Formation of a Heavy-Fermion State in the 2D Periodic Anderson Model

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We study the formation of a heavy-fermion state in the 2D periodic Anderson model. For \( U = 2 \), the density of states, imaginary part of the self-energy and effective magnetic moment all indicate the Kondo screening of local \( f \) electrons, leading to a coherent heavy-fermion state. For \( U = 3 \) and 4, the dominance of RKKY interaction over Kondo screening at low temperatures indicates a magnetic instability at zero temperature. A partial screening of magnetic moments, however, still gives rise to a relatively sharp peak at the Fermi energy in the density of states.

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Since the discovery of the heavy-fermion materials in rare-earth or actinide elements [1,2], a possible dramatic transformation of localized \( f \) electrons to a coherent heavy-fermion state has received considerable attention. Experiments in these materials have exhibited various unusual properties such as the huge coefficient in the magnetic susceptibility, specific heat and so on, which all indicate the formation of a coherent state with a large effective mass. The periodic Anderson model [3] has been considered as the most promising candidate which might be able to describe the anomalous features of these materials. The Hamiltonian for the 2D periodic Anderson model is

\[
H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^+ c_{j\sigma} + \sum_{i\sigma} [V (f_{i\sigma}^+ c_{i\sigma} + c_{i\sigma}^+ f_{i\sigma}) + \epsilon_f f_{i\sigma}^+ f_{i\sigma}] \\
+ U \sum_i (f_{i\uparrow}^+ f_{i\downarrow} - n_{i\uparrow} n_{i\downarrow}) (f_{i\downarrow}^+ f_{i\uparrow} - n_{i\downarrow} n_{i\uparrow}) \\
- \mu \sum_{i\sigma} (c_{i\sigma}^+ c_{i\sigma} + f_{i\sigma}^+ f_{i\sigma}).
\]  

Here \( t \) is the hopping parameter for \( c \) electrons, \( V \) the hybridization energy between \( c \) and \( f \) electrons, and \( \epsilon_f \) the energy level for \( f \) electrons. \( U \) is the Coulomb repulsion energy for \( f \) electrons, \( n_{i\sigma} = (f_{i\sigma}^+ f_{i\sigma}) \) and \( \mu \) is the chemical potential controlling the total electron concentration. \( c_{i\sigma} \) and \( f_{i\sigma} \) are annihilation operators for \( c \) and \( f \) electrons at site \( i \) with spin \( \sigma \), respectively. When the hybridization term is eliminated by means of the equations of motion for \( c \) and \( f \) electrons, the corresponding interacting Green’s functions, \( G_c(\vec{k}, \omega) \) and \( G_f(\vec{k}, \omega) \), are expressed in terms of the self-energy for \( f \) electrons \( \Sigma_f(\vec{k}, \omega) \)

\[
G_c(\vec{k}, \omega) = \frac{1}{\omega - \epsilon_\vec{k} + \mu - \frac{V^2}{\omega - \epsilon_f + \mu - \Sigma_f(\vec{k}, \omega)}},
\]

\[
G_f(\vec{k}, \omega) = \frac{1}{\omega - \epsilon_f + \mu - \frac{V^2}{\omega - \epsilon_\vec{k} + \mu - \Sigma_f(\vec{k}, \omega)}},
\]

where \( \epsilon_\vec{k} = -2t(cos k_x + cos k_y) \) for nearest neighbor hopping. As long as \( f \) electrons are concerned, the interacting Green’s function has the same structure as that for the usual Hubbard model with the inverse of the noninteracting propagator \( [G_f^0(\vec{k}, \omega)]^{-1} \) replaced by \( \omega - \epsilon_f + \mu - \frac{V^2}{\omega - \epsilon_\vec{k} + \mu} \). For later use, we also show the noninteracting \( (U = 0) \) energy dispersion due to hybridization,

\[
E^0_\pm(\vec{k}) = (\epsilon_f + \epsilon_\vec{k} - 2\mu) \pm \sqrt{[\epsilon_f - \epsilon_\vec{k}]^2 + 4V^2}/2.
\]  

Recently the infinite [5] and two [6] dimensional periodic Anderson models for the symmetric case have been studied by using quantum Monte Carlo (QMC) calculations. In these works for a half-filled band, the authors found a strong competition between the Kondo effect [5] and antiferromagnetic order depending on the size of \( V \) and \( U \). Because of its symmetric nature, however, the model can not describe any possible formation of a coherent heavy-fermion state from localized \( f \) electrons. The 2D asymmetric periodic Anderson model has been investigated by McQueen et al. [8] within fluctuation exchange (FLEX) approximation. These authors found a developing density of states near the Fermi energy with decreasing temperature, which was argued as an indication of the Kondo resonance. However, they could not observe a Fermi liquid behavior in the calculations of the self-energy. This is possibly due to the insufficient treatment of strong local correlations and 2D spin fluctuations in the FLEX approximation [10].

