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Transitions from conventional metals and insulators to Kondo metals and insulators

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This paper reports calculations of the spectral weight for the lattice Anderson model, defined on a square (four-site) cluster, by exact diagonalization. The calculations emphasize the change in the density of states as the interaction strength U varies between weak and strong limits. We consider system parameters and occupancies such that the model resembles either a conventional insulator or a conventional metal for weak interactions. Then increasing interaction strength leads in the first case to a Kondo insulator in which there is a gap at the chemical potential between hole and electron states. In the metallic case, several features of the Kondo effect in bulk systems are observed. We also observe the splitting of the f band, leading to the formation of an upper Hubbard band at high energy with some double-site occupancy, while states with two f holes on a site are also separated to form a satellite.

I. INTRODUCTION

In many solids, one finds both nearly free electrons in wide bands and nearly localized electrons in narrow bands associated with unfilled atomic shells. Examples include transition-metal oxides, rare-earth and actinide metals, and heavy-fermion systems. A wide range of physical properties are found: antiferromagnetism occurs, frequently with large atomic moments, but occasionally with small ordered moments. One may find also, mixed-valence, ferromagnetism, low- and high-temperature superconductivity and so on. The lattice Anderson model is probably the simplest theoretical picture which incorporates the essential physics of these systems.[1]

This paper is concerned with the description of the electronic structure of materials of this type through numerical studies of the spectral weight function. We investigate the nondegenerate lattice Anderson model through exact diagonalization calculations on small clusters. The model is defined by the Hamiltonian

$$H=-t\sum_{ij\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}+E_f\sum_{i}n_{fi\sigma}+U\sum_{i}n_{fi\uparrow}n_{fi\downarrow}+V\sum_{i\sigma}(c_{i\sigma}^{\dagger}f_{i\sigma}+f_{i\sigma}^{\dagger}c_{i\sigma}) . \tag{1}$$

The notation is standard. We note that we include only nearest-neighbor c electron hopping and single-site hybridization. If the interaction of the f electrons with each other is neglected, we have a conventional energy-band problem in a very simple form. Usually, one wishes to consider a parameter regime $|V|<|t|$, in which a "c" band centered at $t=0$ of a standard tight-binding form hybridizes with localized "f" levels. The latter are grouped at E_f if $V=0$, but acquire some width through interaction with the "c" states. We will set $t=1$ in all numerical calculations.

In this paper, we shall principally be concerned with numerical studies of the periodic Anderson Model using the exact diagonalization technique on small clusters. Much of the previous work has focused on a description of spin correlations in the ground state. We cite here several calculations of this type.[2–6] Work prior to 1990 has been reviewed by Parlebas.[7]

If the parameters of the Hamiltonian are varied, one encounter different regimes of behavior, which we described in a previous paper.[4] These include doubly occupied f states, mixed-valence (there are two regions), Kondo, and empty f states. In the Kondo region, the f states are singly occupied, although their single-particle energies are lower than those of some of the c states which are doubly occupied. Then one finds correlations between the c and f electron spins. In the limit that there is exactly by one f electron per site, one can treat the f electrons as localized spins which are coupled by an exchange integral J to the c electron spins. In this way, one arrives at the Kondo lattice model, which is related to the periodic Anderson model in much the same way as the t-J model is related to the Hubbard model.

The Hilbert space of the Kondo lattice model on a given cluster is considerably smaller than that of the periodic Anderson model. This permits one to consider systems of larger size. Numerical calculations by several methods have been reported: exact diagonalization, quantum Monte Carlo, and renormalization-group methods have been applied. Some references are also cited below.[8–12] However, the Kondo lattice model can be used only to describe the ground-state and low-energy excitations. The upper part of the Hubbard split f band is omitted. Moreover, it does not have a simple connection to the small U limit of the periodic Anderson model.

Our work here attempts to describe some important characteristics of single-particle states in the periodic Anderson model. This is done through calculations of the spectral weight function and the closely related density of states, which are performed by exact diagonalization methods on a small cluster. Previously,[13] we have considered the model under conditions of strong interactions. We varied E_f for fixed values of U, V, and t and calculated the spectral weight function in the different regimes of behavior mentioned above. Here we consider the spectral weight function as U is varied for fixed E_f, V, and t so that the system passes from weak- to strong-interaction limits. We made two choices of the f level energy, E_f, one of which implies that the system will go with increasing U to the Kondo region in which f levels are singly occupied. The other leads into a mixed-valence region.

