

Topological phase transitions for interacting finite systems

Christopher N. Varney,^{1,2} Kai Sun,^{2,3} Marcos Rigol,¹ and Victor Galitski^{2,3}

¹*Department of Physics, Georgetown University, Washington, DC 20057, USA*

²*Joint Quantum Institute and Department of Physics, University of Maryland, College Park, Maryland 20742, USA*

³*Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA*

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In this paper, we investigate signatures of topological phase transitions in interacting systems. We show that the key signature is the existence of a topologically protected level crossing, which is robust and sharply defines the topological transition, even in finite-size systems. Spatial symmetries are argued to play a fundamental role in the selection of the boundary conditions to be used to locate topological transitions in finite systems. We discuss the theoretical implications of these results, and utilize exact diagonalization to demonstrate its manifestations in the Haldane-Fermi-Hubbard model. Our findings provide an efficient way to detect topological transitions in experiments and in numerical calculations that cannot access the ground-state wave function.

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The discovery of the integer quantum Hall effect¹ provided a new type of quantum phase transition, the topological transition, which does not depend on spontaneous symmetry breaking. In recent years, the interest in topological states of matter and topological transitions was renewed by the discovery of a class of topological insulators with time-reversal symmetry.^{2,3} For noninteracting insulators, it is believed that all possible topologically ordered states have been classified,^{4,5} and the transition between topologically distinct states must feature a closing of the single-particle gap.^{2,3,6} At present, much of the recent development has focused on the role of interactions in topological insulators, specifically the search for interaction-induced topological insulators⁷⁻¹¹ and understanding the nature of quantum phase transitions between different topological classes.¹²⁻²¹

Some of the most important challenges in the study of interacting topological insulators lie in developing a classification scheme and in the difficulty to accurately compute the corresponding topological indices in an interacting system. For a Chern insulator, the standard way of calculating the topological invariant (the Chern number) involves determining the ground-state wave function with twisted boundary conditions^{22,23} or by taking a three-dimensional (3D) integral of the Green's function.²⁴⁻²⁶ Alternatively, it has been proposed that topological order can be ascertained by examining the single-particle gap near the edge states¹³ or the entanglement spectrum.^{27,28} Unfortunately, these approaches are computationally very challenging.

In this Rapid Communication, we show that, for all interacting topological insulators that can be classified by the Chern number, the topological transition is sharply defined in finite-size systems. In contrast to noninteracting infinite systems, where the topological transition is always marked by the closing of the single-particle gap, we show that, for an interacting finite-size system, the interaction-driven topological transition may be characterized by the closing of the excitation gap without necessarily closing the single-particle gap. This closing of the excitation gap can be viewed as a topologically protected level crossing. Next, we show that for models with inversion symmetry the level crossing can only occur for boundary conditions that are invariant under inversion. Based on this finding, we provide a prescription

for efficiently determining the topological transition and, using exact diagonalization, perform a representative study of interacting topological states in the simplest case of a lattice quantum Hall state with broken time-reversal symmetry.

We begin by formulating a general theory that captures such transitions. In contrast to ordinary quantum phase transitions,²⁹ a topological phase transition does not require spontaneous symmetry breaking and can be precisely defined and observed even in finite-size systems. Consider a two-dimensional insulator with Hamiltonian $H(\lambda)$, where λ is a control parameter. Given twisted-boundary conditions,^{30,31} the Chern number can be defined²² as

$$C = \int \frac{d\phi_x d\phi_y}{2\pi i} (\langle \partial_{\phi_x} \Psi^* | \partial_{\phi_y} \Psi \rangle - \langle \partial_{\phi_y} \Psi^* | \partial_{\phi_x} \Psi \rangle), \quad (1)$$

where $|\Psi\rangle$ is the exact many-particle wave function and ϕ_x (ϕ_y) are twists along the x (y) direction. As long as a unique ground state is found for all twisted boundary conditions, the integral of Eq. (1) is quantized to an integer value for any size system. In other words, regardless of the size of the system, we can always define a topological transition between insulators as the place where C changes its value from one integer to another.

