Wave functions of correlated-electron state in the periodic Anderson model

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We investigate the periodic Anderson model by a variational Monte Carlo method. A new wave function is proposed based on the well-known Gutzwiller wave function. We calculate the physical properties using the Monte Carlo algorithm to consider the strong correlation effects. The ground state energy is improved considerably by taking into account electron-hole excitation effects.

Keywords: Periodic Anderson model, Variational Monte Carlo method, Off-diagonal Gutzwiller functions

I. Introduction

Compounds containing rare earth elements belong to the large category of heavy fermions. Heavy fermion materials exhibit many interesting features such as superconductivity, antiferromagnetic metal and paramagnetic metal.[1,2] Many of them are characterized by large specific heat and a huge Pauli susceptibility. These properties indicate a large effective mass of electrons. Some compounds exhibit anomalous transport properties and anomalous temperature dependence of the susceptibility and specific heat near the antiferromagnetic region which are not understood within the normal Fermi liquid theory.[3–5]

Heavy fermions are usually modeled by the periodic Anderson model which contains the conduction electrons and the correlated f electrons. The periodic Anderson model is far from well understood at present. It is not an easy task to calculate the physical quantities for the periodic Anderson model because of the strong correlations among the localized electrons. The periodic Anderson model may include various ground states such as the paramagnetic state, antiferromagnetic state, ferromagnetic state and superconducting state.

The periodic Anderson model has been studied intensively using the quantum Monte Carlo method[6–9] and exact diagonalization.[10–12] The periodic Anderson model brings about a sign problem for the quantum Monte Carlo method even in one dimension. In the diagonalization the tractable system sizes are limited. Therefore we investigate the periodic Anderson model based on a variational Monte Carlo method (VMC).[13] VMC is characterized by a wide applicability from weak to strong correlation region.[14–18] The Gutzwiller function is a simplest and standard wave function for strongly correlated electron systems. Unfortunately, it is not easy to consider the strong correlations even for the simple Gutzwiller function. We can overcome this difficulty by using the Monte Carlo method to evaluate expectation values. Since it seems that the Gutzwiller function fails to keep its validity in the Kondo region, it may be required to improve the Gutzwiller function. Our purpose in this paper is to consider off-diagonal wave functions taking into account the electron-hole excitation effects to describe the heavy fermion state as a first step to improve the Gutzwiller function. We show that the energy is lowered greatly due to the electron-hole excitations.

The paper is organized as follows: In the second section the Hamiltonian and wave functions are presented. The method of calculations is also briefly discussed. We show our results in the subsequent section and the last section is assigned to summary.

II. Hamiltonian and Wave Functions

A. Model and wave functions

The Hamiltonian is given by

$$\begin{aligned} H &= -t \sum_{<ij>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + V \sum_{i\sigma} (c_{i\sigma}^{\dagger} f_{i\sigma} + f_{i\sigma}^{\dagger} c_{i\sigma}) \\ &+ E_f \sum_{i\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} + U \sum_{i} n_{fi\uparrow} n_{fi\downarrow} \\ &= H_0 + U \sum_{i} n_{fi\uparrow} n_{fi\downarrow}, \end{aligned} \tag{1}$$

where $n_{fi\sigma} = f_{i\sigma}^{\dagger} f_{i\sigma}$. $c_{i\sigma}$ ($c_{i\sigma}^{\dagger}$) and $f_{i\sigma}$ ($f_{i\sigma}^{\dagger}$) denote the operators for the conduction electrons and the localized electrons, respectively. V is the hybridization parameter and U is the strength of the Coulomb repulsion. We assume that U is very large compared to the other parameters in this paper. In this paper the energy is measured in units of t. There are two kinds of electrons (c and f) hybridized through the mixing term. If the level of f electrons E_f lies near the Fermi level, we call this case the valence-fluctuation region. The case where the position of E_f is far below the Fermi level is called the Kondo region. In the Kondo region the number of f electrons is close to 1 and the correlation effects are large.

A simplest wave function for this model is the Gutzwiller function given as[13,19–23]

$$\psi_G = \prod_i (1-(1-g)n_{fi\uparrow}n_{fi\downarrow})\psi_0, \tag{2}$$

where ψ_0 is the wave function for non-interacting mixed band:

$$\psi_0 = \prod_{k\sigma}(1+\Gamma_k f^\dagger_{k\sigma}c_{k\sigma})\psi_F. \tag{3}$$

ψ_F denotes the Fermi sea occupied by the conduction electrons up to the Fermi level. The mixing effect is represented by Γ_k which is written as

$$\Gamma^0_k = \frac{2V}{E_f - \epsilon_k + [(\epsilon_k - E_f)^2 + 4V^2]^{1/2}} \tag{4}$$

for the non-interacting band. ϵ_k represents the dispersion of the conduction-electron band. For the Gutzwiller function $\{\Gamma_k\}$ should be regarded as variational parameters. However, it is a hard task to determine Γ_k for each k so that the energy has a minimum. We adopt the following ansatz for Γ_k:

$$\Gamma_k = \frac{2v}{\epsilon_f - \epsilon_k + [(\epsilon_k - \epsilon_f)^2 + 4v^2]^{1/2}}, \tag{5}$$

where ϵ_f and v are variational parameters. It has been shown that Γ_k of this type is well fitted by a variational theory using a linked cluster expansion.[23,24]

Although the Gutzwiller function appears to be very simple, it is not easy to evaluate expectation values for this function. We must employ a linked cluster expansion, the Monte Carlo method or other reliable methods. We use the Monte Carlo method in this paper since we can access to large U using this method.

