Exact Jastrow-Slater wave function for the one-dimensional Luttinger model

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We show that it is possible to describe the ground state of the Luttinger model in terms of a Jastrow-Slater wave function. Moreover, our findings reveal that one-particle excitations and their corresponding dynamics can be faithfully represented only when a Jastrow factor of a similar form is applied to a coherent superposition of many Slater determinants. We discuss the possible relevance of this approach for the theoretical description of photoemission spectra in higher dimensionality, where the present wave function can be straightforwardly generalized and can be used as a variational ansatz, which is exact for the one-dimensional (1D) Luttinger model.

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I. INTRODUCTION

Recently, much progress has been made for understanding the crucial role of strong electron correlation in photoemission spectra, namely, the properties of the one-particle excitations and the corresponding dynamical Green's function.[1,2] This topic has attracted a renewed attention due to the impressive progress in the energy and momentum resolution of angle-resolved photoemission experiments, which confirm spin charge separation in quasi-one-dimensional systems,[3] one of the most important effects induced by strong electron correlation.

From the theoretical point of view, the pioneer work for the dynamical Green's function dates to 1970,[4] which showed the absence of coherence in the strongly correlated regime of the Hubbard model. Later the self-consistent Born approximation[5] was introduced, providing a surprisingly accurate description of the single hole dynamics in lattice models, such as the *t-J* model relevant for high-Tc superconductivity. In this context, P. W. Anderson suggested that the Fermi-liquid picture could be violated not only in one dimension but also in higher dimensionality (D), and especially in 2D. From this speculation, a tremendous amount of work has been devoted to the subject, starting from the reconsideration of the dynamical properties of a single hole in a quantum antiferromagnet,[6–8] and the detailed analysis of the dynamical properties of a single minority spin electron in a bath of fully polarized electrons with opposite spin.[9–12]

Finally, an important progress was achieved by the dynamical mean-field theory (DMFT) that was able to describe the important feature of the Kondo resonance when approaching metal-insulator transition of the half-filled Hubbard model in infinite dimensions.[13,14] In this case it was also shown that the single-particle excitations in the proximity of the Mott transition may be highly nontrivial even in the metallic side. In particular at low energy, a Kondo resonance appears between the expected upper and lower Hubbard bands and determines the coherent quasiparticle weight of the Fermi-liquid metal, which vanishes exactly at the metal-insulator transition. The predictions of DMFT have been confirmed by many experiments. For instance, recently, Mott transition in vanadium oxide was clearly explained.[15] It represents also a theory capable of characterizing the two energy scales found in photoemission experiments of HTc compounds.[16] However, the dynamical properties predicted by this theory are not well understood outside the DMFT formalism. In particular, it should be very important to characterize the anomalous low-energy excitations determining the Kondo resonance from the direct solution of the Schrodinger equation, namely by direct inspection of the eigenfunctions of strongly correlated models such as the Hubbard model or the *t-J* model.

In this work, we consider a much less ambitious task and we use an approach that can provide useful insights on the exact ground-state wave function and excitations. We consider the well-known Jastrow-Slater wave function that has been used successfully in several correlated systems and we focus our analysis in one dimension where analytic calculations are possible and numerical works have confirmed the impressive accuracy of the Jastrow-Slater wave function on several strongly correlated models.[17–19] This wave function can be generally written as a product of a Slater determinant, characterizing free electrons, times the so-called "Jastrow factor" J that appropriately weights the electron configurations (e.g., suppressing the wave function amplitude when the electrons are too close), in order to describe electron correlation. Indeed, by a lengthy but straightforward derivation, we found that the exact ground state (GS) of the Luttinger model can be written as a Jastrow-Slater wave function. Moreover, not only the ground state, but also single-particle excitations can be written in a suitable Jastrow-Slater form. It is interesting that in this case, *many* Slater determinants have to be considered, with an appropriate change of the Jastrow factor. The results we obtained are in perfect agreement with the Luttinger liquid theory in one dimension (1D) and the extension of the wave-function excitations to higher dimensions seem to imply the same Kondo-type resonance scenario obtained by means of DMFT, although at present this is just a speculative conclusion and a further numerical work is necessary to verify it.

This paper is organized as follows: In Sec. II, we review the Luttinger model and later show how the one-dimensional fermionic Luttinger model Hamiltonian can be reduced to a quadratic Bose Hamiltonian by means of the so-called bosonization technique. In Sec. III, we show how the stan-

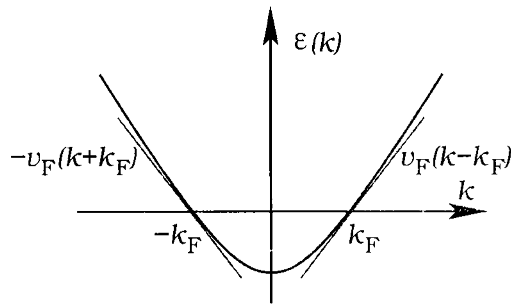

FIG. 1. Linearization of the realistic dispersion of a one-dimensional Fermi system about the Fermi points k_F and $-k_F$.

dard Bogoliubov transformation can be used to diagonalize the quadratic Bose Hamiltonian in order to obtain an exact ground state of the Luttinger model. In Sec. IV, we show that the ground state of the Luttinger model can be rewritten as a Jastrow wave function, whereas in Sec. V, the single-particle excitations of the Luttinger model are given with an explicit Jastrow multi-Slater wave function. Finally in Sec. VI, we study the dynamics of a single particle added to the right branch of the Fermi sea.

