

# Phase diagram of the ionic Hubbard model with density-dependent hopping

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We obtain the quantum phase diagram of the ionic Hubbard model including electron-hole symmetric density-dependent hopping. The boundaries of the phases are determined by crossings of excited levels with particular discrete symmetries, which coincide with jumps of charge and spin Berry phases with a topological meaning. Reducing the magnitude of the hopping terms that do not change the total number of singly occupied sites with respect to the other one, the region of the phase diagram occupied by the fully gapped spontaneously dimerized insulator (which separates the band insulating and Mott insulating phases) is enlarged, particularly for small values of the alternating on-site energy. This result might be relevant for experiments in cold atoms in which topological charge pumping is observed when alternation in the hopping is included.

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## I. INTRODUCTION

Ultracold quantum gases provide a versatile platform as universal quantum simulators of many-body problems [1]. Cold atoms as well as other platforms have been used to study quantized topological charge pumping in driven systems [2]. A time-dependent adiabatic evolution in a closed cycle in a certain space of parameters constitutes a Thouless pump, in which a quantized amount of charge or spin is transported, which is topologically protected [3,4]. The study of Thouless pumps combines various exciting aspects of modern physics, including topological phases, quantum mechanics, metrology [5], and quantum information processing.

Simulating the noninteracting Rice-Mele model [6] with ultracold atoms, quantized charge pumping has been achieved for bosons [7] and fermions [8]. For the fermionic interacting Rice-Mele model, charge pumping has also been studied theoretically [9] using a pump cycle centered at the origin of a two-dimensional parameter space  $(\delta, \Delta)$  explained in Sec. II. In the case of weak enough interaction, the pump cycle encloses two symmetrically located singularities resulting in a pumping of two charges, one for each spin. Notably, the interaction induces an effective repulsion of the singularities while keeping their positions symmetrically disposed. As a consequence, increasing the interaction results in a movement of the singularities towards the frontier of the closed path and when a critical value of the interaction is reached, they are expelled outside from it leading to an abrupt decrease of the quantized charge pumped per cycle from two to zero. This behavior has been recently experimentally observed in an optical lattice [10].

The interacting version of the model (described in detail in Sec. II) is particularly interesting because it also permits the transport of one single charge in the cycle. This has been

explored theoretically (including also spin pumping) [11]. To pump one charge per cycle, a closed path is chosen with its center outside the origin of the parameter space and enclosing one singularity in the trajectory. Therefore, the interaction is used to split the degeneracy of the singularities at the origin in the noninteracting model and permits one to select only one of both inside the loop. Remarkably, this half of the usual Thouless pumping has been recently achieved in a dynamical superlattice of fermionic atoms [12].

A feature of the phase diagram for interacting fermionic models is that it includes regions of the parameter space in which the spin gap vanishes. If in an experimental setup the closed path traverses the spin gapless region, the adiabatic charge pumping results in a challenge for the experiment, because traversing a gapless region with finite velocity necessarily induces transitions from the ground state to excited states.

The goal of this work is to study to what extent the region of the phase diagram occupied by the fully gapped phase can be enlarged. To do so, we study the ionic Hubbard model (IHM), which is a general prototype for the interacting Rice-Mele one, with a density-dependent hopping (DDH). In order to solve the model, we use the method of crossings of excited energy levels based on conformal field theory [13–17], already used in Ref. [18] for the standard IHM. For this model including DDH, the method also coincides with that of jumps of charge and spin Berry phases used in Ref. [19].

The paper is organized as follows. In Sec. II we explain the model and its different phases as the parameters are changed. Furthermore, we provide a description of the Thouless pump and the different types of cycles in the parameter space. Moreover, this section gives a detailed explanation that motivates the inclusion of DDH for enlarging the spin gapless region of the phase diagram. In Sec. III we briefly explain the method of



in the plane  $\delta, \Delta$  that encloses a critical point  $\Delta = \pm\Delta_c$  and passes far from it, necessarily traverses the MI phase, because  $\Delta_c$  and  $\Delta_s$  are very near each other. This case is illustrated at the bottom of Fig. 1. Traversing with a finite velocity, a gapless point produces spin excitations at finite energy, which in turn lead to charge excitations because of the mixing of both sectors at finite energy [26,28]. This leads to oscillations in the charge pumping and loss of quantization with the number of cycles as determined theoretically [11] and experimentally [12]. While the addition of a staggered magnetic field or Ising spin interactions leads to opening of the spin gap and robust charge pumping [11], these terms are not experimentally feasible at present.