In the valence-fluctuation region, the Gutzwiller function is expected to be a good function since the correlations are rather weak. Instead in the Kondo region, the Gutzwiller function turns out to be a poor function and we must go beyond the Gutzwiller function. In this paper we propose the following wave function:

$$\psi = \exp(-\lambda H_0)\psi_G. \tag{6}$$

Since the energy gain due to the hybridization processes is important in the Kondo region, we consider a simplified function of eq.(6),

$$\begin{aligned}\psi^{(1)} &= \exp(-\lambda\sum_{i\sigma}(c^\dagger_{i\sigma}f_{i\sigma} + f^\dagger_{i\sigma}c_{i\sigma}))\psi_G \\ &\equiv \exp(-\lambda H_{mix})\psi_G,\end{aligned} \tag{7}$$

where λ is a variational parameter. We have four variational parameters g, v, ϵ_f and λ. The wave function $\psi^{(1)}$ is called the off-diagonal wave function in this paper. This type of wave functions have been considered for the Hubbard model[25,26] and one can improve the function by a multiplicative operation of the Gutzwiller factor P_G and the off-diagonal kinetic factor $e^{-\lambda H_0}$.[26,27]

We discuss about the physical meaning of the factor $\exp(-\lambda H_{mix})$ briefly. The operator $\exp(-\lambda H_{mix})$ induces electron-hole excitation processes which are considered to improve the Gutzwiller function greatly. In the single impurity Kondo problem the corrections given by the electron-hole excitations are essentially important to discuss the magnetic property based on the Yosida's theory.[28] In order to see how the electron-hole pairs are excited by $\exp(-\lambda H_{mix})$, we examine $\psi^{(1)}$ perturbatively in the manner as

$$\psi^{(1)} = (1-\lambda H_{mix}+\cdots)(1+S+\cdots)\psi_0, \tag{8}$$

where ψ_G is written as $\psi_G = \mathrm{e}^S\psi_0$.[23] The term $H_{mix}S\psi_0$ produces the excitations above the Fermi level.

B. Monte Carlo method

One can employ the Monte Carlo algorithm by Ceperley *et al.* to compute the expectation values of energy for the Gutzwiller function. For the off-diagonal functions, the Monte Carlo method using the auxiliary fields developed in the projector Monte Carlo computations is more efficient to evaluate the physical quantities.[29,30]

The Gutzwiller operator is written as a bilinear form

$$\begin{aligned}P_G &= \prod_i (1-(1-g)n_{fi\uparrow}n_{fi\downarrow}) \\ &= \exp(-\alpha\sum_i n_{fi\uparrow}n_{fi\downarrow}) \\ &= (\frac{1}{2})^N \sum_{\{s_i=\pm1\}} \exp[2a\sum_i s_i(n_{fi\uparrow}-n_{fi\downarrow}) \\ &- \frac{\alpha}{2}\sum_i (n_{fi\uparrow}+n_{fi\downarrow})],\end{aligned} \tag{9}$$

where s_i is the auxiliary field which takes the value of ±1 and N is the number of sites. The numbers a and α are related to g as $\cosh(2a) = \exp(\alpha/2) = (1/g)^{1/2}$. The norm $\langle\psi_G|\psi_G\rangle$ is calculated as

$$\begin{aligned}\langle\psi_G|\psi_G\rangle &= (\frac{1}{2})^{2N}\sum_{\{u_i\}\{s_i\}}\prod_\sigma \\ &\times \langle\psi^\sigma_0|\exp(h^\sigma(u))\exp(h^\sigma(s))|\psi^\sigma_0\rangle,\end{aligned} \tag{10}$$

where ψ^σ_0 is the wave function for the non-interacting mixed band with the spin σ and the potential $h^\sigma(u)$ is given by

$$h^\sigma(u) = 2a\sigma\sum_i u_i n_{fi\sigma} - \frac{\alpha}{2}\sum_i n_{fi\sigma}. \tag{11}$$

Then the weight is written as the sum of determinants,[31]

$$\begin{aligned}\langle\psi_G|\psi_G\rangle &= \mathrm{const}\cdot(\frac{1}{2})^{2N}\sum_{\{u_i\}\{s_i\}}\prod_\sigma \\ &\times \det(\phi^\dagger_\sigma\exp(V^\sigma(u))\exp(V^\sigma(s))\phi_\sigma)\end{aligned} \tag{12}$$

$V^\sigma(s)$ is a diagonal $2N \times 2N$ matrix corresponding to $h^\sigma(s)$, which is given as

$$V^\sigma(s) = \mathrm{diag}(1,\cdots,1,2a\sigma s_1 - \alpha/2,\cdots,2a\sigma s_N - \alpha/2). \quad (13)$$

The first N components show the conduction electron part with no mutual interactions and the second N components show the potential represented by the random fields $\{s_i\}$. ϕ_σ is a $2N \times N_\sigma$ matrix where N_σ is the number of spin-σ electrons. The elements of ϕ_σ are given by

$$(\phi_\sigma)_{ij} = \exp(ir_i \cdot k_j)u_{k_j} \quad (i = 1,\cdots,N; j = 1,\cdots,N_\sigma), \quad (14)$$

$$(\phi_\sigma)_{i+N,j} = \exp(ir_i \cdot k_j)v_{k_j} \quad (i = 1,\cdots,N; j = 1,\cdots,N_\sigma), \quad (15)$$

where u_{k_j} and v_{k_j} are weights of the conduction electrons and the f electrons, respectively:

$$u_{k_j} = 1/(1+\Gamma_{k_j}^2)^{1/2}, \quad v_{k_j} = \Gamma_{k_j}/(1+\Gamma_{k_j}^2)^{1/2}. \quad (16)$$

In the real representation the elements of ϕ_σ are $\cos(r_i \cdot k_j)u_{k_j}$ and $\sin(r_i \cdot k_j)u_{k_j}$ for $i = 1,\cdots,N$; and $\cos(r_i \cdot k_j)v_{k_j}$ and $\sin(r_i \cdot k_j)v_{k_j}$ for $i = N+1,\cdots,2N$. The use of the Monte Carlo procedure enables us to evaluate the expectation values for ψ_G. In order to include the correction to ψ_G given by $\exp(-\lambda H_{mix})$, we consider the determinants

$$\langle\psi^{(1)}|\psi^{(1)}\rangle = (\frac{1}{2})^{2N}\sum_{\{u_i\}\{s_i\}}\prod_\sigma \times \det(\phi_\sigma^\dagger \exp(V^\sigma(u))\exp(-\lambda K_{mix}^\sigma)\exp(-\lambda K_{mix}^\sigma)\exp(V^\sigma(s))\phi_\sigma). \quad (17)$$

K_{mix}^σ is a $2N \times 2N$ matrix given as

$$(K_{mix}^\sigma)_{i,i+N} = 1 \quad (1 \le i \le N), \quad (18)$$

and other elements of K_{mix}^σ vanish. There are four variational parameters g, λ, v and ϵ_f to be determined so that the energy expectation value has a minimum in the parameter space.

