Alternative to Gutzwiller's approach

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An efficient variational procedure to calculate the ground-state properties of the particle-hole symmetric periodic Anderson model is presented. Expectation values are calculated by using an approximate scheme. It is shown that the ground-state energy calculated with the one-site approximation, which essentially is a single-site mean-field approximation, is identical to the corresponding energy obtained by the well-known Gutzwiller wave function using the Gutzwiller approximation. The two-site approximation, in which intersite correlations are explicitly included, is shown to be a better approximation than the Gutzwiller approximation.

I. INTRODUCTION

Most of the current interest[1–9] in the periodic Anderson model stems from its ability to explain to a certain extent the unusual and exciting properties of the heavy fermions and related systems.[10–13] The periodic Anderson model has been studied by various microscopic approaches. Among them, the application of variational methods has led to considerable insight into the problem. The general philosophy behind a variational method is to start from a suitable trial wave function for the ground-state, evaluate the ground-state energy functional, and then determine the inherent parameters by minimizing the energy. The most widely used trial wave function is of the form

$$|\psi_G\rangle = g^D|\psi_0\rangle. \tag{1}$$

It consists of application of the Gutzwiller projector, g^D (to reduce the total number of doubly occupied sites) on the exact wave function, $|\psi_0\rangle$, in the absence of correlations. The calculations with the ansatz are difficult for strongly correlated electron systems because, here, one must deal with an infinite product of operators. To make the calculation tractable one has to follow some approximation scheme. Among the variety of approximate variational schemes that have been used to study the problem, the Gutzwiller approximation[14–20] is the oldest and the most widely used approximation which amounts to the neglect of intersite correlations. Recently, it has been shown that in the limit of large dimensionality, the Gutzwiller approximation becomes exact;[21,22] indeed the intersite correlations decrease if the dimension increases.

In this paper an alternative method simpler than the Gutzwiller method is used to calculate the ground-state energy of the particle-hole symmetric periodic Anderson model. We will show that the one-site ground-state properties evaluated with our variational wave function are identical to those obtained by using the Gutzwiller wave function in terms of the Gutzwiller approximation. This equivalence holds for all values of couplings and in arbitrary dimensions. In the absence of any calculation that treats the average occupation of correlated f electrons self-consistently for the asymmetric periodic Anderson model, comparisions could not be made. However, as shown in Ref. 23 this method considerably simplifies the computations and brings out the role of Coulomb correlations in a very transparent manner. We will also show that the inclusion of intersite correlations gives lower ground-state energy over the one-site and Gutzwiller approximations.

In Sec. II we describe the construction of trial wave function and introduce the method of calculation of the ground-state energy functional using one-site and two-site approximations. In Sec. III we give our results for ground-state energy and comparisons with other methods.

II. FORMALISM

The periodic Anderson model Hamiltonian is given by

$$H = H_0 + U\sum_i n_{fi\uparrow}n_{fi\downarrow}. \tag{2}$$

Here

$$H_0 = \sum_{k,\sigma}\epsilon_k d^\dagger_{k\sigma}d_{k\sigma} + \sum_{i,\sigma}E_f\hat{n}_{fi\sigma} + V\sum_{i,\sigma}(d^\dagger_{i\sigma}f_{i\sigma} + \text{H.c}). \tag{3}$$

U refers to the Coulomb interaction between f-electrons on the same site. The first two terms in Eq. (2) describe the broad conduction band and the nondispersive f level, respectively. The third term describes the hybridization

between f and conduction electrons. The particle-hole symmetry, ($f^\dagger_{i\sigma} \to f_{i\sigma}$, $f_{i\sigma} \to f^\dagger_{i\sigma}$ and $d_{i\sigma} \to d^\dagger_{i\sigma}$, $d^\dagger_{i\sigma} \to d_{i\sigma}$) requires $E_f = -U/2$, the total density of electrons per site, $n = 2$ and the density of both f and d electrons to be 1.

