From Luttinger liquid to Mott insulator: the correct low-energy description of the one-dimensional Hubbard model by an unbiased variational approach

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We show that a particular class of variational wave functions reproduces the low-energy properties of the Hubbard model in one dimension. Our approach generalizes to finite on-site Coulomb repulsion the fully-projected wave function proposed by Hellberg and Mele [Phys. Rev. Lett. 67, 2080 (1991)] for describing the Luttinger-liquid behavior of the doped t–J model. Within our approach, the long-range Jastrow factor emerges from a careful minimization of the energy, without assuming any parametric form for the long-distance tail. Specifically, in the conducting phase of the Hubbard model at finite hole doping, we obtain the correct power-law behavior of the correlation functions, with the exponents predicted by the Tomonaga-Luttinger theory. By decreasing the doping, the insulating phase is reached with a continuous change of the small-q part of the Jastrow factor.

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I. INTRODUCTION

Electrons confined in one-dimensional (1D) systems exhibit peculiar non-Fermi liquid properties, that are by now rather well understood.¹,² Let us just briefly mention some of them which will be useful for what follows. Due to phase-space limitations, particle-hole excitations in single-band 1D models are exhausted by collective charge and spin modes, which are dynamically independent, realizing what is commonly referred to as spin-charge separation. When these modes are gapless, they propagate as acoustic waves (zero-sounds), hence they can be identified by two parameters, the sound velocity \( u_i \) and a dimensionless stiffness \( K_i \), \( i = \rho \) and \( i = \sigma \) for charge and spin modes, respectively. Sometimes however the interaction opens a gap either in one of these sectors, for instance the charge sector in the Hubbard model at half-filling, or in both of them, like in a spontaneously dimerized chain.

Besides spin-charge separation, another manifestation of the 1D non-Fermi liquid behavior is the power-law decay with anomalous exponents of all correlation functions, when both spin and charge modes are gapless, or just some of them, when one of the two modes is gapped. Although these exponents are generically non universal, they all can be expressed in terms of the above mentioned \( K_\rho \) and \( K_\sigma \). Therefore the finite set of parameters \( u_\rho \), \( u_\sigma \), \( K_\rho \) and \( K_\sigma \) is sufficient to characterize completely the asymptotic low-energy behavior of 1D interacting electron models, similarly to the finite number of parameters which identify the low-energy behavior of Landau-Fermi liquids in higher dimensions.³ Indeed, just in analogy with Fermi liquids, this kind of 1D universal behavior was named “Luttinger liquid” by Haldane.⁴,⁵,⁶

In the case of non interacting electrons \( K_\rho = K_\sigma = 1 \). If spin SU(2) symmetry is unbroken and the spin modes are gapless, \( K_\sigma \) remains one as for free fermions even in the presence of interaction and only \( K_\rho \) parametrizes the anomalous exponents. In particular \( K_\rho \) is smaller than one for repulsive interaction, and greater than one otherwise. When both charge and spin sectors are gapless, the asymptotic expressions of the charge and spin equal-time correlation functions are, apart from possible logarithmic corrections,

\[
\langle n(x)n(0) \rangle \sim \frac{K_\rho}{(\pi x)^2} + A_1 \frac{\cos(2k_F x)}{x^{K_\rho+1}} + A_2 \frac{\cos(4k_F x)}{x^{2K_\rho+1}},
\]

\[
\langle S(x) \cdot S(0) \rangle \sim \frac{1}{(\pi x)^2} + B \frac{\cos(2k_F x)}{x^{K_\rho+1}},
\]

where \( n(x) \) and \( S(x) \) are the charge and spin density operators at position \( x \), \( k_F \) is the Fermi momentum, \( A_1 \), \( A_2 \), and \( B \) are model-dependent constants. Analogously the singlet (and triplet) pairing correlations behave as

\[
\langle \Delta^\dagger(x)\Delta(0) \rangle \sim \frac{1}{x^{K_\rho+1}},
\]

