Improved wave function for strongly correlated electronic systems

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A scheme of optimization of a trial wave function in the variational Monte Carlo calculation is developed. It provides a more precise description of the ground state for strongly correlated electronic systems with highly improved trial wave function. A general type of variational wave function constructed from a linear combination of Slater determinants multiplied by Jastrow correlation factors is proposed. They can explicitly contain low-energy fluctuations and long-range correlations. Using this optimization method, we examine the properties of these wave functions by applying them to a one-dimensional Hubbard model for which the exact solution is available for comparison. It is found that these wave functions prove to be substantial improvements compared to the conventional Jastrow-type wave functions.

I. INTRODUCTION

The discovery of high-T_c copper-oxide superconductors has renewed the interest in strongly correlated electronic systems of low dimensions.[1] The Hubbard model is one of the simplest models for such strongly correlated systems. Although much effort has been devoted to elucidating this basic problem by using both analytical and numerical techniques, our understanding is still insufficient.

The variational Monte Carlo (VMC) method is one of the most powerful and transparent approaches for understanding strongly correlated electronic systems. It overcomes the limitation of having to deal with only small-size lattices. In addition, it is quite successful in describing the nature of the correlated systems and provides a deeper insight because of its explicit form of the wave function.

Most VMC studies for strongly correlated electrons have been limited to the Gutzwiller wave function, which takes into account only the on-site correlation.[2,3] Recently, Yokoyama and Shiba have pointed out the need to go beyond the Gutzwiller function and made improvements to estimate some physical quantities using a Jastrow-type wave function for the Hubbard model.[4] It was also shown by several authors that the Jastrow-type wave function has the potential to describe the ground-state properties of a t-J model over the entire phase diagram.[5–7] These wave functions, however, contain only a few variational parameters and are insufficient to understand completely the ground state of strongly correlated systems. Thus, the need to construct better wave functions has been increasing recently.

The conventional procedure for minimizing variational energy, which requires direct evaluation of energies at each mesh point in a variational parameter space, does not allow one to increase the number of parameters and limits improvement of the trial wave function. Therefore, it is very important to develop a method suitable for multiparameter optimization. In this paper, we use Powell's optimization algorithm[8] combined with the fixed sampling in VMC calculations and succeed in extending variational space. This method makes it possible to obtain a more precise description of the ground state of strongly correlated electronic systems.

Another purpose of this paper is to show that, in addition to the improvement in the Jastrow-type correlation factor, low-energy fluctuations play an important role in investigating the ground state of strongly interacting electrons. For this, we propose a new class of variational wave functions that consist of a linear combination of Slater determinants multiplied by Jastrow-type correlation factors. They can explicitly contain low-energy fluctuations such as particle-hole excitations and long-range intersite correlations.

Using this optimization method in VMC calculations, we test the validity of these new wave functions by applying them to the one-dimensional (1D) Hubbard model, for which comparisons of evaluated physical quantities can be made with those by exact solutions or other trial functions. It is shown that these wave functions are superior to other trial functions proposed, particularly for the half-filled band.

This paper is organized as follows. In Sec. II, the general formulation of the optimization procedure is described in detail, and our trial functions are introduced in Sec. III. Section IV provides the results of computations of physical quantities for the 1D Hubbard model. Section V is devoted to a summary and discussions on related problems.

II. FORMULATION

We use the VMC technique to study the ground-state properties of the strongly correlated electronic systems. The variational principle guarantees that it provides an

upper bound for the estimate of ground-state energy of a physical system. Its principal advantage lies in the presumption that the lower the variational estimate of the ground-state energy, the better the wave function, and that reasonable correlations can be introduced directly into the trial functions using physical considerations.

In the VMC method, the expectation values of physical quantities are calculated on the basis of the Metropolis algorithm[9] and the form of trial wave function ψ_T is adjusted so as to arrive at the energy minimum by varying all parameters in ψ_T. One alternative for optimizing ψ_T is to minimize the variance of the variational energy[10,11] $\langle\psi_T|(H-E_R)^2|\psi_T\rangle/\langle\psi_T|\psi_T\rangle$. Minimization of the variance, however, does not always mean the energy minimum and is ambiguous in determining reference energy E_R, which strongly influences the optimization stability. For these reasons we adopt the optimization criterion in which the variational energy is minimized within the statistical error.

