Heavy Quasiparticles in the Anderson Lattice Model

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(Received 4 August 1995)

An exact-diagonalization technique on small clusters is used to study the dynamics of the one-dimensional symmetric Anderson lattice model. Our calculated excitation spectra reproduce key features expected for an infinite Kondo lattice such as nearly localized low-energy spin excitations and extended regions of "heavy-quasiparticle" bands. We show that, in contrast to the hybridization picture, low-energy spin excitations of the nearly localized f-electron system play a key role in the formation of an almost dispersionless low-energy band of heavy quasiparticles.

PACS numbers: 71.27.+a, 71.28.+d, 75.20.Hr

The origin of the anomalous behavior of f-electron compounds is an unresolved issue in the theory of strongly correlated electron systems. Thereby the way in which a periodic array of magnetic ions interacting with a sea of conduction electrons can give rise either to the extreme low-energy scale in the Landau-type quasiparticle bands of heavy-fermion compounds [1,2] or to gaps of apparent many-body origin in the excitation spectra of Kondo insulators [3,4] is not yet understood. On a phenomenological level, heavy-fermion compounds have been described with considerable success by the "renormalized band theory" [1], where the effect of electron correlations is described by the renormalization of on-site energy and hybridization strength of the magnetic ions.

In this Letter we study the Anderson lattice model (ALM), the simplest model relevant for f-electron compounds, by Lanczos diagonalization of small clusters [5], and show that such a renormalized band picture, on one hand, may provide a reasonable phenomenological description of the dispersion relations, but, on the other hand, is not really adequate on a microscopic level: Contrary to the one-particle picture, the heavy quasiparticles may be viewed as loosely bound states of conduction electrons and spin-wave-like excitations of the nearly localized f-electron system. The emerging picture is thus more reminiscent of the spin polaron discussed recently on the basis of a semiclassical treatment of the Kondo lattice [6]. We would like to stress that due to the small size of the clusters our calculations can neither reproduce the exponentially small energy scales present in the Anderson impurity problem nor do they allow for the derivation of an accurate phase diagram. Nevertheless, one may expect that the relative magnitudes of energy scales, and hence the nature of the low lying states, are reproduced correctly by our calculations; in that sense our results for dynamical quantities are complementary to the scaling theories in Ref. [7] or the renormalization group calculations for the ground states of larger systems in Ref. [8].

We consider a tight-binding version of the one-dimensional ALM defined by the Hamiltonian

$$H = -t\sum_{\langle ij\rangle\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{H.c.}) - V\sum_{i\sigma}(c^{\dagger}_{i\sigma}f_{i\sigma} + \text{H.c.}) + U\sum_{i}(n^{f}_{i\uparrow} - \tfrac{1}{2})(n^{f}_{i\downarrow} - \tfrac{1}{2}), \quad (1)$$

where $c_{i\sigma}$ ($f_{i\sigma}$) is the annihilation operator for an electron of spin σ at site i in the c (f) orbitals and $n^{f}_{i\sigma} = f^{\dagger}_{i\sigma}f_{i\sigma}$. Model parameters are hopping strength t between nearest-neighbor c orbitals, mixing V between c and f orbitals, and on-site repulsion U at the f orbitals. The on-site energy of the f orbitals is taken to be $-U/2$, i.e., we consider the "symmetric" case. We focus on electron densities close to "half filling," i.e., $2N_s$ electrons in N_s unit cells (a unit cell contains one c and one f orbital). Restrictions on memory space and computer time necessitate choosing $N_s \leq 6$. To get additional information, we employ twisted boundary conditions (BC) [9,10]. We require $c_{N_s+1\sigma} = e^{i\varphi}c_{1\sigma}$ and $f_{N_s+1\sigma} = e^{i\varphi}f_{1\sigma}$ by introducing an arbitrary phase φ; the allowed momenta are then $k = (2\pi n + \varphi)/N_s$ with $n = 0, \ldots, N_s - 1$. It has been pointed out [11,12] that in the half-filled case finite size effects can be minimized by choosing $\varphi = (N_s/2)\pi$. As will be seen below, the combination of spectra obtained with different values of φ gives remarkably smooth "band structures." However, none of our conclusions to be presented below depend on such an assignment of bands.

