Anderson-Mott transition in a disordered Hubbard chain with correlated hopping

Francesca Battista,[1] Alberto Camjayi,[1] and Liliana Arrachea[1,2]

[1]*Departamento de Física, FCEyN, Universidad de Buenos Aires and IFIBA, Pabellón I, Ciudad Universitaria, 1428 CABA, Argentina*

[2]*International Center for Advanced Studies, ECyT-UNSAM, Campus Miguelete, 25 de Mayo y Francia, 1650 Buenos Aires, Argentina*

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We study the ground-state phase diagram of the Anderson-Hubbard model with correlated hopping at half-filling in one dimension. The Hamiltonian has a local Coulomb repulsion U and a disorder potential with local energies randomly distributed in the interval $(-W, +W)$ with equal probability, acting on the singly occupied sites. The hopping process which modifies the number of doubly occupied sites is forbidden. The hopping between nearest-neighbor singly occupied and empty sites or between singly occupied and doubly occupied sites has the same amplitude t. We identify three different phases as functions of the disorder amplitude W and Coulomb interaction strength $U > 0$. When $U < 4t$ the system shows a metallic phase: (i) only when no disorder is present $W = 0$ or an Anderson-localized phase, (ii) when disorder is introduced $W \neq 0$. When $U > 4t$ the Anderson-localized phase survives as long as disorder effects dominate on the interaction effects, otherwise a Mott-insulator phase (iii) arises. Phases (i) and (ii) are characterized by a finite density of doublons and a vanishing charge gap among the ground state and the excited states. Phase (iii) is characterized by the vanishing density of doublons and a finite gap for the charge excitations.

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I. INTRODUCTION

The idea of inducing electron localization with many-body interactions in fermionic systems was introduced by Mott in the framework of a crystalline array with strong Coulomb interactions [1–3]. As in the case of the usual band insulators, a gap opens in the spectrum of the many-particle system. In this case the origin of this feature is the effect of the interactions rather than the nature of the atomic structure. The Hubbard model constitutes the tight-binding version of this picture. The corresponding Hamiltonian has a hopping term between nearest neighbors in a lattice combined with a local Coulomb interaction [4–6]. The competition between the kinetic energy and the strong correlations represented by these two terms is precisely the origin of the metal-insulator transition proposed by Mott. For this reason, the Hubbard model was thought to be the natural candidate to realize the Mott transition [2]. In bipartite lattices, however, the nesting in the Fermi surface and the relevant umklapp processes at half-filling lead to magnetic instabilities that mask the metallic phase. The ground state is insulating for any value of the Coulomb interaction and, unlike the original Mott picture, it is dominated by strong antiferromagnetic correlations [7]. When the antiferromagnetism is frustrated, several results support the scenario of the metal-insulator Mott transition in this model. This is the case of lattices with frustrating geometries [8], infinite-range hopping, or lattices with an infinite coordination number [9].

The Anderson transition defines a completely different paradigm of metal-insulator transition. The model was introduced [10] to describe the localization of noninteracting single particles due to the introduction of disorder in a crystal potential landscape. The Hamiltonian has a hopping term between nearest-neighbor sites in a lattice with randomly distributed local energies. Unlike the Hubbard model, the insulating phase is gapless. In this phase the electrons get trapped and localized in real space due to the potential landscape [11–14], whereas the metallic phase is stabilized for low strength of disorder in three-dimensional lattices. In lower dimensionality, the ground state is always insulating [15,16].

The combination of Coulomb interaction and local potential disorder defines the disordered Hubbard model, and the outcome of such an interplay is highly nontrivial [14,17–20]. The naive expectation that the combination of two ingredients leading to insulating phases also results in an insulating phase does not apply to this model. In fact, quantum Monte Carlo results in two dimensions [21–23] and results obtained with dynamical mean-field theory in lattices with infinite connectivity [20,24,25] suggest the possibility of a metal-insulator transition in the phase diagram of the Coulomb interaction U vs the strength of disorder W at half-filling. The concept of many-body localization has recently been coined to characterize the effect of disorder in the presence of many-body interactions and has been receiving a lot of attention for some years now [26–33]. Theoretical studies include perturbative calculations [34–36] and numerical simulations [29,30,37–39]. These ideas also are motivating experimental studies not only for solid-state systems, but also in other correlated systems, such as cold atoms and optical lattices [40,41]. In fact, the advances in quantum optics enabled the experimental realization of optical potentials imitating a crystal lattice (optical lattices) [42] with the advantage of having tunable parameters [43–46]. For example, experimental studies of a Hubbard model in three dimensions have been performed using ultracold neutral atoms trapped in an optical lattice [47,48]. The interplay of interaction and disorder is crucial when studying cold atoms in these lattices too [48–51].