For a system with Hamiltonian H, the variational energy as a functional of ψ_T is given by

$$\bar{E}[\psi_T]=\frac{\langle\psi_T|H|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle}=\frac{\int[H\psi_T(\mathbf{R})/\psi_T(\mathbf{R})]w(\mathbf{R})|\psi_C(\mathbf{R})|^2d\mathbf{R}}{\int w(\mathbf{R})|\psi_C(\mathbf{R})|^2d\mathbf{R}}\ , \tag{1}$$

where

$$w(\mathbf{R})=|\psi_T(\mathbf{R})|^2/|\psi_C(\mathbf{R})|^2$$

and $\mathbf{R}$ denotes the coordinates of N_e electrons. An arbitrary function ψ_C is introduced in Eq. (1) for later convenience of computation. In VMC calculations, the integrals over $\mathbf{R}$ are replaced by the importance sampling and then Eq. (1) is written as

$$\bar{E}[\psi_T]\simeq\sum_{\{\psi_C\}}\frac{H\psi_T}{\psi_T}w\Big/\sum_{\{\psi_C\}}w\ , \tag{2}$$

where the sums are taken over a finite set of coordinates of electrons sampled with the probability distribution $|\psi_C|^2$. The weight function w is the relative probability of choosing an electron configuration and exactly compensates the difference between ψ_T and ψ_C in the limit of an infinite number of samples.

To have the energy minimum we must optimize the parameters contained in ψ_T, and we employ the fixed-sample method,[11] where the same distribution function $|\psi_C|^2$ and the same random walk are used during the optimization process to avoid ensemble dependence. This absence of stochastic uncertainty makes it possible to use more efficient search techniques in finding the minimum.

We proceed with the optimization of parameters by successive iterations. This is a practical improvement over the conjugate-gradient method by Powell[8] in the numerical computation. It consists of a sequence of minimizations of $\bar{E}$ along a conjugate set of directions $\mathbf{u}$'s in a variational parameter space. Its essence is as follows, where the dimension of the variational parameter space is N.

We start with a set $\mathbf{C}_0$ of suitably valued parameters in a trial function ψ_T, and put $\psi_C=\psi_T(\mathbf{R};\mathbf{C}_0)$, so that $w=|\psi_T/\psi_C|^2=1$ at first. The conjugate set of directions $\mathbf{u}_i$ is initially set as unit vectors $\mathbf{e}_i$. Then for $i=1,\ldots,N$ we put

$$\mathbf{C}^{(i)}=\mathbf{C}^{(i-1)}+\lambda_i\mathbf{u}_i\ ,$$

where $\mathbf{C}^{(0)}$ is initially set as $\mathbf{C}_0$; with $\psi_T(\mathbf{R};\mathbf{C}^{(i)})$ and $\psi_C(\mathbf{R};\mathbf{C}_0)$ we obtain the temporary minimum of energy by adjusting λ_i at each step. Note that the parameters in ψ_C are unchanged, and now

$$w=|\psi_T(\mathbf{R};\mathbf{C}^{(i)})|^2/|\psi_C(\mathbf{R};\mathbf{C}_0)|^2\neq 1\ .$$

Next, $\mathbf{u}_i$ is replaced by $\mathbf{u}_{i+1}$ for $i=1,\ldots,N-1$ while $\mathbf{u}_N$ is replaced by $\mathbf{C}^{(N)}-\mathbf{C}^{(0)}$, the average direction moved after trying all N possible directions. Then we adjust λ_N in $\mathbf{C}^{(N+1)}=\mathbf{C}^{(N)}+\lambda_N\mathbf{u}_N$ to obtain the new temporary minimum of $\bar{E}$, and $\mathbf{C}^{(0)}$ is replaced by $\mathbf{C}^{(N+1)}$ but the parameters in ψ_C are still unchanged.

Repeating the process above until all parameters converge, we arrive at the best of parameters $\mathbf{C}^{(*)}$. The role of function w is monitoring to check if the change of ψ_T from the initial form ψ_C becomes too large. If the change goes beyond the criterion at $\mathbf{C}^{(k)}$, the optimization procedure must restart with $\psi_T(\mathbf{R};\mathbf{C}^{(k)})$ and $\psi_C(\mathbf{R};\mathbf{C}^{(k)})$ again.

With the repeated cycles of successive minimizations, $\bar{E}$ converges rapidly to the minimum. Notice that the choice of successive directions does not need explicit computation of the gradient of $\bar{E}$ with respect to $\mathbf{C}$ in contrast to Newton's method.

