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# Variational study of the one dimensional $t$–$J$ model: a unified description of the ground state phase diagram

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**Abstract**

We find that the Gutzwiller projected Fermi sea wavefunction (GPWF) has the correct phase structure to describe the kink nature of the doped holes in the ground state of the one dimensional $t$–$J$ model. We find the residual charge correlation beyond the GPWF is well described by an XXZ-type effective Hamiltonian. A Pfaffian-type variational wavefunction with only one parameter is proposed based on this observation and is found to reproduce correctly the global phase diagram and correlation functions of the one dimensional $t$–$J$ model in both the Tomonaga–Luttinger regime and the Luther–Emery regime.

## 1. Introduction

The Gutzwiller projected wavefunctions (GPWFs) are widely used to approximate the ground state of the $t$–$J$ model and the Heisenberg model. In these models, local electronic correlation, as manifested in the no double occupancy constraint of electrons, plays a vital role in determining the low energy physics. Such strong local correlation makes these systems difficult to study analytically. In the variational approach based on GPWFs, these models are first treated in the mean field approximation, in which the local constraint is relaxed to a global one. Then the local constraint is enforced afterwards by the Gutzwiller projection, which simply filters out the unphysical components with doubly occupied sites in the mean field state.

The above variational strategy is used extensively in the study of the high temperature superconductors and quantum antiferromagnets. After many years of efforts, it is now believed that the Gutzwiller projected d-wave BCS state describes well the superconducting state of the high temperature superconductors [1–4]. Quite recently, progress has also been made on the understanding of the quasiparticle properties above such a state [5–8]. The same kind of wavefunction has also been used in recent studies on the exotic orders and exotic excitations of frustrated quantum antiferromagnets [9–12].

An unresolved issue about the GPWF is that it is not clear if the posteriorly executed projection can capture the kinematic effect of the local constraints, even qualitatively. In this paper, we address this issue with the one dimensional $t$–$J$ model. The one

  

dimensional $t$–$J$ model has been studied extensively by a broad band of methods including Bethe-ansatz solution, conformal field theories [13–15], quantum Monte Carlo [16], exact diagonalization [17], and also variational Monte Carlo calculations [18–24]. Many properties concerning the ground state of this model are now well established. This gives us the unique opportunity to judge the validity of a given approximation. The one dimensional $t$–$J$ model is exactly soluble at $J/t = 0$ and $J/t = 2$. For $J/t = 0$, the spin and the charge degree of freedom of the system are totally separated [18]. The spin part is described by the Heisenberg model on the squeezed chain with doped holes removed, while the charge part is described by a noninteracting spinless fermion system. For $J/t = 2$, the system is supersymmetric and it is found that the GPWF provides a fairly accurate approximation for the ground state of the system [15, 22]. For general values of $J/t$ and electron density $n$, the system is a Tomonaga–Luttinger liquid (TLL) below a critical value $J_c/t$ around 2.5. The correlation exponent of the TLL varies continuously with $J/t$ and $n$ [17]. For $J/t > J_c/t$, the system is unstable towards phase separation. For small $n$ and $J/t > 2$, there is also a small region in which the system exhibits a spin gap [21, 24].

The Gutzwiller projected Fermi sea wavefunction and its variants has long been used to describe the ground state of the one dimensional $t$–$J$ model. It is well known that this wavefunction provides an excellent description of the undoped case of the model, namely the spin $\frac{1}{2}$ Heisenberg spin chain [19]. However, the same wavefunction is not that satisfactory for the doped system, except for the supersymmetric case of $J/t = 2$. For example, it fails to predict the TLL behaviour in the small $J/t$ region. A $2k_F$ peak in the spin structure factor is also missed by this wavefunction. Since the wavefunction is parameter free, it also gives no clue on the origin of the spin gap state and the phase separation at large $J/t$.

It is generally believed that the problems with the GPWF originate from the insufficient account of the charge correlation in the system. Along this line of thinking, various kind of Jastrow factor are proposed to remedy the drawbacks of GPWF. For example, Hellberg and Mele introduced a long range Jastrow factor of the form $|F(r_{i\uparrow}, r_{j\downarrow})|^\nu$ and succeed in reproducing the TLL behaviour, where $|F(r_{i\uparrow}, r_{j\downarrow})|^\nu$ is a Slater determinant of all the electron positions [20]. Yokoyama and Ogata found a short range repulsive Jastrow factor is able to restore the $2k_F$ peak in the spin structure factor, while a sufficiently attractive Jastrow factor can cause phase separation [22]. However, both wavefunctions have difficulties in reproducing the correct phase diagram. For example, the spin gap state is missed in both wavefunctions. At the same time, both wavefunctions predict a fully phase-separated state along the boundary of phase separation, which is in fact an oversimplification [17]. More importantly, no understanding on the physical origin of the proposed Jastrow factor is available and it is hard to judge if a similar modification is relevant for a higher dimensional system.

For the sake of possible extension to the higher dimensional case, it is important to know the reason that the simple GPWF fails before any modification on it is made. As mentioned above, it is the residual charge correlation in the system which is responsible for the failure of GPWF. In this paper we make this statement more precise by showing that the GPWF has the correct phase structure to describe the kink nature of the doped holes in the ground state of the one dimensional $t$–$J$ model. In fact, we find the spin structure factor of the GPWF in the squeezed chain coordinate is almost identical to that of a half filled spin chain. Thus the missing $2k_F$ peak in the spin structure factor for small $J/t$ should be recovered if the removed holes are reinserted into the squeezed chain in the right manner.

