Topological phase in a one-dimensional interacting fermion system

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We study a one-dimensional (1D) interacting topological model by means of the exact diagonalization method. The topological properties are first examined with the existence of the edge states at half-filling. We find that the topological phases are not only robust to small repulsive interactions, but also are stabilized by small attractive interactions, and also finite repulsive interaction can drive a topological nontrivial phase into a trivial one while the attractive interaction can drive a trivial phase into a nontrivial one. Next we calculate the Berry phase and parity of the bulk system and find that they are equivalent in characterizing the topological phases. With them we obtain the critical interaction strengths and construct part of the phase diagram in the parameters' space. Finally we discuss the effective Hamiltonian at the large-U limit and provide an additional understanding of the numerical results. These results could be realized experimentally using cold atoms trapped in the 1D optical lattice.

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I. INTRODUCTION

The finding of time-reversal invariant topological insulators (TIs) has become an exciting event in condensed matter physics. Since then many works have been carried out theoretically and experimentally, predicting and verifying the many exotic physical properties exhibited by TIs.[1–3] The key feature of TIs is the existence of the robust edge states determined by the bulk topological property, which can be described by Z_2-valued topological invariants.[4–7] The original definition of TIs is for noninteracting band structures and the relevant physics has been well understood. Thereafter one of the subjects that needs to be explored further is the effects of electron correlations on TIs.

In the situation where many-body interactions exist, the definition of TIs from the topological field theory, which is the presence or absence of a topological term in the effective electromagnetic action, is generally valid.[8] In addition, the method using the Green's functions to construct the topological invariants is also applicable.[9–11] Yet the main difficulty is still to deal with the interactions properly. At the mean-field level, it has been shown that interactions can change the trivial insulators into nontrivial ones.[12–14] It is also been proposed that TIs and new topological phases may appear in the systems with considerable interactions such as $4d$ or $5d$ transition metal oxides.[15,16] Recently, several numerical simulations and analytical works were performed on the interacting two-dimensional Kane-Mele model and studied the interplay of spin-orbit coupling and Coulomb repulsion.[17–25] These studies showed that the Hubbard repulsive interaction can transform the TI of the Kane-Mele model to either the spin liquid phase or antiferromagnetic insulating phase depending on the strength of the spin-orbit coupling. A study using the Lanczos algorithm concludes that the topological properties have already manifested themselves in small systems and therefore can be studied numerically via exact diagonalization (ED) and observed experimentally.[17]

There also appeared works addressing the question of how the presence of interactions changes the classification of the topological phases. For noninteracting systems, five symmetry classes are topologically nontrivial in each spatial dimensionality. This classification has been expected to be also applicable to interacting systems as long as the strength of the interactions is sufficiently small as compared to the gap.[26,27] However, recent studies on a specific one-dimensional (1D) model showed that the free-fermion classification breaks down in the presence of interactions.[28,29] So it is most possible that the interaction does not modify the topological nontrivial classes uniformly.

In this paper, we use the ED to study the effect of interactions in a 1D lattice model which is known to have a topological state in its free form. With the ground-state energies and wave functions, we first calculate the energy and the distribution of the quasiparticle added or removed from the system at half-filling for open boundary conditions (OBC) and periodic boundary conditions (PBC), then we identify the topological phases with the existence of the edge states. The topological features indeed have manifested themselves clearly in the small sizes we can access. We consider both the repulsive and attractive interactions and find the topological phase is robust to repulsive interaction while stabilized by an attractive one when the interaction strengths are small. For the repulsive interaction we find that as its strength is increased, the system undergoes a topological quantum phase transition (TQPT) into a trivial insulator. For attractive interaction it can drive a trivial insulator into a nontrivial one. Then we calculate the Berry phase and the parity of the bulk system, which are equivalent in characterizing the topological property of the system. When the system is in the topological phase they have nontrivial values. With them we obtain the critical interaction strengths and construct part of the phase diagram in the parameters' space. Finally, we discuss the effective Hamiltonian at the large-U limit and provide an additional understanding of the numerical results.

