PHYSICAL REVIEW B

CONDENSED MATTER

THIRD SERIES, VOLUME 48, NUMBER 16 15 OCTOBER 1993-II

Exact-diagonalization study of the spectral-weight functions and the density of states of the lattice Anderson model

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(Received 2 April 1993; revised manuscript received 25 June 1993)

We report numerical calculations of the spectral-weight functions for the lattice Anderson model on small clusters of square and tetrahedral geometry by exact diagonalization. Parameters in the weak-hybridization–strong-interaction sector are considered. The behavior of the f levels is studied as the occupancy varies from the doubly occupied limit to the nearly empty case.

I. INTRODUCTION

There are many physical systems in which wide bands of weakly interacting electron states coexist with strongly interacting, possibly nearly localized electrons in unfilled atomic shells: transition-metal oxides, rare-earth metals, and heavy-fermion systems. A remarkable range of properties can be found among the diverse members of this large class: ferromagnetism; antiferromagnetism, sometimes with large, nearly atomic moments, sometimes with quite small ordered moments, high-temperature and low-temperature superconductivity; mixed valence, enormous electron specific heat at low temperatures and so on. The lattice Anderson model is widely believed to incorporate much of the essential physics of these materials.

An extensive amount of literature exists on this model. At this point, we cite three reviews of aspects of the theory.[1–3]

The theoretical study begins with a band description of the electrons in extended, weakly interacting states (denoted c states). These bands could be obtained from first-principles local-density band calculations but it is often more convenient to consider a parametrized band model. In addition, one has a set of localized orbitals (denoted f). In the atomic limit these are highly degenerate, but several effects, including term structure, spin-orbit coupling, and crystal-field splittings limit the degeneracy under experimentally realizable conditions. The localized and extended orbitals are allowed to hybridize: this gives some itinerancy to the localized electrons while increasing the interaction between electrons in the extended states.

Our objective here is to explore single-particle levels in systems of this type by numerical calculations in which exact solutions are obtained for clusters with a small number of sites (exact diagonalization). This kind of study has been very informative in applications to the Hubbard and $t-J$ models. We list below a few references to such calculations, rather arbitrarily selected, from an already voluminous literature.[4–8]

Exact diagonalization calculations are inherently limited to small clusters by the extremely rapid growth of the dimensionality of the relevant Hilbert space with system size. This problem is even more serious in the case of the Anderson model than in the more frequently studied Hubbard model because of the need to consider more than one orbital per site. In order to have a manageable calculation, we have to drop one of the essential features of real f electron systems: the high degeneracy due to orbital angular-momentum components. It is necessary to limit consideration to a nondegenerate f band. We have an f and a c orbital on each site. In this case, the dimensionality of the Hamiltonian is the same as in the case of a simple Hubbard model with twice the number of sites.

There is another complication: the Lanczos method which is commonly employed to extract a few low-lying eigenvalues of large matrices is inadequate in this case for many interesting values of the parameters. This may occur if there is a large difference in energy between c and f levels. We have observed that the Lanczos method may not give accurate results over a large enough range of energies to describe all the interesting features of the spectral-weight function. As a result, we have to employ a method which obtains all the eigenvalues. These considerations have limited our calculations so far to four-site systems (equivalent to an eight-site simple Hubbard

model). If one is willing to limit the f orbitals to single occupancy (similarly to the $t-J$ approximation to the Hubbard model), one has the Kondo lattice model, and somewhat larger systems (six sites) can probably be studied. We have preferred, however, not to do this, as this would prohibit us from considering interesting satellite structure associated with doubly occupied or completely empty f states.

We have considered four-site systems with two different geometries: a single square and a tetrahedron. The tetrahedron can be considered a better approximation to a three-dimensional structure; and the comparison between results for these two systems gives some insight into what are generic properties of the model, and what may be sensitive to the small size of the system continued.

This paper is organized as follows. The lattice Anderson model is defined in Sec. II and some general features of its behavior as determined from previous exact diagonalization calculations are discussed. Some of the methods of our computations are discussed in Sec. III. Our results are presented in Sec. IV, and Sec. V contains concluding remarks.

II. THE MODEL

We consider here the nondegenerate lattice Anderson model in a basis in which there are two orthogonal orbitals on each site. In a standard notation, the Hamiltonian is

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

The first term of (1) describes c electron hopping between nearest-neighbor sites. In some of our applications, the hybridization interaction has been restricted to electrons on the same site. These restrictions are imposed in order to reduce the number of free parameters of the problem: they are easy to remove if desired. The minus sign in the first term means that the lowest c level will have zero wave vector.