where \( \Delta^\dagger(x) \) creates a singlet (or triplet) pair at position \( x \). Finally, the non-Fermi liquid character of 1D interacting models shows up transparently in the momentum distribution function near the Fermi momentum:

\[
n_k - n_{k_F} \sim -\text{sign}(k - k_F)(|k - k_F|^\theta),
\]

where \( \theta \) is again expressed in terms of \( K_\rho \) through the relation \( \theta = (K_\rho - K_\rho^{-1} - 2)/4 \). For any finite interaction \( K_\rho \neq 1 \), hence the momentum distribution function has a power-law singularity at the Fermi level, in contrast to the finite jump characteristic of Fermi liquids. It is worth mentioning that, for non-frustrated models with repulsive interaction, the insulating phase at half-filling is characterized by all correlation functions decaying exponentially to zero apart from the spin-spin ones, which still decay as a power-law, formally like in (4) with \( K_\rho = 0 \).
The actual value of the parameter \( K \rho \) depends upon the particular microscopic model, through the form and the strength of the interaction as well as the electron doping. For simple Hamiltonians \( K \rho \) can be explicitly calculated by the Bethe ansatz or by exact diagonalization on small systems.

Although analytical techniques, especially bosonization, give important insights into the low-energy properties of 1D systems, both in gapless and in gapped phases, yet they do not provide a simple representation of the ground-state wave function (WF). Even in those simple models which are solvable by Bethe ansatz, the actual ground state WF turns out to be very difficult to interpret and to deal with. In the Hubbard model, for instance, the ground state WF is very involved within the Bethe ansatz formalism and only in the strong-coupling limit it is possible to obtain significant simplifications because of the explicit factorization of the WF into a charge and a spin part. For this reason there have been many attempts aimed to find out approximate variational WFs, which, from one side, could correctly reproduce the peculiar properties of 1D systems but, from the other side, could also give a transparent interpretation of their physical properties. For instance it has been shown that the strong-coupling limit of the Hubbard model, where the on-site Coulomb repulsion \( U \) prohibits doubly occupied sites, is well described by a projected Slater determinant. In particular the large-\( U \) conducting phase at finite hole doping has been found to be properly represented through a fully-projected Gutzwiller WF supplemented by a long-range density-density Jastrow factor. The latter is a crucial ingredient which allows to recover the anomalous power-law behavior of the correlation functions. Indeed any short-range Jastrow factor cannot reproduce the correct Luttinger-liquid behavior since it is unable to affect the low-energy physics. For instance, it is well known that the simple Gutzwiller WF has a finite jump in the momentum distribution function which is certainly incorrect in 1D.

In this paper we generalize this approach to a finite Coulomb repulsion \( U \), namely to the case where charge fluctuations are still allowed. We show that even at finite \( U \) it is possible to design a consistent WF, which can faithfully describe the evolution from the Luttinger-liquid behavior at finite hole doping to the Mott insulating phase at half-filling. Again the crucial ingredient turns out to be a density-density Jastrow factor applied to a simple Slater determinant. More specifically, we apply this variational WF to analyze the single-band Hubbard model. Thanks to the recent improvements in the energy minimization schemes for correlated WFs, the long-range tail of the Jastrow factor can be determined very accurately, without imposing any parametric form, even if the change of its tail may contribute to a very tiny energy gain. We will show that the low-energy properties of the Hubbard model are correctly reproduced within this unbiased variational approach.

The paper is organized as follows: in Sec. II we introduce the model and the physical quantities we are interested in and in Sec. III we present and discuss the results.

### II. THE MODEL

As we previously mentioned, in this work we aim to design a variational WF which is equally accurate for both weak and strong Coulomb repulsion. For sake of simplicity, we will test the quality of this WF in the well-known single-band Hubbard model on a finite chain with \( L \) sites, \( N \) particles and periodic boundary conditions. The Hamiltonian is

\[
H = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + h.c., \tag{5}
\]

where we use the standard notations in which \( c_{i,\sigma} \) (\( c_{i,\sigma}^\dagger \)) destroys (creates) an electron with spin \( \sigma \) at the site \( i \) and \( n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma} \).