II. FORMALISM

We consider the one-dimensional Luttinger model following the work of Lieb and Mattis[20] with the notations given in a later work:[21]

$$H = v_F \sum_k [(k-k_F)\psi_+^\dagger(k)\psi_+(k) - (k+k_F)\psi_-^\dagger(k)\psi_-(k)] + 1/L \int_0^L \int_0^L dx \; dx' u(x-x')N(x)N(x'), \tag{1}$$

where v_F is the Fermi velocity describing a linear band around the Fermi momentum k_F and u is a generic interaction which depends only on the distance between electrons. In this linearization scheme (see Fig. 1), the allowed momenta in the right (+) and left (−) branches satisfy the usual quantization conditions $k = \frac{2\pi}{L} \times$ any integer, valid for periodic boundary conditions, assumed here and henceforth. These two branches are then extended to $-\infty, +\infty$ by means of two fermionic fields $\psi_\pm$ with their appropriate Fourier transforms

$$\psi_\pm(k) = \frac{1}{\sqrt{L}} \int_0^L dx \; e^{ikx}\psi_\pm(x). \tag{2}$$

These fields define a local charge operator $N(x)=N_+(x)+N_-(x)$ by means of the following contributions coming from the right and left branches:

$$\begin{cases} N_+(x) = \psi_+^\dagger(x)\psi_+(x) - \langle \psi_+^\dagger(x)\psi_+(x)\rangle \\ N_-(x) = \psi_-^\dagger(x)\psi_-(x) - \langle \psi_-^\dagger(x)\psi_-(x)\rangle . \end{cases} \tag{3}$$

The basic relations that make the Luttinger model exactly solvable are given by the nontrivial commutation rules of these left and right branches density operators:[20]

$$[N_\pm(q), \; N_\pm(-q)] = \mp \frac{Lq}{2\pi}, \tag{4}$$

where

$$N_\pm(q) = \int_0^L dx e^{-iqx} N_\pm(x). \tag{5}$$

After this important observation, it is possible to represent these density operators in terms of canonically conjugate bosonic fields Φ and Π:[22]

$$\begin{cases} N_+(x) = \frac{1}{\sqrt{4\pi}}[\Pi(x) + \partial_x\Phi(x)] \\ N_-(x) = -\frac{1}{\sqrt{4\pi}}[\Pi(x) - \partial_x\Phi(x)] \end{cases} \tag{6}$$

with

$$[\Phi(x), \; \Pi(x')] = i\delta(x-x'). \tag{7}$$

The total density operator $N(x)$ can be written as

$$N(x) = N_+(x) + N_-(x) = \frac{1}{\sqrt{\pi}}\partial_x\Phi(x). \tag{8}$$

Now it takes just a little more algebra to show that the fermionic Luttinger Hamiltonian [Eq. (1)] can be expressed in terms of these bosonic fields where it assumes the following canonical harmonic form:

$$H = \frac{v_s}{2}\int_0^L dx \left\{ K\Pi^2(x) + \frac{1}{K}[\partial_x\Phi(x)]^2 \right\}, \tag{9}$$

where v_s is the renormalized Fermi velocity and K is the Luttinger parameter that can be simply expressed in terms of v_F and the $k=0$ component of the interaction u.[20,23] In principle, the mapping of Eq. (1) to the harmonic Hamiltonian [Eq. (9)] is exact only if the interaction is assumed to be delta-like, but it can be easily generalized to a momentum-dependent coupling constant u, as it was done for instance in Ref. 20. This canonical form given in Eq. (9) embodies the entire low-energy physics of the so-called Luttinger liquids and due to its simplicity, can be solved explicitly. To this purpose, we introduce Fourier transforms of the bosonic fields:

$$\begin{cases} \Phi_k = \frac{1}{\sqrt{L}}\int_0^L dx\Phi(x)e^{-ikx} \leftrightarrow \Phi(x) = \frac{1}{\sqrt{L}}\sum_k \Phi_k e^{ikx} \\ \Pi_k = \frac{1}{\sqrt{L}}\int_0^L dx\Pi(x)e^{ikx} \leftrightarrow \Pi(x) = \frac{1}{\sqrt{L}}\sum_k \Pi_k e^{-ikx}. \end{cases} \tag{10}$$

By making use of the relations in Eq. (10), Eq. (9) becomes

$$H = \frac{v_s}{2}\sum_k \left[K(\Pi_k\Pi_{-k}) + \frac{1}{K}(k^2\Phi_k\Phi_{-k}) \right], \tag{11}$$

which expresses the Hamiltonian in terms of "normal coordinates," Φ_k and Π_k. Notice that we have essentially reduced the problem to a single harmonic oscillator for each given momentum. The next step merely repeats the procedure carried out for a single harmonic oscillator. We define a set of conjugate creation and annihilation operators:

$$\Phi_k = \frac{1}{\sqrt{2|k|}}[a_k^\dagger + a_{-k}],$$

$$\Pi_k = i\sqrt{\frac{|k|}{2}}[a_{-k}^\dagger - a_k]. \tag{12}$$

Now substituting Eq. (12) into Eq. (11), we obtain the standard quadratic Bose Hamiltonian,

$$H = \sum_k \epsilon_k\left[a_k^\dagger a_k + \frac{1}{2}\right] - \sum_k \frac{\gamma_k}{2}[a_k^\dagger a_{-k}^\dagger + a_k a_{-k}], \tag{13}$$

where the functions γ_k and ϵ_k are given by

$$\epsilon_k = \frac{v_s|k|}{2}\left[K + \frac{1}{K}\right],$$

$$\gamma_k = \frac{v_s|k|}{2}\left[K - \frac{1}{K}\right]. \tag{14}$$

Hamiltonian (13) contains only excitations in a given sector of particle number because in this section, we are interested in determining only the GS.