The Hubbard model with correlated hopping supports a limit with the basic ingredients for a Mott transition. The corresponding Hamiltonian has a local Coulomb interaction U identical to the one of the usual Hubbard model, but the kinetic term is generalized to have different amplitudes (t_a, t_{ab}, t_b) depending on the occupation of the two neighboring sites $\langle ij \rangle$ that intervene in the hopping process with a total number of

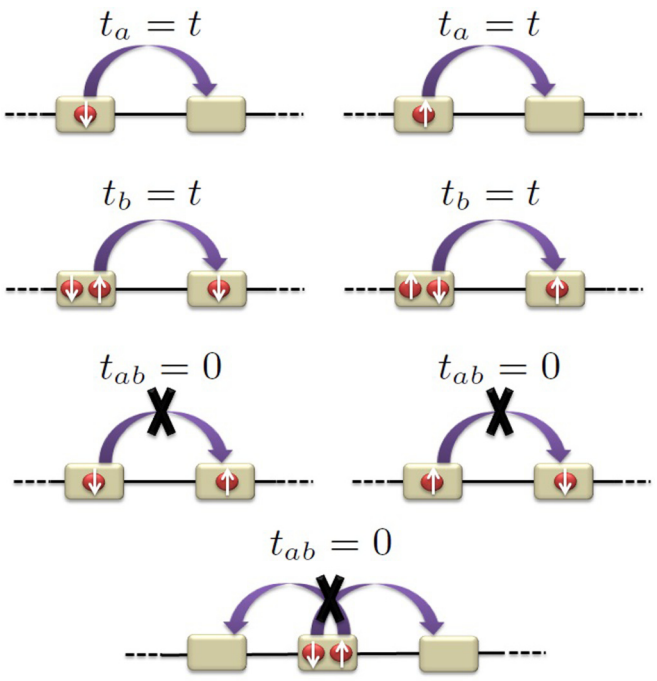

FIG. 1. Schematic of the possible hopping events considered in this paper. The hopping takes place between a singly occupied site and an empty site with amplitude $t_a = t$ or between a single occupied site and a doubly occupied site with amplitude $t_b = t$. The hopping between two singly occupied sites with different spin components to generate a doubly occupied site, and an empty site or vice versa is forbidden $t_{ab} = 0$.

one to three particles, respectively. The corresponding kinetic term reads

$$H(t_a,t_{ab},t_b) = \sum_{\langle ij\rangle,\sigma}^{L} c^{\dagger}_{i,\sigma}c_{j,\sigma}\{t_a(1-n_{i,-\sigma})(1-n_{j,-\sigma}) + t_{ab}[n_{i,-\sigma}(1-n_{j,-\sigma}) + (1-n_{i,-\sigma})n_{j,-\sigma}] + t_b n_{i,-\sigma}n_{j,-\sigma}\} + \text{H.c.} \quad (1)$$

The operators $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) create (annihilate) a $S = 1/2$ fermion with spin component $\sigma = \uparrow, \downarrow$ at the chain site i, and $n_{i,\sigma} = c^{\dagger}_{i,\sigma}c_{i,\sigma}$ is the corresponding number operator. The hopping process that permutes a singly occupied site and an empty site has amplitude t_a. The one permuting a single occupied site and a doubly occupied site has amplitude t_b. The hopping between two singly occupied sites with opposite spins to generate an empty site and a doubly occupied site or vice versa has amplitude t_{ab} (see the sketch of Fig. 1). These terms emerge naturally in the derivation of an effective low-energy model starting from the three-band Hubbard Hamiltonian that describes the Cu-O planes of the superconducting cuprates [52–54]. In some limit, it is equivalent to the so-called extended Hubbard model with a bond-charge interaction which has been investigated in the context of low-dimensional organic superconductors [55–57] as well as in the context of nonconventional superconducting mechanisms, such as hole superconductivity [58,59], η-pairing superconductivity [60,61], mesoscopic transport [62], and quantum information [63,64]. More recently, this model also was investigated in optical lattices and cold atoms [65–70] and was found to provide the effective theory of the Hubbard Hamiltonian in driven lattices [71,72].