Another possibility is to enlarge the region of the SDI phase, separating  $\Delta_c$  and  $\Delta_s$  and performing a pump cycle that avoids the MI phase leading to a fully gapped trajectory in the whole cycle, as shown at the top of Fig. 1. This is in principle possible adding the density-dependent hopping. Such a term in an electron-hole symmetric form has been realized in cold atoms using Floquet engineering [20–25]. The Hubbard model with nearest-neighbor hopping dependent on the occupancy of the sites involved (also called correlated hopping) has been derived and studied as an effective model for the superconducting cuprates [38–40], which leads to enhancement of superconductivity for certain parameters [41–44]. Some studies also include nearest-neighbor repulsion [45,46]. In one dimension, phases with dominating singlet-superconducting correlations appear for some parameters [47–50]. At half filling, it has been found that when the hopping term that changes the number of singly occupied sites [ $t_{AB}$  in Eq. (1)] is larger than the other two, a dimerized phase with a spin gap is favored [13,19,51,52], which is the desired effect.

In conclusion, the critical points of the pump cycles at which the Berry phases jump lie on the line  $\delta = 0$ , because for  $\delta = 0$ , the system has inversion symmetry at each site and as a consequence, the Berry phases can only be either 0 or  $\pi$  (mod  $2\pi$ ). In other words,  $\gamma_c/\pi$  and  $\gamma_s/\pi$  become topological numbers protected by inversion symmetry [35]. In addition, the MI phase in which the spin gap vanishes is also restricted to  $\delta = 0$ . Then to identify a possible cycle that encloses the charge critical point with a ground state separated from the rest of the spectrum in the whole cycle, one can keep  $\delta = 0$ , where all ground-state degeneracies lay. This is what we do in the rest of the work.

### III. METHOD OF CROSSINGS OF EXCITED ENERGY LEVELS

The model in Eq. (1) for  $\delta = 0$  becomes the IHM with electron-hole symmetric DDH. It is interesting to note that the standard IHM (without DDH) is integrable according to numerical studies [33] and in fact it can be solved by Bethe ansatz in some cases [34]. A model with only DDH with  $\Delta = 0$  can also be solved exactly using the Bethe ansatz for particular parameters [53].

In this work, in order to calculate the phase diagram of the model we use the method of crossings of excited energy levels [13–17]. In one dimension, the dominant correlations at large distances determine the thermodynamic phase of the system. In usual cases in which there is no long-range order, one

expects that residual interactions between chains gives rise to this order according to the prevailing long-distance behavior. The idea of the method is that the dominant correlations at large distances correspond to the smallest excitation energies. The crossings of excited levels in appropriate symmetry sectors therefore correspond to phase transitions. The method has been used before for similar models [13,18,19]. For our model, this method and the jumps in the values of the Berry phases give the same information [18], but the crossings of appropriate energy levels is simpler and requires less computational cost.

In terms of jumps in Berry phases, the method can be understood as follows. As explained in the previous section, these jumps correspond to changes in the topological sector of the model which are relevant for charge and spin pumping. The charge Berry phase is the phase accumulated by the ground state, using twisted boundary conditions in which the hopping term at one bond only, is changed by a factor  $e^{i\Phi}$ , as  $\Phi$  varies from 0 to  $2\pi$ . For the spin Berry phase the factor is  $e^{i\Phi}$  for spin up, and  $e^{-i\Phi}$  for spin down [35]. During the cycle, for an even number of sites  $L$ , the ground-state energy is minimized when  $\Phi = \pi$  (antiperiodic boundary conditions) if  $L$  is a multiple of 4, and  $\Phi = 0$  (periodic boundary conditions) for  $L$  even but not a multiple of 4. These boundary conditions are known as closed-shell conditions. The opposite case corresponds to open-shell boundary conditions at which the ground state has a maximum as a function of  $\Phi$ . A jump in any or both Berry phases takes place at parameters for which at this maximum, the ground state becomes degenerate with an excited state with opposite value of the Berry phase [18]. Our method is essentially to identify these crossings separating both states by their properties under discrete symmetries of the model at the specific value of  $\Phi$  where the crossing occurs.

The crossings for both charge and spin transitions are determined using open-shell boundary conditions. The charge transition is determined by a crossing in the ground state of the two singlets of lowest energy with opposite parity under inversion. In the BI phase the ground state is even under inversion, while it is odd in the other two phases. The spin transition between SDI and MI phases, is determined by the crossing of the excited even singlet with lowest energy and the lowest excited odd triplet, which has less energy in the MI phase. In the actual calculation we have not evaluated the total spin  $S$  of the states, but used the parity under time reversal (the singlet is even and the triplet with total spin projection  $S_z = 0$  is odd). All these states have wave vector 0 for  $\Delta \neq 0$ .