Recently we have developed a new approximation scheme for the 2D Hubbard model which shows the essential features of the model [11]. This theory satisfies simultaneously the correct atomic limit for large frequencies (reflected as the correct asymptotic behavior of the self-energy at large \( \omega \)) as well as 2D spin fluctuations due to the Mermin-Wagner theorem [12]. These two features are very important in the study of the 2D periodic Anderson model, in that the screening of local moments by conduction electrons is properly described by the first property and any possible magnetic instability at zero
temperature by the second. One more good feature of our formulation over FLEX approximation or second-order (in $U$) perturbation study is that the dynamical spin susceptibility can be computed accurately by imposing the exact sumrules. In this Letter we present the strong numerical evidence for the formation of a coherent heavy-fermion state from localized $f$ electrons by showing the density of states, low frequency behavior of the self-energy, effective magnetic moment and quasiparticle residue.

In order to compute properly the spin, charge, and particle-particle susceptibilities which govern the interactions between electrons, we impose the following three exact sumrules to them [11,10]:

$$\frac{T}{N} \sum_{q} \chi_{sp}(q) = n - 2 \langle n_{\uparrow} n_{\downarrow} \rangle$$

$$\frac{T}{N} \sum_{q} \chi_{ch}(q) = n + 2 \langle n_{\uparrow} n_{\downarrow} \rangle - n^2$$

$$\frac{T}{N} \sum_{q} \chi_{pp}(q) = \langle n_{\uparrow} n_{\downarrow} \rangle .$$

(4)

$T$ and $N$ are the absolute temperature and number of lattice sites. $q$ is a compact notation for $(\vec{q}, i\nu_n)$ where $i\nu_n$ are either Fermionic or Bosonic Matsubara frequencies. The dynamical spin, charge and particle-particle susceptibilities are calculated by

$$\chi_{sp}(q) = \frac{2\chi_{ph}^0(q)}{1 - U_{sp}\chi_{ph}^0(q)}$$

$$\chi_{ch}(q) = \frac{2\chi_{ph}^0(q)}{1 + U_{ch}\chi_{ph}^0(q)}$$

$$\chi_{pp}(q) = \frac{\chi_{pp}^0(q)}{1 + U_{pp}\chi_{pp}^0(q)} .$$

(5)

$\chi_{ph}^0(q)$ and $\chi_{pp}^0(q)$ are irreducible particle-hole and particle-particle susceptibilities, respectively, which are computed from

$$\chi_{ph}^0(q) = -\frac{T}{N} \sum_{k} G_j^0(k - q) C_j^0(k)$$

$$\chi_{pp}^0(q) = \frac{T}{N} \sum_{k} G_j^0(k - q) C_j^0(k) .$$

(6)

where $G_j^0(k)$ is the noninteracting Green’s function for $f$ electrons defined earlier. $U_{sp}$, $U_{ch}$, and $U_{pp}$ in Eq. 4 are renormalized interaction constants for each channel which are calculated self-consistently by making an ansatz $U_{sp} \equiv U \langle n_{\uparrow} n_{\downarrow} \rangle / \langle (n_{\uparrow} + n_{\downarrow}) \rangle$ [11] in Eq. 4. By defining $U_{sp}$, $U_{ch}$, and $U_{pp}$ this way, the Mermin-Wagner theorem as well as the correct atomic limit for large $\omega$ are satisfied simultaneously [11]. Throughout the calculations we fixed $\varepsilon_f = 0.45$, $V = 1$ and the total electron concentration at 2.25. The unit of energy is $t$ and all energies are measured from the chemical potential $\mu$. We used a $64 \times 64$ lattice in momentum space and performed the calculations by means of well-established fast Fourier transforms (FFT). It should be also noted that we used a real frequency formulation in Eqs. (2)-(6) to avoid any possible uncertainties associated with numerical analytical continuation.