We first consider the single-particle spectral function $A_\gamma(k,\omega)$ defined as a sum $A_\gamma(k,\omega) = A^{-}_{\gamma}(k,-\omega) + A^{+}_{\gamma}(k,\omega)$ of the photoemission spectrum (PES)

$$A^{-}_{\gamma}(k,\omega) = \frac{1}{\pi}\,\widetilde{\delta}\langle\Psi^{N}_{\varphi}| \times \gamma^{\dagger}_{k\sigma}\,\frac{1}{\omega - (H - E^{N}_{\varphi}) - i\epsilon}\,\gamma_{k\sigma}|\Psi^{N}_{\varphi}\rangle, \quad (2)$$

and the inverse photoemission spectrum (IPES)

$$A_\gamma^+(k,\omega) = \frac{1}{\pi}\,\Im\langle\Psi_\varphi^N|\times\,\gamma_{k\sigma}\,\frac{1}{\omega-(H-E_\varphi^N)-i\epsilon}\,\gamma_{k\sigma}^\dagger|\Psi_\varphi^N\rangle, \quad (3)$$

where E_φ^N ($|\Psi_\varphi^N\rangle$) denote the ground state energy (wave function) with N electrons and twisted BC of phase φ. The operator $\gamma_{k\sigma}$ refers to the Fourier transform of the operator for either conduction electrons ($c_{i\sigma}$) or the f electrons ($f_{i\sigma}$). Results for $A_\gamma(k,\omega)$ obtained by the standard Lanczos procedure are given in Fig. 1. One can identify the "upper and lower Hubbard bands" for the f electrons, separated by an energy $\sim U$. They are dispersionless and somewhat broadened, with almost pure f character. In addition to this typical strong-correlation feature, there are two bands which are more reminiscent of noninteracting electrons: One can identify the unrenormalized c-electron band of width $4t$, apparently split into two bands by hybridization with a "renormalized" f level in the middle of the Hubbard gap. This feature results first in a well-defined gap between PES and IPES spectra and second in extended regions of "heavy" bands with apparently pure f character. The dispersion of the two "hybridization bands" as well as the change from almost pure c character to almost pure f character around $\pi/2$ are thereby both roughly consistent with the picture of noninteracting electrons. The spectral weight of the parts with f characters, however, is substantially smaller than in the parts with c character; comparison shows that this asymmetry is the more pronounced the larger the ratio U/V.

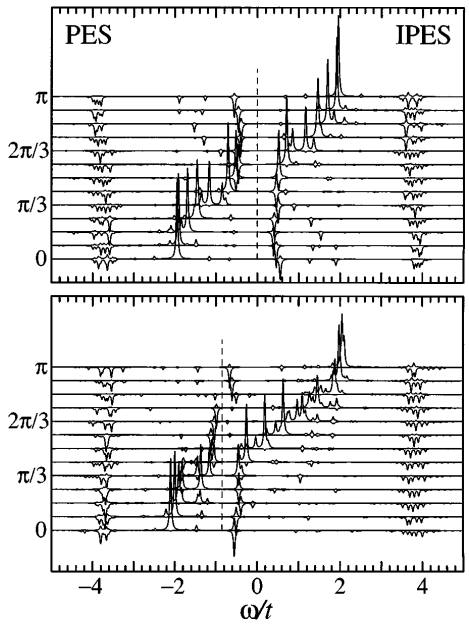

FIG. 1. Single-particle excitation spectra $A_\gamma(k,\omega)$ for $N_s = 6$ with different φ for $V/t = 1$ and $U/t = 6$. The spectra at $k = 0$, $\pi/3$, $2\pi/3$, and π correspond to $\varphi = 0$ (i.e., periodic BC). The f spectra are multiplied by -1 for better distinction, the Lorentzian broadening is $\epsilon = 0.02t$. The upper panel shows the spectra for the half-filled ground state, the lower panel for the ground state with five up and five down electrons (i.e., with two holes). The vertical dashed line shows the chemical potential.

