Analytic calculation of ground-state properties of the one-dimensional *t-J* model with a modified Gutzwiller wave function

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An effective Hamiltonian equivalent to the *t-J* model is derived. We calculate analytically the ground-state energy and correlation functions for a modified Gutzwiller wave function using the technique developed by Metzner, Vollhardt, and Gebhard. We obtain results that are significantly better than those for the usual Gutzwiller wave function, and that are close to the exact results in some cases.

Much of interest in the Hubbard model and its cousin, the *t-J* model, has been stimulated after the suggestion by Anderson[1] that it might describe high-temperature superconductors. Although they are the simplest models for the strongly correlated electron systems, the understanding we have for them is still limited. So far, an exact solution has only been found for the one-dimensional (1D) Hubbard model.[2] There is no exact solution for the *t-J* model even in 1D, except in the supersymmetric[3] ($J=2t$) and other limiting cases, although numerical calculations for clusters have been extensively performed.[4] Analytically, many approximate methods have been developed, such as the slave-boson[5] and the Schwinger-boson[6] mean-field theories as well as their extensions to include fluctuations.[7] The problems with these approaches are associated with the fact that constraints that account for strong correlations can only be treated on average. We will use the Gutzwiller variational approach to deal strictly with these constraints.

Gutzwiller[8] proposed a variational wave function (Gutzwiller wave function, GWF) and suggested an approximate scheme for evaluating expectation values. The Gutzwiller approximation (GA) can result in a metal-insulator transition, as first observed by Brinkman and Rice,[9] and has been applied to many systems.[10] Kotliar and Ruckenstein[11] showed that the GA can be derived as a particular saddle point in the slave-boson approach. There have been many efforts to go beyond the GA using numerical techniques.[12,13] Recently, Metzner and Vollhardt,[14] and Gebhard and Vollhardt[15] calculated analytically the ground-state properties and the correlation functions of the GWF for the 1D Hubbard model. The ground-state properties are, unfortunately, qualitatively inconsistent with the exact solution in the limit of strong correlations. Yokoyama and Ogata[16] showed that the GWF is a good trial function near the supersymmetric point for the 1D *t-J* model, but it still failed to give correct analytic behaviors for correlation functions near k_F. Using the variational Monte Carlo method, Yokoyama and Shiba,[17] and Hellberg and Mele[18] remedied some unsatisfactory features for the Hubbard model by modifying the GWF. Very recently, Hellberg and Mele[19] reported numerical work for the phase diagram of the 1D *t-J* model using the variational approach.

Hard-core bosons are often introduced to represent holes (or spins) for the *t-J* model in conjunction with the slave-boson (or Schwinger-boson) approach. Most approximation schemes end up accounting only on average for the hard-core nature of these bosons. The other constraint that no site is simultaneously occupied by a boson and a fermion is also treated on average. We suggest using a Jordan-Wigner transformation to transform the hard-core boson into a fermion so that the Pauli exclusion principle will automatically ensure that no site is doubly occupied by holes. We then suggest a trial GWF in which double occupancy of the two kinds of fermions (representing holes and spins, respectively) is projected out of the free-fermion wave functions. Both constraints, i.e., no double occupancy by holes or by a hole and a spin are therefore, imposed exactly.

Most calculations that go beyond the GA or GWF are mainly for 1D systems, because the 1D model is relatively easy to explore and the exact solution is available for comparison. It could also share some properties with the 2D systems.[20] The present paper is also restricted to the 1D *t-J* model. We will utilize the techniques developed by Metzner and Vollhardt[14] and Gebhard and Vollhardt[15] to do the analytic calculation of the energy and correlation functions for our trial wave function. We find results that are significantly better than those for the usual GWF. The analytic and approximation-free calculation here might be helpful in the search for a better trial wave function and understanding of electron correlations.

We start by writing the *t-J* Hamiltonian in terms of the hole and one spin variables and introducing our trial wave functions and then we calculate analytically the ground-state energy and correlation functions.

The *t-J* model can be derived from the large-U Hubbard model. In order to get an equivalent Hamiltonian to the *t-J* model, we start from the Hubbard Hamiltonian

$$H=-t\sum_{\langle i,j\rangle}(c_{i,\sigma}^{\dagger}c_{j,\sigma}+\text{H.c.})+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}\ , \tag{1}$$

where $c_{i,\sigma}^{\dagger}(c_{i,\sigma})$, as usual, are the electron creation (annihilation) operators at site i; and $n_{i,\sigma}$ ($\equiv c_{i,\sigma}^{\dagger}c_{i,\sigma}$) are the number operators of electrons. In the large-U limit, one site can be occupied by no more than one particle. The particle concentration in this limit is usually written as $n=n_{\uparrow}+n_{\downarrow}=1-\delta$, with δ the doping.