II. 1D MODEL WITH EDGE MODES

Our starting point is the 1D noninteracting tight-binding model[30]

$$H_0 = \sum_i (M+2B)\Psi_i^\dagger \sigma_z \Psi_i - \sum_{i,\hat{x}} B\Psi_i^\dagger \sigma_z \Psi_{i+\hat{x}} - \sum_{i,\hat{x}} \mathrm{sgn}(\hat{x}) i A \Psi_i^\dagger \sigma_x \Psi_{i+\hat{x}}, \quad (1)$$

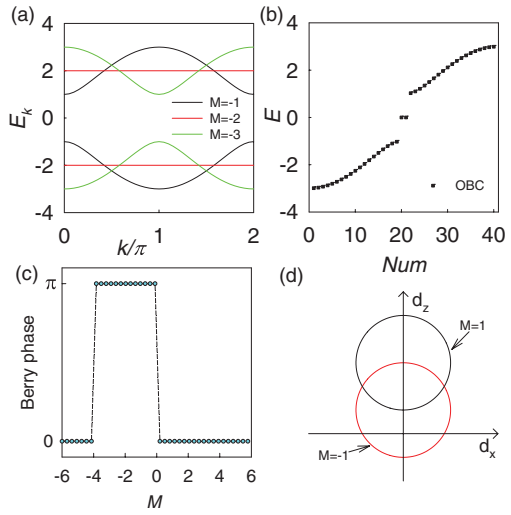

FIG. 1. (Color online) (a) The tight-binding band structure of $\mathcal{H}(k)$. The low-energy excitation is located at k_1 (black line) or k_2 (green line) depending on the parameters. (b) Edge modes in the topological phase ($M=-1$) on a chain of length $N=20$ with OBC. (c) Berry phase of the occupied Bloch state of Eq. (1) at different M. (d) The plot of the curve $[d_x(k),d_z(k)]$ with $k\in[0,2\pi]$. In all figures $B=1$ is set.

where σ_x, σ_z are Pauli matrices and $\Psi_i=(c_{i\uparrow},c_{i\downarrow})^T$ with the $c_{i\uparrow}(c_{i\downarrow})$ electron annihilating operator at the site $\mathbf{r}_i$. The first two terms represent the differences of the on-site potentials and the hopping amplitudes between the up and down electrons, and the third term is due to the spin-orbit coupling. In momentum space Eq. (1) becomes $H_0=\sum_k \Psi_k^\dagger \mathcal{H}(k)\Psi_k$ with $\Psi_k=(c_{k\uparrow},c_{k\downarrow})^T$ the Fourier partner of Ψ_i and

$$\mathcal{H}(k)=[M+2B-2B\cos(k)]\sigma_z+2A\sin(k)\sigma_x.$$

The spectrum of $\mathcal{H}(k)$ consists of two bands,

$$E_k^{(1,2)}=\pm\sqrt{[M+2B-2B\cos(k)]^2+[2A\sin(k)]^2}.$$

Usually the two bands are dispersive, but when the parameters satisfy $-M/2=B=A$ the bands are flat. For $M=0$ ($M=-4B$) bands 1 and 2 touch at the Dirac point $k_1=0$ ($k_2=\pi$), while for other values a gap $\Delta=\min\{2|M|,2|M+4B|\}$ opens up at the Dirac point k_1 or k_2. At half-filling, depending on the values of the parameters A, B, and M the system can be a trivial insulator or a nontrivial insulator with edge modes. In the following we take B positive and set $A=1$ as the energy scale.

