Interplay of local order and topology in the extended Haldane-Hubbard model

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We investigate the ground-state phase diagram of the spinful extended Haldane-Hubbard model on the honeycomb lattice using exact diagonalization (ED) and a mean-field (MF) variational approach. This model, governed by both onsite and nearest-neighbor interactions, can result in two types of insulators with finite local order parameters, either with spin or charge ordering. Besides, a third one, a topologically non-trivial insulator with non-local order is manifest. We test expectations of previous analyses in spinless versions asserting that once a local order parameter is formed, the topological characteristics of the ground-state, associated with a finite Chern number, are no longer present, resulting on a topologically trivial wave-function. Here, at the largest cluster accessible to ED, we unveil a regime displaying both charge density ordering accompanied by an SU(2) symmetry broken phase with Chern number $C = 1$. This phase, however, is not present in the MF variational method, and is a warning of the systematic finite-size effects that can affect conclusions obtained in small clusters.

I. INTRODUCTION

Topological phases, which evade the paradigm of the conventional Landau-Ginzburg’s theory of spontaneously broken symmetries associated to the onset of a local order parameter, has been paramount to characterize and classify a large class of materials [1–3]. In the past few years, the classification of topologically ordered states in non-interacting systems is believed to be complete [4, 5]. Nonetheless, interacting topological models are expected to display much richer phenomena [6], as for example, antiferromagnetic topological insulating states [7–10] or interaction-driven topological Mott insulators, in otherwise topologically trivial models [11–18]. Some of these results, obtained via mean-field methods, have been disputed [19–23], but two-dimensional systems with quadratic band-crossings, and weak interactions, may yet allow the observation of interaction-induced non-trivial topology [24–30].

In the scope of strong interactions, topologically ordered states were seen to be absent when the system develops either charge or magnetic ordering [31–41]. Recently, however, a new class of exotic states has been shown, where in an interacting spinful version of the Haldane model it is possible to observe spontaneous SU(2) symmetry breaking. This is manifested as one spin species yet remaining topological, whereas the other turns trivial upon the increasing of a control parameter, resulting in a phase with Chern number equals to one [42–44].

In this paper, we further investigate the possibilities that finite local order parameters can coexist with a topological phase, obtaining the phase diagram of the half-filled spinful Haldane model (see Fig. 1), in the presence of both on-site and nearest-neighbor repulsive interactions on a honeycomb lattice. Sufficient local interactions are known to spontaneously induce SU(2) symmetry breaking [45, 46] resulting in an antiferromagnetic (Mott) insulator, whereas its nearest-neighbor counterpart induces a charge density wave (CDW) insulator if large enough, associated with a discrete (inversion) symmetry breaking. Our main finding is that, in general, when the development of either order occurs, the topological characteristics of the wave-function, encoded on a finite Chern number, are no longer present. Exceptions to this, however, may occur in the finite lattices one investigates the model on, and is unclear whether they might occur in the thermodynamic limit. [47]

One of the main challenges in investigating the interplay of topology and interactions is to unbiasedly compute the ground-state properties, and thus the topological invariants for the model of interest. If the model lacks time-reversal symmetry, as the Haldane-Hubbard model, quantum Monte Carlo (QMC) methods are largely limited due to the presence of severe sign problem [48–50]. Cluster dynamical mean-field theory (DMFT), on the other hand, has been very successful [42, 51, 52], but the necessity to employ QMC as an impurity solver, also limits the low temperature regime with larger cluster sizes, where again, a vanishing average sign is detrimental to simulations [52]. Density matrix renormalization methods are also particularly reliable in investigating topological properties, but more easily applicable to ladder or cylinder geometries if beyond one-dimension [21, 53–57]. We have chosen instead the exact diagonalization (ED), where in spite of the small lattice sizes amenable to computations, has been proven to be extremely useful in characterizing topological interacting systems [27, 31, 32, 58, 59]. In particular, previous investigations indicate that on a honeycomb lattice, clusters with reciprocal lattices containing the $K$ high-symmetric point are able to grasp the fundamental critical features

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owing to the closing of the excitation gap at this point during the topological phase transition [31, 32]. To put these results in perspective, we complement with a mean-field analysis of the model, qualitatively corroborating the onset of the ordering depending on the interaction parameters.

The presentation is organized as follows: In Sec. II, we introduce the model and all the quantities we use to characterize the different phases. Section III and IV, respectively, presents the results using ED and MF, respectively. Lastly, Sec. V summarizes and discusses the results.

