Exact Solution of a Hubbard Chain with Bond-Charge Interaction

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We obtain the exact solution of a general Hubbard chain with kinetic energy t, bond-charge interaction X, and on-site repulsion U with the only restriction $t = X$. At zero temperature and half filling, the model exhibits a Mott transition at $U = 4t$. In the metallic phase and near half filling, superconducting states are part of the degenerate ground state and are favored for small U if the system is slightly perturbed.

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The exact solutions, particularly those obtained using the Bethe ansatz, have brought a very important progress in the understanding of strongly correlated systems. However, the conditions for integrability using the Bethe ansatz are very restrictive, and only a limited class of realistic models can be solved with this technique [1]. Because of the importance of the exact solutions in clarifying the effect of different physical ingredients and as a test of approximations, the search for exact solutions has been recently extended to other models and techniques, in spite of the fact that in some cases the model or the parameters are rather unrealistic [2–8].

The model we consider is a particular case of the following Hamiltonian:

$$H = H_U + H_t$$
$$= U\sum_i n_{i\uparrow}n_{i\downarrow} + \sum_{\langle ij\rangle\sigma} c^\dagger_{j-\sigma}c_{i-\sigma}\{t_{AA}(1-n_{i\sigma})(1-n_{j\sigma}) + t_{AB}[n_{i\sigma}(1-n_{j\sigma}) + (1-n_{i\sigma})n_{j\sigma} + t_{BB}n_{i\sigma}n_{j\sigma}\}. \quad (1)$$

H has been derived as an effective one-band Hamiltonian for the description of cuprate superconductors [9]. Similar models including in some cases the nearest-neighbor repulsion V have been studied by several authors [4,5,8–13]. If $t_{AA} + t_{BB} - 2t_{AB} = 0$, the three-body term of H_t vanishes, and H reduces to the model considered by Hirsch and Marsiglio, in the framework of their theory of "hole superconductivity" [10]. Following Ref. [8], we call the coefficients of the one- and two-body parts of H_t as $t_{AA} = -t$ and $t_{AB} - t_{AA} = X$, respectively. In the weak-coupling case $0 < X \ll t$, a standard BCS-type mean-field approximation [10] and a renormalization-group analysis in the one-dimensional (1D) continuum-limit theory [13] show that a small positive X gives rise to an effective attractive interaction for a particle density $n > 1$, while this interaction is repulsive for $n < 1$, and vanishes at half filling. This situation cannot be extended to the case $X = t$, since for these parameters ($t_{AB} = t_{AA} + t_{BB} = 0$) H_t is symmetric under an electron-hole transformation and the physics for densities n and $2 - n$ should be the same. Thus, it is of interest to study this case. This is one of the goals of this Letter. Strack and Vollhardt studied the model for these parameters (including V) at half filling and argued that this case corresponds to a physically relevant range of parameters [8].

The study of the Mott transition also makes the case $t_{AB} = 0$ appealing, because of the suppression of antiferromagnetic correlations. This avoids the problem of having to distinguish between a Mott insulator, in which the particles become localized as a consequence of strong on-site repulsion, and an antiferromagnetic insulator, in which a weak interaction opens a gap in a nested Fermi surface. The latter is the case of the Hubbard model in bipartite lattices. Studies of the Mott transition in these cases are restricted to the paramagnetic phase [14–16]. Other studies have taken nonbipartite lattices [17] or systems in which the noninteracting Fermi surface has no nesting [18,19]. In the large U limit, the model of Eq. (1) becomes equivalent to a generalized t-J model [20] with hopping t_{AA} (t_{BB}) for $n < 1$ ($n > 1$), correlated hopping t^2_{AB}/U, and antiferromagnetic exchange interaction $J = 4t^2_{AB}/U$, which vanishes for $t_{AB} = 0$.

In this Letter we obtain the exact solution of Hamiltonian (1) for a chain with open boundary conditions under the only restriction $t_{AB} = |t_{AA}| - |t_{BB}| = 0$. We also discuss the effect of a finite t_{AB} on the basis of our Lanczos results for finite chains. Strack and Vollhardt obtained the exact ground state for $t_{BB} = -t_{AA} = t$, for arbitrary dimension including the nearest-neighbor repulsion V, but only for $n = 1$ and two regimes of parameters in which all particles are static in the ground state [8]. Both regimes of parameters have been enlarged by Ovchinikov [8]. In 1D and for $V = 0$ we are able to obtain all eigenstates for arbitrary filling, particularly in a third regime of parameters in which the dynamical part of the Hamiltonian H_t plays an important role in the ground state.