Once the fully optimized wave function $\psi_T(\mathbf{R};\mathbf{C}^{(*)})$ is obtained, it is used in evaluating the physical quantities with another VMC run.

III. TRIAL WAVE FUNCTION

In this section, we present a new class of variational wave functions for strongly interacting lattice fermions. A single Slater determinant composed of single-particle states multiplied by the Jastrow-type two-body correlation factor is fairly common in the variational theory. The Gutzwiller wave function, which is a prototype of the trial function of this type, has been extensively used for strongly correlated systems.[2,3,6,12] However, it is unsatisfactory on many points, since it involves only the on-site correlation, and various attempts to extend the variational parameter space have been made. For the Hubbard model, Yokoyama and Shiba[4] introduced the attractive correlation between empty and doubly occupied sites in the half-filled case, and a Jastrow-type intersite correlation in the non-half-filled case, to be multiplied respectively by the Gutzwiller function. For the t-J model, repulsive or attractive Jastrow-type correlations with a Gutzwiller projector are proposed by several authors.[5-7] In addition, spin-spin, as well as spin-fermion, correlations are included in Jastrow-type functions for other strongly correlated models.[13-15]

However, these trial wave functions can reproduce only a fraction of the true ground-state energy. The pri-

mary deficiency of the single Slater determinant expression is the inadequate treatment of the low-energy fluctuations. We include them in our wave function in more general ways. For this purpose, we begin with a linear combination of Slater determinants, each of which corresponds to an n-particle excited state ($n=0,1,2,\ldots$),

$$\psi=\left[1+\sum h^{\mu}_{\nu}c^{\dagger}_{\mu s}c_{\nu s}+\sum h^{\mu\nu}_{\tau\rho}c^{\dagger}_{\mu s}c^{\dagger}_{\nu s'}c_{\tau s}c_{\rho s'}+\cdots\right]\psi_0 \tag{3a}$$

$$\equiv\sum_{k=0}\psi^{(k)}\ , \tag{3b}$$

where ψ_0 is an uncorrelated Slater determinant composed of single-particle states, $\psi^{(k)}$ corresponds to each term in Eq. (3a), and Greek indices denote either wave vector or lattice site, depending on the method of representation. ψ represents the configuration interaction in either momentum space or real space. In the latter case, multisite correlation in off-diagonal form, which needs rearrangement of particle configurations in both hopping and interacting processes, can be easily introduced.

If the sums in Eq. (3) are taken over all possible configurations, the expansion is complete in a given Hilbert space. The exact solution would be obtained by diagonalizing $\langle\psi^{(l)}|H|\psi^{(k)}\rangle$ in this case. However, this is not practical except for very small lattice sizes. In practice, the expansion is truncated, and an approximate wave function can be obtained. After some selections from the terms in Eq. (3) and classifying them into diagonal and off-diagonal terms, we arrive at the following trial wave function as a subset of ψ:

$$\psi_t=\left[1+h\sum_{ij\sigma}Fc^{\dagger}_{i\sigma}c_{j\sigma}\right]F\psi_F\ , \tag{4}$$

where $c_{j\sigma}$ ($c^{\dagger}_{j\sigma}$) annihilates (creates) an electron with spin σ on the jth lattice site, ψ_F denotes a filled Fermi sea, and the coefficient h is determined variationally. A correlation factor of diagonal form, F, is introduced into ψ_t in order to take into account site-dependent correlations in $c^{\dagger}_{i\sigma}c_{j\sigma}\psi_F$ as well as in ψ_F. Particle-hole excitations are explicitly contained in ψ_t. With this wave function, we can explicitly express the successive hopping of electrons.

We examine this wave function by applying it to the 1D Hubbard model, which is not only one of the simplest models for strongly correlated electrons, but also a candidate for a realistic model of superconducting copper oxides. The Hamiltonian is given as

$$H=-t\sum_{\langle ij\rangle\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\ , \tag{5}$$

where the notation is a standard one. In the following, we take the lattice constant as the unit of distance. In order to simplify our calculations, we restrict the transfers of electrons in ψ_t to the nearest neighbor in accordance with the Hamiltonian (5).