For the particle-hole symmetric case, the ground-state wave function in the absence of Coulomb correlations is given by

$$|\psi_{U=0}\rangle = \prod_{k<k_f,\sigma} \left(\alpha'_{k\sigma} d^\dagger_{k\sigma} - \beta'_{k\sigma} f^\dagger_{k\sigma}\right)|0\rangle. \tag{4}$$

Here,

$$\alpha'_{k\sigma} = \frac{\sqrt{(\epsilon_k^2 + 4V^2)^{1/2} - \epsilon_k}}{\sqrt{2}(\epsilon_k^2 + 4V^2)^{1/4}} \tag{5}$$

and

$$\beta'_{k\sigma} = \frac{\sqrt{(\epsilon_k^2 + 4V^2)^{1/2} + \epsilon_k}}{\sqrt{2}(\epsilon_k^2 + 4V^2)^{1/4}}. \tag{6}$$

At finite values of U, the physical space for the correlated electrons may be simply written as a tensor product over four possible states, singly occupied with spin up and down, doubly occupied, and empty, at each lattice site i. To take correlations into account, we introduce an operator P_i on the starting wave function. The starting wave function, $|\psi_{uc}\rangle$, is the exact ground-state wave function for the $U = 0$ problem with variational functions $\alpha'_{k\sigma}$ and $\beta'_{k\sigma}$ replaced by the appropriate variational functions $\alpha_{k\sigma}$ and $\beta_{k\sigma}$. The new variational functions also satisfy the constraint $\alpha^2_{k\sigma} + \beta^2_{k\sigma} = 1$. The trial ground-state wave function for the correlated problem is given by

$$|\psi_c\rangle = \prod_i \psi_{ci} = \prod_i P_i |\psi_{uc}\rangle. \tag{7}$$

The most general form of the operator P_i is given by

$$P_i = a - b n_{fi\uparrow} n_{fi\downarrow} + c n_{fi\uparrow} + d n_{fi\downarrow}, \tag{8}$$

where a, b, c, and d are variational parameters that depend on U, V, and conduction electron bandwidth. For the paramagnetic case considered in this work, $c = d$.

For finite values of U, due to the hybridization between d and f electrons, the density of f and d electrons per site is not conserved. However, it is reasonable to demand the conservation of total electron density per site.

$$\left\langle \sum_\sigma n_{f i\sigma} + d^\dagger_{i\sigma} d_{i\sigma} \right\rangle_{ci} = \left\langle \sum_\sigma n_{f i\sigma} + d^\dagger_{i\sigma} d_{i\sigma} \right\rangle_{uc}, \tag{9}$$

where $\langle O\rangle_{ci}$ means $\langle\psi_{ci}|O|\psi_{ci}\rangle/\langle\psi_{ci}|\psi_{ci}\rangle$ and $\langle O\rangle_{uc}$ means $\langle\psi_{uc}|O|\psi_{uc}\rangle/\langle\psi_{uc}|\psi_{uc}\rangle$. Equation (9), using translational invariance, gives either $c = b/2$ or $c = -(2a - b)/b$. In order to have the correct limiting value for the operator P_i at $U = 0$, only the relevant solution is $c = b/2$ and $a = 1$. Correspondingly, we obtain

$$P_i = 1 + b/2(n_{fi\uparrow} + n_{fi\downarrow} - 2n_{fi\uparrow} n_{fi\downarrow}). \tag{10}$$

The ground-state energy functional for the periodic Anderson model is

$$E_g = \frac{\langle\psi_c|H|\psi_c\rangle}{\langle\psi_c|\psi_c\rangle}. \tag{11}$$

Here H and $|\psi_c\rangle$ are given by Eqs. (2) and (7), respectively.

The calculation of ground-state energy, Eq. (11), presents a complicated many-body problem, therefore, in this paper, we perform the calculation by using one-site and two-site approximations.

A. One-site approximation

In the one-site approximation we replace $\langle n_{fi\sigma} n_{fj\sigma'} \cdots\rangle_{uc}$ by $\langle n_{fi\sigma}\rangle\langle n_{fj\sigma'}\rangle_{uc}\cdots$, here $i \neq j \neq \cdots$. Physically, such an approximation amounts to neglect of intersite correlations.

The various matrix elements appearing in Eq. (11), obtained by using one-site approximation, translational invariance, and spin symmetry are given by

$$\langle d^\dagger_{i\sigma} f_{i\sigma}\rangle_c = R^{\rm os}\langle d^\dagger_{i\sigma} f_{i\sigma}\rangle_{uc}, \tag{12}$$

$$\langle f^\dagger_{i\sigma} d_{i\sigma}\rangle_c = R^{\rm os}\langle f^\dagger_{i\sigma} d_{i\sigma}\rangle_{uc}, \tag{13}$$

$$\langle f^\dagger_{i\uparrow} f_{i\uparrow} f^\dagger_{i\downarrow} f_{i\downarrow}\rangle_c = C^{\rm os}\langle f^\dagger_{i\uparrow} f_{i\uparrow} f^\dagger_{i\downarrow} f_{i\downarrow}\rangle_{uc}, \tag{14}$$

where $R^{\rm os}$ is given by

$$R^{\rm os} = \left[\frac{8 + 4b}{8 + b(4 + b)}\right] \tag{15}$$

and

$$C^{\rm os} = \frac{8}{8 + b(4 + b)}.$$

The ground-state energy, after substituting $\alpha_{k\sigma}$ and $\beta_{k\sigma}$ obtained from the minimization of the energy functional by imposing the constraint $\alpha^2_{k\sigma} + \beta^2_{k\sigma} = 1$ through a Lagrange multiplier $\lambda_{k\sigma}$, is given by

$$E_g/N = \frac{1}{N}\sum_{k<k_f,\sigma} \lambda^-_{k\sigma} - U/2 + 2U/[8 + b(4 + b)]. \tag{16}$$