Now we adiabatically vary λ from λ_1 to λ_2 . If the excitation gap remains finite during this procedure for all twisted-boundary conditions, the value of the Chern number must remain invariant because the topological index is quantized to integer numbers for gapped systems. This observation immediately implies that if the topological index changes its value, then the excitation gap $\Delta_{\text{ex}}^{(1)} = E_1 - E_0$, with E_0 (E_1) the energy of the ground (first-excited) state, must vanish for some twisted-boundary condition at the topological transition. In direct contrast to an ordinary quantum phase transition, where finite-size effects in general result in a finite-size gap, this phenomenon of a vanishing excitation gap remains even in finite-size systems, where the vanishing of $\Delta_{\text{ex}}^{(1)}$ implies the existence of a level crossing between the lowest two states. We emphasize here that this level crossing is required by the topological properties of the ground-state wave functions, and thus we refer to it as a topologically protected level crossing.

Identifying this topologically protected level crossing point, in principle, requires the computation of excitation gaps

for every twisted-boundary condition. This difficulty can be avoided if we focus on a special class of topological transitions where (a) the system has space-inversion symmetry and (b) the topological index changes by an odd number at the transition. These two conditions are satisfied in a large class of topological transitions [including the Haldane-Fermi-Hubbard (HFH) Hamiltonian,¹³ which we investigate below as a test model]. With space-inversion symmetry, the excitation gap at (ϕ_x, ϕ_y) must coincide with its partner $(-\phi_x, -\phi_y)$. At the topological transition point, this symmetry relation implies that if the gap closes at some (ϕ_x, ϕ_y) , then $(-\phi_x, -\phi_y)$ also has a level crossing. Consequently, there are in general an even number of level crossings and the Chern number must change by an even integer. In order for the Chern number to change by an odd value at the transition point, the level crossing must occur at one of the boundary conditions which are their own space-inversion partners: $(0,0)$, $(\pi,0)$, $(0,\pi)$, and (π,π) . Thus, we only need to examine the excitation gap for these high-symmetry boundary conditions to identify the topological transition. In addition, systems with higher rotational symmetry can simplify this further.³¹

Finally, we emphasize that the existence of a level crossing is a necessary condition for a topological transition, instead of a sufficient one. By naively looking at the excitation gap, one cannot distinguish the topological phase transition from an accidental level crossing. However, if one knows that the topological index does change, e.g., by calculating the Chern number or by the use of limiting arguments, then the level crossing must be associated with the topological transition.

To demonstrate the physics described above, we use a thick-restart Lanczos algorithm³² to study a model which has a lattice quantum Hall state with broken time-reversal symmetry.⁶ Here, we consider the HFH Hamiltonian¹³

$$H = -t_1 \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{H.c.}) - t_2 \sum_{\langle\langle ij \rangle\rangle} (e^{i\phi_{ij}} c_i^\dagger c_j + \text{H.c.}) + V \sum_{\langle ij \rangle} n_i n_j \quad (2)$$

on a honeycomb lattice at half-filling, where c_i^\dagger (c_i) are the fermion creation (annihilation) operators at site i and $n_i = c_i^\dagger c_i$ is the corresponding number operator. Here t_1 (t_2) are the nearest-neighbor (next-nearest-neighbor) hopping amplitudes, V is a repulsive nearest-neighbor interaction, and the next-nearest-neighbor hopping term has a complex phase $\phi_{ij} = \pm\phi$ corresponding to loops in the anticlockwise (clockwise) direction. In what follows, we restrict our study to clusters whose symmetry in momentum space contains the zone corner $\mathbf{k} = K$, as justified in Ref. 13. Also note that we set the unit of energy $t_1 = 1$ and the definitions of all the observables are presented in the Supplemental Material.³¹

For small V the system is a gapped topological insulator, which has a unique ground state and a finite gap $\Delta_{\text{ex}}^{(1)}$. In the limit $V \rightarrow \infty$, the system turns into a topologically trivial charge-density-wave (CDW) insulator in which all of the particles are all located on one sublattice. Here, the system has a doubly degenerate ground state, i.e., $\Delta_{\text{ex}}^{(1,2)} = 0$, and two finite gaps: the excitation gap $\Delta_{\text{ex}}^{(2)} = E_2 - E_0$, where E_2 is the energy of the second excited state, and single-particle gap