Next, we consider the correlation factor for the half-filled case (i.e., $n_e=N_e/N_s=1$, N_s is the total number of sites) where the Mott-Hubbard-type metal-insulator transition[16] is an important problem. It is pointed out that attractive correlation between empty and doubly occupied sites has an important effect in this case.[4,17] We include it in the correlation factor in long-range form:

$$F_H=\prod_{[ij]}[1-\{1-\eta(r_{de})\}d_ie_j]\ , \tag{6}$$

where $d_i=n_{i\uparrow}n_{i\downarrow}$, $e_j=(1-n_{j\uparrow})(1-n_{j\downarrow})$, and $[ij]$ denotes a d-e pair. When η takes the same value for all r_{de} (distance between the empty and doubly occupied sites), F_H reduces to the Gutzwiller projector. For large U/t, it is expected that the weight of the state having doubly occupied sites decays rapidly with r_{de}. Thus, the function η is approximated as

$$\eta(r_{de})=\begin{cases}\eta_1 & \text{if } r_{de}=1\\ \eta_2 & \text{if } r_{de}=2\\ \alpha/r_{de}^{\beta} & \text{otherwise}\ .\end{cases} \tag{7}$$

We note that only the nearest-neighbor correlation between the empty and doubly occupied sites was considered in the previous VMC studies.[4,18]

Equations (4), (6), and (7) constitute our trial wave function for the half-filled Hubbard model:

$$\psi_H=\left[1+h\sum_{\langle ij\rangle\sigma}F_Hc^{\dagger}_{i\sigma}c_{j\sigma}\right]F_H\psi_F\ . \tag{8}$$

As a result, we have five variational parameters, i.e., h, η_1, η_2, α, and β. They are optimized by the method stated in Sec. II.

The second case is the less-than-half-filled system ($n_e<1$), where the problem of the stability of the Tomonaga-Luttinger Fermi liquid state[19,20] is very important in the strong-coupling regime. In the presence of many empty sites, a crucial defect in the previous studies is the lack of precise description of the long-range intersite correlation. We take the following long-range correlation factor of Jastrow type:

$$F_Q=\prod_{ij}\prod_{\sigma\sigma'}[1-\{1-\xi(r_{ij})\}n_{i\sigma}n_{j\sigma'}]\ , \tag{9}$$

where $r_{ij}=|r_i-r_j|$ is the distance between the ith and jth sites, and we assume the form of function $\xi(r_{ij})$ to be

$$\xi(r_{ij})=\begin{cases}\xi_l & \text{if } r_{ij}=l\quad(l=0,\ldots,6)\\ \exp(-\gamma/r_{ij}) & \text{if } r_{ij}\geq 7\ .\end{cases} \tag{10}$$

Thus, the degree of freedom in variational parameter space is fairly large compared to that in Ref. 4. Equations (4), (9), and (10) constitute our trial wave function for the less-than-half-filled Hubbard model as

$$\psi_Q=\left[1+h\sum_{\langle ij\rangle\sigma}F_Qc^{\dagger}_{i\sigma}c_{j\sigma}\right]F_Q\psi_F\ , \tag{11}$$

in which nine variational parameters are contained, i.e., h, $\xi_0,\ldots,\xi_6$, and γ. When ξ is restricted to the on-site correlation ξ_0 only, then F_Q reduces to the Gutzwiller projector. Note that when $\xi_0=0$ we deal with the subspace without a doubly occupied site for the Hubbard model with $U=\infty$. We take the quarter filling ($n_e=\frac{1}{2}$) as a typical example of a less-than-half-filled system.

IV. RESULTS

We present the results of our VMC calculations where comparisons with those by exact solutions and other trial wave functions are made. We consider the 1D Hubbard chain with 50 sites for the half-filled band, and with 60 sites for the quarter-filled band under the periodic boundary condition. In these cases, no degeneracy occurs in ψ_F. The variational parameters are determined by the optimization procedure stated in Sec. II. Once the fully optimized wave function is obtained, we use it to evaluate the total energy, spin- , and charge-correlation functions in Fourier-transformed form,

$$S(k)=\frac{1}{4N_s}\sum_{ij} e^{ik(r_i-r_j)}\langle (n_{i\uparrow}-n_{i\downarrow})(n_{j\uparrow}-n_{j\downarrow})\rangle \ , \tag{12}$$

$$C(k)=\frac{1}{N_s}\sum_{ij} e^{ik(r_i-r_j)}\{\langle (n_{i\uparrow}+n_{i\downarrow})(n_{j\uparrow}+n_{j\downarrow})\rangle - \langle n_{i\uparrow}+n_{i\downarrow}\rangle\langle n_{j\uparrow}+n_{j\downarrow}\rangle\} \ , \tag{13}$$

and the momentum-distribution function

$$n(k)=\tfrac{1}{2}\sum_{ij\sigma} e^{ik(r_i-r_j)}\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle \ . \tag{14}$$