Here

$$\lambda^\pm_{k\sigma} = \epsilon_k/2 \pm \left[(\epsilon_k/2)^2 + \tilde{V}^{\rm os^2}\right]^{1/2}, \tag{17}$$

$\tilde{V}^{\rm os} = VR^{\rm os}$, and b is determined from the variational requirement, $\partial E_g/\partial b = 0$.

At this point it would be interesting to compare the ground-state energy functional [Eq. (16)] with the Gutzwiller energy functional.[24] The Gutzwiller energy functional is given by

$$E_g^{\rm Gutz}/N = \frac{1}{N}\sum_{k<k_f,\sigma} \lambda^-_{k\sigma} - U/2 + Ud^f, \quad (18)$$

where $\lambda^-_{k\sigma}$ is same as given by Eq. (17), but with $\tilde{V}^{\rm os}$ replaced by $\tilde{V}_{\rm Gutz} = V[8d^f(1-2d^f)]^{\frac{1}{2}}$ and d^f is a variational parameter, determined by minimizing the energy. Now, If we put $d^f = 2/[8+b(4+b)]$ in Eq. (18), then we find that our energy functional [Eq. (16)] becomes identical to the Gutzwiller energy functional [Eq. (18)]. Furthermore, since both approaches search for the minimum of the ground-state energy in the same parameter space, they must give the same results at the point of minimum.

B. Two-site approximation

In the two-site approximation we include correlations on two sites by using

$$\langle n_{fi\sigma} n_{fj\sigma}\rangle_{uc} = \langle n_{fi\sigma}\rangle_{uc}\langle n_{fj\sigma}\rangle_{uc} - F_{ij}F_{ji}, \quad (19)$$

where

$$F_{ij} = \langle f^\dagger_{i\sigma} f_{j\sigma}\rangle_{uc} = \frac{1}{N}\sum_{k<k_F} e^{ik(R_i-R_j)}\langle n_{fk\sigma}\rangle_{uc}. \quad (20)$$

Calculation of various matrix elements was carried out by assuming that R_i and R_j in Eq. (20) are nearest neighbors, translational invariance and spin symmetry. The two-site results for expectation values are given by

$$\langle d^\dagger_{i\sigma} f_{i\sigma}\rangle_c = R^{\rm ts}\langle d^\dagger_{i\sigma} f_{i\sigma}\rangle_{uc}, \quad (21)$$

$$\langle f^\dagger_{i\sigma} d_{i\sigma}\rangle_c = R^{\rm ts}\langle f^\dagger_{i\sigma} d_{i\sigma}\rangle_{uc}, \quad (22)$$

$$\langle f^\dagger_{i\uparrow} f_{i\uparrow} f^\dagger_{i\downarrow} f_{i\downarrow}\rangle_c = C^{\rm ts}\langle f^\dagger_{i\uparrow} f_{i\uparrow} f^\dagger_{i\downarrow} f_{i\downarrow}\rangle_{uc}, \quad (23)$$

where

$$R^{\rm ts} = 4(2+b)\left(8+4b+b^2\right)/A, \quad (24)$$

$$C^{\rm ts} = \left[2\left(8+4b+b^2\right) - 32\,b\,F_{ij}^4(4+b)\right]/A, \quad (25)$$

$$A = \left(8+4\,b+b^2\right)^2 + 16b^2(4+b)^2F_{ij}^4. \quad (26)$$

Once again, the variational functions $\alpha_{k\sigma}$ and $\beta_{k\sigma}$ are determined from minimization of the ground-state energy functional by imposing the constraint $\alpha^2_{k\sigma} + \beta^2_{k\sigma} = 1$ through a Lagrange multiplier $\lambda_{k\sigma}$. The minimum of the energy is given by

$$E_g^{\rm ts}/N = \frac{1}{N}\sum_{k<k_f,\sigma}\left(\lambda^-_{k\sigma} + x_{k\sigma}n_{fk\sigma}\right) - U/2 + UC^{\rm ts}/4, \quad (27)$$

where

$$\lambda^\pm_{k\sigma} = \tfrac{1}{2}\left\{(\epsilon_k - x_{k\sigma}) \pm \left[(\epsilon_k + x_{k\sigma})^2 + 4\tilde{V}^{\rm ts2}\right]^{1/2}\right\}, \quad (28)$$

$$x_{k\sigma} = \cos[k\times(R_i-R_j)]\left\{4y_\sigma\frac{\partial\tilde{V}^{\rm ts}}{\partial F_{ij}} - \frac{\partial C}{\partial F}\right\}, \quad (29)$$