The method is expected to be very accurate. In particular, for the model with only DDH and on-site repulsion  $U$  [Eq. (1) with  $\Delta = \delta = 0$ ], the phase diagram obtained from jumps in the Berry phases practically coincides with that obtained from bosonization at several densities for small values of  $U$ , for which bosonization is expected to be quantitatively valid [52].

To determine the phase diagram we have set  $t_{AB} = 1$  as the unit of energy. Then for a given value of  $t_{AA}$  and  $\Delta$  we have calculated the values of  $U$  that correspond to the charge ( $U_c$ ) and spin ( $U_s$ ) transitions using the method of crossings of energy levels for all even number of sites  $L$  in the range  $6 \leq L \leq 14$ . The results were extrapolated to  $L \rightarrow \infty$  using a quadratic polynomial in  $1/L$ . Examples of the extrapolation are shown

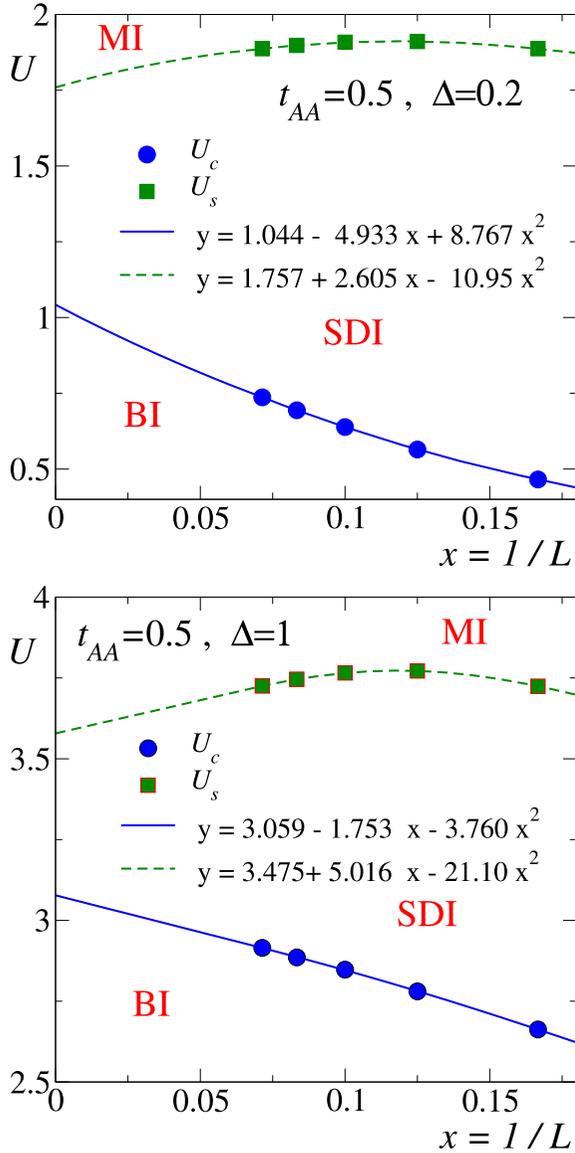


FIG. 2. Critical values of  $U$  for the charge and spin transitions for  $t_{AB} = 1$ , and other parameters indicated inside each figure.

in Fig. 2. The curves fit the data well and the finite-size effects are in general small, except for the charge transition for small values of  $\Delta$ . In any case, a deviation of the value of  $U_c$  for  $\Delta = 0.2$  for up to 20% is very unlikely from the trend of the curve and does not modify our conclusions. Calculations with  $L = 16$  are possible, but they are very time-consuming and lead to a modification of the extrapolated values of  $U_c$  by less than 1% in the region of interest of small  $\Delta$ .