The ground-state and thermodynamic properties of this model were studied through exact diagonalization calculations for a four-site tetrahedral cluster in Ref. 9. Similar calculations also involving spectral-weight functions and including Coulomb repulsion between f electrons were reported by Reich and Falicov.[10] Other numerical calculations have been presented concerning different geometries.[11–14] We shall focus attention here on the strong-interaction–weak-hybridization sector of parameter space; $U>t>V$ (but we do not consider infinite U). In this sector, the distinction between c and f states remains clear in the interacting system except for ranges of parameter values where strong hybridization occurs.

It will be helpful in understanding the results of the calculations described below to indicate different regions of behavior as E_f is increased from a large negative value.[9] (Only positive values of U are considered.) Let $E_c^{(0)}$ denote the lowest energy of the c states.

(i) $E_f+U<E_c^{(0)}$. In this region, we have doubly occupied f states. If the number of electrons is greater than that required to fill all the f levels, some c states will be occupied; otherwise they are empty.

(ii) $E_c^{(0)}<E_f+U<E_c^{(1)}$. Mixed valence behavior occurs as the system varies from $f^{(2)}$ configurations on each site to $f^{(1)}$. In the model, mixed valence will persist until E_f has risen to the point at which the c levels below E_f+U can accommodate enough electrons so the f band is only half full with one f electron per site. For example, if there are two electrons per atom, in case (i) both will be in f states, and mixed valence will persist until one electron per atom has been transferred to c states. At this point, we suppose that c states are occupied up to $E_c^{(1)}$.

(iii) $E_f+U>E_c^{(1)}$ and $E_f<E_c^{(1)}$. This is the Kondo region in which one electron per atom is in f states, and one in c states. The system avoids large repulsive energy by forming local moments on each site. The c electrons couple with these moments. Both the c and f bands are nearly half full.

(iv) $E_c^{(1)}<E_f<E_c^{(2)}$. This is the upper mixed valence in which sites transform from $f^{(1)}$ to $f^{(0)}$, and which persists until E_f rises to an energy $E_c^{(2)}$ at which all f electrons have transferred to c states.

(v) $E_f>E_c^{(2)}$. All f states are empty.

We shall, in considering the spectral-weight function, follow mainly the procedures of Ref. 5. Since the object of the work is to see what happens to single-particle states in the presence of interactions, we begin by diagonalizing the Hamiltonian with $U=0$. This can be done analytically. In this way, we obtain the single-particle eigenstates

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

in which $|fi\rangle(|ci\rangle)$ is a single-particle state in which there is a single $f(c)$ electron on site i, and γ is an index which combines "band" and wave vector. The notation which is commonly employed in the case of the one-band Hubbard model in which the single-particle states are specified by $\mathbf{k}$ only is not adequate here: there are two single-particle states of each $\mathbf{k}$. We use the states $|\varphi_\gamma\rangle$ to define the creation and annihilation operators $c_\gamma^{\dagger}$, c_γ.

We have considered in this paper two systems: A square and a tetrahedron. In the case of the square, we have considered only single-site hybridization, as this enables us to avoid introduction of an additional free parameter. In this case, the single-particle states and their energies 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),

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

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

We have considered the tetrahedron for hybridization

(strength V) on nearest-neighbor sites, and with $-t$ in the first term of (1) replaced by $+t$. These choices maintain continuity with our previous work described in Ref. 8. In this case, there are only two states, one not degenerate with Γ_1 symmetry corresponding to $\mathbf{k}=(0,0,0)$,

$$E=\tfrac{1}{2}\{E_f+3t\pm[(E_f-3t)^2+36V^2]^{1/2}\}\ , \tag{4a}$$

and the other, triply degenerate case of symmetry Γ_4, corresponding to $\mathbf{k}=(\pi,0,0)$; $(0,\pi,0)$ and $(0,0,\pi)$,

$$E=\tfrac{1}{2}\{E_f-t\pm[(E_f+t)^2+4V^2]^{1/2}\}\ . \tag{4b}$$

If V is negligible, the f levels are at E_f. The c levels of the square are located at $-2t$, 0, and $2t$ for Eqs. (3a), (3b), and (3c), respectively. The Γ_1 c level for the tetrahedron is at $3t$, and the Γ_4 is at $-t$.

