# Variational Wave Functions and Ground-State Properties in the One-Dimensional $t$-$J$ Model

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Ground-state properties of the one-dimensional $t$-$J$ model are studied by using exact diagonalization of small systems and compared with those found with Gutzwiller-Jastrow-type variational functions. Near the supersymmetric case ($J/t=2$), the Gutzwiller wave function is an extremely good trial function for all electron densities. It reproduces momentum distribution and correlation functions of the exact ground state except for critical behaviors. For $J/t<2$ ($>2$), the ground-state properties are well described by Jastrow functions with repulsive (attractive) intersite correlations.

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Variational theory is one of the most powerful methods for understanding strongly correlated electron systems. The Gutzwiller wave function (GWF) [1] has been extensively used in the Hubbard model and $t$-$J$ model; however, it is always difficult to see to what extent it reproduces the true ground state. Therefore comparison to the exact results obtained in one-dimensional (1D) systems is particularly important. It also gives us an overview of the problem from a different angle and can yield important insights to higher-dimensional systems. In this paper we study ground-state properties in the 1D $t$-$J$ model obtained in the exact diagonalization and analyze them in the light of GWF. The $t$-$J$ model itself is also an important model for its close relationship to the high-temperature superconductivity [2,3].

In the subspace with no double occupancy the 1D $t$-$J$ model is defined as

$$H=-t\sum_{j\sigma}(c_{j\sigma}^{\dagger}c_{j+1\sigma}+c_{j+1\sigma}^{\dagger}c_{j\sigma}) +J\sum_{j}(\mathbf{S}_j\cdot\mathbf{S}_{j+1}-\tfrac{1}{4}n_jn_{j+1}). \quad (1)$$

Henceforth we take $t=1$. This Hamiltonian was originally introduced as an effective Hamiltonian of the Hubbard model in the strong-coupling regime [2,4]; so far most variational studies were directed to the small-$J$ region (equivalently large-$U$ Hubbard model). The numerical [4,5] and analytical [6] studies showed that the GWF is unsatisfactory in describing the properties in the less-than-half-filled case, although it is excellent for the Heisenberg chain where there is no density fluctuation. Some of the unsatisfactory features were remedied by modifying the GWF [7,8]. On the other hand, quite recently Tomonaga-Luttinger liquid behavior [9] (small-$J$ region) and a phase separation (large-$J$ region) have been studied without using variational functions. The critical exponents of the long-range behaviors of correlation functions were calculated exactly for the supersymmetric case [10,11] ($J=2$) and numerically for the other cases [12]. However, the global features of physical quantities such as the momentum distribution function $n(k)$ and the spin (charge) correlation function $S(k)$ [$N(k)$] have not been studied. The relationship to the variational functions is quite interesting. We will show that the GWF is an extremely good variational wave function for the supersymmetric case. Furthermore, the Gutzwiller-Jastrow-type wave functions successfully describe the behavior of the 1D $t$-$J$ model in the whole phase diagram including phase separation [12,13].

Figure 1 shows $n(k)$ and $S(k)$ obtained in the small-cluster diagonalization for various values of $J$ in the quarter-filled case ($n=0.5$). Singularities appear at $k_F$ in $n(k)$ and $2k_F$ in $S(k)$. Their dependence on $J$ is consistent with the behavior of the exponent $K_\rho$ which in-