The model has the property that if the number of electrons is exactly equal to the product of the number of sites times the number of orbitals ("half filled"), there is a gap at the Fermi energy.[2] The simulation then refers to an insulator, and as U increases, we study the development of the system from a conventional insulator into an unconventional one (a Kondo insulator if we go into the Kondo region). To simulate a metallic case, we add an additional electron, so that there is no gap in the $U=0$ limit. Then increasing U leads from a conventional metal to an unconventional Kondo or mixed-valence metal.

Our simulations are, of course, restricted to quite small systems. We consider four sites arranged as a square. Since there are two orbitals per site, the dimension of the Hilbert space of the model is the same as that of an eight site one band Hubbard model. We could work with a larger system (six or eight sites) were we to restrict the f levels to exactly single occupancy, as in the Kondo lattice model mentioned above, or if we were only interested in the ground state. In that case, one could use the Lanczos algorithm which makes calculations for systems with up to eight sites possible using the full periodic Anderson model.[14] However, the investigations we report here require results over a large range of energies, and we have found that the usual Lanczos method often becomes inaccurate. The present calculations are based on complete diagonalization of the Hamiltonian. Because the system is so small, we emphasize what we believe to be generic properties of the model which are qualitatively independent of system size.

The remainder of this paper is organized as follows. Our notation, and some (known) properties of the spectral weight function are summarized in Sec. II. Our results are described in Sec. III. Finally, the work is summarized in Sec. IV.

II. SINGLE-PARTICLE STATES AND THE SPECTRAL WEIGHT FUNCTION

In this paper, we consider, as mentioned above, a ring (square) of four sites. Only single-site hybridization is considered. The calculation begins by diagonalizing the Hamiltonian of Eq. (1) with $U=0$, which is done analytically. We obtain the single-particle eigenstates

$$|\varphi_\gamma\rangle=\sum_i(\alpha_{i\gamma}|fi\rangle+\beta_{i\gamma}|ci\rangle)\ . \tag{2}$$

Here $|fi\rangle(|ci\rangle)$ is a single-particle state in which there is a single $f(c)$ electron on site i, and γ is a composite index which combines band number and wave vector. Note that, in contrast with the more familiar case of the Hubband model it is not adequate to use the wave vector $\mathbf{k}$ alone: there are two states for each $\mathbf{k}$. The states $|\varphi_\gamma\rangle$ are used to define the creation and annihilation operators $c_\gamma^\dagger, c_\gamma$.

The energies of the single-particle states are

$$\mathbf{k}=(0,0);\quad E=\tfrac{1}{2}\{E_f-2t\pm[(E_f+2t)^2+4V^2]^{1/2}\}\ , \tag{3a}$$

$\mathbf{k}=(\pi,0)$ and $(0,\pi)$ (doubly degenerate),

$$E=\tfrac{1}{2}\{E_f\pm[E_f^2+4V^2]^{1/2}\}\ , \tag{3b}$$

$$k=(\pi,\pi),\quad E=\tfrac{1}{2}\{E_f+2t\pm[(E_f-2t)^2+4V^2]^{1/2}\}\ . \tag{3c}$$

The spectral weight function is given by

$$A_{\gamma\sigma}(E)=\sum_m\{Z^{(h)}_{\gamma\sigma,m}\delta[E-E_g(N)+E_m(N-1)+\mu]+Z^{(e)}_{\gamma\sigma,m}\delta[E-E_m(N+1)+E_g(N)+\mu]\}\ . \tag{4}$$

In this equation, g designates the ground state of the N particle system, m designates an arbitrary state of the $N-1$ or $N+1$ particle system, and μ is the chemical potential. The quantities Z are the squares of matrix elements,

$$Z^{(h)}_{\gamma\sigma,m}=|\langle\psi_m^{N-1}|c_{\gamma\sigma}|\psi_g^N\rangle|^2\ , \tag{5a}$$

$$Z^{(e)}_{\gamma\sigma,m}=|\langle\psi_m^{N+1}|c^\dagger_{\gamma\sigma}|\psi_g^N\rangle|^2\ . \tag{5b}$$