We employ the Monte Carlo algorithm in which a new configuration is generated by the motion of a single particle and/or by the interchange of two particles with opposite spin. We collect typically 2×10^4 samples for the optimization of the variational parameters and $3\times(10^4-10^5)$ samples for the evaluation of the observables. To keep the statistical independence of these samples, we take long enough thermalization and sampling intervals to achieve a reasonable acceptance ratio.

The optimization of the variational parameters was well accomplished with convergence rapid enough to handle a large parameter space. The optimal values of variational parameters show the following general behaviors: For the half-filled band, η in Eq. (7) decays rapidly with r_{de} and η_1 decreases with increasing U/t, as expected. As an example, the minimum energy is realized for $\eta_1\sim0.5$, $\eta_2\sim0.4$, $\alpha\sim0.6$, and $\beta\sim0.4$ for $U/t=4$. For $n_e=\frac{1}{2}$, ξ in Eq. (10) gradually increases toward unity with r_{ij} and the on-site correlation ξ_0 decreases with increasing U/t. This suggests that the correlation by the prefactor F_Q is repulsive in the quarter-filled case. For example, the optimal values of $\xi_0\sim0.3$ and $\xi(r_{ij})$ with $r_{ij}\geq1$ are between 0.7 and 1 for $U/t=4$. In both cases, the optimal value of h monotonically increases with U/t, leading to the virtual process causing the exchange coupling by the successive hopping of electrons. In the following, we present the results of the physical quantities evaluated with the optimized wave functions.

A. Half-filled band

We start with the results of the total energy per site, E, in the half-filled case. In Fig. 1, the total energy for ψ_H is plotted as a function of U/t, and is compared with those for the Gutzwiller function ψ_G and the exact solution for the infinite systems by Bethe ansatz.[21] The present value of variational energy is greatly improved, particularly for a large value of U/t, and is fairly close to the exact one. The agreement is within $\sim6\%$. Notice that a sizable lowering of the energy is achieved compared to the Gutzwiller function in the whole U/t region. For a large U/t regime, the energy of ψ_G departs appreciably from that by the exact solution, in contrast to ψ_H. In fact, the perturbation expansion from the strong-coupling limit[22] shows that the exact energy behaves as $E\propto -t^2/U$ while ψ_G leads to $E\propto -t^2/[U\ln(U/t)]$ for $U/t\to\infty$, as shown by the analytic calculation.[23] The Gutzwiller wave function includes only the on-site correlation, in which the weights of electron configurations are not effectively classified by their mobility or r_{de}, i.e., all configurations with a given number of doubly occupied sites have the same weight in the subspace. On the other hand, a large fraction of the true ground-state energy is recovered by our trial wave function ψ_H, in which the particle-hole excitation, together with the long-range correlation between empty and doubly occupied sites, is properly included.

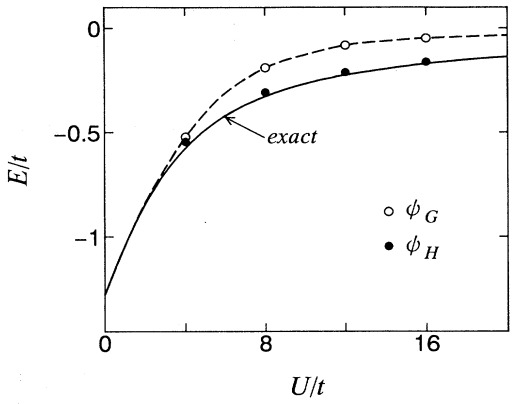

FIG. 1. Total energy per site of the 1D half-filled Hubbard model as a function of U/t, evaluated by VMC calculations with ψ_H (filled circles). A comparison is made with those by ψ_G (open circles) and the exact solution (Ref. 21) from the Bethe ansatz for the infinite systems (solid line).