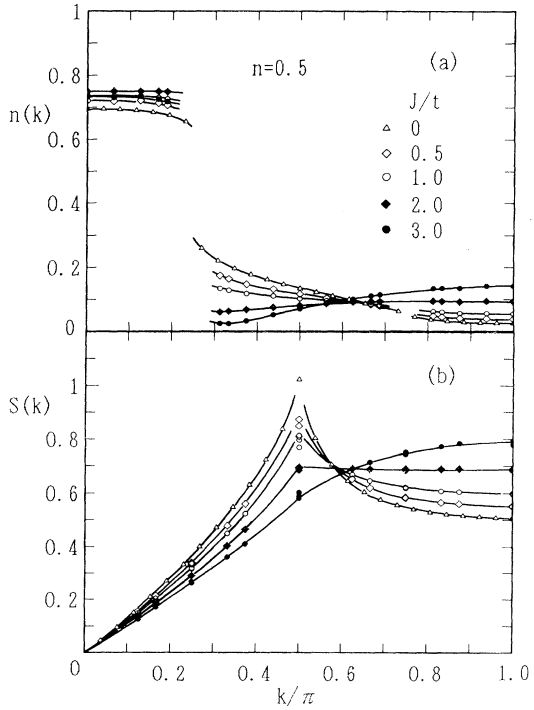


FIG. 1. (a) The momentum distribution function and (b) the spin-correlation function for the quarter-filled case at $J=0.5$, 1.0, 2.0, and 3.0 obtained in the exact diagonalization of the systems with 4, 8, 12, and 16 sites. For $J=0$, we show the result in the wave function for the $U\rightarrow\infty$ Hubbard model with 52 sites [14].

creases from $\frac{1}{2}$ as $J$ increases [12]. For example, $n(k)$ has a power-law singularity at $k_F$ with an exponent $(K_\rho-1)^2/4K_\rho$. For small values of $J$, the correlation functions resemble the results in the large-$U$ Hubbard model [14]. As $J$ increases, however, they lose this behavior. Near the supersymmetric case ($J=2$), the system behaves similarly to the noninteracting case, where $n(k)$ has a jump at $k_F$ and $S(k)$ and $N(k)$ become flat in $k>2k_F$. This corresponds to the fact that the exponent $K_\rho$ becomes 1 near $J=2$ ($J\sim 2.3$ for $n=0.5$) [12], and the leading term of the singularity becomes the same as in the noninteracting case. It is worthwhile noticing, however, that the Green's function does not have a pole even in this case, because the spin and charge velocities are different.

Next we estimate the ground-state energy. The ground state is always singlet and nondegenerate, if we choose periodic (antiperiodic) boundary conditions for $N/2$ =odd (even), respectively ($N$ is the electron number) [12,14]. Under these boundary conditions, the energy converges smoothly to the thermodynamic limit. For $n=0.5$ we calculate the ground-state energies in 4-, 8-, 12-, and 16-site clusters and fit the results by the formula $E/N_a=\epsilon_\infty+C_1/N_a^2+C_2/N_a^4+C_3/N_a^6$ ($N_a$ is the number of sites). Figure 2(a) shows the fitted values of $\epsilon_\infty$. In the region $J\geq 3.4$ the energies cannot be fitted by this formula, because the system phase separates in this region. To check the convergence, we calculated another series of singlet energies by using different boundary conditions, i.e., antiperiodic ones for $N/2$ =odd and vice versa [15]. Fitting of the data by the same formula gives another estimate of $\epsilon_\infty$. (In this case $C_1>0$, while the former fitting gives $C_1<0$.) We find the difference of $\epsilon_\infty$ between the two estimates is very small ($\Delta\epsilon_\infty<10^{-6}t$) [16].

