Character of the phase transitions in the Haldane-Hubbard model with inversion-breaking ionic potentials

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Using the exact-diagonalization (ED) approach, we revisit the ground-state phase diagram of the Haldane-Hubbard model on the honeycomb lattice with staggered sublattice potentials, and further study the character of transitions between different phases by examining the lower-lying energy levels, excitation gaps, structure factors and fidelity metrics. The phase diagram includes the band insulator, Mott insulator and two Chern insulator (CI) phases with Chern number \( C = 2 \) and \( C = 1 \). We observe some clues of second-order phase transition between the two CI phases, while all the other phase transitions are found to be first-order ones. The mean-field method provide a similar phase diagram with ED, even though we can not identify the phase-transition style.

I. INTRODUCTION

As the most important concept in condensed matter physics, the Landau-Ginzburg theory describes the phase transition of matter that is caused by the spontaneous breaking of a certain symmetry [1]. While the discovery of the integer quantum Hall effect in a two-dimensional electron gas under strong magnetic field provided an extra paradigm to characterize quantum states [2]. In the past few decades, the topological properties have thus begun to play an increasingly important role as a new standard for the classification of a large class of materials [3–6], and the topological ordered states in non-interaction systems have been completely classified based on time-reversal, particle-hole, chiral and crystal symmetries [7–10].

In the interacting systems, the correlation effect of electrons is excepted to give rise to more intriguing and richer phenomena [11]. A famous example is the fractional quantum Hall state, which allows the existence of quasiparticle excitations that carry fractional charge and have fractional statistics due to strong repulsion among electrons [12–14]. Secondly, the electronic interactions may directly lead to the so-called topological Mott insulator via a dynamically generated spin-orbit coupling [15–23]. Despite some of these mean-field results remain controversial [24–28], interaction-induced topological states may still be observed in two-dimensional systems with quadratic band crossing and weak interactions [29–36]. Finally, the coexistence of the topological and locally ordered states have also been largely investigated by introducing interaction to topological systems [37–42]. For example, an exotic phase with one of the spin components in the Hall state and the other one in a localized state can emerge in the spinful Haldane-Hubbard model with inversion-breaking ionic potentials [39–42].

In this paper, we adopt the exact diagonalization (ED) and mean-field (MF) methods to study the spinful Haldane-Hubbard model at half-filling and zero temperature. By tuning the strength parameters of the staggered sublattice potential \( \Delta \) and the on-site Coulomb interaction \( U \), we further explore its ground-state phase diagram. Our results are similar to those obtained by Vanhala et al. [39], and the intermediate phases with the Chern number \( C = 1 \) can be also observed. Here, we aim to identify the phase-transition styles by analyzing the energy levels, excitation gaps, structure factors and fidelity metrics in ED results, which gives unbiased ground-state information in finite-size systems. Some clues of second-order phase transition appears between the two topological phases with \( C = 1 \) and \( C = 2 \), while other phase boundaries are found to be first-order ones. The mean-field (MF) theory provides similar phase diagram with ED, however, the character of phase transitions is hardly to identify owing to the single-particle approximation.

The presentation is organized as follows: In Sec. II, we introduce the model and all the quantities we use to characterize the different phases. Sections III presents the results of the exact diagonalization and mean field methods. Lastly, Sec. IV summarizes and discusses the results.

II. MODEL AND MEASUREMENTS

We write the Hamiltonian of the Haldane-Hubbard model as

\[
\hat{H}_k = -t_1 \sum_{\langle i,j \rangle, \sigma} (\hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + H.c.) - t_2 \sum_{\langle \langle i,j \rangle \rangle, \sigma} (e^{i\phi_{ij}} \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + H.c.)
\]  

(1)
and the local part
\[
\hat{H}_l = - U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \Delta \sum_{i,\sigma} \text{sgn}(i) \hat{n}_{i,\sigma}.
\] (2)

Here, \( \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} \) creates (annihilates) an electron at site \( i \) of the honeycomb lattice with spin \( \sigma \) = \( \uparrow \) or \( \downarrow \), and \( \hat{n}_{i,\sigma} \equiv \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} \) is the number operator. \( t_1 \) \( (t_2) \) is the nearest-neighbor (next-nearest-neighbor) hopping constant; \( U \) is the on-site interaction strength; \( \Delta \) is the staggered potential. \( \text{sgn}(i) \) equals +1 for sublattice A and −1 for sublattice B, respectively. The complex phase \( \phi_{i,j} = \phi (-\phi) \) in the clockwise (anticlockwise) loop is added to the second hopping term. Throughout the paper, we focus on the ground-state phase diagram at half-filling.

