

Exact Bond Ordered Ground State for the Transition between the Band and the Mott Insulator

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We derive an effective Hamiltonian H_{eff} for an ionic Hubbard chain, valid for $t \ll U, \Delta$, where t is the hopping, U is the Coulomb repulsion, and Δ is the charge-transfer energy. H_{eff} is the minimal model for describing the transition between the band insulator (BI) ($\Delta - U \gg t$) and the Mott insulator (MI) ($U - \Delta \gg t$). Using spin-particle transformations [Phys. Rev. Lett. **86**, 1082 (2001)], we map H_{eff} ($U = \Delta$) into an SU(3) antiferromagnetic Heisenberg model whose exact ground state is known. In this way, we show rigorously that a spontaneously dimerized insulating ferroelectric phase appears in the transition region between the BI and the MI.

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It is well known that the insulating state can have different origins. The simplest case is the band insulator (BI) since it is one of the possible solutions for noninteracting electrons moving in a periodic potential. In particular, the BI occurs when the number of particles per unit cell is even, so the bands are either full or empty. The other traditional example of insulating state is the Mott insulator (MI). In this case, the charge localization is just a consequence of the local Coulomb interaction U between the electrons. The charge gap of the BI is just the band gap. In the case of the MI, this gap is a function of the Coulomb repulsion and goes asymptotically to U in the strong coupling limit. These two insulating states have completely different properties. For instance, the BI's are paramagnets while the MI's, in general, are antiferromagnets. This observation raises the following question: What happens when a system evolves continuously from the BI to the MI state?

To find an answer to this question has been the main motivation for studying the ionic Hubbard model (IHM) during the last ten years. The IHM was originally proposed in the 1980s to describe the neutral-ionic transition in mixed stack charge-transfer organic crystals [1,2]. This model is a Hubbard Hamiltonian on a bipartite lattice with different diagonal energies for the two sublattices. The difference between both energies is Δ . During the 1990s, there was a renewed interest in the IHM due to the potential applications to the description of the ferroelectric (FE) perovskites [3–5]. At half filling, the ground state of the IHM is an ionic or BI for $\Delta \gg U$ and a MI for $U \gg \Delta$. Field theory arguments in one dimension pointed out the existence of an intermediate bond ordered insulating (BOI) phase for $\Delta \ll U \ll t$ [5]. For $t \ll U, \Delta$, perturbation theory clearly describes the BI ($t \ll \Delta - U$) and the MI ($t \ll U - \Delta$) [2], including the charge dynamics of the latter [6]. However, perturbation theory diverges in the transition region and no insight is provided for the BOI. The numerical solutions of finite

chains [7–10] have difficulties and contradictory conclusions were reported. The reason will become clear after deriving the main result of the present Letter.

Contrary to the cases of the BI and the MI states, no exact solution having long range bond ordering is known for the transition regime. Finding an exact ground state is not only crucial to prove the existence of the BOI phase rigorously but also to understand its microscopic origin and fundamental properties. This result becomes even more important if we consider that the BOI phase is an electronically induced spin-Peierls instability that generates a FE state out of the spin-singlet dimer pairs. In particular, a bond ordered FE state was observed in the pressure-temperature phase diagram of the prototype compound, tetrathiafulvalene-*p*-chloranil [11,12]. In addition, as it was pointed out by Egami *et al.* [3], the microscopic origin of the FE transition in covalent perovskite oxides like BaTiO₃ is still unclear. It is known that a picture based on static Coulomb interactions and the simple shell model is inadequate to describe some FE properties [13]. The exact result presented here demonstrates that when an ionic insulator gets close to a charge-transfer instability (strong covalency), an electronic mechanism for ferroelectricity takes place.