II. MODEL AND MEASUREMENTS

We study the extended Haldane-Hubbard model (EHHM), which is a combination of the Haldane model [60] and the extended Hubbard model on the honeycomb lattice [61, 62],

\[
\hat{H} = - t_1 \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + H.c.) - t_2 \sum_{\langle i,j \rangle, \sigma} (e^{i\phi_{ij}^\dagger} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + H.c.) + U \sum_n \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + V \sum_{\langle i,j \rangle, \sigma, \sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}.
\]

Here, \(\hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}\) represents the electronic creation (annihilation) operator at site \(i\) with spin \(\sigma = \uparrow, \downarrow\), and \(\hat{n}_{i,\sigma} = \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}\), the corresponding number operator. \(t_1 \) (\(t_2\)) denotes the nearest-neighbor (next-nearest-neighbor) hopping energy scale; \(U\) and \(V\) are the on-site and nearest-neighbor interactions, respectively. A complex phase \(\phi_{ij} = \pm \phi\) representing the loops in the clockwise (anticlockwise) directions is added to the next-nearest-neighbor hopping term. This phase, if chosen such that \(0 < \phi < \pi\), originates a model which breaks time-reversal symmetry. In the non- and weak-interacting regimes, the ground-state can thus be characterized by a topological invariant, the Chern number [60]. Throughout the paper, we focus on the ground-state phase diagram of Eq. (1), at half-filling, with periodic boundary conditions (PBC), using both exact diagonalization and mean-field techniques, in lattices containing \(N\) unit cells (and \(2N\) sites). Below, we briefly describe their methodology and how the observables are computed.

A. Exact diagonalization in real space

By employing periodic boundary conditions, we make use of translational-symmetries, reducing the Hilbert space size by a factor of \(N\). We proceed with a large scale diagonalization, where we apply either Arnoldi [63] or Krylov-Schur methods [64, 65] to extract the ground-state, and a few excited states of Eq. (1), for lattices with up to \(N = 9\), i.e., 18 sites. As will later become clear, such lattice sizes are essential for the analysis, since clusters with a reciprocal lattice that contain the zone corner (\(K\) high-symmetry point) could exhibit the characteristic first-order phase transition from the topological to the topologically trivial phase, while others may miss this feature, displaying it as a second-order one [31, 52]. In the next section, we report results for clusters encompassing both cases, and this will become more evident.

The characterization of the quantum phase transition is done via computing different quantities, such as the ground-state fidelity metric, the charge and spin structure factors, and the Chern number. The first is defined as [66–68]

\[
g(x, \delta x) = \frac{2}{N} \left(1 - \frac{|\langle \Psi_0(x) \rvert \Psi_0(x + \delta x) \rangle|^2}{\delta x^2}\right),
\]

where \(x\) represents the interaction parameters \(U\) or \(V\), and \(|\psi_0(x)\rangle \langle \psi_0(x + \delta x)\rangle\) the ground-state of \(\hat{H}(x)\) \([\hat{H}(x + \delta x)]\). This quantity is expected to produce a diverging peak with the system size, and has been routinely used to characterize different phase transitions, since it makes no underlying assumptions about the associated order parameter [32, 69–71]. In what follows, we set \(\delta x = 10^{-3}\) for either \(x = U\) or \(V\).

To probe the onset of the different local orders, with either spin-density wave (SDW) or charge-density wave (CDW), we define structure factors in a staggered fashion

\[
S_{SDW} = \frac{1}{N} \sum_{i,j} (-1)^\eta (\hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}),
\]

\[
S_{CDW} = \frac{1}{N} \sum_{i,j} (-1)^\eta (\hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}) (\hat{n}_{j,\uparrow} + \hat{n}_{j,\downarrow}),
\]

with \(\eta = 0 \) (\(\eta = 1\)) if sites \(i\) and \(j\) are in the same (different) sublattice, i.e., A or B.

The topological invariant is quantified by the Chern number. If using twisted boundary conditions (TBC) [72], it can be defined as an integration over the Brillouin zone [73],

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

with \(|\Psi\rangle\) being the many-particle wave function, and \(\phi_x, \phi_y\) the twisted phase along the \(x\) (\(y\)) direction. Provided there are no degeneracies in the ground-state, Eq. (4) results in an \(\mathbb{Z}\) integer number. An immediate drawback is that this expression requires the computation of derivatives and integrals of the wave-function with respect to the continuous variable. It has been shown, however, to already converge to the true Chern number if using a sufficiently discretized version [32, 74, 75]. In what follows, we report results using a mesh of \(6 \times 6\) phases \((\phi_x, \phi_y)\) over the Brillouin zone. A comparison with finer meshes is exemplified in the Appendix A.
B. Mean-field method in momentum space

To constrain the results obtained via ED, we report in Sec. IV mean-field (MF) calculations. For that, we employ a two-site unit cell computing the corresponding fields in momentum space, owing to the translational invariance of the problem. We choose $\mathbf{a}_1 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2})$ and $\mathbf{a}_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2})$ as the basis vectors in real space; their counterparts in reciprocal space are $\mathbf{b}_1 = \frac{1}{a}(-2\pi, \frac{2\pi}{\sqrt{3}})$ and $\mathbf{b}_2 = \frac{1}{a}(2\pi, \frac{2\pi}{\sqrt{3}})$. By introducing the operators $a^\dagger_{\mathbf{k}, \sigma}$ and $b^\dagger_{\mathbf{k}, \sigma} = \frac{1}{\sqrt{\mathcal{N}}} \sum_{i \in \mathcal{A}} c^\dagger_{i, \sigma} e^{i \mathbf{k} \cdot \mathbf{r}_i}$, and $b^\dagger_{\mathbf{k}, \sigma} = \frac{1}{\sqrt{\mathcal{N}}} \sum_{i \in \mathcal{B}} c^\dagger_{i, \sigma} e^{i \mathbf{k} \cdot \mathbf{r}_i}$, the Hamiltonian (1) can be expressed as follows:

$$
\hat{H} = \hat{H}_0 + \hat{H}_1,
$$

with,

$$
\hat{H}_0 = \sum_{\mathbf{k}, \sigma} \left( m_{+}(\mathbf{k}) a^\dagger_{\mathbf{k}, \sigma} a_{\mathbf{k}, \sigma} + m_{-}(\mathbf{k}) b^\dagger_{\mathbf{k}, \sigma} b_{\mathbf{k}, \sigma}
- t_1 g(k) a^\dagger_{\mathbf{k}, \sigma} b_{\mathbf{k}, \sigma} - t_1 g^*(k) b^\dagger_{\mathbf{k}, \sigma} a_{\mathbf{k}, \sigma} \right),
$$

and,

$$
\hat{H}_1 = \frac{U}{\mathcal{N}} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}, \uparrow} c^\dagger_{\mathbf{k}', -\mathbf{q}, \downarrow} c_{\mathbf{k}', \downarrow} c_{\mathbf{k}, \uparrow}
+ \frac{V}{\mathcal{N}} \sum_{\mathbf{q}} \sum_{\sigma, \sigma'} g(\mathbf{q}) a^\dagger_{\mathbf{k}+\mathbf{q}, \sigma} a_{\mathbf{k}, \sigma} b^\dagger_{-\mathbf{q}, \sigma'} b_{\mathbf{k}', \sigma'},
$$

where $g(\mathbf{k}) = 1 + e^{-i \mathbf{k} \cdot \mathbf{a}_1} + e^{-i \mathbf{k} \cdot \mathbf{a}_2}$, and $m_{\pm}(\mathbf{k}) = -2t_2 \left| \cos(\mathbf{k} \cdot \mathbf{a}_1 \mp \phi) + \cos(\mathbf{k} \cdot \mathbf{a}_2 \pm \phi) + \cos(\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2) \pm \phi) \right|$.

After a mean field decoupling of the four-fermion terms (including both Hartree and Fock terms), we arrive at the following mean-field Hamiltonian

$$
\hat{H}_{MF} = \hat{H}_0 + \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} \begin{pmatrix} 
\xi^a_{\sigma}(\mathbf{k}) & \xi^a_{\sigma'}(\mathbf{k}) & \xi^b_{\sigma}(\mathbf{k}) & \xi^b_{\sigma'}(\mathbf{k}) \\
\xi^a_{\sigma'}(\mathbf{k}) & \xi^a_{\sigma'}(\mathbf{k}) & \xi^b_{\sigma}(\mathbf{k}) & \xi^b_{\sigma}(\mathbf{k}) \\
\xi^b_{\sigma}(\mathbf{k}) & \xi^b_{\sigma}(\mathbf{k}) & \xi^a_{\sigma'}(\mathbf{k}) & \xi^a_{\sigma'}(\mathbf{k}) \\
\xi^b_{\sigma'}(\mathbf{k}) & \xi^b_{\sigma'}(\mathbf{k}) & \xi^a_{\sigma'}(\mathbf{k}) & \xi^a_{\sigma}(\mathbf{k}) 
\end{pmatrix} \psi_{\mathbf{k}}
$$

where we have used the spinor notation $\psi^\dagger_{\mathbf{k}} = [a^\dagger_{\mathbf{k}, \uparrow}, b^\dagger_{\mathbf{k}, \uparrow}, a^\dagger_{\mathbf{k}, \downarrow}, b^\dagger_{\mathbf{k}, \downarrow}]$ as a basis for each lattice momentum $\mathbf{k}$. Now, by making use of the variational mean-field approach, we end up with the following set of mean-field equations, which complemented by the charge conserva-

$$
\xi^a_{\sigma}(\mathbf{k}) = -\frac{V}{\mathcal{N}} \sum_{\mathbf{q}} g(\mathbf{k} - \mathbf{q}) [a^\dagger_{\mathbf{q}, \sigma'} a_{\mathbf{q}, \sigma}]_{MF},
$$

$$
\xi^a_{\sigma} = U n^a_{\sigma} + 3V \sum_{\sigma'} n^b_{\sigma'},
$$

$$
\xi^b_{\sigma} = U n^b_{\sigma} + 3V \sum_{\sigma'} n^a_{\sigma'},
$$

$$
\varepsilon^a_{\sigma} = -\frac{U}{\mathcal{N}} \sum_{\mathbf{q}} (a^\dagger_{\mathbf{q}, \sigma} a_{\mathbf{q}, \sigma})_{MF},
$$

$$
\varepsilon^b_{\sigma} = -\frac{U}{\mathcal{N}} \sum_{\mathbf{q}} (b^\dagger_{\mathbf{q}, \sigma} b_{\mathbf{q}, \sigma})_{MF},
$$

with densities $n^a_{\sigma} = \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} (a^\dagger_{\mathbf{q}, \sigma} a_{\mathbf{q}, \sigma})_{MF}$ and $n^b_{\sigma} = \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} (b^\dagger_{\mathbf{q}, \sigma} b_{\mathbf{q}, \sigma})_{MF}$. In the expressions above, the averages $\langle \cdots \rangle_{MF}$ are taken in the grand-canonical ensemble by accounting for the Boltzmann factor in the mean-field Hamiltonian.