The physical origin of the residual charge correlation can be easily seen if one reformulates the GPWF in terms of the slave boson theory [25, 26]. In the slave boson theory, the constrained electron operator is decomposed as $\hat{c}^\dagger_{i,\sigma} = f^\dagger_{i,\sigma} b_i$, in which $f^\dagger_{i,\sigma}$ is a spin $\frac{1}{2}$ neutral fermion called a spinon and $b_i$ is a spinless charge 1 boson called a holon. The local constraint now

takes the form of an equality, $\sum_\sigma f^\dagger_{i,\sigma} f_{i,\sigma} + b^\dagger_i b_i = 1$. In terms of the slave boson theory, the GPWF corresponds to a state with all holons condensed into the zero momentum state. However, the holon is not a true boson but a hard core boson as a result of the local constraint. For a general value of $J/t$, there is also an effective attraction between the holons caused by the exchange term of the $t$–$J$ model. Thus an XXZ-type effective Hamiltonian should be a good approximation for the residual charge correlation.

Based on these observations, a Pfaffian-type variational wavefunction is proposed for the ground state of the one dimensional $t$–$J$ model. This wavefunction, which has only one parameter, reproduces well the global phase diagram of the model, including the Luther–Emery (LE) phase in the small $n$ and large $J/t$ region. It is found that this wavefunction also reproduces well various correlation functions of the system and provides a refined picture for the phase separation at large $J/t$.

The paper is organized as follows. Section 2 is devoted to the investigation of the properties of the GPWF. In section 3, the new variational scheme and the Pfaffian-type wavefunction are introduced. The phase diagram and correlation functions determined from this new variational wavefunction are presented in section 4. Section 5 summarizes the paper and includes a discussion on related issues.

## 2. The GPWF

The one dimensional $t$–$J$ model reads

$$\mathcal{H} = -t \sum_{i,\sigma} (\hat{c}^\dagger_{i\sigma} \hat{c}_{i+1,\sigma} + \text{h.c.}) + J \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \tfrac{1}{4} n_i n_{i+1}), \tag{1}$$

in which $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha\beta} \hat{c}^\dagger_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} \hat{c}_{i\beta}$ and $n_i = \sum_\alpha \hat{c}^\dagger_{i\alpha} \hat{c}_{i\alpha}$. The electron in this model is subjected to the constraint of no double occupancy

$$\sum_\alpha \hat{c}^\dagger_{i\alpha} \hat{c}_{i\alpha} \leqslant 1. \tag{2}$$

The ground state of the one dimensional $t$–$J$ model is governed by a well defined phase structure. This can be most easily seen at half filling when the system reduces to the Heisenberg spin chain. For the Heisenberg model, it is well known that the ground state satisfies the Marshall sign rule [27, 28]. The rule says that the ground state wavefunction is real in the Ising basis and its sign is given by $(-1)^{N_\downarrow}$ up to a global phase, where $N_\downarrow$ denotes the number of down spins in the even sublattice. This sign rule is a manifestation of the antiferromagnetic spin correlation in the ground state. With such a sign rule, one easily verify that $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \leqslant 0$ for $i$ and $j$ belonging to different sublattices and $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \geqslant 0$ for $i$ and $j$ belonging to the same sublattice.

The ground state at finite doping is governed by a similar sign rule. It can be easily checked that all matrix elements of the $t$–$J$ Hamiltonian are negative definite in a wavefunction that satisfies the Marshall sign rule on the squeezed chain. The squeezed chain is the chain from which the sites occupied by the doped holes are removed. This can be seen by noting that the motion of holes in this model does not disturb the spin configuration on the squeezed chain. Thus, the ground state of the one dimensional $t$–$J$ model should satisfy such a modified Marshall sign rule. With such a modified Marshall sign rule, one easily see that the holes in the ground state behave as an antiphase domain wall for spin.

Now we show that the GPWF satisfies the Marshall sign rule on the squeezed chain. The GPWF reads

$$|\text{GPWF}\rangle = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) |\text{FS}\rangle, \tag{3}$$

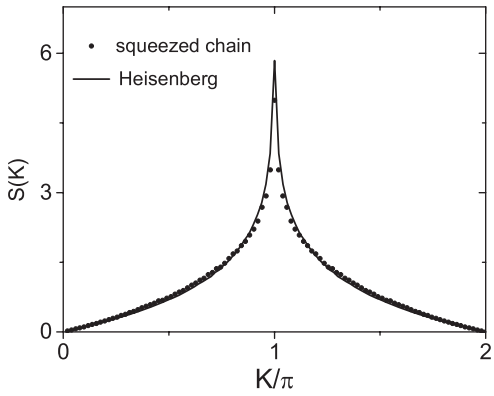


**Figure 1.** Spin structure factor of the GPWF in the squeezed coordinate as compared with that of a half filled spin chain. The calculation is done on a 204 site lattice which is quarter filled.

in which $|\mathrm{FS}\rangle$ denotes the simple Fermi sea. In the natural basis $\prod_{i,j} c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow}|0\rangle$, the amplitude of the GPWF is given by the following Vandermont determinant:

$$\Psi(\{i\},\{j\}) = \psi_{\mathrm{PW}} \prod_{\alpha<\beta} (Z_{i_\alpha} - Z_{i_\beta}) \prod_{l<m} (Z_{j_l} - Z_{j_m}), \tag{4}$$

in which $\psi_{\mathrm{PW}} = \exp[-\mathrm{i}k_{\mathrm{F}}(\sum_\alpha i_\alpha + \sum_l j_l)]$ is a plane wave factor and $Z_{i_\alpha} = \exp(\mathrm{i}\frac{2\pi i_\alpha}{N})$ and $Z_{j_l} = \exp(\mathrm{i}\frac{2\pi j_l}{N})$ are chord coordinates of up spins and down spins.