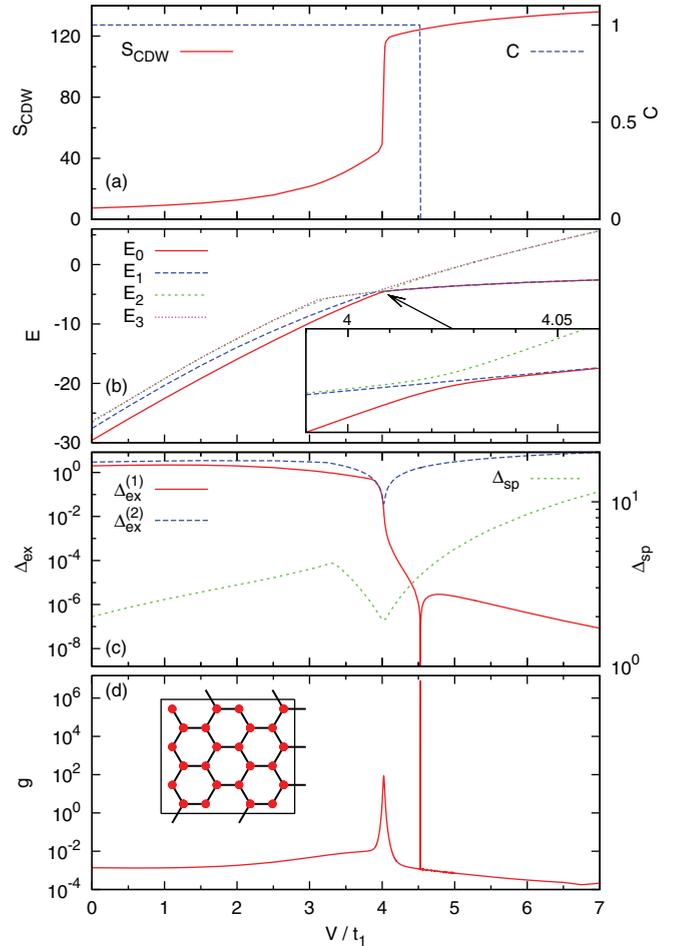


FIG. 1. (Color online) (a) CDW structure factor S_{CDW} and Chern number C , (b) ground-state energy E_0 and first three excited state energies (E_1 , E_2 , and E_3) with an inset that shows a closeup view of the avoided level crossing at $V = V_C$, (c) excitation gaps $\Delta_{\text{ex}}^{(1,2)}$ and a single-particle gap Δ_{sp} , and (d) fidelity metric $g(V, \delta V)$ with $\delta V = 10^{-4}$ as a function of the interaction strength V/t_1 for the 24C cluster [see the inset of (d)], and parameters $t_1 = 1.0$, $t_2 = 0.8$, and $\phi = \pi/2$. Note that this cluster does not possess all of the symmetries present in the infinite system.

Δ_{sp} , which is the energy required to add or remove a particle from the system.³¹ In general, the onset of CDW order and the change in the topological index may occur at different interaction strengths V_C and V_T , respectively, opening up a topological Mott-insulating region. For this Hamiltonian, we observe two cases that are related to the symmetry of the cluster: (1) $V_C < V_T$ and (2) $V_C = V_T$.

Figure 1 depicts the properties of the HFH Hamiltonian for the 24C cluster [see the inset in Fig. 1(d)] with parameters that typify the case $V_C < V_T$. In Fig. 1(a), we show the CDW structure factor³¹ and the Chern number. Here the jump in the structure factor marks the CDW transition at $V_C = 4.022 \pm 0.001$. In addition to the CDW transition, the topological index also changes its value as V increases, and we identify the topological transition at $V_T = 4.5281 \pm 0.0001$.

Next, we show the four lowest-energy states in Fig. 1(b), with an inset focusing on the avoided level crossing at $V = V_C$. In addition, there is a topologically protected level crossing

