Variational description of Mott insulators

Manuela Capello,1,2 Federico Becca,1,2 Michele Fabrizio,1,2,3 Sandro Sorella,1,2 and Erio Tosatti1,2,3

1 International School for Advanced Studies (SISSA), Via Beirut 2-4, I-34014 Trieste, Italy
2 INFN-Democritos National Simulation Centre, Trieste, Italy.
3 International Centre for Theoretical Physics (ICTP), P.O. Box 586, I-34014 Trieste, Italy.
(Dated: March 22, 2022)

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.

PACS numbers: 71.10.Fd, 71.10.Pm, 71.27.+a, 71.30.+h

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, 3, 4, 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. [2] 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 this defects by allowing H-D correlations just on nearest neighbor sites, [2, 6] 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 of a metallic behavior. [2]

In this Letter we show that this plan can be accomplished with success. In particular, we demonstrate for a specific one-dimensional (1D) model that: (i) non-trivial insulating WFs with or without symmetry breaking do exist; (ii) the MIT, so far well described only in infinite dimensions, [2] is accessible variationally even in finite dimensions. We consider the 1D $t-t'$ Hubbard model

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

(1)

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

Bosonisation [10] and density-matrix renormalization group calculations [11, 12] predict that the ground state at half-filling is an insulator with gapless spin excitations...
with the BCS energy spectrum

$E_q = \frac{\Delta_q}{\sqrt{\epsilon_q^2 + \Delta_q^2}}$, and

$\Delta_q = \Delta_1 \cos(q) + \Delta_2 \cos(2q) + \Delta_3 \cos(3q)$, $\Delta_1$, $\Delta_2$, and $\Delta_3$ being variational parameters. Obviously $|BCS\rangle$ reduces to the Fermi sea for $\Delta_q = 0$. The operator $\mathcal{P} = \mathcal{J} \mathcal{P}_N$, where $\mathcal{P}_N$ projects onto the subspace with fixed number of electrons $N = L$ and $\mathcal{J}$ is the Jastrow factor:

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

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 remark that, in presence of a magnetic flux $\phi \neq 0$, the Jastrow term can acquire a non-centrosymmetric 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, \[13\] will play a relevant role in determining the response to $\phi$. In practice we find it more convenient to discriminate the Mott insulator from the metal through correlation functions which can be calculated in absence of flux, as it is very unhandy to follow the changes of the variational WF due the presence of $\phi$.

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, $w_{i,j} = |w_{i,j}|(-1)^{|i-j|}$. 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

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Spin and charge properties of the C050 WF (top panels), the C051 WF (middle panels), and the C150 WF (bottom panels). Left panels: $N_q/q$ (triangles) and $S_q/q$ (circles) as a function of $q$ for $L = 500$. Right panels: $D_2^z$, $Z_c$, 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: $A_0 = 0.03$, $A_2 = 0.17$ (C050 and C051), $m = 0$, $A_2 = 8.4 \times 10^{-3}$ (C150), $\Delta_1 = 2t$, $\Delta_2 = 1.7t$ (C150 and C050), and $\Delta_1 = \Delta_2 = \Delta_3 = 0$ (C051).
}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{Energy per site $\epsilon$ 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: $Z_s$ for the GWF+$J$ (full circles) and for the GWF (open circles), lines are three parameter fits.
}
\end{figure}
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 to fulfill variationally the f-sum rule. Indeed, if we denote the variational energies of \(|\Psi\rangle\) by \(E_0\) and of \(n_q \langle \Psi \rangle\) by \(E_q\), then we can prove for the optimized \(v_{i,j}\)'s that

\[
\lim_{q \to 0} (E_q - E_0) = \frac{q^2}{2 N_q} \frac{\langle \Psi \mid \sum_{k,\sigma} \partial^2 c_{k,\sigma}^\dagger c_{k,\sigma} \mid \Psi \rangle}{\langle \Psi \langle \Psi \rangle}.
\]

where \(N_q = \langle \Psi | n_{-q} n_q \langle \Psi / \langle \Psi \langle \Psi \rangle\) is the equal-time density-density correlation function. On the assumption that our variational WF \(|\Psi\rangle\) gives a fair description of the actual ground state WF, Eq. 14 allows to infer the behavior of the long wavelength charge excitation spectrum by just analysing 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 \(N_q \sim N_q^0 / (1 + N_q^0 q^2)\). 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 \(\Delta\’s\), it is possible to optimize the full WF by recent developments in the variational Monte Carlo technique. Yet, to afford larger scale simulations, we also assume an analytic parametrization of \(v_{i,j}\):