Now we exchange the up spin at site $i_1$ and the down spin at site $j_1$. The resultant change in phase is given by

$$\Delta\Phi = \arg\left( \prod_{\alpha>1} \frac{Z_{i_\alpha} - Z_{j_1}}{Z_{i_\alpha} - Z_{i_1}} \prod_{l>1} \frac{Z_{j_l} - Z_{i_1}}{Z_{j_l} - Z_{j_1}} \right). \tag{5}$$

Since $|Z| = 1$, $\arg(\frac{Z_{i_\alpha} - Z_{j_1}}{Z_{i_\alpha} - Z_{i_1}})$ is nothing but the angle in the segment $Z_{i_1} - Z_{j_1}$ in the unit circle. Noting the fact that in a circle the angles in the same segment equal one another and the sum of the opposite angles of quadrilaterals equals $\pi$, one easily finds that $\Delta\Phi = N_c\pi$, in which $N_c$ denotes the number of electrons between site $i_1$ and site $j_1$. Taking into account the sign due to fermion exchange, one finds the change in phase is in accordance with the modified Marshall sign rule. Following essentially the same steps, one can also verify the case of exchanging a hole and an electron.

Thus the GPWF has the right phase structure to describe the ground state of the one dimensional $t$–$J$ model and the kink nature of the doped holes in it. In fact, this conclusion can be made even stronger. In figure 1, we plot the spin structure factor of the GPWF in the squeezed coordinate and compare it with that of a half filled spin chain. We see that the two are almost identical with each other. Since the spin degree of freedom is described exactly by a Heisenberg model on the squeezed chain at $J/t = 0$, while the GPWF provides an exceedingly good approximation for $J/t = 2$, it is natural to expect the same behaviour to hold for arbitrary $J/t$ and $n$.

Two conclusions follow directly from the above reasoning. First, since the spin correlation on the squeezed chain is already well described by the GPWF, the missing $2k_{\mathrm{F}}$ peak in the spin structure factor should be recovered if the removed holes are correctly reinserted into the squeezed chain, or the missing $2k_{\mathrm{F}}$ peak should be attributed to the residual charge correlation in the system. Second, since the squeezed spin chain picture is argued to hold for arbitrary

$J/t$ and $n$, a single wavefunction may suffice to describe the whole phase diagram of the one dimensional $t$–$J$ model, including the spin gap phase at small $n$ and large $J/t$.

## 3. The new variational scheme

The origin of the residual charge correlation can be most easily seen by reformulating the GPWF in terms of the slave boson theory. In the slave boson theory, the constrained electron operator is decomposed as $\hat{c}^{\dagger}_{i,\sigma} = f^{\dagger}_{i,\sigma} b_i$, in which $f^{\dagger}_{i,\sigma}$ represents the fermionic spinon and $b_i$ represents the bosonic holon. In terms of these slave particles, the $t$–$J$ model reads

$$\begin{aligned}
&\mathcal{H} = \mathcal{H}_t + \mathcal{H}_J \\
&\mathcal{H}_t = -t \sum_{i,\sigma} (f^{\dagger}_{i,\sigma} f_{i+1,\sigma} b^{\dagger}_{i+1} b_i + \text{h.c.}) \\
&\mathcal{H}_J = \frac{J}{2} \sum_i b_i b^{\dagger}_i b_{i+1} b^{\dagger}_{i+1} \left( \mathbf{S}^f_i \cdot \mathbf{S}^f_{i+1} - \frac{1}{4} n^f_i n^f_{i+1} \right),
\end{aligned}$$

in which $\mathbf{S}^f_i = \frac{1}{2} \sum_{\alpha\beta} f^{\dagger}_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} f_{i\beta}$ and $n^f_i = \sum_{\alpha} f^{\dagger}_{i\alpha} f_{i\alpha}$. The no double occupancy constraint now takes the form of an equality

$$\sum_{\alpha} f^{\dagger}_{i\alpha} f_{i\alpha} + b^{\dagger}_i b_i = 1. \tag{6}$$

When the local constraints equation (6) is exactly satisfied, the factor $b_i b^{\dagger}_i b_{i+1} b^{\dagger}_{i+1}$ appearing in $\mathcal{H}_J$ plays no role and can be neglected.

In the mean field treatment, an RVB order parameter $\chi = \sum_{\alpha} \langle f^{\dagger}_{i+1\alpha} f_{i\alpha} \rangle$ is introduced to decompose the interaction term. At the same time, the local constraint is relaxed to a global one. The mean field Hamiltonians for the spinon and the holon part read [26]

$$\begin{aligned}
&\mathcal{H}^f = -\left( tx + \frac{3J\chi}{8} \right) \sum_{i\sigma} (f^{\dagger}_{i,\sigma} f_{i+1\sigma} + \text{h.c.}) \\
&\mathcal{H}^b = -t\chi \sum_i (b^{\dagger}_i b_{i+1} + \text{h.c.}),
\end{aligned}$$

in which $x$ is the hole density. The mean field ground state is given by the product of the spinon Fermi sea and the holon Bose condensate

$$|\Phi\rangle = (b^{\dagger}_{k=0})^{N_{\text{h}}} \prod_{k \leqslant k_{\text{F}}} f^{\dagger}_{k\uparrow} f^{\dagger}_{k\downarrow} |0\rangle. \tag{7}$$

When this state is projected into the subspace that satisfies the constraint equation (6), we get the GPWF.

In the mean field theory, the holon is a free boson and condenses in the ground state. However, due to the local constraint, the holon is actually a hard core boson which cannot condense in one spatial dimension. The uncondensed nature of the hard core boson in 1D originates from the kinematic effect of the local constraint. Due to this constraint, the Hilbert space for the one dimensional hard core boson system becomes disconnected at the single particle level. We note for comparison that the Hilbert space of the spinon part is still connected even when the local constraint is enforced. Thus the holon should be treated as a hard core boson rather than a free boson.