The topological property of the system can be understood in terms of the Berry phase in k space, which is $\gamma=\oint \mathcal{A}(k)dk$ with the Berry connection $\mathcal{A}(k)=i\langle u_k|\frac{d}{dk}|u_k\rangle$ and $|u_k\rangle$ the occupied Bloch state.[32,33] The numerical result is shown in Fig. 1(c). It shows the Berry phase γ mod 2π gets a nonzero value π for $-4B<M<0$. We also have performed a numerical diagonalization of H_0 on a chain with OBC. In accordance with the above argument, we find a pair of zero modes appearing in the gap when the Berry phase of the system is π [Fig. 1(b)].

We notice that when the Berry phase is π the masses at the two Dirac points k_1 and k_2 have different signs [i.e., $M(M+4B)<0$]. This can also serve as a criterion of the topological property in the system. The reason can be understood from the low-energy Hamiltonians governing the excitations in the vicinity of the Dirac points.[30,31,34,35] By linearizing $\mathcal{H}(k)$ near k_1 and k_2 we obtain two Dirac Hamiltonians

$$\begin{aligned} h_k^1&=2A\sigma_x k+M\sigma_z,\\ h_k^2&=-2A\sigma_x k+(M+4B)\sigma_z. \end{aligned} \tag{2}$$

For $-4B<M<0$ the masses at the Dirac points exhibit opposite signs, while for $M>0$ and $M<-4B$ the masses at the Dirac points exhibit the same signs. In the following we show that the two cases correspond to two phases with different topological properties. We consider a junction between the two phases running along a line in real space (suppose $-4B<M<0$ for $x<0$ and $M>0$ for $x>0$). So the mass of h_k^1 necessarily undergoes a sign change across the $x=0$ boundary. Such a soliton mass profile is known to produce a massless state in the associated Dirac equation, localized near the boundary. Specifically, a Dirac equation

$$[2A(-i)\sigma_x\partial_x+\sigma_z m(x)]\phi(x)=E\phi(x)$$

with $m(x\to-\infty)<0$ and $m(x\to\infty)>0$ has a gapless solution

$$\phi(x)=e^{-\frac{1}{2A}\int_0^x m(x')dx'}\begin{pmatrix}1\\ i\end{pmatrix}$$

localized at the boundary with zero energy. Since the $M>0$ phase can be continually connected to the $M=\infty$ phase which is a trivial insulator, the phase for $-4B<M<0$ has a nontrivial topological property. The above argument is similar when $M<-4B$ for $x>0$ in the junction. So through the relative signs at the Dirac points we can obtain the same condition for the nontrivial topological phase.

Furthermore, we can write $\mathcal{H}(k)=\mathbf{d}(k)\cdot\vec{\sigma}$, where $d_x(k)=2A\sin(k)$, $d_y(k)=0$, and $d_z(k)=M+2B-2B\cos(k)$. The pair $[d_x(k),d_z(k)]$ forms a closed loop in the plane when k changes from 0 to 2π. If the system has nontrivial topological properties, the loop will contain the origin point of the plane [Fig. 1(d)]. It is also consistent with the former arguments.

III. EFFECT OF THE HUBBARD INTERACTION

To study the effect of the interaction, we add the Hubbard term $H_1=U\sum_i n_{i\uparrow}n_{i\downarrow}$ to Eq. (1). This term changes the single electron Hamiltonian Eq. (1) to a many-body one. For the noninteracting case, the topological property can be directly read from the presence of the edge states in the gap of the single electron energy spectrum. However, in the presence of interaction, there is no longer a single electron state. Then how can we identify the topological property of the system?

