Variational study of the spin-gap phase of the one-dimensional *t-J* model

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We propose a correlated spin-singlet-pair wave function to describe the spin-gap phase of the one-dimensional t-J model at low density and large J/t. In addition to having singlet pairs, this wave function has a Jastrow factor with a variational parameter ν. Several correlation functions are calculated by using the variational Monte Carlo method. The result shows the expected long-range behavior of the Luther-Emery phase with the Luttinger exponent K_ρ related to ν, $K_\rho = 1/2\nu$. [S0163-1829(96)05638-X]

High-temperature superconductivity (HTSC) has continued to be one of the important current issues in the field of condensed matter physics. It is generally believed that the two-dimensional (2D) t-J model is a good working model for the theory of HTSC, which involves the basic interactions of the copper-oxygen planes. However, recently the one-dimensional (1D) version of the model has received much attention. Inspired by the unusual normal-state properties of high-temperature superconductors (HTS's), Anderson[1] proposed that HTS may be described as the Tomonaga-Luttinger liquid[2] (TLL) instead of the conventional Landau's Fermi liquid. Since the TLL is well studied in the 1D model, many of its properties give us useful references in the study of the 2D model. For example, the shift of the characteristic momentum from $2k_F$ to $2k_F^{\rm SF}$ of spinless fermions (SF's) in the density-density correlation function has been used to argue for spin and charge separation.[3,4] Recently, there has been more experimental evidence for a spin-gap phase[5] in HTS's. So far there is no good account of this phase from the 2D model. It turns out that there is also a phase with a spin gap in the 1D model. Recent studies[6,7] have identified this phase as the Luther-Emery (LE) phase.[8] A more careful study of this phase in 1D would help us to gain insight into dealing with the 2D model. In this paper we will present a wave function that catches the essence of this LE phase.

The 1D t-J model is defined as

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

with the constraint of no double occupancy. By diagonalizing the 16-site chain, Ogata *et al.*[10] have found two phases in the phase diagram of the 1D t-J model. For very large J/t holes and spins phase separate. With decreasing J the system is described as a TLL which exhibits power-law correlations with exponents characterized by a single parameter K_ρ. For the TLL there is no gap in both spin and charge excitations. In addition to the momentum distribution, the important correlation functions, such as the spin-spin, density-density, and pair-pair, functions all have power-law decay:

$$\langle S_z(r)S_z(0)\rangle \sim A_0 r^{-2} + A_1\cos(2k_F r) r^{-\lambda_S} + A_2\cos(4k_F r) r^{-\lambda_4}, \tag{2}$$

$$\langle N(r)N(0)\rangle \sim B_0 r^{-2} + B_1\cos(2k_F r) r^{-\lambda_N} + B_2\cos(4k_F r) r^{-\lambda_4}, \tag{3}$$

$$P(r) = \langle \Delta^\dagger(r)\Delta(0)\rangle \sim C_0 r^{-\lambda_P}, \tag{4}$$

where $\Delta(i) = C_{i\uparrow}C_{i+1\downarrow} - C_{i\downarrow}C_{i+1\uparrow}$, and some of the exponents are $\lambda_S = K_\rho + 1$, $\lambda_N = K_\rho + 1$, and $\lambda_P = 1/K_\rho + 1$.

Using the ground-state projection method, two groups[6,7] have recently found a third phase, the Luther-Emery[8] (LE) phase with a nonzero spin gap in the region of low electron density and high interaction strength. Due to the spin gap, the spin-spin correlation function decays exponentially with distance. It has similar power-law correlation functions for density-density and pair-pair functions as the TLL but with different exponents $\lambda_N = K_\rho$ and $\lambda_P = 1/K_\rho$.