III. CALCULATIONAL PROCEDURES

The spectral-weight function is given by

$$\begin{aligned}A_{\gamma,\sigma}(E)=\sum_m\{&|\langle\psi_m^{N-1}|c_{\gamma,\sigma}|\psi_g^N\rangle|^2\\&\times\delta[E-E_g(N)+E_m(N-1)+\mu]\\&+|\langle\psi_m^{N+1}|c_{\gamma,\sigma}^\dagger|\psi_g^N\rangle|^2\\&\times\delta[E-E_m(N+1)+E_g(N)+\mu]\}\ .\end{aligned} \tag{5}$$

In this equation, g designates the ground state of the N-particle system, and m designates an arbitrary state of either the $N-1$- or $N+1$-particle system. The quantity μ is the chemical potential and γ designates a single-particle state, including both $\mathbf{k}$ and band index (i.e., c or f). Here, we will number the single-particle states in order of increasing energy according to Eqs. (3) and (4). For a four-site system with two orbitals per site, γ runs from 1 to 8. In the present problem, A does not depend on spin σ, so we will drop that label.

In an infinite system, the sum over m becomes an integral, and A is continuous. For a small system, A obviously cannot be plotted directly, and many authors simply replace the δ function by a Lorentzian of unit area and some small, arbitrary width. Although we see no objection to this procedure, a different representation is used here which focuses on the matrix elements in (5). We use the notation

$$Z_\gamma(E)=|\langle\psi_m^{N-1}|c_{\gamma,\sigma}|\psi_g^N\rangle|^2 \tag{6a}$$

for holes and

$$Z_\gamma(E)=|\langle\psi_m^{N+1}|c_{\gamma,\sigma}^\dagger|\psi_g^N\rangle|^2 \tag{6b}$$

for electrons. The energy E referenced in Eqs. (6) is determined by the relevant δ function in Eq. (5), and thus implicitly incorporates the m index. The Z_γ are residues of the single-particle Green's function. Each Z_γ is a positive quantity ≤ 1. The limiting case $Z_\gamma=1$ corresponds to the concentration of the entire spectral weight on a single state m, which is characteristic of a system of noninteracting particles.

Frequently, one wishes to consider the density of states

$$n(E)=\sum_{\gamma\sigma}A_{\gamma\sigma}(E)\ . \tag{7}$$

As a convention, we will actually consider only a single spin, omitting a factor of 2. We then define a related quantity Z (no index) by

$$Z(E)=\sum_\gamma Z_\gamma(E)\ . \tag{8}$$

We note that

$$\int_{-\infty}^{\infty}A_\gamma(E)dE=\sum_m Z_\gamma(E_m)=1\ , \tag{9}$$

from commutation relations. The integral must include all energies. However, because $\sum_\gamma c_\gamma^\dagger c_\gamma$ is the operator representing the total number of particles the summed quantity $Z(E)$ sums to N for electron and hole states separately. The chemical potential μ is determined from

$$\mu=\tfrac{1}{2}[E_g(N+1)-E_g(N-1)]\ . \tag{10}$$

Our procedure is to investigate only a limited set of values of U and V, but to vary E_f so that the system passes through the different regions mentioned in Sec. II. Variation of E_f causes the number of c and f electrons to vary, even though the total number of electrons is fixed ($N=8$ for all the calculations reported here), and thus has effects somewhat similar to variation of the occupancy or "doping" in one-band Hubbard model calculations.

IV. RESULTS

We describe our results in each of the five regions mentioned in Sec. II. In all cases, the initial occupancy is half full (eight electrons). The ground sate of the half-full system is always a spin singlet; the first excited state is always a triplet. The excitation energy of this state can be considered to specify a spin gap. It is always smaller than the excitation energy of the lowest singlet excited state, which can be regarded as defining a charge gap. The ground state of both the $N-1(7)$ and $N+1(9)$ electron systems has $S=\frac{1}{2}$. The charge gap refers to the lowest excited state with this spin, and the spin gap to the excitation energy of the lowest state with $S=\frac{3}{2}$. In most cases, the charge gap is smaller than the spin gap (the $N=9$ case for the tetrahedron offers some exceptions).

(i) Full f bands. We made calculations for $E_f=-9$, $U=5$, $V=0.1$, and $V=0.5$ for the square. The spin and charge gaps are large, and nearly equal because both spin and charge excitations require promotion of an electron into the c states above the f bands. We find sharp electron, quasiparticle peaks, with negligible subsidiary structure, located close to but slightly above the positions determined from Eqs. (3). The states of a single hole also give rise to strong quasiparticle peaks, located at energies approximately E_f+U. There is no significant subsidiary structure close to the principal peaks. Equations (3) and (4) do not accurately describe the location of the peaks since they are displaced upward by U from E_f; but if E_f is replaced by E_f+U in Eqs. (3) and (4), the actual peak position and those estimated in a single-particle approximation agree rather well. The result is that a single-

particle picture of f band holes is valid, provided E_f is suitably corrected.