The correlated hopping Hubbard Hamiltonian can be solved exactly in one dimension (1D) in two limits. One corresponds to the usual Hubbard model where $t_a = t_b = t_{ab}$, which can be solved by Bethe ansatz [73]. The other solvable case is $|t_a| = |t_b| = t$ and $t_{ab} = 0$ [74,75]. At half-filling, when the Coulomb interaction U overcomes a critical value U_c, the ground state corresponds to an insulator with an energy gap increasing linearly with U. It is interesting to note that for $t_{ab} = 0$ the antiferromagnetic correlations are inhibited completely. Hence, the insulating phase has the characteristic of an ideal Mott insulator in the sense that it does not have any magnetic order. Below the critical value U_c, the system is gapless and has the characteristics of a normal metal.

The aim of this paper is to investigate the phase diagram of the correlated Hubbard model in the exactly solvable limit of Ref. [74] at half-filling with an additional term in the Hamiltonian that represents a disordered potential for the singly occupied sites. The model is introduced in Sec. II. In Sec. III we present the methodology to investigate the ground state of this Hamiltonian. Results are presented in Sec. IV, and Sec. V is devoted to a summary and conclusions.

II. MODEL

We study a disordered Hubbard model with correlated hopping. The corresponding Hamiltonian is

$$H = H_K + H_U, \quad (2)$$

where

$$H_K = H(t,0,t) + \sum_{i,\sigma}^{L} \epsilon_i n_{i,\sigma}(1-n_{i,-\sigma}),$$
$$H_U = U\sum_{i}^{L} n_{i,\uparrow}n_{i,\downarrow}. \quad (3)$$

The Hamiltonian H_K represents the kinetic term characterized by hopping processes between nearest-neighbor sites $\langle ij\rangle$ of the lattice. It corresponds to Eq. (1) with $t_{ab} = 0$ and identical amplitudes for t_a and t_b as indicated in the sketch of Fig. 1. This is precisely the exactly solvable limit where the hopping process changing the number of occupied sites and introducing antiferromagnetic correlations is forbidden [74,75]. In addition to the correlated hopping, there is a disorder potential characterized by local random energies $-W < \epsilon_i < W$ (third term) which acts on the singly occupied sites. The homogeneous case corresponds to the limit $W = 0$, which is the exactly solvable case. The Hamiltonian H_U describes the Coulomb repulsion with $U > 0$, which acts only on doubly occupied sites.

As in the case studied in Refs. [74,75] we can verify that the number of doubly occupied sites $N_d = \sum_i n_{i,\uparrow}n_{i,\downarrow}$ is conserved $[H,N_d] = 0$. Hence, the particles can exist in the lattice in the form of single fermions or doublons. The latter are defined by pairs of particles with different spins occupying the same site. The number of each of these species is conserved separately. The total number of particles also is conserved and

can be expressed as $N = N_f + 2N_d$, where N_f is the number of the unpaired particles. The role of U is equivalent to a chemical potential for the doublons.

In the limit of $W = 0$ and $|t_a| = |t_b| = t$, studied in Refs. [74,75], the ground state at half-filling ($N = L$) displays a Mott transition at the critical value of $U_c = 4t$. For $U > U_c$ the ground state corresponds to a zero energy state where all the sites of the lattice are occupied by a single particle. This state is characterized by $N_d = 0$, and the kinetic energy is zero ($\langle H_K \rangle = 0$) and is 2^L degenerate due to all the possible spin orientations. As it does not have any special magnetic order it fits to the picture of the Mott insulator. In this phase, there is a gap between the ground state and the lowest-energy excited state in the charge sector, which depends linearly on U. For $U < U_c$ the energy gap closes, the ground state is in a degenerate metallic phase with states containing superconducting order in the manyfold, and it is characterized by $\langle H_K \rangle \neq 0$ and $N_d \neq 0$.