Variational approaches have been very successful in the study of the phase diagram. In particular, Hellberg and Mele[9] (HM) have shown that the TLL is very well represented by a wave function with long-range Jastrow correlations. The HM wave function is defined as

$$|\text{HM}\rangle = \prod_{i>j}\left[\frac{L}{\pi}\sin\left(\frac{\pi}{L}(r_i - r_j)\right)\right]^\nu \Phi_F, \tag{5}$$

where r_i denotes the hole position, L is the total number of sites, and Φ_F is the projected ideal Fermi gas wave function. The holes repel each other when ν is positive and attract otherwise. HM also showed that with tuning ν for different J/t and densities this wave function can reproduce the phase diagram of the 1D t-J model. Not only is the energy quite accurate, it also produces the correct power-law correlations that are the signatures of the TLL. Specifically they have found

$$K_\rho = \frac{1}{2\nu + 1}. \tag{6}$$

However $|\text{HM}\rangle$ fails to predict the spin-gap phase[6,7] which is a LE phase instead of a TLL.

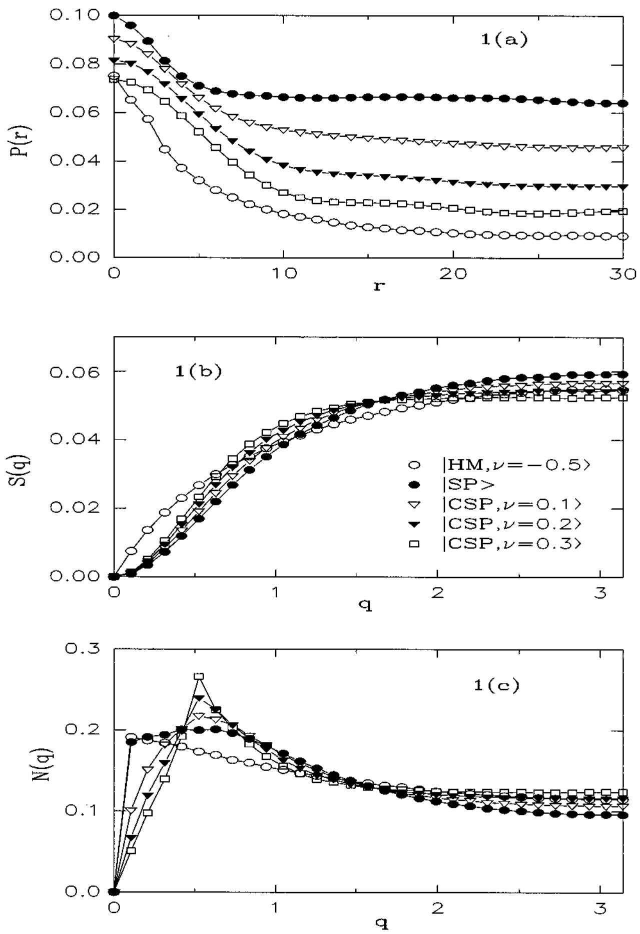

FIG. 1. Variational Monte Carlo results of (a) pairing correlations (shown in real space), (b) spin, and (c) density structure factors of $|\mathrm{HM},\nu=-0.5\rangle$ and $|\mathrm{CSP}\rangle$ for several different ν. The system has 10 electrons in 60 sites. Symbols are defined in (b).

In the study of the spin-gap phase, using the exact pairing wave function of two electrons in an infinite chain as a basis, Chen and Lee[6] (CL) proposed a singlet-pair (SP) wave function

$$|\mathrm{SP}\rangle = P_d\left[\sum_{n=1}^{\infty} h^{n-1} b_n^+\right]^{N_e/2} |0\rangle, \tag{7}$$

where $h=2t/J$, N_e is the total number of electrons, P_d is the projection operator that forbids two particles occupying the same site, and the operator $b_n^+ = \Sigma_i C_{i\uparrow}^+ C_{i+n\downarrow}^+ - C_{i\downarrow}^+ C_{i+n\uparrow}^+$. Without any tuning parameters CL showed that $|\mathrm{SP}\rangle$ has lower energy than $|\mathrm{HM}\rangle$ and more significantly it has the correct short-distance spin-spin correlation which characterizes the LE phase. However, with increasing particle density there will be correlations among pairs and holes. And more seriously, $|\mathrm{SP}\rangle$ is of a particular form of the projected BCS wave function [or resonance valence bond (RVB)], and hence produces a long-range pairing order, which is inconsistent with the LE phase with a power-law correlation in pairing. Taking h as a tuning parameter will not help to suppress the long-range order.

