Strong-coupling limit of the Kondo problem

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We examine the low-temperature properties of a single magnetic impurity in a metal, for an arbitrary ratio of the Kondo coupling to the bandwidth, and arbitrary band filling, using the slave-boson technique. For sufficiently strong coupling, we find that true bound states of conduction electrons and the magnetic impurity appear. Then, the corrections to χ and γ take small *negative* values. In the regime where the conduction band is nearly empty, we find a zero-temperature phase transition between a singlet binding phase and a free-local-moment phase.

The spin-$\frac{1}{2}$ Kondo single-impurity model[1] describes the interaction of a local moment and a band of conduction electrons. The Hamiltonian contains two energy scales, the conduction-electron bandwidth D and the Kondo exchange J. In the limit $J \ll D$, the low-energy physics can be expressed in terms of a single energy scale, the Kondo temperature $T_K \simeq De^{-(J/D)}$ and the thermodynamic quantities are universal scaling functions when expressed in terms of the Kondo temperature. This regime has been analyzed extensively using various renormalization-group methods,[2] Fermi-liquid theory,[3] and more recently slave-boson methods.[4–6] The limit $J \gg D$ has been discussed qualitatively by Nozières,[7] who pointed out that no universality is expected in this case and calculated χ and γ in perturbation theory in D/J. He also explained how bound states of conduction electrons and spins form in this limit, and how these results combined with the renormalization group flows can be used to understand the weak-coupling physics.

In this paper we focus on the strong-coupling limit per se, and ask how does the formation of the Nozières bound state affect the conduction electrons. We use the functional integral approach of Read and Newns[4] to obtain a description of the low-temperature properties of the Kondo Hamiltonian, which are valid for arbitrary values of J/D and the band-filling factor. This is important since, as in the two-impurity Kondo problem,[5] there are interesting physical features in the particle-hole asymmetric case that disappear in the particle-hole symmetric situation. There are several motivations for this study. The strong-coupling situation may be realized by putting a magnetic impurity in a narrow-band metallic host.

Disorder and correlations cause a band narrowing effect near the metal-insulator transition,[8] while the bare Kondo exchange is increased by the localization of the wave functions, and so the model can yield some useful insights into the physics of local moments interacting with conduction electrons near the metal-insulator transition.

The Anderson lattice model in different parameter regions describes heavy fermions (HF's) and the high-temperature superconductors (HTS's).[9] This lattice problem has been investigated with the functional integral approach. The analysis of Ref. 9 shows that the HTS's are in a regime which corresponds to strong Kondo coupling (i.e., the copper-oxygen superexchange is comparable to the oxygen bandwidth). The HF system, on the other hand, is in a weak Kondo coupling limit. It has been shown that in the weak-coupling limit the functional integral approach gives the essentially correct physics of the single impurity,[4] lending credibility to the extension of this method to treat the lattice HF problem. It is then useful to check whether the functional integral method gives also the correct strong-coupling physics (including the presence of a Nozières bound state) in the impurity limit to gauge the reliability of the natural extensions of this method to the lattice.

In this paper, we consider the N-channel Coqblin-Schrieffer Hamiltonian,[10] which represents the limit of the corresponding one-impurity Anderson model, in situations where the valence fluctuations can be ignored. This Hamiltonian is a generalization of the single-impurity Kondo model given by

$$H=\sum_{k,M}\varepsilon_k c^\dagger_{kM}c_{kM}+\frac{J}{N}\sum_{k,k',M,M'}c^\dagger_{k'M'}f^\dagger_M f_{M'}c_{kM}\ , \tag{1}$$

where c_{kM} and f_M represent the band electrons and f electrons, respectively.

The number of electrons in the localized f level is fixed to be $n_f=\sum_M f^\dagger_M f_M=Q_0$. In the original Coqblin-Schrieffer model, as considered by Read and Newns,[4] $Q_0=1$ is a constant independent of N. However, in order to obtain a truly N-independent mean-field theory which is exact at $N\to\infty$, we follow Ref. 6 and set $Q_0=N/2$. We will argue that this large-N limit captures correctly the weak- and the strong-coupling physics.

Here we use the functional integral formulation of the model problem,[4,6] to explore its behavior for arbitrary J/D and band filling. In this approach, a new field $s(\tau)$ is introduced in order to decouple the interaction term, and the constraint $n_f=N/2$ is enforced by introducing a Lagrange multiplier field $\lambda(\tau)$. After the fermions are integrated out, the fields s and λ can be determined in the saddle-point approximation (mean-field theory), where the time dependence is ignored, by finding the minimum of the effective action.