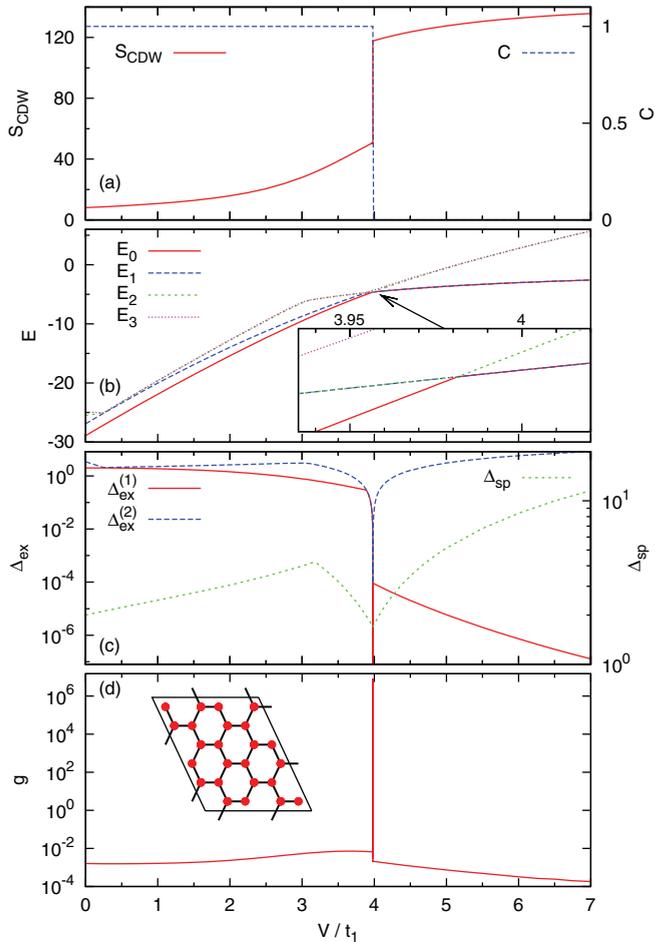


FIG. 2. (Color online) (a) CDW structure factor S_{CDW} and Chern number C , (b) ground-state energy E_0 and first three excited state energies (E_1 , E_2 , and E_3) with an inset that shows a closeup view of the level crossing at $V = V_C = V_T$, (c) excitation gaps $\Delta_{\text{ex}}^{(1,2)}$ and a single-particle gap Δ_{sp} , and (d) fidelity metric as a function of the interaction strength V/t_1 for the 24D cluster [see the inset of (d)] and the same parameters as Fig. 1.

at $V = V_T$ (not visible). This can be seen more clearly in Fig. 1(c), where we show the single-particle gap Δ_{sp} and excitation gaps $\Delta_{\text{ex}}^{(1)}$ and $\Delta_{\text{ex}}^{(2)}$. Here Δ_{sp} and $\Delta_{\text{ex}}^{(2)}$ both have a pronounced minimum at $V = V_C$, where both gaps are expected to vanish in the thermodynamic limit. The topological transition, on the other hand, is characterized by a vanishing excitation gap $\Delta_{\text{ex}}^{(1)}$, not necessarily by the vanishing of the single-particle gap. This is in direct contrast to Ref. 18, which claims that the topological transition is connected to the minimum of the single-particle gap. In addition, we emphasize that, for all of the clusters we studied, the closing of the excitation gap at the topological transition always takes place for the periodic boundary condition case $\phi_x = \phi_y = 0$ (Ref. 31).

One natural consequence of the level crossing seen in Fig. 1(c) can be observed in the fidelity metric³¹ $g(V, \delta V)$, which has been shown to be a sensitive indicator of quantum phase transitions.^{13,33–36} We illustrate this quantity in Fig. 1(d). While the CDW transition is marked by a peak with finite width (independent of δV) indicative of a traditional (first-order) phase transition, the topological transition is characterized by

a singular point where the overlap goes to zero, and the fidelity metric has a singular peak with height $2/N(\delta V)^2$ and width $\sim \delta V$, where N is the number of sites. Here we emphasize that because there is a topologically protected level crossing, this singular behavior of the fidelity metric will always occur for a topological transition. Due to the singular nature of this peak, numerical calculations of g may easily miss this feature, instead observing a jump discontinuity.¹³

The second case, $V_C = V_T$, is more representative of the model in the infinite limit. Indeed, for any cluster which preserves the full symmetry of the honeycomb lattice we find that $V_C = V_T$ for all parameters studied. In Fig. 2, we show the properties of the 24D cluster [see the inset in Fig. 2(d)] with the same parameters as in Fig. 1. In Fig. 2(a), the CDW transition, marked by the jump in the structure factor, and the change in the Chern number both occur at $V = V_C = V_T = 3.9813 \pm 0.0001$. As a result, there is a level crossing [shown in Fig. 2(b)] which is topologically protected and the ground state is triply degenerate. This threefold degeneracy becomes evident by examining the excitation gaps $\Delta_{\text{ex}}^{(1)}$ and $\Delta_{\text{ex}}^{(2)}$ [Fig. 2(c)], which both approach zero as $V \rightarrow V_T$. In the fidelity metric [Fig. 2(d)], we see only the singular peak associated with the topological transition. In general, we find that the two features do coexist, with the CDW fidelity peak becoming much sharper and, in many cases, completely obscured by the singular peak at the topological transition.