The change of $A_\gamma(k,\omega)$ with hole doping is at first sight completely consistent with the picture of noninteracting electrons [13]: The chemical potential seems to shift into the heavy band, so that a kind of Fermi surface emerges, and upper and lower Hubbard bands remain unaffected. In addition to this rigid-band-like behavior, however, there is also a modification of the "light" parts of the band structure, far from E_F: c-type spectral weight is transferred from PES to IPES near $\pi/2$, i.e., the Fermi momentum for a half-filled band of unhybridized conduction electrons. The change of $A_c(k,\omega)$ thus is reminiscent of *unhybridized* conduction electrons. On a phenomenological level, this could be reproduced if one assumed that the renormalized f-level energy is pinned near the chemical potential of $N - N_s$ unhybridized conduction electrons, i.e., the Fermi energy of a "frozen-core" band structure.

We now want to clarify the nature of the heavy-band states. Important information can be obtained from the momentum distribution function $n_{\gamma\sigma}(k) = \langle\gamma_{k\sigma}^\dagger\gamma_{k\sigma}\rangle$; more precisely, we study the change of $n_{\gamma\sigma}(k)$ upon removing one electron. In a six-unit-cell system, we evaluate the difference $\Delta n_{\gamma\sigma}(k)$ between the $n_{\gamma\sigma}(k)$ in the lowest state with five down-spin and six up-spin electrons at the total momentum $k_{\rm tot}$ and the $n_{\gamma\sigma}(k)$ of the ground state at half filling. We choose $k_{\rm tot}$ such that the single-hole state belongs to the heavy part of the band. In the hybridization model, the creation operators in the lower hybridization band would read $a_{k\sigma}^\dagger = u_k c_{k\sigma}^\dagger + v_k f_{k\sigma}^\dagger$, so that $\Delta n_{c\uparrow}(k) = 0$, $\Delta n_{c\downarrow}(k) = -|u_k|^2\delta_{k,-k_{\rm tot}}$, $\Delta n_{f\uparrow}(k) = 0$, and $\Delta n_{f\downarrow}(k) = -|v_k|^2\delta_{k,-k_{\rm tot}}$. Since one may expect $u_k \approx 0$ and $v_k \approx 1$ in the heavy band, the electron is removed only from the f species with spin down and at $k = -k_{\rm tot}$. The calculated results for $\Delta n_{\gamma\sigma}(k)$ are shown in Fig. 2, where we note the following features, almost all of which are in contrast to these predictions: (i) Independently of the actual momentum $k_{\rm tot}$ of the single-hole state, c electrons of both spin directions are removed at the two k_F^c. (ii) The resulting loss of up-spin electrons is compensated by an almost k-independent spin polarization of the f electrons. (iii) As the only agreement with the hybridization model there is an extra "dip" in $n_{f\downarrow}(k)$ for $k = -k_{\rm tot}$, which however diminishes rapidly in magnitude for decreasing V/U. These results establish first of all that the "heavy quasiparticle" is predominantly a "missing c electron" with only a small admixture of f character (for large U/V). By contrast, the pure f character of the lower Hubbard band suggests that it is in this band where an f electron is missing. We thus have an energy separation of c-like and f-like degrees of freedom (of order $U/2$), in contrast to the hybridization scenario. However, there must be some mechanism which renders the missing c electron "invisible" in $A_c(k,\omega)$ when k is in the heavy band.