We will show in the next section that the present model for $U = 0$ can be mapped to the usual spinless Anderson model [10]. Therefore, the ground state of H is clearly an Anderson gapless localized state for arbitrarily low strength of the disorder $W \neq 0$. Since the number of doublons does not contribute to the kinetic energy, it is also clear that for those parameters where the ground state has $N_d \neq 0$, the system may be in an Anderson-like localized phase with a finite number of doublons. This is expected to happen also when the effect of disorder is introduced while $U < U_c$. The question that arises is about the nature of the Mott phase as disorder is introduced for $U > U_c$. The investigation of this phase is the main goal of the present paper.

III. METHOD

In order to find the spectrum of H we follow a similar procedure to the one introduced in Refs. [74,75]. We focus on open boundary conditions and start by mapping the Hamiltonian H_K to a spinless Anderson Hamiltonian with N_f particles in L sites. To this end it is convenient to express the different states of a given lattice site in terms of the following representation: $|0\rangle \to e_i^\dagger|0\rangle \equiv |\circ\rangle$, $c_\sigma^\dagger|0\rangle \to f_{i,\sigma}^\dagger|0\rangle \equiv |\sigma\rangle$, $c_\uparrow^\dagger c_\downarrow^\dagger|0\rangle \to b_i^\dagger|0\rangle \equiv |\bullet\rangle$. Here $f_{i\sigma}$ is fermionic whereas e_i and d_i are bosonic operators that obey the following constraint:

$$e_i^\dagger e_i + d_i^\dagger d_i + \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} = 1, \tag{4}$$

which implies that a given site may have only one type of boson ($\circ$ or $\bullet$) or fermion with only one type of spin component ($\uparrow$ or $\downarrow$). We substitute this representation in H_K and focus on $|t_a| = |t_b| = t$ [76]. The resulting Hamiltonian reads

$$H_K = t \sum_{\langle ij\rangle,\sigma} [f_{j\sigma}^\dagger f_{i\sigma}(e_i^\dagger e_j + d_i^\dagger d_j) + \text{H.c.}] + \sum_{i\sigma} \epsilon_i f_{i\sigma}^\dagger f_{i\sigma}. \tag{5}$$

This model has two SU(2) local symmetries. The usual spin-1/2 symmetry with generators,

$$S_i^z = (f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow})/2, \quad S_i^+ = f_{i\uparrow}^\dagger f_{i\downarrow}, \quad S_i^- = f_{i\downarrow}^\dagger f_{i\uparrow}, \tag{6}$$

and the η-pairing symmetry with generators,

$$\eta_i^z = \left(1 - \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} - 2d_i^\dagger d_i\right)\Big/2, \quad \eta_i^+ = e_i^\dagger d_i,$$
$$\eta_i^- = d_i^\dagger e_i. \tag{7}$$

Here we notice that states $\circ$ and $\bullet$ of the η-pairing symmetry are akin to $\uparrow$ and $\downarrow$ of the usual spin symmetry. Interestingly, we can verify

$$[H_K, S_i^+] = [H_K, S_i^-] = [H_K, \eta_i^+] = [H_K, \eta_i^-] = 0. \tag{8}$$

Therefore, we can work in the subspace corresponding to the highest weight representation of these SU(2) algebras. This is equivalent to working in the subspace where all the fermions have $\uparrow$ spin and all the bosons are $\circ$. We can diagonalize the Hamiltonian in this subspace and then, due to (8), we know that each eigenstate $|\psi_m\rangle$ will be degenerate with states resulting from the application of all the lowering operators $S_i^-|\psi_m\rangle$ and $\eta_i^-|\psi_m\rangle$.

For a fixed number of particles N and a given number of doublons N_d, these eigenstates have a degeneracy $2^{N_f} \times C(N - N_f, N_d)$ with $C(N - N_f, N_d)$ being the combinatory number. This is due to the different spin orientations of the unpaired particles and the different possibilities for allocating the doublons in the $N - N_f$ lattice sites which are not occupied by the unpaired fermions. The eigenenergies of H for $U = 0$ only depend on N_f. More precisely, these eigenenergies for $U = 0$ are those of N_f spinless fermions in a lattice with L sites and a disorder potential profile ϵ_i. For $U \neq 0$ we notice that the Coulomb interaction acts like a chemical potential for the doublons. Then, we must add to the eigenenergies of H_K the quantity UN_d.