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The exact solution of the model is greatly facilitated by its symmetries. In any dimension for $t_{AB} = 0$, $[H_t, H_U] = 0$ and the number of doubly occupied sites is conserved [8]. Also, as in the case of the model of Essler, Korepin, and Schoutens [5], for $t_{AB} = 0$, H_t commutes not only with the total spin, but also with the following generators of another SU(2) algebra:

$$\eta = \sum_{i=1}^{L} c_{i\downarrow} c_{i\uparrow}, \qquad \eta^\dagger = \sum_{i=1}^{L} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger,$$
$$\eta_z = \sum_{i=1}^{L} \left(\tfrac{1}{2} - \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} \right), \tag{2}$$

where L is the number of sites. This allows us to construct eigenstates of minimum energy which possess off-diagonal long-range order for sufficiently small values of U and $|n - 1|$.

The solution of the chain is obtained by mapping H_t into a tight-binding model of spinless fermions. To obtain this mapping it is convenient to write H in a slave-boson representation. We represent the four possible states at site i: $|0\rangle$, $c_{i\sigma}^\dagger|0\rangle$, $c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger|0\rangle$, by $e_i^\dagger|0\rangle$, $f_{i\sigma}^\dagger|0\rangle$, $d_i^\dagger|0\rangle$ (pictorially ○, ↓ or ↑ and ●), respectively, using two bosons to represent the empty (○) and doubly occupied (●) sites and two fermions (↑ and ↓) to describe the singly occupied sites. The Hamiltonian takes the form

$$H = U \sum_i d_i^\dagger d_i + t_{AA} \sum_{\langle ij \rangle_\sigma} f_{j\sigma}^\dagger f_{i\sigma} e_i^\dagger e_j - t_{BB} \sum_{\langle ij \rangle_\sigma} f_{j\sigma}^\dagger f_{i\sigma} d_i^\dagger d_j$$
$$+ t_{AB} \sum_{\langle ij \rangle} \left[f_{j\uparrow}^\dagger f_{i\downarrow}^\dagger (e_i d_j + e_j d_i) + \text{H.c.} \right], \tag{3}$$

with the constraints $e_i^\dagger e_i + d_i^\dagger d_i + \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} = 1$. When $t_{AB} = 0$, the numbers $N_\sigma = \sum_i f_{i\sigma}^\dagger f_{i\sigma}$, $N_e = \sum_i e_i^\dagger e_i$ and $N_d = \sum_i d_i^\dagger d_i$ are separately conserved. Note also that in a bipartite lattice, changing the phase of the bosons e_i or d_i by -1 in one sublattice changes the sign of t_{AA} or t_{BB}, respectively. Thus we can choose these signs arbitrarily. Taking $-t_{AA} = t_{BB} = t > 0$ as in Ref. [8], H_t takes the form

$$H_t = -t \sum_{\langle ij \rangle \sigma} \left[f_{j\sigma}^\dagger f_{i\sigma} \left(e_i^\dagger e_j + d_i^\dagger d_j \right) + \text{H.c.} \right]. \tag{4}$$

In a chain with open boundary conditions also, the *order* of the bosons and that of the fermions along the chain are separately conserved: H_t permutes the order of a fermion and a boson which are nearest neighbors, but two bosons or two fermions cannot be permuted. For a given number of fermions $N_f = N_\uparrow + N_\downarrow$, let us numerate the L sites, N_f fermions, and $N_b = N_e + N_d = L - N_f$ bosons with similar sequence (for example, from left to right) using the labels i, j, and m, respectively. Then, any state with a definite number of particles on each site can be written as

$$|\psi_l\rangle = \prod_{m=1}^{N_b} \left\{ B(m) e_{i(m)}^\dagger + [1 - B(m)] d_{i(m)}^\dagger \right\}$$
$$\times \prod_{j=1}^{N_f} \left\{ F(j) f_{i(j)\uparrow}^\dagger + [1 - F(j)] f_{i(j)\downarrow}^\dagger \right\} |0\rangle. \tag{5}$$

Here $i(m)$ is the position of the mth boson in the sequence [its inverse, defined on the set of sites for which $n_{bi} = e_i^\dagger e_i + b_i^\dagger b_i = 1$ is simply $m(i) = \sum_{l=1}^{i} n_{bl}$], and $i(j)$ has a similar meaning for the fermions. $B(m) = 1$ if the mth boson is an "empty" one and zero otherwise. Similarly in terms of the spin of the fermions $F(j) = 1/2 + S_{i(j)}^z$. The products are ordered throughout with increasing labels to the right. As an example, the state $|\psi_l\rangle = ○\,\uparrow\downarrow\,○●\,\uparrow\uparrow\downarrow\,●\ldots$ and any other state $|\psi_{l'}\rangle$ such that $\langle\psi_l| H_t |\psi_{l'}\rangle \neq 0$ have $B(1) = B(2) = 1$, $B(3) = B(4) = 0$, $F(1) = F(3) = F(4) = 1$, and $F(2) = F(5) = 0$.