In this Letter, we first derive an effective Hamiltonian, H_{eff} , for the limit $U \gg t$ and $\Delta \gg t$ of an extended IHM that includes a nearest-neighbor Coulomb repulsion V . By means of the generalized spin-particle transformations introduced in Refs. [14–16], we map H_{eff} into an anisotropic SU(3) antiferromagnetic Heisenberg model that becomes isotropic for $U = \Delta$ and particular values of the other parameters. The isotropic model is exactly solvable [17–19] and is also equivalent to the biquadratic $S = 1$ Heisenberg model. The exact ground state is a dimerized spin system that becomes a BOI when translated back to the original fermionic variables.

We start by considering an IHM with an additional Coulomb interaction V between nearest neighbors:

$$H = -t \sum_{i,\sigma} (f_{i+1\sigma}^\dagger f_{i\sigma} + \text{H.c.}) + \frac{\Delta}{2} \sum_i (-1)^i n_i + U \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right) + V \sum_i (n_i - 1)(n_{i+1} - 1), \quad (1)$$

where $n_{i\sigma} = f_{i\sigma}^\dagger f_{i\sigma}$, $n_i = \sum_\sigma n_{i\sigma}$, and $t > 0$. Note that $\Delta > 0$ is the diagonal energy difference between sites in different sublattices.

We consider only the half-filled case $\rho = 1$, i.e., one particle per site. If $t = 0$, the ground state of H is a nondegenerate BI for $U < \Delta + 2V$. There is only *one* low-energy state per site: the odd sites are doubly occupied and the even sites are empty (see Fig. 1). For $U > \Delta + 2V$ the ground state is a degenerate MI (one particle per site) and the low-energy subspace has *two* states per site due to the spin degeneracy. When t is finite and small, far from the transition region the low-energy Hamiltonian of the MI is a Heisenberg model and the degeneracy is lifted in favor of a spin-density wave [2,6] (see Fig. 1). However, to describe the transition region, we need to include *three* states per site in the low-energy subspace \mathcal{H}_0 . In order to construct an effective Hamiltonian in \mathcal{H}_0 , it is convenient to perform an electron-hole transformation for the odd sites:

$$\begin{aligned} c_{i\uparrow}^\dagger &= -f_{i\downarrow}, & c_{i\downarrow}^\dagger &= f_{i\uparrow}, & \text{for odd } i; \\ c_{i\sigma}^\dagger &= f_{i\sigma}^\dagger, & & & \text{for even } i. \end{aligned} \quad (2)$$

After this transformation, H becomes invariant under a translation of one lattice space ($i \rightarrow i + 1$). The low-energy subspace \mathcal{H}_0 is now defined as the set of states with no double occupancy on any site. This constraint can be incorporated by defining the constrained fermion operators: $\tilde{c}_{i\sigma}^\dagger = c_{i\sigma}^\dagger (1 - c_{i\bar{\sigma}}^\dagger c_{i\bar{\sigma}})$ and $\tilde{c}_{i\sigma} = (\tilde{c}_{i\sigma}^\dagger)^\dagger$. In addition, to connect our low-energy theory with spin Hamiltonians (see below), we introduce the following transformation:

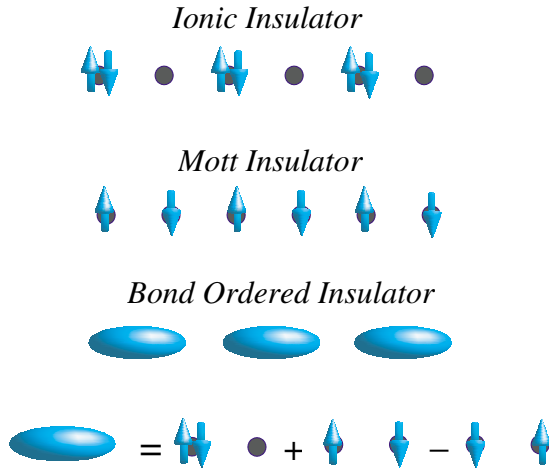


FIG. 1 (color online). Schematic plot of the different ground states of H_{eff} .