Another source of the residual charge correlation is provided by the superexchange term of the $t$–$J$ model. When two electrons are next to each other, they enjoy an attraction due to the superexchange. This attraction is not captured by the mean field order parameter $\chi$ and should be reintroduced.

Combining these considerations, the residual charge correlation beyond the GPWF should be described by the following XXZ-type effective Hamiltonian:

$$\mathcal{H}_v = -\sum_i (\hat{b}_i^\dagger \hat{b}_{i+1} + \text{h.c.}) - v \sum_i \hat{b}_i^\dagger \hat{b}_{i+1}^\dagger \hat{b}_{i+1} \hat{b}_i, \tag{8}$$

in which $\hat{b}_i^\dagger$ is the operator for the hard core boson and $v$ is the rescaled attraction. If we denote the ground state of $\mathcal{H}_v$ as $\Lambda_v$, then $\mathrm{P_G}\Lambda_v|\mathrm{GPWF}\rangle$ should be a good variational wavefunction for the one dimensional $t$–$J$ model.

Although $\mathcal{H}_v$ is exactly soluble [29], an explicit form for $\Lambda_v$ is available only in limited cases. For $v = 0$, $\Lambda_v$ is nothing but the Hellberg–Mele Jastrow factor with $\nu = 1$. For $v = 1$, $\Lambda_v$ is a constant and our proposed wavefunction reduces to the GPWF. At quarter filling, $\mathcal{H}_v$ exhibits particle–hole symmetry. In [30], we show that a Hellberg–Mele-type variational wavefunction provides an exceedingly good description for the ground state of the XXZ model in the $S^z = 0$ sector. However, away from the particle–hole symmetric point, the Hellberg–Mele wavefunction ceases to be a good approximation.

For general values of $v$ and boson density, we have to resort to approximation. Through the Jordan–Wigner transformation, the XXZ Hamiltonian can be rewritten as

$$\mathcal{H}_v = -\sum_i (c_i^\dagger c_{i+1} + \text{h.c.}) - v \sum_i c_i^\dagger c_{i+1}^\dagger c_{i+1} c_i, \tag{9}$$

in which $c_i^\dagger$ is a spinless fermion. For this Hamiltonian, we adopt the BCS approximation to decouple the interaction term. The BCS ground state for the spinless fermion reads

$$\prod_{k>0} (u_k + v_k c_k^\dagger c_{-k}^\dagger)|0\rangle, \tag{10}$$

in which $\frac{v_k}{u_k} = \frac{\Delta_k}{\epsilon_k + E_k}$, $\Delta_k = \Delta \sin(k)$, $\epsilon_k = -2\cos(k) - \mu$ and $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$. Here $\Delta$ is the BCS gap for the spinless fermion and is treated as the only variational parameter in our theory (the chemical potential $\mu$ can be determined by the density equation and is not an independent parameter). In real space, the BCS state for the spinless fermion reads

$$|\Lambda\rangle = \left( \sum_{i,j} f_{i,j} c_i^\dagger c_j^\dagger \right)^{\frac{N_\mathrm{h}}{2}} |0\rangle, \tag{11}$$

in which

$$f_{i,j} = \sum_{k>0} \frac{v_k}{u_k} \sin(k(i-j)).$$

When $|\Lambda\rangle$ is expanded in the Fock basis of the spinless fermion, the amplitude $\psi$ is given by the Pfaffian of a $N_\mathrm{h} \times N_\mathrm{h}$ antisymmetric matrix $\bar{f}$ with matrix elment $f_{i,j}$ [31],

$$\psi = \mathrm{Pf}(\bar{f}) = \sum_{i_k < j_k; i_1 < i_2 \cdots < i_{\frac{N_\mathrm{h}}{2}}} (-1)^p \prod_{k=1}^{\frac{N_\mathrm{h}}{2}} f_{i_k, j_k}, \tag{12}$$

where $i_k$ and $j_k$ denote the coordinates of the hole and the sum is over all possible coverings of the hole coordinates $\{(i_1, j_1), (i_2, j_2), \cdots, (i_{\frac{N_\mathrm{h}}{2}}, j_{\frac{N_\mathrm{h}}{2}})\}$ such that $i_k < j_k$ and $i_1 < i_2 \cdots < i_{\frac{N_\mathrm{h}}{2}}$. $p$ is the parity of the permutation of the $\frac{N_\mathrm{h}}{2}$ hole coordinates

$$\begin{pmatrix} 1 & 2 & 3 & 4 & \cdots & N_\mathrm{h}-1 & N_\mathrm{h} \\ i_1 & j_1 & i_2 & j_2 & \cdots & i_{\frac{N_\mathrm{h}}{2}} & j_{\frac{N_\mathrm{h}}{2}} \end{pmatrix}.$$

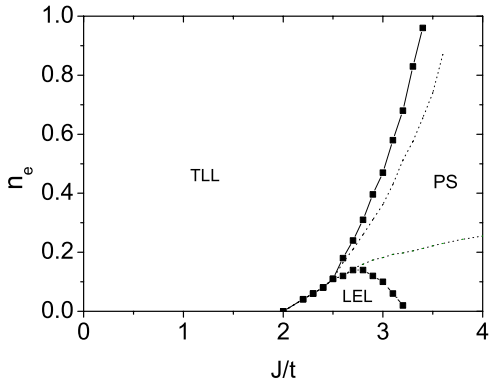


**Figure 2.** Ground state phase diagram of the one dimensional $t$–$J$ model determined from the Pfaffian-type variational wavefunction. The dotted lines indicate the boundaries for the existence of locally stable phases. Here TLL denotes the Tomonaga–Luttinger liquid and LEL denotes the Luther–Emery liquid, while PS denotes the phase separated state.