III. EXACT SOLUTION OF THE MODEL BY BOGOLIUBOV TRANSFORMATION

We will use the following unitary transformation which is the standard Bogoliubov transformation to diagonalize Eq. (13):

$$U = e^{iS}, \tag{15}$$

where S has been obtained in Ref. 20:

$$S = i\sum_{q>0} \theta_q a_q^\dagger a_{-q}^\dagger + \text{H.c.}.$$

It is easy to show that

$$U a_q U^\dagger = \cosh(\theta_q)a_q + \sinh(\theta_q)a_{-q}^\dagger. \tag{16}$$

It follows immediately that the transformed Hamiltonian $H \to UHU^\dagger$ assumes the diagonal form

$$UHU^\dagger = \sum_{k|E_k\rangle 0}\left(E_k a_k^\dagger a_k + \frac{\epsilon_k}{2}\right), \tag{17}$$

where

$$E_k = \sqrt{\epsilon_k^2 - \gamma_k^2} = v_s|k|. \tag{18}$$

This can only be possible provided

$$\tanh(\theta_k) = -\frac{\gamma_k}{\epsilon_k + \sqrt{\epsilon_k^2 - \gamma_k^2}}, \tag{19}$$

namely that θ_k does not depend on the momentum k and is simply given in terms of the Luttinger parameter K,

$$e^{-2\theta_k} = K.$$

After this unitary transformation, the ground state cannot contain any boson excitation because $E_k > 0$, implying that in this representation, the ground state coincides with the vacuum $|0\rangle$, namely the noninteracting Fermi sea $|FS\rangle$, the unique state of the Luttinger model corresponding to the vacuum of the canonical operators a_k $(a_k|FS\rangle = 0, \ \forall k)$.

It follows that in the original representation, the GS of the Bose Hamiltonian is simply given by $U|FS\rangle$ and can be written in the following general form up to an irrelevant normalization constant:

$$|GS\rangle = \exp\left\{\sum_{q>0} f_q a_q^\dagger a_{-q}^\dagger\right\}|FS\rangle. \tag{20}$$

Here, f_q is a function whose analytic form will be determined in what follows. In order to determine f_q, we notice that $Ua_kU^\dagger$ must annihilate the GS $U|FS\rangle$ $\forall k$. After substituting $U|FS\rangle$ with the ansatz [Eq. (20)] and by means of Eq. (16), we obtain a simple equation

$$a_{-k}^\dagger[\cosh(\theta_k)f_k + \sinh(\theta_k)]|GS\rangle = 0 \tag{21}$$

which can be solved to get

$$f_k = -\tanh(\theta_k) = \frac{\gamma_k}{\epsilon_k + \sqrt{\epsilon_k^2 - \gamma_k^2}}. \tag{22}$$

By replacing the quantities ϵ_k and γ_k from Eq. (14) into Eq. (22), we obtain the pairing function in terms of the Luttinger interaction parameter K:

$$f_k = \frac{\sqrt{K} - \frac{1}{\sqrt{K}}}{\sqrt{K} + \frac{1}{\sqrt{K}}}. \tag{23}$$

When $K=1$ (i.e., in the noninteracting regime), the pairing function f_k correctly vanishes, and the ground state is just the Fermi sea $|FS\rangle$.

IV. GROUND STATE OF THE LUTTINGER MODEL BY THE JASTROW-SLATER WAVE FUNCTION

In this section, we show that the ground state of the Luttinger model is a Jastrow-Slater wave function, i.e., ground state (20) can be rewritten as a Jastrow wave function $|\psi_J\rangle$:

$$|\psi_J\rangle = e^{-1/2\Sigma_q v_q N_q N_{-q}}|FS\rangle, \tag{24}$$

where $|FS\rangle$ is the free Fermi sea,

$$N_q = i\frac{q}{\sqrt{\pi}}\Phi_q = iq\sqrt{\frac{1}{2\pi|q|}}(a_q^\dagger + a_{-q}), \tag{25}$$

and v_q are the momentum-dependent parameters.

Henceforth we assume that $v_q \geq 0$ and that $v_q = 0$ for $q = 0$, because the total charge $\int_0^L dx N(x)$ is conserved. In this way we will obtain the analytic form of the Jastrow parameters (v_q) as functions of the pairing amplitude f_q, by requiring that

$$e^{-\{\Sigma_{q>0}v_q N_q N_{-q}\}}|FS\rangle = R_\alpha e^{\{\Sigma_{k>0} f_k a_k^\dagger a_{-k}^\dagger\}}|FS\rangle, \quad (26)$$

where R_α is an overall constant which depends only on f_q. In the following derivation we do not even need to assume that the pairing function f_k is constant.

Let us first introduce the Hubbard Stratonovich transformation for the Jastrow factor:

$$e^{-\{\Sigma_{q>0}v_q N_q N_{-q}\}} = \int \prod_{q>0} \frac{dz_q}{\pi} e^{-|z_q|^2 + \sqrt{v_q}(z_q N_q - z_q^* N_{-q})}. \quad (27)$$

Using Eq. (25), the right-hand side of the above equation simplifies to

$$e^{-\{\Sigma_{q>0}v_q N_q N_{-q}\}} = \int \prod_{q>0} \frac{dz_q}{\pi} e^{-|z_q|^2 + A_q + B_q}, \quad (28)$$

where

$$A_q = iq\sqrt{\frac{v_q}{2\pi|q|}}(a_q^\dagger z_q + a_{-q}^\dagger z_q^*), \quad (29)$$

$$B_q = iq\sqrt{\frac{v_q}{2\pi|q|}}(a_{-q} z_q + a_q z_q^*). \quad (30)$$

Now using the Baker-Haussdorf-Campbell formula $e^{A_q+B_q} = e^{A_q}e^{B_q}e^{-1/2[A_q,B_q]}$ (valid if $[A_q,[A_q,B_q]] = [B_q,[A_q,B_q]] = 0$ as in this case), the commutator in the previous expression can be explicitly evaluated and it is a constant:

$$-\frac{1}{2}[A_q,B_q] = -\frac{|v_q||q|}{2\pi}|z_q|^2. \quad (31)$$

On the other hand, $e^{B_q}|FS\rangle = |FS\rangle$ because all nonvanishing powers of B_q annihilate the vacuum. Thus, we obtain the following equation after applying operator (28) to $|FS\rangle$:

$$e^{-\{\Sigma_{q>0}v_q N_q N_{-q}\}}|FS\rangle = \int \prod_{q>0} \frac{dz_q}{\pi} e^{-|z_q|^2(1+\alpha_q)} e^{A_q}|FS\rangle, \quad (32)$$

where

$$\alpha_q = \frac{|q|v_q}{2\pi} > 0. \quad (33)$$

By performing the remaining simple Hubbard-Statonovich transformation integral we obtain

$$|\psi_J\rangle = R_\alpha e^{-\Sigma_{q>0}\alpha_q/1+\alpha_q a_q^\dagger a_{-q}^\dagger}|FS\rangle,$$

where

$$R_\alpha = \prod_{q>0} \frac{1}{1+\alpha_q}. \quad (34)$$

Notice that this constant can be infinite if v_q does not decay sufficiently fast for large q. The divergence in the infinite product can generally be removed by introducing a large momentum cutoff, e.g., $|q| < \Lambda_{\rm cut}$, and taking into account that R_α is just an overall normalization constant that does not change any physical expectation value even when the cutoff is sent to infinity.