In Fig. 3, we show the t_2 - V phase diagrams for clusters from 12 to 24 sites. In general, the system is a topological insulator (TI) at weak-coupling and a topologically trivial CDW insulator at strong-coupling. For clusters without sixfold rotational symmetry [Figs. 3(a)–3(c)], we find a region of parameter space with a coexistence of topological and CDW order. For clusters with sixfold rotational symmetry [Fig. 3(d)], we find that the CDW and topological transitions always coincide. As this symmetry is present in the thermodynamic

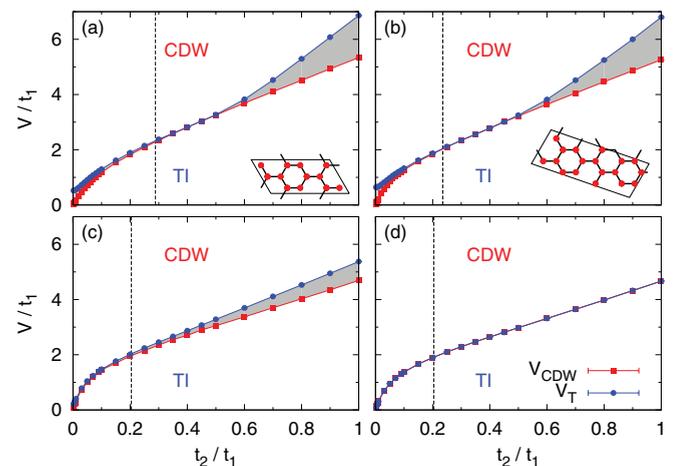


FIG. 3. (Color online) t_2 - V phase diagram for the (a) 12A, (b) 18C, (c) 24C, and (d) 24D clusters with parameters $t_1 = 1.0$ and $\phi = \pi/2$. The red squares indicate the onset of CDW order, and the blue circles indicate the topological transition. The shaded region marks the coexistence of CDW and topological order. All points to the vertical line are dominated by strong finite-size effects. Illustrations of the 12A and 18C clusters are shown as insets in the corresponding panel.

limit, and given the reduction we see in the region where CDW and topological order coexist as we increase the size of the clusters without that symmetry, we conclude that the topological CDW insulator phase does not exist in this model in the thermodynamic limit. In addition, we find no evidence for a topologically trivial insulating phase without CDW order.¹⁸

It is known that, at $t_2 = 0$, the system exhibits a semimetal-CDW transition at finite V in the thermodynamic limit. However, in Fig. 3, we observe a sudden decrease in V_C for small t_2 , resulting in a very small value of V_C at $t_2 = 0$. This apparent contradiction is due to finite-size effects, which become dominant as $V, t_2 \rightarrow 0$. In this region, the single-particle gap becomes very small ($\sim t_2$), so much larger systems (with sizes larger than the inverse gap) need to be studied to accurately determine the phase boundaries. To highlight this observation, we mark the onset of strong finite-size effects ($t_2 = L^{-1}$) by a dashed line in Fig. 3, where L is the linear size of the system. The drop of V_C takes place in the regime with strong finite-size effects ($t_2 < L^{-1}$). As the system size increases, the region with $t_2 < L^{-1}$ is pushed to $t_2 = 0$, so the sudden drop of V_C at small t_2 disappears in the thermodynamic limit, resulting in a finite V_C in the limit $t_2 \rightarrow 0$.

In summary, we have shown that the closing of the excitation gap is a signature of the topological transition in interacting systems. This topologically protected level crossing exists even in finite-size systems, and the resulting singular behavior at the transition can be observed in quantities such as the fidelity metric. When coupled with the use of spatial symmetries to simplify the choice of boundary conditions, this phenomenon provides an efficient scheme for locating the topological transition which can be straightforwardly generalized to time-reversal invariant topological insulators and fractional topological states. Aside from a few special cases,^{37,38} our findings provide a generic methodology to locate a topological transition in interacting finite-size systems via an experimentally measurable quantity. Consequently, this allows for the study of topological phases and transitions in cold-atom experiments and computational approaches in which the ground-state wave function is not accessible.

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