Weak structure in the density of states which is strongly hybridization dependent is found, well separated from the quasiparticle peaks, at excitation energies about $|E_f|+|E_c|$ (measured with respect to μ). This structure was not apparent in our results for $V=0.1$ but is present for $V=0.5$. Apparently, as the hybridization increases, the ground state has some probability of having virtual f holes and excited c electrons. A single-particle removal can then lead to a state in which two f holes are present on the same site (and a c electron is present as well).

(ii) Lower mixed valence region. In this region, the upper half of the Hubbard split f band increasingly overlaps the c states. We made calculations for the square at $E_f=-7$ and -5, $V=0.1$ *and* 0.5, $U=5$ for the square, and $E_f=-6$, $V=0.5$, $U=5$ for the tetrahedron.

In the square, for $E_f=-7$, the $k=0$ lowest c state of $E=-2$ is degenerate with the upper half of the f levels; consequently there is strong hybridization between the f and c levels with $k=0$. A similar situation occurs in the tetrahedron, except that it is the triply degenerate c levels at $E=-1$ which are degenerate with the upper f levels, so that these levels mix. Strong quasiparticle peaks are associated with the hybridized level and the other f levels on the hole side; on the electron side there are quasiparticle peaks associated with the upper hybridized level and the remaining c levels. Perhaps the most interesting feature is that the lower Hubbard band at E_f can be seen, although the peaks are rather weak. The normal ground state has only a single hole in the f levels. When an additional electron is removed, there are both normal states in which the f holes avoid each other, and other states in which two f holes are on the same site. These states form the lower Hubbard band. Approximately 10% of the hole spectral weight is associated with this band. Also, it is quite narrow, the width being only about 10–20 % of what would be expected from single-particle c-f hybridization according to Eqs. (3).

The electron states for this choice of parameter are quite simple. There are three (the expected number) strong quasiparticle peaks with only very weak subsidiary structure. The one closest to the Fermi energy is a strongly hybridized c-f combination; the upper two are only weakly hybridized and are located at the expected positions from Eqs. (3).

When E_f is increased to -5 (for the square) the c states with $\mathbf{k}=(\pi,0),(0,\pi)$ hybridize strongly with the corresponding states in the upper half of the split f band. The positions and strengths of the peaks in the density of states are shown in Fig. 1.

In this, and other graphs to follow, the zero of energy is taken at the chemical potential; hole states appear at negative energies, and electron states at positive energies. The quantity $|E|$ is the excitation energy: the amount of energy that has to be added to the system to remove an electron, or to add one. Starting at large negative energies we see states around $E=-5$ which are associated with the lower f band; i.e., states in which two holes are on the same site. Approximately 30% of the hole spectral weight is in this band. The lowest c state appears at

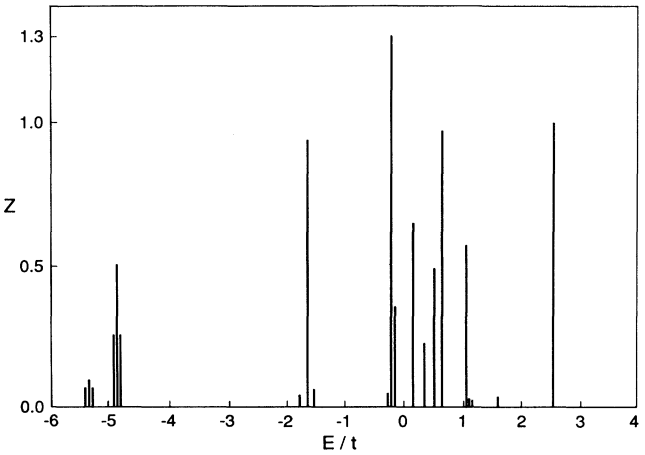

FIG. 1. Bar graph representation of the density of states in terms of the quantity Z [Eqs. (6) and (8)]. The separation in energy of some closely spaced contributions has been increased for clarity of presentation. Square geometry, $E_f=-5.0$, $V=0.5$, $U=5$.

$E=-1.62$. This state, which has $\mathbf{k}=\mathbf{0}$, is represented by a strong quasiparticle peak of strength near maximum. It is accompanied by two weak peaks of different symmetries which can quantitatively be regarded as representing weak interaction broadening the peak.