In order to calculate the expectation value the Monte Carlo samples are generated by the importance sampling with the weight function $|w| = |w_\uparrow w_\downarrow|$ where

$$w_\sigma = \det(\phi_\sigma^\dagger \exp(V^\sigma(u)\exp(-\lambda K_{mix}^\sigma)\exp(-\lambda K_{mix}^\sigma)\exp(V^\sigma(s))\phi_\sigma). \quad (19)$$

Following the standard algorithm for QMC,[29] the ratio of $|w| = |w_\uparrow w_\downarrow|$ is calculated to determine whether we accept or reject a new configuration when we update the Ising variable from old s_i to the new s_i'.[27]

III. Physical Properties of Off-Diagonal Wave Functions

A. Comparison with exact results

First let us check the validity of our method in small clusters. In Table I we show the ground-state energy obtained by our method and by the exact diagonalization for $N = 8$. ΔE is defined by $\Delta E = E - E(V = 0)$ where E is the ground-state energy and $E(V = 0)$ is the energy for $V = 0$. The Table I indicates that the energy obtained by $\psi^{(1)}$ is close to the exact value. We obtain $\psi^{(2)}$ if we improve $\psi^{(1)}$ further by multiplying the exponential factors again:

$$\psi^{(2)} = \exp(-\lambda' H_{mix})\exp(-\alpha' D) \times \exp(-\lambda H_{mix})\exp(-\alpha D)\psi_0, \quad (20)$$

where $D = \sum_i n_{fi\uparrow}n_{fi\downarrow}$ and λ', α', λ and α are variational parameters. Apparently $\psi^{(2)}$ is a nice function to consider the ground-state energy. In this paper we consider $\psi^{(1)}$ in order to reduce the number of variational parameters.

In Table II we show the nearest neighbor spin correlations as well as the energy to compare with the exact diagonalization for $N = 6$. The spin correlation functions are defined by

$$S_{ff}(\ell) = \langle(n_{fi\uparrow} - n_{fi\downarrow})(n_{fi+\ell\uparrow} - n_{fi+\ell\downarrow})\rangle, \quad (21)$$

$$S_{fc}(\ell) = \langle(n_{fi\uparrow} - n_{fi\downarrow})(n_{ci+\ell\uparrow} - n_{ci+\ell\downarrow})\rangle, \quad (22)$$

where $n_{ci\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. In Figs.1 and 2 we compare the spin correlation functions with the exact results obtained by the diagonalization for $N = 6$, where the spin structure factor is defined by

$$S_{ff}(q) = \frac{1}{N}\sum_{ij}\exp[iq(R_i - R_j)]\langle(n_{fi\uparrow} - n_{fi\downarrow})(n_{fj\uparrow} - n_{fj\downarrow})\rangle. \quad (23)$$

The parameters are $N_e = 10$, $V = 0.5$, $E_f = -2$ and $U = 10$ for Fig.1 and $N_e = 12$, $V = 0.5$, $E_f = -2$ and $U = 10$ for Fig.2. Obviously $\psi^{(1)}$ well reproduces the behaviors of spin correlation functions.

TABLE I. Ground state energy for the periodic Anderson model with $N = 8$ and $N_e = 12$. The parameters are given by $V = 0.5$, $E_f = -3.0$ and $U = 10.0$ for $t = 1$. The boundary condition is antiperiodic. The expected statistical error is the last digit is in parentheses.

	Energy	ΔE	g	v	ϵ_f	λ	g'	λ'
exact	-31.93	-0.539						
ψ_G	$-31.69(1)$	-0.30	0.02	0.1	-1.8	–	–	–
$\psi^{(1)}$	$-31.88(1)$	-0.49	$\sim 9 \times 10^{-5}$	0.082	-1.78	0.14	–	–
$\psi^{(2)}$	$-31.91(1)$	-0.52	$\sim 9 \times 10^{-5}$	0.056	-1.78	0.09	0.01	0.1

TABLE II. Ground state energy and nearest neighbor correlation functions for the periodic Anderson model. The parameters are given by $N = 6$, $V = 0.5$, $E_f = -2$ and $U = 10.0$. The boundary condition is periodic.

	N_e	Energy	ΔE	$S_{ff}(\ell = 1)$	$S_{fc}(\ell = 0)$	g	v	ϵ_f	λ
exact	10	-18.796	-0.796	0.0405	-0.1706	–	–	–	–
ψ_G	10	-18.50	-0.50	0.019	-0.22	0.272	0.2	-1.3	–
$\psi^{(1)}$	10	-18.63	-0.63	0.024	-0.20	$\sim 2 \times 10^{-4}$	0.12	-1.3	0.06
exact	12	-20.325	-0.325	-0.804	-0.040	–	–	–	–
ψ_G	12	-20.13	-0.13	-0.58	-0.090	0.023	0.17	-0.78	–
$\psi^{(1)}$	12	-20.30	-0.30	-0.61	-0.034	$\sim 10^{-4}$	0.07	-0.84	0.064

B. Results for the half-filled case

In this section we consider the 1D half-filled periodic Anderson model. The parameters are given by $V = 0.5$, $E_f = -1.0$ and $U = 10$ in units of t. First we show the variational results for the Gutzwiller function. In order to find the variational parameters for which the energy has a minimum, we calculate the energy-expectation values for various values of v, g and ϵ_f. In Figs.3(a)-3(c) the energy-expectation values are shown as a function of ϵ_f for fixed v and g for $N = 40$ and $N_e = 80$. In Fig.4 we show the momentum distribution functions for the f and conduction electrons defined as

$$n_f(k) = \frac{1}{2}\sum_\sigma \langle f^\dagger_{k\sigma} f_{k\sigma}\rangle, \tag{24}$$

$$n_s(k) = \frac{1}{2}\sum_\sigma \langle c^\dagger_{k\sigma} c_{k\sigma}\rangle, \tag{25}$$

respectively. These quantities indicate that the ground state is insulating. In Fig.5 the spin and charge correlation functions are shown; the spin correlation function is defined by eq.(23) and the charge correlation function is defined as

$$C_{ff}(q) = \frac{1}{N}\sum_{ij} \exp[iq(R_i - R_j)][\langle (n_{fi\uparrow} + n_{fi\downarrow})(n_{fj\uparrow} + n_{fj\downarrow})\rangle - \langle n_{fi\uparrow} + n_{fi\downarrow}\rangle\langle n_{fj\uparrow} + n_{fj\downarrow}\rangle], \tag{26}$$

for the f electrons. The spin and charge correlation functions for the conduction electrons are similarly defined. The figure indicates a large antiferromagnetic correlation for the f electrons showing a peak at $q = \pi$. We have calculated correlation functions for $N = 41$ and $N_e = 82$ (for optimum parameters) since the periodic boundary condition is favorable to estimate them.