The variational ansatz for the ground state WF is

\[
|\Psi_N\rangle = \mathcal{J}(D), \tag{6}
\]

where \( \mathcal{J} \) is a Jastrow factor and \( |D\rangle \) an uncorrelated Slater determinant, that, for simplicity, we assume to be the \( N \)-electron Fermi sea of the tight-binding model with dispersion \( \epsilon_k = -2t \cos k \). Since spin SU(2) is unbroken, there is no need to introduce a spin-spin Jastrow factor, because a free-electron determinant already provides the correct value \( K_\sigma = 1 \). Therefore, in order to preserve all the symmetries of the Hamiltonian, \( \mathcal{J} \) is a purely density-density correlator written in term of the density operator \( n_i = \sum_\sigma c_{i,\sigma}^\dagger c_{i,\sigma} \) as

\[
\mathcal{J} = \exp \left[ -\frac{1}{2} \sum_{ij} v_{ij} n_i n_j \right],
\]
where, due to translation and inversion symmetry, \( v_{ij} \) can be described by using \( L/2 \) independent variational parameters \( v(|i-j|) = v_{ij} \); in particular, \( v(L/2) \) can be set to zero since, due to the conservation of the total number of particles, \( v_{ij} \to v_{ij} + \text{const} \) provides only an irrelevant normalization factor in the WF.

A more sophisticated possibility would have been to choose \(|\mathcal{D}\rangle\) as the ground state of a mean-field BCS Hamiltonian projected onto a fixed number of particles. For the simple Hubbard model of Eq. (4), the latter ansatz leads to a slightly lower energy, without modifying the low-energy properties, and, therefore, it will not be considered in the following. It should be mentioned, however, that in presence of a large next-nearest-neighbor hopping term, a gap in the BCS mean field Hamiltonian may open, leading to translational symmetry breaking at half-filling or to a phase of singlet pairs with dominant superconducting correlations at finite doping.\(^{18,19}\)

Summarizing, all the variational parameters are contained in the Jastrow coefficients \( v(|i-j|) \) for all the \( L/2 \) independent distances in real space and are calculated by a full energy minimization, without assuming any particular parametric form.

Important quantities to assess the nature of the ground state are the static structure factor for the charge:

\[
N_q = \frac{\langle \Psi_N | n_{-q} n_q | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle},
\]

and similarly for the spin:

\[
S_q = \frac{\langle \Psi_N | S^z_{-q} S^z_q | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle},
\]

where \( n_q \) and \( S^z_q \) are the Fourier transform of the local density and spin operators.

Another quantity that gives information on the WF is the quasiparticle weight:

\[
Z_k = \frac{|\langle \Psi_{N-1} | c_{k,\sigma} | \Psi_N \rangle|^2}{\langle \Psi_N | \Psi_N \rangle \langle \Psi_{N-1} | \Psi_{N-1} \rangle},
\]

where \(|\Psi_N\rangle\) and \(|\Psi_{N-1}\rangle\) are the WFs with \( N \) and \((N-1)\) particles, \( c_{k,\sigma} \) is the annihilation operator of a particle of momentum \( k \) and spin \( \sigma \). The \((N-1)\)-particle state is obtained by the \( N\)-particle one by removing an electron from the Slater determinant, i.e., \(|\Psi_{N-1}\rangle = \mathcal{F} c_{k,\sigma} |\mathcal{D}\rangle\). In a Fermi liquid \( Z_k \) is finite in the thermodynamic limit signaling the existence of coherent quasiparticles. On the contrary a non-Fermi liquid phase without quasiparticles is identified by a vanishing \( Z_k \).
III. RESULTS AND DISCUSSION