$$\begin{aligned} \tilde{c}_{i\downarrow}^\dagger &\rightarrow -\tilde{c}_{i\downarrow}^\dagger & \text{for } i = 4n & \text{ and } i = 4n + 1; \\ \tilde{c}_{i\uparrow}^\dagger &\rightarrow -\tilde{c}_{i\uparrow}^\dagger & \text{for } i = 4n + 2 & \text{ and } i = 4n + 1. \end{aligned} \quad (3)$$

The high-energy subspace \mathcal{H}_1 consists of all states that have at least one double occupied site. The only term of H that mixes \mathcal{H}_0 and \mathcal{H}_1 is the hopping term t . By means of a second order canonical transformation that eliminates the terms proportional to t , we obtain the following effective Hamiltonian for the low-energy spectrum of H :

$$\begin{aligned} H_{\text{eff}} &= t \sum_{i,\sigma} (\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{i+1,\sigma}^\dagger + \text{H.c.}) + \frac{\Delta - U}{2} \sum_i \tilde{n}_i \\ &+ J \sum_i \left(s_i^z s_{i+1}^z - s_i^x s_{i+1}^x - s_i^y s_{i+1}^y - \frac{1}{4} \tilde{n}_i \tilde{n}_{i+1} \right) \\ &- V \sum_i (1 - \tilde{n}_i)(1 - \tilde{n}_{i+1}), \end{aligned} \quad (4)$$

where $\tilde{n}_i = \sum_\sigma \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma}$ and $s_i^\alpha = 1/2 \sum_{\tau,\tau'} \tilde{c}_{i\tau}^\dagger \sigma_{\tau\tau'}^\alpha \tilde{c}_{i\tau'}$ with $\alpha = \{x, y, z\}$ (σ^ν are the Pauli matrices). The exchange interaction $J = 2t^2/(U + \Delta - V)$ comes from a second order process in the hopping t . In this derivation we have neglected the second order three-site hopping term. The negative sign for the xx and yy interactions is just a consequence of the gauge transformation of Eq. (3).

If $t \sim V$ and $\Delta - U \gg t$, the ground state of H_{eff} is the empty state that corresponds to the BI in the original language. For $U - \Delta \gg t$, the ground state has one particle per site. By eliminating states with empty sites with another canonical transformation, H_{eff} reduces to the Heisenberg model that describes the strong coupling limit of the MI. We are interested in the transition regime $U \sim \Delta$. To analyze this case, we allow J to vary independently of the other parameters. In other words, we consider H_{eff} as an independent minimal model for describing the transition between the BI and the MI.

To exploit the symmetries of H_{eff} , it is convenient to use the generalized Jordan-Wigner transformations introduced in Refs. [14–16]. In particular, for this case it is appropriate to rewrite H_{eff} in terms of the hierarchical SU(3) language [16]. To this end, we need to map the constrained fermion operators in one sublattice (say A) into SU(3) spins in the fundamental or “quark” representation [15,16]:

$$S(j) = \begin{pmatrix} \frac{2}{3} - \tilde{n}_j & K_j^\dagger \tilde{c}_{j\uparrow} & K_j^\dagger \tilde{c}_{j\downarrow} \\ \tilde{c}_{j\uparrow}^\dagger K_j & \tilde{n}_{j\uparrow} - \frac{1}{3} & \tilde{c}_{j\uparrow}^\dagger \tilde{c}_{j\downarrow} \\ \tilde{c}_{j\downarrow}^\dagger K_j & \tilde{c}_{j\downarrow}^\dagger \tilde{c}_{j\uparrow} & \tilde{n}_{j\downarrow} - \frac{1}{3} \end{pmatrix}, \quad (5)$$

where K_j is the kink operator [14]:

$$K_j = \exp \left[i\pi \sum_{k < j} \tilde{n}_k \right] \quad (6)$$

that transmutes the statistics. The components $S^{\mu\nu}$ are generators of the $su(3)$ algebra with commutation relations $[S^{\mu\mu'}(j), S^{\nu\nu'}(j)] = \delta_{\mu'\nu'} S^{\mu\nu}(j) - \delta_{\mu\nu'} S^{\nu\mu'}(j)$. We also make use of the conjugated or “antiquark” representation

$$\tilde{S}(j) = \begin{pmatrix} \frac{2}{3} - \bar{n}_j & -\bar{c}_{j\downarrow}^\dagger K_j & -\bar{c}_{j\uparrow}^\dagger K_j \\ -K_j^\dagger \bar{c}_{j\downarrow} & \bar{n}_{j\downarrow} - \frac{1}{3} & \bar{c}_{j\uparrow}^\dagger \bar{c}_{j\downarrow} \\ -K_j^\dagger \bar{c}_{j\uparrow} & \bar{c}_{j\downarrow}^\dagger \bar{c}_{j\uparrow} & \bar{n}_{j\uparrow} - \frac{1}{3} \end{pmatrix} \quad (7)$$

to describe the degrees of freedom of the B sublattice. Equations (5) and (7) are generalizations of the Jordan-Wigner transformations to $SU(3)$ spins [15,16]. The resulting H_{eff} is as an anisotropic $SU(3)$ Heisenberg model with an applied “magnetic field”:

$$H_{\text{eff}} = \sum_{i \in A, \mu, \nu} J_{\mu\nu} S^{\mu\nu}(i) \tilde{S}^{\nu\mu}(i+1) - B \sum_i S^{00}(i), \quad (8)$$

with $J_{00} = -V$, $J_{01} = J_{02} = -t$, $J_{11} = J_{12} = J_{22} = -J/2$, $J_{\mu\nu} = J_{\nu\mu}$, and $B = 2V/3 - J/3 + U/2 - \Delta/2$. Note that this model connects $SU(3)$ spins in the A sublattice with the conjugate $SU(3)$ spins (antiquark representation) in the B sublattice. Let us now consider $V = J/2 = t$ and $U = \Delta$. For this line in the space of parameters H_{eff} is an *isotropic $SU(3)$ antiferromagnetic Heisenberg model* that is invariant under staggered conjugate $SU(3)$ rotations, \mathcal{R} and \mathcal{R}^\dagger , on sublattices A and B , respectively. This model is integrable [17–19] and the exact solution is a spin-dimerized ground state. In the original language this is equivalent to saying that the charge and the spin are both dimerized (bond ordering). The exact ground state energy per site is $e_0/t = -1.796864\dots$. The value of the gap is $\Delta/t = 0.173178$, a rather small value, and the correlation length $\xi = 21.0728505\dots$ is very large [19]. This explains the numerical difficulties for identifying this phase.

To relate the dimerization in $SU(3)$ and the bond ordering of the fermionic variables, we need just to translate the corresponding order parameter from the $SU(3)$ language back to our original fermionic language. The spin-dimer $SU(3)$ order parameter is [20,21]

$$D = |h_{i-1,i} - h_{i,i+1}|, \quad (9)$$

where $h_{i-1,i} = |i-1, i\rangle\langle i, i-1|$ is a projector on the $SU(3)$ singlet spin state, $|i-1, i\rangle$, at the bond $(i-1, i)$. Note, in addition, that $h_{i-1,i}$ is the isotropic $SU(3)$ Heisenberg Hamiltonian for the same bond. In the fermionic language, $|i-1, i\rangle$ has the following expression:

$$|i-1, i\rangle = \frac{1}{\sqrt{3}} (1 - \bar{c}_{i-1\uparrow}^\dagger \bar{c}_{i\downarrow}^\dagger - \bar{c}_{i-1\downarrow}^\dagger \bar{c}_{i\uparrow}^\dagger) |0\rangle. \quad (10)$$