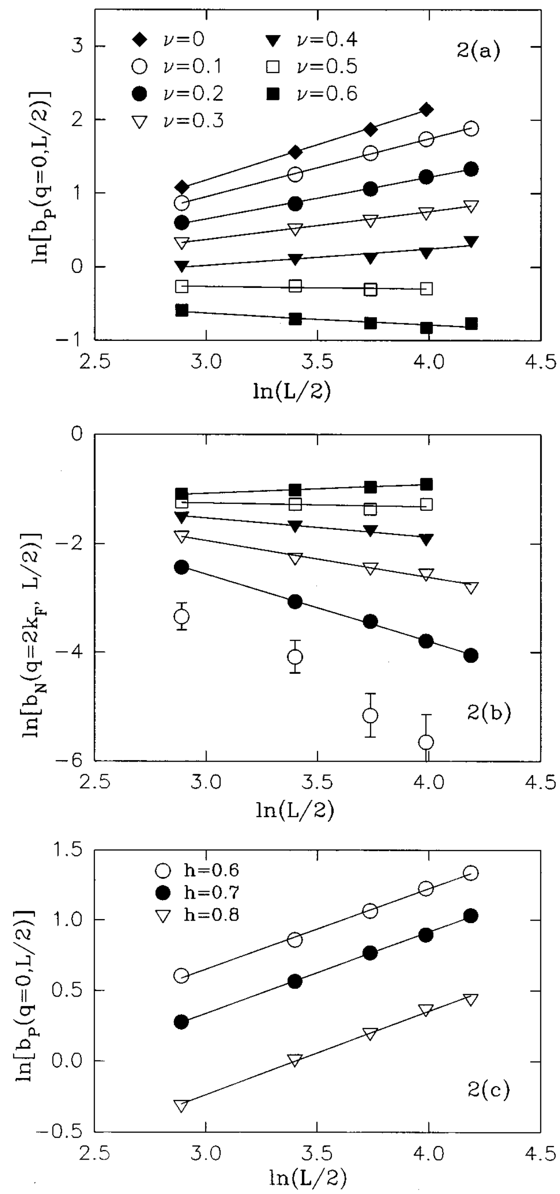

FIG. 2. Finite-size scaling of the quantities (a) $b_P(L/2)$ and (b) $b_N(L/2)$ as defined in Eqs. (9) and (10) for $|\mathrm{CSP}\rangle$ with a fixed $h=0.6$. The electronic density is fixed at $n_e=\frac{1}{6}$ for lattice sizes ranging from $L=36$ to 132. The solid lines are the results of linear fits of the data points. The slopes of the lines in (a) and (b) give $1-\lambda_P$ and $1-\lambda_N$, respectively. (c) is similar to (a) but for a fixed $\nu=0.2$ and various h.

TABLE I. Critical exponents λ_P (λ_N) of pairing (density) correlations for $|\mathrm{CSP}\rangle$ with various variational parameters ν. The numbers in the parentheses show the error in the last digit. The last row is the predicted values of K_ρ by Eq. (11).