The superscripts (h) and (e) denote holes and electrons, respectively. For an added electron, the energy E of a peak in the spectral weight function is the energy above the Fermi energy at which an extra electron can propagate. For holes, $-E$ is the energy which must be added to the system to remove an electron or propagate a hole. The Z's are residues of the single-particle Green's function, and each is a positive quantity ≤ 1. The limiting case, $Z_{\gamma\sigma,m}=1$ corresponds to the concentration of the entire spectral weight on one (many body) state m, which is characteristic of noninteracting particles. The density of states is defined by

$$n(E)=\sum_{\gamma\sigma}A_{\gamma\sigma}(E)\ . \tag{6}$$

The spectral weight functions are normalized to unity if integrated over all energies, i.e., including both hole and electron energies.

$$\int_{-\infty}^{\infty}A_{\gamma\sigma}(E)dE=1\ . \tag{7}$$

If we consider electron $(E>0)$ and hole $(E<0)$ energy ranges separately, we have

$$\sum_\gamma\int_0^\infty A_{\gamma\sigma}(E)dE=\sum_\gamma\langle\psi_g^N|1-c^\dagger_{\gamma\sigma}c_{\gamma\sigma}|\psi_g^N\rangle=2N_S-n_\sigma\ , \tag{8a}$$

where n_σ is the number of electrons of spin σ in the system, and N_S is the number of sites. Also,

$$\sum_\gamma\int_{-\infty}^0 A_{\gamma\sigma}(E)=\sum_\gamma\langle\psi_g^N|c^\dagger_{\gamma\sigma}c_{\gamma\sigma}|\psi_g^N\rangle=n_\sigma\ . \tag{8b}$$

Not only are Eqs. (8a) and (8b) useful for checking numerical calculations, they tell us something about the effects of "doping". At half filling (assuming N_S is even) the ground state is a singlet (this is known from previous calculations[2-7]) and $n_\sigma = n_{-\sigma} = N_S$. Now let us add one electron with spin up ($\sigma = \uparrow$). Then the integrated weight for electrons of spin ↑ is $N_S - 1$, and that for holes is $N_S + 1$. In other words, the spectral weight is increased in the hole region of the spectrum and decreased in the electron region. Obviously, the opposite occurs if an electron is removed from the system.

We determine the chemical potential by

$$\mu(N) = \tfrac{1}{2}[E_g(N+1) - E_g(N-1)] \ . \qquad (9)$$

This result follows from consideration of a limited "grand" cannonical ensemble in which only states with $N-1$, N, and $N+1$ particles are included.[3]

Note that if $N = 2N_S$ (half filling, singlet ground state), the spectral weight functions for ↑ and ↓ spins are the same and the spin index on A is unnecessary and may be dropped. This is not the case for $N = 2N_S + 1$. Let, in this case, $n_\uparrow = n_\downarrow + 1$. If we add another electron of ↑ spin, only triplet states are contributed to A; but if we add one of ↓ spin, both singlet and triplet states contribute. Similar considerations apply if $N = 2N_S - 1$.

III. RESULTS

In our calculations, the hopping parameter t was fixed at 1.0. Most of the calculations employed a hybridization parameter of 0.50. Two values of the f electron energy, $E_f = -3.0$ and 0.0 were considered. The single-particle level structure from Eqs. (3) is shown in Fig. 1. In the case of $E_f = -3.0$, the f levels lie below the c levels; for $E_f = 0.0$, the f levels are in the middle of the c distribution and the levels with $k = (\pi, 0)$, and $(0, \pi)$ show strong f-c hybridization. We made calculations for values of the interaction parameter ranging from $U = 0.1$ (weak interaction) to 8.0 (strong interaction), and for electron numbers $N = 8$ (half filling) and $N = 9$. The half-filled case simulates an insulator for all U; the other resembles a metal. The strong interaction limit in the case of $E_f = -3.0$ leads to (roughly) singly occupied f levels when U is large (Kondo region); while $E_f = 0.0$ leads to mixed valence.

