Calculation of the ground state of the one-dimensional two-impurity Anderson model

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By means of the method of fermion coherent state, a one-dimensional two-impurity Anderson model is studied systematically. In the framework of Fermi-liquid theory, we analytically obtain the expression of the ground-state energy and quantitatively calculate the ground-state energy of the two-impurity system when the energy band is in the half-filling or under half-filling case. When the average number of electrons per site n is well away from half filling, a quick dropping of the binding energy per electron is obtained as a function of the coupling V. Also, the beneficial conditions for the two impurities to enter the metallic host are given. [S0163-1829(99)05643-X]

I. INTRODUCTION

In a many-body system, the properties of the magnetic impurities embedded in an electron gas have been a subject of considerable interest.[1–4] This is largely because the understanding of two such impurities is a starting point to understand the magnetic properties of the heavy fermion materials.[5] To attack these many-body problems, there are some widely used techniques: numerical renormalization method,[6] well-controlled quantum Monte Carlo stimulations,[7] and the coupled cluster method[8] (CCM) as well as a Lanczos finite-matrix truncation scheme,[9] which have been applied to the single-impurity periodic one-dimensional (1D) Anderson model. Some other theoretical work on heavy fermion materials are mainly focused on perturbative approximations, such as random phase approximation.

The main purpose of the present paper is to propose a method to investigate a 1D two-impurity system. In fact, this method may also be used on a broad class of many-body fermion systems by constructing the fermion coherent state. We generalize the phonon coherent state method put forward by Davydov[10] and developed by Wang *et al.*[11] to a fermion system and analytically get the expression of the ground-state energy of such a system. The key advantage of our method is that we can quantitatively calculate the ground-state energy of a two-impurity fermion system, the energy band of which is in the half-filling or under half-filling case. The effectiveness of such a method proves the applicability of Fermi-liquid theory to such important problems with strong interaction and forms the basis for understanding more general cases about strong-correlation systems.

II. THE MODEL

We consider the 1D two-impurity Anderson model in the absence of direct hopping between impurities, which comprises two orbitals representing two impurities, positioned at $x_1 = x/2$ and $x_2 = -x/2$, coupled to noninteracting conduction electrons representing the metallic host. Its Hamiltonian is

$$H = \sum_{k\mu} \epsilon_k c^+_{k\mu} c_{k\mu} + \sum_{j\mu} \epsilon_d d^+_{j\mu} d_{j\mu} + V \sum_{jk\mu} (d^+_{j\mu} c_{k\mu} e^{ikx_j} + \text{H.c.}) + U \sum_j d^+_{j\uparrow} d^+_{j\downarrow} d_{j\downarrow} d_{j\uparrow}, \quad (1)$$

where the Fermi operator $c^+_{k\mu}$ creates a conduction electron with momentum k, spin σ, and energy ϵ_k, the operator $d^+_j (j = 1,2)$ creates an electron at the impurity orbital at position x_j with the localized energy level ϵ_d, V is the coupling between the conduction states and each impurity and U is the Coulomb repulsion energy between opposite-spin electrons occupying the same impurity which is set to zero for simplicity.

Before we generalize the phonon coherent state method[10] to fermion system, the validity of the concept of Landau Fermi liquid is needed. It is well known that the clean Q1D systems shows the Luttinger liquid behavior, but that even the slightest amount of impurities restores the Fermi surface.[12] This means that the 1D two-impurity Anderson system we now are discussing is Fermi liquid. We believe, therefore, the important concept of Fermi liquid is still valid here. Now, we introduce the hole operators $h_{k\mu}$ and $h^+_{k\mu}$. Below the Fermi level E_F, we set

$$c^+_{k\mu} \equiv h_{k\mu} \quad c_{k\mu} \equiv h^+_{k\mu}, \quad (k \leqslant k_F), \quad (2)$$

where k_F is Fermi vector. The preceding simplified Hamiltonian then becomes

$$H=\sum_{k\mu}\theta(k-k_F)\epsilon_k+\sum_{k\mu}\theta(k-k_F)\epsilon_k c^+_{k\mu}c_{k\mu}$$
$$-\sum_{k\mu}\theta(k_F-k)\epsilon_k h^+_{k\mu}h_{k\mu}+\sum_{j\mu}\epsilon_d d^+_{j\mu}d_{j\mu}$$
$$+V\sum_{jk\mu}\{e^{ikx_j}[\theta(k-k_F)d^+_{j\mu}c_{k\mu}+\theta(k_F-k)d^+_{j\mu}h^+_{k\mu}]$$
$$+\text{H.c.}\}. \tag{3}$$