Next we consider the off-diagonal function $\psi^{(1)}$. We show the energy expectation values in Figs.6(a)-6(d) to obtain a minimum in the parameter space. We show the energy as a function of g in Fig.7 where the energy expectation values are obtained after optimization for other variational parameters. The energies are shown in Table III for comparison with the Gutzwiller function. Obviously the energy is improved appreciably due to the off-diagonal correlation factor, which is suggestive of the importance of the intersite correlation effect. It should be noted that the optimum value of g is very small for $\psi^{(1)}$. This is because we can get energy gain due to the exponential correlation factor for small g suppressing the double occupancy. The momentum distribution functions are presented in Fig.8. The spin correlation function $S_{ff}(q)$ shown in Fig.9 indicates that the antiferromagnetic spin correlation is enhanced due to electron-hole excitation corrections taken into account by the off-diagonal factor. A comparison is made favorably with the results by QMC for the spin correlation function and the hybridization energy in Table III. The results are characterized by the feature that in spite of a large energy gain due to the multiplicative operation by $\exp(-\lambda H_{mix})$ the correlation functions are not so changed. The energy gain is mainly due to the hybridization energy. These results and the comparison with the exact diagonalization suggest that $\psi^{(1)}$ is a reasonable wave function for the one-dimensional periodic Anderson model.

C. Results for the non-half-filled case

Let us turn to the non-half-filled case. The parameters are given by $N = 40$, $N_e = 70$, $V = 0.5$ and $U = 10$ for the periodic boundary condition. The position of f electrons is set to be $E_f = -1$ and $E_f = -3$ in units of t. The ground state is considered to be metallic for less than half-filling. First, the results for the Gutzwiller function are shown. Following the similar manner mentioned

TABLE III. Ground state energy for 1D half-filled case with $N = 40$ and $N_e = 80$. The parameters are given by $V = 0.5$, $E_f = -1.0$ and $U = 10.0$. The boundary condition is chosen to be antiperiodic. r_{mix} denotes $r_{mix} = E_{mix}(U)/E_{mix}(U = 0)$ and $E_{mix} = E_{mix}(U) = V \sum_{i\sigma} \langle c^{\dagger}_{i\sigma} f_{i\sigma} + h.c. \rangle$. $E_{mix}(U = 0)$ denotes the expectation value for $U = 0$. QMC results are for the symmetric case in which $t = 1$, $V = 1$, $U = 6$ and $N = 12$ for $S_{ff}(\ell = 1)$[7] and $t = 0.5$, $V = 0.375$, $U = 3$ and $N = 16$ for r_{mix}.[9]

	Energy	ΔE	$S_{ff}(\ell = 1)$	$S_{fc}(\ell = 0)$	E_{mix}	r_{mix}	g	v	ϵ_f	λ
ψ_G	$-92.55(0)$	-1.57	$-0.51(1)$	$-0.10(1)$	$-5.50(0)$	0.22	0.02	0.14	-0.3	–
$\psi^{(1)}$	$-93.36(1)$	-2.38	$-0.54(1)$	$-0.067(1)$	$-6.19(0)$	0.24	$\sim 10^{-4}$	0.07	-0.2	0.07
QMC			~ -0.3			~ 0.25				

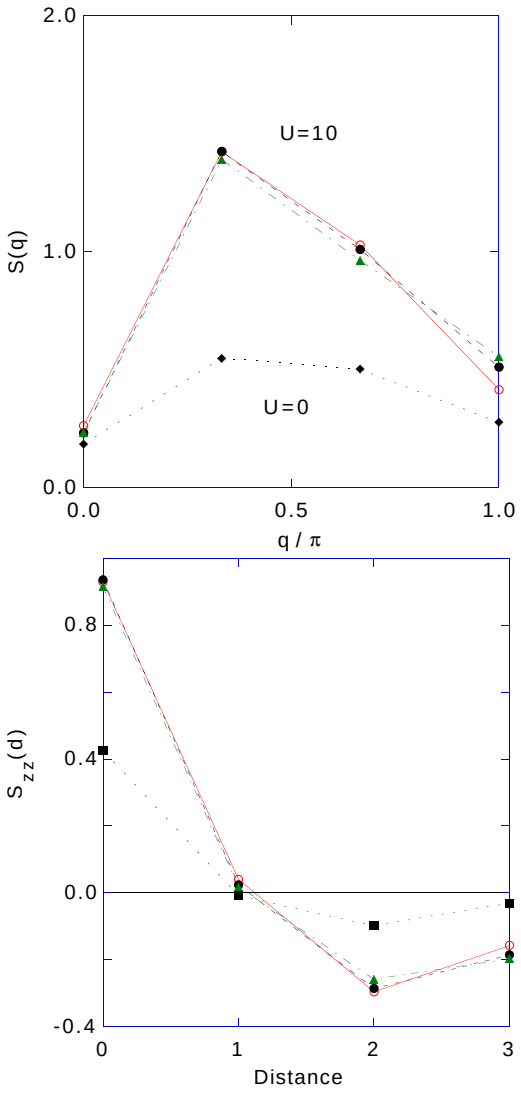

FIG. 1. f-electron spin correlation functions for $N = 6$, $V = 0.5$, $E_f = -2$, $U = 10.0$ and $N_e = 10$ with the periodic boundary condition. $S_{ff}(q)$ for (a) and $S_{ff}(\ell)$ for (b). The open circles represent exact results, triangles represent the data by the Gutzwiller function, and filled circles represent the data by $\psi^{(1)}$. The diamonds show a non-interacting behavior.

