Formation of a Coherent Heavy Electron State in the Anderson Lattice Model

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We present self-consistent calculations for the self-energy, thermodynamic potential, and magnetic susceptibility of the 2D asymmetric Anderson lattice Hamiltonian, in the fluctuation exchange approximation. For parameters that yield a large local moment, a narrow peak at the Fermi energy grows out of an otherwise smooth density of states as the system is cooled. The height of the peak reaches a maximum and then decreases, signaling the onset of coherence. The susceptibility shows a similar temperature dependence.

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The f electrons in heavy-electron metals undergo an unusual transformation with decreasing temperature, apparently changing continuously from a lattice of independent local moments exchange-coupled with a band of conduction electrons, to an extremely narrow hybridized band of highly renormalized itinerant quasiparticles [1]. Among the issues raised by this scenario are the identification of the processes controlling the formation of the coherent itinerant state, the relation of this transformation to the compensation of local f moments in the single (or dilute) impurity Kondo problem, and the character of the low-temperature quasiparticles.

The Anderson lattice model is believed to provide a paradigm for this transformation. In its simplest form, the model contains a single spin-degenerate f level of energy e_f at each lattice site and a tight-binding conduction band with nearest-neighbor hopping matrix element t. Conduction and f electrons on the same site hybridize with energy V, and two f electrons on the same site have Coulomb energy U. The Hamiltonian is

$$H = -t\sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma} + \sum_{i\sigma}\{V(f^\dagger_{i\sigma}c_{i\sigma} + c^\dagger_{i\sigma}f_{i\sigma}) + e_f n^f_{i\sigma} - h\sigma(n^c_{i\sigma} + n^f_{i\sigma})\} + U\sum_i n^f_{i\uparrow}n^f_{i\downarrow}\,, \tag{1}$$

where $c_{i\sigma}$ ($f_{i\sigma}$) annihilates a conduction (f) electron at site i with spin σ, and h describes the coupling of the electron spins to a homogeneous magnetic field.

Much work on the Anderson lattice Hamiltonian has focused on the limit of infinite U, using methods originally developed for the single-impurity Anderson model [2]. The observation that thermodynamic properties of the single impurity problem are reproduced accurately by second-order (in U) perturbation theory for the self-energy [3] has aroused renewed interest in perturbation theory for the lattice model.

One approach to perturbation theory for the self-energy is to make a straightforward expansion in U, with diagrams evaluated using the $U = 0$ Green's function. Another approach is to expand in terms of skeleton diagrams evaluated with the Green's function containing the approximate self-energy being calculated [4]. In addition to relative computational simplicity, the first approach has the virtue that it includes all contributions of a given order in U, which prevents errors due to cancellations between included and excluded terms of the same order. The second approach has the advantage that it can describe situations where the difference between the interacting and noninteracting excitation spectra matters, and if the self-energy is calculated from a "conserving approximation," the self-consistent solution will respect all symmetry derived conservation laws [5]. There is no *a priori* way to choose between these approaches, but the dramatic changes with temperature in the low-energy excitation spectra of the heavy-electron metals suggest a self-consistent approach. Previous workers have recognized that the Green's functions used to calculate the self-energy must include the Hartree self-energy (which shifts the bare f level), but have not treated other contributions self-consistently [6].

We have carried out fully self-consistent calculations for the 2D asymmetric Anderson lattice Hamiltonian in the fluctuation exchange approximation (FEA), beginning from the diagrammatic expansion for the thermodynamic potential in terms of the fully renormalized Green's function G and self-energy Σ [4],

$$\Omega(T,\mu,h) = -\,\mathrm{Tr}\,[\Sigma G + \ln(-G_0^{-1} + \Sigma)] + \Phi[G]\,. \tag{2}$$

Here Tr denotes a generalized trace over all arguments of the Green's function, G_0 is the Green's function of the noninteracting system, and $\Phi[G]$ is a set of Feynman diagrams whose functional derivative with respect to G generates the skeleton-diagram expansion for Σ. With the spin-quantization axis along the field, the Green's functions and self-energies are spin diagonal, and because the Hubbard interaction acts only between f electrons, Φ is a functional of the f-electron Green's function G_f alone and only the f-electron self-energy Σ_f is nonzero. This greatly simplifies the solution of Dyson's equation

for G [7].

