Gutzwiller Variational Approximation to the Heavy-Fermion Ground State of the Periodic Anderson Model

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A variational wave function for the Kondo-lattice limit of the periodic Anderson model is evaluated with a Gutzwiller approximation. We obtain a characteristic energy from this coherent wave function of the Kondo form but with a different exponent in the case of finite degeneracy. The effective mass and charge and spin susceptibilities are evaluated, and only in the case of large degeneracy and not too small hybridization strength is a heavy-Fermi-liquid state stable against magnetic order.

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The highly unusual behavior of the heavy-electron metals[1] has stimulated attempts to derive this behavior starting from the periodic Anderson model in the Kondo limit. In this Letter we present a variational method based on a hybridized wave function in which the doubly occupied f-electron configurations are projected out. To treat the projection operators we use an extension of Gutzwiller's method.[2] This results in an effective one-electron Hamiltonian to describe the low-energy quasiparticle states in which the hybridization matrix element is renormalized and the f level shifted in energy. We obtain from our coherent wave function a characteristic energy which has a Kondo form and whose exponent agrees with that of the single-site Kondo problem in the limit of large orbital degeneracy. Our method resembles that of Brandow[3] who obtained an effective Hamiltonian from a diagrammatic technique. Functional integration techniques have also led to a similar effective Hamiltonian.[4] On phenomenological grounds Razafimandimby, Fulder, and Keller[5] proposed a similar model. Our results differ significantly from these authors. We find that a paramagnetic heavy Fermi-liquid state is stable only if the orbital degeneracy is relatively large and the bare hybridization matrix element is not too weak. The renormalizations have simple physical interpretations and are determined self-consistently by a variational method which can be generalized to more realistic models. Further, our results show that there is close analogy to the single-band almost-localized models[6] proposed for ^{3}He[7] and these systems.[8]

The analogy to ^{3}He has been proposed previously on general grounds.[9] Lastly we should mention a previous approach using Gutzwiller methods by Varma.[10] He reported on the basis of numerical calculations that the ground state in this limit had nonintegral valence. Our analytic results show a Kondo form for the deviation from integral valence. We give explicit results for the effective mass and charge and spin susceptibilities.

The periodic Anderson-model Hamiltonian is

$$H_A=\sum_{\mathbf{k}\sigma}\epsilon_k c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\sum_{\mathbf{k}l\sigma}V_{\mathbf{k}l}(c^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}l\sigma}+f^{\dagger}_{\mathbf{k}l\sigma}c_{\mathbf{k}\sigma})+E_f\sum_{il\sigma}n_{il\sigma}+\frac{1}{2}U\sum_{\substack{i\\ l\sigma\neq l'\sigma'}}n_{il\sigma}n_{il'\sigma'}. \tag{1}$$

The conduction-band dispersion $\epsilon(k)$ is chosen as linear ranging from -1 to $+1$. In the Kondo limit, the bare f-level energy $E_f<0$ and the on-site Coulomb repulsion U is large ($U\rightarrow\infty$). The hybridization matrix element is $V_{\mathbf{k}l}$ (chosen as k independent for simplicity) and the degeneracy of the f level, N_f, is assumed to be even, $N_f=2L$. The total number of electrons, n, is taken as $1<n<2$.

In the single-site Kondo problem a variational wave function[11] which mixes the states with the f level occupied and a hole in the conduction band with each other through a state with the f level empty and the conduction band filled was used to treat the spectroscopic response.[12] An extension to the lattice problem was proposed by Brandow[3] with the wave function written as a projection operator to remove doubly occupied sites operating on a one-electron hybridized-band wave function. The key problem is how to treat the projection operator. Brandow[3] used a diagrammat-

ic technique to derive an effective Hamiltonian. Here we use an extension of the Gutzwiller technique[2] with important differences from his result. In the Gutzwiller approximation for a single-band Hubbard model the effect of correlations is to renormalize the kinetic energy by a factor, q, calculated from the classical statistical weighting factors (see Vollhardt[7]).