Now by a direct comparison with Eq. (26), we obtain that the Jastrow wave function ψ_J is the ground state of the Luttinger model if and only if

$$\frac{\alpha_q}{1+\alpha_q} = -f_q = \frac{\frac{1}{\sqrt{K}} - \sqrt{K}}{\sqrt{K} + \frac{1}{\sqrt{K}}}. \quad (35)$$

It follows immediately from the above equation that for $K < 1$, the ground-state momentum dependence of the Jastrow parameters can be expressed as

$$v_q = \frac{\pi}{|q|}\left(\frac{1}{K} - 1\right). \quad (36)$$

Remark: From Eq. (36), it follows immediately that when $K=1$ (corresponding to the free theory), $v_q = 0\ \forall\ q$ and hence $|\psi_J\rangle$ reduces to $|FS\rangle$ which is the ground state of the free theory.

V. SINGLE-PARTICLE EXCITATIONS BY A JASTROW MULTI-SLATER WAVE FUNCTION

In general, not only the ground state but all the eigenstates of the Luttinger Hamiltonian can be written in a Jastrow multi-Slater form with appropriate Jastrow factors. To this purpose, let us consider that an eigenstate of the noninteracting Luttinger model $|FS_k\rangle$ (defined later) can be transformed onto an exact eigenstate of the interacting Luttinger model $(K \neq 1)$ by means of the unitary transformation $U = e^{iS}$ [defined in the previous chapter in Eq. (15)], namely,

$$|\psi_k\rangle = e^{iS}|FS_k\rangle. \quad (37)$$

Here, $|FS_k\rangle$ is a suitable excited state in the free theory with an extra particle added to the right branch slightly above the Fermi momentum (as we are interested in low-energy excitations only). This excited state can be expressed as

$$|FS_k\rangle = \int_0^L dx\ \ e^{-ikx}\psi_+^\dagger(x)|FS\rangle. \quad (38)$$

The right-moving operator $\psi_+^\dagger(x)$ after integration over x creates a state, namely, a noninteracting Slater determinant with an extra particle added to the right branch and with total momentum $k + k_F$.

The eigenstate $|\psi_k\rangle$ defined in Eq. (37) can be expressed exactly in the following generalized Jastrow-Slater form (see Appendix A for a detailed derivation):

$$|\psi_{J,h}\rangle = \int_0^L dx \exp\left[-\frac{1}{2}\sum_q v_q N_q N_{-q}\right] \times \exp\left[\sum_q h_q e^{iqx} N_q\right]\psi_+^\dagger(x) e^{-ikx}|FS\rangle. \quad (39)$$

A. Remark

In Appendix A, we establish the dependence of h_q on the interaction parameter K. It can be shown that when $K=1$

(corresponding to the free theory), $v_q=0$, $h_q=0$ and the excited state $\psi_{J,h}$ reduces to $|FS_k\rangle$ which is a single determinant. Generally, when $K\neq 1$, $h_q\neq 0$ and in this case the excited state $\psi_{J,h}$ represents a multideterminant Jastrow correlated state, very similar to the Edward's ansatz used for the single spin-flip state of the ferromagnetic Hubbard model described in Sec. I.[9] Our derivation shows that this ansatz is exact for the Luttinger model. Strictly speaking, the number of determinants required to describe the ansatz is infinite because in Eq. (39), the variable x is continuous and a Slater determinant is required in general for each value of x. In practice, however, we can go back to a lattice discretized version of the Luttinger model where the position of an electron is discretized and therefore for generic lattice models, the number of determinants required for describing the present ansatz should scale as the number of lattice sites. In this respect, our result does not simply mean that one-particle excitations of the Luttinger liquid can be expressed as linear superpositions of Slater determinants (this implication would be trivial because any state can be expressed in this way), but provides an important restriction to the form of the wave function because the number of Slater determinants used in this ansatz remains much smaller than the dimension of the Hilbert space.

B. Spectral property of the Luttinger liquid: The quasiparticle weight

With this formalism, one can recover most of the exact results obtained with the conventional bosonization technique since we have represented the ground state and the one-particle excitations using a different (but equivalent) functional form. For instance, we evaluated the quasiparticle weight for the Luttinger liquid determined by the ground state and the lowest one-particle excitation. Our calculation obtained with Jastrow-Slater wave functions implies that the quasiparticle weight vanishes in the thermodynamic limit according to the power law $Z\sim L^{-\theta}$, where $\theta=(K+K^{-1}-2)/2$. This result ties in perfectly with Luttinger liquid theory.[20,24]

VI. ONE-PARTICLE DYNAMICS

The above result can be extended to represent the quantum mechanical time evolution e^{iHt} of any one-particle state in a suitable time-dependent Jastrow-Slater form. In particular, we apply to the ground state written as $e^{iS}|FS\rangle$ the operator $\int_0^L dx\ e^{-ikx}\psi_+^\dagger(x)$ that creates a fermion with momentum $k+k_F$ in the right branch. In this section we determine the exact time-evolved state

$$|\Psi(t,k)\rangle = e^{iHt}\int_0^L dx\ \ e^{-ikx}\psi_+^\dagger(x)e^{iS}|FS\rangle \tag{40}$$

in terms of a generalized Jastrow-Slater form. This form is similar to what we obtained for the one-particle excitation $|\psi_k\rangle$ in the previous section. Since all the single-particle excitations have the same two-body Jastrow potential v_q, it is reasonable to expect the following ansatz:

$$|\Psi_{JhC}(k,t)\rangle = \int_0^L dx\ \ C(t)e^{-ikx}\exp\left[-\frac{1}{2}\sum_q v_q N_q N_{-q}\right] \times \exp\left[\sum_q h_q(t)e^{iqx}N_q\right]\psi_+^\dagger(x)|FS\rangle. \tag{41}$$

Indeed this is the exact time-evolved state within the Luttinger model Hamiltonian provided the functions $h_q(t)$ are chosen appropriately (see Appendix B).