Now let us compare the above results with the GWF: $P_d\Phi_F=\prod_j(1-n_{j\uparrow}n_{j\downarrow})\Phi_F$, where $\Phi_F$ is a simple Fermi sea. The variational Monte Carlo (VMC) method [4,5] was used to evaluate expectation values for the systems with $N/2$ =odd under the periodic boundary conditions. Sample numbers and sampling intervals are taken so as to reduce statistical fluctuations enough. In Fig. 2(b), we compare the total energy of the GWF with that of the Bethe ansatz (BA) at $J=2$. It is surprising that two results almost coincide for any value of $n$ in the scale of this figure. In fact, for the half-filled or the Heisenberg case ($n=1$), the energy of the GWF, $E(\mathrm{GWF})=-\frac{1}{2}[(3/\pi)\mathrm{Si}(\pi)+1]=-1.384235\ldots$ [4,6], is extremely close to the exact result, $E(\mathrm{BA})=-2\ln 2=-1.386294\ldots$. For $n=0.5$, analytic expressions obtained in Ref. [6] give $E_t=-0.574632\ldots$ and $E_J=-0.164230\ldots J$. At $J=2$ the total energy becomes $E(\mathrm{GWF})=-0.903092\ldots$, which is quite close to the exact one: $E(\mathrm{BA})=-0.903649\ldots$. The difference is only 0.06%, which is better than the half-filled case. Furthermore, by solving the two-electron problem, we can show that the ground-state wave function is given by $|\Psi\rangle=P_d c_{k=0\uparrow}^\dagger c_{k=0\downarrow}^\dagger|0\rangle$ at $J=2$. This means that the GWF is exact in the low-density limit. In fact, the total energies of the GWF and BA coincide up to the order of $n^3$; $\epsilon_\infty=-2n+\pi^2n^3/12+O(n^4)$. This is consistent with the fact that the critical exponent $K_\rho$ approaches 1 for $n\to 0$. This Fermi-liquid state is nothing but the GWF.

As shown in Fig. 3, physical quantities in the GWF also almost coincide with those in the true ground state. It is remarkable that the ground state of the $t$-$J$ model

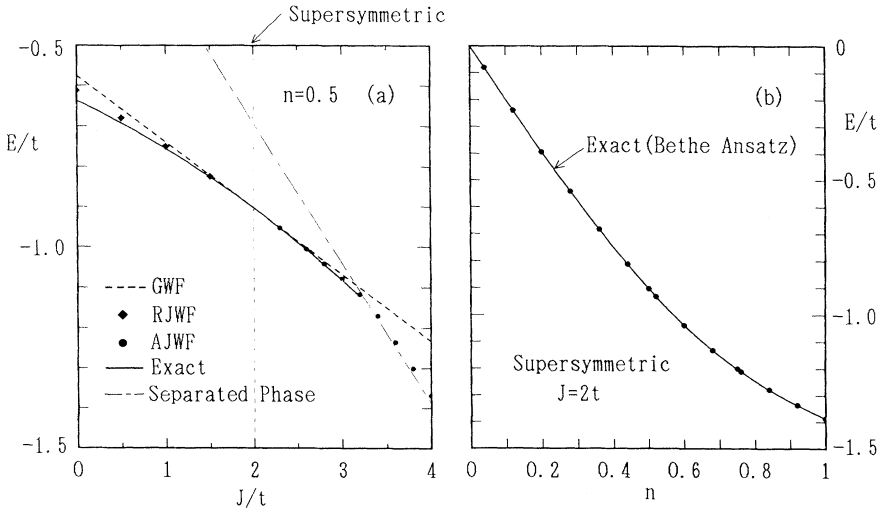


FIG. 2. (a) Total energy as a function of $J/t$ at $n=0.5$. Extrapolated values ($N_a\to\infty$) of the exact diagonalization, the energy of the fully phase-separated state, and variational energies of the three types of variational functions are compared. (b) Comparison of the total energy per site in the 1D $t$-$J$ model between the Gutzwiller wave function (solid circles) and Bethe ansatz for $J=2$ as a function of electron density. In the VMC calculations systems with 50–100 sites are used.