The states of the basis with highest weight can be mapped to the states of N_f spinless fermions. Therefore, the problem of diagonalizing the Hamiltonian H_K can be mapped to diagonalizing the Anderson Hamiltonian in L sites with N_f spinless particles, which can be represented by a tridiagonal matrix with diagonal elements ϵ_i, $i = 1, \ldots, L$ and band elements t. The single-particle eigenenergies of this problem are the eigenvalues of that matrix e_j, $j = 1, \ldots, L$, and the N_f-particle energies are

$$E_m^{(N_f)} = \sum_{j=1}^{N_f} e_{m(j)}, \tag{9}$$

with $m = 1, \ldots, C(L, N_f)$. These correspond to fill in N_f of the L single-particle states, labeled with $m(j)$, $j = 1, \ldots, N_f$ with only one particle, in consistency with the Pauli principle. The eigenenergies of the N-particle states with N_f single fermions and N_d doublons are obtained easily for any value of U from

$$E_m^{(N)} = E_m^{(N_f)} + UN_d, \qquad N = N_f + 2N_d. \tag{10}$$

Hence, all the eigenenergies for the system with N particles can be obtained by considering all the eigenenergies (10) with all combinations of numbers of free particles and doublons ranging from $N_f = 0$, $N_d = N/2$ to $N_f = N$, $N_d = 0$, satisfying the constraint of adding to a total number of particles N as indicated in (10).

In order to investigate the phase diagram of this model at half-filling ($N = L$) we follow the procedure described above in chains with different size L's for several values of U and 2000 realizations of the local energies ϵ_i, which are randomly distributed with equal probability within the interval $(-W, W)$. We focus on the charge gap between the ground state and the first charge excitation,

$$\Delta = E_1 - E_0, \tag{11}$$

where E_0 and E_1 are the ground-state energy and the first excited state, respectively, of the N particles in the L-site chain. Typically, the two associated eigenstates differ in one doublon. We also analyze the average over the density of doubly occupied sites,

$$d = N_d/L. \tag{12}$$

To evaluate the phase diagram, we perform finite-size scaling with sizes $L \leqslant 1200$ and extrapolate the results to the thermodynamic limit.

IV. RESULTS

As discussed in Sec. II we do no expect any metallic phase at half-filling $N = L$ in the present model when $W \neq 0$. For $U = 0$ and finite W this model is equivalent to the Anderson model, which is always in a localized phase in 1D. In the limit where $W = 0$, the system is in a metallic phase for $U < 4t$, characterized by a finite density of doublons $d \neq 0$ and a vanishing value of the charge gap $\Delta = 0$. Instead, for $U > 4t$ the ground state is in the Mott-insulator phase with $d = 0$ and a finite energy gap Δ. The ground-state energy for $U = W = 0$ is in the subspace with $N_f = N/2$ and $N_d = N/4$. As U increases keeping $W = 0$, d decreases and vanishes at the critical value of $U = 4t$ where the Mott transition takes place, whereas in the thermodynamic limit where $L \to \infty$, $\Delta = 0$. In the Mott-insulator phase, for $U > 4t$, Δ becomes finite.

In what follows, we analyze the behavior of the density of doublons d and Δ in the presence of disorder. The average over 2000 disorder realizations of these two quantities is shown in Fig. 2 for a finite-size lattice. For $W = 0$ we can distinguish the characteristics of the Mott transition above described. The (small) finite value of Δ for $U < 4t$ is due to finite-size effects and it extrapolates to zero as the lattice size $L \to \infty$. For $W \neq 0$ within the range of $U < 4t$ we see the same qualitative behavior for d and Δ. We identify the phase within this region of parameters with Anderson localization as an extension of the limiting case where $U = 0$ and $W \neq 0$. A dramatic change in the behavior of the two quantities shown in Fig. 2 is, instead, observed as a function of W starting from the Mott-insulator phase at $U > 4t$. We see that the averaged density of doublons d increases from zero whereas Δ decreases as W increases. In Fig. 3 we show the behavior of Δ and d as functions of W for fixed values of the Coulomb interaction U. We focus on the regime with $U > 4t$. We study chains of different sizes and extrapolate to the thermodynamic limit. These results indicate the existence of a critical value W_c such that for $W < W_c$ the density of doublons is vanishingly low and extrapolates to zero as $1/L \to 0$, whereas for $W > W_c$ the density of doublons becomes finite and increases as a function of W. This change in the behavior of the density of doublons as a function of W