A Pfaffian is a square root of the determinant of a antisymmetric matrix of even order[3] and can be calculated easily.

Thus our variational wavefunction for the one dimensional $t$–$J$ model is given by

$$\Psi = \mathrm{Pf}(\bar{f})|\mathrm{GPWF}\rangle, \tag{13}$$

in which $\mathrm{Pf}(\bar{f})$ is the Pfaffian for the holes. This wavefunction has only one variational parameter, $\Delta$. This parameter describes in a mean field manner the effective attraction between the holes, which are now spinless fermions.

## 4. Results

### *4.1. Ground state phase diagram*

The ground state phase diagram determined from the Pfaffian-type wavefunction is presented in figure 2. To obtain the phase diagram, we have calculated the energy of the Pfaffian-type variational wavefunction with the variational Monte Carlo (VMC) method [32] and optimized with respect to the only variational parameter $\Delta$. Our calculation is done on a 100 site $t$–$J$ chain with period boundary condition. To satisfy the closed-shell condition, the electron number is limited to be $4n + 2$. When the optimized parameter as a function of $J/t$ and the electron density $n_e$ is known, the energy and other correlation functions of the system can be calculated, from which the ground state phase diagram can be determined.

The phase diagram contains three distinct phases. These phases are characterized by their distinct physical correlations. In the TLL regime, both charge and spin excitation are gapless and both the charge and the spin structure factor exhibit linear behaviour in the long wavelength limit. In the LEL phase, the charge excitation remains gapless while the spin excitation spectrum opens a gap. The gap in the spin excitation spectrum results in a qualitative

[3] Through the Jordan–Wigner transformation, a hard core boson system with even number of particles and periodic boundary condition maps into a spinless fermion system with anti-periodic boundary condition. Such a change of boundary condition is essential for the pairing of the spinless fermion. The Pfaffian wavefunction, which is the unique ground state of the BCS mean field Hamiltonian for the spinless fermion system, is positive definite up to a global sign. This can be seen by noting that the off-diagonal matrix elements of the mean field Hamiltonian are negative definite in a basis in which the creation operators for the spinless fermions are ordered according to their coordinates in the one dimensional lattice.

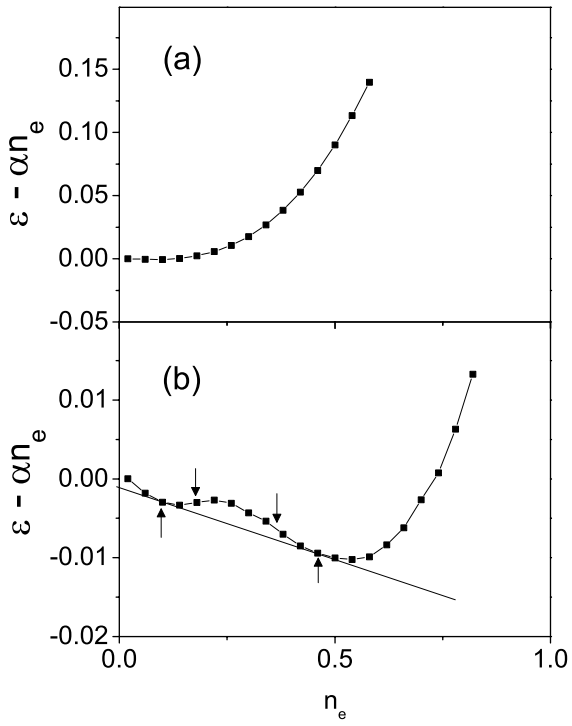


**Figure 3.** Variational energy per site $\epsilon$ as a function of the electron density $n_e$ for $J/t = 2$ (a) and $J/t = 3$ (b). For clarity's sake, a linear decreasing background of the energy is subtracted. $\alpha = \frac{d\varepsilon}{dn_e}|_{n_e \to 0}$ is the initial slope of the energy curve. The arrows above the curve indicate the locations of the inflexion points, while the arrows below the curve indicate the locations of the tangency points. The phase boundaries are determined from these points as explained in the text.

change in the behaviour of the spin structure factor in the long wavelength limit which then exhibits a quadratic dependence on the momentum (see below for more details). In the phase separated (PS) regime, the system is either locally unstable with a negative compressibility, or globally metastable with respect to charge modulation.

For small and intermediate values of $J/t$, the system is in the TLL phase in which both charge and spin excitation are gapless. For larger values of $J/t$, the system is unstable towards phase separation. At small $n_e$ and large $J/t$, there is a small region in which the system exhibits a spin gap. In the spin gap phase, the charge excitation is still gapless. Following the convention, this phase is termed the Luther–Emery liquid.

The phase boundaries are determined as follows. To illustrate the idea, we plot the variational energy as a function of the electron density for $J/t = 2$ and $J/t = 3$ in figure 3. For $J/t = 2$, the energy curve is concave everywhere so that a homogenous phase is globally stable for all electron densities. For $J/t = 3$, a convex region appears at intermediate values of electron density in the energy curve. In this case, the boundaries for the globally stable phases are given by the two tangency points shown in the figure, while the boundaries for the locally stable phases are given by the two inflexion points.

For electron density that lies between the two tangency points, the system is unstable towards phase separation. The densities of the phase separated phases are given by two tangency points. For $2.5 < J/t < 3.2$, the system phase separates into a hole rich phase and an electron rich phase. For $3.2 < J/t < 3.4$, the hole rich phase is replaced by a empty

phase. For $J/t > 3.4$, a fully phase separated state is realized in which the electron rich phase is replaced by a half filled spin chain.