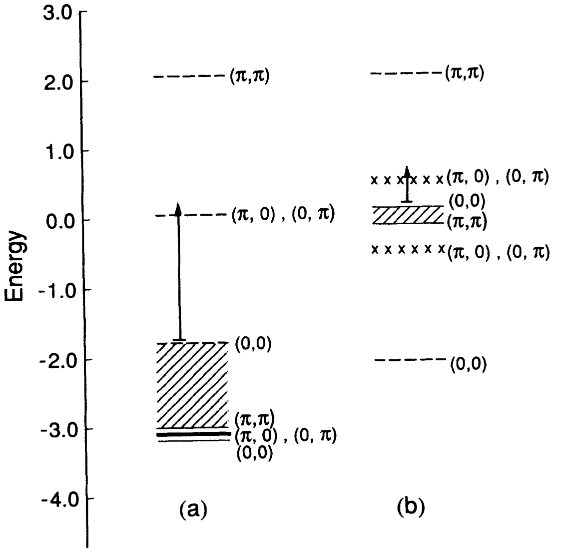

FIG. 1. Single-particle energies (a) $E_f = -3.0$, (b) $E_f = 0.0$. Solid lines, f levels; dashed lines, c levels; crosses strongly hybridized c-f levels. The **k**'s are indicated in parentheses. The degenerate levels $(\pi, 0)$ and $(0, \pi)$ are represented by heavier lines. The gap in the half-filled case is indicated by hatching. The arrows show the motion of the chemical potential, μ in the metallic case, $N = 9$. The foot of the arrow shows μ for $U = 0.1$, the head indicates μ for $U = 8.0$.

A. Insulating case

For the geometry considered, the half-filled condition corresponds, in the weak-interaction limit, to an insulating situation. However, there are significant differences in the two cases considered. For $E_f = -3.0$, we see from Fig. 1 that there is a rather large gap separating a narrow f band from a broad c band. For $E_f = 0.0$, however, the $U = 0$ gap is fairly small; separating an occupied f level with $k = (\pi, \pi)$ from an unoccupied one with $k = (0, 0)$. This structure with strongly hybridized c-f levels above and below the gap, occurs in the middle of widely spaced c levels. In this case, there would not be a gap in the absence of hybridization.

One way to characterize the effect of interaction in these systems is through the f state occupation. Table I lists the number of f electrons per site, n_f, for several different values of U. It will be seen that for $E_f = -3$, there are nearly $2f$ electrons per site when U is small. The small difference from 2 is due to hybridization. It is interesting that n_f remains significantly larger than 1 even for $U = 2$. This is discussed below. As U continues to increase n_f becomes close to 1, the Kondo situation. However, for $E_f = 0.0$, n_f is close to 1 at $U = 0$, and decreases, remaining smaller than 1 as U increases, corresponding to mixed valence.

In the presence of interaction, the gap $\Delta(N)$ in an N electron system, may be defined by

$$\Delta(N) = E_g(N+1) - 2E_g(N) + E_g(N-1) \ . \qquad (10)$$

We tabulate Δ in Table II for several values of U.

In the case of $E_f - 3.0$, we see that the gap decreases with U, but not monotonically. The gap is larger for $U = 4$ than for 2, but is smaller for $U = 8$ than 4. For $E_f = 0.0$, the gap is initially much smaller, increases with

TABLE I. Number of f electrons per site, n_f, for insulating ($N = 8$) and metallic ($N = 9$) cases.

U	n_f $E_f = -3.0$		n_f $E_f = 0.0$	
N	8	9	8	9
0.1	1.886	1.926	0.975	1.204
0.5	1.827	1.891	0.886	1.087
1.0	1.714	1.821	0.821	0.978
2.0	1.472	1.659	0.767	0.896
4.0	1.077	1.112	0.739	0.865
8.0	0.978	0.995	0.727	0.855

TABLE II. Gap at the chemical potential for the half-filled band. Note that all energies are ratios with respect to the hopping parameter t, which has been set to unity.

U	$E_f=-3.0$	$E_f=0.0$
0	1.257	0.236
0.1	1.178	0.238
0.5	0.886	0.274
1.0	0.596	0.336
2.0	0.314	0.346
4.0	0.399	0.333
8.0	0.239	0.255

U, reaches a maximum in the neighborhood of $U=2$, and for larger U, approaches values similar to those for $E_f=-3.0$.

It is interesting to consider the role of hybridization in establishing a gap. First, consider the occupancy of levels in the absence of any hybridization. Then the f levels will be fully doubly occupied for

$$E_f < -U + E_c^{(0)} , \tag{11a}$$

where $\Delta E_c^{(0)}$ is the lowest level in the c "band" (-2 in the present case). If E_f is larger than this, some electrons will transfer from f to c states. If E_f rises to the point where

$$E_f = -U + \Delta E_c , \tag{11b}$$

where ΔE_c is the energy required to add one more electron to the c band if $N/2-1$ are already present, all the f states are singly occupied. In a bulk system, ΔE_c is the Fermi energy of the c electrons. In the model we use here, $\Delta E_c^{(1)}=0$ in the absence of hybridization. Thus, in this model, when $U>3$, we expect to have two electrons in the degenerate c states of $k=(0,\pi)$ and $(\pi,0)$, which can accommodate four. Thus, there is no gap in the Kondo region in the absence of hybridization. In the case $E_f=0.0$, leading to mixed valence, the f states are degenerate with the c levels with $k=(\pi,0)$ and $(0,\pi)$, and there is again no gap (for any U) in the absence of hybridization.