$\tilde{V}^{\rm ts} = VR^{\rm ts}$ and y_σ is given by

$$y_\sigma = \frac{1}{N}\sum_k \frac{\tilde{V}^{\rm ts}}{\left[(\epsilon_k + x_{k\sigma})^2 + \tilde{V}^{\rm ts2}\right]^{1/2}}. \quad (30)$$

III. RESULTS AND DISCUSSIONS

Although the method described in this paper can be used in any dimension, for simplicity and comparison with other approaches, we have taken a one-dimensional model $\epsilon_{k\sigma} = -2t\cos(ka)$. Here a is the nearest-neighbor distance. The values of parameters used are t=0.5 eV, $V/2t = 0.375$, and $|R_i - R_j|/a = 1$. The ground-state energy calculated by using one-site [Eq. (16)] and two-site approximations [Eq. (27)] is shown in Fig. 1. The ground-state energy obtained by quantum Monte Carlo[9] and renormalization group[5] are also shown in Fig. 1.

We find that the energy calculated using the wave function Eq. (7) and one-site approximation are exactly the same as that obtained[24] by the Gutzwiller wave function in terms of Gutzwiller approximation. However, it should be noted that the equivalence of the variational wave function Eq. (7) with the one-site approximation and the Gutzwiller wave function with the Gutzwiller approximation holds for arbitrary dimensions and is independent of the values of U, V, t and form of the conduction electron dispersion [see discussion below Eq. (17)].

A variational principle gives an upper bound on the

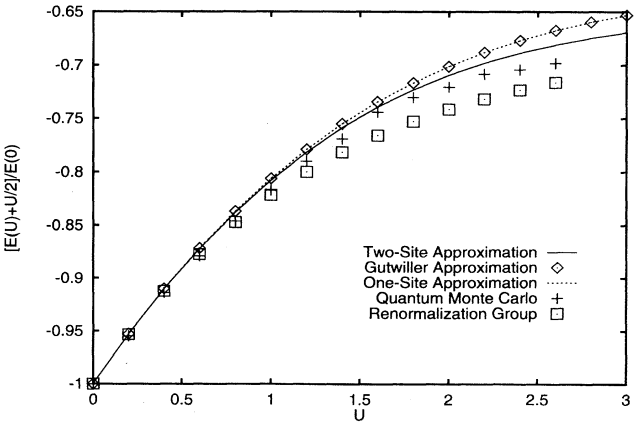

FIG. 1. $[E(U) + U/2]/|E(0)|$ vs U for the symmetric periodic Anderson model with $V/2t$=0.375. $E(U)$ is the ground-state energy per site and $E(0)$ is the ground-state energy at $U = 0$. Our two-site ground-state energy is lower than the Gutzwiller (Ref. 24).

ground-state energy and therefore, provides a criterion for the quality of the wave function. Figure 1 clearly shows that for large values of $U/2t$ the two-site ground-state energy is lower than the one-site energy and the Gutzwiller energy. Hence, the two-site approximation is a more faithful representation of the ground-state properties of the particle-hole symmetric periodic Anderson model.

Numerical calculations[9,5] have clearly indicated the presence of short-ranged magnetic correlations in the ground-state. However, in this paper we have considered only the paramagnetic case. It would be interesting to include the possibility of antiferromagnetic correlations in the trial wave function to study the ground-state properties of the periodic Anderson model.

In this paper we have studied the ground-state properties of the particle-hole symmetric Anderson model, using a variational wave function in which the correlations were included by the introduction of an operator. The calculation of the expectation values is a very difficult task. For this purpose, the calculations were performed by using one-site and two-site approximations. In the former case, complete agreement with the Gutzwiller method was obtained. The two-site results show appreciable improvement over the Gutzwiller method. Possible strengths of this method are as follows: (i) It can be used to study more complicated models involving strong electron correlations; (ii) it can be straightforwardly generalized to study more complicated wave functions; (iii) a variety of intersite spin correlations can be included; and (iv) the crystal structure effects can also be studied.

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