The important role of the Jastrow factor has been already discussed by Hellberg and Mele in the context of the 1D $t-J$ model. In this case, it is possible to show analytically that the momentum distribution function of the variational WF has an algebraic singularity at $k_F$, with an exponent related to the strength of the Jastrow factor. Recently, we have shown that in the 1D Hubbard model a suitable long-range Jastrow can also drive a metallic Slater determinant into an insulating phase and that, in the limit of small momenta, the Fourier transform of the Jastrow parameters $v_q$ are related to the charge-structure factor. In particular, in the conducting regime and for small momenta a random-phase-approximation (RPA) expression holds:

$$N_q \sim \frac{N_q^0}{1 + 2v_qN_q^0},$$

where we indicate with $N_q^0$ the charge structure factor of the WF without $\mathcal{J}$. For a conducting Slater determinant, like the free-electron state, $N_q^0 = |q|/\pi$ for small $q$. For a non-vanishing hole doping $\delta$ and interaction $U/t$, by optimizing the variational WF, we obtain that the Jastrow factor is singular, i.e., $v_q \sim 1/|q|$. This fact is crucial to recover the correct low-$q$ behavior of $N_q$, whose linear slope is renormalized by the interaction, leading to $N_q \sim K_{\rho} |q|/\pi$. Therefore, the Jastrow factor has to be intrinsically long-range. According to the RPA expression, a more singular Jastrow term $v_q \sim 1/|q|^2$ is needed to bring the system into the insulating phase at half-filling. In 1D, such a Jastrow factor leads to a confined phase, where perturbation theory does not apply, and, therefore, also the RPA is expected to fail. Nonetheless, it turns out that, also within the insulating phase, the small-$q$ behavior of $N(q)$ is qualitatively reproduced by Eq. (10) and a more accurate empirical expression is given by:

$$N_q \sim \frac{N_q^0}{1 + \beta v_q N_q^0},$$

where $\beta > 2$ is a constant that strongly depends upon the electronic interaction. In Fig. 4, we report $\beta$ for different values of the ratio $U/t$ at half-filling, and, for comparison, also at quarter-filling, where the value $\beta = 2$ is recovered, according to Eq. (10). In the half-filled insulating phase, although for $q \to 0$ we have that $N_q \sim q^2$, the coefficient of the quadratic term is not simply related to the Jastrow factor. In this case, it is important to emphasize that the presence of the singular Jastrow factor $v_q \sim 1/|q|^2$ determines a qualitative change of the static structure factor $N(q)$ even at large momenta $q \sim 2k_F = \pi$. In fact, the charge structure factor $N^0(q)$ for the free Fermi gas is characterized by a cusp at $q \sim 2k_F$, which is responsible of the well-known Friedel oscillations in a metal and the RPA expression cannot remove this feature. On the other hand, a true insulating phase does not possess this singularity and, indeed, as shown in Fig. 2, the charge structure factor $N(q)$ for the WF containing a singular Jastrow factor shows a smooth behavior around $q \sim \pi$. This clearly indicates the non-perturbative and highly non-trivial effect implied by the formation of a confined state in this correlated WF between empty sites (holons) and doubly occupied ones (doubilons).

In order to demonstrate that the WF is able to capture the Luttinger-liquid metallic properties, we consider the quarter-filling case. In Fig. 3, we show the charge and spin structure factor for different values of $U/t$. For small momenta, the linear slope of $N_q$ is renormalized with respect to the non-interacting value, leading to $N_q \sim K_{\rho} |q|/\pi$. On the other hand, the small-$q$ behavior of $S_q$ is not affected by the interaction and we have that $S_q \sim |q|/4\pi$. Notice that, in the presence of a strong interaction, the two singularities at $2k_F$ and $4k_F$ are clearly visible in $N_q$, whereas in $S_q$ only the singularity at $2k_F$ can be detected. From the small-$q$ linear part of $N_q$, it is possible to extract the value of $K_{\rho}$ (see Table I), which is in very good agreement with the exact one. It is important to emphasize that the relationships among exponents of different correlation functions are correctly reproduced by our variational WF. Indeed, we can compare the value of the exponent $\theta$ found from a direct evaluation of the quasiparticle weight at $k = k_F$, i.e., $Z_k \sim 1/L^\theta$ (see Fig. 4), with the one obtained with $\theta = (K_{\rho} + K_{\rho}^{-1} - 2)/4$ by using the value of $K_{\rho}$ extracted from the linear slope of $N_q$. As reported in Table I, we obtain an excellent agreement for the values of the interaction $U/t$ considered. Finally, we can also calculate the singlet pairing correlations:

$$P(r) = \frac{1}{L} \sum_i \langle \Psi_N | \Delta_{i+r} \Delta_i | \Psi_N \rangle,$$
TABLE I: Critical exponents for the 1D Hubbard model at quarter-filling: $K_p$ is found from the low-$q$ behavior of $N_q$, $\theta_c = (K_p + K_p^{-1} - 2)/2$, and $\alpha$ is found by fitting $Z_\theta$ with $Z_\theta \sim 1/L^\alpha$. The last two columns refer to the critical exponent of the pairing correlations: $\alpha$ is found from the pairing correlation at the maximum distance $P(L/2) \sim 1/L^\alpha$ and $\alpha_c = K_p^{-1} + 1$. In the first column, we report the exact value of $K_p$.

| $U/t$ | $K_p^{\text{exact}}$ | $K_p$ | $\theta_c$ | $\alpha$ | $\alpha_c$ |
|-------|-----------------------|-------|-------------|----------|----------|
| 4     | 0.711                 | 0.705(3) | 0.031(5) | 0.031(3) | 2.1(1)  | 2.42(6) |
| 10    | 0.594                 | 0.595(3) | 0.078(5) | 0.072(3) | 2.4(1)  | 2.68(9) |
| 18    | 0.551                 | 0.550(3) | 0.097(5) | 0.092(3) | 2.5(2)  | 2.82(9) |

In order to calculate the exponent $\alpha$, we report in Fig. 6 (right panel), the case of doping the exact relation $\alpha = K_p^{-1} + 1$. Nonetheless, the results reported in Table I are rather satisfactory and not too far from the ones obtained with $\alpha = K_p^{-1} + 1$. In the first column, we report the exact value of $K_p$.

\[ \Delta_i = c_{i,\uparrow}^\dagger c_{i+1,\downarrow} - c_{i+1,\uparrow}^\dagger c_{i,\downarrow} \]  

where $\Delta_i$ creates a singlet pair of electrons at nearest neighbors. In order to calculate the exponent $\alpha$ related to the decay of $P(r) \sim 1/r^\alpha$, we consider the pairing correlation at the maximum distance $P(L/2)$ for different sizes, see Fig. 3. In this case, the signal is very small and a precise determination of the critical exponent is quite difficult. Nonetheless, the results reported in Table I are rather satisfactory and not too far from the ones obtained with the exact relation $\alpha = K_p^{-1} + 1$.

Let us now consider how the insulating case is reached by decreasing the hole concentration. First of all, it should be mentioned that, not too close to the insulating phase at half-filling, the charge and spin structure factor have small size effects and, therefore, reliable calculations are possible even without using too large $L$. As an example, we report in Fig. 4 (right panel), the case of doping $\delta = 2/11$, where we can see that there are no appreciable differences in $N_q$ from $L = 22$ to $L = 154$.