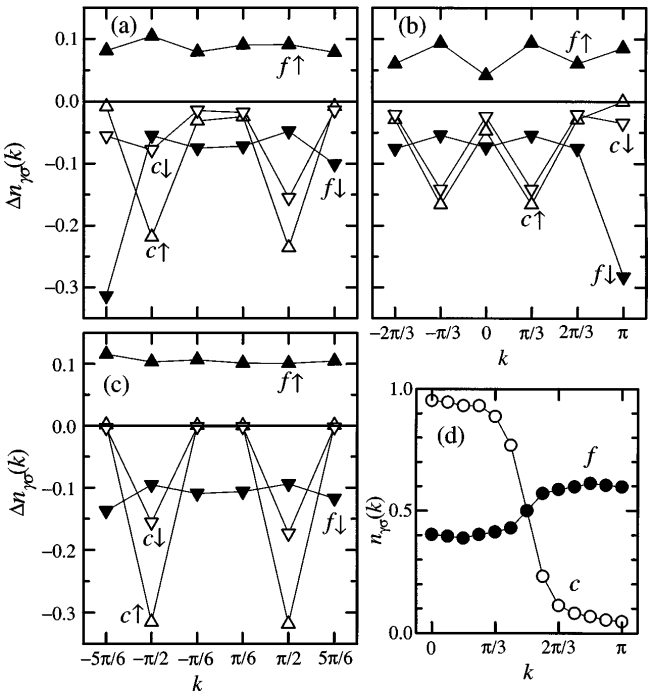

FIG. 2. Difference $\Delta n_{\gamma\sigma}(k)$ between zero-hole and one-hole ground states at $U/t = 6$: (a) $V/t = 1$, $k_{\rm tot} = 5\pi/6$, $\varphi = \pi$ (i.e., antiperiodic BC); (b) $V/t = 1$, $k_{\rm tot} = \pi$, $\varphi = 0$; (c) $V/t = 0.5$, $k_{\rm tot} = 5\pi/6$, $\varphi = \pi$. As a reference, $n_{\gamma\sigma}(k)$ for the zero-hole ground state at $V/t = 1$ is shown in (d).

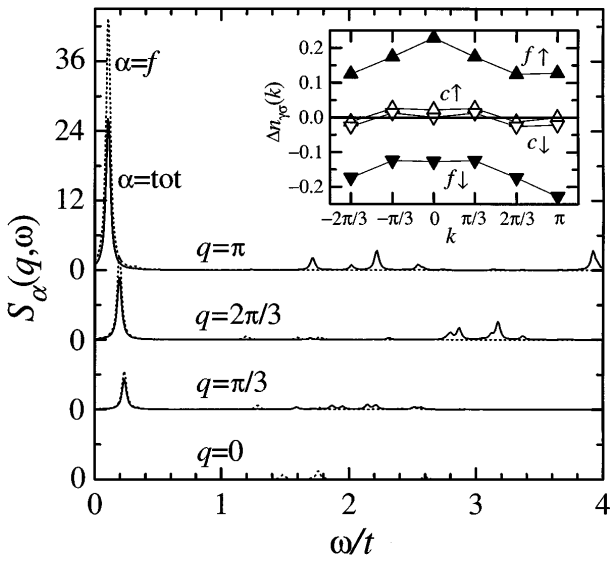

FIG. 3. Spin-excitation spectra $S_\alpha(q,\omega)$ for $V/t = 1$ and $U/t = 6$, $\varphi = 0$. The Lorentzian broadening $\epsilon = 0.02t$. Inset shows the change of $n_{\gamma\sigma}(k)$ due to the spin excitation.