Around $E=0$, we find several states which involve the strongly hybridized c and f states of $\mathbf{k}=(\pi,0)$ and $(0,\pi)$. In addition, there are more weakly hybridized (mostly f) states of the other symmetries. There is a small gap at the Fermi energy which separates electron and hole states. This is quite close in size to the charge gap in the states of the half-filled system, and substantially larger than the spin gap. It is proportional to V as one expects from a hybridization-induced splitting of a degeneracy. In the case of an added hole, the c-f complex contains only one electron; so that we have a relatively conventional quasiparticle picture with both strongly hybridized and upper f band states available in a narrow energy range. An added electron appears to lead to a more strongly interacting situation in which the available states are spread over a wider range of energies. A simple quasiparticle picture is then more questionable.

At higher energies ($E=2.5$), we encounter the upper c state [$\mathbf{k}=(\pi,\pi)$]. There is a single strong quasiparticle peak of nearly maximum strength with weak subsidiary structure spread over a fairly wide range.

The lower mixed valence region situation we investigated in the tetrahedron seems to be qualitatively entirely consistent with the picture presented above for the square. We do not describe it in detail.

(iii) Kondo region: the lower f band is fully occupied, and the c states are half full. Because of the degeneracies of the partly filled c states, both square and tetrahedral geometries would be expected to correspond to metallic systems. However, there is a gap at the Fermi energy between electron and hole states which is approximately proportional to V^2. The formation of a hybridization induced gap at the Fermi energy seems to be consistent

with theoretical expectations.[15,16] The $n=8$ half filled ground state shows in both cases strong antiferromagnetic first-neighbor f-spin correlations (stronger in the square), while the same site spin correlations between c and f electrons are in both cases strongly antiferromagnetic. The analog of the Kondo temperature in these small systems is probably the excitation energy of the first triplet state, the spin gap. It was shown in Ref. 8 that the antiferromagnetic spin correlations are disrupted on this energy scale; while the high density of spin rearrangement states at low energies will produce incoherent behavior at high temperatures. Here we consider only the ground (coherent) state of the parent system.

In this case, we show the density of states for both the square (with $E_f=-2.4$, $V=0.5$, $U=5$) in Fig. 2, and the tetrahedron (with $E_f=-3.0$, $V=0.5$, $U=5$) in Fig. 3. The positions of the major peaks in the spectral weight and the residues Z_γ are listed for the square with the parameters above in Table I. We did not choose symmetric values ($E_f=-U/2$) in order to try to avoid features specific to that case. In both cases, the spin gap is small ($0.0075t$ in the square, 0.220 in the tetrahedron). The charge gap is larger (0.185, square; 0.332, tetrahedron). In both cases, as the energy E is increased one first encounters the lower half of the Hubbard split f band; then some c states (the Fermi energy falls in this range), while at higher energies one encounters both additional, empty c states, and the upper half of the split f band. We number the spectral weight functions in order of increasing energy of the underlying hybridized single-particle states according to Eqs. (3).

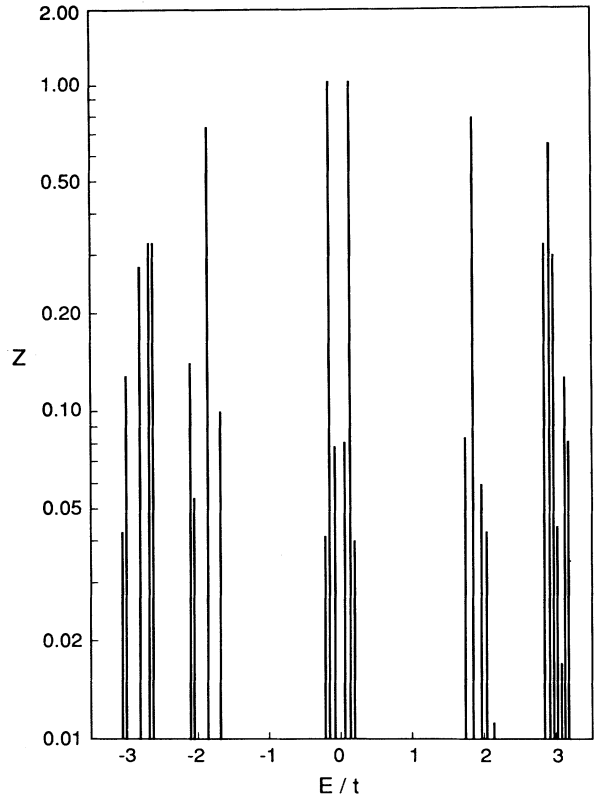

FIG. 2. Density of states in the Kondo region. Square geometry, $E_f=-2.4$, $V=0.5$, $U=5$.