The resulting saddle-point equations can be written as

$$-\int \frac{d\varepsilon}{\pi} n_F(\varepsilon) \operatorname{Im} g_f(\varepsilon+i\eta)=\frac{1}{2}, \tag{2}$$

$$\int \frac{d\varepsilon}{\pi} n_F(\varepsilon) \operatorname{Im}[g_0(\varepsilon+i\eta) g_f(\varepsilon+i\eta)]=\frac{1}{J}, \tag{3}$$

where

$$g_f(z)=[z-\varepsilon_f-s_0^2\, g_0(z)]^{-1}, \tag{4}$$

$$g_0(z)=\sum_k [z-\varepsilon_k]^{-1}. \tag{5}$$

Here, s_0 and $i\varepsilon_f$ are the saddle-point values of the fields $s(\tau)$ and $\lambda(\tau)$, respectively, and

$$n_F(\varepsilon)=[1+\exp\{(\varepsilon-\mu)/T\}]^{-1}$$

is the Fermi function.

To make progress analytically, without losing the physics of bound-state formation, we need a simple model of a bounded density of states. We use

$$\rho(\varepsilon)=(2/\pi D^2)\Theta(D-|\varepsilon|)\sqrt{D^2-\varepsilon^2},$$

and the correspondent conduction-electron Green's function is[11,12]

$$g_0(z)=\int d\varepsilon \frac{\rho(\varepsilon)}{z-\varepsilon}=\frac{2}{z+\sqrt{z^2-D^2}}. \tag{6}$$

We consider first the particle-hole symmetric situation, i.e., $\mu=0$. Then $\varepsilon_f=0$, and we only need to consider the second saddle-point equation to determine s_0 as a function of J. The bound states appear as roots of the equation

$$\varepsilon_0=\varepsilon_f+\operatorname{Re}[s_0^2 g_0(\varepsilon_0)], \tag{7}$$

which fall outside the band. Here $\varepsilon=\varepsilon_0$ is the position of the bound state. Since $\operatorname{Re}[g_0(\varepsilon)]=(2/D^2)\varepsilon$ for $|\varepsilon|\le D$, we obtain a simple result that bound states appear for $\Delta>D$, i.e., when the resonance width exceeds the bandwidth. With the above form of $g_0(\varepsilon)$, the integrals are difficult to evaluate analytically over the whole range of parameters, but we can easily analyze the limiting cases of weak and strong coupling. At weak coupling ($J \ll D$), only a resonance of width $\Delta=\pi s_0^2\rho=D\exp\{-1/\rho J\}$ is found, in agreement with previous work. On the other hand, for strong coupling ($J \gg D$), two bound states appear at $\varepsilon=\pm\varepsilon_0$, with $\varepsilon\approx s_0$. In this limit, the saddle-point equation for s_0 reduces to $s_0=\frac{1}{2}J$ so that we find a bound (and an antibound) state at $\varepsilon\approx\pm\frac{1}{2}J$. If we recall that the Coqblin-Schrieffer model (that we consider) and the Kondo model differ by a potential scattering term of the form $H_p=-\frac{1}{4}Jn_c$, we see that the obtained bound states indeed correspond to the triplet and singlet bound states (of energies $\frac{1}{4}J$ and $-\frac{3}{4}J$, respectively) in agreement with the results of Nozières.[7]

Once the parameters ε_f and s_0 are determined, the low-temperature thermodynamic and transport properties can be determined from the saddle-point Hamiltonian, and are controlled by the scattering phase shift of the quasiparticles at the Fermi energy. The T matrix is given by $s_0^2\, g_f(\varepsilon+i\eta)$ and the phase shift takes the form

$$\delta(\varepsilon)=\arctan\left[\frac{\Delta(\varepsilon)}{\Sigma_R(\varepsilon)+\varepsilon_f-\varepsilon}\right], \tag{8}$$

where $\Delta(\varepsilon)\equiv\pi s_0^2\rho(\varepsilon)$ and $\Sigma_R(\varepsilon)\equiv\operatorname{Re}[s_0^2\, g_0(\varepsilon)]$. As an illustration, we plot $\delta(\varepsilon)$ for a half-filled band ($\mu=0$) in Fig. 1, in the limits of weak and strong coupling. Note that for strong coupling the derivative of the phase shift at the Fermi surface $\delta'(\varepsilon)$ becomes negative. This is important for thermodynamics since both the susceptibility χ and the linear coefficient of the specific heat $\gamma=C/T$ are proportional to $\delta(\varepsilon=\mu)$. In particular, for a half-filled band ($\mu=0$), we find

$$\delta'(0)=\frac{1}{Z_R(0)\Delta}, \tag{9}$$

where the renormalization coefficient Z_R is defined by

$$Z_R(\varepsilon)=\left[1-\frac{\partial}{\partial\varepsilon}\Sigma_R(\varepsilon)\right]^{-1}. \tag{10}$$