Since hybridization is required to produce a gap in the Kondo region (as well as in the case of mixed valence), it is natural to refer to the gap as a hybridization gap. Early numerical calculations[2] (and ours are in agreement) showed that the gap was proportional to V^2 for small V, as would be expected. It may then seem confusing to find that a gap is present in the Kondo lattice model, which apparently contains no hybridization. Hybridization has simply been hidden by including it in the exchange coupling of c spins and localized f spins through the cannonical transformation leading from the Anderson lattice to the Kondo lattice.[15]

Figure 2 shows the density of states for $E_f=-3.0$ and $U=0.5$. This illustrates the weak interaction limit. The diagram shows the high density of states associated with the f levels, separated by a significant gap from the c levels, which are represented by the three well separated peaks for $E>0$. The figure is drawn with the zero of energy being the chemical potential, μ. In fact, the f levels have moved up in energy by about 0.4 with respect to their position in Fig. 1.

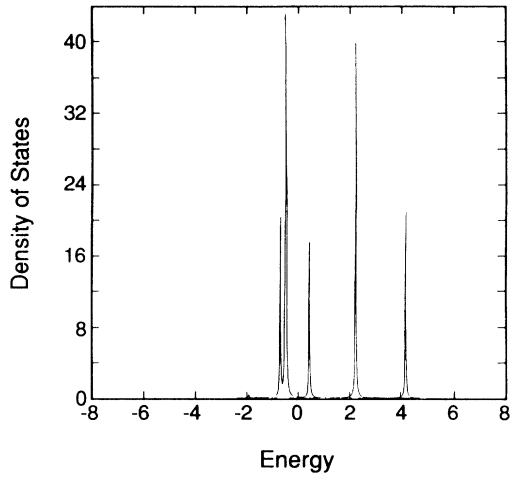

FIG. 2. Density of states for the conventional insulator $E_f=-3.0$, $V=0.5$, $U=0.5$. An artificial, Lorentzian broadening of 0.10 has been included.

As U increases, the f electron energies and the chemical potential rise, crossing the lowest c level and moving toward the c levels with $k=(\pi,0)$ and $(0,\pi)$ near $E=0$ (in Fig. 1). Figure 3 shows the density of states for $E_f=-3.0$, $U=8$, which is strongly in the Kondo region. In this case, the chemical potential is quite close to $E=0$ in Fig. 1, so that the energy scales of Figs. 1 and 3 have, to graphical accuracy, a common origin. The pattern of levels shown in Fig. 3 is quite different from that of Fig. 1 as a result of the continued rise in the f energies, showing the pronounced Hubbard splitting of the f band, and the appearance of satellite structure at negative energies (in Fig. 3) in which there are two f holes on a site.

The peak at the highest energy (near $E=E_f+U=5$) represents the upper half of the Hubbard split f band. This region, which in a high-resolution drawing would show several peaks for each $\mathbf{k}$, contains about 46% of the

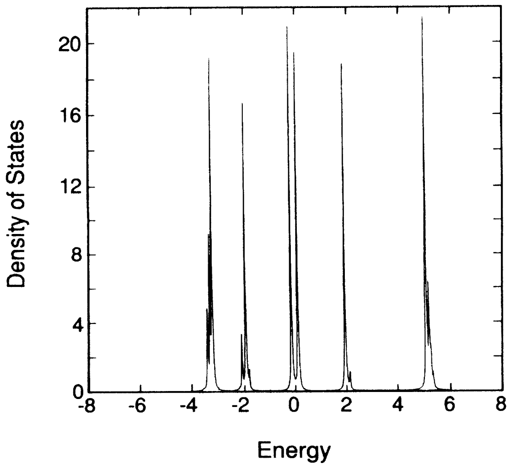

FIG. 3. Density of states for the Kondo insulator: $E_f=-3.0$, $V=0.5$, $U=8.0$.

total electron spectral weight (i.e., 46% of the spectral weight for $E>0$). Coming down in energy, we encounter a peak at $E=2$ of (nearly) unit spectral weight associated with the c states of $k=(\pi,\pi)$, little altered in position from that shown in Fig. 1. Near $E=0$, we find three levels one for each $\mathbf{k}$, too closely spaced in energy to be resolved in the drawing, which define the upper portion of the gap. Most of the spectral weight here is associated with the degenerate c states of $k=(\pi,0)$, $(0,\pi)$, which remain close to the position in Fig. 1. However, the weight (Z) of the members of this pair is roughly 0.5 each, instead of 1.