To extend the method to a two-band model we proceed in two steps. First, we fix the number of f electrons, n_f, and then we project out the doubly occupied states keeping n_f fixed. The variational wave function is

$$|\Psi\rangle = P_{n_f} P |\Psi_0\rangle, \tag{2}$$

where $|\Psi_0\rangle$ is a one-electron hybridized-band wave function and P and P_{n_f} are the projection operators which remove double occupancy and fix the number of f electrons. The operator P is treated by renormalizing all hopping processes by a factor $q(n_f, L)$. In Eq. (1), a hopping process involves two factors of V, and so V is renormalized by a factor $q^{1/2}$. The result is an effective Hamiltonian for a fixed n_f,

$$H_{\text{eff}}(n_f) = \sum_{\mathbf{k}\sigma} [\epsilon_k c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_l \tilde{V}_{\mathbf{k}l\sigma} (c^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}l\sigma} + f^\dagger_{\mathbf{k}l\sigma} c_{\mathbf{k}\sigma}) + \sum_l E_f f^\dagger_{\mathbf{k}l\sigma} f_{\mathbf{k}l\sigma}], \tag{3}$$

with $\mathbf{V}_{\mathbf{k}l\sigma} = q_{l\sigma}^{1/2}(n_f, L) V_{\mathbf{k}l}$. In this $U \to \infty$ limit, q is simply given by the ratio of occupation number factors for the correlated and uncorrelated wave functions. In the correlated wave function an f electron with quantum numbers $l\sigma$ can hop onto another site only if it has no f electrons, while in an uncorrelated wave function the only requirement is that it does not have an $l\sigma$ electron. The result is

$$q_{l\sigma}(n_f, L) = (1 - n_f)/(1 - n_{fl\sigma}), \tag{4}$$

where $n_{fl\sigma}$ is density of $l\sigma$ electrons. Note that because of the denominator this renormalization factor is different from that obtained by Brandow[3] and others,[4] except as $L \to \infty$, when $n_{fl\sigma} \approx \frac{1}{2} L \to 0$. The denominator can be justified in several ways. First, in a completely spin-polarized state with $L = 1$, $q = 1$ as it should, since this limit is a one-electron problem. A second way is to take the ratio of the kinetic energy of a small number of holes in the lower Hubbard band as $U \to \infty$ to the kinetic energy of the uncorrelated problem. Using the exact results of Brinkman and Rice[13] we can verify Eq. (4) to 10%–20%.

The density n_f is to be determined by minimizing the expectation value of $H_{\text{eff}}(n_f)$. Instead of fixing n_f it is more convenient to go over to the equivalent of a grand canonical ensemble and introduce an f-electron chemical potential μ_σ (or self-energy μ_σ), leading to an effective Hamiltonian

$$K_{\text{eff}} = H_{\text{eff}} - \sum_{\mathbf{k}l\sigma} \mu_\sigma f^\dagger_{\mathbf{k}l\sigma} f_{\mathbf{k}l\sigma}, \tag{5}$$

where we have restricted ourselves to the oribtal paramagnetic case (i.e., all orbitals occupied equally). With the assumption that V_l is l independent, K_{eff} can be diagonalized at once. Only the symmetric combination of the f levels hybridizes, and the other $L - 1$ orbital combinations are unhybridized. The hybridized bands have an energy

$$\xi_{k\pm,\sigma} = \tfrac{1}{2}\{\epsilon_k + E_f - \mu_\sigma \pm [(\epsilon_k - E_f + \mu_\sigma)^2 + 4L\tilde{V}_\sigma^2]^{1/2}\} \tag{6}$$

The + (−) label refers to the upper (lower) hybridized band. We should point out that the assumption that $V_{\mathbf{k},l}$ is a constant is too simple since in this case l is not conserved in the hopping process and only the symmetric combination of orbitals is hybridized and effectively $L = 1$. In fact, there is conservation of angular momentum around the axis in a hopping process[14,15] and this requires that the orbital combination that hybridizes is essentially $\mathbf{k}$ dependent. The form (4) for q assumes l conservation in hopping processes and so is consistent with the latter. However, in calculating the energy we will simplify and replace $|V_{\mathbf{k},l}|$ by an average value.