As for this latter issue, we note that the spin polarization of the f electrons suggests the presence of a spin excitation. We therefore consider the spin-excitation spectrum

$$S_\alpha(q,\omega) = \frac{1}{\pi}\,\Im\langle\Psi_\varphi^N|\times S_{\alpha q}^- \frac{1}{\omega - (H - E_\varphi^N) - i\epsilon} S_{\alpha q}^+|\Psi_\varphi^N\rangle, \quad (4)$$

where $S_{\alpha q}^+$ is the Fourier transform of either the total-spin raising operator $c_{i\uparrow}^\dagger c_{i\downarrow} + f_{i\uparrow}^\dagger f_{i\downarrow}$ ($\alpha = $ tot) or the f-electron-spin raising operator $f_{i\uparrow}^\dagger f_{i\downarrow}$ ($\alpha = f$). The calculated spectra (see Fig. 3) show strong low-energy peaks with negligible dispersion, which probably are the (almost) local singlet-triplet excitations expected for a Kondo lattice. In $S_f(q,\omega)$, these low-energy peaks are enhanced, whereas the smaller peaks at higher energies are suppressed: Obviously, the spin flip on an f electron in the ground state to excellent approximation produces another eigenstate. There is a pronounced k dependence of the peak intensity, similar to spin waves in an antiferromagnet. One may assume that this reflects the antiferromagnetic spin correlations due to the RKKY-type interaction. We also study the change of the momentum distribution of the half-filled system due to a spin excitation; more precisely, we consider the difference between the momentum distribution for the lowest state with $S_z = 1$ and momentum π [i.e., the final state for the low-energy peak in $S_\alpha(q,\omega)$] and that for the ground state. This difference is shown in the inset of Fig. 3. Whereas the c electrons remain virtually unaffected by the spin excitation, there is an almost k-independent polarization of the f electrons, as one would expect it for a quantum spin system without charge degrees of freedom. Again we find a remarkable degree of separation of the c- and f-electron "subsystems," which may also provide a natural explanation for the strongly different spin and charge excitations found in previous studies [8,11,12,14–19] of Kondo insulators.

Let us now combine the above results to obtain a simple picture of the heavy states. Since they represent the parts of the PES or IPES spectrum with the lowest excitation energy, let us consider the limit $V \to 0$ and ask: How can we remove or add an electron so as to lower the energy most efficiently? In the half-filled ground state there is on the average one f electron per unit cell, with only a small admixture of the empty or doubly occupied f site. Removing or adding an f electron will on the average raise the energy by $U/2$, and thus is unfavorable. Accordingly, the state $f_{k\sigma}|\Psi_\varphi^N\rangle$, which would be the most natural ansatz within the hybridization picture, has only small overlap with the true "heavy state," particularly in the strong correlation case (i.e., small V/U). One measure for the weight of this state in the ground state would be the "depth" of the dip in $n_{f\sigma}(k)$. On the other hand, a c electron can be removed or added with practically no cost in energy if that is done near k_F^c. Next, the f-electron spin excitations with their small excitation energies offer a way to dispose of "excess momentum" with almost no cost in energy. This suggests to remove or add the c electron always at k_F^c, and transfer the excess momentum to an f-spin excitation. This picture immediately explains the reduction of $n_{f\sigma}(k_F^c)$, as well as the spin polarization of the f-electron system due to the accompanying f-spin excitation. We are thus led to the following ansatz for a

holelike heavy state,

$$|\Psi(k)\rangle = \left\{ u_k f_{-k\downarrow} + \sum_{k_F^c} v_{k_F^c} [c_{k_F^c\downarrow} S_f^z(k + k_F^c) - c_{k_F^c\uparrow} S_f^+(k + k_F^c)] \right\} |\Psi_\varphi^N\rangle . \quad (5)$$