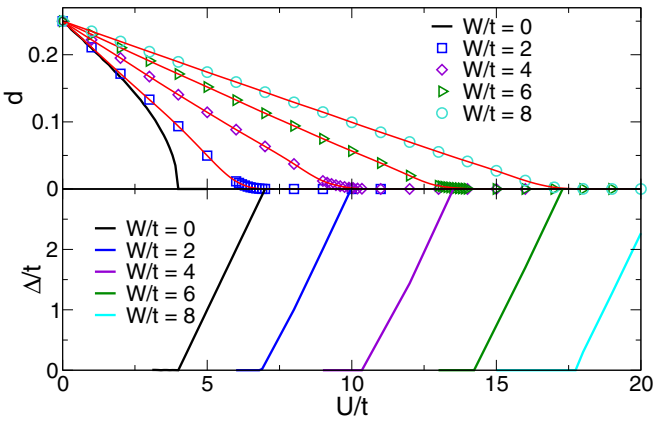

FIG. 2. (Top) Density of doublons d and (bottom) gap between the ground state and the first excited state, Δ as functions of the Coulomb interaction U for different values of disorder potential $W = 0,2,4,6,8$. The two quantities are averaged over 2000 realizations of disorder in a lattice with $L = N = 1200$. All the energies are expressed in units of the hopping parameter t.

is accompanied by a change in the behavior of Δ as a function of W. In fact, for $W < W_c$ we find that Δ extrapolates to a finite value in the thermodynamic limit, whereas $\Delta \to 0$ for $W > W_c$. These features are consistent with a transition from a Mott-insulator phase to an Anderson-localized phase at W_c.

The inferred phase diagram is shown in Fig. 4. The line separating the Mott-insulator from the Anderson-localized phases is evaluated calculated from the criteria of vanishing Δ and vanishing d in the thermodynamic limit. Polynomial extrapolations of Δ and d as functions of $1/L$ have been carried out with sizes up to $L = 1200$. The two estimates agree within the numerical precision. The same procedure can be followed to get the exact solution away from half-filling. In this case,

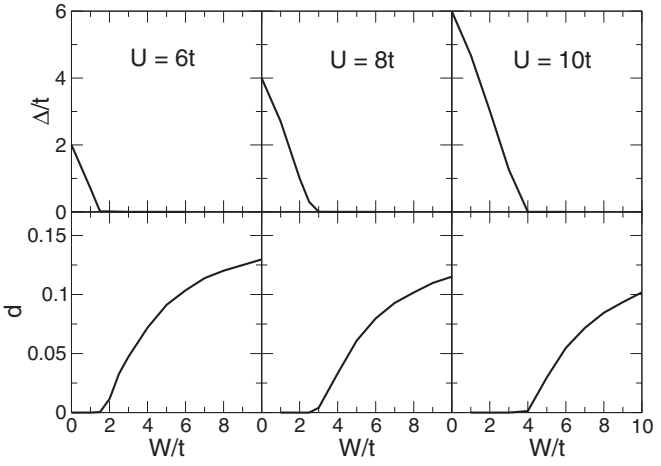

FIG. 3. Top panels: Energy gap value as a function of the parameter W for (left) $U = 6t$; (center) $U = 8t$; and (right) $U = 10t$. Bottom panels: Disorder-averaged density of doublons $d = N_d/L$ for the same values of U. All these data correspond to extrapolations to the thermodynamic limit from chain sizes $L \leqslant 1200$ and averaging over 2000 realizations of disorder.