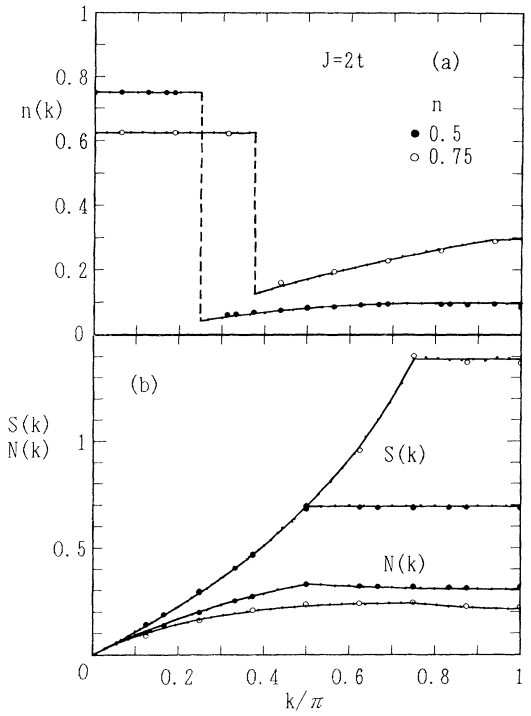


FIG. 3. Comparison of (a) the momentum distribution function and (b) the spin and charge correlation functions between the GWF (solid line) and the exact diagonalization (open and solid circles) at $J=2$. The analytic expressions have been obtained in Ref. [6]. Here we show the results of VMC calculations in 60- and 72-site systems with $5\times10^4$ samples. The VMC results are in good agreement with the analytic expression within an error of the order of the linewidth. For the diagonalization, the data in $N_a=4$, 8, 12, and 16 sites for $n=0.5$ and $N_a=8$ and 16 sites for $n=0.75$ are shown.

has an enhancement of $n(k)$ in the vicinity of $\pi$, which was considered before as a pathological behavior of the GWF [5]. It can be shown that this enhancement originates from the correlated electron motion, $\langle c_{i\sigma}^{\dagger}c_{j\sigma}(1-n_{i-\sigma})(1-n_{j-\sigma})\rangle_0$. All these results show that the GWF is an extremely good trial function to describe globally the 1D $t$-$J$ model at $J=2$, although it is not the exact ground state; the GWF is basically a Fermi liquid and has a discontinuity $\sqrt{1-n}$ at $k=k_F$ in $n(k)$, while the exact solution gives a power-law singularity. (As mentioned above, $K_\rho=1$ at $J\sim2.3$. However, we will see shortly that the Jastrow factor lowers the energy at that parameter.) In order to describe these power-law behaviors around $k_F$, it seems necessary to introduce low-energy excited states around the Fermi surface into the trial wave function. In this connection Hellberg and Mele [8] have introduced a holon wave function to obtain the power-law singularity at $J=0$.

The $J$ dependence of the variational energy in Fig. 2(a) shows that the GWF is very good in the vicinity of the supersymmetric case. It is possible to speculate this reason. An up-spin electron, for example, can hop to a neighboring site with the same amplitude $t=J/2$ independent of the neighboring state (hole or down-spin electron). This fact makes the up-spin part of the wave function similar to the Fermi sea, in which the up spins move freely without any correlations to the down spins.

Incidentally, it was proved [17] that the GWF in the half-filled case is the exact ground state of a Heisenberg model with an exchange coupling falling off as the inverse square of the distance. The present results suggest that the GWF can be a ground state of a similar supersymmetric model even for $n<1$. Actually, a recent investigation [18] has proved that the GWF is the exact ground state of a Hamiltonian with $J_{ij}=2t_{ij}\propto r_{ij}^{-2}$ for any $n$.

In the following we study Jastrow-type wave functions to describe the $t$-$J$ model away from $J=2$. We take into account the spin-independent charge-density correlation:

$$\Psi=\prod_{jl}\prod_{\sigma\sigma'}\{1-\eta(|r_j-r_l|)\}n_{j\sigma}n_{l\sigma'}\}\Phi_F\,. \tag{2}$$

For the $t$-$J$ model, the conditions $\eta(0)=0$ and $\eta(\infty)=1$ have to be satisfied. We use the following functions:

$$\eta(r)=\begin{cases}(2/\pi)\arctan(r/\zeta), & \text{(a) RJWF},\\ 1, & \text{(b) GWF},\\ 1+\alpha/r^{\beta}, & \text{(c) AJWF},\end{cases} \tag{3}$$

for $r\neq0$, and $\zeta$, $\alpha$, and $\beta$ are positive variational parameters. Form (a), which is referred to as a repulsive Jastrow wave function (RJWF), includes intersite repulsive correlation and thus prefers configurations with electrons mutually apart. In the limit $\zeta\to0$, it is reduced to the GWF (b). An attractive Jastrow wave function (AJWF) with the correlation factor (c) favors local configurations with electrons close to each other. It is reduced to the GWF when $\alpha\to0$ and it represents a fully phase-separated state when $\alpha\to\infty$. Comparing with RJWF and AJWF, we may regard the GWF as a "free-electron" state in that there is no amplitude modification from the noninteracting state except for the exclusion of doubly occupied sites.