In the inspiration of phonon coherent state,[10] we introduce the fermion coherent state

$$|\rangle=\exp\Bigg[\sum_{k_1\mu_1k_2\mu_2}\alpha_{\mu_1\mu_2}(k_1,k_2)\theta(k_1-k_F)\theta(k_2-k_F)$$
$$\times c^+_{k_1\mu_1}c^+_{k_2\mu_2}+\sum_{k_1\mu_1k_2\mu_2}\beta_{\mu_1\mu_2}(k_1,k_2)$$
$$\times\theta(k_F-k_1)\theta(k_F-k_2)h^+_{k_1\mu_1}h^+_{k_2\mu_2}$$
$$+\sum_{j_1\mu_1j_2\mu_2}\gamma_{j_1\mu_1j_2\mu_2}d^+_{j_1\mu_1}d^+_{j_2\mu_2}$$
$$+\sum_{k_1\mu_1k_2\mu_2}\eta_{\mu_1\mu_2}(k_1,k_2)\theta(k_1-k_F)\theta(k_F-k_2)c^+_{k_1\mu_1}h^+_{k_2\mu_2}$$
$$+\sum_{k_1\mu_1j_2\mu_2}\lambda_{\mu_1j_2\mu_2}(k_1)\theta(k_1-k_F)c^+_{k_1\mu_1}d^+_{j_2\mu_2}$$
$$+\sum_{k_1\mu_1j_2\mu_2}\xi_{\mu_1j_2\mu_2}(k_1)\theta(k_F-k_1)h^+_{k_1\mu_1}d^+_{j_2\mu_2}\Bigg]|\rangle_0, \tag{4}$$

where $\alpha_{\mu_1\mu_2}(k_1,k_2),\beta_{\mu_1\mu_2}(k_1,k_2),\gamma_{j_1\mu_1j_2\mu_2},\eta_{\mu_1\mu_2}(k_1,k_2),$ $\lambda_{\mu_1j_2\mu_2}(k_1),\xi_{\mu_1j_2\mu_2}(k_1)$ are variational functions with

$$\alpha_{\mu_1\mu_2}(k_1,k_2)=-\alpha_{\mu_2\mu_1}(k_2,k_1)$$
$$\beta_{\mu_1\mu_2}(k_1,k_2)=-\beta_{\mu_2\mu_1}(k_2,k_1) \tag{5}$$
$$\gamma_{j_1\mu_1j_2\mu_2}=-\gamma_{j_2\mu_2j_1\mu_1}$$

and will be determined consistently from the itinerant equations below. $|\rangle_0=\Pi_{k\mu}\theta(k_F-k)c^+_{k\mu}|0\rangle$ is the ground state of noninteracting fermion system. Here, $|0\rangle$ is the true vacuum state.

The fermion coherent state has the properties of

$$c_{k\mu}|\rangle=\Bigg\{\sum_{k_2\mu_2}2\theta(k_2-k_F)\alpha_{\mu\mu_2}(k,k_2)c^+_{k_2\mu_2}$$
$$+\sum_{k_2\mu_2}\theta(k_F-k_2)\eta_{\mu\mu_2}(k,k_2)h^+_{k_2\mu_2}$$
$$+\sum_{j_2\mu_2}\lambda_{\mu j_2\mu_2}(k)d^+_{j_2\mu_2}\Bigg\}|\rangle \tag{6}$$