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 [43, 44].

A. Exact diagonalization in real space

By using the translational symmetries in periodic boundary condition, we reduce the size of Hilbert space by a factor of \( N \) \( (N = 6 \) for our 12A lattice, see Ref. [38]), and apply the Arnoldi [45] method to obtain the ground state and several low-lying excited states. The reciprocal lattices of this 12A cluster contain the \( K \) high-symmetry point, which is crucial to grasp the critical features because the closing of the excitation gap occurs at this point during the topological phase transition [37, 44].

Several properties can be used to characterize the quantum phase transition. Among them, the ground-state fidelity metric is defined as [46–48]:
\[
g(U, \Delta U) \equiv \frac{2}{N} \left[ 1 - \frac{|\langle \Psi_0(U) | \Psi_0(U + \Delta U) \rangle|}{(\Delta U)^2} \right],
\] (3)

with \( |\psi_0(U)\rangle \) \( (|\psi_0(U + \Delta U)\rangle) \) being the ground state of \( \hat{H}(U) \) \( [\hat{H}(U + \Delta U)] \). In what follows, we set \( \Delta U = 10^{-3} \). In finite-size systems, this quantity is expected to exhibit a large and sharp peak or discontinuity for the first-order transition, while there is a wider and smaller “hump” for the second-order one [38, 44, 49].

The spin-density wave (SDW) and charge-density wave (CDW) structure factors can be used to characterize the Mott insulator (MI) and band insulator (BI), respectively. We define them in a staggered fashion as follows:
\[
S_{\text{SDW}} = \frac{1}{N} \sum_{i,j} (-1)^\eta \langle \hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow} \rangle \langle \hat{n}_{j,\uparrow} - \hat{n}_{j,\downarrow} \rangle,
\]
\[
S_{\text{CDW}} = \frac{1}{N} \sum_{i,j} (-1)^\eta \langle \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow} \rangle \langle \hat{n}_{j,\uparrow} + \hat{n}_{j,\downarrow} \rangle,
\] (4)

where \( \eta = 0 \) \( (\eta = 1) \) indicates that sites \( i \) and \( j \) are in the same (different) sublattice.

The topological invariant is quantified by the Chern number. Given the twisted boundary conditions [50], it can be defined as [51],
\[
C = \int \frac{d\phi_x d\phi_y}{2\pi i} \left( \langle \partial_{\phi_x} \Psi^* \partial_{\phi_y} \Psi \rangle - \langle \partial_{\phi_y} \Psi^* \partial_{\phi_x} \Psi \rangle \right),
\] (5)

where \( |\Psi\rangle \) is the ground-state wave function, and \( \phi_x \) \( (\phi_y) \) is the twisted phase along the \( x \) \( (y) \) direction. To avoid the integration which cost huge computational resources, we instead use a sufficiently discretized version, which has been shown to converge to the result of Eq. (5) [37, 52, 53]. In fact, a mesh of \( 6 \times 6 \) phases \( (\phi_x, \phi_y) \) over the Brillouin zone is sufficiently enough to guarantee the convergence.

B. Mean-field method in momentum space

To contrast the results obtained via ED, we employ a variational mean-field method in momentum space to repeat the phase diagram. The details of this method can be seen in Ref. [38], here we just show the definitions of the CDW and SDW order parameters,
\[
\mathcal{O}_{\text{CDW}} = \left| \langle n^a_{\uparrow} + n^b_{\uparrow} \rangle - \langle n^b_{\downarrow} + n^a_{\downarrow} \rangle \right|,
\]
\[
\mathcal{O}_{\text{SDW}} = \frac{1}{2} \left( \langle \vec{S}_a \rangle_{\text{MF}} - \langle \vec{S}_b \rangle_{\text{MF}} \right),
\] (6)

where \( \vec{S}_i = \frac{1}{2} \sum_{\alpha \beta} c_{i\alpha}^\dagger \vec{\sigma}_{\alpha \beta} c_{i\beta} \) and \( \vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z) \) is the vector of spin-1/2 Pauli matrices. Similarly to ED, we use the discrete formulation in its multiband (non-Abelian) version to compute the Chern number [52].