VII. DISCUSSION

The most important outcome of this work is that it is possible to obtain an essentially exact description of the low-energy properties of one-dimensional correlated models by means of a Jastrow-Slater wave function. Indeed, we have shown that the ground state of the Luttinger model, the well-known and accepted model for describing low-energy physics in one dimension, can be written exactly as a long-range Jastrow factor applied to the uncorrelated Fermi sea.

In addition, not only the ground state of the Luttinger model but also single-particle excitations can be described by the Jastrow wave function. In this case however, the Jastrow factor is applied to many Slater determinants. Thus, unlike the nondegenerate ground state which is just a Jastrow-Slater single determinant, the excited state has an intrinsic multideterminant character. This multideterminant state reflects the effect of inserting a single particle to the ground state of the Luttinger model. The wave function for the system with an extra particle changes drastically in form within the Jastrow-Slater ansatz, i.e., from a single determinant to a multideterminant state. The dynamical properties of the Luttinger liquid were also formulated within the Jastrow-Slater wave function. More specifically, the dynamics of a single particle added to the ground state of the Luttinger model can be expressed as a Jastrow multi-Slater state, with time-dependent and complex Jastrow factors.

To avoid confusion, we remark here that this is just a new alternative point of view of the well-known exact solution of the Luttinger model in one dimension. However, it is important to emphasize that the Jastrow-Slater wave-function approach can be easily extended to higher dimensionality and indeed, a long-range Jastrow factor applied to a Slater determinant has been used widely for electronic simulations based on the so-called quantum Monte Carlo technique.[25] However, the present form of a multideterminant Jastrow factor, which we have shown to be a necessary ingredient to deal with the single-particle excitation spectrum of the Luttinger model, has never been used before to the best of our knowledge. This form is particularly important in one dimension, in order to destroy the quasiparticle weight and determine the non-Fermi-liquid behavior. Therefore, we expect that the extension of this wave function to higher dimensionality may lead to a deeper understanding of the photoemission spectrum of strongly correlated materials like high-temperature superconductors which display unconventional behavior.[26,27] In these systems, the photoemission spectrum is still controversial and unexplained. For instance, the strong momentum dependence in angle-resolved photoemission experiments[28–30] with Fermi arcs or hole pockets cannot be easily reproduced with the conventional single determinant Jastrow-Slater ansatz for the single-particle excitations.[26] On the contrary, the extension of the wave function defined in Eq. (39) to higher dimensionality provides a variational ansatz containing more variational freedom for the excitations [e.g., h_q in Eq. (39)], which may lead to more accurate results and possibly better agreement with experiments. Obviously, a systematic variational Monte Carlo study outside the scope of this work is necessary to confirm this interesting possibility.

Finally, we would like to comment on the possible explanation of the Kondo resonance in the spectral weight of a metal, predicted by DMFT in infinite dimensions. In our approach, the wave function of an added particle with momentum k can be viewed as a coherent superposition of Slater determinants with a real space defect located at each space position x [see Eq. (39)]. The excitation described in Eq. (39) is very similar to old types of wave functions[9] and previous approaches to consider the single hole dynamics.[21] The common feature of this approach with the Kondo problem is that the single-particle (or -hole) excitation acts like a real space impurity in the frame where the extra particle is taken fixed. The impurity problem is a peculiar characteristic of the Kondo model fixed point and therefore, we expect that the Jastrow-Slater approach should be able to introduce another energy scale, the Kondo one, in the problem of the photoemission spectrum, very similarly to the DMFT scenario. Again also in this case, numerical work is necessary to verify this issue.

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APPENDIX A: DETAILED DERIVATION OF THE SINGLE-PARTICLE EXCITED STATE

We report below the detailed derivation of the single-particle excited wave function. Although it may appear cumbersome and elaborated, it is indeed very simple conceptually. All one-particle excitations, as well as the ansatz state [Eq. (39)], can always be normal ordered according to the following obvious rule. (i) The fermionic operator $\psi_+^\dagger(x)$ is always the leftmost one. (ii) After that all bosonic terms can be ordered in the normal way: the creation operators $a_q^\dagger$ to the left and the destructions a_q to the right positions. (iii) In this way all the destruction operators a_q disappear because they have to be applied to the vacuum and the final expression drastically simplifies.

Indeed after the above three steps, it is easy to convince ourselves that one can generally obtain, both from the exact excitation [Eq. (37)] and the ansatz [Eq. (39)], similar expressions containing, after the fermionic operator, a Gaussian form of operators $a_q^\dagger$ applied to the vacuum. In this way, it is possible to match the two expressions.