$$d_{j\mu}|\rangle=\Bigg\{\sum_{j_2\mu_2}2\gamma_{j\mu j_2\mu_2}d^+_{j_2\mu_2}$$
$$-\sum_{k_1\mu_1}\theta(k_1-k_F)\lambda_{\mu_1j\mu}(k_1)c^+_{k_1\mu_1}$$
$$-\sum_{k_1\mu_1}\theta(k_F-k_1)\xi_{\mu_1j\mu}(k_1)h^+_{k_1\mu_1}\Bigg\}|\rangle \tag{7}$$

$$h_{k\mu}|\rangle=\Bigg\{\sum_{k_2\mu_2}2\theta(k_F-k_2)\beta_{\mu\mu_2}(k,k_2)h^+_{k_2\mu_2}$$
$$-\sum_{k_1\mu_1}\theta(k_1-k_F)\eta_{\mu_1\mu}(k_1,k)c^+_{k_1\mu_1}$$
$$+\sum_{j_2\mu_2}\xi_{\mu j_2\mu_2}(k)d^+_{j_2\mu_2}\Bigg\}|\rangle \tag{8}$$

Inserting Eq. (3) into the Schrödinger equation $H|\rangle=E|\rangle$ in terms of the properties (6)–(8), and equating the coefficients of the terms of $|\rangle,c^+c^+|\rangle,c^+d^+|\rangle,c^+h^+|\rangle,$ $h^+h^+|\rangle,h^+d^+|\rangle,d^+d^+|\rangle$ on both sides of the Schrödinger equation under the approximation to neglect terms of higher rank more than two operators operating on $|\rangle$, we have the following seven coupled equations

$$E=E_0-V\sum_{j_1k_1\mu_1}\theta(k_F-k_1)e^{-ik_1x_{j_1}}\xi_{\mu_1j_1\mu_1}(k_1) \tag{9}$$

$$2\epsilon_{k_1}\alpha_{\mu_1\mu_2}(k_1,k_2)+V\sum_{j_2}e^{-ik_2x_{j_2}}\lambda_{\mu_1j_2\mu_2}(k_1)$$
$$+V\sum_{j_3k_3\mu_3}e^{-ik_3x_{j_3}}\lambda_{\mu_2j_3\mu_3}(k_2)\eta_{\mu_1\mu_3}(k_1,k_3)=0,$$
$$(k_1>k_F,\ k_2>k_F) \tag{10}$$

$$\epsilon_{k_1}\beta_{\mu_1\mu_2}(k_1,k_2)-V\sum_{j_3k_3\mu_3}\theta(k_F-k_3)e^{-ik_3x_{j_3}}\xi_{\mu_1j_3\mu_3}(k_1)$$
$$\times\beta_{\mu_3\mu_2}(k_3,k_2)=0,\quad (k_1<k_F,\ k_2<k_F) \tag{11}$$

$$2\epsilon_d\gamma_{j_1\mu_1j_2\mu_2}+V\sum_{k_1}\theta(k_1-k_F)e^{ik_1x_{j_1}}\lambda_{\mu_1j_2\mu_2}(k_1)$$
$$-2V\sum_{j_3k_3\mu_3}\theta(k_F-k_3)e^{-ik_3x_{j_3}}\gamma_{j_3\mu_3j_1\mu_1}\xi_{\mu_3j_2\mu_2}(k_3)=0 \tag{12}$$

$$(\epsilon_{k_1}-\epsilon_{k_2})\eta_{\mu_1\mu_2}(k_1,k_2)-V\sum_{j_1}e^{-ik_1x_{j_1}}\xi_{\mu_2j_1\mu_1}(k_2)$$
$$+2V\sum_{j_3k_3\mu_3}\theta(k_F-k_3)e^{-ik_3x_{j_3}}\lambda_{\mu_1j_3\mu_3}(k_1)\beta_{\mu_3\mu_2}(k_3,k_2)$$
$$+V\sum_{j_3k_3\mu_3}\theta(k_F-k_3)e^{-ik_3x_{j_3}}\xi_{\mu_2j_3\mu_3}(k_2)\eta_{\mu_1\mu_3}(k_1,k_3)$$
$$=0,\quad (k_1>k_F,k_2<k_F) \tag{13}$$