A. Existence of the edge states

Generally for a finite chain of N sites, the full Hilbert space of the system has dimension 4^N. Since in the Hamiltonian H_0+H_1 the total particle number is conserved, we can get the ground-state energy and wave function of a system with a fixed number of electrons using ED. Then we can define the energy of the quasiparticle added to a system with n electrons as $\Delta E_n=E_{n+1}^0-E_n^0$, where E_n^0 is the ground energy of a system with n particles. Similarly to the noninteracting case, if the

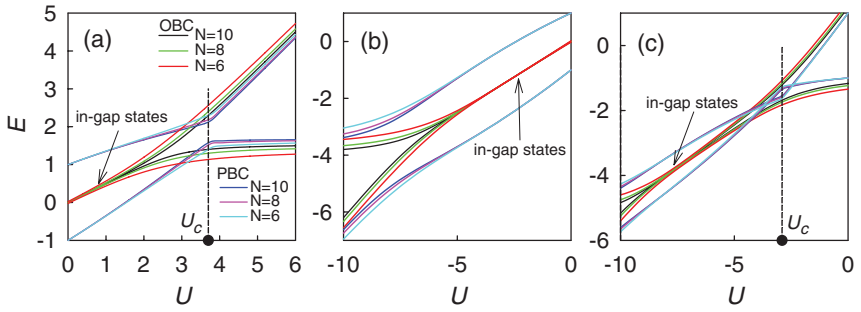

FIG. 2. (Color online) The energies of the quasiparticles added or removed from the half-filling system with OBC and PBC. (a, b): the phase at $U = 0$ is topological ($M = -1$); (c) the phase at $U = 0$ is trivial ($M = 1$). The critical interactions U_c in (a) and (c) can be accurately determined from the parity of the ground-state wave function. Here $B = 1$.

system has a nontrivial topological property, there appear states in the gap of the quasiparticle energy spectrum (QPES) as the boundary condition changes from PBC to OBC. Since this definition can be continually connected to the single electron case, we expect it to be valid at least for the small-U cases.

First we consider the effect of repulsive interaction. Figure 2(a) shows the results of starting from a system with a nontrivial topological property. Similar to the noninteracting case, we are concerned about the electron added or removed from the half-filling system. It shows that the energies of the quasiparticles added or removed appear in the gap when U is below a critical value U_c. At small U the two in-gap modes have exactly the same values. Due to the finite-size effect, when U approaches the critical value, the energies of the two modes is separated by a gap. When U is beyond U_c, the in-gap modes disappear and evolve into the bulk ones. The result clearly shows that the topological phase survives in the presence of a small repulsive interaction and a TQPT is driven by a finite repulsive interaction. We also study the case of starting from a trivial insulator and find that no in-gap modes appear when the repulsive interaction is added.

Next we turn to study the effect of attractive interaction. The calculations are straightforward and the results are shown in Figs. 2(b) and 2(c). In Fig. 2(b) the attractive interaction is introduced into a system with a nontrivial topological property. It shows that the existence of the in-gap modes persist to quite large strengths. Then as the strength is further increased, the in-gap modes continuously evolve into bulk ones. In Fig. 2(c) we show the result of introducing the attractive interaction to a trivial insulator. We find that when the strength reaches a critical value U_c, the in-gap modes begin to appear in the gap of QPES, indicating that the attractive interaction can drive a trivial phase into a nontrivial one. Then the in-gap modes persist till the strength becomes very large when they evolve into bulk ones. This behavior is very similar to that of disorder.[36,37]

Till now by identifying the in-gap states in the QPES, we show the effects of the repulsive and attractive Hubbard interactions in the topological phase. In the noninteracting systems, the in-gap mode is also referred to as the edge mode due to the fact that they mainly distribute near the edges of the chain. Similarly in the interacting case we can also calculate the distribution of the in-gap mode to study its nature. Using the many-body wave functions, the distribution of the electron added can be defined as $\Delta n_i = \langle \psi^0_{n+1} | \hat{n}_i | \psi^0_{n+1} \rangle - \langle \psi^0_n | \hat{n}_i | \psi^0_n \rangle$, where $\hat{n}_i = c^\dagger_{i\uparrow} c_{i\uparrow} + c^\dagger_{i\downarrow} c_{i\downarrow}$ is the electron number operator on site i and ψ^0_n is the ground-state wave function of the system with n electrons. The results at different U and M are shown in Fig. 3. Since the electrons added or removed at half-filling have exactly the same distributions, only one of them is shown. In Fig. 3(a), we start from a system with a nontrivial topological property. As expected at $U = 0$ the in-gap state mainly distributes near the edges. As we increase the strength of the repulsive interaction, the distribution begins to evolve from the ends to the bulk. Though the result is greatly affected by the finite-size effect, the distribution at $U < U_c$ is still clearly distinct from that at $U > U_c$ (U_c is about $3 \sim 4$), indicating the different topological properties existing in the system. Next we add attractive interaction to the above system and the result is shown in Fig. 3(b). As the strength increases, the topological phase is first stabilized, manifested by the increase of the components near the ends. Then the distribution