Once convergence for the free energy has been achieved, we can compute the CDW and SDW order parameters

$$
\mathcal{O}_{CDW} = \left| \langle n^a_\uparrow + n^a_\downarrow \rangle - \langle n^b_\uparrow + n^b_\downarrow \rangle \right|,
$$

$$
\mathcal{O}_{SDW} = \left| \frac{1}{2} \langle \langle \mathbf{S}_\uparrow \rangle - \langle \mathbf{S}_\downarrow \rangle \rangle \right|,
$$

where $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha, \beta} c^\dagger_{i, \alpha} \sigma_{\alpha, \beta} c_{i, \beta}$, and $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ is the vector of spin-1/2 Pauli matrices. Even though we compute other order parameters related to different broken symmetry phases, these two turned out to be the most stable. For the calculation of the Chern number, we use the discrete formulation in its multiband (non-Abelian) version [74]. In what follows, $t_1$ is set to be the unit of energy and $t_2 = 0.2$. We further fix the Haldane phase $\phi$ to $\pi/2$, in order to maximize the Chern insulating (CI) phase [31, 60].

III. RESULTS OF THE EXACT DIAGONALIZATION CALCULATION

We start by directly presenting the phase diagram [Fig. (1)] obtained via ED using four different clusters 18A, 16B, 12A and 12C [see Fig. 1(f)], and the particular characterization of each phase will be presented afterwards. These clusters are selected in such a way that they are able to accommodate a Néel state (i.e., they are bipartite if considering PBC), and we notice that clusters 12A and 12X also exhibit the K-point as a valid momentum-point in the reciprocal lattice, unlike clusters 12C and 16X [Fig. 1(e)]. These can result in systematic finite-size effects, as we argue below.

The phase diagrams are characterized by phases with the formation of a local order parameter as a result of the interactions: large-$U$ and $V$, result in SDW and CDW phases, respectively. At the regime of weak-interactions,
a topologically-nontrivial CI phase with Chern number \( C = 2 \) distributes at a closed area. That is, the parent spinful non-interacting model possess a ground-state characterized by a topological invariant which survives in the presence of both interactions, as long as they are sufficiently small or compete, preventing the onset of the formation of a local order parameter. The transition to a charge-ordered phase is fairly consistent across the different system sizes, whereas the one to a spin-ordered one suffers from slightly larger finite-size effects. These finite-size effects are not merely related to the number of sites in the lattice but rather if the cluster under study contains or not the \( K \)-point in its reciprocal lattice. For that reason, clusters 12A and 18A present a quantitatively similar SDW transition, while for 12C and 16B this transition is systemically deviated to smaller on-site interactions \( U \).

These phase diagrams are constructed from the analysis of several quantities mentioned in Sec. II. In order to display all relevant features, we focus on a typical line with \( V = 1 \), which successively crosses the CDW, CI and SDW phases when increasing \( U \) from \( U = 0 \) to \( U = 10 \). The results are shown in Fig. 2 for cluster 18A on the left panels, whereas the right panels display the corresponding quantities for cluster 16B. The lattices with 12-sites present similar results as their larger counterparts, in what concerns the presence or absence of the the previously mentioned \( K \)-point.

To start, we characterize the type of the transition, by analyzing the low-lying energy spectrum dependence across the different phases. The first four energy levels, i.e., \( E_\alpha \) with \( \alpha = 0, 1, 2, 3 \) (\( E_0 \) is the ground-state energy) are plotted in Figs. 2 (a) and 2 (e). A careful inspection shows that level crossings occur at the two phase boundaries (CDW-CI and CI-SDW) for the 18A cluster, resulting in first order phase transitions. These are absent in the 16B cluster, and we reemphasize the carefulness required in selecting lattices with the most suitable point-group symmetries. These crossings are more easily indentified if defining the excitation gaps \( \Delta_{ex}^{(\alpha)} = (E_\alpha - E_0) / L \), as shown in Figs. 2 (b) and 2 (f) for \( \alpha = 1 \) and 2, and clusters 18A and 16B, respectively. In the CI-SDW transition for the 18A cluster, owing to the fact that the ground-state is non-degenerate, a vanishing \( \Delta_{ex}^{(1)} \) precisely marks the phase boundary.