The convex region of the energy curve diminishes to zero at about $J/t = 2.5$. The phase boundary between the TLL phase and the LEL phase for $J/t < 2.5$ is determined by examining the infrared behaviour of the spin structure factor $S(q)$. In the spin gap phase, $S(q)$ should be quadratic at small $q$, while in the TLL phase a linear behaviour is expected [33]. For the charge excitation, a similar criterion exists on the density structure factor $N(q)$.

The existence of the LEL phase is quite unexpected from the point of view of the mean field theory. In the mean field theory, the spinon is still described by a filled Fermi sea, which is by definition gapless. However, after Gutzwiller projection the spinon gets entangled with the holon. Such an entanglement changes drastically the spin correlation of the system.

### *4.2. Correlation functions*

Four correlation functions are evaluated in this work. They are the momentum distribution function defined as

$$n(k) = \frac{1}{2N}\sum_{i,j,\sigma}\langle c^{\dagger}_{i\sigma}c_{j\sigma}\rangle \mathrm{e}^{\mathrm{i}k(r_i-r_j)}, \tag{14}$$

the spin structure factor defined as

$$S(k) = \frac{4}{N}\sum_{i,j}\langle S^z_i S^z_j\rangle \mathrm{e}^{\mathrm{i}k(r_i-r_j)}, \tag{15}$$

the charge structure factor defined as

$$C(k) = \frac{1}{N}\sum_{i,j}(\langle n_i n_j\rangle - \langle n_i\rangle\langle n_j\rangle)\mathrm{e}^{\mathrm{i}k(r_i-r_j)}, \tag{16}$$

and the pair correlation function defined as

$$P(k) = \frac{1}{N}\sum_{i,j}(\langle \Delta^{\dagger}_i \Delta_j\rangle \mathrm{e}^{\mathrm{i}k(r_i-r_j)}), \tag{17}$$

in which $\Delta_i$ is the annihilation operator for a nearest neighbouring pair

$$\Delta_i = \frac{1}{\sqrt{2}}(c_{i\uparrow}c_{i+1\downarrow} - c_{i\downarrow}c_{i+1\uparrow}). \tag{18}$$

First we present the result for the TLL phase. The correlation functions for $J/t = 0, 1$ and 2 at quarter filling are shown in figure 4. For comparison's sake, we also plot the result calculated from the Hellberg–Mele wavefunction. From the figure we see that the correlation functions calculated from the Pfaffian-type wavefunction are almost identical with that calculated from the Hellberg–Mele wavefunction, apart from the small deviations due to critical fluctuations. Since the Pfaffian is derived from a BCS mean field approximation in which a gap opens up, the residual charge correlation described by it is short ranged. Thus the Pfaffian-type wavefunction should exhibit Fermi-liquid behaviour, as is clear in figure 4. To recover the critical fluctuations, one should go beyond the mean field approximation.

For $J/t > 2$, the Pfaffian-type wavefunction becomes less satisfactory for the quarter filled system. In figure 5, we plot the correlation functions of the quarter filled system at $J/t = 2.5$ and 3, the latter of which is very close to the boundary of phase separation. Near the boundary of phase separation, the Hellberg–Mele wavefunction starts to develop charge instability, as is clear from figure 5. This tendency is missed by the Pfaffian-type wavefunction. Instead, a structure at $2k_{\mathrm{F}}$ remains evident in the correlation functions. This is to be expected, since

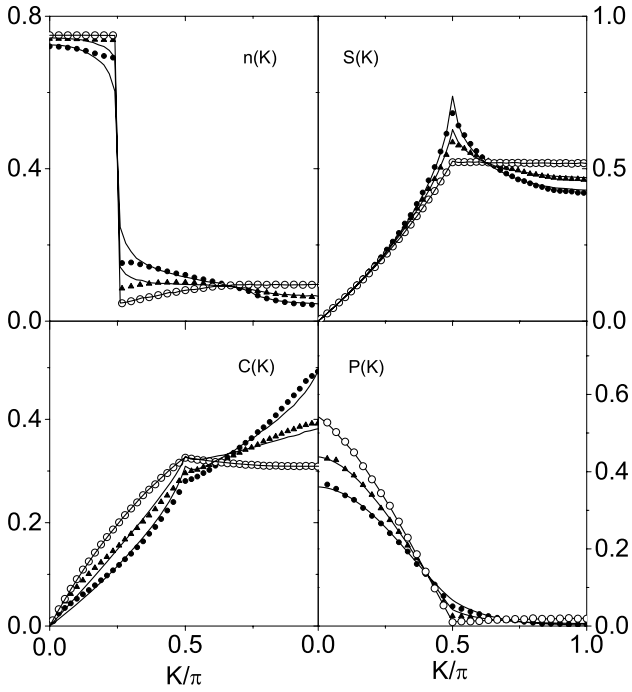


**Figure 4.** The momentum distribution function $n(k)$, the spin structure factor $S(k)$, the charge structure factor $C(k)$, and the singlet pairing correlation function $P(k)$ at quarter filling for $J/t = 0$ (filled circle), $J/t = 1$ (filled triangle), and $J/t = 2$ (open circle). The solid lines denote the results calculated from the Hellberg–Mele variational wavefunction.

we start from a fermionic description of the residual charge correlation. In fact, it is quite amazing that the BCS approximation remains a good approximation for $J/t$ as high as 2.5 (the optimized value for the BCS gap $\Delta$ is approximately given by $J/t$ at quarter filling).

To quantify the above discussion, we plot in figure 6(a) the relative error in the variational energy for both the Pfaffian-type wavefunction and the Hellberg–Mele wavefunction. For small $J/t$, the energy of the Pfaffian-type wavefunction is slightly lower than that of the Hellberg–Mele wavefunction. For larger value of $J/t$, the ordering is reversed. However, both wavefunctions give good estimates for the ground state energy before phase separation.