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

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 \(Z_c = \langle \Psi | \exp \left( \sum_{i,j} j s_i^z s_j^z \right) | \Psi \rangle / \langle \Psi \langle \Psi \rangle\). In the thermodynamic limit, for 1D systems, \(|Z_c| \to 0\) for a metal and \(|Z_c| \to 1\) for an insulator.

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 also the spin excitations are 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” \(Z_s = \langle \Psi | \exp \left( \sum_{i,j} j s_i^z s_j^z \right) | \Psi \rangle / \langle \Psi \langle \Psi \rangle\), \(|Z_s| \to 0\) 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 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. Remarkably, even if the C0S0 BCS WF is not explicitly dimerized, after application of the Jastrow factor, 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 de-
we show the behavior of \( \Delta \) Mott insulator.

One electron band for an insulator- into a perfectly good shown in Fig. 2. Remarkably the long range Jastrow correction, \( \text{WF} \) is equally accurate both at weak and at large \( U/t \), as shown in Fig. 4.

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 \( |Z_c| \rightarrow 0 \) by increasing \( L \), and an insulating phase, where \( |Z_c| \rightarrow 1 \) for \( L \rightarrow \infty \). 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. 3b).

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: \( \Delta_q \) connects only different sublattices (i.e., \( \Delta_q = 0 \)), making \( E_q \) gapped. 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 \( \Delta_q \neq 0 \), although \( |\Delta_q| \) is small, hence \( S_q \sim q^2 \), corresponding to an exponentially decaying spin-spin correlations. By increasing \( U/t \) and entering into the insulating phase there is a fast increase of \( \Delta_2 \), 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 non trivial phase diagram comprising different phases and a MIT. We argue that similar variational WFs with \( v_q \sim 1/q^2 \) could describe non-trivial Mott insulating phases in higher dimensions too, giving the possibility to improve realistic descriptions of Mott insulating compounds. We also believe these wave functions to hold a great potential promise for future attacks to the superconducting phases that result by doping Mott insulators.

This work was partially supported by INFM, by MIUR (COFIN 2003), by FIRB RBAU017S8R004, and by FIRB RBAU10LX5H. F.B. was supported by an INFM research position. We acknowledge useful discussions with C. Castellani, A. Parola, and G. Santoro.

---

[1] N.F. Mott, Proc. Phys. Soc. (London) 62, 416 (1949).
[2] M.C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963).
[3] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. 56, 1490 (1987).
[4] M. Dzierzawa et al., Helv. Phys. Acta 70, 124 (1997).
[5] F. Gebhard, Phys. Rev. B 41, 9452 (1990).
[6] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. 59, 3669 (1990).
[7] P. Fazekas and K. Penc, Int. J. of Mod. Phys. B 1, 1021 (1988).
[8] See however: H. Yokoyama et al., cond-mat/0308264.
[9] A. Georges et al., Rev. Mod. Phys. 68, 13 (1996).
[10] M. Fabrizio, Phys. Rev. B 54, 10054 (1996).
[11] R. Arita et al., Phys. Rev. B 57, 10324 (1998); K. Kuroki et al., J. Phys. Soc. Jpn. 66, 3371 (1997).
[12] S. Daal and R.M. Noack, Phys. Rev. B 61, 1646 (2000).
[13] A.J. Millis and S.N. Coppersmith, Phys. Rev. B 43, 13770 (1991).
[14] L. Reatto and G.V. Chester, Phys. Rev. 155, 88 (1967).
[15] S. Sorella, Phys. Rev. B 64, 024512 (2001).
[16] R. Resta, Phys. Rev. Lett. 80, 1800 (1998).
[17] S. Sorella et al., Phys. Rev. Lett. 88, 117002 (2002).
[18] C. Gros et al., Phys. Rev. B 36, 381 (1987).