The CDW-CI transition, on the other hand, is better characterized by the vanishing of the second excitation gap, \( \Delta_{ex}^{(2)} \). The reason behind this is that in the CDW phase, the ground-state is two-fold degenerate in the thermodynamic limit (and nearly degenerate in the finite cluster we deal with), with a level crossing occurring between \( E_2 \) and \( E_0 \) (or \( E_1 \)) as the transition is approached. In contrast, in the 16B cluster, such many-body gaps never close, but the transitions can be yet pinpointed by peaks in the fidelity metric \( g \), displayed in Fig. 2 (h). In turn, for the 18A cluster [Fig. 2 (d)] a proper peak is missing (a discontinuity is instead observed) precisely due to the fact the transition is first order, and one needs a resolution of the control parameter (in this case \( U \)) that is small enough to capture the very narrow \( \delta U \)-dependent peak, \( g_{peak} \). Again for the 16A cluster, the 'hump' depicting the CI-SDW transition becomes wider and smaller in magnitude for larger \( V \), making the characterization of this transition more challenging [see dashed lines in Figs. 1(b) and 1(d)], and thus amounting for the difference between the phase diagrams of clusters containing or not the \( K \)-point.

Lastly, we report in Figs. 2 (c) and 2 (g) the structure factors corresponding to each order, CDW and SDW, which display a characteristic discontinuous behavior as similarly found elsewhere for other models manifesting a transition between topologically non-trivial and trivial phases [27, 31, 32]. The inset in Fig. 2 (c) shows the extensive nature of \( S_{CDW} \) and \( S_{SDW} \) within each phase, by contrasting the 18A cluster with its counterpart that also contains the \( K \)-point in its reciprocal space, the lattice.
FIG. 2. Four lowest-lying energy levels $E_{\alpha}$ [(a) and (e)], excitation gaps $\Delta E^{(\alpha)\alpha}$ [(b) and (f)], structure factors $S$ [(c) and (g)] and the fidelity metric $g$ [(d) and (h)] of the extended Haldane-Hubbard model with $V = 1$ on the 18-sites (left panels) and 16-sites (right panels) clusters. First order phase transitions are only seen for the 18A cluster (see text). The inset in panel (c) includes the structure factors for the cluster 12A, highlighting the extensive nature of the corresponding correlators sum within the ordered phases.

12A.

Back to the phase diagram in Fig. 1, we are now in position to characterize the phase that displays a non-local order parameter, the topologically non-trivial Chern insulating phase. We present in Fig. 3 an overlay of the computed Chern number, using a discrete version of Eq.(4) [See also App. (A)], and the original boundaries for the phases presented in Fig. 1. For the clusters 12C and 16B, a $C = 2$ phase gives way to a $C = 0$ (thus topologically trivial) roughly at the same positions as the fidelity peak signal the CI-SDW phase transition, at large-$U$ values. For the CDW phase, on the other hand, such change of the topological-invariant number is not seen in the ranges of $V$’s computed, but in the spinless version of the present model, such coexistence of a $C \neq 0$ with a local order parameter has been attributed to the fact that $K$ is not in the set of $k$-points available for some finite clusters, precisely as here [31, 32].

The most interesting features of this computation are thus the ones that come from the calculation in clusters 12A and 18A, which contain the $K$ in its reciprocal lattice. Although for the 12A case [Fig. 3(c)] the computed Chern number closely follows the general belief that once the local order parameters develop the topological characteristics vanish, results from cluster 18A [Fig. 3(a)] are much richer. In this case, we find that in part of the CDW phase, at smaller $U$ values, there is a coexistence regime of a finite CDW order with the presence of a SU(2) symmetry-breaking $C = 1$ phase. A physical interpretation of this result is that in such area of the phase diagram one pseudospin component of the spinful model remains topologically non-trivial whereas the other does not. Whether this coexistence will also occur in the thermodynamic limit is not clear, in special in view of the fact that the cluster 18A does not possess all point group symmetries of the honeycomb lattice, albeit clearly possessing one of the essential ingredients, the manifestation of the $K$-point physics. In Appendix A, we further present more details on the numerical computation of the Chern number, in particular for this lattice size, supporting the results displayed in Fig. 3(a).

IV. RESULTS OF THE MEAN-FIELD CALCULATION

To contrast the previous results, and to further understand finite-size discrepancies in the ED results for the Chern number, we now report the outcomes when casting the interactions in a mean-field form [see Sec. II]. The phase diagram, constructed by taking into account the onset of the order parameters $\mathcal{O}_{\text{CDW}, \text{SDW}}$ [Eq.(9)], is shown in Fig. 4 (a) on $180 \times 180$ and $30 \times 30$ lattices. We first notice that the finite-size effects are rather small, and
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V. SUMMARY AND DISCUSSION

We studied the extended Haldane-Hubbard model in the honeycomb lattice, at unity filling. Depending on the magnitude of the repulsive interactions (either on-site or nearest-neighbor) the ground-state displays insulating behavior, with the presence of phases with finite local order parameters, as charge-density and (antiferromagnetic) spin-density waves, in addition of a topological phase, with its resulting non-local order parameter associated to a topological invariant. Besides, the transitions among all such different phases are first order, when computed with ED [76]. This picture is numerically inferred in small lattices employing the exact diagonalization, and complemented by a variational mean-field analysis. In the former method, due to the small system sizes amenable to computations, some of the clusters may not display all the point group symmetries of the lattice in the thermodynamic limit. For that reason, we must caution that some of the results we display might suffer from systematic finite size effects. Among those, a surprising result is the manifestation of a SU(2) symmetry breaking, where the appearance of a $C = 1$ phase concurs with a charge density wave in a large part of the phase diagram, when dealing with the largest cluster manageable to ED calculations. Such phase is absent in the variational mean-field results, but could be potentially revisited with a larger number of sites in the unit cell, at the expense of introducing a much larger number of fields to be converged [54].

