Variational Description of Mott Insulators

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The Gutzwiller wave function for a strongly correlated model can, if supplemented with a long-range Jastrow factor, provide a proper variational description of Mott insulators, so far unavailable. We demonstrate this concept in the prototypical one-dimensional $t - t'$ Hubbard model, where at half-filling we reproduce all known phases, namely, the ordinary Mott undimerized insulator with power-law spin correlations at small t'/t, the spin-gapped metal above a critical t'/t and small U, and the dimerized Mott insulator at large repulsion.

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Since Mott's original proposal [1] the correlation-driven metal-Mott insulator transition (MIT) has attracted rising interest, renewed by the discovery of novel strongly correlated materials. On the verge of becoming Mott insulators, many systems display very unusual properties, high-T_c superconductivity being one spectacular example. While understanding Mott insulators and MITs is conceptually simple, calculations constitute a hard and long-standing problem. Conventional electronic structure methods, such as Hartree-Fock (HF) or density functional theory in the local density approximation (LDA) cannot describe MITs, unless one allows for some kind of symmetry breaking. The standard example is long-range static magnetic order in the unrestricted HF, local-spin density, or LDA + U approximations. This device works by effectively turning the MIT into a conventional metal-band insulator transition, thus masking the essence of the Mott phenomenon, where a charge gap appears quite independently of spin order. The fact that most known Mott insulators are, indeed, accompanied at low temperatures by some symmetry breaking, usually of magnetic type, further encourages the (wrong) surmise that it is not possible to describe any Mott insulator without a symmetry breaking.

Another useful and popular approximation that may invite the same conclusion is based on the variational Gutzwiller wave function (GWF) and its various generalizations [2–5]. The GWF is the simplest way to improve a symmetry-unbroken, hence metallic, Slater determinant by partly projecting out the expensive double-occupancy charge configurations. In principle, were the projection complete, the GWF would, indeed, describe a Mott insulator devoid of symmetry breaking. Full projection, however, means zero band-energy gain, generally incorrect, except for infinite on-site repulsion. For finite projection, appropriate at finite repulsion, the GWF unfortunately describes a metallic state in any finite dimensional lattice, at least as long as the uncorrelated Slater determinant state is metallic [3]. To obtain an insulator, one is forced once again to Gutzwiller project an artificially symmetry-broken determinant wave function (WF). The main drawback of the GWF can be immediately recognized if one recalls Mott's original description of a correlation-driven insulator. Let us consider for simplicity the single-band Hubbard model at half filling. First of all, it is clear that the system must even in the insulating phase allow for charge fluctuations around the mean value, implying some doubly occupied (doublon, D) and empty (holon, H) sites, or it would jeopardize all band-energy gain. However, in order to describe an insulator, D and H have to be bound; otherwise, any infinitesimal electric field could induce electric current. This spatial correlation among expensive charge configurations is exactly what is missing in the conventional GWF. There have been several attempts to cure these defects by allowing H-D correlations just on nearest neighbor sites [6,7], with only partial success. It is actually suggested by our previous discussion that long-range H-D correlations should be a fundamental ingredient of a realistic insulating WF; otherwise, there would always exist a finite probability for H and D to escape from one another, signaling a metallic behavior [8].

In this Letter we show that this plan can be accomplished with success. In particular, we demonstrate for a specific one-dimensional (1D) model the following: (i) nontrivial insulating WFs with or without symmetry breaking do exist; (ii) the MIT, so far well described only in infinite dimensions [9], is accessible variationally even in finite dimensions. We consider the 1D $t - t'$ Hubbard model

$$\mathcal{H} = -t\sum_{i,\sigma} c^{\dagger}_{i,\sigma} c_{i+1,\sigma} + \text{H.c.} + t'\sum_{i,\sigma} c^{\dagger}_{i,\sigma} c_{i+2,\sigma} + \text{H.c.} + U\sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \tag{1}$$

where $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) creates (destroys) an electron with spin σ on-site i and $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$. In the following we assume t and t' are positive.