$$(\epsilon_{k_1}+\epsilon_d)\lambda_{\mu_1 j_1 \mu_2}(k_1)+2V\sum_{j_2} e^{-ik_1 x_{j_2}}\gamma_{j_2\mu_1 j_1\mu_2}$$
$$+2V\sum_{k_2}\theta(k_2-k_F)e^{ik_2 x_{j_1}}\alpha_{\mu_1\mu_2}(k_1,k_2)$$
$$+V\sum_{j_3 k_3\mu_3}\theta(k_F-k_3)e^{-ik_3 x_{j_3}}\lambda_{\mu_1 j_3\mu_3}(k_1)\xi_{\mu_3 j_1\mu_2}(k_3)$$
$$-2V\sum_{j_3 k_3\mu_3}\theta(k_F-k_3)e^{-ik_3 x_{j_3}}\gamma_{j_3\mu_3 j_1\mu_2}\eta_{\mu_1\mu_3}(k_1,k_3)$$
$$=0, \quad (k_1>k_F) \tag{14}$$

$$(\epsilon_d-\epsilon_{k_1})\xi_{\mu_1 j_1\mu_2}(k_1)-Ve^{ik_1 x_{j_1}}\delta_{\mu_1\mu_2}$$
$$-V\sum_{k_2}\theta(k_2-k_F)e^{ik_2 x_{j_1}}\eta_{\mu_2\mu_1}(k_2,k_1)$$
$$+4V\sum_{j_3 k_3\mu_3}\theta(k_F-k_3)e^{-ik_3 x_{j_3}}\gamma_{j_3\mu_3 j_1\mu_2}\beta_{\mu_3\mu_1}(k_3,k_1)$$
$$+V\sum_{j_3 k_3\mu_3}\theta(k_F-k_3)e^{-ik_3 x_{j_3}}\xi_{\mu_1 j_3\mu_3}(k_1)\xi_{\mu_3 j_1\mu_2}(k_3)$$
$$=0, \quad (k_1<k_F) \tag{15}$$

where $E_0=\Sigma_{k\mu}\hbar^2k^2/2m\,(k<k_F)$ is Fermi level of free-electron gas in the normal state.

III. NUMERICAL CALCULATION

Theoretical work on the 1D two-impurity Anderson model has either considered half-filling case, or concerned the situations well away from half filling. However, very little work concerned the close vicinity of half filling, a situation of considerable interest, in particular in view of the physics of impurities in Anderson model. If we define n as the average number of fermions per site, the three cases mentioned above mean $n\approx 1$, $n<1$, and $n\to 1$ but $n\neq 1$. With our model, it is very convenient to consider preceding three different cases and discuss the different behaviors.

For an 1D two-impurity electron gas, infinite length of system will lead to ineffectiveness of impurity. As a result, in order to observe the comparatively apparent effects in 1D two-impourity electron gas system, we just study the finite 1D lattice case. By taking the periodic boundary condition,

$$k=\frac{2\pi n}{L}, \quad (n=1,2,\ldots,N), \tag{16}$$

where L is the length of quantum wire, N is the number of lattice, we calculate the ground-state energy at half filling or under half-filling case. Now, we demonstrate our numerical results and give the explanations.

(a) At first, we define the binding energy ΔE as the difference between the ground-state energy E of impurity system and that of free electron gas in the normal state. If $\Delta E<0$, it means that it is possible theoretically for impurities to form a stable system in which the ground-state energy of two-impurity system is lower than that of free-electron gas and is a benefit for impurities to mix with the electron gas in the lattice. In the opposite situation it will be impossible to form a stable system. The coupling between the conduction electrons and d electrons reflects mainly the stability of such system. The stronger the coupling, the lower ground-state energy will be. In Figs. 1(a) and 1(b), we show the calculated binding energy per electron $\Delta E/N$ as a function of coupling constant V due to different n. From the figures, we notice that, (i) The 1D two-impurity system is more stable with the coupling V increasing. That is, the increasing of coupling V is benefit for the impurities entering the 1D metallic host. (ii) The average number of electrons per site n means the height of Fermi surface and the amount of filling electrons in energy band, which reflects many physical properties of alloys. All the electrons in a 1D-ordered lattice (we call it metallic host) move communally, which has the characteristic of extended state. When ordered lattice is doped by few impurities, the periodicity of lattice is destroyed locally and some electrons or holes will be trapped in the impurities. The electrons moving locally near the impurities have the characteristic of localized state. When a 1D-ordered lattice has the average number of electrons per site $n\approx 1$, the electrons will have high momentum. Then they will have less opportunities to be trapped by the localized state associated with the impurities than $n<1$ in which electrons have low momentum. That is, the binding energy as $n<1$ is lower than that in the case of $n\approx 1$. As is well illustrated by Figs. 1(a) and 1(b).