The Hamiltonian (1) can be transformed into a negative-U Hubbard model by the following canonical transformation[21]

$$c_{i,\downarrow}^{\dagger}=\exp(i\mathbf{Q}\cdot\mathbf{R}_i)\bar{c}_{i,\downarrow}\ ,\quad c_{i,\uparrow}^{\dagger}=\bar{c}_{i,\uparrow}^{\dagger}\ ,$$
$$C_{i,\downarrow}=\exp(-i\mathbf{Q}\cdot\mathbf{R}_i)\bar{c}_{i,\downarrow}^{\dagger}\ ,\quad c_{i,\uparrow}=\bar{c}_{i,\uparrow}\ , \tag{2}$$

where $\exp(i\mathbf{Q}\cdot\mathbf{R}_i)=1$ for $\mathbf{R}_i$ at A sublattice and -1 for $\mathbf{R}_i$ at B sublattice. The Hamiltonian (1) becomes

$$H=-t\sum_{\langle i,j\rangle}(\bar{c}_{i,\sigma}^{\dagger}\bar{c}_{j,\sigma}+\text{H.c.})-U\sum_i\bar{n}_{i,\uparrow}\bar{n}_{i,\downarrow}+U\sum_i\bar{n}_{i,\uparrow}\ . \tag{3}$$

If $n_{\uparrow}=n_{\downarrow}=(1-\delta)/2$ for the original particles, we have that $\bar{n}_{\uparrow}=(1-\delta)/2$ and $\bar{n}_{\downarrow}=(1+\delta)/2$, so that there are more down-spin particles than up-spin ones for the transformed particles. In the large U case, all up-spin particles will be paired with $N(1-\delta)/2$ down-spin particles, or else there will be an energy cost U for each unpaired particle, as seen from (3). There is a gap U between the upper and lower bands. In the lower band, we have $N(1-\delta)/2$ pairs and δN unpaired particles. We introduce the fermion operators h_i for the unpaired particles and the operators $b_i^{\dagger}=c_{i,\uparrow}^{\dagger}\bar{c}_{i,\downarrow}^{\dagger}$ for pairs, which can be shown to satisfy the hard-core boson commutation relation. For each site there are three possible states, which are $b_i^{\dagger}|0\rangle$, $h_i^{\dagger}|0\rangle$, and $|0\rangle$. The usual second-order perturbation theory then gives the effective Hamiltonian of (3) as

$$\begin{aligned}H=&-t\sum_{\langle i,j\rangle}[h_i^{\dagger}h_jb_j^{\dagger}b_i+h_i^{\dagger}h_j(1-N_i^b)(1-N_j^b)+\text{H.c.}]\\&-J\sum_{\langle i,j\rangle}[b_i^{\dagger}b_j(1-N_i^h)(1-N_j^h)-N_i^bN_j^b-N_i^bN_j^h]\\&-J\sum_i b_i^{\dagger}b_i\ ,\end{aligned} \tag{4}$$

where $J-4t^2/U$, $N_i^b-b_i^{\dagger}b_i$, and $N_i^h-h_i^{\dagger}h_i$. The terms involving more than two sites have been neglected in (4). A similar effective Hamiltonian valid in the case of $J\rightarrow 0$ was derived earlier by Batiev.[22] The Hamiltonian (4) should be an alternative description of the usual t-J model.

In one dimension, one can transform hard-core bosons into fermions by the Jordan-Wigner transformation

$$b_j=f_j\exp\left[i\pi\sum_{l<j}f_l^{\dagger}f_l\right]\ . \tag{5}$$

The previous restricted Hilbert space is now equivalent in the new fermionic variables to the condition that no site is doubly occupied. We use the Gutzwiller projector to take into account this constraint. Denoting h_i by $d_{i\uparrow}$ and f_i by $d_{i\downarrow}$, the variational wave function has the familiar form

$$|\psi\rangle=\prod_i[1-(1-g)n_{i\uparrow}^dn_{i\downarrow}^d]|\phi\rangle\ , \tag{6}$$

where $|\phi\rangle$ is taken to be the free-fermion sea of $d_{i\uparrow}$ and $d_{i\downarrow}$, and $g=0$ here.

