Interaction-driven polarization shift in the t - V - V' lattice fermion model at half filling: Emergent Haldane phase

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We study the t - V - V' model in one dimension at half filling. It is known that for large enough V fixed, as V' is varied, the system goes from a charge-density wave into a Luttinger liquid, then a bond-order phase, and then a second charge-density wave phase. We find that the Luttinger liquid state is further split into two, separating parts with distinct values of the many-body polarization Berry phase. Inside this phase, the variance of the polarization is infinite in the thermodynamic limit, meaning that even if the polarization differs, it would not be measurable. However, in the gapped phases on each side of the Luttinger liquid, the polarization takes a different measurable value, implying topological distinction. The key difference is that the large- V' phases are link-inversion symmetric, while the small- V' one is site-inversion symmetric. We show that the large- V' phase can be related to an $S = 1$ spin chain, and exhibits many features of the Haldane phase. The lowest lying states of the entanglement spectrum display different degeneracies in the two cases, and we also find string order in the large- V' phase. We also study the system under open boundary conditions, and suggest that the number of defects is related to the topology.

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I. INTRODUCTION

Topological condensed-matter systems constitute an active research area. Topological band insulators are well understood [1–3]. Quantum phase transitions occur when the relevant topological invariant ($\mathbb{Z}$ or $\mathbb{Z}_2$) undergoes a finite change at a gap closure *point*. These systems also obey the bulk-boundary correspondence principle, which predicts the existence of edge states in the topologically nontrivial phases.

Recently, attention has focused [3–13] on interacting systems. An early result is the Haldane conjecture [14–16], which is based on a field-theoretical mapping of the Heisenberg model to a continuum one, and states that $S = 1$ spin chains are topologically nontrivial and exhibit spin- $\frac{1}{2}$ edge states. A useful scheme to visualize this state of affairs is the Affleck, Kennedy, Lieb, and Tasaki (AKLT) wave function, also known as the valence bond solid (VBS), a model for $S = 1$ systems. Recently Oshikawa [17] extended the AKLT wave function to arbitrary integer spin models. Pollmann *et al.* [9] showed that topological protection is present only in odd- S systems, and the protecting symmetries are time reversal, dihedral rotation, and link inversion.

The generalization of the idea of a topological invariant to the many-body case is also a crucial question, since topological invariants [1–3] in noninteracting systems are integrals over Bloch states of a periodic system. Manmana *et al.* [10] define an invariant using the single-particle Green's function and the chiral symmetry operator. The invariant obtained this way reduces to the known invariant if the system is noninteracting. In the interacting case, topological edge states can arise in three ways: poles or zeros in the Green's function (single-particle effects) or spontaneous symmetry breaking at the edge (many-body effect). The latter is not necessarily picked up by a topological invariant defined based on the single-particle Green's function. The polarization Berry phase reduces to the Zak phase when a noninteracting system is considered; however, in the interacting case it is a genuine many-body expectation value.

In this paper we study the one-dimensional t - V - V' interacting lattice model of spinless fermions. t denotes the hopping parameter, V the nearest neighbor interaction, and V' the next nearest neighbor interaction. It is known [18] that at large enough V a scan in V' will find four phases: charge-density wave (CDW-1), Luttinger liquid (LL), bond-order (BO) phase, and a different charge-density wave (CDW-2) phase. Our central finding is that at a critical V'_c the LL phase is split into two parts. For $V' < V'_c$ the Berry phase is zero, for $V' > V'_c$ it is π . In the LL phase, in the thermodynamic limit, the variance of the polarization diverges with system size, thus the different polarization averages are not measurable (expected for a gapless phase). However, on the different sides of the LL phase, the phases are such that the polarizations

are measurable, and the discrete difference between the two implies [19,20] topological distinction. In particular we find that the CDW-2 exhibits parallels to a Haldane phase [14,15]. We show this via a mapping of our original Hamiltonian to an $S = 1$ spin model, by calculating the entanglement spectrum, and by showing that hidden antiferromagnetic (HAFM) order as well as finite range string correlation, as defined by den Nijs and Rommelse [21], is present. We also analyze the system with open boundary conditions, with particular emphasis on defects which occur in ordered states as a result of the introduction of boundaries. Our results here suggest that the number of defects in a particular ordered phase may be connected to the value of the topological invariant.

The paper is organized as follows. In Sec. II the t - V - V' model is presented, as well as its connection to integer- S quantum spin chains. In Sec. III the polarization amplitude is introduced. It is shown that link inversion gives rise to a non-trivial Berry phase, and several variants of the Lieb-Schultz-Mattis [22] (LSM) theorem pertinent to our study are derived. In Sec. IV our numerical results are presented and in Sec. V we conclude our work.