In the FEA, Φ is [8, 9]

$$\Phi = \tfrac{1}{4}U[n_f^2 - (n_\uparrow^f - n_\downarrow^f)^2] + \tfrac{1}{2}\mathrm{Tr}[\ln(1 - \Pi_{\uparrow\uparrow}\Pi_{\downarrow\downarrow})] + \mathrm{Tr}[\ln(1 - \Pi_{\downarrow\uparrow}) + \Pi_{\downarrow\uparrow} + \tfrac{1}{2}\Pi_{\downarrow\uparrow}^2] + \mathrm{Tr}[\ln(1 + \Pi_{pp}) - \Pi_{pp} + \tfrac{1}{2}\Pi_{pp}^2] , \quad (3)$$

which generates Hartree-Fock and second-order self-energies, plus contributions from exchanged longitudinal spin fluctuations and density fluctuations, transverse spin fluctuations, and singlet pair fluctuations. The susceptibility bubbles are given by

$$\Pi_{pp}(\mathbf{r}, \tau) = UG_{f\uparrow}(\mathbf{r}, \tau)G_{f\downarrow}(\mathbf{r}, \tau), \quad (4)$$

$$\Pi_{\sigma\sigma'}(\mathbf{r}, \tau) = -UG_{f\sigma'}(\mathbf{r}, \tau)G_{f\sigma}(-\mathbf{r}, -\tau) . \quad (5)$$

For the results presented below, the contribution to Φ from spin fluctuations is within 10% of that from the second-order diagram; contributions from pair fluctuations and from density fluctuations are smaller by factors of roughly $-1/4$ and $-1/10$, respectively.

We calculate Σ_f using an algorithm originally developed for the Hubbard model [10], on a 32×32 lattice with spot checks on lattices as large as 128×128, and using a frequency cutoff at least 6 times the unhybridized conduction band width, $W = 8t$.

The magnetic susceptibility $\chi(T)$ was found from the slope of $\mathrm{Tr}[\sigma_z G]$ versus h for small fields (typically $0.005t$ and $0.01t$); this calculation of $\chi(T)$ is equivalent to solving an integral equation for the response function with irreducible vertices comprising particle-particle and particle-hole bubble chains and Aslamazov-Larkin-type diagrams [11].

The retarded self-energy on the real axis was obtained from N-point Padé approximants [12], and used to construct the spectral functions and quasiparticle dispersion relations along symmetry directions in the Brillouin zone. The densities of states were found from Padé continuations of the $\mathbf{k}$-summed imaginary-frequency Green's functions. These self-energies and densities of states are insensitive to variations in the order of the approximant over a wide range of N, and satisfy sum rules to better than 1% accuracy.

For the calculations reported here, we used $\mu = 1.8t$, $V = t$, and $\tilde{e}_f = 1.5t$, where $\tilde{e}_f = e_f + \frac{1}{2}U(n_\uparrow^f + n_\downarrow^f)$ is the ($h = 0$) Hartree-renormalized f level. With these parameters the total f density and c density are approximately $n_f = 1.05$ and $n_c = 1.52$, and vary by less than 2% for $0 < U < 4t$ at fixed temperature and by approximately 0.5% for $0.002 < T/t < 0.25$ at $2t \le U \le 4t$; differences between temperature dependences at fixed $\tilde{e}_f$ and at fixed e_f are thus insignificant. We note in passing that for $W \sim 1$ eV our lowest temperature corresponds to ~ 3 K. The noninteracting density of states is shown in Fig. 1(a) (here and subsequently, energies are measured from μ). The Fermi energy sits in a region of large density of states (DOS), but is not coincident with any sharp structure.