We start in Fig. 1 by studying the density of states (Fig. (a)) and imaginary part of the self-energy at the Fermi surface for $U = 2$, $\varepsilon_f = 0.45$ and $V = 1$ with decreasing temperature. The long-dashed, dashed, dotted and solid curves denote $T = 1/16$, 1/64, 1/256 and 1/1024, respectively. The inset in (a) shows the density of states for $T = 1/1024$ in the wide range of frequency axis.

![Figure 1](image_url)

**FIG. 1.** (a) Density of states and (b) imaginary part of the self-energy at the Fermi surface for $U = 2$, $\varepsilon_f = 0.45$ and $V = 1$ with decreasing temperature. The long-dashed, dashed, dotted and solid curves denote $T = 1/16$, 1/64, 1/256 and 1/1024, respectively. The inset in (a) shows the density of states for $T = 1/1024$ in the wide range of frequency axis.

In order to establish a more firm ground that this is indeed due to the screening of magnetic moments by conduction electrons, we show the effective magnetic moment defined as $T\chi_{sp}(0, 0)$ upon decreasing the temperature (filled circles in Fig. 2(a)). Below $T = 1/128$, the effective magnetic moment vanishes linearly in temperature, a clear indication of the Kondo screening. Above this temperature, it deviates significantly from a straight line and appears gradually saturating at high tempera-
The quasiparticle residue is almost isotropic throughout the Fermi surface. In Fig. 2(b) we present the drastic change of the quasiparticle dispersion in the upper branch, $E_0^\text{sp}(\vec{k})$ in Eq. 3, where the Fermi energy stays. The interacting quasiparticle dispersion becomes dramatically flattened along the directions $(0, 0) - (\pi, \pi)$ and $(0, \pi) - (0, 0)$, leading to a heavy effective mass as well as large density of states at the Fermi energy. It is of interest to notice that the interacting energy band appears separated into $f$ electron (lower band) and $c$ electron (upper band) dominating parts, which is absent in the noninteracting band.

In order to understand the role of $U$ in the one and two particle properties, we also performed the calculations for $U = 3$ and 4 with all the other parameters unchanged. In both cases, we found the indication of a ferromagnetic instability with decreasing temperature, which is signaled by a divergent behavior of $\chi_{sp}(\vec{q}, 0)$ at $\vec{q} = (0, 0)$ in Fig. 3. Note that there is no finite temperature phase transition in two dimensions due to the Mermin-Wagner theorem. The inset clearly shows $\chi_{sp}(0, 0) \sim \exp(constant/T)$ at low temperatures. This magnetic instability happens because the RKKY interaction between $f$ electrons becomes dominating over the Kondo screening for large $U$.

In Fig. 4 we present the density of states (Fig. 4(a)) and imaginary part of the self-energy (Fig. 4(b)) for $U = 3$, $T = 1/2048$ (solid curves) and $U = 4$, $T = 1/290$ (dotted curves). These temperatures are the lowest ones for each $U$ where we found the convergent solutions for $U_{sp}$ in our numerical calculations. The inset in (a) shows the density of states in the wide range of frequency axis. Due to 2D strong spin fluctuations at low temperatures, the spectral weight is significantly suppressed in the low frequency regime (inset in Fig. 4(a)), compared with that for $U = 2$ (inset in Fig. 4(a)). To our surprise, a relatively sharp peak is still persisting at the Fermi energy even in the presence of strong spin fluctuations. In order to understand the nature of this peak, we computed the scattering rates in Fig. 4(b). $\text{Im}\Sigma(\vec{k}_F, \omega)$ shows a small dip at the Fermi energy in a large scattering background, which is different from the case for $U = 2$. This local minimum of the scattering rates at the Fermi energy is responsible for the sharp structure in the density of states. This feature comes from a partial screening of $f$ electrons by conduction electrons for the following reason. In the critical region the imaginary part of the spin susceptibility becomes singular like $\text{Im}\chi_{sp}(\vec{q}, \nu) \sim \delta(\nu - \Omega)$ near $\vec{q} = (0, 0)$ for a ferromagnetic case. $\Omega$ is the characteristic spin fluctuation energy which is less than $10^{-2}$ for the parameters used for $U = 3$ and 4. Hence, the imaginary part of the self-energy near the Fermi energy is given by