Next, we show the results of spin- and charge-correlation functions in Fig. 2 for some values of U/t. The charge fluctuation $C(k)$ tends to be suppressed by the correlation effect as shown in comparison with $U/t=0$. On the other hand, the spin-correlation function $S(k)$ is considerably enhanced at $k=\pi$, indicating well-known long-range antiferromagnetic correlation. The $U/t\to\infty$ limit of the half-filled Hubbard model corresponds to the $S=\frac{1}{2}$ antiferromagnetic Heisenberg model for which the exact result[24] of $S(k)$ is available for small system sizes ($N_s=26$). The present result of $S(k)$ for $U/t=16$ is fairly close to the exact one, as shown in Fig. 2.

Let us now discuss the result of the momentum-distribution function. The inclusion of only the nearest-neighbor correlation between empty and doubly occupied sites[4] into ψ_G leads to an insufficient description of $n(k)$ for small U/t. In this case, $n(k)$ has an apparent jump at

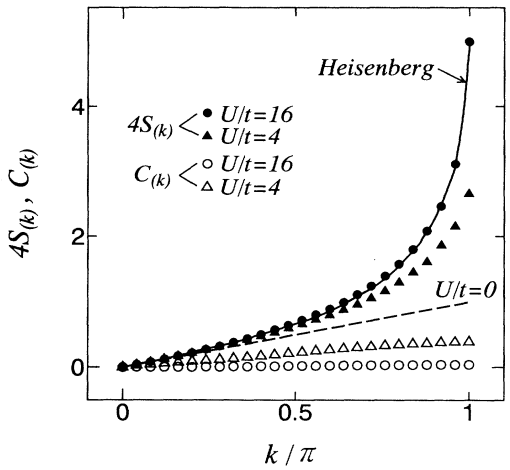

FIG. 2. Spin- and charge-correlation functions $S(k)$ and $C(k)$ for the half-filled case at $U/t=0$ (broken line), 4 (triangles), and 16 (circles). Filled symbols represent $4S(k)$, while open ones represent $C(k)$. Note $4S(k)$ is equal to $C(k)$ when $U/t=0$. The exact result of $4S(k)$ for the 1D and $S=\frac{1}{2}$ Heisenberg model (Ref. 24) is also shown (solid line).

the Fermi surface leading to metallic behavior. This will not be true in our model. At half filling, an insulating state is expected for which $n(k)$ has no discontinuity at k_F. The present result shows a reasonable improvement, as shown in Fig. 3. An insulating behavior expected for the half-filled band is recovered for large U/t: It seems that $n(k)$ is a smoothly decreasing function and the data near k_F are well fitted with a linear function. These are consistent with the result by the boundary condition integration technique.[25] Moreover, the perturbation calculation for the half-filled Hubbard model in the strong-coupling limit[26] gives the explicit form

$$n(k)=\frac{1}{2}+\frac{4t\ln 2}{U}\cos k+O[(t/U)^3]\ . \tag{15}$$

The VMC result for $U/t=16$ agrees well with Eq. (15), as shown in Fig. 3. Therefore, ψ_H represents an insulating state in the strong-coupling regime.

For $U/t=4$, we have also calculated $n(k)$ using the wave function $\psi'_H=F_H\psi_F$, which includes only the correlation between empty and doubly occupied sites, i.e., $h=0$ in ψ_H. The result is shown by the open triangles in Fig. 3. Comparison with the result for ψ_H with the optimal value of $h\sim 1$ (closed triangles) shows that the particle-hole excitation has a crucial effect in the improvement of $n(k)$. However, the question remains as to whether or not the discontinuity at $k=k_F$ for small U/t vanishes in the limit of an infinite number of lattice sites. The introduction of long-range transfers of electrons in ψ_H may be necessary, although we have restricted the transfers to the nearest neighbor.

B. Less-than-half-filled band

This subsection shows the result for the less-than-half-filled case evaluated with the fully optimized trial function in the form of Eq. (11). We consider the quarter-filled ($n_e=\frac{1}{2}$) Hubbard model with $N_s=60$ as a typical example of a less-than-half-filled system.