A similar phase has been described in the Haldane-Hubbard model in the presence of a staggered potential $\Delta$, sandwiched in between the standard antiferromagnetic Mott insulating phase at large onsite interactions, and a band-insulating one, at similarly large magnitudes of $\Delta$ [42, 43][77]. In what concerns such SU(2) symmetry broken phases, whether or not they are a result of systematic finite-size effects, is yet elusive. In practice, the smallest finite lattice displaying all the complete set of point group symmetries is a lattice with 24 sites [22]. Our largest cluster with 18 sites possesses a reduced (by the application of translational symmetries) Hilbert space $D \simeq 262 \cdot 10^6$ states, whereas for that lattice, $D \approx 609 \cdot 10^6$, much beyond the current capabilities of cutting edge exact diagonalization schemes. Another possibility, however, is the usage of DMRG methods in wide ladders, which is amenable to tackle a much larger number of sites, and has been used in the past to investigate problems that simultaneously feature topological aspects and interactions [21, 78]. This will be left for future studies.

ACKNOWLEDGMENTS

FIG. 4. (a) The phase diagram of Eq. 1 under the mean-field approximation. (b) A line-cut of the phase diagram at $V = 1$, showing the local order parameters $O_{\text{CDW}}$ and $O_{\text{SDW}}$ together with the corresponding Chern number $C$. Panels (c) and (d) display the smallest band gap $\Delta(k)$ along the lines $U = 2$ and $V = 0.5$, respectively, and are highlighted by the dotted lines in panel (a).
Appendix A: The $C = 1$ phase for cluster 18A

We argue in Sec. III that for the case of the 18A cluster, the Chern number in parts of the CDW phase displays a surprising value of $C = 1$, i.e., a spontaneous symmetry breaking occur, in line with what has been found in related spinful models possessing a checkerboard potential instead [42, 43]. To better understand this result, we describe in more details the procedure we follow in order to compute the topological invariant. The calculation is based on the prescription presented in Refs. [32, 74], where a discretized version of Eq. 4 is employed. For that, we introduce twisted boundary conditions [72, 73], in which the many-body ground-state $|\Psi_{\phi_x,\phi_y}^{0}\rangle$ is obtained on a torus $\{\phi_x, \phi_y\} \in [0, 2\pi)$. In the numerical computations, this range is discretized in $N_x$ and $N_y$ intervals, resulting in $\phi_x = \frac{2m\pi}{N_x}$ and $\phi_y = \frac{2n\pi}{N_y}$, with the integers $m, n$ chosen such that $m \in [0, N_x)$ and $n \in [0, N_y)$, and the ground-state in such points is specified as $|\Psi_{m,n}^{0}\rangle$.

As a result, the discrete version of the Berry curvature can be written as,

$$\tilde{F}_{m,n} = -i \log \left( \frac{U_{m,n}^x U_{m+1,n}^y}{U_{m,n+1}^x U_{m,n}^y} \right),$$

(A1)

where the complex numbers $U_{m,n}^{x(y)}$ are the normalized overlaps of the wave-functions in consecutive points of the patched torus,

$$U_{m,n}^x = \frac{\langle \Psi_{m,n}^0 | \Psi_{m+1,n}^0 \rangle}{\langle \Psi_{m,n}^0 | \Psi_{m,n+1}^0 \rangle}, \quad U_{m,n}^y = \frac{\langle \Psi_{m,n}^0 | \Psi_{m,n+1}^0 \rangle}{\langle \Psi_{m,n}^0 | \Psi_{m,n+1}^0 \rangle},$$

(A2)

with $\tilde{F}_{m,n}$ chosen in the branch $(-\pi, \pi]$.

Finally, the topological invariant is thus written as a normalized summation of the Berry curvatures,

$$C = \sum_{m,n} \frac{\tilde{F}_{m,n}}{2\pi},$$

(A3)

which, for a sufficiently large discretization $N_{x,y}$, converges to the correct Chern number.