1. First step: Simplification of the ansatz $|\psi_k\rangle$

In order to apply e^{iS} to the fermion field $\psi_+^\dagger(x)$ we follow Ref. 20 that have derived that

$$e^{iS}\psi_+^\dagger(x)e^{-iS} = \psi_+^\dagger(x)\exp\left[\sum_q e^{iqx}(h_q^{LM}a_q^\dagger + h_{-q}^{LM}a_{-q})\right], \tag{A1}$$

where for $q>0$,

$$h_q^{LM} = i\sqrt{\frac{2\pi}{|q|L}}(\cosh\theta_q - 1),$$

$$h_{-q}^{LM} = i\sqrt{\frac{2\pi}{|q|L}}\sinh\theta_q. \tag{A2}$$

We can use Eq. (A1) to simplify the exact excitation $|\psi_k\rangle$ given by Eq. (37):

$$|\psi_k\rangle = \int_0^L dx\ e^{-ikx}e^{iS}\psi_+^\dagger(x)e^{-iS}e^{iS}|FS\rangle$$
$$= \int_0^L dx\ \psi_+^\dagger(x)\exp\left[\sum_q e^{iqx}(h_q^{LM}a_q^\dagger + h_{-q}^{LM}a_{-q})\right]e^{iS}|FS\rangle. \tag{A3}$$

We recall that the ground state of the Luttinger model, apart from a normalization constant, is given by

$$|GS\rangle = e^F|FS\rangle, \tag{A4}$$

where

$$F = \sum_{q>0} f_q a_q^\dagger a_{-q}^\dagger. \tag{A5}$$

In this way we obtain

$$|\psi_k\rangle = R_\alpha\int_0^L dx\psi_+^\dagger(x)e^F\exp\left[\sum_q e^{iqx}e^{-F}(h_q^{LM}a_q^\dagger + h_{-q}^{LM}a_{-q})e^F\right] \times|FS\rangle.$$

Finally by using

$$e^{-F}a_pe^F = f_pa_{-p}^\dagger + a_p,$$

$$e^{-F}a_p^\dagger e^F = a_p^\dagger, \tag{A6}$$

and applying again $e^{A+B}=e^Ae^Be^{-1/2[A,B]}$ with $A=\Sigma_q(h_q^{LM}+f_qh_{-q}^{LM})e^{iqx}a_q^\dagger$ and $B=\Sigma_qh_q^{LM}e^{-iqx}a_q$ we obtain

$$|\psi_k\rangle = C\int_0^L e^{-ikx}dx\ \psi_+^\dagger(x)e^F\exp\left[\sum_q (h_q^{LM}+f_qh_{-q}^{LM})a_q^\dagger e^{iqx}\right] \times|FS\rangle,$$

$$C = \exp\left(1/2\sum_q h_q^{LM}(h_q^{LM}+f_qh_{-q}^{LM})\right). \tag{A7}$$

2. Second step: Simplification of the ansatz $|\psi_{Jh}\rangle$

Also the ansatz ψ_{LJ} can be recast in a form similar to Eq. (A7) using even simpler algebra because the Jastrow depends only on the total density operator N_q, with commutation rules

$$[N_q, N_{q'}] = 0, \tag{A8}$$

$$[N_q, \psi_+^\dagger(x)] = \frac{1}{\sqrt{L}} e^{-iqx} \psi_+^\dagger(x). \tag{A9}$$

In this way it is easy to derive the following useful relations:

$$e^{-1/2\Sigma_q v_q N_q N_{-q}} \psi_+^\dagger(x) \;\; e^{1/2\Sigma_q v_q N_q N_{-q}} = \psi_+^\dagger(x) \exp - \left[\sum_q \frac{v_q}{\sqrt{L}} \left(e^{iqx} N_q + \frac{1}{2\sqrt{L}} \right) \right],$$

$$e^{\Sigma_q h_q N_q e^{iqx}} \psi_+^\dagger(x) \;\; e^{-\Sigma_q h_q N_q e^{iqx}} = \psi_+^\dagger(x) \exp\left[\sum_q \frac{h_q}{\sqrt{L}} \right].$$

With the above relations we can bring the operator $\psi_{(x)=e^{ik_F x}\psi_+^\dagger(x)}$ (as all the left branch states are occupied for momenta $p \simeq k_F$ as we assume) in the leftmost side of Eq. (39) and obtain

$$|\psi_{J,h}\rangle = \exp\left[\sum_q \left(\frac{z_q^{(1)}}{\sqrt{L}} \right) \right] \times \int_0^L dx \;\; \psi_+^\dagger(x) e^{-ikx} \exp\left[\sum_q z_q^{(2)} e^{iqx} N_q \right] \times \exp\left[-\frac{1}{2} \sum_q v_q N_q N_{-q} \right] |FS\rangle, \tag{A10}$$

where

$$z_q^{(1)} = h_q - \frac{v_q}{2\sqrt{L}} \tag{A11}$$

and

$$z_q^{(2)} = h_q - \frac{v_q}{\sqrt{L}}. \tag{A12}$$

Our ansatz can be further simplified by implementing the condition which enabled us to obtain the Jastrow parameter in terms of the pairing function, namely:

$$\exp\left[-\frac{1}{2} \sum_q v_q N_q N_{-q} \right] |FS\rangle = R_\alpha e^F |FS\rangle, \tag{A13}$$

where F has been previously defined in Eq. (A5). Now we can replace $N(q)$ in terms of canonical operators as in Eq. (25) and we can perform similar steps as before, namely:

$$|\psi_{Jh}\rangle = R_\alpha \exp\left[\sum_q \left(\frac{z_q^{(1)}}{\sqrt{L}} \right) \right] \int_0^L dx \;\; \psi_+^\dagger(x) e^{-ikx} \times \exp\left[\sum_q \frac{iqz_q^{(2)} e^{iqx}}{\sqrt{2\pi|q|}} (a_q^\dagger + a_{-q}) \right] e^F |FS\rangle.$$

This can be also written as

$$|\psi_{Jh}\rangle = R_\alpha \exp\left[\sum_q \left(\frac{z_q^{(1)}}{\sqrt{L}} \right) \right] \int_0^L dx \;\; \psi_+^\dagger(x) e^{-ikx} \times e^F \exp\left[\sum_q \frac{iqz_q^{(2)} e^{iqx}}{\sqrt{2\pi|q|}} \times e^{-F} (a_q^\dagger + a_{-q}) e^F \right] |FS\rangle.$$