II. MODEL HAMILTONIAN

The t - V - V' model already has a long history [18,23–25]. While evidence for the four different phases was known since the early study [23], the precise phase diagram was only established recently by Mishra *et al.* [18] The Hamiltonian of the t - V - V' model is

$$\hat{H} = \sum_{i=1} (-t[\hat{c}_{i+1}^\dagger \hat{c}_i + \text{H.c.}] + V \hat{n}_i \hat{n}_{i+1} + V' \hat{n}_i \hat{n}_{i+2}). \quad (1)$$

We take t as the energy scale. The Hamiltonian can be mapped [23] onto a spin- $\frac{1}{2}$ chain, via a Jordan-Wigner transformation:

$$\hat{H} = \sum_{i=1}^L (-t[s_i^+ s_{i+1}^- + s_i^- s_{i+1}^+] + V s_i^{(z)} s_{i+1}^{(z)} + V' s_i^{(z)} s_{i+2}^{(z)}). \quad (2)$$

It is obvious that dihedral π -rotation symmetry is a symmetry of the t - V - V' Hamiltonian. Rotation of each spin by π around a chosen axis, x , y , or z , returns $\hat{H}$ to itself. Time reversal and link inversion are also symmetries of $\hat{H}$. In Ref. [9] these three symmetries were found to be the ones protecting the topological Haldane phase in odd- S spin chains.

The canonical example of the topological Haldane phase is the $S = 1$ Heisenberg model. Crucial insight into the behavior of this model can be gained via the AKLT variational state whose elementary components are $S = \frac{1}{2}$ sites, but it is constructed in such a way that pairs of AKLT sites correspond to a true site of the $S = 1$ system. This construction is also mentioned by Manmana *et al.* [10] to relate one-dimensional fermion models (or $S = \frac{1}{2}$ models) to $S = 1$ spin models in the example they use, which is a Su-Schrieffer-Heeger (SSH) type model [26] with a Hubbard interaction.

We can proceed in an analogous manner in the t - V - V' model. We divide the Hamiltonian in Eq. (2) into two

pieces:

$$\begin{aligned} \hat{H}_\bullet &= \sum_{i=1}^{\frac{L}{2}} (-t[s_{2i}^+ s_{2i-1}^- + s_{2i}^- s_{2i-1}^+] + V s_{2i}^{(z)} s_{2i-1}^{(z)}) \\ \hat{H}_{\bullet\bullet} &= \sum_{i=1}^{\frac{L}{2}} (-t[s_{2i}^+ s_{2i+1}^- + s_{2i}^- s_{2i+1}^+] + V s_{2i}^{(z)} s_{2i+1}^{(z)}) \\ &\quad + V' \sum_{i=1}^{\frac{L}{2}} (s_{2i-1}^{(z)} s_{2i+1}^{(z)} + s_{2i}^{(z)} s_{2i+2}^{(z)}). \end{aligned} \quad (3)$$

Note that $\hat{H}_\bullet$ consists of uncoupled pairs of sites. As in the AKLT procedure, we express $\hat{H}_\bullet$ in an $S = 1$ (truncated) basis: $|\uparrow\rangle = |\uparrow\uparrow\rangle$, $|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, and $|\downarrow\rangle = |\downarrow\downarrow\rangle$. In this basis $\hat{H}_\bullet$ becomes an onsite $S = 1$ term,

$$\hat{H}_\bullet = \sum_{i=1}^{\frac{L}{2}} (2V + t)(S_i^{(z)})^2 - (t + V)\frac{L}{2}. \quad (4)$$

$\hat{H}_{\bullet\bullet}$ turns out to be a pairing term of the form

$$\hat{H}_{\bullet\bullet} = \sum_{i=1}^{\frac{L}{2}} \left(-\frac{t}{2} [\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+] + (V + 2V') \hat{S}_i^{(z)} \hat{S}_{i+1}^{(z)} \right). \quad (5)$$

The Hamiltonian $\hat{H}_{\bullet\bullet} + \hat{H}_\bullet$ was studied [17] in detail in the context of the Haldane phase. The symmetries which protect [9] the Haldane phase in odd- S systems, namely, time reversal, dihedral rotation, and link inversion, are all present in this Hamiltonian, and HAFM and string order [21] are also exhibited. While this Hamiltonian is a mapping based on a truncated basis (the $S = 0$ states are missing), below we show that this is not relevant; a Haldane phase is still exhibited, since the additional terms account for states of $S_z = 0$.