On the negative energy side of the gap, we encounter a mirror image (roughly) of the states just above the gap, again with most of the spectral weight (0.5 each) being in the $k=(\pi,0)$, $(0,\pi)$ pair. The c state of $k=(0,0)$, which is accompanied by considerable subsidiary structure (interaction broadening) produces the peak near $E=-2$. The lowest-energy peaks in the range $-3.6<E<-3.2$ are associated with the states in which two f holes are on the same site. These states would form a satellite peak in a photoemission experiment. Here, they have about 45% of the total hole spectral weight (spectral weight for $E<0$).

Although Eqs. (8a) and (8b) require, in the half-filled case in which $n_\sigma=N_S$, the total spectral weight for electrons and holes is the same, this does not apply to the individual components associated with particular single-particle states. For example, at $U=8$, 95% of the integrated spectral weight associated with the $k=(0,0)$ "c" type state is in the hole region, and 74% of that is associated with the peak near $E=-2$. This state has changed from an unoccupied to an occupied state as U increased, but it has remained essentially a noninteracting single-particle state. Similarly, the $k=(\pi,\pi)$ "c" state remains a single-particle state in the unoccupied (conduction-band) region. The spectral weight associated with the c states of $k=(\pi,0)$ and $(0,\pi)$ is split into the two peaks adjacent to the gap. We think that reduced spectral weight in the gap region (about $\frac{1}{2}$ that expected in a conventional insulator) is one of the characteristic features of the Kondo insulator.

The spectral weight associated with the f states is quite diffuse, with about half being associated with holes and half with electron states. This is an obvious consequence of the Hubbard splitting of the f levels.

Figure 4 shows the density of states for $E_f=0.0$ and $U=4$. In this case, our simulation refers to a mixed-valence insulator. Starting at high energy, we encounter in the neighborhood of $E=4$, the upper half of the split f band. The peak close to $E=2$ is associated with the c state with $k=(\pi,\pi)$. The gap region shows a highly asymmetric distribution of states. The peak on the positive-energy side is principally associated with the doubly degenerate strongly hybridized states of $k=(\pi,0)$, and $(0,\pi)$ plus the "f" state of $k=(0,0)$. The spectral weight in this region has been reduced in comparison with that for small U by the formation of the upper Hubbard "f" band.

On the hole side, we encounter first the f state of $k=(\pi,\pi)$, a weak f state with $k=(0,0)$, split from the one above $E=0$, and then a complex of three states deriving from the lower hybridized states of $k=(\pi,0)$, and $(0,\pi)$ (see Fig. 1). The lowest-energy peak is associated with the "c" state of $k=(0,0)$. There is no low-energy satellite structure associated with two hole f states (in contrast with Fig. 3). The choice of E_f has forced these states into the energy range between $E=-1$ and $E=0$. The result is a complicated upper valence band while the conduction band has remained simple in comparison.

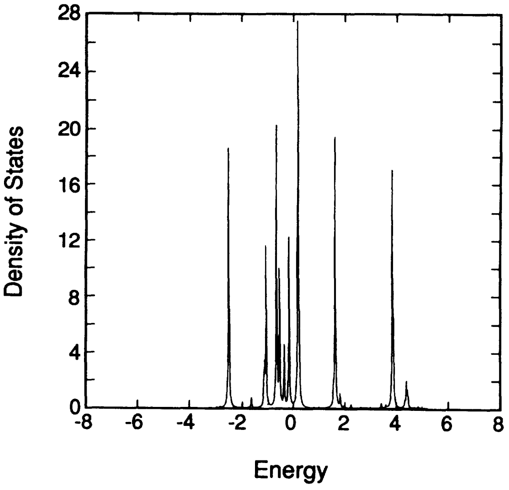

FIG. 4. Density of states for the mixed-valence insulator: $E_f=0.0$, $V=0.5$, $U=4.0$.