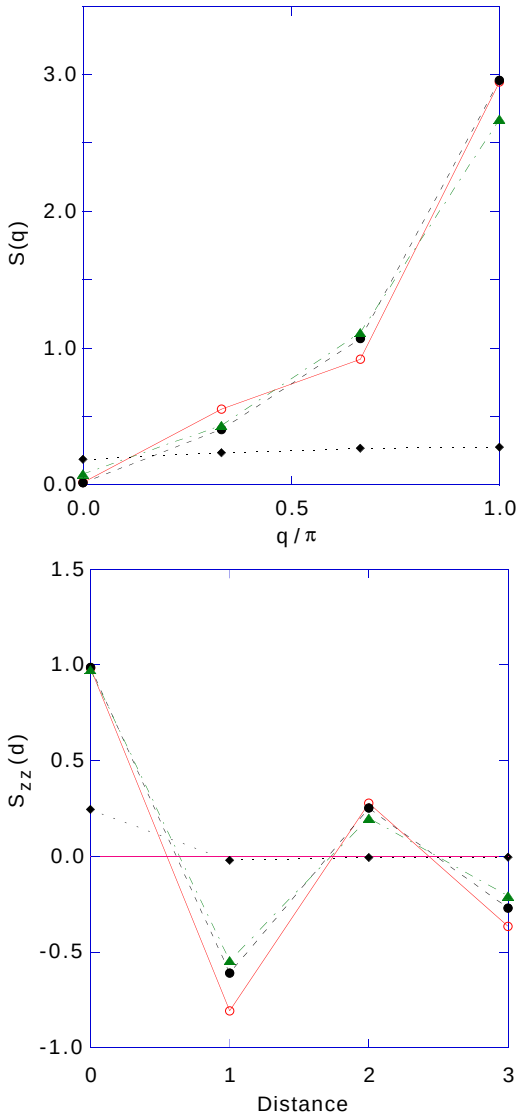

FIG. 2. f-electron spin correlation functions for $N = 6$, $V = 0.5$, $E_f = -2$, $U = 10.0$ and $N_e = 12$ (half-filled case) with the periodic boundary condition. The symbols are as in Fig.1.

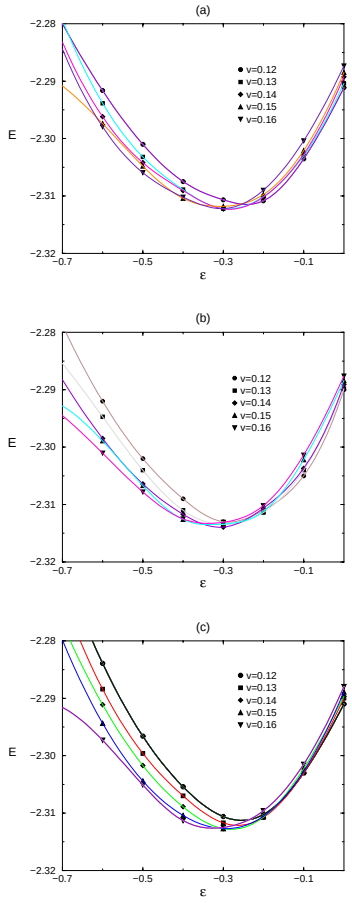

FIG. 3. Energy expectation values as a function of $\epsilon \equiv \epsilon_f$ for the Gutzwiller function at half-filling. $g = 0.01$ for (a), 0.02 for (b) and 0.03 for (c). The parameters in the Hamiltonian are given by $V = 0.5$, $E_f = -1$ and $U = 10$.

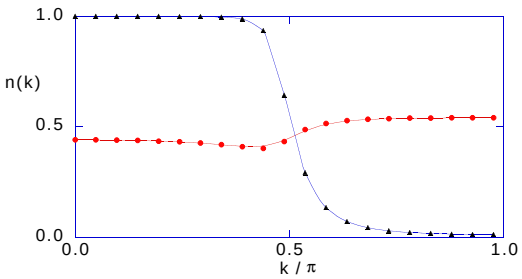

FIG. 4. The momentum distribution function for the f (circles) and conduction electrons (triangles) at half-filling.

above the optimum variational parameters are found as $g = 0.03$, $\epsilon_f = -0.8$ and $v = 0.24$ for $E_f = -1$, as is shown in Fig.10(a) where the energy is optimized for ϵ_f and v. For $E_f = -3$ the energy in Fig.10(b) has a broad minimum for small g. Our optimum parameters are $g = 0.0006$, $\epsilon_f = -0.9$ and $v = 0.007$. The energy gain compared to the case $V = 0$ is estimated to be 0.146/40=0.00365 per site which is very small compared to V^2/E_f. This suggests that the Gutzwiller function should be improved in the Kondo region. The momentum distribution functions are presented in Figs.11(a)

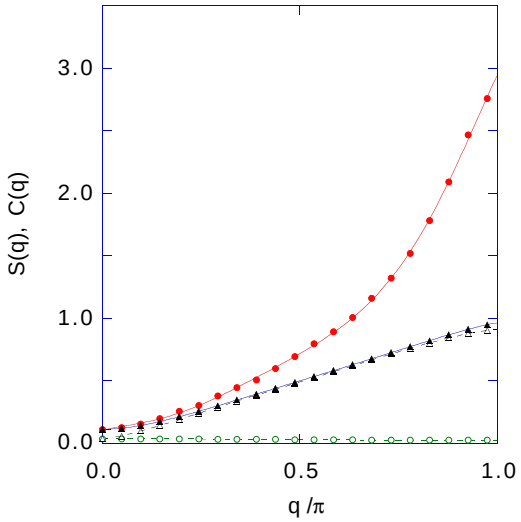

FIG. 5. The spin and charge structure functions for the f (circles) and conduction electrons (triangles) at half-filling. Filled and open symbols correspond to the spin and charge correlation functions, respectively.

and 11(b). The momentum distribution functions are characterized by a metallic behavior as indicated by a jump at the Fermi wave number and suggestive of the importance of the correlation effect. The momentum distribution function for the conduction electrons also has small non-zero distribution above the Fermi level (for $|k| > k_F$) for $\psi^{(1)}$. The spin correlation function shown in Figs.12(a) and 12(b) has a peak away from $q = \pi$ and is highly enhanced for the f electrons. The structure of spin correlation function is understood as a sum of two contributions; one is the inter-band contribution and the other is the intra-band contribution.[13] In the Kondo region the correlation functions exhibit similar behaviors to those for the Kondo lattice.[22]