Finally, using the relations in Eq. (A6) and the fact that $a_q|FS\rangle = 0 \;\forall q$, we obtain

$$|\psi_{Jh}\rangle = C_{Jh} \int_0^L dx \;\; \psi_+^\dagger(x) e^{-ikx} e^F \times \exp\left[\sum_q \frac{iqz_q^{(2)}(1+f_q) e^{iqx}}{\sqrt{2\pi|q|}} a_q^\dagger \right] |FS\rangle, \tag{A14}$$

where

$$C_{Jh} = R_\alpha \exp\left[\sum_q \left(\frac{z_q^{(1)}}{\sqrt{L}} - \frac{|q|}{4\pi} z_q^{(2)} z_{-q}^{(2)} (1+f_q) \right) \right].$$

We are now in the position to match the two states $|\psi_{Jh}\rangle$ and $|\psi_k\rangle$ using Eqs. (A14) and (A7), respectively. Indeed, apart from an irrelevant constant, the ansatz $|\psi_{Jh}\rangle$ is an exact excited state of the Luttinger model, if the following condition is satisfied:

$$\frac{iqz_q^{(2)}(1+f_q)}{\sqrt{2\pi|q|}} = h_q^{LM} + f_q h_{-q}^{LM}. \tag{A15}$$

Since $z_q^{(2)}$ is linear in h_q, the above equation is a simple linear equation that can be solved for the unknown quantity h_q.

APPENDIX B: DETAILED DERIVATION OF THE REAL TIME EVOLUTION FOR THE JASTROW-SLATER WAVE FUNCTION

1. Simplification of the state Ψ_{JhC}

This can be obtained by applying the same derivation described in Sec. II, with slightly different notations. Therefore the final expression is

$$|\Psi_{JhC}\rangle = \int_0^L dx e^{-ikx} \psi_+^\dagger(x) C_{Jh}(t) C(t) \times e^F \exp\left[\sum_q \frac{iqz_q^{(2)}(1+f_q) e^{iqx}}{\sqrt{2\pi|q|}} a_q^\dagger \right] |FS\rangle,$$

$$C_{Jh}(t) = R_\alpha \exp\left[\sum_q \left(\frac{z_q^{(1)}}{\sqrt{L}} - \frac{|q|}{4\pi} z_q^{(2)} z_{-q}^{(2)} (1+f_q) \right) \right]. \tag{B1}$$

Here,

$$z_q^{(2)}(t) = h_q(t) - \frac{v_q}{\sqrt{L}} \tag{B2}$$

and

$$z_q^{(1)}(t) = h_q(t) - \frac{v_q}{2\sqrt{L}}. \tag{B3}$$

2. Simplification of the propagated state $|\Psi_t\rangle$

This is a quite cumbersome and complicated derivation. We sketch how to obtain the final expression of this section. One writes the propagator:

$$e^{iHt} = e^{iS}e^{iH_0t}e^{-iS}. \tag{B4}$$

Then one makes the effort to bring to the left the operator $\psi^\dagger(x)$ using Eq. (A1) also for obtaining the expression of $e^{-iS}\psi^\dagger e^{iS}$ which is the same result of Eq. (A1) (derived for $e^{iS}\psi_+^\dagger e^{-iS}$) with $\theta_q \to -\theta_q$, namely

$$h_q^{LM}(\theta_q) \to \bar{h}_q^{LM} = h_q^{LM}(-\theta_q).$$

Moreover we have to use that

$$e^{iH_0t}\psi_+^\dagger(x)e^{-iH_0t} = \int dx' \left(\sum_p \frac{1}{L} e^{ip(x-x')+iv_spt} \right) \psi_+^\dagger(x'), \tag{B5}$$

$$= \psi_+^\dagger(x + v_s t), \tag{B6}$$

$$e^{iH_0t}a_q^\dagger e^{-iH_0t} = e^{iE_qt}a_q^\dagger, \tag{B7}$$

and also the fact that

$$e^{iS}e^{iH_0t}a_q^\dagger e^{-iH_0t}e^{-iS} = e^{iHt}e^{iS}a_q^\dagger e^{-iS}e^{-iHt}$$
$$= e^{iE_qt}\cosh(\theta_q)a_q^\dagger + e^{-iE_qt}\sinh(\theta_q)a_{-q},$$

where $E_q = v_s|q|$ is not changed by the interaction. Then we arrive at the final result by using that $e^{iH_0t}|FS\rangle = |FS\rangle$, repeated applications of the Baker-Haussdorf-Campbell formula, and little extra effort such as

$$e^{\alpha a_q}e^{\beta a_q^\dagger} = e^{\beta a_q^\dagger}e^{\alpha a_q}e^{\alpha\beta}$$

[a relation that determines the constant $C_{1,2}(t)$ below]:

$$|\Psi(k,t)\rangle = MC_1C_2(t)C_{12}(t)\int_0^L dx \;\; e^{-ikx}\psi_+^\dagger(x + v_s t)$$
$$\times \exp\left\{ \sum_q e^{iqx}[(h_q^{LM} + f_q h_{-q}^{LM})e^{iqv_st} + B_q(t)]a_q^\dagger \right\}$$
$$\times e^F|FS\rangle,$$

where

$$B_q(t) = \bar{h}_q^{LM}[e^{iE_qt}\cosh(\theta_q) + e^{-iE_qt}f_q\sinh(\theta_q)],$$

$$C_{1,2}(t) = \exp\left[\sum_q h_q^{LM}e^{-iqv_st}B_q(t) \right],$$

$$M = \exp\left[1/2\sum_q (\bar{h}_q^{LM})^2 \right],$$

$$C_1 = \exp\left[1/2\sum_q h_q^{LM}(h_q^{LM} + h_{-q}^{LM}f_q) \right],$$

$$C_2(t) = \exp\left[1/2\sum_q e^{-iE_qt}\bar{h}_{-q}^{LM}\sinh(\theta_q)B_q(t) \right],$$

where the constant M follows from the normal order of

$$\exp\left[\sum_q e^{iqx}(\bar{h}_q^{LM}a_q^\dagger + \bar{h}_{-q}^{LM}a_{-q}) \right],$$

the constant C_1 follows from the normal ordering of

$$e^{-F}\exp\left[\sum_q e^{iq(x+v_st)}(h_q^{LM}a_q^\dagger + h_{-q}^{LM}a_{-q}) \right]e^F$$

and $C_2(t)$ from the normal ordering of

$$e^{-F}\exp\left\{ \sum_q e^{iqx}\bar{h}_q^{LM}[e^{iE_qt}\cosh(\theta_q)a_q^\dagger + e^{-iE_qt}\sinh(\theta_q)a_{-q}] \right\}e^F,$$

which can be made explicit by using simple manipulations already introduced in the previous section [see Eq. (A6)].