In addition to exact diagonalization of the Hamiltonian [Eq. (1)], we also perform auxiliary calculations. We construct a variational wave function, which can be viewed as the marriage of the AKLT wave function with the Baeriswyl variational wave function [27,28]. In the AKLT scheme an $S = 1$ site is considered as two spin- $\frac{1}{2}$ sites. Bonds connecting different $S = 1$ sites are taken to be in singlet states. A projector is applied to the $S = 1$ sites themselves, projecting them into $S_z = 1, 0, -1$ states.

In our case, we start with an ordered state for $V' \rightarrow \infty$, a state with alternating pairs of occupied and unoccupied sites, 11001100..., and apply the projector

$$\exp(-\alpha \hat{H}_V^{(0)}), \quad (6)$$

where $H_V^{(0)}$ is the Hamiltonian without the second-nearest neighbor coupling term, but including the hopping energy and the nearest neighbor coupling term. α is a variational parameter. The projector is only applied between bonds connecting an occupied and an unoccupied site (10 or 01). The wave function is represented in tensor network notation of Ref. [29] in part (c) of Fig. 5, where a comparison of the energies of this scheme with exact diagonalization results is also shown. The results indicate that this wave function provides an accurate description of the system.

In our study of the system with open boundary conditions, we also complement our exact diagonalization results with a cluster mean-field theory calculation. Here clusters of four sites are solved exactly, but the inter-cluster couplings are considered at the mean-field level. We do this for the case of open boundary conditions, meaning that the mean-field parameters for each cluster vary as a function of the position of the cluster in the lattice.

III. POLARIZATION AMPLITUDE, SYMMETRY ANALYSIS, AND TOPOLOGICAL ANALOGY

Topological invariants for noninteracting systems [30–33] are quantities derived from geometric phases [34,35]. Of particular importance is the Zak phase, a type of geometric phase, which arises when the crystal momentum is varied across the Brillouin zone. This geometric phase is unique to systems with periodic boundary conditions. The path in the Brillouin zone is not cyclic (open path Berry phase), but the endpoints are related via a symmetry transformation. The Zak phase is the topological invariant sensitive to the transition [36,37] in the SSH model [26], and it has a straightforward many-body generalization [38,39] (a single-point Berry phase [40]). Recently, Marks *et al.* [19] also used the many-body generalization of the polarization Berry phase [38,39] to study a topologically nontrivial interacting model.

For our calculations with periodic boundary conditions, we define the polarization amplitude

$$Z_q = \langle \Psi | \hat{U}_q | \Psi \rangle, \quad (7)$$

$$\hat{U}_q = \exp(i2\pi q \hat{X}/L).$$

where $\hat{X} = \sum_{x=1}^L x \hat{n}_x$. The operator $\hat{U}_q$ is known as the total momentum shift operator. In terms of Z_q the polarization [38,41] of a system with filling p/q per unit cell can be written as

$$P = \frac{L}{2\pi q} \text{Im} \ln Z_q. \quad (8)$$

This expression can be shown [36,38] to be consistent with the modern theory of polarization. The variance [39] of the total position as well as higher order cumulants [42] can also be derived [43], under the assumption that Z_q is the analog of a characteristic function, defined on a discrete set of points (q takes only integer values). The polarization of Resta [38] is the first moment of this characteristic function, while the variance of Resta and Sorella [39] is the second cumulant. Both can be obtained [43] via finite difference derivatives with respect to q . Recently, Z_q was intensively studied [41,43–48] as a source of information about quantum phase transitions and the associated finite size scaling. In this work, exploiting the fact that Z_q is a characteristic function, we analyze its Fourier transform,

$$P(x) = \sum_{q'=0}^{L-1} \exp\left(-i\frac{2\pi}{L}q'x\right) Z_{q'}, \quad (9)$$

understood to be the polarization distribution of the system, defined over the lattice positions $x = 1, \dots, L$. The summation index s runs over all components of the polarization

amplitude $Z_{q'}$. The Aligia and Ortiz [41] correction is automatically considered. For example, if a system has half filling, $p/q = 1/2$, then there will be no odd- q' contributions, and $P(x)$ will have two peaks within one supercell (see Figs. 2 and 4).