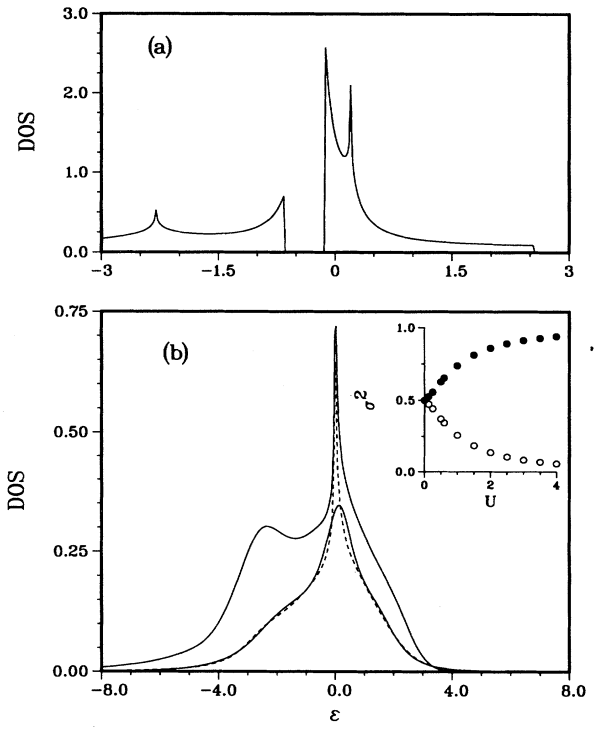

FIG. 1. (a) The noninteracting total density of states with $\tilde{e}_f = 1.5t$, $V = t$, and $\mu = 1.8t$. (b) The interacting total (upper solid) and f-electron (dashed) densities of states with $U = 2t$ and $T = t/64$, and the f-electron density of states (lower solid) for $T = t/4$. The inset shows the f-site local spin (•) and charge (○) fluctuations as a function of U. Here and in all subsequent figures the unit of energy is t, energies are measured from μ, and the DOS are for a single spin.

The f-site local spin and charge fluctuations can be found from the density of doubly occupied sites,

$$D_f = \langle n_{i\uparrow}^f n_{i\downarrow}^f \rangle ,$$

$$\sigma_S^2 = \langle (n_{i\uparrow}^f - n_{i\downarrow}^f)^2 \rangle = n_f - 2\,D_f , \quad (6)$$

$$\sigma_C^2 + n_f^2 = \langle (n_{i\uparrow}^f + n_{i\downarrow}^f)^2 \rangle = n_f + 2\,D_f ,$$

and we get D_f from a numerical U derivative of Ω. The inset to Fig. 1(b) shows σ_S^2 and σ_C^2 as a function of U for $T = t/64$. In the remainder of this paper we focus on $U = 2t$ and $U = 4t$, which yield large local moments. We note that the corresponding single-impurity Kondo temperatures are $T_K \approx t/30$ and $T_K \approx t/250$; the latter is near the lowest temperature accessible to our calculations for $U = 4t$. Self-consistency is essential to the results presented here: for $T = t/32$, the FEA evaluated with G_0 is unstable for $U > 0.6$.

Figure 1(b) shows the total and f densities of states for $U = 2t$ and $T = t/64$. The noninteracting hybridization gap has disappeared on account of the large (and essentially temperature independent) scattering rate for