Bosonization [10] and density-matrix renormalization group calculations [11,12] predict that the ground state at

half filling is an insulator with gapless spin excitations (labeled $C0S1$, where $CnSm$ indicates a state with n gapless charge modes and m gapless spin modes) for $t'/t \lesssim 0.5$, a spin-gapped metal ($C1S0$) with strong superconducting fluctuations for $t'/t \gtrsim 0.5$ and small U/t, and a fully gapped spontaneously dimerized insulator ($C0S0$) for $t'/t \gtrsim 0.5$ and large U/t. Dimerization is characterized by the discrete order parameter $D_d^2 = \lim_{|i-j|\to\infty} |\chi(i-j-1) - 2\chi(i-j) + \chi(i-j+1)|$, where $\chi(i-j) = 9\langle S_i^z S_{i+1}^z S_j^z S_{j+1}^z\rangle$ gives the dimer-dimer correlation function of spin rotationally invariant WFs, S_i^z being the spin operator along the z axis at site i.

The $C1S0$ metallic phase suggests a variational WF built out of BCS, namely

$$|\Psi\rangle = \mathcal{P}|\mathrm{BCS}\rangle = \mathcal{P}\exp\Big(\sum_q f_q c_{q,\uparrow}^\dagger c_{-q,\downarrow}^\dagger\Big)|0\rangle, \qquad (2)$$

where $|\mathrm{BCS}\rangle$ is the ground state of a BCS Hamiltonian with gap function Δ_q and dispersion $\epsilon_q = -2t\cos(q) + 2t'\cos(2q) - \mu$, μ being the free electron chemical potential. The pairing function is defined by $f_q = \Delta_q/(\epsilon_q + E_q)$, with the BCS energy spectrum $E_q = \sqrt{\epsilon_q^2 + \Delta_q^2}$, and $\Delta_q = \Delta_1\cos(q) + \Delta_2\cos(2q) + \Delta_3\cos(3q)$, Δ_1, Δ_2, and Δ_3 being variational parameters. Obviously, $|\mathrm{BCS}\rangle$ reduces to the Fermi sea for $\Delta_q = 0$. The operator $\mathcal{P} = J\mathcal{P}_N$, where $\mathcal{P}_N$ projects onto the subspace with a fixed number of electrons $N = L$ (L being the number of sites) and J is the Jastrow factor:

$$J = \exp\Big(\sum_{i,j}\frac{1}{2}v_{i,j}(n_i - 1)(n_j - 1) + w_{i,j}h_i d_j\Big), \qquad (3)$$

where $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ is the density operator, $d_i = n_{i,\uparrow}n_{i,\downarrow}$ the doublon operator, and $h_i = (1 - n_{i,\uparrow})(1 - n_{i,\downarrow})$ the holon one. We note that, in the presence of a magnetic flux $\phi \neq 0$, the Jastrow term can acquire a noncentrosymmetric component, $w_{i,j} - w_{j,i} \neq 0$. While the centrosymmetric part $w_{i,j} + w_{j,i}$ turns out to be less crucial than $v_{i,j}$ for the $\phi = 0$ ground state, the odd component $w_{i,j} - w_{j,i}$, which is zero at zero flux and had not been included so far [13], plays a relevant role in determining the response to ϕ. In practice we find it more convenient to discriminate the Mott insulator from the metal through correlation functions which can be calculated in the absence of flux, as it is very unhandy to follow the changes of the variational WF due the presence of ϕ.

Numerically we find that the optimized $v_{i,j}$ is smooth as a function of the distance $|i-j|$, while $w_{i,j}$ is staggered, $w_{i,j} = |w_{i,j}|(-1)^{|i-j-1|}$. Although $w_{i,j}$ improves the accuracy, it does not change qualitatively the nature of the WF, which is mainly determined by $v_{i,j}$, as we discuss below. For this reason most of the results are obtained with $w_{i,j} = 0$. Indeed, since $(n_i - 1)(n_j - 1) = h_i h_j + d_i d_j - h_i d_j - d_i h_j$, then $v_{i,j} < 0$ implies H-H (D-D) long-range repulsion and H-D long-range attraction. The latter embodies the binding of H and D, while the repulsion prevents accumulation of H-D pairs. That is just the desired type of correlations missing in the GWF.

We notice that optimization of the Jastrow factor allows one to fulfill variationally the f-sum rule. Indeed, if we denote the variational energies of $|\Psi\rangle$ by $\mathcal{E}_0$ and of $n_q|\Psi\rangle$ by $\mathcal{E}_q$, then we can prove for the optimized $v_{i,j}$'s that

$$\lim_{q\to 0}(\mathcal{E}_q - \mathcal{E}_0) = \frac{q^2}{2N_q}\frac{\langle\Psi|\frac{1}{L}\sum_{k,\sigma}\partial_k^2\epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma}|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \qquad (4)$$