Due to half filling, all Z_q for q odd are zero. In the limiting cases $V \rightarrow \infty$ and $V' \rightarrow \infty$ the nonzero Z_q take the following values [43]: while $Z_q = 1$ for the former, Z_q alternates between ± 1 for the latter. We can also generally demonstrate the role of link-inversion symmetry by generalizing a result of Zak [35] to the many-body case. In Zak's original paper [35] it was argued that the Zak phase takes a trivial value (zero) in the case of inversion symmetry about a lattice site, while a nontrivial value is taken if the inversion symmetry is about the bond-center (π) (also known as link-inversion symmetry). Zak showed this by first expressing the Zak phase,

$$\gamma_{\text{Zak}} = \frac{i2\pi}{a} \int_0^{2\pi} dk \langle u_k | \partial_k | u_k \rangle, \quad (10)$$

using Wannier functions $w(x)$ as

$$\gamma_{\text{Zak}} = \frac{2\pi}{a} \int_{-\infty}^{\infty} x |w(x)|^2 dx. \quad (11)$$

In Eqs. (10) and (11) a denotes the size of the unit cell and $w(x)$ is the Wannier function for some band. If the system obeys reflection symmetry about a lattice site, then $w(-x) = \pm w(x)$, leading to $\gamma = 0$ (equivalent to shifts by 2π). The case of link-inversion symmetry, $w(-x+a) = \pm w(x)$, leads to $\gamma = \pi$.

Our task is to generalize this argument to the many-body case. Our starting point is the phase of the many-body polarization expression derived by Resta [38,39], applied to a half-filled system [41] (filling $n = p/q$, where $p = 1$, $q = 2$):

$$\Gamma = \text{Im} \ln Z_2 = \text{Im} \ln \langle \Psi | \hat{U}_2 | \Psi \rangle. \quad (12)$$

We apply a site-centered reflection to the total momentum shift operator,

$$\hat{R}_s \hat{U}_2 \hat{R}_s^{-1} = \exp(i4\pi \hat{R}_s \hat{X} \hat{R}_s^{-1}/L) = \hat{U}_2. \quad (13)$$

In this case the site around which reflection was performed was chosen to be the one at the origin. It is easily seen that $\Gamma = -\Gamma = 0$. We now apply a reflection operator around a bond center, using

$$\hat{R}_s \hat{X} \hat{R}_s^{-1} = \sum_x (L-x+1) \hat{n}_x, \quad (14)$$

leading to the result $\Gamma = \pi$. This result was also shown for matrix product states which are not “cat states” (superposition of two states not connected by any local operator) in Ref. [9]. Our proof above is entirely general.

It is also possible to prove an analogous version of the LSM theorem, in which link inversion versus site inversion plays the crucial role, and is therefore relevant to our model. The original LSM theorem shows that spin chains behave qualitatively differently, depending on the spin being integer or half integer. In our case, the distinction depends on whether a model exhibits site or link-inversion symmetry.

We start with a ground state $|\Psi_0\rangle$ of a model whose Hamiltonian consists of a hopping of the type in Eq. (1), and

some coordinate dependent interaction term. We construct a new state

$$|\Psi_1\rangle = \hat{U}_1 |\Psi_0\rangle. \quad (15)$$

The energy of this state compared to the ground state is

$$E_1 - E_0 = -t[\cos(2\pi/L) - 1] \sum_i \langle \Psi_0 | \hat{c}_i^\dagger \hat{c}_{i+1} | \Psi_0 \rangle. \quad (16)$$

In the thermodynamic limit, the $E_1 \rightarrow E_0$, but $|\Psi_1\rangle$ may not be a state that is different from $|\Psi_0\rangle$. To show this, apply the different inversion operators ($\hat{R}_s, \hat{R}_b$) and time reversal symmetry, as

$$\begin{aligned} \hat{R}_s \hat{T} \hat{U}_1 \hat{T}^{-1} \hat{R}_s^{-1} &= \hat{U}_1 \\ \hat{R}_b \hat{T} \hat{U}_1 \hat{T}^{-1} \hat{R}_b^{-1} &= -\hat{U}_1. \end{aligned} \quad (17)$$

The state $|\Psi_1\rangle$ is even if the system is site-inversion symmetric, while it is odd in the case of bond-inversion symmetry. The two possibilities arising from these results are the following. In the thermodynamic limit, there may be a gapless excitation which is odd with respect to bond inversion; alternatively, bond inversion symmetry may be spontaneously broken with degenerate ground states with a gap above each.