\[
\text{Im}\Sigma_f(\vec{k}_F, \omega) \sim \sum_{\vec{q}} \int d\nu \text{Im}\chi_{sp}(\vec{q}, \nu)[B(\nu) + F(\nu - \omega)] \times \text{Im}G^R_f(\vec{k}_F - \vec{q}, \omega - \nu) \\
\sim \sum_{\vec{q}} \frac{1}{2} \frac{(\epsilon_f - \epsilon_{kF - \vec{q}})}{(\epsilon_f - \epsilon_{kF - \vec{q}}^2 + 4V^2)}
\]
Im\(\Sigma(k, \omega)\) self-energy at the noninteracting Fermi surface for \(\varepsilon_V\) and of states in the wide range of frequency axis. A peak at \(\omega = 1\) with \(V = 1\) gives rise to larger scattering rates at \(\omega \neq 0\) than those at \(\omega = 0\), leading to a small dip at the Fermi energy. This is in turn responsible for a relatively sharp peak in the density of states. Hence, a peak at \(\omega = 0\) in the density of states for \(U = 3\) and 4 is caused by mixing of f and c electrons, that is, a partial screening of local moments by conduction electrons. To confirm this argument, we also calculated the density of states and imaginary part of the self-energy by increasing \(\varepsilon_V\) for \(U = 4\) and \(T = 1/290\) with increasing \(V\). \(V = 1, 1.25\) and 1.5 are denoted as the solid, dotted and dashed curves, respectively.

\[ \times \delta(\omega - E_{sp}^{\uparrow}(\vec{k}_F - \vec{q})) . \]  

Since \(\text{Im}\chi_{\text{sp}}(\vec{q}, \nu)\) shows a nearly divergent behavior in the small region with the radius of approximately \(\pi/16\) from the origin in our calculations, the summation of \(\vec{q}\) is over this area. Due to the mixture of f and c electrons through \(V\), generally the hybridized band \(E_{sp}^{\uparrow}(\vec{k})\) has some dispersion or slope at the noninteracting Fermi surface. Because of this feature, the contributions from \(\vec{q} \neq (0, 0)\) give rise to larger scattering rates at \(\omega \neq 0\) than those at \(\omega = 0\), leading to a small dip at the Fermi energy in the scattering rates. This is in turn responsible for a relatively sharp peak in the density of states. Hence, a peak at \(\omega = 0\) in the density of states for \(U = 3\) and 4 is caused by mixing of f and c electrons, that is, a partial screening of local moments by conduction electrons. To confirm this argument, we also calculated the density of states and imaginary part of the self-energy by increasing the hybridization strength \(V\) with all the other parameters including the total electron concentration fixed. As mixing \((V)\) is increased, the scattering rates from spin fluctuations are more suppressed near the Fermi energy in Fig. 3(b). The distance between the local maximum and the dip is given by the value \(E_{sp}^{\uparrow}(\vec{k}_F - \vec{q})\) at \(q = \pi/16\) for all three different \(V\). In a hypothetical situation where \(E_{sp}^{\uparrow}(\vec{k}) = \text{constant}\) (no mixing) and the same \(\text{Im}\chi_{\text{sp}}(\vec{q}, \nu)\) is taken, the scattering rates would be maximum at the Fermi energy, leading to a pseudogap instead of a peak in the density of states.

In summary, the formation of a coherent heavy-fermion state in the 2D periodic Anderson model has been studied on the basis of the recently developed theory for the Hubbard model. For \(U = 2\), the growing density of states and rapidly vanishing scattering rates near the Fermi energy as well as linearly vanishing (in temperature) effective magnetic moment below a characteristic temperature, strongly support the Kondo screening of f electrons, leading to a heavy-fermion state. For \(U = 3\) and 4, the dominance of RKKY interaction over Kondo screening at low temperatures indicates a magnetic instability at zero temperature. The persistence of a peak at \(\omega = 0\) even in the presence of strong spin fluctuations is due to a partial screening of f electrons by conduction electrons.

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\[ \text{FIG. 4. (a) Density of states and (b) imaginary part of the self-energy at the noninteracting Fermi surface for } \varepsilon_F = 0.45 \text{ and } V = 1 \text{ with } U = 3, T = 1/2048 \text{ (solid curves) and } U = 4, T = 1/290 \text{ (dotted curves). The inset in (a) shows the density of states in the wide range of frequency axis.} \]

\[ \text{FIG. 5. (a) Density of states and (b) imaginary part of the self-energy at the noninteracting Fermi surface for } \varepsilon_F = 0.45, U = 4 \text{ and } T = 1/290 \text{ with increasing } V. \text{ } V = 1, 1.25 \text{ and } 1.5 \text{ are denoted as the solid, dotted and dashed curves, respectively.} \]

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