ν	0.1	0.2	0.3	0.4	0.5	0.6
λ_P	0.21(2)	0.43(3)	.62(2)	0.77(8)	1.03(4)	1.16(8)
λ_N		2.3(4)	1.63(8)	1.32(8)	1.06(8)	0.84(5)
K_ρ	5	2.5	1.667	1.25	1.0	0.833

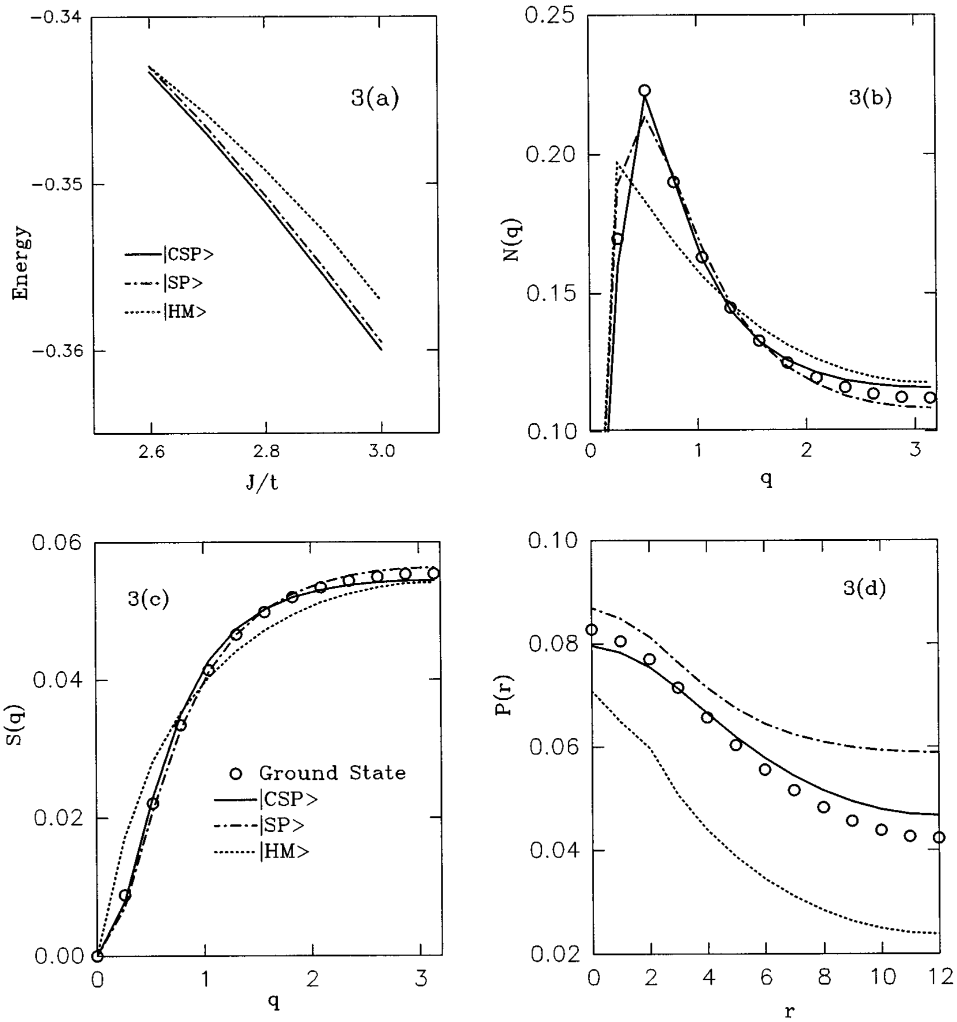

FIG. 3. (a) Variational energies, (b) density, and (c) spin structure factor, as well as (d) pairing correlation of the *t*-*J* model for $|\mathrm{CSP}\rangle$, $|\mathrm{SP}\rangle$, and $|\mathrm{HM}\rangle$ at the density $n_e = 1/6$. The variational parameters are optimized for $J/t = 2.8$. We take $h = 2t/J$ for both $|\mathrm{CSP}\rangle$ and $|\mathrm{SP}\rangle$, and $\nu = 0.08$ and -0.5 for $|\mathrm{CSP}\rangle$ and $|\mathrm{HM}\rangle$, respectively. The lines and symbols are labeled in (c). This system with 4 electrons in a 24-site chain is also exactly diagonalized by the Lanczos method and these exact results are shown as the circles.