One model analyzed by Manmana *et al.* [10] was a spinful SSH model [26] with a Hubbard interaction. In the case of this model, it is also possible to highlight the role of inversion symmetry, via a relevant analog of the LSM theorem. Let us write the model in the following form:

$$\hat{H} = \sum_{i,\sigma} [(-J\hat{c}_{i,\sigma}^\dagger \hat{a}_{i,\sigma} - J'\hat{d}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \text{H.c.}) + U\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}]. \quad (18)$$

$\hat{c}_{i,\sigma}^\dagger$ ($\hat{d}_{i,\sigma}^\dagger$) are creation operators on the different sublattices. It is sufficient to consider one spin channel, and define a momentum shift operator of the form

$$\hat{U} = \exp \left(i \frac{2\pi}{L} \sum_{j=1}^L j (\hat{n}_{j,\uparrow}^{(c)} + \hat{n}_{j,\uparrow}^{(d)}) \right). \quad (19)$$

One can use this operator to construct a state $|\Psi_1\rangle = \hat{U} |\Psi_0\rangle$, and the energy difference will be

$$E_1 - E_0 = J'[\cos(2\pi/L) - 1] \sum_i \langle \Psi_0 | \hat{c}_{i,\uparrow}^\dagger \hat{c}_{i+1,\uparrow} | \Psi_0 \rangle. \quad (20)$$

Equation (17) holds, meaning that a bond-inversion symmetric system will have a degenerate ground state.

The basis used to construct $\hat{H}_\bullet$ and $\hat{H}_{\bullet\bullet}$ is a truncated one; the state $S = 0, M = 0$ is missing. Still, we can formulate a theorem of the Lieb-Schultz-Mattis type, as was done above. The relevant operator is

$$\hat{U} = \exp \left(i \frac{2\pi}{L} \sum_{j=1}^L j (\hat{S}_j^z + S) \right). \quad (21)$$

If one applies the steps above to a fixed S spin model (applying link inversion and time reversal), the result is a sign change in $\hat{U}$ for an odd- S model, but no sign change for an even- S model. This is consistent with the results of Ref. [9]. The fact that the basis is a truncated one for our case makes no difference, since other states are $S = 0$ states, and the maximum spin a site can be is $S = 1$.

FIG. 1. Phase diagram of the t - V - V' model at half filling. The phase lines separating the charge-density wave (CDW), Luttinger liquid (LL), bond-order (BO), and second charge-density wave (CDW-2) phases were determined by Mishra *et al.* [18]. The thick dashed line inside the LL phase indicates the main finding of this paper, where the polarization undergoes a discrete change. Along this line the polarization distribution is flat. The maximum of the polarization undergoes a discrete shift along this line (Fig. 3). The asterisks at $V/t = 6$ indicate the cases for which the polarization is shown in part (a) of Fig. 3.

IV. EXACT DIAGONALIZATION RESULTS

The results of Mishra *et al.* [18] for the phase diagram are shown in Fig. 1. The phase lines separate a charge-density wave (CDW-1), a LL, a bond-order phase, and a second charge-density wave (CDW-2) phase. Our main result is that in addition to the known [18] phase diagram, we find the dashed line inside the LL phase which separates phases in which the polarization (average of the polarization distribution) differs by one-quarter of a supercell (see Fig. 2). Along the transition line the polarization distribution, $P(x)$, is flat, and the line separates regions of the V/t - V'/t parameter space in which the polarization maxima differ by a quarter of a supercell. Since the filling with respect to number of unit cells is $1/2$, $\frac{L}{4\pi} \text{Im} \ln Z_2$ corresponds to the polarization [41]. Part (a) of Fig. 3 shows the reconstructed distribution $P(x)$ for selected points along the line $V/t = 6$ with different values

FIG. 2. Heat map of the polarization distribution $P(x)$ as a function of V'/t , $V/t = 6.0$. Exact diagonalization calculations with periodic boundary conditions.

FIG. 3. (a) polarization distributions for systems indicated by asterisks in Fig. 1: $V/t = 6$; $V'/t = 2.0, 2.4, 2.59, 2.8, 3.6$. The points are in the phases CDW, LL (below polarization switch, $V'/t < 2.59$), LL (where polarization switch occurs), LL (above polarization switch, $V'/t > 2.59$), BO, respectively. The position of the polarization maximum undergoes a discrete change at $V'/t = 2.59$. Exact diagonalization calculations with periodic boundary conditions. (b) Size scaling exponent of the variance of the polarization. Arrows indicate the four cases shown in Fig. 4.

of V'/t below, at, and above the transition point (points are indicated in the main figure with asterisks, upper panel). The transition in this case occurs at $V' \approx 2.59t$, where $P(x)$ is entirely flat. The positions of the two maxima both shift at the transition point.

Figure 4 shows the distributions $P(x)$ for different system sizes for four cases. The distributions are scaled by the system size on the x axis to enable comparison. Two cases which are in the LL phase are shown ($V' = 2.4, 2.8$), as well as two other cases in the two different CDW phases ($V' = 1.0$ and $V' = 6.0$). The CDW distributions show sharp peaks, whereas in the LL phase the distributions have smeared out maxima. We also calculated the size scaling exponent of the variance of the polarization, shown in part (b) of Fig. 3. The variance was calculated according to the procedure in Ref. [43].