We consider first a paramagnetic state. The hybridized quasiparticle bands are shown in Fig. 1. In the special case $n = 2$, the lower (−) band is completely filled and the system is insulating. When $1 < n < 2$ the lower band is partially filled up to a Fermi wave vector k_F and the system is metallic. The total

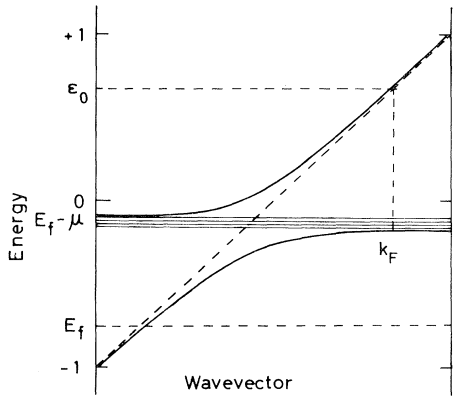

FIG. 1. The energy level structure for the case of L degenerate bands and value of $n = 1.8$. Only the symmetric combination of f levels hybridizes with the conduction band (see text). All f levels are moved up to by an energy $(-\mu)$ so that the number of f electrons is n_f which has a value $n_f \lesssim 1$.

number of f electrons is given by

$$n_f = N^{-1} \sum_{k<k_F,\sigma} \frac{\epsilon_k - E_f + \mu_\sigma}{2[(\epsilon_k - E_f + \mu_\sigma)^2 + 4L\tilde{V}_\sigma^2]^{1/2}} + \frac{1}{2}, \tag{7}$$

where N is total number of sites and the energy per site is

$$N^{-1}\langle H_{\rm eff}\rangle = N^{-1} \sum_{k<k_F,\sigma} \xi_{k-,\sigma} + \sum_\sigma \mu_\sigma n_{f\sigma}. \tag{8}$$

In the weak hybridization limit, it suffices to work to leading logarithmic order. Then the energy can be evaluated as a function of n_f and by use of Eq. (7), to eliminate μ, we get

$$N^{-1}\langle H_{\rm eff}(n_f)\rangle = \epsilon_0^2/2 + (E_f - \epsilon_0)n_f + n_f^2/2 - \tfrac{1}{2} - L\tilde{V}^2 \ln[n_f(1+\epsilon_0 - n_f)/L\tilde{V}^2], \tag{9}$$

where $\epsilon_0 = \epsilon_{kF}$ (see Fig. 1). Minimizing with respect to n_f gives

$$1 - n_f = \frac{\epsilon_0(2L-1)}{2L^2V^2} \exp\left[\frac{-(2L-1)(\epsilon_0 - E_f - 1)}{2L^2V^2}\right]. \tag{10}$$

This optimum value has an exponential form similar to that in the single-site Kondo problem. In leading logarithmic accuracy only the exponent can be compared. For $L = 1$, the exponent is a factor of 2 smaller than the single-site Kondo exponent, while as $L \to \infty$ it agrees.

The condensation energy, E_c, defined as the energy difference per site between the hybridized and unhybridized problems in the leading logarithmic accuracy is

$$E_c = [(1 + E_f - \epsilon_0)/(2L-1) - \tfrac{1}{2}](1-n_f)^2. \tag{11}$$

Note that $E_c \propto (1-n_f)^2$. However, the characteristic energy to be compared to the Kondo temperature will be proportional to $1-n_f$, just as in a superconductor the characteristic energy is the energy gap and not the condensation energy per site.

The specific heat is given by the density of quasiparticle states which from Eq. (6) is

$$N_0 = 2\frac{(\epsilon_0 + E_f + \mu)^2}{qLV^2} = \frac{2}{qLV^2}. \tag{12}$$

Since it involves q^{-1}, as expected, and also the ratio of the conduction bandwidth to the hybridization energy, it can be very large. The denominator corresponds to an effective Fermi temperature or Kondo temperature which is the characteristic energy of the system.

Next we consider the charge susceptibility, χ_c. A change in the total number of electrons in this problem is just a change in the filling parameter ϵ_0. If we calculate the second derivative of the total energy with respect to ϵ_0, the leading term comes from the change in the unhybridized term in Eq. (9), and the correction from the change in the condensation energy is small in the Kondo limit. In other words, when we make a change in the total electron density the number of f electrons will hardly change, $1-n_f$ will remain small, and the hybridized quasiparticle bands will ride with the change in filling factor. As a result the parameter F_0^s must be very large since it must cancel the large effective-mass term in Eq. (12) to give a charge susceptibility of the conduction band,

$$\chi_c = 1 \text{ and } F_0^s \approx 2/qLV^2. \tag{13}$$

This result emphasizes the many-body character of the mass enhancement and the strong residual interactions between the quasiparticles tending to suppress s-wave superconductivity.