At first we show the dependence of the total energy on U/t together with the result of ψ_G and the Bethe ansatz solution[27] in Fig. 4. By setting $\xi_0=0$, the $U=\infty$ Hubbard model is easily realized in the subspace where the double occupation of a site is forbidden. The ground-state energy is considerably improved as compared to ψ_G in the whole U/t region. The difference in energy between the VMC result with ψ_Q and the exact one is less

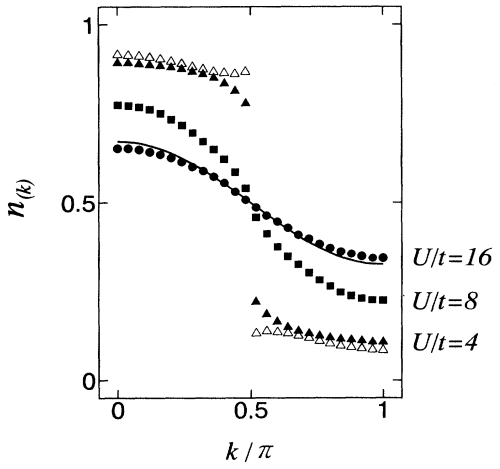

FIG. 3. Momentum-distribution function $n(k)$ in the half-filled case evaluated by VMC calculations with ψ_H is shown for $U/t=4$ (filled triangles), 8 (filled squares), and 16 (filled circles), in comparison with the result of perturbational t/U expansion (Ref. 26) for $U/t=16$ (solid line). We also show the result of $n(k)$ for $U/t=4$ evaluated by VMC calculations with $\psi'_H=F_H\psi_F$, i.e., $h=0$ in ψ_H (open triangles).

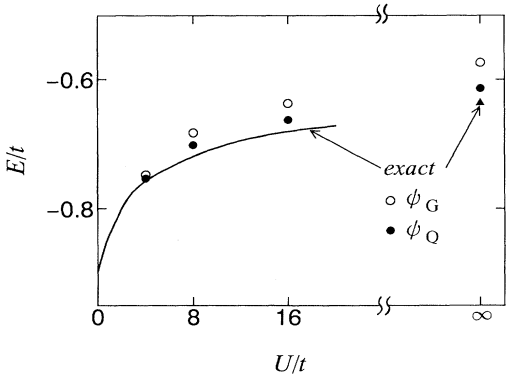

FIG. 4. Total energy per site using ψ_Q as a function of U/t for the quarter-filled Hubbard chain (filled circles). They are compared with those by ψ_G (open circles), and the exact solution for infinite systems (Ref. 27) (solid line). At $U/t=\infty$, the value of exact solution $-2\sin(n_e\pi)/\pi$ with $n_e=\frac{1}{2}$ is represented by a triangle.

than $\sim 4\%$ while for ψ_G the difference is less than $\sim 10\%$. This may be understood as follows. The competition between the on-site repulsive interaction and the kinetic term should tend to keep electrons apart. Therefore, the projection weights for spin configurations such as $|\cdots +0-0\cdots\rangle$, $|\cdots +-000+\cdots\rangle$, etc., must be differentiated. This situation is correctly described in our trial function with h and ξ but lacking in ψ_G.

In Fig. 5, spin- and charge-correlation functions are shown. The spin-correlation function $S(k)$ exhibits a sharp cusp at $k=2k_F$, indicating that spin correlations at $2k_F$ are dominant at long-length scales, while $C(k)$ is fully suppressed. As U/t decreases, this cusp is suppressed. At $U/t=\infty$, an exact calculation of $S(k)$ and $n(k)$ has been carried out based on the Bethe ansatz wave function for small system sizes.[24] The overall behavior of our $S(k)$ is similar to the exact one for $U/t=\infty$.

Finally, we discuss the momentum-distribution function. The ground state of the Hubbard model, as well as the t-J model, belongs to a general class of interacting Fermi systems known as Tomonaga-Luttinger liquids,[19,20] while ordinary metals are well described by the Landau theory of Fermi liquids. In the Tomonaga-Luttinger liquids, the momentum-distribution function exhibits a power-law singularity near k_F in contrast to a discontinuity for ordinary metals.

Figure 6 shows our result of $n(k)$ for several values of U/t. One notices a strong singularity at $k=k_F$ and a weak singularity at $k=3k_F$. For $U/t=\infty$, the overall behavior of $n(k)$ is similar to the exact one[24] except for $k\simeq k_F$. It seems that there is a finite discontinuity at the Fermi surface, and the Tomonaga-Luttinger behavior expected for the ground state is not recovered. There may be room for further improvement of the wave function for the partially filled band; an improved choice of parameters $\xi(r)$ with long-range nature must to be made in order to accurately describe low-energy properties.