The variance was calculated by first obtaining the first cumulant,

$$C_1 = \frac{L}{4\pi} \ln Z_2, \quad (22)$$

and then defining

$$\tilde{Z}_q = Z_q \exp\left(-\frac{i2\pi q}{L} C_1\right). \quad (23)$$

Using $\tilde{Z}_q$ we define the variance as

$$C_2 = -\frac{L^2}{4\pi^2 q^2} (\tilde{Z}_2 + \tilde{Z}_{-2} - 2\tilde{Z}_0), \quad (24)$$

which amounts to a discrete second derivative of $\tilde{Z}_q$. Although the Resta-Sorella formula defines the variance based on the logarithmic derivative of Z_q , we found (here and also in Ref. [43]) that in exact diagonalization, where the system

FIG. 4. Polarization distributions as a function of the rescaled coordinate x/L for systems with $V/t = 6$ and different values of V'/t . For $V'/t = 1.0$ and $V'/t = 6.0$ (CDW-1 and CDW-2 phases, respectively) the polarization distributions exhibit sharp peaks, which sharpen with system size. For the cases $V'/t = 2.4$ and $V'/t = 2.8$, on either side of the polarization switch, there are no sharp peaks, and the distributions exhibit negligible size dependence. The scaling exponent of the variation of the polarization is indicated by arrows in part (b) of Fig. 3. Exact diagonalization calculations with periodic boundary conditions.

sizes are small, the above procedure proved more suitable. The variance for a given set of parameters was obtained for different system sizes, and the size scaling exponent was calculated by fitting the variance as a function of system size L to the function $f(L) = \alpha L^\gamma$. The results are shown in part (b) of Fig. 3.

Clearly, the two LL phases exhibit $\gamma = 2$, meaning that the variance of the polarization scales as the square of the system size for both cases. This also means that the polarization distributions in the LL phase flatten as $L \rightarrow \infty$. They behave similarly to the phase transition line within the LL phase shown in Fig. 1. Even though finite systems exhibit a fixed average polarization, since the variance diverges with system size, it will not be an experimentally measurable quantity. In contrast, both insulating phases show a γ near 1.

The following picture emerges. The gapless LL phase, in which the polarization distribution is flat in the limit of large system size, separates gapped phases in which the polarizations differ by a quarter of a lattice constant. This corresponds to a shift in Zak phase of π , exactly as in the case of the SSH model. However, unlike in that model, the topologically distinct phases are not separated by one phase transition point. Instead, they are separated by the entire LL phase. In the finite system, the LL phase exhibits a topological phase line, on either side of which the polarization distribution is distributed according to a Gaussian whose variance diverges with system size. In the insulating phases on either side, the distributions are peaked and have finite variances; even in the thermodynamic limit, the polarization therefore is measurable.

Parts (a) and (b) of Fig. 5 shows two graphs of low-lying states of the entanglement spectrum for a system with $V/t = 6$ as a function of V'/t for two different entanglement cuts.

FIG. 5. (a) and (b) Low lying states of the entanglement spectrum for a system with $V/t = 6$ as a function of V'/t . In the small CDW-1 phase the degeneracy of the lowest lying state is 2, while in the CDW-2 phase it is 4. These numbers are indicated on the graphs. The upper of these two graphs is a system with $L = 24$ with an entanglement cut into a subsystem ($L = 12$) and environment ($L = 12$). The lower one of the upper two graphs is a system with $L = 24$ with an entanglement cut into a subsystem ($L = 11$) and environment ($L = 13$). Exact diagonalization calculations with periodic boundary conditions. (c) Comparison of energies for a tensor network variational calculation and exact diagonalization. The variational wave function is drawn in the tensor network notation of Ref. [29]. Both calculations use periodic boundary conditions.

The system consists of $L = 24$ sites with periodic boundary conditions. In one case (uppermost graph) the entanglement cut is taken at half the system ($L_s = 12$ and the environment is $L_e = 12$ which is traced out), while in the middle panel the entanglement cut is taken such that the subsystem size is $L_s = 11$ and the environment (traced out) is 13 sites. In both graphs, the lowest lying state is twofold degenerate in the CDW-1 phase, while it is fourfold degenerate in the CDW-2 phase. In the $L_s = 12$ case the two states in the CDW-1 phase form a basis for a two-dimensional irreducible representation of the link-inversion operator. The four states in the CDW-2 phase form a basis for two two-dimensional irreducible representations of the link inversion operator. For the $L_s = 11$ case the two degenerate states on the CDW-1 side form two identity representations of the site-inversion operator, while on the CDW-2 side, we find, again, two two-dimensional representations thereof.