#### IV. RESULTS

In Fig. 3, we compare the phase diagram of the standard IHM with that in which the hopping terms that do not alter the total number of singly occupied sites  $t_{AA} = t_{BB}$  is reduced. For fixed  $\Delta$  the system is a BI for low  $U$  and a MI for large  $U$ . Both phases are separated by a narrow region of the SDI phase. Increasing  $U$ , the charge transition at  $U = U_c$  (with a jump in  $\gamma_c$  from 0 to  $\pi$  [18]) corresponds to the change from

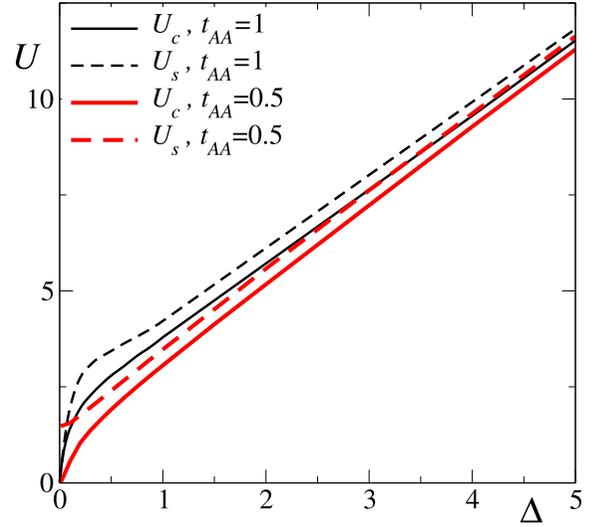


FIG. 3. Phase diagram of the IHM with DDH in the  $\Delta, U$  plane for  $t_{AB} = 1$ , and two values of  $t_{AA} = t_{BB}$ . The region between the full and dashed lines corresponds to the SDI.

the BI to the SDI, and at the spin transition for  $U = U_s$  (with a jump in  $\gamma_c$  from 0 to  $\pi$  [18]) the SDI changes to the MI.

For  $\Delta \gtrsim 3t_{AB}$  the width of the SDI phase is of the order of a fraction of  $t_{AB}$ . Naturally, keeping the three hopping terms equal  $t_{\alpha\beta} = t$  and reducing  $t$ , the SDI phase shrinks and both  $U_c, U_s \rightarrow 2\Delta$  for  $t \rightarrow 0$ . It is therefore noticeable that reducing only  $t_{AA} = t_{BB}$ , the extension of the SDI phase is increased for  $\Delta > 3t_{AB}$  and by about 15% for  $\Delta = 5t_{AB}$ .

As is apparent in Fig. 4, this effect is more dramatic for  $\Delta < 0.2t_{AB}$ . In fact, contrary to the case of equal  $t_{\alpha\beta} = t$ , there is a finite spin gap for small  $U$  even at  $\Delta = 0$  when  $t_{AB} > t_{AA} = t_{BB}$ . This result has been found before [13,19,51,52] and can be understood from analytical calculations using bosonization [51,52] which coincide very well with numerical calculations [19] for small values of  $U$ .

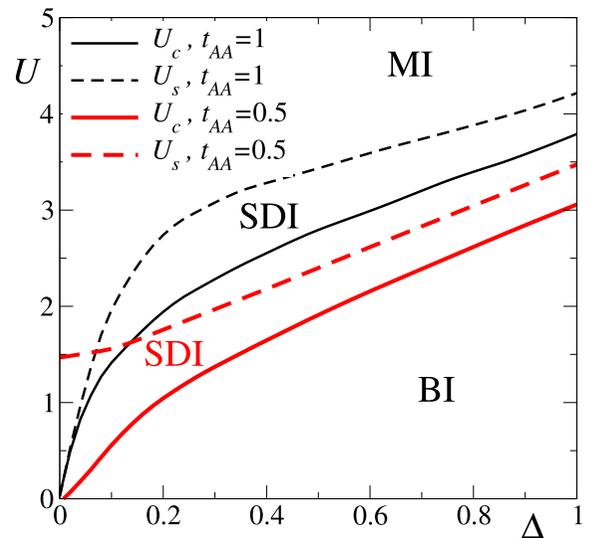


FIG. 4. Same as Fig. 3 in a smaller region of  $\Delta$ .

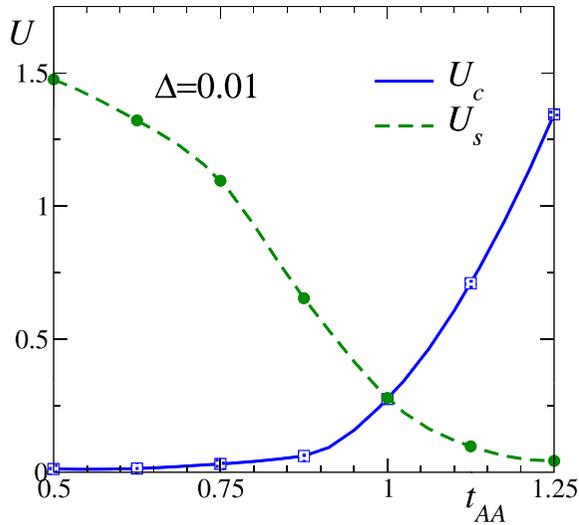


FIG. 5. Critical values of  $U$  at the charge and spin transitions as a function of  $t_{AA} = t_{BB}$  for  $t_{AB} = 1$  and  $\Delta = 0.01$ .