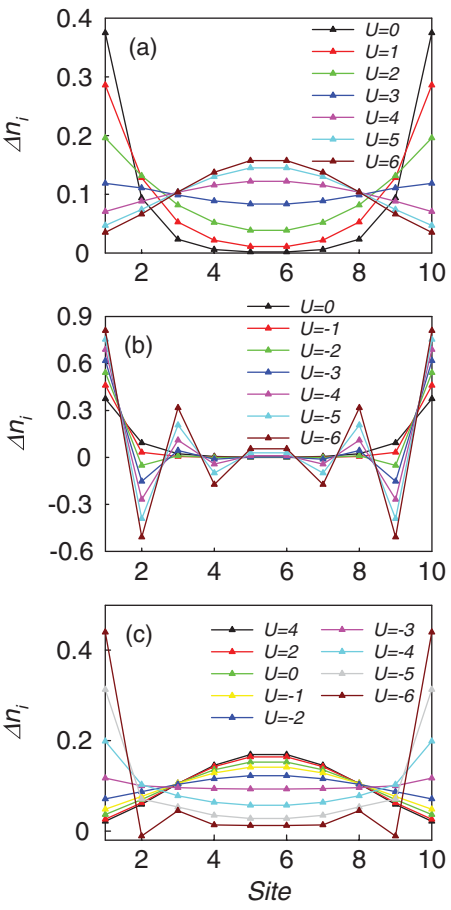

FIG. 3. (Color online) The distribution of the quasiparticles added or removed from the half-filling system with OBC. (a, b) $M = -1$; (c) $M = 1$. Here $B = 1$ and the system size $N = 10$.

begins to oscillate between positive and negative values. The occurrence of the negative value is due to the many-body effect. The amplitude of the oscillation decays from the end to the bulk and as the strength is further increased, the decay becomes slower, so the in-gap state begins to disappear, indicating the system is experiencing a TQPT. We also start from a trivial insulator and the result is shown in Fig. 3(c). It shows that in the presence of the repulsive interaction the distribution still mainly concentrates in the bulk, while after the attractive interaction is added the distribution begins to evolve from the bulk to the ends. The dramatic change occurs at $U = -3$ when the distribution shows a sign of edge one. The estimated critical value $-3 \sim -2$ is in good consistent with U_c in Fig. 2(c). Then as the strength of the attractive interaction is further increased the distribution shows a similar behavior as that in Fig. 3(b). These results are consistent with those obtained from the QPES.

B. Topological properties of the bulk system

Till now we have examined the topological phase in the interacting system with the existence of the edge states. It is known that their existence is due to the bulk topological properties. So in the following we will calculate the Berry phase of the ground state of the interacting system at half-filling using the twisted boundary conditions.[33,38,39] It can be defined as

$$\gamma = \oint i \langle \psi_\theta | \frac{d}{d\theta} | \psi_\theta \rangle,$$

where θ is the twisted boundary phase which takes values from 0 to 2π and ψ_θ is the corresponding ground-state many-body wave function at half-filling. To compare with the previous results, we first study the Berry phases associated with Fig. 2. We find that the Berry phase γ mod 2π has the value π and 0 for $U < U_c$ and $U > U_c$ (see Fig. 2).