We also calculated the entanglement spectrum (for a system with $L = 24$ and an entanglement cut at half the system) for the variational ansatz shown in Fig. 5. Since the symmetry is explicitly broken in this variational wave function, there are four different ways to choose such an entanglement cut. Each different cut gives rise to one low-lying state in the entanglement spectrum, consistent with the fourfold degeneracy of the CDW-2 phase found via exact diagonalization.

In Fig. 6 we show quantities related to HAFM ordering. By hidden antiferromagnetic (AFM) order we mean [17] the following. Once sites are paired, as was done to construct the

FIG. 6. (a) Probability of being in a real-space configuration not consistent with $S = 1$ hidden antiferromagnetic order. (b) String order correlation function for different V'/t . The system size is $L = 24$. Nearest neighboring sites were paired. $V/t = 6$. Exact diagonalization calculations with periodic boundary conditions.

truncated Hamiltonian in Sec. II, the z component of the spin of the paired sites are calculated (if both sites are occupied, $S_z = +$; if one site of the two is occupied, $S_z = 0$; if both sites are empty, $S_z = -$). In hidden AFM order $+$ and $-$ sites must alternate, possibly with 0 sites in between. An example of such a configuration is $+000 - + - 00 + 0 - \dots$ (a configuration in the space of paired sites). In the upper panel of Fig. 6 the fraction of configurations *not* consistent with hidden AFM order are shown. We see that in the CDW-1 and CDW-2 states, the overwhelming majority of configurations are consistent with hidden AFM. It is only in the ungapped region (mainly the LL phase) where configurations not consistent with hidden AFM are found.

The lower panel of Fig. 6 shows the string order correlation function of den Nijs and Rommelse [21], which is of the form

$$C(r = k - j) = \left\langle S_j^z \exp \left(i\pi \sum_{l=j+1}^{k-1} S_l^z \right) S_k^z \right\rangle. \quad (25)$$

The CDW-1 state displays a rapidly decaying correlation function, while the CDW-2 state show ordering. For the former, definite conclusions are difficult to draw, due to the small system size, but it appears that there is a decay in the string correlation function.

Manmana *et al.* [10] analyzed the bulk-boundary correspondence principle in an interacting topological system, a spin-dependent SSH model with Hubbard on-site interaction. This model is presented as an example of symmetry breaking at the edges, as opposed to single-particle topological edge states corresponding to poles or zeros of the single-particle Green's function. Symmetry breaking at the edges is a many-body phenomenon to which the single-particle Green's function based topological invariant is not necessarily sensitive.

Their analysis is not directly applicable to our model due to the finite range of the interactions. We are not able to take a dimerized limit. Instead, we investigate the nature of the order parameter, focusing on the defects which arise when the

FIG. 7. Real space density for four cases: (a) $V/t = 6$, $V'/t = 0$, (b) $V/t = 6$, $V'/t = 8$, (c) $V/t = 500$, $V'/t = 0$, and (d) $V/t = 0$, $V'/t = 500$. Open boundary conditions. The system size is $L = 24$.

boundary conditions are open. The density distribution for our interacting system with open boundary conditions is shown for four cases in Fig. 7 under open boundary conditions. The upper two plots show CDW-1 ($V/t = 6$, $V'/t = 0$) and CDW-2 ($V/t = 6$, $V'/t = 8$) examples, while the bottom two show nearly completely ordered CDW-1 and CDW-2 cases. The completely ordered states are interesting because each one is adiabatically connected to all states on the same side of the LL region. All distributions in Fig. 7 invert around the midpoint, meaning that the left edge can be related to the right edge via link-inversion symmetry. In Fig. 8 the density distributions are shown for the nearly completely ordered CDW-1 and CDW-2 states based on a four-site cluster mean-field calculation with open boundary conditions. In each case one particular

FIG. 8. Real space density calculated via cluster-mean-field theory for two cases, (a) $V/t = 500$, $V'/t = 0$ and (b) $V/t = 0$, $V'/t = 500$, under open boundary conditions. The system size is $L = 40$.