For weak coupling $Z_R(0)\approx 1$ and so $\delta'(0)\approx 1/\Delta$, and we get large positive enhancements in agreement with previous work. In the opposite limit, $Z_R(0)$

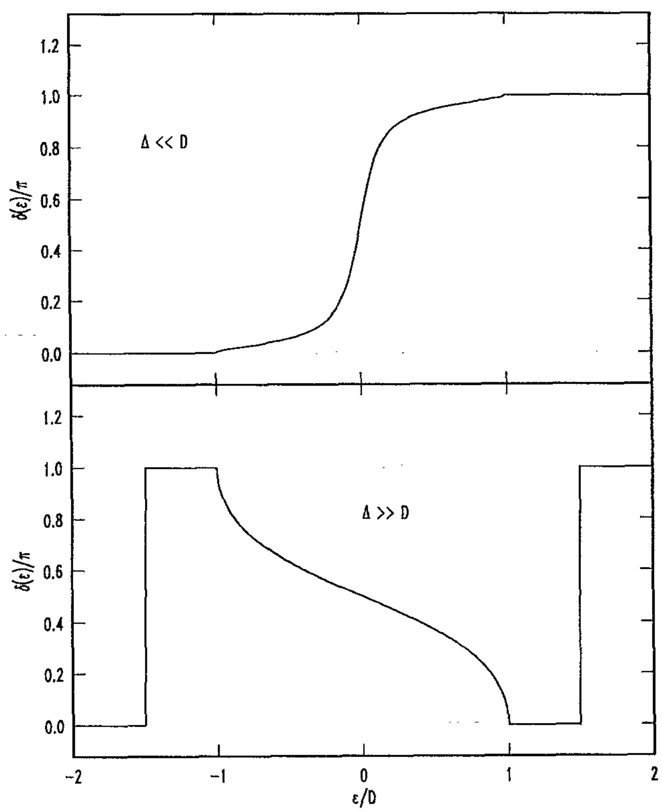

FIG. 1. Phase shift as a function of energy for the half-filled band case. The top figure depicts the situation at weak coupling where a resonance state is formed at $\varepsilon_0\approx 0$, and the phase shift changes from 0 to π as the resonance is crossed. The bottom figure shows the phase shift in the case of strong coupling where two bound states appear outside the band. Note how the slope $\delta(\varepsilon)$ assumes a negative value inside the band leading to a decrease of χ and γ.

$=(1-\Delta/D)^{-1}\approx -D/\Delta$, giving $\delta'(0)\approx -1/D$, resulting in a (small) *decrease* in χ and γ. The negative sign of $\delta'(0)$ results from the fact that Z_R *changes sign*, which for the present band-structure model and at half filling occurs precisely at bound-state formation $\Delta=D$.

Away from half filling ($\mu\neq 0$) there is no particle-hole symmetry and $\varepsilon_f\neq 0$. For arbitrary ε_f and s_0 the saddle-point equations can only be solved numerically, but we gain insight into the qualitative behavior of the solutions by considering some limiting situations. Let us begin by considering the empty band case ($\mu<-D$). At first sight, this appears to be a trivial scenario, since there are no band electrons and we expect no Kondo effect. However, at *sufficiently strong* coupling J, a bound state can form at energy $\varepsilon_0<\mu$, so that an electron from the reservoir will be "absorbed" into the bound state in order to compensate the local moment. For $\mu<-D$, only contributions from the poles of $g_0(z)$ will contribute to the integrals, and Eq. (2) gives $Z_R(0)=\frac{1}{2}$, or

$$s_0^2=\frac{-1}{\mathrm{Re}g_0'(\varepsilon_0)}, \tag{11}$$

where $g_0'(\varepsilon)\equiv(\partial/\partial\varepsilon)g_0(\varepsilon)$. Similarly, Eq. (3) gives

$$-g_0(\varepsilon_0)=2/J . \tag{12}$$

The last equation determines (implicitly) the bound-state energy ε_0 as a function of J. Since the contributions vanish unless $\varepsilon<\mu$, we find that a nontrivial solution exists only for

$$J\geq J_c(\mu)=-2/g_0(\mu) . \tag{13}$$

Otherwise, we have only the trivial solution $s_0=0$, $\varepsilon_f=\mu$ (which always exists). In order to determine the relative stability, we have also calculated the free energy of the solutions. For the nontrivial (singlet) solution, we find $(1/N)F_S=\frac{1}{2}\varepsilon_0-\mu$, and $(1/N)F_{\mathrm{LM}}=-\frac{1}{2}\mu$ for the trivial (free-local-moment) solution. Since at $J=J_c(\mu)$, the bound state is located precisely at the Fermi energy $\varepsilon_0^c=\mu$, we conclude that the two solutions have equal energy *at* the phase boundary, while the singlet solution is stable (has lower energy) at $J>J_c(\mu)$.