We note that

$$\langle\psi|d_{i\uparrow}^{\dagger}d_{j\uparrow}(1-N_{i\downarrow}^d)(1-N_{j\downarrow}^d)|\psi\rangle\equiv\langle\psi|d_{i\uparrow}^{\dagger}d_{j\uparrow}|\psi\rangle\ .$$

We can therefore rewrite (4) for the trial function (6) as

$$\begin{aligned}H=&-t\sum_{\langle i,j\rangle}(d_{i\uparrow}^{\dagger}d_{j\uparrow}d_{j\downarrow}^{\dagger}d_{i\downarrow}+\text{H.c.})-t\sum_{\langle i,j\rangle}(d_{i\uparrow}^{\dagger}d_{j\uparrow}+\text{H.c.})\\&-J\sum_{\langle i,j\rangle}(d_{i\downarrow}^{\dagger}d_{j\downarrow}-N_{i\downarrow}^dN_{j\downarrow}^d-N_{i\downarrow}^dN_{j\uparrow}^d)-J\sum_i n_{i\downarrow}^d\ ,\end{aligned} \tag{7}$$

which is the effective Hamiltonian we will discuss below.

In this paper we will take $n_{\uparrow}^d=n_{\downarrow}^d$, which implies $\delta=\frac{1}{3}$. It is only in this case that expectation values can easily be evaluated analytically. Nevertheless, certain general features of our approach can be identified from this specific case.

The ground-state energy $E=\langle\psi|H|\psi\rangle$ can be expressed as

$$\begin{aligned}\frac{E}{N}=&-t\frac{1}{N}\sum_q\varepsilon[n_{q,\uparrow}^d-\langle S_d^+(q)S_d^-(-q)\rangle]\\&-\frac{J}{2}\frac{1}{N}\sum_q\varepsilon_q[n_{q,\downarrow}^d-\langle\rho_{\downarrow}^d(q)\rho_{\downarrow}^d(-q)\rangle\\&-\langle\rho_{\uparrow}^d(q)\rho_{\downarrow}^d(-q)\rangle]-J(1-\delta)/2\ ,\end{aligned} \tag{8}$$

where $\rho_{\sigma}^d(1)=\sum_k d_{k+q,\sigma}^{\dagger}d_{k,\sigma}$ and $\varepsilon_q=2\cos q$. It can be easily shown that

$$\begin{aligned}&\langle S_d^+(q)S_d^-(-q)\rangle=C_d^{SS}(q)/2\ ,\\&\langle\rho_{\downarrow}^d(q)\rho_{\downarrow}^d(-q)\rangle=[C_d^{SS}(q)+C_d^{NN}(q)]/4+(n_{\downarrow}^d)^2\delta_{q,0}\ ,\\&\langle\rho_{\uparrow}^d(q)\rho_{\downarrow}^d(-1)\rangle=[C_d^{SS}(q)-C_d^{NN}(q)]/4+n_{\uparrow}^dn_{\downarrow}^d\delta_{q,0}\ .\end{aligned} \tag{9}$$

Here C_d^{SS} and C_d^{NN} are, respectively, the pseudospin and density correlation functions of d particles, and are defined by

$$\begin{aligned}&C_d^{SS}(q)=\langle S_d^z(q)S_d^z(-q)\rangle-(S^z)^2\delta_{q,0}\ ,\\&C_d^{NN}(q)=\langle\rho^d(q)\rho^d(-q)\rangle-(\rho^d)^2\delta_{q,0}\ ,\end{aligned} \tag{10}$$

where $S_d^z(q)\equiv\rho_{\uparrow}^d(q)-\rho_{\downarrow}^d(q)$ and $\rho^d(q)=\rho_{\uparrow}^d(q)+\rho_{\downarrow}^d(q)$. $C_d^{SS}(q)$ and $C_d^{NN}(q)$ have already been found analytically in Ref. 15, and for convenience, we list them here

$$C_d^{SS}(q)=\begin{cases}-\ln(1-Q)\ , & 0\le|Q|\ge\bar{n}\\ -\ln(1-\bar{n})\ , & \bar{n}\le|Q|\le 1\ ;\end{cases}$$

$$C_d^{NN}(q)=\begin{cases}Q\left[1-\frac{1}{2}\ln\frac{F(\bar{n}-Q)}{F(\bar{n})}\right]\ , & 0\le|Q|\le 2(1-\bar{n})\\ 2(1-\bar{n})+\frac{Q}{2}\ln\frac{F(n'-Q)}{F(\bar{n}-Q)}\ , & 2(1-\bar{n})\le|Q|\le\bar{n}\\ 2(1-\bar{n})+\frac{Q}{2}\ln\frac{F(n'-Q)}{F(Q-\bar{n})}+\ln F(Q-\bar{n})\ , & \bar{n}\le|Q|\le 1\ .\end{cases} \tag{11}$$