FIG. 9. (a) Proportion of configurations in the ground state wavefunction with number of defects in the ordered state with a given parity. In the CDW-1 cases ($V/t = 6$, $V'/t = 0$, $V/t = 20$, $V'/t = 0$, both CDW-1) the weight of configurations with an odd number of defects is shown, whereas in the CDW-2 cases ($V/t = 6$, $V'/t = 8$, $V/t = 0$, $V'/t = 20$, both CDW-2) the weight of configurations with an even number of defects is shown. (b) average number of defects (appropriate to CDW-1 or CDW-2) and the variance (error bars) in the ground state. The legend applies to both upper and lower panels. Both calculations are exact diagonalization with open boundary conditions.

symmetry broken state exists at each edge. In the middle the system has to “connect” between the different symmetry broken states at the edges. For the CDW-1 case one (or an odd number of) defect(s) is needed, while in the CDW-2 case two (or an even number of) defect(s) are required. The defects are indicated by the arrows on the figure. The parameters in the two cases were chosen so as to be deep in the CDW-1 (large- V) and the CDW-2 (large- V') phases, respectively. The system aims to maximize ordering; however, it also has to connect between the two different ordered states at the boundaries, while at the same time maximizing the respective order parameter. For this reason, the number of defects in each case is the minimum (one for CDW-1, two for CDW-2).

Defects can be located anywhere on the lattice, and the quantum ground state can be a superposition of states with different numbers of defects in different places. Figure 9 shows the weight of configurations with an odd (even) number of defects for the CDW-1 (CDW-2) case in the ground state wave function. In these calculations, the ground state wave function was obtained in real space. In each real-space component the defects were counted as follows. In the CDW-1 case, there are two ordered states, $1010\dots$ or $0101\dots$, where 0 represents an empty site and 1 an occupied one. If the leftmost site is filled, we assume that segment of the system is in the former; if not, then it is in the latter. We then check, starting from the leftmost site and going right, whether the configuration deviates from this ordered state. For example, if the configuration is $10100\dots$, the fifth site exhibits a defect. After a defect is encountered, we reset

the ordered state accordingly, and look for the next defect. We use a similar scheme for the CDW-2 state, except there the possible ordered states are 11001100..., 01100110..., 10011001..., and 00110011.... This means that the first two sites determine an ordered state. When a defect is encountered the resetting to a new ordered state is based on the defect site and the one before it. The defects counted are of the types indicated in Fig. 8. As the system size increases, the weight of configurations with odd (even) number of defects approaches unity in the CDW-1 (CDW-2) ground state. The lower panel of Fig. 9 shows the average number of defects and its variance for the four cases. The number of defects increases linearly with system size.

As mentioned above, it is difficult to construct a model in this case which identifies the edge state. In the example of Manmana *et al.* [10] the model was one in which dimerization was possible, and in this limit the analysis is not much more difficult than for the noninteracting SSH model. In our case, for the CDW-2, such a limit does not exist; however, we can make conjectures based on the results above. Symmetry breaking occurs at the edges in such a way that different symmetry broken ordered states are realized at the different boundaries. In order to connect the two boundaries, an odd number of defects is necessary in the CDW-1 phase, and the number of defects needs to be even in the CDW-2 phase. This may be a common scenario in ordinary symmetry broken systems, but, most importantly, it coincides with the findings of Manmana *et al.* [10]. In the case of symmetry breaking at the edges in a topological interacting system, a localized edge state may not be easily identifiable, since it is a many-body state, not a single-particle one, and it is possible that the number of defects which connect symmetry broken ordered states on opposite ends of the chain is of topological origin, in this case related to the quantized value of the polarization. This is a conjecture here; it is based on analyzing the observed patterns of the numerical simulations.

V. CONCLUSION

The main criterion for topological insulation is the topological invariant assuming nontrivial values. In noninteracting systems the invariant undergoes a finite change at a gap closure point. Topologically distinct phases are separated by gap closure points or quantum phase transitions.

In the t - V - V' model, for fixed V large enough to start in a charge-density wave phase, as V' is increased a Luttinger liquid phase is encountered. Passing through this phase, there is a bond-order phase followed by a new charge-density wave. The many-body polarization single-point Berry phase changes discontinuously inside the Luttinger liquid phase at a critical V' . However, in contrast to noninteracting systems, this change in the topological invariant occurs inside a gapless phase. Inside the gapless Luttinger liquid phase the variance of the polarization diverges with system size, meaning that the Berry phase is undefined inside this whole region. In short, topologically distinct phases are separated not by a quantum phase transition point, as in noninteracting systems, but by the Luttinger liquid phase itself. The topological phase was shown to be a Haldane phase, exhibiting hidden antiferromagnetic order and finite string correlation.

The model we studied can be realized experimentally in cold atoms in an optical lattice setting [49]. The degree of control in such an experiment places strongly correlated one-dimensional models within reach [50]. Particularly pertinent to our study is that the geometric phase [34,35] which gauges the transition can also be directly [51] measured.

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