Second, the off-diagonal wave function is investigated for $E_f = -1$ and -3. The energy is shown in Figs.13(a) and 13(b) where the energy is optimized for ϵ_f and v. The optimum parameters are shown in Table IV. A large energy gain is obtained by our wave function even in the Kondo region. The momentum distribution function are shown in Figs.14(a) and 14(b). Although the 1D periodic Anderson model may belong to the class of the Luttinger liquid,[32] we approximately analyze the correlation effect following the standard Fermi liquid relations:[13]

$$\begin{aligned} \Delta n_f(k_F) &= n_f(k_F - 0) - n_f(k_F + 0) \\ &= (1 + \frac{V^2}{(\epsilon_{k_F} - \mu)^2} - \frac{\partial \Sigma(k_F, \omega)}{\partial \omega}|_{\omega=0})^{-1}, \end{aligned} \tag{27}$$

$$\begin{aligned} \Delta n_s(k_F) &= n_s(k_F - 0) - n_s(k_F + 0) \\ &= \frac{V^2}{(\epsilon_{k_F} - \mu)^2} \Delta n_f(k_F), \end{aligned} \tag{28}$$

where $\Delta n_f(k_F)$ and $\Delta n_s(k_F)$ are jumps of $n_f(k)$ and $n_s(k)$ at $k = k_F$, respectively, and μ is the chemical potential. The many-body enhancement factor

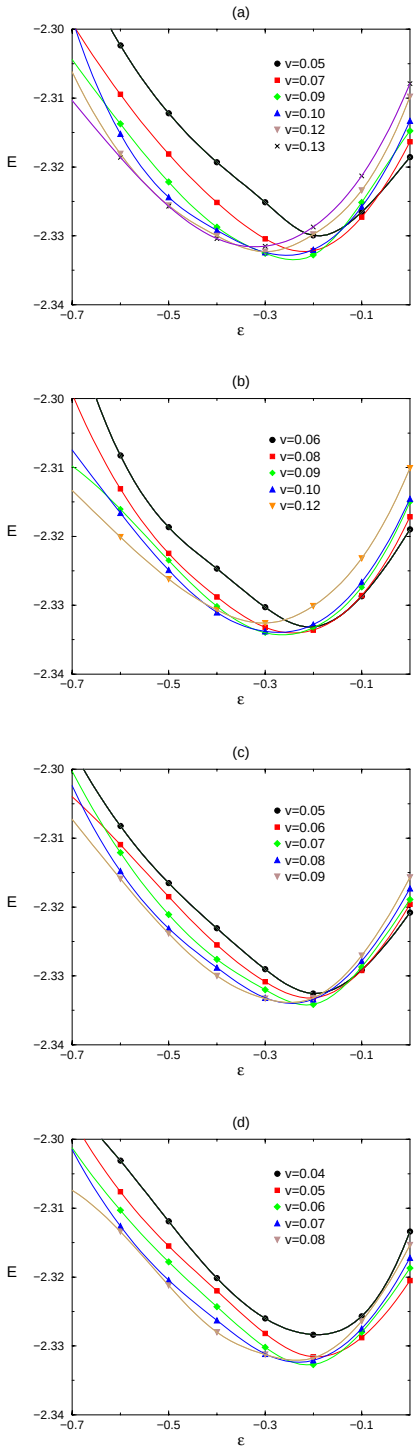

FIG. 6. Energy expectation values as a function of $\epsilon \equiv \epsilon_f$ for $\psi^{(1)}$ at half-filling. $g = 10^{-4}$ is fixed and $\lambda = 0.05$ for (a), 0.06 for (b), 0.07 for (c) and 0.08 for (d).

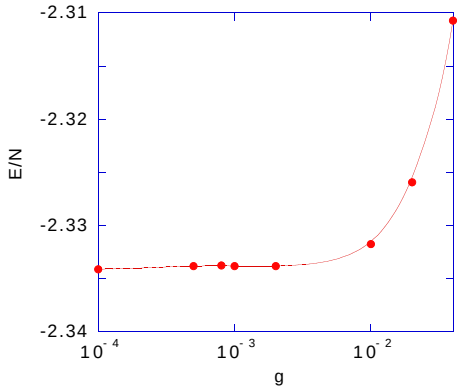

FIG. 7. Energy expectation values as a function of g for $\psi^{(1)}$ at half-filling.

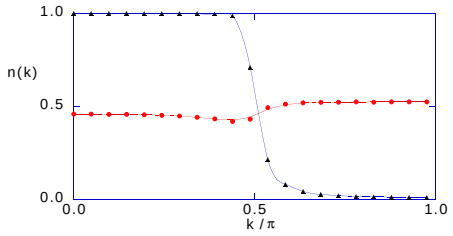

FIG. 8. The momentum distribution function for $\psi^{(1)}$ at half-filling.

$-\partial\Sigma(k_F,\omega)/\partial\omega$, where $\Sigma(k_F,\omega)$ the f-electron self-energy, is presented in Table V as well as $\Delta n_f(k_F)$ and $\Delta n_s(k_F)$. The enhancement factor can be as large as several hundreds in the Kondo region. We present the spin correlation functions in Figs.15(a) and 15(b). The features are essentially similar to those obtained for the Gutzwiller function, which may reflect the one dimensionality of the model.

IV. Summary

We have proposed a new wave function for the periodic Anderson model. The wave function is improved by considering multiplicative operations of the off-diagonal operators starting from the Gutzwiller function. Our wave

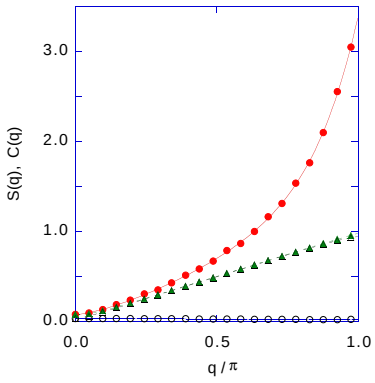

FIG. 9. The spin and charge structure functions for $\psi^{(1)}$ at half-filling.

TABLE IV. Ground state energy for 1D non-half-filled case with $N = 40$ and $N_e = 70$. The parameters are given by $V = 0.5$, $U = 10.0$ and $E_f = -1.0$ and -3.0. The boundary condition is chosen to be periodic. r_{mix} denotes $r_{mix} = E_{mix}(U)/E_{mix}(U=0)$ and $E_{mix} = E_{mix}(U)$.