In the doped region, the system is always conducting, $N_q$ having a linear behavior for small momenta, with a slope that depends upon $U/t$ and $\delta$. For sufficiently small hole doping, it turns out that the linear regime is limited to a small window around $q = 0$, whereas for larger momenta, $N_q$ acquires a finite curvature, see Fig. 7 (left panel). The two different regimes are separated by the singularity at $q = 4k_F = 2\pi\delta$, and, therefore, by decreasing $\delta$, the width of the linear regime shrinks, the slope being almost constant. Therefore, we arrive at the empirical result:

\[ N_q \sim \frac{K_p |q|}{\pi} \Theta(4k_F - q) + (c + q^2) \Theta(q - 4k_F), \]  

where $k_F = (1 - \delta) \pi/2$, $\Theta(x)$ indicates the Heaviside step function and $c$ is a constant determined by imposing continuity of $N_q$ at $q = 4k_F$. This singular behavior, with the kink at $q = 4k_F$, is entirely due to correlation and it is compatible with the exact result that $K_p$ remains finite, more precisely $K_p \sim 1/2$, for $\delta \to 0$. It is important to stress that, by approaching half-filling, the width of the linear regime shrinks with doping and reduces to zero for $\delta \to 0$.

For completeness, we report in Fig. 7 the form of the Jastrow factor at half-filling and for small concentration of holes considered in Fig. 8. Starting from the insulating phase, upon doping, $v_q$ moves away from $v_q \sim 1/q^2$, and becomes less singular, i.e., $v_q \sim 1/|q|$. Clearly, at very small doping, the size effects affect the small-$q$ part, and, in particular, for the smallest momentum we can have some deviations from the expected $v_q \sim 1/|q|$ behavior.

The correct minimization of the Jastrow factor is particularly important for having an accurate description of $Z_k$, especially when approaching half-filling. Indeed, in this case, the Jastrow factor for one hole is considerably different from the insulating one for small $q$’s (see Fig. 8), and one has to optimize both WFs with $N$ and $(N - 1)$ particles. This difference can be appreciated by considering $\Sigma_L = 1/L \sum_{q \neq 0} v_q$, which diverges linearly with the system size $L$ if $v_q \sim 1/q^2$ and, instead, diverges only logarithmically if $v_q \sim 1/q$. In Fig. 8 we report $\Sigma_L$ as
a function of $L$ for the insulating state and for the one-hole case: the difference between the two cases clearly demonstrates the different behavior of $v_q$ for small momenta. By a careful minimization of both the WFs, it is possible to recover the result that $\theta = 1/2$ independently of $U/t$. Indeed, upon increasing $U/t$, our variational WF gives a rather accurate description of the insulating phase, the size effects being strongly reduced due to the small correlation length expected at large $U/t$. In this limit, we obtain a reasonable good agreement with the exact exponent for the quasiparticle weight (see Fig. 9): $\theta = 0.60 \pm 0.05$ and $\theta = 0.55 \pm 0.05$ for $U/t = 10$ and $U/t = 18$, respectively. On the other hand, it should be mentioned that a naive calculation with a singular Jastrow $v_q \sim 1/q^2$ for both WFs would lead to a wrong exponential behavior of the quasiparticle weight.

In conclusion, we have shown that an accurate description of the charge and spin properties of the 1D Hubbard model is possible within the simple variational ansatz given by Eq. (10). The main ingredient of the variational WF is represented by a singular density-density Jastrow factor, whose long-range part determines the low-energy behavior of the correlation functions and can be found by optimization of the energy. In the conducting regime, the small-$q$ Fourier transform of the density-density Jastrow term diverges like $v_q \sim 1/|q|$, implying the correct renormalization of the charge structure factor for small momenta, i.e., $N_q \sim K_q|q|/\pi$. By approaching the insulating phase and by decreasing the hole doping, the Jastrow factor modifies its small-$q$ part and, eventually, it acquires a more singular behavior like $v_q \sim 1/q^2$. Within this context, it is possible to obtain a consistent scenario, where we recover the correct relationships among the exponents of different physical quantities. Obviously, our approach works due to the quality of the variational ansatz in 1D. Despite the difficulty to define very accurate WFs in higher spatial dimensions, the possibility to obtain the correct low-energy description of a Hamiltonian by using a simple optimization of the energy is very appealing and work is in progress for the generalization of this ansatz to two-dimensional systems, where no exact solutions are available.

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