The particular features of the phase diagram for small  $\Delta$ , render it possible to perform time evolutions around a critical point for the charge transition that transport a quantized unit of charge per cycle with open charge and spin gaps in the whole cycle, like the pump cycle shown at the top of Fig. 1. For example for  $\Delta = 0.2$ ,  $t_{AB} = 1$ , and  $t_{AA} = t_{BB} = 0.5$ , we find  $U_c = 1.044$  and  $U_s = 1.757$ . Performing a time-dependent cycle in either plane  $(\delta, \Delta)$  or  $(\delta, U)$  with the center at the charge critical point (with  $\delta = 0$ ) and the amplitude in  $\Delta$  of about  $\pm 0.2$  or in  $U$  near  $\pm 0.5$ , the cycle never reaches the MI phase and therefore, the spin gap is always open. One point that should be taken into account is that the spin transition is of the Kosterlitz-Thouless type, and therefore the spin gap is exponentially small in the SDI phase near the transition boundary [19]. Therefore it might be convenient to move the time cycle away from the MI-SDI boundary, keeping the critical point inside the cycle.

In the previous figures we have taken  $t_{AA} = t_{BB} = t_{AB}/2$ . In Fig. 5 we show how the values of  $U$  at both transitions change with  $t_{AA} = t_{BB}$  for a small value of  $\Delta$ . We can see that the change is more rapid for  $t_{AA}$  near  $t_{AB}$  and the increase in  $U_s$  is already large for  $t_{AA}/t_{AB} = 3/4$ .

When  $t_{AA}/t_{AB}$  exceeds 1 for a significant amount,  $U_c$  becomes larger than  $U_s$  giving rise to a new phase in between. A detailed study of the properties of this phase is beyond the scope of the present work. For  $\Delta = 0$ , studies with bosonization indicate that this region corresponds to a Tomonaga-Luttinger liquid (gapless) phase with triplet

superconducting and bond spin-density wave correlations dominating at large distances [19,51,52]. However,  $\Delta$  is a relevant perturbation that can substantially modify the physics. In principle, a long-range charge-density wave is expected that opens a charge gap. However, numerical studies in the model with  $\Delta = 0$  but adding nearest-neighbor repulsion  $V$ , which also favors a charge-density wave, indicate that the charge gap still vanishes for small values of  $V$  [46].

## V. SUMMARY AND DISCUSSION

We have calculated the quantum phase diagram of the ionic Hubbard model, including electron-hole symmetric density-dependent hopping, which corresponds to Eq. (1) with  $\delta = 0$  and  $t_{AA} = t_{BB} < t_{AB}$ , using the method of crossings of excited energy levels in rings of up to 14 sites.

The model has three phases: the BI, the MI, and a narrow region of the SDI in between. The BI and SDI are fully gapped except at the transition points between them at  $\Delta = \pm \Delta_c$ , which lead to topological singularities at the points  $(0, \pm \Delta_c)$  in the two-dimensional space  $(\delta, \Delta)$ . Therefore an adiabatic cycle in this space which encloses one of these singularities leads to a Thouless pumping of one charge per cycle.

Nevertheless, since the region of the SDI is very narrow, experimental pump cycles with cold atoms that surround only one of the charge critical points, for which quantized pumping is observed, usually cross the MI region in which the spin gap is closed, leading to transition to excited states and loss of adiabaticity and quantized charge transport after the first pump cycle [12].

We obtain that a reduction of  $t_{AA} = t_{BB}$  with respect to  $t_{AB}$ , increases the region of the phase diagram occupied by the fully gapped SDI phase, particularly for  $|\Delta| < t_{AB}$  and  $U < 2t_{AB}$ . This result is of possible relevance to experiments similar to the above mentioned. Floquet engineering renders it possible to achieve the region  $t_{AA} = t_{BB} < t_{AB}$  [20–25], and therefore enlarge the region of the gapped SDI phase.

To confirm the possibilities of this proposal, it would be useful to calculate the spin gap and the internal charge gap between even and odd singlets in the SDI phase. This would require a study of longer chains using, for example, density-matrix renormalization group. It would also be useful to simulate the time dependence in pumping cycles similar to the ones suggested here, using infinite time-evolving block decimation.

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