where $N_q = \langle\Psi|n_{-q}n_q|\Psi\rangle/\langle\Psi|\Psi\rangle$ is the density-density correlation function. On the assumption that our variational WF $|\Psi\rangle$ gives a fair description of the actual ground state WF, Eq. (4) allows one to infer the behavior of the long-wavelength charge excitation spectrum by just analyzing the charge structure factor N_q of $|\Psi\rangle$. Namely, if $N_q \sim q$, there should exist gapless charge modes, while if $N_q \sim q^2$ charge excitations are presumably gapped. In turn N_q is determined by the structure factor of the uncorrelated BCS WF, N_q^0, and by the Fourier transform of $v_{i,j}$, v_q, through $N_q \sim N_q^0/(1 + N_q^0 v_q)$ [14]. Since N_q^0 tends to a constant value for $q \to 0$, the long-wavelength behavior of N_q is actually determined by the singular behavior of v_q, $v_q \sim 1/q$, or $v_q \sim 1/q^2$ implying $N_q \sim q$ or $N_q \sim q^2$, respectively. In other words the long-range Jastrow factor not only restores gauge invariance, $\lim_{q\to 0}N_q = 0$, but also filters out either the metallic or the insulating component of the uncorrelated WF by an unbiased minimization of the energy.

Despite the large number of variational parameters, $v_{i,j}$'s, $w_{i,j}$'s as well as Δ's, it is possible to optimize the full WF by recent developments in the variational Monte Carlo technique [15]. Yet, to afford larger scale simulations, we also assume an analytic parametrization of $v_{i,j}$:

$$v_{i,j} = -\frac{1}{L}\sum_q \cos[q(i-j)]\frac{A}{\sqrt{\sin^2(q/2) + m^2} - m}, \qquad (5)$$

with A and m variational parameters, with m playing the role of the inverse Mott-localization length: $m = 0$ or $m > 0$ implying, respectively, metallic, $v_q \sim 1/q$, or insulating, $v_q \sim 1/q^2$, behavior.

Besides the small-q behavior of the charge structure factor N_q, another quantity which can discriminate between a metal and an insulator is a "rigidity" defined through $Z_c = \langle\Psi|\exp(\frac{2\pi i}{L}\sum_j j n_j)|\Psi\rangle/\langle\Psi|\Psi\rangle$. In the thermodynamic limit, for 1D systems, $|Z_c| \to 0$ for a metal and $|Z_c| \to 1$ for an insulator [16].

For what concerns the spin modes, we argue that their behavior is determined by the BCS spectrum E_q, namely, if E_q is gapless, then the spin excitations are also gapless and the spin structure factor $S_q \sim q$, whereas, if $\min(E_q) > 0$,

the spin excitation spectrum has a gap and $S_q \sim q^2$. This is supported by the direct calculation of the generalized spin rigidity $Z_s = \langle\Psi|\exp(\frac{4\pi i}{L}\sum_j j S^z_j)|\Psi\rangle/\langle\Psi|\Psi\rangle$, $|Z_s| \to 0$ for a spin-gapless WF, and $|Z_s| \to 1$ for a spin-gapped WF.

First of all, we now prove that the WF (2) with an appropriate choice of parameters is able to describe $C0S1$, a Mott insulator with no symmetry breaking, as well as $C0S0$, a spontaneously dimerized insulator, and $C1S0$, a spin-gapped metal. In Fig. 1, we show how the three possible cases $C0S1$, $C1S0$, and $C0S0$ can be actually realized. The two WFs corresponding to $C0S0$ and $C0S1$ are, indeed, insulating even though the average density of H (D) is finite. Moreover, we note that, unlike the uncorrelated BCS WF, the correlated variational WF in the $C1S0$ phase is not superconducting, as it should, of course, be in 1D, thanks to the long-range Jastrow factor [17]. Remarkably, even if the $C0S0$ BCS WF is not explicitly dimerized, after application of the Jastrow factor (3), a finite dimerization order parameter emerges. As in the liquid-solid transition of helium, it is typical of Jastrow functions to describe phase transitions in two-body correlation functions, without an explicit symmetry breaking in the one-body properties.