As anticipated [7], the GWF is unstable against the RJWF for the small-$J$ region; that is, the total energy in RJWF, $E(\zeta)=E_t(\zeta)+E_J(\zeta)$, has a minimum at finite $\zeta$. The critical value $J_G^R$ at which the GWF becomes stable can be obtained from the behavior of $E(\zeta)$ near $\zeta=0$. We find $E_t(\zeta)=-0.575-0.058\zeta$ and $E_J(\zeta)=-0.164J+0.029\zeta J$ for small $\zeta$ at $n=0.5$. This means that the GWF ($\zeta=0$) is unstable for $J<2.0$. The $\zeta$ dependence is because the electrons tend to keep apart from each other as $\zeta$ increases. In this way, we find $J_G^R\sim2.0\pm0.1$ for $n=0.3$, 0.5, and 0.833.... In the region $J<J_G^R$, the minimum appears at $\zeta\sim1.6$ (for $J/t=0$), 1.2 (0.5), 0.7 (1.0), 0.4 (1.5), and 0 (2.0) for $n=0.5$. The repulsive interaction represented by the magnitude of $\zeta$ becomes weaker with increasing $J$. The energies are considerably improved on the GWF, which are shown in Fig. 2(a). Correlation functions $S(k)$, $N(k)$, and $n(k)$ of the opti-

mized RJWF agree fairly well with the diagonalization results. Note that the RJWF still represents the metallic state and has a jump of $n(k)$ at $k_F$. In the AJWF, $E_J$ becomes lower and $E_t$ becomes higher as $\alpha$ increases, because the amplitude of configurations with electrons located next to one another increases. By studying the small-$\alpha$ behavior, we obtain the critical value $J_G^A \sim 2.0$ ($n=0.5$) at which GWF becomes unstable against the AJWF. Searching the energy minimum in the $\alpha$-$\beta$ plane, we obtain the optimized energy in $J>2$ [Fig. 2(a)]. The minimum occurs at $\alpha<10$ for $J\leq 3.2$ and $\alpha>10$ for $J>3.4$. In the latter case, $E_t$ goes to 0 and $E_J$ becomes the energy of the spin system for $\beta=0.625\sim 1$, which is nothing but a sign of the phase separation. Detailed analysis shows that the critical value $J_c=3.3$, which is in good accordance with the diagonalization result [12]. This phase separation in AJWF is also confirmed through the charge correlation function $\langle n_i n_j\rangle$ in real space. It approaches the value of the fully phase-separated state, $\langle n_i n_j\rangle = n-|i-j|/N_a$ for $\alpha>10$. The spin-correlation function becomes considerably similar to the Heisenberg chain in this region.

To summarize, the ground state of the 1D $t$-$J$ model changes its characteristics from RJWF to GWF and finally to AJWF. For $J<2$, $E_t$ is dominant and there is repulsive correlation between electrons; for $J>2$, the situation is reversed. This behavior is consistent with the appearance of a region with dominant superconducting correlation ($K_\rho>1$) which was found in the exact diagonalization. Near $J=2$, the two are well balanced, and a kind of "noninteracting" state well represented by the GWF is realized. Although the present wave functions do not give correct exponents, the ground-state properties are reproduced fairly well. In the 2D $t$-$J$ model, we can also show that the ground state of two electrons is given by the "GWF" at the supersymmetric case, as in the 1D case. This strongly suggests that the GWF can be a good trial function near $J=2$ in 2D as well, which requires more investigation.

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