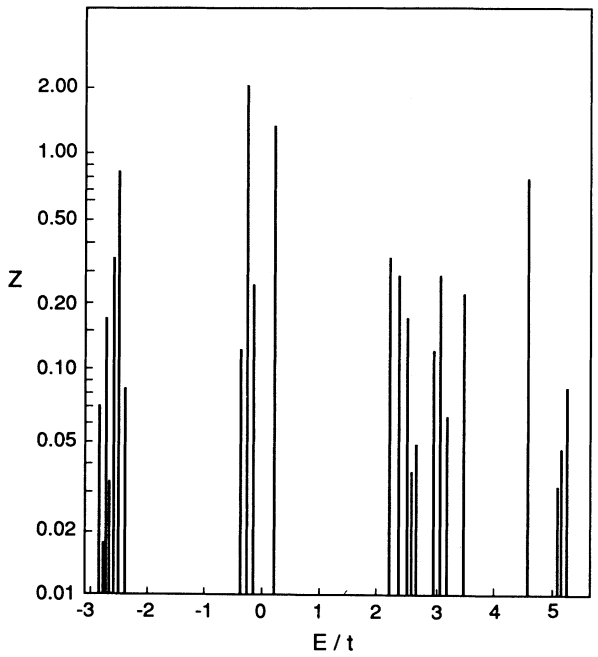

FIG. 3. Density of states in the Kondo region. Tetrahedral geometry, $E_f=-3.0$, $V=0.5$, $U=5$.

Inspection of Table I shows that the spectral weights associated with the single-particle eigenstates are not restricted to a single energy. Each eigenstate is present to some extent in both hole and electron regions of energy, although the proportions are quite different. The lowest eigenstate (1) emphasizes holes, the highest (8) electrons, while the other are significantly distributed over both. The most strongly hybridized states (1 and 5) have substantial residues at energies corresponding to both c and f levels. If we combine contributions from the different single-particle states, to give a representation of the density of states (Figs. 2 and 3) we see that there are strong peaks at energies corresponding to the c states, with significant subsidiary structure corresponding to interaction broadening. We interpret this as supporting a quasiparticle description of c states. However, the picture in the upper and lower f band regions is not so clear. There is, in each of the two f band regions, a predominant peak for each $\mathbf{k}$. The energy separations of the peaks are rather small, corresponding, as expected, to narrow bands. In some cases there is substantial subsidiary structure which suggests the possibility of larger broadening. It is not clear whether dispersing features would be observable in angle-resolved measurements of photoemission satellite peaks from similar bulk systems. About 40% of the hole spectral weight is associated with the lower f band for the parameters considered in both the square and the tetrahedron. The same proportion applies to the electron spectral weight in the upper f band in the square while this proportion is about 20% in the tetrahedron.

TABLE I. Energies and residues Z_γ [Eqs. (6a) and (6b)]. Square geometry, $E_f=-2.4$, $V=0.5$, $U=5$.

	$\mathbf{k}=(0,0)$			$\mathbf{k}=(\pi,0)$			$\mathbf{k}=(\pi,\pi)$	
E	Z_1	Z_5	E	Z_2	Z_6	E	Z_4	Z_8
3.127	0.011	0.003	3.145	0.043	0	3.378	0.013	0
3.119	0.013	0.004	2.999	0.018	0	3.128	0.115	0.011
2.975	0.234	0.068	2.865	0.327	0.002	3.111	0.003	0
2.080	0.032	0.008	2.256	0.006	0	2.857	0.314	0.062
1.739	0.066	0.016	2.106	0.007	0	2.112	0.013	0.106
0.164	0.068	0.010	2.094	0.009	0	1.889	0.008	0.782
			1.955	0.032	0	0.191	0.035	0.006
			0.183	0.153	0.397			
−0.192	0.037	0.004	−0.184	0.012	0.538	−0.164	0.070	0.009
−1.862	0.432	0.304	−1.919	0.032	0.008	−1.701	0.092	0.006
−2.081	0.026	0.114	−2.076	0.010	0.002	−2.042	0.051	0.003
−2.690	0.047	0.366	−2.225	0.010	0.002	−2.832	0.264	0.013
−2.982	0.030	0.097	−2.699	0.276	0.044	−2.979	0.023	0.001
			−2.883	0.010	0.002			
			−3.004	0.037	0.005			

(iv) Upper mixed valence region. As E_f increases, electrons transfer from the lower f band into the c states. The number of states in the upper f band gradually diminishes. We have made several calculations in this region: for the square with $U=5$ and $V=0.5$, we have considered $E_f=0$, 1, and 2, and in the tetrahedron with the same U and V, we have considered $E_f=0$, 1, 2, and 3. The results have many similarities, and we consider it sufficient to discuss only two cases.