	E_f	Energy	ΔE	$S_{ff}(\ell=1)$	$S_{fc}(\ell=0)$	E_{mix}	r_{mix}	g	v	ϵ_f	λ
ψ_G	-1	$-89.77(0)$	-2.67	$-0.12(1)$	$-0.15(1)$	$-9.40(0)$	0.395	0.03	0.24	-0.8	–
$\psi^{(1)}$	-1	$-90.58(0)$	-3.48	$-0.13(1)$	$-0.11(1)$	$-9.24(0)$	0.388	$\sim 10^{-4}$	0.14	-0.8	0.07
ψ_G	-3	$-167.25(0)$	-0.14	$-0.15(2)$	$-0.0016(1)$	$-0.29(0)$	0.021	$\sim 6\times10^{-4}$	0.007	-0.9	–
$\psi^{(1)}$	-3	$-168.91(0)$	-1.81	$-0.15(2)$	$-0.004(3)$	$-3.78(0)$	0.26	$\sim 3\times10^{-5}$	0.004	-0.9	0.09

TABLE V. Physical quantities that contain information on the correlation effects for 1D non-half-filled case with $N = 40$ and $N_e = 70$. The parameters are given by $V = 0.5$, $U = 10.0$ and $E_f = -1.0$ and -3.0. The boundary condition is chosen to be periodic. $\Delta n_f(k_F)$ and $\Delta n_s(k_F)$ denote the jumps in $n_f(k)$ and $n_s(k)$, respectively, at $k = k_F$. n_f is the number of f electrons. $-\partial\Sigma(k_F,\omega)/\partial\omega$ is the many-body enhancement factor evaluated through the Fermi liquid relation. q is the enhancement factor obtained using the Gutzwiller approximation given by $q = [(1-n_f)/(1-n_f/2)]^{1/2}$.

	E_f	Δn_f	Δn_s	n_f	v	ϵ_f	$-\partial\Sigma(k_F,\omega)/\partial\omega$	q^{-1}
ψ_G	-1	0.29	0.031	0.859	0.24	-0.8	2.3	2.0
$\psi^{(1)}$	-1	0.23	0.024	0.886	0.14	-0.8	3.2	2.2
ψ_G	-3	0.0044	0.00013	0.999	0.007	-0.9	226	22
$\psi^{(1)}$	-3	0.0034	0.00023	0.997	0.004	-0.9	293	13

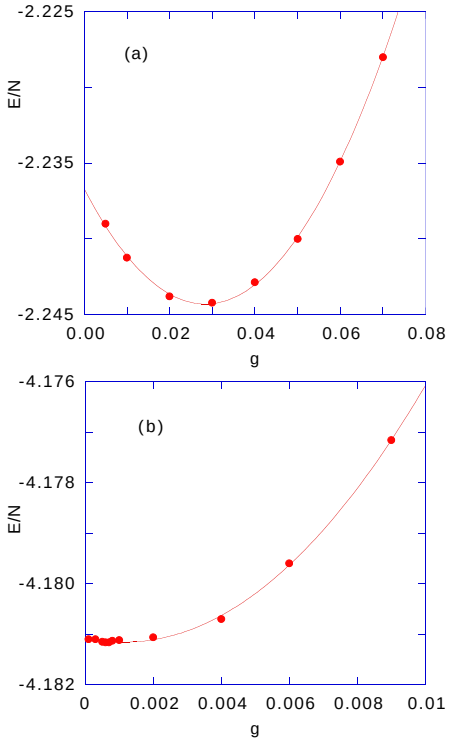

FIG. 10. The energy as a function of g for the Gutzwiller function for $E_f = -1$ (a) and $E_f = -3$ (b) for non-half-filled case. $N = 40$, $N_e = 70$, $V = 0.5$ and $U = 10$. The variational parameters v and ϵ_f are optimized for each g.

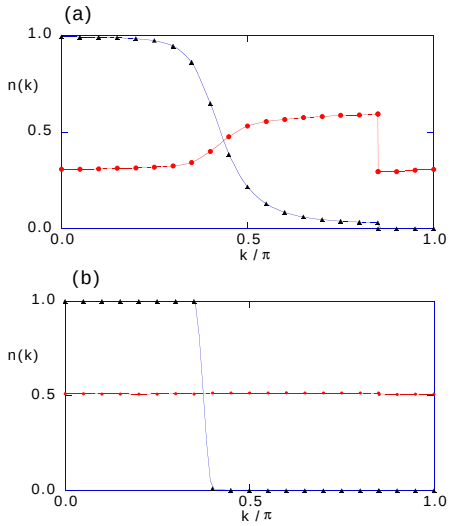

FIG. 11. The momentum distribution function for the Gutzwiller function for $E_f = -1$ (a) and $E_f = -3$ (b). $N = 40$, $N_e = 70$, $V = 0.5$ and $U = 10$.

function is simplest one among the non-trivial functions as a first step toward a development of the variational theory for the Anderson model. The multiplicative operation considered in this paper is regarded to produce the electron-hole excitation corrections to the Gutzwiller function. The expectation values are evaluated using the Monte Carlo algorithm with the auxiliary fields.

An application is made to investigated the 1D periodic Anderson model. It has been shown that the energy is lowered greatly due to the off-diagonal operation. The off-diagonal operation produces only small effects to the correlation functions, which means that the correlation functions are basically determined by the zeroth approximation given by the Gutzwiller function in 1D dimension.

In the Kondo region the Gutzwiller function gives a poor estimate for the energy expectation value as indicated by the property that the energy lowering is very small. This suggests an instability of the ground state against the ordered states with the ferromagnetic or antiferromagnetic long range ordering in the Kondo region if the calculations are based on the Gutzwiller function.