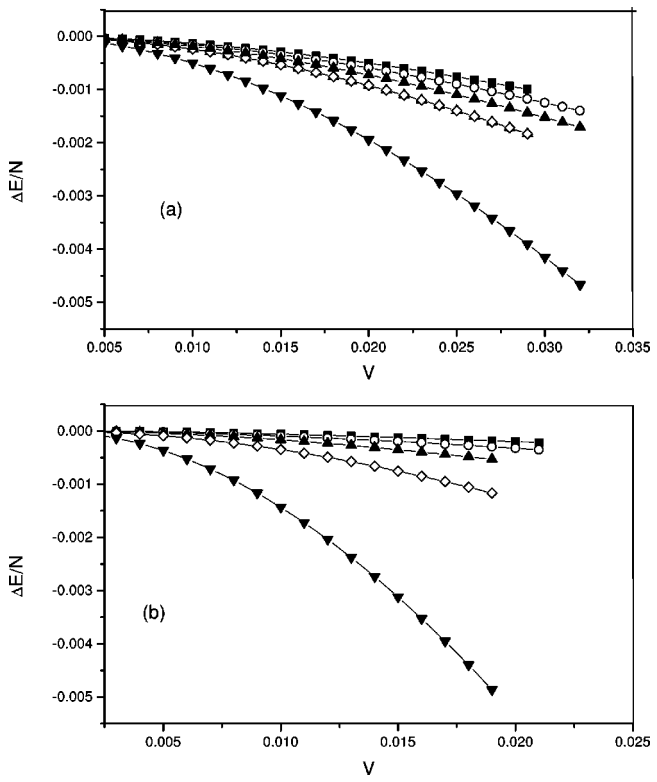

FIG. 1. The binding energy per electron $\Delta E/N$ as a function of the coupling V between orbital electrons and conduction ones. They are given for several different values of average number of electrons per site n (a) $N=16$, $L=4$ nm. Solid squares, $n=1$; open circles, $n=7/8$; solid up triangles, $n=3/4$; open diamonds, $n=5/8$; solid down triangles, $n=3/8$. (b) $N=24$, $L=10.08$ nm. Solid squares, $n=1$; open circles, $n=5/6$; solid up triangles, $n=2/3$; open diamonds, $n=1/2$; solid down triangles, $n=1/3$. We take the distance between two impurities as $x=\pi/2k_F$, which is used in this paper.

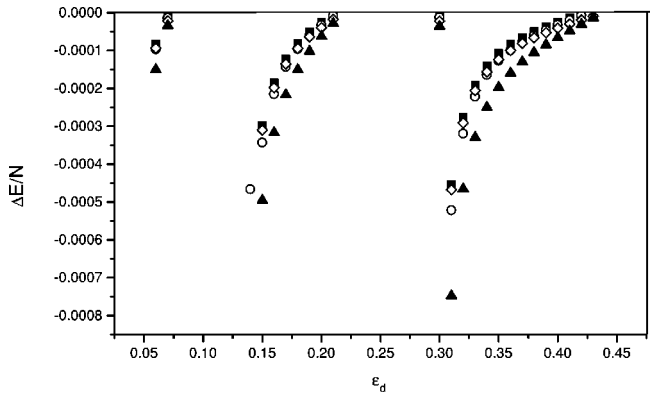

FIG. 2. The binding energy per electron $\Delta E/N$ with the parameters $N=16$, $L=4$ nm as a function of the energy of localized energy level ϵ_d for different average number of electrons per site n. Solid squares, $n=1$; open circles, $n=7/8$; open diamonds, $n=3/4$; solid up triangles, $n=5/8$.