A necessary condition for the validity of this method is that the first excitation gap $\Delta_{ex}^{(1)}$ is always finite along the torus formed by the phases $\{\phi_x, \phi_y\}$, i.e., the phases do not result in a gap closing, otherwise the Berry curvature defined above would display a singularity. In Fig. 5, left panels, we show an example of $\Delta_{ex}^{(1)}(\phi_x, \phi_y)$ when patching $\{\phi_x, \phi_y\}$ using $N_x = N_y = 6$. The four consecutive

$\Delta_{ex}^{(1)}$s are chosen across a cut in the phase diagram with $V = 1.5$ and onsite interactions $U = 2.0, 2.5, 3.0$ and 3.5. In this range, the computed Chern number from Eq. A3 is given, respectively, by $C = 1, 0, 0$ and 2. From $U = 2$ to $U = 2.5$, although gaps are all finite in $\{\phi_x, \phi_y\}$ (and much larger than the tolerance on the convergence set in the Krylov-Schur diagonalization), the corresponding Berry curvatures present a systematic change, see two top right panels in Fig. 5. In turn, the second change of the Chern number along this $V = 1.5$ line is less surprising, and is related to the first order phase transition, when the nearly-degenerate doublet of states in the CDW phase crosses the third lowest eigenvalue in the Hamiltonian, entering in the Chern insulating phase.

We have further tested the unexpected $C = 1$ to $C = 0$
transition for other values of $V$, but it results in similar outcomes. Another possibility that may explain such SU(2) symmetry broken phase on cluster 18A is related to the small number of patches $N_{x,y}$ used in the calculation of the topological invariant. Figure 6 displays a direct comparison of the Berry curvature for a typical point in the phase diagram that resulted in $C = 1$: $(U,V) = (2,2)$. Increasing the number of patches from $N_{x,y} = 6$ to $12$ does not alter the computed Chern number, so this technical aspect is not responsible for its appearance in this finite cluster.

FIG. 6. The Berry curvature normalized by $2\pi$, $\tilde{F}_{m,n}/2\pi$, for the cluster 18A with parameters $U = 2$ and $V = 2$, along the TBC torus $\{\phi_x, \phi_y\}$. In (a), $N_{x,y} = 6$, whereas in (b) $N_{x,y} = 12$. General features are maintained albeit the much finer mesh in the latter, and the resulting Chern number is $C = 1$ in both cases [See Fig. 3(a)].

[1] T. Zhang, Y. Jiang, Z. Song, H. Huang, Y. He, Z. Fang, H. Weng, and C. Fang, “Catalogue of topological electronic materials,” Nature 566, 475 (2019).
[2] M. G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B. A. Bernevig, and Z. Wang, “A complete catalogue of high-quality topological materials,” Nature 566, 480 (2019).
[3] F. Tang, H. C. Po, A. Vishwanath, and X. Wan, “Comprehensive search for topological materials using symmetry indicators,” Nature 566, 486 (2019).
[4] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, “Classification of topological insulators and superconductors in three spatial dimensions,” Phys. Rev. B 78, 195125 (2008).
[5] A. Kitaev, in Advances in Theoretical Physics: Landau Memorial Conference, edited by V. Lebedev and M. Feigelman, AIP Conf. Proc., Vol. 1134 (AIP, Melville, NY, 2009), p. 22.
[6] M Hohenadler and F F Assaad, “Correlation effects in two-dimensional topological insulators,” Journal of Physics: Condensed Matter 25, 143201 (2013).
[7] R. S. K. Mong, A. M. Essin, and J. E. Moore, “Antiferromagnetic topological insulators,” Phys. Rev. B 81, 245209 (2010).
[8] C. Fang, M. J. Gilbert, and B. A. Bernevig, “Topological insulators with commensurate antiferromagnetism,” Phys. Rev. B 88, 085406 (2013).
[9] T. Yoshida, R. Peters, S. Fujimoto, and N. Kawakami, “Topological antiferromagnetic phase in a correlated Bernevig-Hughes-Zhang model,” Phys. Rev. B 87, 085134 (2013).
[10] S. Miyakoshi and Y. Ohta, “Antiferromagnetic topological insulator state in the correlated Bernevig-Hughes-Zhang model,” Phys. Rev. B 87, 195133 (2013).
[11] S. Raghu, X.-L. Qi, C. Honerkamp, and S.-C. Zhang, “Topological Mott insulators,” Phys. Rev. Lett. 100, 156401 (2008).
[12] J. Wen, A. Rüegg, C.-C. Joseph Wang, and G. A. Fiete, “Interaction-driven topological insulators on the kagome and the decorated honeycomb lattices,” Phys. Rev. B 82, 075125 (2010).
[13] J. C. Budich, R. Thomale, G. Li, M. Laubach, and S.-C. Zhang, “Fluctuation-induced topological quantum phase transitions in quantum spin-Hall and anomalous-Hall insulators,” Phys. Rev. B 86, 201407 (2012).
[14] A. Dauphin, M. Müller, and M. A. Martin-Delgado, “Rydberg-atom quantum simulation and Chern-number characterization of a topological Mott insulator,” Phys. Rev. A 86, 053618 (2012).
[15] C. Weeks and M. Franz, “Interaction-driven instabilities of a Dirac semimetal,” Phys. Rev. B 81, 085105 (2010).
[16] L. Wang, X. Dai, and X. C. Xie, “Interaction-induced topological phase transition in the Bernevig-Hughes-Zhang model,” Europhys. Lett. 98, 57001 (2012).
[17] A. Rüegg and G. A. Fiete, “Topological insulators from complex orbital order in transition-metal oxides heterostructures,” Phys. Rev. B 84, 201103 (2011).
[18] K.-Y. Yang, W. Zhu, D. Xiao, S. Okamoto, Z. Wang, and Y. Ran, “Possible interaction-driven topological phases in (111) bilayers of LaNiO3,” Phys. Rev. B 84, 201104 (2011).
[19] Noel A. García-Martínez, A. G. Grushin, T. Neupert, B. Valenzuela, and E. V. Castro, “Interaction-driven phases in the half-filled spinless honeycomb lattice from exact diagonalization,” Phys. Rev. B 88, 245123 (2013).
[20] M. Daghofer and M. Hohenadler, “Phases of correlated spinless fermions on the honeycomb lattice,” Phys. Rev. B 89, 035103 (2014).
[21] J. Motruk, A. G. Grushin, F. de Juan, and F. Pollmann, “Interaction-driven phases in the half-filled honeycomb lattice: An infinite density matrix renormalization group study,” Phys. Rev. B 92, 085147 (2015).
[22] S. Capponi and A. M. Läuchli, “Phase diagram of interacting spinless fermions on the honeycomb lattice: A comprehensive exact diagonalization study,” Phys. Rev. B 92, 085146 (2015).
[23] D. Scherer, M. M. Scherer, and C. Honerkamp, “Correlated spinless fermions on the honeycomb lattice revisited,” Phys. Rev. B 92, 155137 (2015).
[24] K. Sun, H. Yao, E. Fradkin, and S. A. Kivelson, “Topological insulators and nematic phases from spontaneous symmetry breaking in 2d fermi systems with a quadratic band crossing,” Phys. Rev. Lett. 103, 046811 (2009).
in the extended fermionic Hubbard model on the hexagonal lattice," Phys. Rev. B 98, 235129 (2018).