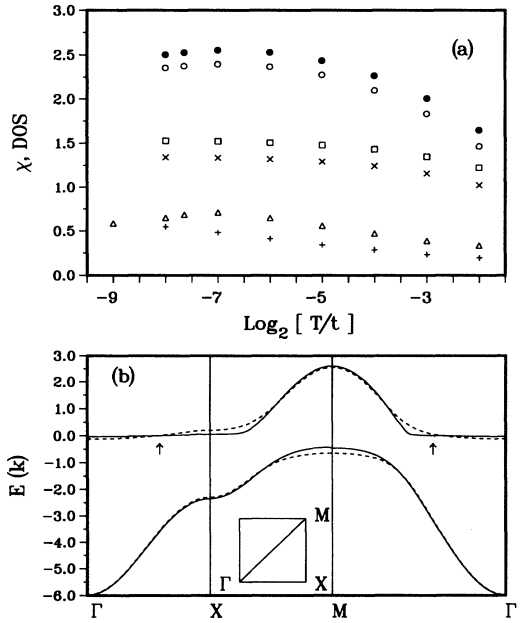

FIG. 2. (a) The f-electron density of states at $\varepsilon = 0$ for $U = 2t$ ($\triangle$) and $U = 4t$ (+) together with the total and f-electron spin susceptibility for $U = 2t$ ($\bullet$ and $\circ$) and $U = 4t$ ($\square$ and $\times$). (b) The bare (dashed) and renormalized (solid) band structures for $T = t/32$ along high-symmetry directions in the Brillouin zone. The small arrows indicate the approximate location of the renormalized Fermi surface.

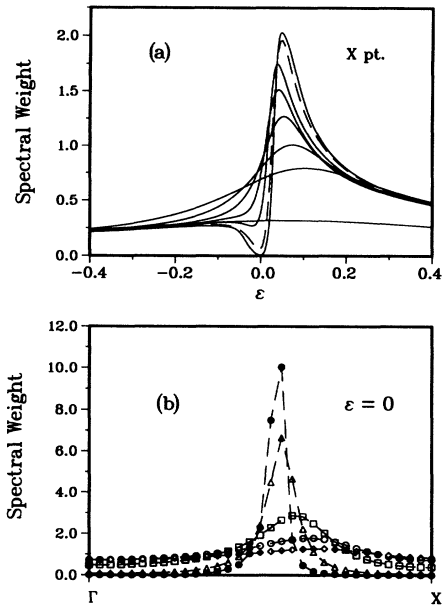

FIG. 3. The spectral function (a) at X as a function of energy for T decreasing (corresponding to peak heights increasing) by factors of 2 between $t/4$ and $t/512$; and (b) at $\varepsilon = 0$ as a function of $\mathbf{k}$ along ΓX for $T = t/512$ ($\bullet$), $t/256$ ($\triangle$), $t/128$ ($\square$), $t/64$ ($\circ$), and $t/32$ ($\diamond$).

electrons near the gap edges. The most prominent feature is a sharp peak near $\varepsilon = 0$ in the f-electron density of states, which develops as the temperature is reduced from $T = t/4$, for which the f density of states is also shown. From Fig. 2(a) we see that for $U = 4t$ the DOS at $\varepsilon = 0$ grows down to $T = t/256$, but for $U = 2t$ it reaches a maximum at $T \approx t/128$ and then decreases [13]. The temperature dependence of the f-electron contribution to the magnetic susceptibility is qualitatively similar.

The turnover with decreasing T of the $\varepsilon = 0$ DOS for $U = 2t$ signals a crossover from incoherent local moments to a coherent quasiparticle band. Figure 2(b) shows the bare band structure and the renormalized "band structure" obtained from the zeros of the real part of the denominator of the Green's function at $T = t/32$ with $U = 2t$. As expected, these renormalized "bands" are significantly flattened near the Fermi energy. On the scale of Fig. 2(b) the bands at lower temperatures would be essentially indistinguishable from those shown for $T = t/32$, but the Fermi velocities decrease with decreasing temperature over the full range of temperatures studied. At $T = t/256$ the ratio of the Fermi velocities of the noninteracting and interacting ($U = 2t$) systems is 4.7 along ΓX and 7.9 along ΓM.