Here $F(x)=1-x$, $Q\equiv q/\pi$, $n'\equiv 2-\bar{n}$, and $\bar{n}=(1+\delta)/2$. $n_{q\sigma}^d$ in Eq. (8) has also been formulated in Ref. 14 and can be determined by a recursive calculation. From these expressions and (8), we obtain the energy

$$E/N=-2\alpha t-\beta J\ . \tag{12}$$

We find $\alpha=0.2603$ and $\beta=0.2565$. For the usual GWF, $\alpha_G=0.2448$ and $\beta_G=0.4896$. Using the Bethe ansatz and perturbation theory for small J, Ogata and Shiba[23] obtained $\alpha_B=0.2757$ and $\beta_B=0.2554$. Compared with the exact solution, the present result is better than that for the usual GWF.

In our description, the kinetic energy of the up-spin electrons is given by the second term in the first brackets of (8), which is equal to $-\alpha' t=-0.2758t$. It is surprising that α' equals, to within numerical accuracy, α_B, the value obtained using the Bethe ansatz, implying that we have a very good description for the motion of up-spin electrons in the small-J limit. We analyze this result as follows. The electron kinetic term is usually written as $T=-\sum_{q,\sigma}\varepsilon_q n_\sigma(q)$, with $n_\sigma(q)$ the electron distribution function. We can formally write the kinetic term in (8) as $\bar{T}=-t\sum_{q,\sigma}\varepsilon_\sigma \bar{n}_\sigma(q)$, where $\bar{n}_\sigma(q)$ is a pseudoelectron-distribution function, as will be briefly discussed later. $\bar{n}_\sigma(q)$ is shown in Fig. 1. $\bar{n}_\uparrow(q)$ (the solid curve) is a continuous function at the Fermi surface, whereas in the usual GWF case the distribution function, shown by the dashed curve in Fig. 1, has a jump at the Fermi surface. As the real electron distribution function $n_\sigma(q)$ is continuous at the Fermi surface, the kinetic energy of up-spin electrons in the present description is expected to be better. However, for down-spin electrons, $\bar{n}_\downarrow(q)$ given by the first term in the first brackets of (8) is the same as the distribution function of the usual GWF (the dashed curve of Fig. 1). It will fail to give a good energy, as observed by Metzner and Vollhardt[14] for the Hubbard model in the strong correlation limit.

The real electron spin-correlation function $C_R^{SS}(q)$ and the density correlation function $C_R^{NN}(q)$ can be defined in a similar way to (10). It is easily shown that $C_R^{SS}(q)$ and $C_R^{NN}(q)$ have the following relations with the pseudospin and density correlation functions $C_d^{SS}(q)$ and $C_d^{NN}(q)$:

$$C_R^{SS}(q)=[C_d^{SS}(q)+9C_d^{NN}(q)]/4 \; , \qquad C_R^{NN}(q)=[C_d^{SS}(q)+C_d^{NN}(q)]/4 \; . \tag{13}$$

Figure 2 shows the spin-correlation functions for the usual GWF (dashed curve) and for our wave function (solid curve). $C_R^{SS}(q)$ has a sharp cusp at $q=2k_F$, and decreases as q increases, in contrast to the q-independent behavior for the usual GWF. This feature is qualitatively in agreement with the Monte Carlo simulations.[23] This means we have a rather good description for correlations of spins and holes at short range (i.e., large q). However, for small q, $d^2C_R^{SS}/dq^2>0$, not less than zero, as seen in the numerical calculations. This unpleasant feature is a result of the asymmetry of the trial wave function for up- and down-spin states.

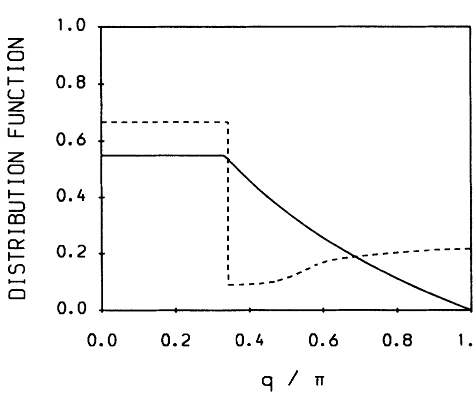

FIG. 1. The distribution function used for the kinetic energy. The solid line and the dashed line correspond to up- and down-spin electrons, respectively.