Although the Hellberg–Mele wavefunction provides a good description for the quarter filled system, it fails badly at low electron density. On the other hand, the Pfaffian-type wavefunction describes quite well the physics in the low density regime, including the spin gap phase at large $J/t$. To illustrate this point, we plot in figure 6(b) the error in variational binding energy for a single pair of electrons calculated from both wavefunctions. From the figure we see that the Pfaffian-type wavefunction is almost exact for all values of $J/t$ in the low density limit. We think this explains why the spin gap phase can be correctly reproduced by the Pfaffian-type variational wavefunction.

Now we present the correlation functions for the LEL phase at small $n_e$ and large $J/t$. In figure 7, the correlation functions for $J/t = 2.8$ and $n_e = 0.06$, a system deeply inside the LEL phase, are plotted. As mentioned above, the spin gap manifests itself in the quadratic behaviour of the spin structure factor in the small $q$ limit.

In the LEL phase, Chen and Lee introduced a correlated spin-singlet-pair wavefunction [21]. This wavefunction describes a dilute gas of electronic Cooper pairs. Our wave-

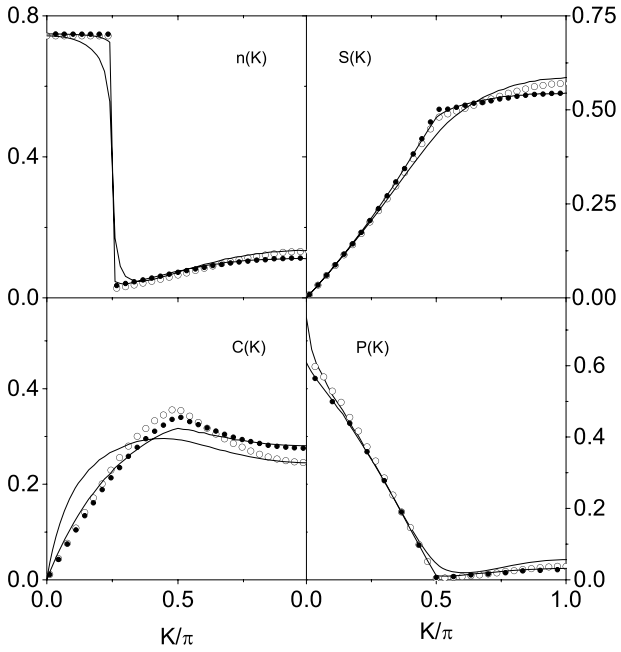


**Figure 5.** The correlation functions at quarter filling for $J/t = 2.5$ (filled circle) and $J/t = 3$ (open circle). The solid lines denote the results calculated from the Hellberg–Mele variational wavefunction.

function differs qualitatively from their wavefunction. This is evident from the long wavelength behaviour of the charge structure factor. The charge structure factor calculated from the Pfaffian-type wavefunction exhibits a linear behaviour in the long wavelength limit, indicating a linear dispersion in the charge excitation spectrum, while the charge structure factor calculated from the Chen–Lee wavefunction approaches a constant value in the long wavelength limit, indicating a quadratic dispersion in the charge excitation spectrum. Thus the Pfaffian-type wavefunction describes an interacting gas of Cooper pairs while the Cooper pairs in the Chen–Lee wavefunction are more like a free gas. At the same time, there is an artificial ODLRO in the Chen–Lee wavefunction. To suppress such an artificial ODLRO, additional correlation should be introduced into the wavefunction [21, 24]. The Pfaffian-type wavefunction is free from such an artifact.

## 5. Summary and discussion

In this paper, we have carried out a variational study of the one dimensional $t$–$J$ model. We find the failure of the simple GPWF should be attributed to the residual charge correlation. Reformulating the GPWF in terms of the slave boson theory, we find that the residual charge correlation should be described by an XXZ-type effective Hamiltonian. Based on this observation, a Pfaffian-type variational wavefunction is proposed for the one dimensional $t$–$J$ model. We find that this wavefunction, which has only one variational parameter, reproduces correctly the global phase diagram and the corresponding correlation functions of the one dimensional $t$–$J$ model.

In the TLL regime, the correlation functions calculated from the Pfaffian-type wavefunction follow closely that calculated from the Jastrow-type wavefunctions proposed by

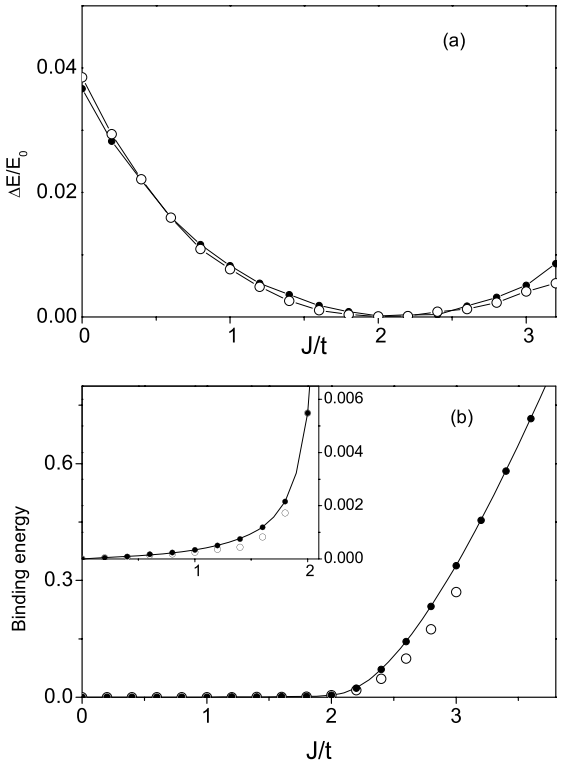


**Figure 6.** (a) Relative error in variational energy at quarter filling calculated from the Pfaffian-type wavefunction (filled circle) and the Hellberg–Mele wavefunction (open circle). The lines are guides to the eye. (b) Absolute error in variational binding energy for a single pair of electrons calculated from the Pfaffian-type wavefunction (filled circle) and the Hellberg–Mele wavefunction (open circle). The solid line gives the exact binding energy. The inset shows an expanded view of the $0 < J/t < 2$ region. The exact value of the ground state energy is taken from [22].