B. Metallic case

The lowest state of either an added electron or of a hole is a spin singlet, and the first excited state is a spin triplet. The integrated spectral weight at the chemical potential μ (electrons and holes combined) and the excitation energies of the first triplet states are given in Table III for a value of $E_f(-3.0)$ leading into the Kondo region for large U, and in Table IV for $E_f=0.0$ corresponding to mixed valence. Results for some specific U are described in more detail below.

The density of states for $E_f=-3.0$, $U=0.5$ (but $N=2N_S+1$) is shown in Fig. 5. This is quite similar qualitatively to that of Fig. 2, except that the chemical

TABLE III. Combined integrated spectral weight at the chemical potential ($Z=Z^{(e)}+Z^{(h)}$); E_x^h, energy of first triplet excited state of an added hole; E_x^e, energy of first triplet state of an extra electron. Calculations were made for $E_f=-3.0$, $V=0.5$.

U	Z	E_x^h	E_x^e
0.0	2.00	1.257	1.874
0.1	2.00	1.174	1.861
0.5	2.00	0.863	1.788
1.0	1.99	0.537	1.623
2.0	1.84	0.178	0.989
5.0	0.21	0.008	0.015
8.0	0.09	0.003	0.003

TABLE IV. Combined integrated spectral weight at the chemical potential ($Z=Z^{(e)}+Z^{(h)}$); E_x^h, energy of first triplet excited state of an added hole; E_x^e, energy of first triplet excited state of an added electron. Calculations were made for $E_f=0.0$, $V=0.5$.

U	Z	E_x^h	E_x^e
0.0	2.00	0.236	0.382
0.1	1.99	0.214	0.338
0.5	1.84	0.147	0.190
1.0	1.42	0.102	0.091
2.0	0.95	0.069	0.031
4.0	0.73	0.051	0.013
8.0	0.64	0.044	0.008

potential is now in the middle of the peak associated with the c state of $k=(0,0)$. The structure is accurately described by the single-particle levels of Fig. 1.

However, there is one difference hidden in the artificially broadened peaks of Fig. 5. There is a small exchange splitting referring to singlet and triplet states. The outer "c" electron resides in a $k=(0,0)$ state outside a singlet core. Hence if an additional electron is added leading to double occupancy of this state, a singlet must be formed; likewise, if the outer electron is removed, the result must be a singlet. However, if an electron is added to or removed from other states, both singlets and triplets may be formed. The splitting of the upper c states ($E>0$) is quite small [0.002 for $k=(\pi,0)$; $(0,\pi)$, and 0.0007 for $k=(\pi,\pi)$] and ferromagnetic in sign: the triplets are at lower energy than the singlet. The splittings of the hole states are larger, though still small [0.05 for $k=(\pi,\pi)$, $(\pi,0)$, and $(0,\pi)$; 0.03 for $k=(0,0)$] and antiferromagnetic: the singlets are at lower energy than the triplets.

We now turn to the case $E_f=-3.0$, $U=8$ for which the density of states is shown in Fig. 6 (which may also be compared with Fig. 3). The chemical potential has moved into the region of the $k=(\pi,0)$; $(0,\pi)$, states in Fig. 1. As in the case of the Kondo insulator discussed above, f spectral weight has been significantly redistributed to the upper Hubbard band (near $E=5$) and to the low-energy satellite region below $E=-3$. The c states near $E=\pm2$ are present in the form of multiple split peaks at these energies.

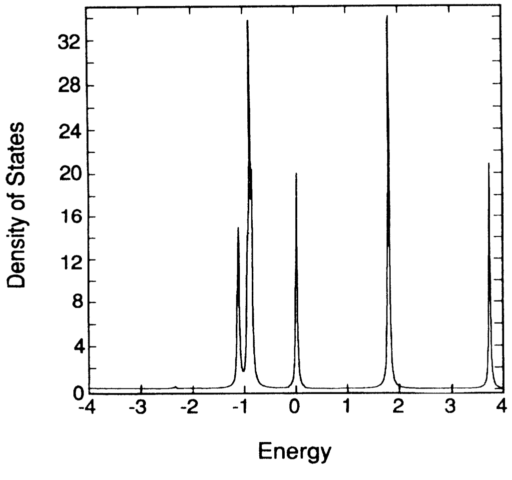

FIG. 5. Density of states for the conventional metal: $E_f=-3.0$, $V=0.5$, $U=0.5$.