In terms of the original f fermions [see Eqs. (2) and (3)], this is a linear combination of an on-site singlet and a nearest-neighbor singlet state that is illustrated at the bottom of Fig. 1. Xian showed that $D = 0.4216D_0$, where D_0 is the value of D for a perfect dimerized state [20]. Replacing Eq. (10) in (9), it becomes clear that D is a BOI order parameter. From a calculation of the charge Berry phase [7] we obtain that the shift in polarization of the two possible perfect dimerized states (see the bottom of Fig. 1) relative to the MI is $\pm e/6$. Equation (10) shows that the dimer formation is just a consequence of the charge-

transfer instability between the two sublattices. In this sense, this exact ground state unveils the fundamental role of *covalency* for the stabilization of a bond ordered FE state [3,11,12]. This is not only relevant to describe one dimensional systems like tetrathiafulvalene-*p*-chloranil [11,12] but is also helpful to gain a deeper understanding of the FE transition of covalent perovskites [3].

Using another set of transformations that connect the constrained fermions with $SU(2)$ $S = 1$ spins [14],

$$\begin{aligned} S_j^+ &= \sqrt{2}(\bar{c}_{j\uparrow}^\dagger K_j + K_j^\dagger \bar{c}_{j\downarrow}), & S_j^- &= \sqrt{2}(K_j^\dagger \bar{c}_{j\uparrow} + \bar{c}_{j\downarrow}^\dagger K_j), \\ S_j^z &= \bar{n}_{j\uparrow} - \bar{n}_{j\downarrow}, \end{aligned} \quad (11)$$

we can also write $H_{\text{eff}}(V = J/2 = t)$ as an $S = 1$ biquadratic Heisenberg model [15] with a single-ion anisotropy:

$$H_{\text{eff}}(V = J/2 = t) = -t \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 + E \sum_i (S_i^z)^2, \quad (12)$$

where $E = (\Delta - U)/2$. The strength of the anisotropy term is determined by the difference $\Delta - U$. If E is large and positive ($\Delta \gg U$), the spin system has an easy plane anisotropy. Each site is most of the time in the $S^z = 0$ state, which means that the magnetization is perpendicular to the z axis. The ground state is nondegenerate (there is no broken symmetry) and corresponds, in the original language, to the *band insulator*. If E is large and negative ($U \gg \Delta$), the system has a strong easy axis anisotropy and each site is in the $S^z = \pm 1$ state; i.e., the local magnetization is parallel to the z axis. The ground state is critical due to the antiferromagnetic correlations which characterize the MI. In between, for $U = \Delta$, we have demonstrated that there is a dimerized state which corresponds to the BOI. In terms of the original variables, the strong quantum fluctuations that appear in the proximity of the charge-transfer instability break the Z_2 inversion symmetry by increasing the strength of one bond relative to the next one.

The $S = 1$ version of H_{eff} also provides a simple way of studying the low-energy excitations of our exact bond ordered state. The excitations of a dimerized spin $1/2$ chain are spinons that carry a spin $S = 1/2$. In the same way, the excitations of our $S = 1$ dimer state are $S = 1$ spinons. Each spinon is a soliton or antiphase boundary for the Z_2 spin-dimer order parameter. The two regions with opposite dimerization are separated by a local $S = 1$ defect which is attached to the antiphase boundary. In terms of the original language, the $S_z = 0$ spinons correspond to $s = 0$ solitons (charge excitations), while the $S_z = \pm 1$ spinons are $s = 1/2$ solitons (spin and charge excitations). From Eqs. (2) and (12), the total charge operator relative to half filling is $Q = \sum_{i \in A} (S_i^z)^2 - \sum_{i \in B} (S_i^z)^2$. For a general dimerized solution with arbitrary E we have on each site $\langle (S_i^z)^2 \rangle = 1 - \alpha$ with $\alpha = 1/3$ for the exact solution at $E = 0$. When the defect is localized on site j (the extension of the defect does not affect the charge or spin of the excitations