Because of the properties of Eq. (4) and the open boundary conditions, the 1D model has an extremely rich symmetry structure, including L SU(2) symmetries which are the local versions of those previously mentioned. There is one usual spin SU(2) algebra related to each of the N_f fermions and a "local pairing" SU(2) algebra related with each boson. As an example it can be easily verified that $(H_t e_{i(m)}^\dagger d_{i(m)} - e_{i(m)}^\dagger d_{i(m)} H_t)|\psi_l\rangle = 0$, where $e_{i(m)}^\dagger d_{i(m)}$ is a raising operator. Thus one can separately diagonalize H_t in each subspace of definite values of $B(m)$ and $F(j)$. For fixed N_f there are 2^L subspaces, and the size of each one is $\binom{L}{N_f}$. The raising and lowering operators establish a one to one correspondence between each state of one of these subspaces and the corresponding one of another subspace, and H_t takes the same form in all these subspaces. In the subspace of the highest weight of all SU(2) algebras [all $B(m) = F(m) = 1$], the solution of H_t for given N_f is easily obtained. The eigenstates written in the original representation have the form

$$|\psi_e^0\rangle = \prod_{j=1}^{N_f} c_{k_j\uparrow}^\dagger |0\rangle, \qquad c_{k\uparrow}^\dagger = \left(\frac{2}{L+1} \right)^{1/2} \sum_i \sin(ki) c_{i\uparrow}^\dagger, \tag{6}$$

where the possible values of $k(L + 1)/\pi$ are positive integers. These eigenstates can be extended to any values of $B(m)$ and $F(j)$ using the lowering operators:

$$|\psi_e\rangle = \prod_{i=1}^{L} \Big(n_{fi} \left\{ F(j_i) + [1 - F(j_i)] c_{i\downarrow}^\dagger c_{i\uparrow} \right\}$$
$$+ (1 - n_{fi}) \left\{ B(m_i) + [1 - B(m_i)] c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \right\} \Big) |\psi_e^0\rangle, \tag{7}$$

where $n_{fi} = n_i(2 - n_i)$, $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$, $j_i = \sum_{L=1}^{i} n_{fi}$, and $m_i = i - j_i$.

Equations (6) and (7) also describe all the eigenstates of $H = H_t + H_U$. The latter term reduces the degeneracy to $2^{N_f}\binom{N_b}{N_d}$ and adds UN_d to the energy.

For each particle density n, the ground state of H is obtained by minimizing the energy with respect to the density of doubly occupied sites $d = N_d/L$ and taking the lowest N_f values of k in Eq. (6), with the constraint $nL = 2dL + N_f$. The result is very simple. In the thermodynamic limit three regimes can be distinguished depending on the values of U/t and the particle density n (see Fig. 1). Also three regions of values of U/t can be separated (for $n = 1$ and $|U| > 4t$ the ground state

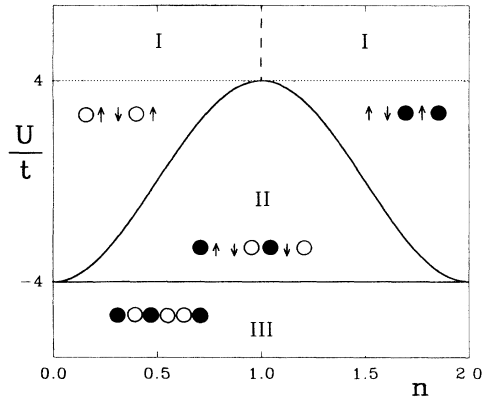

FIG. 1. Scheme for the ground state of the model as a function of U/t and particle density. On the dashed line the system is a Mott insulator.

was already obtained by Ovchinikov extending previous results of Strack and Vollhardt [8]):

(a) $U > 4t$. This region lies inside what we call regime I: for $n \leq 1$ the physics is the same as that of a spinless model. The ground state expectation value $\langle H_U \rangle = 0$ and

$$d = 0, \qquad e(n) = -\frac{2t}{\pi} \sin(n\pi), \tag{8}$$

where $e(n)$ is the energy density. For $n \geq 1$, from electron-hole symmetry $d = n - 1$, $e(n) = U(n-1) + e(2-n)$. For $n = 1$, $\langle H_t \rangle = \langle H_U \rangle = 0$ and the system is an insulator with energy gap $U - 4t$.