To check the quality of the variational WF (2) for the Hamiltonian (1), we start by considering the case of $t' = 0$, which allows us a direct comparison with exact Bethe *ansatz* results. For the reasons we mentioned previously, the GWF gives a rather poor variational description of the half-filled Hubbard model for $U \gg t$. In this limit an alternative procedure is commonly adopted. It is known that for $U \gg t$ the half-filled Hubbard model transforms by a Schrieffer-Wolff transformation e^{iS} into a Heisenberg model. Therefore, instead of using the GWF, it is more convenient to use $e^{iS}|\Psi_G\rangle$, where $|\Psi_G\rangle$ is the *fully projected* GWF. In that case, one searches for the optimal uncorrelated WF which, after complete projection, minimizes the average of $e^{-iS}\mathcal{H}e^{iS}$, namely, of a Heisenberg Hamiltonian. Practically one is forced to expand $e^{iS} \simeq 1 + iS$, which limits the applicability of this WF to the large U/t regime [18]. On the contrary, our WF is equally accurate both at weak and at large U/t, as shown in Fig. 2. Remarkably, the long-range Jastrow correlations turn a fully metallic Fermi sea—the worst case one-electron band for an insulator—into a perfectly good Mott insulator.

Going back to the $t - t'$ Hubbard model, in Fig. 3 we show the behavior of $|Z_c|$ and D_d for $t'/t = 0.75$. By increasing U/t, $|Z_c|$ shows a sudden increase, and we can easily discriminate between the metallic phase, where $|Z_c| \to 0$ by increasing L, and an insulating phase, where $|Z_c| \to 1$ for $L \to \infty$. Moreover, in the latter case, the MIT is, indeed, accompanied by a spontaneous dimerization, marked by a finite dimer order parameter D_d; see Fig. 3(b).

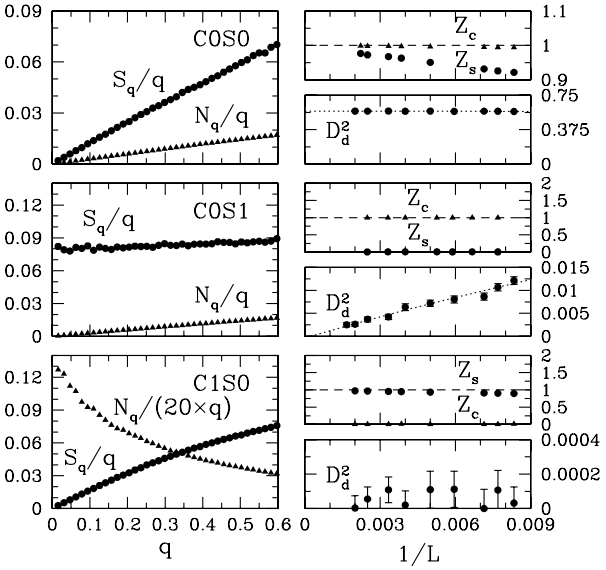

FIG. 1. Spin and charge properties of the $C0S0$ WF (top panels), the $C0S1$ WF (middle panels), and the $C1S0$ WF (bottom panels). Left panels: N_q/q (triangles) and S_q/q (circles) as a function of q for $L = 400$. Right panels: D_d^2, Z_c, and Z_s as a function of $1/L$. The dotted line is a three parameter fit, and the dashed line marks the value 1. The parameters of the WF are $Am = 0.33$, $A^2 = 0.17$ ($C0S0$ and $C0S1$), $m = 0$, $A^2 = 8.4 \times 10^{-3}$ ($C1S0$), $\Delta_1 = 2t$, $\Delta_2 = 1.7t$ ($C1S0$ and $C0S0$), and $\Delta_1 = \Delta_2 = \Delta_3 = 0$ ($C0S1$).

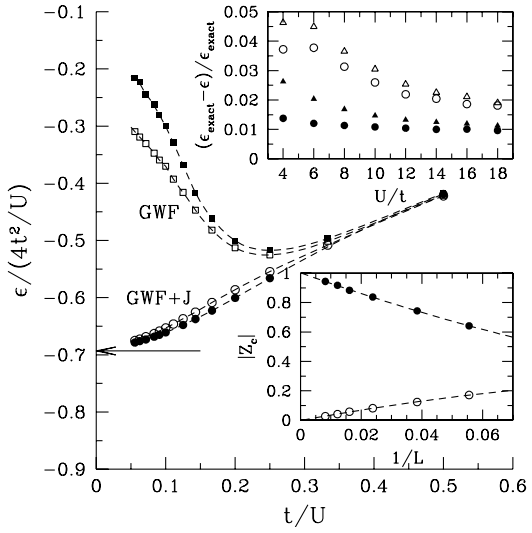

FIG. 2. Energy per site ϵ for the simple GWF ($L = 18$, empty squares, and $L = 82$, full squares) and for the WF with long-range density-density Jastrow (GWF + J) ($L = 18$, empty circles, and $L = 82$, full circles), for $t' = 0$. The Slater determinant is a simple Fermi sea, with $\Delta_q = 0$. The arrow indicates the exact energy per site of the Heisenberg model, and the lines are guides to the eye. Top inset: accuracy of the WF with all the density-density Jastrow independently minimized (same symbols as before) and with the analytic parametrization ($L = 18$, empty triangles, and $L = 82$, full triangles). Bottom inset: Z_c for the GWF + J (full circles) and for the GWF (open circles); lines are three parameter fits.