[63] R. B. Lehoucq, D. C. Sorensen, and C. Yang, “Arpack users guide: Solution of large scale eigenvalue problems by implicitly restarted arnoldi methods.” (1997).

[64] S. Balay, S. Abhyankar, M. F. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, A. Dener, V. Eijkhout, W. D. Gropp, D. Karpeyev, D. Kaushik, M. G. Knepley, D. A. May, L. C. McInnes, R. T. Mills, T. Munson, K. Rupp, P. Sanan, B. F. Smith, S. Zampini, H. Zhang, and H. Zhang, “PETSc Web page,” https://www.mcs.anl.gov/petsc (2019).

[65] V. Hernandez, J. E. Roman, and V. Vidal, “SLEPc: A scalable and flexible toolkit for the solution of eigenvalue problems,” ACM Trans. Math. Software 31, 351 (2005).

[66] P. Zanardi and N. Paunković, “Ground state overlap and quantum phase transitions,” Phys. Rev. E 74, 031123 (2006).

[67] L. Campos Venuti and P. Zanardi, “Quantum critical scaling of the geometric tensors,” Phys. Rev. Lett. 99, 095701 (2007).

[68] P. Zanardi, P. Giorda, and M. Cozzini, “Information-theoretic differential geometry of quantum phase transitions,” Phys. Rev. Lett. 99, 100603 (2007).

[69] M.-F. Yang, “Ground-state fidelity in one-dimensional gapless models,” Phys. Rev. B 76, 180403 (2007).

[70] C. J. Jia, B. Moritz, C.-C. Chen, B. Sriram Shastry, and T. P. Devereaux, “Fidelity study of the superconducting phase diagram in the two-dimensional single-band Hubbard model,” Phys. Rev. B 84, 125113 (2011).

[71] R. Mondaini, P. Nikolić, and M. Rigol, “Mott-insulator–superconductor transition in a two-dimensional superlattice,” Phys. Rev. A 92, 013601 (2015).

[72] D. Poilblanc, “Twisted boundary conditions in cluster calculations of the optical conductivity in two-dimensional lattice models,” Phys. Rev. B 44, 9562 (1991).

[73] Q. Niu, D. J. Thouless, and Y.-S. Wu, “Quantized Hall conductance as a topological invariant,” Phys. Rev. B 31, 3372 (1985).

[74] T. Fukui, Y. Hatsugai, and H. Suzuki, “Chern numbers in discretized Brillouin zone: Efficient method of computing (spin) Hall conductances,” J. Phys. Soc. Japan 74, 1674 (2005).

[75] Y.-F. Zhang, Y.-Y. Y., Y. Ju, L. Sheng, R. Shen, D.-N. Sheng, and D.-Y. Xing, “Coupling-matrix approach to the Chern number calculation in disordered systems,” Chinese Phys. B 22, 117312 (2013).

[76] In mean-field, however, the continuous closing of the gap (on a small scale of the control parameter) is suggestive of a second order transition.

[77] In special, we highlight that the ED results presented in Ref. [42] are obtained for a lattice equivalent to cluster 16B, which is prone in missing fundamental features of the phase diagram, in particular the first order nature of the transitions, as we show in the text.

[78] P. W. Klein, A. G. Grushin, and K. Le Hur, “Stochastic Chern number from interactions and light response,” (2020), arXiv:2002.01742 [cond-mat.str-el].