(b) $U < -4t$. This region coincides with regime III. Here (for an even number of particles) all particles are paired, all pairs are static ($\langle H_t \rangle = 0$), and

$$d = n/2, \qquad e(n) = Un/2. \tag{9}$$

(c) $-4t \leq U \leq 4t$. In this region there are two critical densities n_1 and n_2 defined by $n_i = (1/\pi)\arccos(-U/4t)$ and $n_1 \leq 1 \leq n_2 = 2 - n_1$. For $n \leq n_1$ or $n \geq n_2$ the physics corresponds to regime I and the ground state, and its energy was described above. Instead, for $n_1 < n < n_2$ the system is inside regime II. This regime is the only one in which empty, single, and double occupancy at any site is possible, and the competition between H_t and H_U is apparent in the ground state. The double occupancy and energy are given by

$$d = \frac{n - n_1}{2}, \quad e(n) = Ud - \frac{1}{2\pi}(16t^2 - U^2)^{1/2}. \tag{10}$$

In regimes II and III the system is at the borderline of phase separation and also of superconductivity. Eigenstates with off-diagonal long-range order (ODLRO) are part of the degenerate ground state. To show this, let us take an eigenstate $|\psi_g\rangle$ of the form of Eq. (7), with N_d doubly occupied sites, which belongs to the ground state. The state $|\psi\rangle = \eta^{N_d}|\psi_g\rangle$ with η given by Eq. (2) is clearly different from zero [it is obtained from $|\psi_g\rangle$ putting all $B(m) = 1$ in Eq. (7)] and is also an eigenstate of H_t with the same eigenvalue as that of $|\psi_g\rangle$. Also $|\psi\rangle$ is a highest-weight state of the η-pairing SU(2) algebra [Eq. (2)]. Similarly the state $|\psi_{N_d}\rangle = (\eta^\dagger)^{N_d}|\psi\rangle$ is an eigenstate of H_t with the same eigenvalue, and an eigenstate of H with the same energy as the original state $|\psi_g\rangle$. In Ref. [5], it is shown that $|\psi_{N_d}\rangle$ in the thermodynamic limit ($L \to \infty$ with $d = N_d/L$ constant) has ODLRO if $d \neq 0$ and $1 + d - n = N_e/L \neq 0$.

The model has a metal-insulator transition at $U_c = 4t$. The four-boson theory of Kotliar and Ruckenstein [15] in the mean-field approximation gives $U_c = 16t/\pi$ [9] in good agreement with the exact value. The approximation also gives a reasonably accurate U_c for the infinite-dimensional Hubbard model [16].

The form of the Hamiltonian in the representation of Eq. (3) suggests that addition of a small t_{AB}, such that it can be treated in second-order perturbation theory, introduces antiferromagnetic correlations between nearest-neighbor fermions and allows the permutation of nearest-neighbor bosons d and e, increasing their mobility and favoring superconductivity. We have solved numerically the model for $t_{BB} = |t_{AA}| = 1$, $t_{AB} = 0.2$, and $L = 10$. In the case $t_{AA} = -1$, for $1/2 < n \leq 1$, the model exhibits phase separation for $U > U_s$ with $U_s \sim 1$ for $n \sim 3/4$ and $U_s = 0$ for $n = 1$, while for $U < U_s$ the system behaves as a Tomonaga–Luttinger liquid (TLL) [21]. For $n < 1/2$ the TLL behavior is observed for all values of U. Within the TLL regime, the evaluation of the compressibility, the Drude weight, and the spin and charge velocities allowed us to derive the correlation exponent K_ρ [21]. The resulting values indicate that the dominant correlations are the superconducting ones for $1/2 < n < 1$ and the charge-charge ones for $n < 1/2$. In the case $t_{AA} = t_{BB} = 1$, there is no phase separation. For $1/2 < n < 3/2$ and small values of U, the system is a TLL with dominant superconducting correlations. For $n = 1$ there is a transition to an insulating phase for $U \sim 3.5$.

In this Letter we have solved exactly a Hubbard chain including bond-charge repulsion for a particular value of the latter. The model displays a Mott transition at half filling, and in two regimes of parameters the ground state contains superconducting states. Numerical results show that superconductivity is favored by a small perturbation for not too large on-site Coulomb repulsion.

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