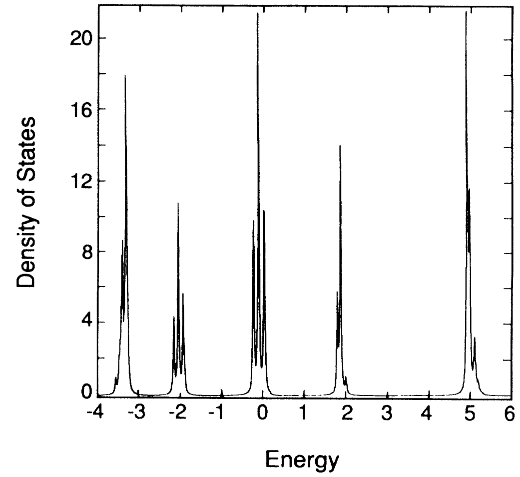

FIG. 6. Density of states for the Kondo metal: $E_f=-3.0$, $V=0.5$, $U=8.0$.

There are two special features: The lowest-energy state of an added electron or the highest state of a hole is a singlet of $k=(0,0)$, predominately f character, and of rather small combined integrated spectral weight (0.09). Most of the f spectral weight associated with $k=(0,0)$ is in other regions of the spectrum, but a small portion has accompanied the chemical potential. The small spectral weight implies that this state is a highly correlated many-body state. The lowest excited state on the electron side is a spin triplet belonging to $k=(\pi,0)$, $(0,\pi)$. This is mostly c like with much larger integrated weight (about 0.5). The excitation energy is quite small (only 0.003). This implies that the spin correlations of the ground state will be broken at quite low temperatures, leading to a Curie-Weiss magnetic susceptibility. The features of a singlet ground state and low-temperature breakup of spin correlations characterize Kondo behavior, and justify our characterization of our model as a Kondo metal, although the energy scale is not necessarily that encountered in real metals.

We have made similar calculations in the mixed valence region, $E_f=0.0$. The densities of states are quite similar to those shown previously, and we do not present a separate figure. The spectral weight at the chemical potential (Table IV) is much larger for large U in the mixed valence region than in the Kondo region. The triplet electron and hole excitation energies are small for large U, but are bigger than in the Kondo region. At high energy, there is, first, the upper f band, then the broadened c state of $k=(\pi,\pi)$. Near $E=0$, the chemical potential is in a complex peak involving a $k=0$ spin singlet state of primarily f character and strongly hybridized spin triplets belonging to $k=(\pi,0)$ $(0,\pi)$. For either an added electron or a hole, the lowest state is a spin singlet with the first excited state being the triplets, as discussed previously. The spectral weight of the singlet is much larger than in the Kondo region, indicating greater single-particle character. In the case of a hole, the lowest excited state is also a spin triplet belonging to $k=(\pi,\pi)$ with a triplet of $k=(\pi,0)$, $(0,\pi)$ close by. A major difference between the spectra in the mixed-valence region and that in the Kondo region is that there is no region of states at negative energies below the lowest c states in which two holes are on the same site. As in the insulating case, shown in Fig. 4, this structure is spread over a range of energies between the lowest c state and the chemical potential.

IV. SUMMARY

We have carried out exact diagonalization calculations for the lattice Anderson model defined on a four site, square cluster. These computations emphasize the development of the density of states as one passes from the weak interaction (smaller) limit to strong interactions. Parameters of the model were chosen so that in two cases, the strong interaction limit is in the Kondo region, and two lead into mixed valence. Occupancies were chosen so that both insulating and metallic behavior occur.

For a half-filled band case, the system resembles an insulator for all interaction strengths U; however, the gap can result either simply from the placement of the f levels below the c levels so that they are doubly occupied, or from removal of accidental degeneracies by hybridization when the f levels are in the middle of the c levels. As U increases, the f states become singly occupied, and the existence of a gap requires hybridization.

In the metallic case, the lowest single-particle state is a singlet. The integrated spectral weight of this state is rather small for large U, indicating strong correlations. The first excited state is a triplet, with a small excitation energy. These features will lead to behavior analogous to that encountered in the analysis of the Kondo effect in bulk systems.

Increasing interaction strength leads to a splitting of the f band. States in which there is a double occupancy of f orbitals rise to high energies, where they form the upper Hubbard band. This band acquires spectral weight from lower levels, which can only be singly occupied. There are also levels with binding energies close to the bare f level energy in which two f holes are on the same site.

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