Here $S_f^z(q)$ is the z-spin operator for the f electrons with momentum transfer q, and u_k and v_k are (variational) parameters. The state [Eq. (5)] has momentum k, z spin $1/2$, and total spin $S = 1/2$; i.e., the spins of f-electron excitation and c-electron hole maximally compensate each other. This is reminiscent of the "quenching" of a Kondo-impurity spin due to bound-state formation. The variational parameters in (5) are determined from the requirement that $|\Psi(k)\rangle$ has norm 1 and maximum overlap with the exact heavy state with momentum k. Figure 4 shows the overlap $|\langle\Psi(k)|\Psi_\varphi^{N-1}\rangle|^2$ for different values of V/t and U/t at $k = 5\pi/6$; here $|\Psi_\varphi^{N-1}\rangle$ denotes the exact heavy state, and $|\Psi(k)\rangle$ is given in Eq. (5). For comparison, the overlap of the state $f_{-k\downarrow}|\Psi_\varphi^N\rangle$ (normalized to unity) with $|\Psi_\varphi^{N-1}\rangle$ is also shown (in the hybridization picture, the latter quantity would be 1). While the "bare f electron" is a good approximation only in the small U/V case, the overlap of the state in Eq. (5) is $>90\%$, for all parameter values, so that we find a good description of the heavy-band states in the strong correlation region.

In summary, we have studied the single-particle spectral function and dynamical spin-correlation function for finite clusters of the Anderson lattice model at or near half filling. Despite the necessarily rather coarse energy scales available in the clusters, our results do reproduce key features expected for infinite Kondo lattices, namely, extended heavy bands and almost dispersionless low-energy spin excitations. On a phenomenological level, the low-energy parts of the spectral function can be described reasonably well by a renormalized band picture where an "effective f level" pinned to the frozen-core Fermi energy mixes with the conduction band. This picture, however, has not much significance beyond a purely phenomenological level: There is a clear separation between the low-energy hybridization bands which correspond to a missing (or extra) c electron and the two Hubbard bands which correspond to a missing (or extra) f electron. The heavy quasiparticles rather have the character of loosely bound states between a conduction electron at the Fermi momentum of the unhybridized conduction-electron system and spin-wave-like excitation of the f-electron lattice which acts very much like a pure quantum-spin system.

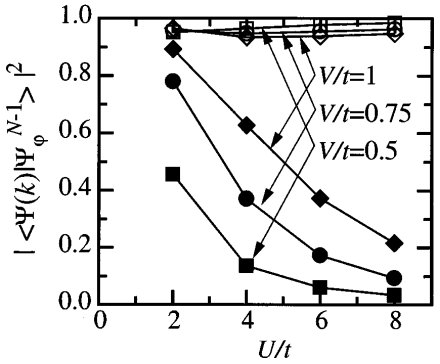

FIG. 4. Overlap of the state given by Eq. (5) (white symbols) and the state $f_{-k\downarrow}|\Psi_\varphi^N\rangle/\langle\Psi_\varphi^N|f_{-k\downarrow}^\dagger f_{-k\downarrow}|\Psi_\varphi^N\rangle^{1/2}$ (black symbols) with the exact heavy state $|\Psi_\varphi^{N-1}\rangle$ at $k = 5\pi/6$ and $\varphi = \pi$ as functions of U/t.

Since the "spin polaron bands" are formed by bound states, rather than by true hybridization, it seems natural to assume that the breaking of the bound states will completely remove the heavy parts of the band structure and leave behind only the frozen-core Fermi surface. Since the heavy quasiparticles involve the spin compensation of f excitation and c hole, it is moreover clear that they can be broken by a magnetic field. Then, the breaking of the heavy polarons by a magnetic field and the corresponding collapse of the Fermi surface to the frozen-core volume appears as a natural explanation for the so-called metamagnetic transition associated with the "itinerant-to-localized" nature of f electrons [20].

We thank S. Haas for useful conversations. This work was supported by Priority-Areas Grants from the Ministry of Education, Science, and Culture of Japan, the New Energy and Industrial Technology Development Organization (NEDO), and the Office of Naval Research under Grant No. ONR-N00014-93-1-0495. Support of R. E. by the European Community is acknowledged. Computations were carried out in Nagoya University, Institute for Molecular Science, and the Cray C90 at Pittsburgh Supercomputer Center.

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