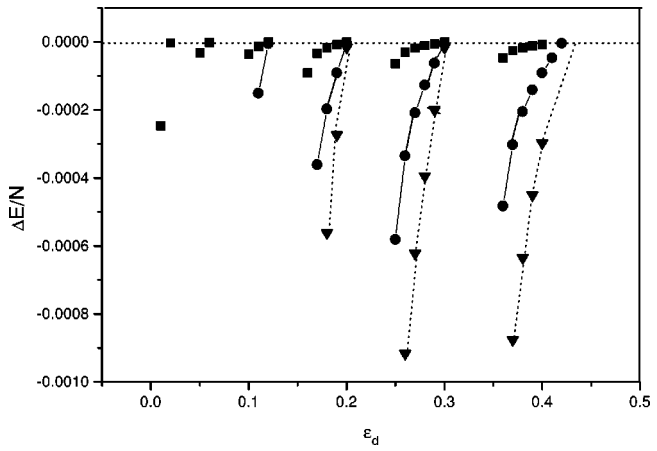

FIG. 3. The binding energy per electron $\Delta E/N$ shown as a function of the energy of localized orbitals ϵ_d for different V in the case of half filling. We take $N=24$, $L=12.48$ nm. Squares, $V=0.0015$; circles, $V=0.005$; down triangles, $V=0.01$.

From the figures, we also can see that, at the case of half filling or close vicinity of half filling, the binding energy per electron decreases linearly and slowly with V. But such process will become more remarkable as the situations well away from half filling is satisfied. Such as in Fig. 1(b), when $n=1/3$, the quickly dropping of $\Delta E/N$ with V manifests the binding energy per electron is more sensitive than $n\approx 1$.

(b) Now let us discuss the influence of the localized energy level ϵ_d on the ground-state energy. When V is set, there are two competition effects. On the one hand, as the energy of the localized energy level $\epsilon_d>0$, the state of the orbital electrons induced by the impurities will be partially localized, which will increase the energy of system and is harmful for the impurities to be stable. On the other hand, the interaction of the orbital electrons and conduction ones will decrease the energy of system, which is helpful for the impurity system to be stable. The mutual competition of the above two effects makes the situation more complex. From the Fig. 2, we can see, in some regions, such as $\epsilon_d \in [0.01,0.05]$, $[0.08,0.14]$, and $[0.22,0.29]$, that it is impossible for two impurities to mix with the metallic host to form a stable system. In the stable region, we can see clearly there is also the feature mentioned above that the binding energy per electron decreases with the declining of n. With the increasing of ϵ_d, the region suitable for the two impurities to enter the metallic host is larger companying with $\Delta E/N$ drops heavily. Particularly, when $\epsilon_d=0.29$, the $\Delta E/N$ drops abruptly from -1×10^{-4} to -8×10^{-3} and then increases little by little with ϵ_d. In Fig. 3, we plot the binding energy per electron versus ϵ_d with different V. A very typical feature is that $\Delta E/N$ varies more precipitously with the increasing of V for the coupling between the orbital electrons and conduction ones is helpful for the system's stability. The other feature same as Fig. 2 is that there also exist some regions impossible for the 1D two-impurity Anderson system to be steady.

IV. CONCLUSION

To summarize, in this paper we have studied the problem of the 1D two-impurity Anderson model by means of the fermion coherent state. Through calculating the binding energy per electron, we can judge what conditions will be favorable for the impurities mixing with the metallic host. Generally speaking, the increasing of the coupling between the orbital electrons and the conduction electrons is beneficial for the impurity and the metallic host to mix together. The binding energy per electron decreases linearly and slowly with V in the case of half filling or in the vicinity of half filling. To the system whose energy band is well away from half filling, our numerical calculations show that, its binding energy per site decreases more quickly.

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