Yokoyama and Ogata [22]. This indicates that our wavefunction is describing the same physics as the Yokoyama–Ogata wavefunction in the TLL regime. However, in the LEL regime, our wavefunction differs qualitatively from the correlated spin-singlet pair wavefunction proposed by Chen and Lee and is free from the artificial ODLRO [21]. As compared with these earlier studies, our approach provides a clearer picture of the underlying physics, which is important for possible generalization to the study of higher dimensional systems. Moreover, it provides a unified picture for the TLL phase and the LEL phase with a single wavefunction. In our formulation, the evolution from the TLL phase to the LEL phase can be understood in terms of the BCS to BEC crossover of the spinless fermion system.

The critical behaviour of the one dimensional $t$–$J$ model is not correctly described by the Pfaffian-type wavefunction. This is to be expected since the Pfaffian factor is derived from a BCS-type mean field treatment. To recover the correct critical behaviour, one should go beyond the mean field approximation for the treatment of the effective XXZ model.

It is interesting to note how the spin correlation is affected by the charge degree of freedom in the one dimensional $t$–$J$ model. Through the investigation of the phase structure of the ground state wavefunction, we find the doped holes behave as anti-phase domain walls for the spin correlation. We find further that the spin degree of freedom of the system is well approximated by a half filled spin chain in the squeezed coordinates throughout the phase

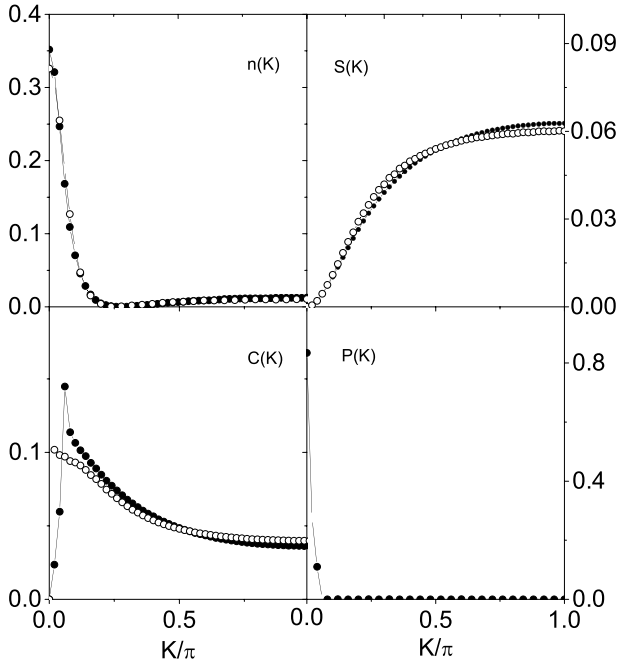


**Figure 7.** Correlation functions for $J/t = 2.8$ and $n_e = 0.06$, a system deeply inside the spin gap phase. The closed symbols denote the results calculated from the Pfaffian-type wavefunction, while the open symbols denote the results calculated from the Chen–Lee wavefunction. No attempt is made to compare the pair correlation function since the Chen–Lee wavefunction exhibits an artificial ODLRO.

diagram. For small electron density, the effect of the charge degree of freedom on the spin part can be so drastic as to induce a gap in the excitation spectrum of the latter. This spin gap is beyond the mean field description and should be attributed to the strong entanglement of the spin and the charge degree of freedom in the projected subspace.

It is also interesting to note the effect of the local constraint for this system. In conventional GPWF, the effect of the local constraint is taken into account subsequently by filtering out the unphysical components. We find that this procedure may fail when the kinematic effect of the local constraint is essential for establishing (or, more accurately, destroying) the mean field correlation in the unprojected state. The one dimensional $t$–$J$ model provides a particular example of this type. In the one dimensional $t$–$J$ model, the Hilbert space for the charge degree of freedom is disconnected at the single particle level due to the local constraint. When the local constraint is relaxed, the connectivity of the Hilbert space for the charge degree of freedom is changed in a qualitative manner. Such a change in the connectivity of the Hilbert space is responsible for the appearance of the Bose condensation of the charged particle in the mean field theory and is ultimately responsible for the failure of the GPWF to describe the Tomonaga–Luttinger behaviour of the system.

A full account of the residual charge correlation in the $t$–$J$ model should also include the attractive contribution due to the exchange term. In the mean field treatment, the exchange term is decoupled in the $f^\dagger_{i\sigma} f_{j\sigma}$ channel, which cannot account for such a charge correlation effect. We find this attraction counteracts the effect of the local constraint and cancels it out around $J/t = 2$. This explains the excellency of the GPWF at the supersymmetric point.

In two spatial dimensions, the kinematic effect of the local constraint should be less dramatic since the connectivity of the Hilbert space is not affected by the local constraint. This can also be seen from the fact that the two dimensional XXZ model does undergo Bose condensation at zero temperature. However, it is much more subtle to analyse the interplay between the spin and charge degrees of freedom in two spatial dimensions since the two frustrate each other. Thus, the validity of the simple GPWF in two dimensions remains to be seen.

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