The Hamiltonian $\mathcal{H}(k)$ possesses the symmetry implemented by a unitary transformation

$$\sigma_z \mathcal{H}(k) \sigma_z = \mathcal{H}(-k). \tag{3}$$

The symmetry is similar to the inversion symmetry except that there is an additional sign when it is performed on the spin-down electron. Thus we can define the parity of the wave function ψ_n^0. In the basis of a fixed number of electrons, $\psi_n^0 = \sum_i \phi_i |i\rangle$ with $|i\rangle$ denoting the ith n-electrons basis. Under the inversion transformation, $\mathcal{P}\psi_n^0 = \sum_i \phi_i \mathcal{P}|i\rangle = \sum_i \phi_i \epsilon_i |j\rangle_i = \pm\psi_n^0$, where $\mathcal{P}|i\rangle = \epsilon_i |j\rangle_i$ and $\epsilon_i = \pm 1$ depending on the times of exchanging the fermion operators. We calculate the parities of the ground- and the first-excited states associated with Fig. 2 and the results are shown in Fig. 4. It shows that at half-filling there is a gap between the two states even in the presence of the interactions and the gap may be eliminated at the critical strength U_c where the parity also changes its sign.

We also find that the parity is the same as the Berry phase to characterize the bulk topological properties since they both change their values at the same critical value U_c. From either one the accurate values of the critical interactions can be obtained, such as $U_c = 3.66$ in Fig. 2(a) and $U_c = -2.86$ in Fig. 2(c). We want to mention that in some cases, such as at the large attractive interaction though the in-gap states disappear, the Berry phase or the parity of the ground state does not change their values. These cases are beyond our discussion because the ground states become degenerate and the systems are not insulators any more.

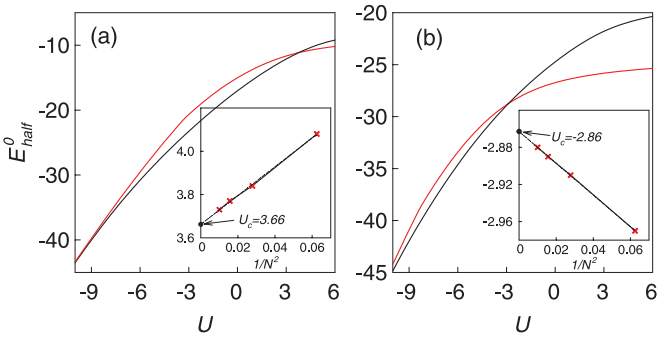

FIG. 4. (Color online) The energies and parities of the ground- and the first-excited states. (a) $M = -1$ and (b) $M = 1$. The red (black) curve has the parity value $-1(1)$. In both figures $B = 1$ and $N = 8$.

From these calculations, we can get part of the phase diagram in the parameters' space, as shown in Fig. 5. Figure 5(a) is in the (M,U) plane. It shows that at each value of B the curve is symmetric about $M = -2B$ and the behaviors are similar as M is far from $-2B$. When M approaches $-2B$, the property is different depending on the value of B. For $B < 1$, the critical interaction gets its maximum at $M = -2B$. While for $B > 1$ the results become complex and depend greatly on the system sizes, so no definite conclusions are made. Figure 5(b) is in the (M,B) plane. At $U = 0$ the topological phase is in the area restricted by the lines $M = 0$ and $B = -M/4$. Its size is shrunk by the repulsive interaction and broadened by the attractive one. Corresponding to the results in Fig. 5(a) at a fixed B of each curve the sum of