In view of the power-law correlation produced by the Jastrow factor in $|\mathrm{HM}\rangle$, a natural way to modify the wave function $|\mathrm{SP}\rangle$ in order to correctly represent the pairing correlation in the LE phase is to add the Jastrow factor to $|\mathrm{SP}\rangle$. This new trial function denoted as $|\mathrm{CSP}\rangle$ is

$$|\mathrm{CSP}\rangle = \prod_{i>j} \left[\frac{L}{\pi} \sin\left(\frac{\pi}{L} (r_i - r_j) \right) \right]^{\nu} |\mathrm{SP}\rangle. \tag{8}$$

Here we present our results of $|\mathrm{CSP}\rangle$ by using the variational Monte Carlo method. The closed-shell boundary condition is used for all the data presented in this paper. The correlation functions either in real space or in Fourier space are shown in Fig. 1 for various ν. The pairing correlation function is defined in Eq. (4). The variational parameter is $h = 2/3$ for $J/t \simeq 3$ at the electron density $n_e = 1/6$. Open circles are the results of $|\mathrm{HM}\rangle$ with $\nu = -0.5$ which is the optimal wave function within $|\mathrm{HM}\rangle$ in the spin-gap region of the 1D *t*-*J* model. Comparing the variational energies among several wave functions for $J/t = 3$ we find that the lowest energy is obtained by $|\mathrm{CSP}\rangle$ with $\nu = 0.1$ (open triangles). Figure 1(a) shows that in this region of J/t, $|\mathrm{HM}\rangle$ underestimates the pairing correlation as compared to the $|\mathrm{CSP}\rangle$. This has been pointed out in previous studies using the ground-state projection method.[6,7] On the other hand, the long-distance behavior of the pairing correlation of $|\mathrm{SP}\rangle$ ($\nu = 0$, solid circle) seems to lead to a long-range pair ordering as mentioned above. With a nonzero ν the long-range behavior has changed and we will show below that it has the power-law dependence as expected from the LE phase.

Spin $[S(q)]$ and density $[N(q)]$ structure factors are plotted in Figs. 1(b) and 1(c), respectively, with the same parameters as in Fig. 1(a). It is easy to show that $S(q)$ should be quadratic at small q if there is a gap in spin excitations.[11] This indeed has been found in Fig. 1(b) for $|\mathrm{SP}\rangle$ and $|\mathrm{CSP}\rangle$. More interestingly, this behavior is quite robust, and it hardly changes with the variation of the exponent ν in contrast to the drastic changes occurring in pairing and density correlations. The reason, we believe, is that the wave functions $|\mathrm{SP}\rangle$ and $|\mathrm{CSP}\rangle$ only have short-range pairs. This preserves the spin gap even in the presence of strong density fluctuations induced by the Jastrow correlation factor.

As shown in Fig. 1(c) $|\mathrm{HM}, \nu = -0.5\rangle$ has the maximum of $N(q)$ at $2\pi/L$. This indicates that the system is close to the phase separation. However, for the LE phase one would expect a sharp peak at $2k_F$ and even a divergent one if $K_\rho < 1$. For $|\mathrm{SP}\rangle$ the maximum is indeed at $2k_F$ but it is quite broad. As for $|\mathrm{CSP}\rangle$ we find that the peak becomes sharper and sharper as ν increases. The size of the peak also grows with ν. By using finite-size scaling we find that the peak diverges with the lattice size for $\nu > 0.5$ (see below).