We note that the "excitonic order parameter" s_0, which vanishes in the free-local-moment (FLM) phase, assumes a *finite* value

$$s_0^c(\mu)=[|g_0'(\mu)|]^{-1/2} \tag{14}$$

at the transition, so that we have a *first-order* transition line. As $\mu\to -D$ (approaches the band edge), $s_0^c(\mu)\to 0$, and the first-order transition line ends at the tricritical point M, located at $\mu=-D$ and $J_M=D$. The resulting phase diagram is presented in Fig. 2.

The nature of the transition at $\mu=-D$ and $J<D$ can be elucidated by considering the case of a nearly empty band, i.e., μ infinitesimally above the band edge $-D$. The analysis of Eqs. (2) and (3) shows that in that case no bound states are found, but a resonance appears at $\varepsilon_0\approx\mu$ and of width $\Delta(\mu)\approx\delta\mu\exp\{-1/\rho(\mu)\}$, with $\delta\mu\equiv\mu+D$ being the distance from the band edge. Thus, the order parameter $s_0(\mu)\sim\sqrt{\Delta(\mu)}$ vanishes *continuously* as the band edge is approached, so for $J<D$ we have a *second-order* phase-transition line (shown by a heavy line in Fig. 2).

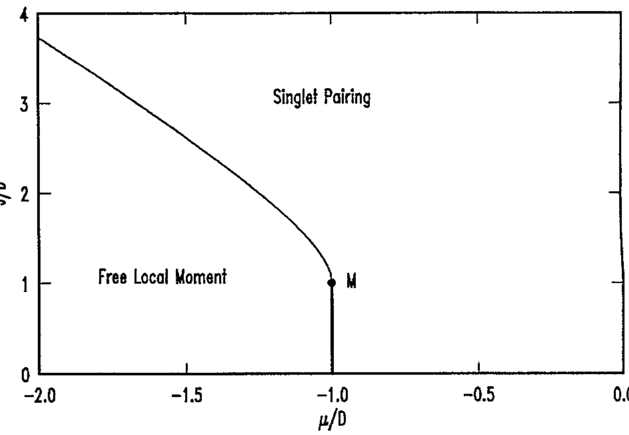

FIG. 2. Phase diagram as a function of the chemical potential μ and the impurity-electron interaction J. The phase transition separating the singlet phase and the free-local-moment phase changes from first order (discontinuous in s_0) for $\mu/D<-1$ to second order (continuous) at the tricritical point M. The phase diagram is shown only for $\mu\leq 0$ since it is symmetric (a mirror image) for $\mu\geq 0$ due to particle-hole symmetry.

The phase shift $\delta(\varepsilon)$ can assume only the values 0, $\pi/2$, or π outside the band, and we find $\delta'(\mu)=0$ in the singlet phase, signaling that χ and γ vanish (at $T=0$) in that case. In the FLM phase $\delta'(\mu)=\infty$ which is in agreement with the fact that χ and γ diverge as $T\to 0$ for free local moments. For a partially filled band ($\mu>-D$), the behavior of χ and γ is qualitatively similar as at half filling, with large positive enhancements at weak coupling and small negative corrections in the strong-coupling limit.

It is interesting to note that even in the empty band singlet phase, where χ and γ vanish at $T=0$, we can expect *large* positive corrections at finite temperatures of the order

$$T_K^{\mathrm{eff}}=F_{\mathrm{LM}}-F_S . \tag{15}$$

Since $T_K^{\mathrm{eff}}\to 0$ as $J\to J_c(\mu)$, we find an effective Kondo temperature that vanishes everywhere along the transition line separating the singlet and the local-moment phase. This result is surprising, since the transition occurs at $J_c(\mu)\leq D$, i.e., at intermediate or strong coupling where the Kondo exchange is large. In a system with a finite concentration of impurities we expect a phase transition between two different insulating phases, one having a Curie-like susceptibility, and the other a Pauli value. We propose to look for this effect in II-IV-based magnetic semiconductor heterostructures, where the two-dimensionality provides a finite density of states at the bottom of the band.

In summary, we have examined the behavior of a single magnetic impurity in a metal, for general electron-impurity interaction, using a large-N slave-boson approach. In the weak-coupling limit this approach was known to give the main features of the exact solution:

large enhancements of the specific heat and magnetic susceptibility, and resonant scattering at the Fermi level. In contrast, we have shown here that for sufficiently strong coupling, true bound states of conduction electrons and the magnetic impurity appear, while the corrections to χ and γ change sign to take up small *negative* values. As the empty band limit is approached, we find additional phase transitions separating the singlet binding phase from the free-local-moment phase. The effective Kondo temperature T_K^{eff} is found to vanish everywhere along the transition line, although this can occur at arbitrarily strong coupling.

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