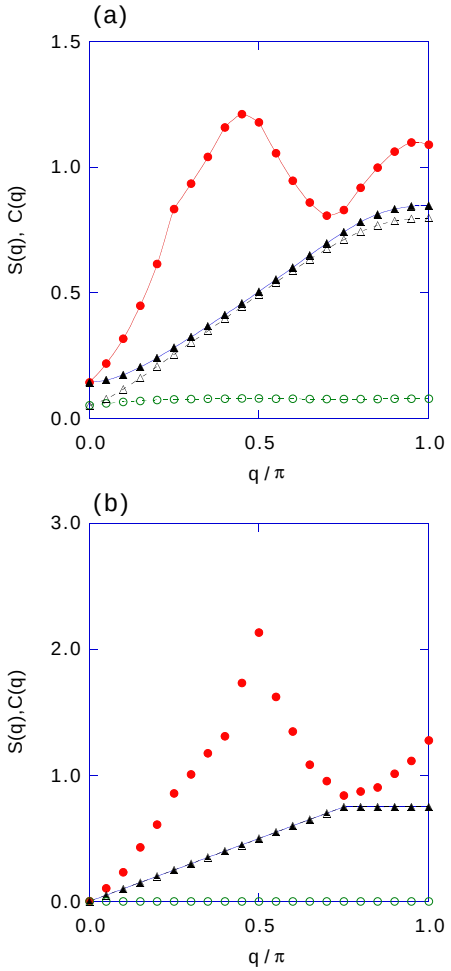

FIG. 12. The spin and charge structure functions for the Gutzwiller function for $E_f = -1$ (a) and $E_f = -3$ (b). Circles and triangles denote the f-electron and conduction electron correlation functions, respectively. Filled and open symbols correspond to spin and charge correlation functions, respectively. The parameters in the Hamiltonian are $N = 40$, $N_e = 70$, $V = 0.5$ and $U = 10$.

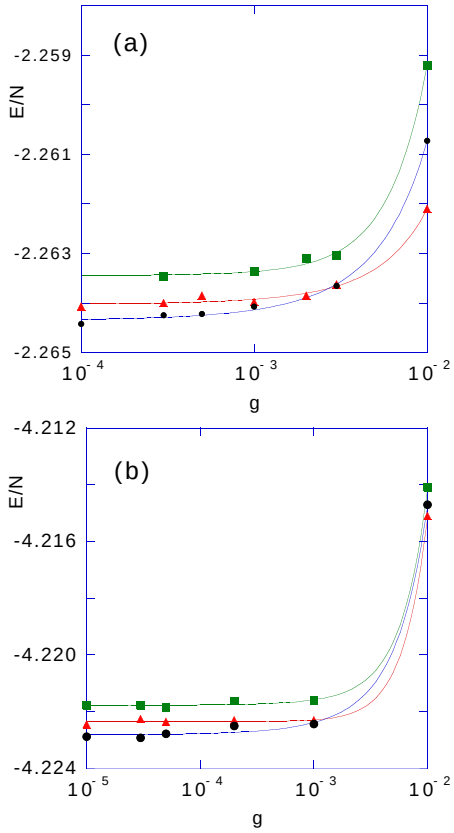

FIG. 13. The energy as a function of g for $\psi^{(1)}$ for $E_f = -1$ (a) and $E_f = -3$ (b) where $N = 40$, $N_e = 70$, $V = 0.5$ and $U = 10$. v and ϵ_f are optimized to obtain a minimum of energy. For (a) $\lambda = 0.06$ (triangles), 0.07 (circles) and 0.08 (squares). For (b) $\lambda = 0.08$ (triangles), 0.09 (circles) and 0.10 (squares).

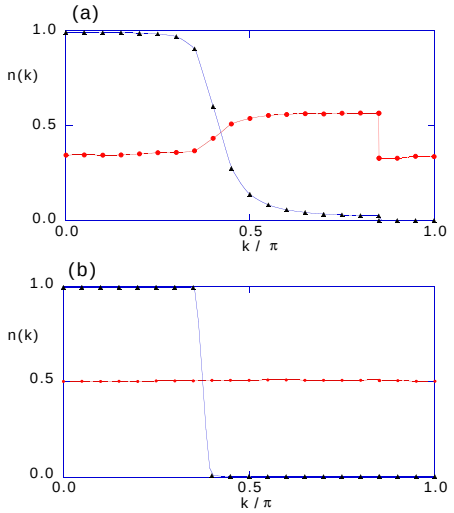

FIG. 14. The momentum distribution function for $\psi^{(1)}$ for $E_f = -1$ (a) and $E_f = -3$ (b) where $N = 40$, $N_e = 70$, $V = 0.5$ and $U = 10$.

The phase diagram of the ground state should be investigated taking account of the off-diagonal correlation factors since the energy lowering is appreciably large. Following the work in this paper an application to examine an instability against various ordering states deserves an intensive investigation. Higher order off-diagonal functions may be necessary to consider the ground state more exactly. The 2D or 3D models must be investigated as more realistic models in the future. Applications to other models such as the orbitally-degenerate periodic Anderson model, the two-impurity Anderson model[33–37] and the d-p model (three-band Cu-O model)[38] are also possible.

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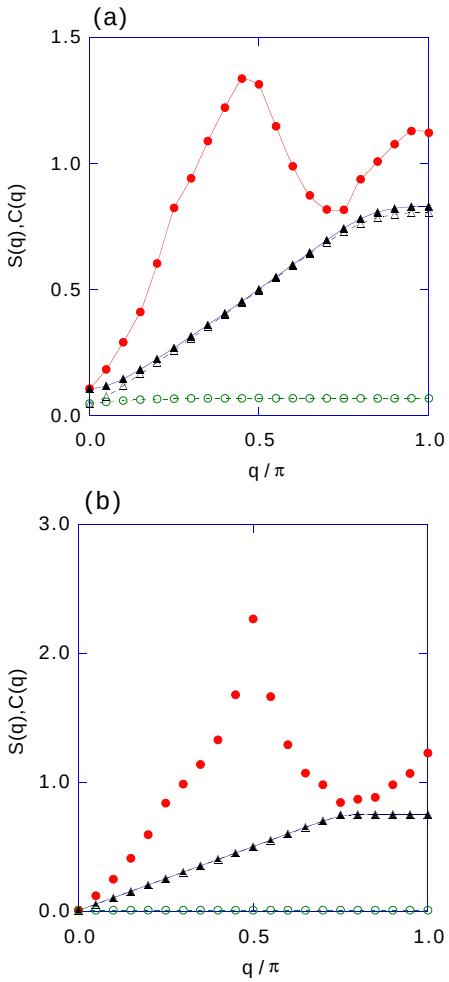

FIG. 15. The spin and charge structure functions for $\psi^{(1)}$ for $E_f = -1$ (a) and $E_f = -3$ (b) where $N = 40$, $N_e = 70$, $V = 0.5$ and $U = 10$. Circles and triangles denote the f-electron and conduction electron correlation functions, respectively. Filled and open symbols correspond to spin and charge correlation functions, respectively.

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