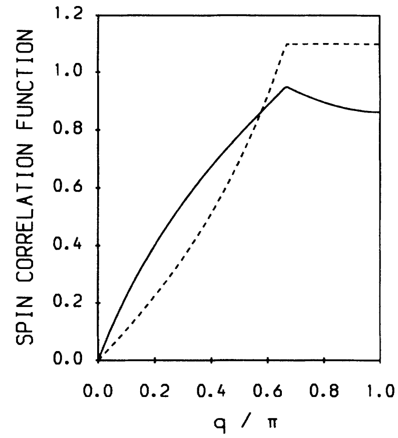

FIG. 2. The spin correlation function $C_R^{SS}(q)$. The present result (solid curve) is compared with that for the usual GWF.

The density correlation function can be easily shown to be equal to the hole-hole correlation function $C_R^{HH}(q)$.[13] For $J\to 0$, the hole correlation is just the density correlation of the free spinless fermions, the exact result for which is shown in Fig. 3 by the dotted curve. The density correlation functions of the present work and the usual GWF are shown by the solid and the dashed curves. The density correlation we obtain is close to the exact result, and is much better than that for the usual GWF.

Now we briefly discuss the electron momentum distribution. In the present description, an up-spin electron is actually represented by a fermion and a boson [or a fermion with a phase given by (5)]. The momentum distribution function $n_\uparrow(k)$ is

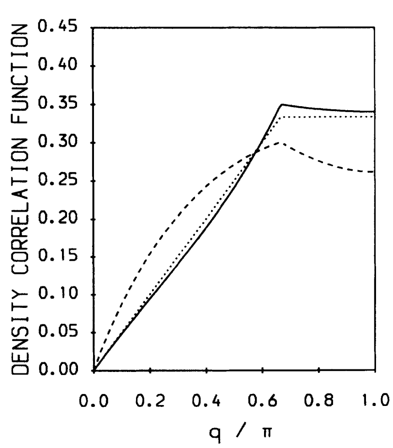

FIG. 3. The density correlation function $C_R^{NN}(q)$. The present result (solid curve) is compared with the exact result (dotted curve) of $J\to 0$ and that for the usual GWF (dashed curve).

$$n_\uparrow(k)=\frac{1}{N}\sum_{jl}\langle c_{j\uparrow}^{+}c_{l\uparrow}e^{i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{R}_l)}\rangle=\frac{1}{N}\sum_{jl}\left\langle h_j^\dagger h_l f_l^\dagger\left\{\exp\left[-i\pi\left[\sum_{n<l}f_n^\dagger f_n-\sum_{n'<j}f_{n'}^\dagger f_{n'}\right]\right]\right\}f_j\right\rangle e^{i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{R}_l)} , \quad (14)$$

which would usually need to be calculated numerically. A very similar expression has been evaluated by Weng *et al.*[24] who obtained, using the bosonization technique, $n(k)$, which agrees with the exact result for the limit $J\to 0$

$$n(k)\sim n(k_F)-c|k-k_F|^{1/8}\,\mathrm{sgn}(k-k_F) . \quad (15)$$

On this basis we would expect that $n_\uparrow(k)$ calculated from Eq. (14) should give reasonable results. In contrast, the momentum distribution for down-spin electron $n_\downarrow(k)$ is

$$n_\downarrow(k)=1-\langle h_{Q+k}^\dagger h_{Q+k}\rangle-\frac{1}{N}\sum_{jl}\left\langle h_j^\dagger h_l f_l^\dagger\left\{\exp\left[-i\pi\left[\sum_{n<l}f_n^\dagger f_n-\sum_{n'<j}f_{n'}^\dagger f_{n'}\right]\right]\right\}f_j\right\rangle e^{i(\mathbf{Q}\,\mathbf{k})\cdot(\mathbf{R}_j-\mathbf{R}_l)} . \quad (16)$$

As there is a jump at $Q+k=k_F$ for $\langle h_{Q+k}^\dagger h_{Q+k}\rangle$, there will be a discontinuity for $n_\downarrow(k)$.

In this paper we have derived an effective Hamiltonian equivalent to the *t-J* model. This Hamiltonian is represented by one kind of boson and one kind of fermion. Applying the Gutzwiller projection to these two kinds of particles, we have obtained analytically the energy and the spin and density correlation functions. Our trial wave function, though simple, improved the usual Gutzwiller wave function and could produce almost perfect properties in some cases, such as the energy for electrons with one kind of spin and the density correlation function. However, for the other spin (say, down-spin) electrons, our wave function, based on the same approximation as the usual Gutzwiller wave function, failed to give a good description. The trial wave function proposed by Hellberg and Mele[18] has the correct spin symmetry. But there are still some deviations of the energy they obtained from the exact one. From the present study we find that projecting out the double occupancy of a site by a spin and a hole can give good results for the energy. A trial function with not only this feature but also with the correct spin symmetry would be interesting. This is planned to be the subject of further investigation.

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