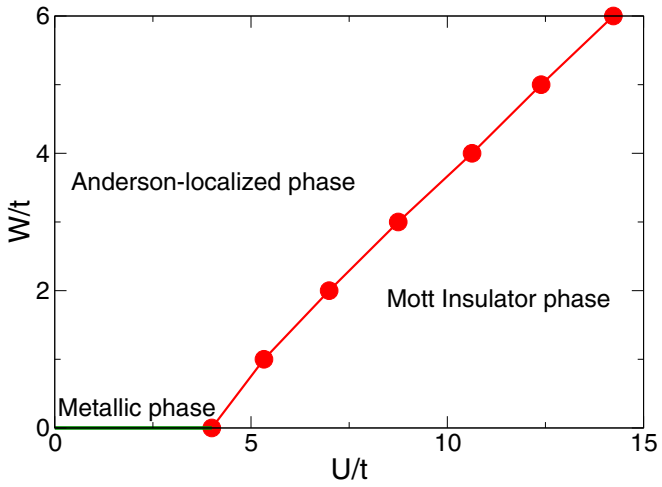

FIG. 4. Phase diagram of the disordered Hubbard model with correlated hopping at half-filling $N = L$ in 1D. The phases are as follows: (i) metallic phase for $W = 0$ and $U < 4t$, (ii) Anderson-localized phase for $W \neq 0$ and $U < 4t$ as well as for $W > W_c$ and $U > 4t$, and (iii) a Mott-insulator phase for $W < W_c$ and $U > 4t$. Phases (i) and (ii) are characterized by $d \neq 0$ and $\Delta = 0$. Phase (iii) is characterized by $d = 0$ and $\Delta \neq 0$. The line separating the Mott-insulator from the Anderson-localized phases corresponds to $\Delta = 0$ and $d = 0$ in the thermodynamic limit. The size of the symbols is proportional to the uncertainty on the numerical data.

the system is in the metallic phase for $W = 0$ for any value of U whereas it localizes for an arbitrarily low strength of W.

Before closing this section, we briefly comment on the similarities and differences between the phase diagram of the disordered Hubbard model with correlated hopping in 1D studied in the present paper and the phase diagram of the disordered Hubbard model at half-filling in higher dimensions described by dynamical mean-field theory (DMFT). In the latter case, a phase diagram with the same phases identified in Fig. 4 has been derived [24,25,77]. In fact, the main underlying characteristic shared by the model we study here and the DMFT description of the Hubbard model is the absence of antiferromagnetic correlations. In our case, this is an intrinsic property of the model, whereas in the mean-field solutions this is encoded in the approximation of the momentum-independent self-energy. In the present 1D case, the metallic phase is confined to $W = 0$, whereas in the higher-dimensional DMFT cases, it also extends to a region with finite W. It is also interesting to stress that the Mott phase can be identified by the change in the behavior of the double occupancy. The double occupancy as a good order parameter to characterize the transition from a metallic to the Mott-insulating phase, akin to the magnetization in the Ising model, was introduced in Ref. [18]. This idea also was followed in Landau theory for the DMFT-Mott transition in Ref. [19] where the Mott-insulating phase is characterized by a few numbers of doubly occupied sites, whereas the metallic one is identified as a liquid rich in doubly occupied sites. This is precisely the case for the model studied here. In our case, the fact that the Mott-insulating phase is defined by an exactly vanishing number of doublons is due to the fact that the number of doubly occupied sites is a conserved quantity in the correlated-hopping Hamiltonian.

V. CONCLUSIONS

We have analyzed the phase diagram of the correlated Hubbard model with disorder at half-filling in 1D. The different phases are summarized in Fig. 4. Without disorder the model has a metallic and a Mott-insulator phase. Our results indicate that the metallic phase becomes unstable and localizes as in the Anderson model for an arbitrarily low disorder strength. This phase is characterized by a vanishing gap in the charge excitations and a finite density of doublons in the ground state. Instead, the Mott-insulator phase, which is characterized by a vanishing density of doublons in the ground state and a finite charge gap, becomes stable up to a critical strength of disorder where a phase transition to an Anderson-localized state takes place. The possibility for clearly identifying these two insulating phases makes this model appealing for further theoretical studies and to be realized in optical lattices and cold atoms. Several interesting issues remain to be investigated further in the future, in particular, the possible emergence of a metallic phase for finite disorder strength in systems of higher dimensionality and the role of antiferromagnetic and charge-density wave correlations, which could be introduced by means of an extra correlated hopping process and nearest-neighbor Coulomb interactions, generalizing the model of Refs. [78,79] with the addition of disorder.

Although the experimental realization of the disordered correlated hopping model in the limit we studied here is not obvious in solid-state real materials, its implementation in optical lattices is within the scope of current experiments [80–82]. Different mechanisms for the experimental implementation of disorder in these systems have been reported [49,83,84]. In particular, in Ref. [84], the disorder has been introduced by means of localized impurity atoms. In the case that the latter are spin polarized, they would magnetically couple only to the singly occupied sites of the lattice under investigation, which would correspond to a realization of the type of disorder we are considering in the present paper.

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