{\sigma,i+1,j}, P_{\sigma,i+1,j}\right] \\
+ \left[P_{\sigma,i,j+1}, P_{\sigma,i,j+1}\right] + \left[P_{\sigma,i,j-1}, P_{\sigma,i,j+1}\right] \right).
\]

Note that due to periodic boundary conditions in BZ, \(P_{\sigma,L_x+1,j} = P_{\sigma,1,j}\) and \(P_{\sigma,i,L_y+1} = P_{\sigma,i,1}\). Then the
Chern number is approximated as

\[ C_{\sigma} = \frac{1}{2\pi i} \int_{\text{B.Z.}} \text{Tr} \left( P_{\sigma} dP_{\sigma} \wedge dP_{\sigma} \right) \]

\[ \approx \frac{1}{2\pi i} \sum_{i,j=1}^{N} \frac{P_{\sigma,i,j}}{4} \left( [P_{\sigma,i+1,j}, P_{\sigma,i,j+1}] + [P_{\sigma,i,j+1}, P_{\sigma,i-1,j}] + [P_{\sigma,i-1,j}, P_{\sigma,i,j-1}] + [P_{\sigma,i,j-1}, P_{\sigma,i+1,j}] \right). \quad (B4) \]

Under such a construction, the evaluation of the spin Chern number might be subject to finite-size effects and an integral Chern number is not guaranteed. However, as we have presented in this paper, the approach is still useful in characterizing topological phase transitions which involve Chern number variations.