In addition to establishing the power-law behavior for density-density and pair-pair correlations we must also find a relation between their exponents. In order to extract the exponents of the power-law correlations we consider the finite-size scaling behavior of the following quantities:[12]

$$b_P(L/2) = P(q=0) - P(q=2\pi/L) \tag{9}$$

and

$$b_N(L/2) = 2N(q=2k_F) - N(q=2k_F+2\pi/L) - N(q=2k_F-2\pi/L), \tag{10}$$

where $P(q)$ is the Fourier transform of $P(r)$. In Fig. 2(a) we plot $\log[b_P(q=0,L/2)]$ versus $\log(L/2)$ to obtain the exponent $1-\lambda_P$ as the slope of the linear fit of the data. A similar analysis of $b_N(q=2k_F, L/2)$ gives the exponent $1-\lambda_N$. We have used lattice sizes ranging from $L=36$ to 132. The successful fit of the data supports our conclusion of power-law behavior in pairing and density correlations. The exponents obtained in these plots are tabulated in Table I. We find that the relation $\lambda_P = 1/\lambda_N$ is satisfied with the data in Table I, i.e., the scaling relation expected for the LE phase is recovered.[13] Additionally we find that within the error bars the variational parameter ν is related to the critical exponent K_ρ of the LE phase in a simple relation[14]

$$K_\rho = \frac{1}{2\nu}. \tag{11}$$

Correspondingly we have $\lambda_N = 1/2\nu$ and $\lambda_P = 2\nu$.

The finite-size scaling of pairing correlations for a given $\nu(=0.2)$ and various h is shown in Fig. 2(c). We find that all the data fit to lines of the same slope and hence of the same exponent. Therefore we conclude that the long-range power-law correlations are controlled by the Jastrow factors, irrespective of the parameter h which controls the short-range properties.

Having established $|\mathrm{CSP}\rangle$ as a good wave function to describe the LE phase, now we like to investigate if it is also a proper wave function to faithfully represent the ground state. The variational energies of $|\mathrm{HM}\rangle$, $|\mathrm{SP}\rangle$, and $|\mathrm{CSP}\rangle$ at the density $n_e = 1/6$ are shown in Fig. 3(a). We observe that $|\mathrm{CSP}\rangle$ and $|\mathrm{SP}\rangle$ are very close in energy for large J/t. By using the power method[6] we find that the variational energy of $|\mathrm{CSP}\rangle$ is about 0.3% above the ground-state energy. Although $|\mathrm{CSP}\rangle$ and $|\mathrm{SP}\rangle$ have similar energies, they have significant differences in their long-range correlations as indicated above. In Figs. 3(b)–3(d) we show the density and spin structure factors and pairing correlations for $|\mathrm{HM}\rangle$, $|\mathrm{SP}\rangle$, and $|\mathrm{CSP}\rangle$ optimized for the t-J model with $J/t=2.8$. This system contains 4 electrons in a 24-site chain. For this system the exact ground state can be obtained by the Lanczos diagonalization method. Results for the ground state are shown as the open circles in Fig. 3. We find that for the spin correlation $|\mathrm{CSP}\rangle$ and $|\mathrm{SP}\rangle$ have similar quadratic behavior at small q and agree with the exact result very well. However, for density and pairing correlations $|\mathrm{CSP}\rangle$ describes much better than $|\mathrm{SP}\rangle$. We have also looked at the overlap of these three trial wave functions with the exact ground state. They are 0.984, 0.982, and 0.914 for $|\mathrm{CSP}\rangle$, $|\mathrm{SP}\rangle$, and $|\mathrm{HM}\rangle$, respectively. The excellent consistency between the correlations of the ground state and $|\mathrm{CSP}\rangle$ and the substantial overlap of the two wave functions support the expectation of the LE phase

In conclusion, we have presented a wave function to describe the LE phase in 1D. This wave function $|\mathrm{CSP}\rangle$ has correlated spin-singlet pairs. This is established by using the variational Monte Carlo method. The wave function shows exponential dependence for the spin-spin correlation and power-law behavior in density-density and pair-pair correlations. By finite-size scaling we established the relation of the variational parameter ν to the exponent K_ρ, $K_\rho = 1/2\nu$. Comparing with the exact ground state of a small lattice we showed that $|\mathrm{CSP}\rangle$ describes very well the ground-state properties of the spin-gap phase of the 1D t-J model.

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[14] This relation has been conjectured by C. S. Hellberg (private communication).