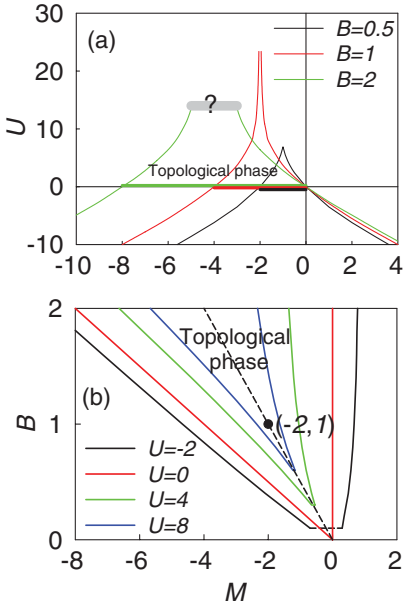

FIG. 5. (Color online) The phase diagram in (M,U) and (M,B) planes. The system size $N = 8$.

the two corresponding M's is $-4B$ and when $U > 0$ and $B < 1$ the tips of the curves fall on the line $B = -M/2$. We notice that $(M, B) = (-2, 1)$ is a special point where the noninteracting system exhibits flat bands. Here at the large repulsive interaction the ground- and the first-excited states also become degenerate and the Berry phase and parity of the ground state keep the same value all the way.

C. Effective Hamiltonian at large-U limit

To understand the phase diagram better, it is helpful to study the system at the large-U limit, when the effective Hamiltonian is[40]

$$H_{\text{eff}} = -\sum_i \left(J_x \sigma_i^x \sigma_{i+1}^x + J_y \sigma_i^y \sigma_{i+1}^y + J_z \sigma_i^z \sigma_{i+1}^z\right) + \sum_i (M + 2B)\sigma_i^z, \tag{4}$$

where $J_x = (B^2 - A^2)/U$, $J_y = (B^2 + A^2)/U$, and $J_z = -J_x$. When $A = B$ it is $H_{\text{eff}}^1 = -J \sum_i \sigma_i^y \sigma_{i+1}^y + Jg \sum_i \sigma_i^z$ with $J = \frac{2B^2}{U}$ and $g = \frac{(M+2B)U}{2B^2}$, which is the quantum Ising model.[41] By tuning the dimensionless coupling g, H_{eff}^1 exhibits a quantum phase transition and the critical point is exactly at $|g| = 1$. For $-\frac{2B^2}{U} - 2B < M < \frac{2B^2}{U} - 2B$, the ground state is twofold degenerate and possesses long-range correlations in the magnetic order parameter σ_y, while beyond the above range of M it is in a quantum paramagnetic state. This naturally explains the degeneracy at $B = -M/2 = 1$ for the large repulsive interaction.

IV. CONCLUSION

To conclude, we study the effect of interactions in a 1D topological model by means of the ED method. The topological features have already manifested themselves clearly in the small sizes the calculations can access. Our studies focus on the half-filling system. We examine the topological phases with the existence of the edge states, which are exhibited from the energy and distribution of the electron added to or removed from a system at half-filling and with OBC. We show that the topological phase is robust to small interactions and the finite repulsive interaction can drive a topological nontrivial phase into a trivial one while the attractive interaction can drive a trivial phase into a nontrivial one.

We calculate the Berry phase and the parity of the ground-state wave function to study the bulk topological properties. The Berry phase and the parity have an intrinsic connection and are equivalent to describe the topological properties due to the symmetry in our model. In the cases where the edge state exists, the Berry phase has nontrivial value π. At the TQPT points the Berry phase and the parity change their values. From them we determine the critical interactions and construct part of the phase diagrams in the parameters' space.

These results demonstrate the existence of the topological phases in 1D interacting fermion systems. Though the model we use is artificial, it may be constructed experimentally using cold atoms trapped in the optical lattice, which allows one to directly simulate ideal and tunable models. At present ultracold Fermi gases in a truly 1D regime can be realized using strong optical lattices and the interactions can be tuned between the repulsive and attractive ones by means of Feshbach resonances.[42] With these developments some of the basic phenomena in the interacting fermion systems are being studied. In addition, there have appeared some studies which suggested methods to mimic the effect of spin-orbit coupling and to produce topological states of matter in cold-atom systems.[43–45] So it is very hopeful that these results are tested in cold-atom experiments.

ACKNOWLEDGMENTS

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