Lastly, we turn to the magnetic susceptibility, χ_s. In the single-site problem a j-coupling scheme may be appropriate and has been widely used,[12,14] but in the periodic lattice problem it is not so obvious that the bands should be simply described in this manner. Therefore, we will use simply a constant g factor and neglect any orbital magnetic moment. The inverse of the spin susceptibility is given by the second derivative of the energy with respect to the magnetization, m. Taking the first derivative of the energy given by the expectation value of Eq. (3) we get that the magnetic field corresponding to a given value of m is

$$B = \frac{\partial}{\partial m}\langle H_{\rm eff}\rangle = \tfrac{1}{2}\{m - \tfrac{1}{2}(\mu_\uparrow - \mu_\downarrow) - \tfrac{1}{2}[(\epsilon_0 + m - E_f + \mu_\uparrow)^2 + 4L\tilde{V}_\uparrow^2]^{1/2} + \tfrac{1}{2}[(\epsilon_0 - m - E_f + \mu_\downarrow)^2 + 4L\tilde{V}_\downarrow^2]^{1/2}\}. \tag{14}$$

Note that although $\tilde{V}_\sigma$ has an important m dependence through q_0 it gives no contribution since $\langle H_{\rm eff}\rangle$ is sta-

tionary with respect to $n_{f\sigma}$ and μ_σ. However, it enters the second derivative leading to the result

$$\frac{1}{\chi_s}=\frac{2}{N_0}-\left[\frac{\partial\mu_\uparrow}{\partial m}+\frac{2qLV^2}{2L-1}\frac{\partial n_{f\uparrow}}{\partial m}\right]. \tag{15}$$

The term which includes the derivatives of μ and n_f determines another Landau parameter, F_0^a. By differentiating the minimization conditions for $\mu_\uparrow$ and $n_{f\uparrow}$, we obtain for the Wilson ratio in the Kondo limit

$$\frac{\chi_s}{\frac{1}{2}N_0}=\left[1-\frac{4L-3}{(2L-1)^2}-\frac{2L}{(2L-2)^2}\ln\frac{\epsilon_0}{qLV^2}\right]^{-1}. \tag{16}$$

First, we note that for $L=1$, $\chi_s<0$ always. Therefore the energy decreases with increasing m, i.e., the paramagnetic state is unstable towards a magnetic ordering. Our treatment is only for uniform magnetic states and the actual magnetic order will be determined by the detailed structure of the conduction-band, Ruderman-Kittel-Kasuya-Yosida interaction. For $L=1$, the paramagnetic state is stable only in other limits such as in the limit of a small n_f or in an extreme mixed-valence regime. However, when L is large the paramagnetic state can be stable ($\chi_s>0$) even in the Kondo regime. The condition is $2L\geqslant(\epsilon_0-E_f-1)/LV^2$, where we have used Eq. (10) to rewrite the logarithmic term in Eq. (15). The quantity ϵ_0-E_f-1 is the depth of the bare f level from the Fermi energy, and $\frac{1}{2}\pi LV^2$ is the width of the virtual level in the single-site problem. This ratio governs the crossover between Kondo and mixed-valence regimes. This result that orbital degeneracy is essential to stabilize the paramagnetic state agrees with the conclusions of Coleman,[15] Read, Newns, and Doniach,[4] and Yamada, Yosida, and Hanzawa.[16] Note, however, that our model is still too simple to give us a reliable criterion for real systems.

In this Letter we presented a variational approach to the periodic Anderson model in the Kondo limit. Significant intersite interaction effects are found and our results agree with single-site Kondo results only in the limit of large orbital degeneracy of the f level. A paramagnetic heavy Fermi-liquid state is stable only in this limit and for not too weak hybridization otherwise, and in particular for a doubly degenerate f level, a magnetic state is favored. The heavy Fermi-liquid state can be viewed as an almost localized Fermi liquid in which the deviation from integral valence is very small.[8] ^{3}He, on the other hand, has been succesfully described by the almost localized Fermi-liquid model by use of the limit of integral valence but with a small number of doubly occupied and empty sites.[7] This makes clear the origin of the analogy between the two systems which has been proposed previously[9] on intuitive grounds. Note that in both systems there are similar strong interactions between the quasiparticles.

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