If we examine the single-particle spectral functions, however, we conclude that these curves cannot be interpreted as coherent quasiparticle bands, except for $U = 2t$ with $T < t/128$. Figure 3(a) shows the temperature dependence of the spectral function $A(\mathbf{k}, \varepsilon)$ at the X point, which is well away from the Fermi surface along ΓX. It is apparent that this point (and presumably all other points along ΓX as well) contributes substantial spectral weight at $\varepsilon = 0$ for all temperatures above $T = t/128$. We also plot the $\varepsilon = 0$ spectral weight along the ΓX direction in Fig. 3(b). Both plots clearly demonstrate that a quasiparticle interpretation of the renormalized band structure is meaningful only for $T < t/128$. Formation of the coherent state is controlled by competition between the spectral width of the f electrons and the bandwidth of the f-derived quasiparticle bands, both of which decrease with decreasing temperature. Although for $U = 2t$ the "coherence temperature" and Kondo temperature are roughly comparable, we do not see how to relate the physics of the Kondo effect to the competition between the two temperature-dependent energy scales in our calculation.

The momentum dependence of the self-energy, shown in Fig. 4, is weak at high temperatures, as expected for independent local moments, and becomes significant as coherence is established. The particle-hole bubble $\Pi_{\downarrow\uparrow}(\mathbf{q}, 0)$ at $\mathbf{q} = \mathbf{0}$ has a similar T dependence to the full susceptibility, while the bubble at the X point follows $\Pi_{\downarrow\uparrow}(\mathbf{0}, 0)$ closely down to $T = t/128$, but continues to increase at lower temperatures, perhaps indicating an incipient antiferromagnetic transition.

The quasiparticle renormalization factor decreases

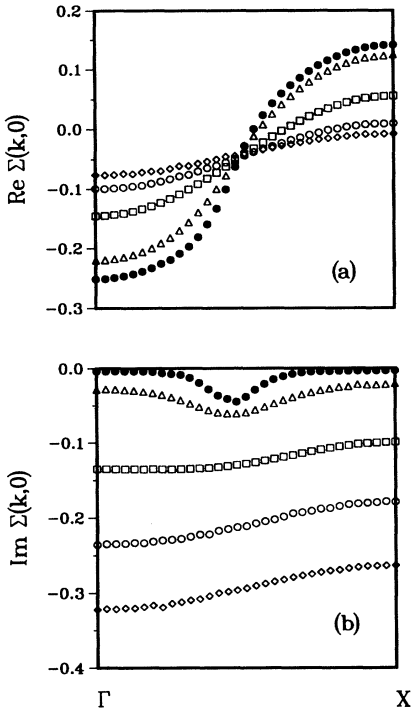

FIG. 4. The temperature dependence of (a) Re $\Sigma_f^R(\mathbf{k},0)$ and (b) Im $\Sigma_f^R(\mathbf{k},0)$ for $\mathbf{k}$ along ΓX and for temperatures as listed in Fig. 3(b).

with temperature down to $T = t/512$ on the Fermi surface along both ΓX and ΓM. The temperature dependence of $\mathrm{Im}\,\Sigma_f^R(\mathbf{k}_F, \varepsilon = 0)$ is significantly stronger than the $T^2 \ln T$ expected for a 2D Fermi liquid at all temperatures that we studied, and the frequency dependence is not of the form $\varepsilon^2 \ln|\varepsilon|$, but more nearly resembles the anomalous frequency dependence of $\mathrm{Im}\,\Sigma^R(\mathbf{k}_F, \varepsilon)$ observed in FEA calculations for 2D Hubbard models very near half-filling or with van Hove singularities close to the Fermi surface [14]. While we do not observe 2D Fermi liquid behavior, we cannot rule out the possibility that a Fermi liquid will form at lower temperatures.

In summary, using the fluctuation exchange approximation, we have observed a crossover between a lattice of incoherent local moments and a band of renormalized itinerant quasiparticles in a 2D Anderson lattice model with $U = 2t$. The magnetic susceptibility bubble has its maximum at the X point, which raises the possibility of an incipient antiferromagnetic transition. We are exploring this question using conserving calculations of the response to a staggered field.

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