It is clear therefore that, exactly as in the previous section, the above state can be written as a generalized Jastrow Slater of the form Ψ_{JhC}, with appropriate choice of the complex time-dependent function $h_q(t)$ and time-dependent constant $C(t)$. Indeed after the simple replacement in the dummy integration in dx of $x+v_st \to x$ [notice that we are using PBC and therefore $\psi_+^\dagger(x+L) = \psi_+^\dagger(x)$] so that the integration domain can be shifted by arbitrary constants, we obtain the following simple conditions to match:

$$C(t)C_{Jh}(t) = e^{ikv_st}MC_1C_2(t)C_{12}(t), \tag{B8}$$

$$\frac{iqz_q^{(2)}(t)(1+f_q)}{\sqrt{2\pi|q|}} = e^{-iqv_st}[(h_q^{LM} + f_q h_{-q}^{LM})e^{iqv_st} + B_q(t)], \tag{B9}$$

whereas the density term in the Jastrow factor is always characterized by the same v_q given by Eq. (36).

[1] C. Kim, A. Y. Matsuura, Z.-X. Shen, N. Motoyama, H. Eisaki, S. Uchida, T. Tohyama, and S. Maekawa, Phys. Rev. Lett. **77**, 4054 (1996).

[2] C. Kim, Z.-X. Shen, N. Motoyama, H. Eisaki, S. Uchida, T. Tohyama, and S. Maekawa, Phys. Rev. B **56**, 15589 (1997).

[3] B. J. Kim, H. Koh, E. Rotenberg, S.-J. Oh, H. Eisaki, N. Motoyama, S. Uchida, T. Tohyama, S. Maekawa, Z.-X. Shen, and C. Kim, Nat. Phys. **2**, 397 (2006).

[4] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).

[5] C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).

[6] D. Poilblanc, T. Ziman, H. J. Schulz, and E. Dagotto, Phys. Rev. B **47**, 14267 (1993).

[7] B. I. Shraiman and E. D. Siggia, Phys. Rev. B **42**, 2485 (1990).

[8] S. Sorella, Phys. Rev. B **46**, 11670 (1992).
[9] D. M. Edwards, Prog. Theor. Phys. Suppl. **101**, 453 (1990); W. von der Linden and D. M. Edwards, J. Phys.: Condens. Matter **3**, 4917 (1991).
[10] H. Castella and X. Zotos, Phys. Rev. B **47**, 16186 (1993).
[11] S. Sorella, Phys. Rev. B **49**, 12373 (1994).
[12] N. Prokof'ev and B. Svistunov, Phys. Rev. B **77**, 020408(R) (2008).
[13] Antoine Georges, Gabriel Kotliar, Werner Krauth, and Marcelo J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[14] Avraham Schiller, Pradeep Kumar, Rainer Strack, and Dieter Vollhardt, Phys. Rev. B **51**, 8337 (1995).
[15] P. Limelette, A. Georges, D. Jrome, P. Wzietek, P. Metcalf, and J. M. Honig, Science **302**, 89 (2003).
[16] M. Le Tacon, A. Sacuto, A. Georges, G. Kotliar, Y. Gallais, D. Colson, and A. Forget, Nat. Phys. **2**, 537 (2006).
[17] C. S. Hellberg and E. J. Mele, Phys. Rev. Lett. **67**, 2080 (1991).
[18] M. Capello, F. Becca, M. Fabrizio, S. Sorella, and E. Tosatti, Phys. Rev. Lett. **94**, 026406 (2005).
[19] M. Capello, F. Becca, S. Yunoki, M. Fabrizio, and S. Sorella, Phys. Rev. B **72**, 085121 (2005).
[20] D. C. Mattis and E. H. Lieb, J. Math. Phys. **6**, 304 (1965). $\varphi(p)$ in the notations of this Ref. is equal to θ_p of our notations.
[21] S. Sorella and A. Parola, Phys. Rev. B **57**, 6444 (1998).
[22] S. Eggert and I. Affleck, Phys. Rev. B **46**, 10866 (1992).
[23] K. V. Pham, M. Gabay, and P. Lederer, Phys. Rev. B **61**, 16397 (2000).
[24] J. Voit, Rep. Prog. Phys. **57**, 977 (1994).
[25] D. M. Ceperley and B. J. Alder, J. Chem. Phys. **81**, 5833 (1984).
[26] S. Yunoki, E. Dagotto, and S. Sorella, Phys. Rev. Lett. **94**, 037001 (2005).
[27] M. R. Norman and C. Pepin, Rep. Prog. Phys. **66**, 1547 (2003).
[28] M. R. Norman, H. Ding, M. Randeria, J. C. Campuzano, T. Yokoya, T. Takeuchi, T. Takahashi, T. Mochiku, K. Kadowaki, P. Guptasarma, and D. G. Hinks, Nature (London) **392**, 157 (1998).
[29] Nicolas Doiron-Leyraud, Cyril Proust, David LeBoeuf, Julien Levallois, Jean-Baptiste Bonnemaison, Ruixing Liang, D. A. Bonn, W. N. Hardy, and Louis Taillefer, Nature (London) **447**, 565 (2007).
[30] K. Shen, F. Ronning, D. H. Lu, F. Baumberger, N. J. C. Ingle, W. S. Lee, W. Meevasana, Y. Kohsaka, M. Azuma, M. Takano, H. Takagi, and Z.-X. Shen, Science **307**, 901 (2005).