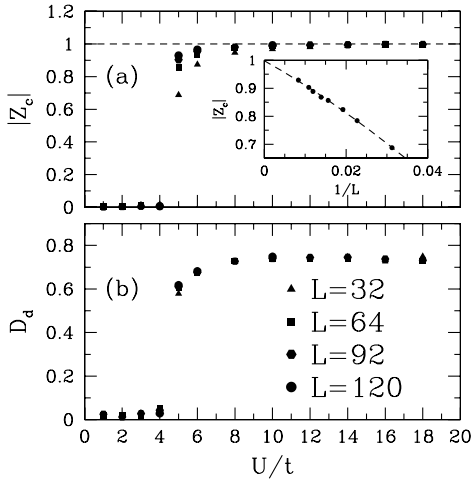

FIG. 3. (a) $|Z_c|$ as a function of U/t for $t'/t = 0.75$ and different sizes. (b) The same for the dimer order parameter D_d. The $v_{i,j}$'s are independently minimized; very similar results are obtained with the parametrization of Eq. (5). Inset: The size scaling of $|Z_c|$ for $U/t = 5$; the dashed line is a three parameter fit.

The variational phase diagram for the half-filled $t - t'$ Hubbard model is finally shown in Fig. 4. In the region of $t'/t \lesssim 0.5$ and $U > 0$, we find no evidence of a phase transition, apart from finite-size effects at small U/t. The best variational state has $N_q \sim q^2$, indicating a charge gap and $S_q \sim q$, gapless spin excitations: Δ_q connects only different sublattices (i.e., $\Delta_2 = 0$), making E_q gapless. For $t'/t \gtrsim 0.5$, there is a clear MIT at finite U/t between a spin-gapped metal, stable for small U/t, and a dimerized insulator, stable at large U/t. In the metallic phase, the variational WF has $N_q \sim q$, E_q gapped, with $\Delta_2 \neq 0$, although $|\Delta_q|$ is small; hence, $S_q \sim q^2$, corresponding to exponentially decaying spin-spin correlations. By increasing U/t and entering into the insulating phase, there is a fast increase of Δ_2, with E_q always fully gapped, and $v_q \sim 1/q^2$. In this phase, therefore, $N_q \sim q^2$ and $S_q \sim q^2$. Although the variational WF does not explicitly break translational symmetry, there is a finite dimerization in the thermodynamic limit. Remarkably, this is due to the concomitant effect of a singular Jastrow $v_q \sim 1/q^2$ and a gapped BCS spectrum E_q.

In conclusion, it is possible to describe a Mott insulator by a variational WF based on a metallic Fermi sea which includes, besides a partial Gutzwiller projector, a long-range density-density Jastrow term. The accuracy of the WF is verified in a one-dimensional $t - t'$ Hubbard model at half filling, which has a nontrivial phase diagram comprising different phases and a MIT. We argue that similar variational WFs with $v_q \sim 1/q^2$ could describe nontrivial Mott insulating phases in higher dimensions too, giving the possibility to improve realistic descriptions of Mott insulating compounds. We also believe these WFs to hold a great potential promise for future attacks to the superconducting phases that result by doping Mott insulators.

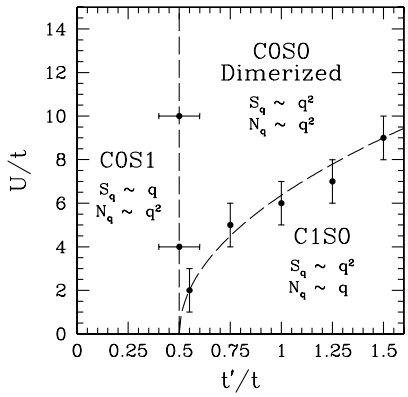

FIG. 4. Variational phase diagram of the 1D $t - t'$ Hubbard model. The error bars take into account finite-size effects, and dashed lines are guides to the eye.

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