First, we consider the tetrahedron with $E_f=0$. The residues $Z_\gamma(E)$ relating to the individual spectral weights for $\mathbf{k}=(0,0,0)$ (labeled Γ_1) and $\mathbf{k}=(\pi,0,0)$ (labeled Γ_4, this case is triply degenerate) are given in Table II. The single-particle states are numbered in order of increasing energy. The lowest single-particle state is a hybridized Γ_4 with energy, measured from μ, of -1.34. The spectral function for the case shows a strong peak close to this energy with additional structure near the energy of the upper Γ_4 and a weaker peak near that of the upper Γ_1. Finally, there is a peak at considerably higher energy ($\sim U$) in the upper f band. The upper Γ_4 has peaks in the same positions with different amplitude. The spectral weight of the lowest Γ_1 is strongly concentrated on two states at energies close to those obtained from (4a); the upper Γ_1 has, in addition, a strong peak in the upper f band. We note that the upper f band corresponds to states with two f electrons on the same site. About 17% of the electron spectral weight is in these levels. Our results for this geometry agree qualitatively with those of Reich and Falicov[10] (who considered different occupancies and parameters).

In Fig. 4 we show a representation of the density of states for square geometry with $E_f=1.0$. In this case also there are major peaks near the energies of single-particle states obtained from Eqs. (3a) and (3b), measured with respect to μ (here, $\mu=1.16$). The four groups of peaks can be accounted for in this way. All $\mathbf{k}$ values are represented in closely spaced peaks in the upper f band ($E-\mu\sim U$). The subsidiary structure associated with the major quasiparticle peaks is rather weak (peak height of 10% or less than the principal ones). Roughly 20% of the electron spectral weight is associated with the upper f band.

(v) Empty f bands. When E_f is such that the f levels are higher than the c states, we return to a simple situation, as was also the case when the f levels were full. We made calculations for $E_f=3.0$ for the square and $E_f=4.0$ for the tetrahedron (both with $V=0.5$ and $U=5$). The results show strong quasiparticle peaks for both holes and electrons at energies close to those obtained from Eqs. (3) and (4). The hole peaks differ by less than 1% from unit magnitude. The electron peaks are a

TABLE II. Energies and residues Z_γ [Eqs. (6a) and (6b)]. Tetrahedral geometry, $E_f=0.0$, $V=0.5$, $U=5$.

	Γ_4			Γ_1	
E	Z_1	Z_5	E	Z_4	Z_8
5.988	0.096	0.024	5.533	0.004	0.260
4.197	0.009	0.002	4.190	0.005	0.022
3.116	0.056	0.018	3.232	0.529	0.284
0.352	0.409	0.311			
−1.084	0.022	0.224	−0.352	0.443	0.373
−1.325	0.353	0.394	−1.901	0.017	0.025
−1.898	0.030	0.001			

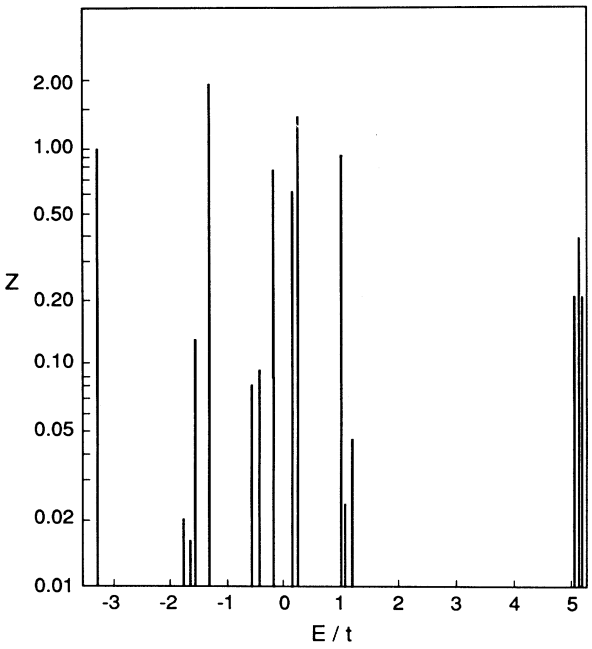

FIG. 4. Density of states in the upper mixed valence region. Square geometry, $E_f = 1.0$, $V = 0.5$, $U = 5$.

few percent less than unity. In this case there are weak peaks, most probably strongly dependent on the hybridization strength at higher energies.

There are two general features of the results presented in detail above that deserve additional comment: (1) the relative spectral intensity associated with the upper and lower portions of the split f band, and (2) the adequacy of the single-particle description of c-f hybridization used in Eqs. (3) and (4).