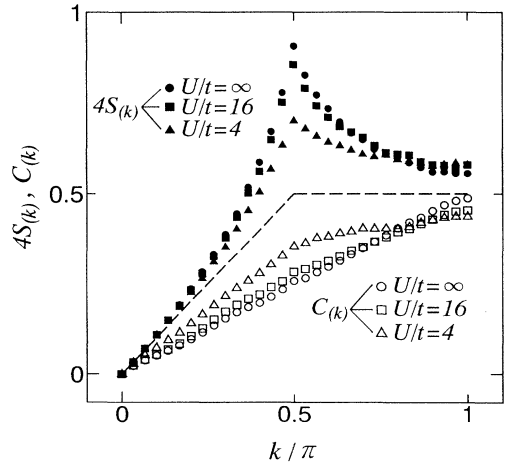

FIG. 5. Spin- and charge-correlation functions $S(k)$ and $C(k)$ for the quarter-filled case. The selected values of U/t are 0 (broken line), 4 (triangles), 16 (squares), and ∞ (circles).

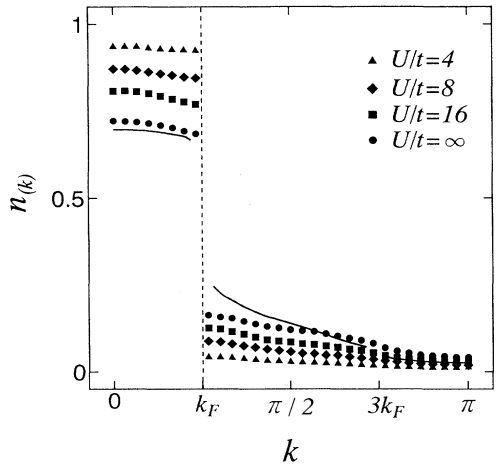

FIG. 6. Momentum-distribution functions for $U/t=4$ (triangles), 8 (diamonds), 16 (squares), and ∞ (circles) in the quarter-filled case. The exact result (Ref. 24) by Bethe ansatz for $U/t=\infty$ is also shown (solid line).

V. SUMMARY AND DISCUSSION

In this paper we have developed an optimization method for VMC calculations. With this method, it has become possible to utilize wave functions with a large number of variational parameters. The method mentioned here can be used to obtain a more precise description of the ground state for strongly correlated electronic systems with wave functions superior to those with only a few parameters used in previous VMC calculations.

We have proposed a new type of variational wave function, which is constructed of a linear combination of Slater determinants multiplied by Jastrow-type correlation factors. They can explicitly contain low-energy fluctuations such as particle-hole excitations. We have examined these wave functions by applying them to the 1D Hubbard model.

For the half-filled band, we have introduced the long-range attractive correlation between empty and doubly occupied sites into the variational wave function. The results of total energy, correlation functions, and momentum-distribution functions for large U/t show good agreement with results achieved through exact solutions.

For the less-than-half-filled case, we have employed the trial wave function in which Jastrow-type long-range intersite correlation is multiplied by a linear combination of Slater determinants. With this wave function, the energy and correlation functions are close to the exact one obtained by Bethe ansatz. The behavior of $n(k)$ near k_F remains a problem.

In order to investigate the metal-insulator transition or power-law singularity in more detail, we need a systematic analysis of the singularity of $n(k)$ near the Fermi surface in the thermodynamic limit. However, it is difficult to completely determine the singularity of $n(k)$ at k_F, since numerical calculations are carried out for finite-size systems. The finite-size corrections for the thermo-

dynamic limit, such as the boundary-condition integration technique,[25] may be useful for extracting essential information from numerical studies of finite clusters. In addition, our results are within the limits of the trial wave function, which includes various assumptions. Further refinements of the trial functions seem to be required, especially for the non-half-filled band. When other correlation effects that recover the true low-energy behavior of the charge excitations are involved, further improvement is expected to achieve correct Luttinger-liquid behavior. In fact, for t-J and $U=\infty$ Hubbard models, a particular form of long-range correlations in the Jastrow factor has been shown to lead to the characteristic behavior of Tomonaga-Luttinger liquids.[5,7,28]

An application of the present method with some modifications to the t-J model is also interesting because of the close connection with high-T_c superconductors. Fortunately, the present optimization procedure for the multiparameter system is flexible enough to extend the variational parameter space for any system. These are left for future research.

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