III. RESULTS AND ANALYSIS

The phase diagrams in the parametric space \((U, \Delta)\) obtained from ED and MF are displayed in Figs. 1(a) and 1(b), respectively. Actually, they are roughly same as those in Ref. [39]: the CI phase with \( C = 2 \) in the small
state and one excited state in Figs. 2(a) and 2(e), excitation gap vanishing in Figs. 2(b) and 2(f), discontinuities of the CDW and SDW structure factors in Figs. 1(c) and 2(g), as well as sharp peaks in the fidelity metrics $g$ in Figs. 2(d) and 2(h).

Instead, some clues of second-order phase transitions appears at $U = 4.8$ and $\Delta = 2.0$ between the $C = 1$ and $C = 2$ phases. Rather than a level crossing, the two lowest energy levels approaches to each other at this point, as detailed in the inset of Fig. 2(a). Correspondingly, the decreasing of the excitation gap $\Delta_{\text{ex}}^{(1)}$ occurs instead of gap vanishing, see Fig. 2(b). The slowly changing of structure factors and a smaller "hump" in fidelity metric can be also observed in Figs. 2(c) and 2(d), respectively. All these features indicates a second-order transition close to this critical point.

However, for the critical point located at $U = 8.5$ and $\Delta = 2.0$, we do not have any evidence about the character of transition except for the changing of Chern number. We thus speculate this narrow region, i.e., the $C = 1$ phase between the $C = 2$ and MI phases, to be a finite-size effect. To further verify our idea, we show the contour plots of $S_{\text{SDW}}, S_{\text{CDW}}, g$ and $\Delta_{\text{ex}}^{(1)}$ as a function of $U$ and $\Delta$ in Figs. 3(a), 3(b), 3(c) and 3(d), respectively. We find that except for this region, all the other phase boundaries identified by the Chern number have a very good correspondence with the change of their structure factors, the peak or "hump" of the fidelity metrics and the first excitation gaps. This disagreement has been also observed in Refs. [37, 38, 49] and can be attributed to the finite-size effect.

Back to the phase diagram of MF method in Fig. 1(b), we show more details with parameter $\Delta = 1.6$ ($\Delta = 4.0$)
in the left (right) panel of Fig. 4. The results of the Chern number \(C\), the CDW and SDW order parameters \(O_{\text{CDW}}\) and \(O_{\text{SDW}}\) are displayed in Figs. 4(a) and 4(b). For the case of \(\Delta = 1.6\), the Chern number changes from 0 to 2 and to 0 as \(U\) increases. The result of \(O_{\text{SDW}}\) becomes finite and the CDW structure factor decreases more rapidly when the system goes into the \(C = 1\) phase. For \(\Delta = 4.0\), similar behavior happens at the transition point between the BI and \(C = 1\) phases. We further display the smallest band gap \(\Delta(k)\) in Figs. 4(c) and 4(d) with \(\Delta = 1.6\) and \(\Delta = 4.0\), respectively. On the \(20 \times 20\) lattice, the minimums appear together with the changing of Chern numbers and they turn to be gap closings as the lattice size increases to \(180 \times 180\). In our opinion, these features can not be used to discuss the character of phase transitions. However, the MF method provide similar phase diagram with ED results.

**IV. SUMMARY AND DISCUSSION**

To summarize, we studied the spinful Haldane-Hubbard model at half-filling on the honeycomb lattice by the ED and MF methods. By tuning the on-site interaction strength \(U\) and staggered sublattice potential \(\Delta\), the ground state exhibits a rich phase diagram, which includes the BI (CDW) and MI (SDW) phases with finite local order parameters, as well as two topologically nontrivial phases with Chern number \(C = 2\) and \(C = 1\). In the ED results, we observed the energy-level crossings, the discontinuities of structure factors and the sharp peaks of fidelity metric at both BI and MI phase boundaries, signaling a first-order phase transition. While some clues of second-order transition (such as the energy-level approaching, the slowly changing of structure factors and a small “hump” of fidelity metric) are observed between the two topological phases. In the MF method, however, the character of transitions can not be identified from the relevant properties, even though it provides a similar phase diagram with ED.

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