In regard to the division of spectral intensity we observe that the sum rules mentioned in Sec. III specify a fixed value (N) for the sum of the quantities Z_γ over all energies and single-particle states for electrons and holes separately, regardless of the values of any of the system parameters. In regions (i) and (v) (full and empty f bands), these sum rules are essentially exhausted by a single state for each γ, as one expects for a noninteracting system. However in both mixed valence regions and the Kondo region, the f band is split by (roughly) U. In the lower mixed valence region the upper f band hybridizes with c states; while the lower f band can be regarded as a satellite. As E_f increases, the number of f holes increases, and spectral weight is transferred from the hybridized "normal" band to the satellite as the number of opportunities to have more than one f hole on a given site increases. In the Kondo region, the lower f band is close to full, and the upper, empty. The spectral weight associated with the single-particle eigenstates is distributed over a large range of energies. Then, as one moves into the upper mixed valence region, the lower f band hybridizes and the upper one is empty. The spectral weight associated with the upper f band gradually diminishes as the f state occupancy in the hybridized band decreases with increasing E_f.

A major objective of exact diagonalization many-body calculations is to give some indication of the importance of corrections to a noninteracting single-particle theory. In the present problem, we would consider a noninteracting single-particle picture to be valid if the spectral-weight function for each single-particle state were to show a single peak of unit magnitude ($Z_\gamma \sim 1$) at an energy determined from Eqs. (3) and (4). This is essentially what occurs in the empty f band region (v). In the full f band region (i), we see immediately that we must replace E_f by $E_f + U$ in Eqs. (3) and (4). This gives quite good although not exact results for the peak positions.

However, in the mixed valence and Kondo regions there are serious problems. As we see in the tables the two spectral functions with the same $\mathbf{k}$ have peaks at the same energies, in both electron and hole regions of energy, and also in the lower and (or) upper Hubbard split f bands. One has to conclude that the single-particle description of hybridized bands has broken down, although a quasiparticle description of the excitations may still be useful. The single-particle approach is guaranteed to be correct as $U \to 0$, but in this work we are concerned with relatively large U. A first approximation as to the essential physics seems to be to consider hybridization with two f levels (at E_f and $E_f + U$), i.e., to take account first of the Hubbard splitting. This is certainly reasonable since, in the model sector considered here, $U \gg V$.

We have tested calculations of this type, and found that a reduced $V (V \to V/\sqrt{2})$ is desirable. In this way, we can come much closer to reproducing the positions of the main peaks. But we have not found quantitative agreement. The question modification of hybridization in the presence of U is a very important one for the band theory of cerium, rare earth, and actinide metals and compounds. It has been extensively discussed previously.[17] We hope that the availability of exact results, although restricted to small systems, will be a stimulus to further investigations.

V. CONCLUSIONS

We have investigated the spectral-weight function of the nondegenerate lattice Anderson model defined on small (four site) clusters of square and tetrahedral geometries through exact diagonalization calculations. We emphasize the strong-interaction–weak-hybridization sector. A half-filled band situation was considered. We vary the f electron energy for fixed U, V so that five different regions of behavior are obtained. The differences between the results for the different geometries are not major, and seem to result from differences in the single-particle level structure.

When the f bands are either empty or full, there is strong evidence not only that a quasiparticle picture is valid but that a one-electron calculation can give quantitatively accurate energies. The situation is more complex in both mixed valence regions and in the Kondo region. Then the f band is always split by roughly U. In the lower mixed valence region, the upper half of the split f band hybridizes with the c levels; the lower part, which contains states in which two f holes are on the same site,

is a satellite of the sort observed in photoemission experiments. In the Kondo region, the lower f band is full, the upper is empty, and the c levels are also half full. There are strong quasiparticle peaks near the Fermi energy; away from it there is a subsidiary structure suggesting broadening in a large system. In the upper mixed valence region, the lower f band hybridizes with the c levels; the upper band, where there would be two f electrons on a site, contains possible excited states. The number of states in this band decreases with the number of f electrons in the lower band. In these ranges one finds a small gap at the Fermi energy whose magnitude increases as the hybridization V if there is a degeneracy of levels in the absence of V, and as V^2 (for small V) otherwise.

We observe that a single-particle calculation of hybridization does not accurately locate the position of quasiparticle peaks in the mixed valence and Kondo region, and does not accurately describe the hybridization evident in the spectral-weight function. The important problem of the modification of hybridization by the electron interaction requires further quantitative investigation.

ACKNOWLEDGMENTS

The research performed at LSU was supported in part by the National Science Foundation under Grant No. DMR 91-20166. Some of the computations were performed at the National Center for Supercomputing Applications, Urbana, Illinois. We are grateful for their support.

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