because they are topological invariants) we have $\langle (S_i^z)^2 \rangle = 0, 1$. Since the defect separates two regions with opposite dimerization, it is easy to check that the $s = 0$ solitons (antisolitons) have charge $Q = \pm(1 - \alpha)$ while the charge of the $s = 1/2$ solitons (antisolitons) is $Q = \pm\alpha$. For $E = 0$, both excitations are degenerate as a consequence of the SU(3) invariance. These excitations coincide with those obtained by Fabrizio *et al.* [5], who treat the bosonized IHM as a phenomenological Ginzburg-Landau energy functional. The magnitude α is proportional to their jump in the charge field. In particular, the $s = 1/2$ excitations interpolate between an ordinary electron near the BI-BOI boundary ($\alpha = 1$, $E > 0$) and a spinon near the BOI-MI boundary ($\alpha = 0$, $E < 0$).

In order to obtain an exact ground state of H_{eff} we used a value of $J = 2t$ which is beyond the region allowed by perturbation theory. Therefore, to connect our exact solution with the IHM, it is important to discuss the effect of reducing the value of J . In addition, since most of the previous papers do not include the V term, it is also important to analyze its effect. A simple first order estimation of the energy change for the three competing phases, $\delta E_{\text{BI}} = \delta U/2 + t$, $\delta E_{\text{MI}} = 2t \ln 2$, and $\delta E_{\text{BOI}} = \delta U/6 - 5e_0 t/9$, when J and V are reduced to zero, indicates that the BOI survives if the difference $U - \Delta$ is simultaneously increased to a value of order t . This conclusion is supported by different numerical results [7–9] that report a bond ordered ground state of $H(V = 0)$ for the same region of parameters ($U - \Delta \sim t$ and $U, \Delta \gg t$). These observations suggest that our exact solution is continuously connected with the BOI phase which was numerically found in the IHM.

In summary, we have derived an effective low-energy Hamiltonian, H_{eff} , for the $U, \Delta \gg t$ limit of the IHM. H_{eff} is a minimal model to describe the BI to MI transition. Its simple form and the fact that it operates in a reduced Hilbert space of local dimension $D = 3$ provide a new framework to understand this transition. Using the spin-particle transformations introduced in Refs. [15,16], we mapped H_{eff} into an anisotropic SU(3) antiferromagnetic Heisenberg model. By increasing the value of J beyond the region allowed by perturbation theory, we have shown that there is an exactly solvable SU(3) invariant point for $U = \Delta$ and $V = J/2 = t$. In this way, we demonstrated the existence of a bond ordered phase for the transition regime between the BI and the MI. The large value of the correlation length $\xi = 21.0728505 \dots$ explains the numerical difficulties for detecting this phase in finite size systems. This exact solution provides an answer to the question that was formulated in the introduction: in the transition regime the system resolves the competition between the BI and the MI by creating a rather local resonance which can be visualized on each dimer as a linear combination of a unit cell of the BI and a nearest-neighbor singlet that is related with the MI (see Fig. 1). One of the most important physical consequences

of this nontrivial phenomenon is the generation of a new mechanism for ferroelectricity [3] that should be relevant for ionic insulators which are close to a charge-transfer instability. This result should motivate a careful reexamination of the ferroelectricity in covalent materials.

In addition to the SU(3) mapping, we used a second spin-particle transformation [14] that maps the constrained fermions into $S = 1$ SU(2) spins. In this new language $H_{\text{eff}}(V = J/2 = t)$ is a biquadratic Heisenberg model with a single-ion anisotropy along the z axis which is proportional to $\Delta - U$. The transitions among the BI, BOI, and MI phases have been reinterpreted in the $S = 1$ language. We have also shown that the $S = 1$ version of H_{eff} provides the most natural frame to understand the low-energy excitations of the BOI. These excitations are solitons that carry a fractional charge and spin $s = 0$ or $s = 1/2$. The relevance of these results illustrates the elegance and the potential of the generalized spin-particle transformations introduced in Refs. [14–16].

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