Kondo effect in Fermi systems with a gap: A renormalization-group study

Kan Chen
Department of Computational Science, National University of Singapore, Singapore 119260

C. Jayaprakash
Department of Physics, The Ohio State University, Columbus, Ohio 43210

(Received 26 June 1997)

We present the results of a Wilson renormalization-group study of the single-impurity Kondo and Anderson models in a system with a gap in the conduction-electron spectrum. The behavior of the impurity susceptibility and the zero-frequency response function, $T\langle\langle S_z;S_z\rangle\rangle$ are discussed in the cases with and without particle-hole symmetry. For the case of no particle-hole symmetry, we find a transition, as the bandgap Δ increases, from a singlet ground state (when $\Delta \ll T_K$, where T_K is the Kondo temperature) to a doublet ground state (when $\Delta \gg T_K$). But there is no such transition for the case with particle-hole symmetry: the ground state is always a doublet. In addition, for the asymmetric Anderson model the correlation functions, $\langle \vec{S}\cdot\vec{\sigma}(0)\rangle$, $\langle n_d\rangle$, and $\langle n_d(2-n_d)\rangle$ are computed. [S0163-1829(98)05205-9]

I. INTRODUCTION

The properties of a magnetic impurity in a semiconductor or an insulator are of interest for a variety of reasons. In a normal Fermi system a spin-$\frac{1}{2}$ impurity yields logarithmic temperature dependences in the impurity susceptibility and the resistivity at high temperatures; at low temperatures the magnetic moment is quenched.[1,2] The existence of a sharp Fermi surface and the concomitant occurrence of (low-energy) particle-hole pairs play an important role in understanding the behavior of the model. Thus it is interesting from a theoretical point of view to understand whether the Kondo effect persists and under what conditions quenching occurs in a system with a gap and determine the behavior quantitatively. We also note that the Anderson impurity has been studied in the context of the logarithmic temperature dependence of the conductivity of trans-polyacetylene;[4] the system was modeled by a continuum Hamiltonian proposed by Takayama, Lin-Liu, and Maki[5] that exhibits a gap due to Peierls distortion. The impurity model was investigated using a Hartree-Fock closure of the equation of motion. In addition, a variety of Kondo and valence fluctuating insulators (modeled theoretically by a Kondo or Anderson lattice) such as SmB_6 and $Ce_3Bi_4Pt_3$ among others provide another motivation for studying the single-impurity problem in a system with a gap.

In this paper we present the results of our study of the Kondo and Anderson impurities in a system with a gap. We apply Wilson's (numerical) renormalization-group (RG) technique using a variant of a numerical tridiagonalization method devised by us earlier[6] and provide results for both the susceptibility and zero-frequency response functions. We also discuss a simple effective Hamiltonian that allows us to understand the physics underlying our results.

We begin with a summary of previous work on the problem; in the next section we provide a brief sketch of the technique that is described in detail in the literature;[3] in the following section we describe the results of our numerical calculations, and in the final section we discuss the effective Hamiltonian description of our results.

We begin with a brief overview of previous work. The calculations were done by Ogura and Saso[9–11] and Takegahara *et al.*[12,13] Ogura and Saso used a $1/N$ expansion of the degenerate Anderson model and found a transition to leading order in $1/N$: the ground state was a triplet (magnetic) when the gap E_g was greater than twice the Kondo temperature T_K and a nonmagnetic singlet for smaller gaps. In their quantum Monte Carlo (QMC) simulations they found indications of a similar transition even for the symmetric Anderson model;[9] for the asymmetric model they obtained a transition between the different ground states at approximately $E_g \approx 3T_K$. We note that their QMC computations were limited to temperatures above $T_K/10$.

Takegahara, Shimizu, and Sakai[12,13] used both quantum Monte Carlo simulations and the numerical renormalization-group method of Wilson. They considered the symmetric Anderson model and found that at low temperatures the susceptibility follows a Curie law resulting from an unquenched magnetic moment. They observed the crucial difference between symmetric and asymmetric Anderson models cases; when particle-hole symmetry is obeyed the moment remains unquenched for all nonzero values of the gap, while there is a transition in the asymmetric case. They also used the Wilson numerical renormalization group to follow the spectrum of the low-energy states but not the susceptibility. It is difficult to use their version of the numerical RG formulation to calculate low-temperature (much less than the band gap) properties of the model.

The importance of the particle-hole symmetry breaking has been emphasized recently[14] in the context of the Kondo problem with a pseudogap.[8] In this work the impurity susceptibility for the case of a Kondo system with a gap was also calculated using the Wilson renormalization-group method: in the particle-hole symmetric case the impurity retains its moment in the ground state for all J; in the presence of potential scattering the moment is completely quenched provided that $\Delta \ll T_K$. These results are in agreement with those of Takegahara *et al.*[12,13] However, Yu and Guerrero[15],

who studied an Anderson impurity in a semiconducting host using the density-matrix renormalization technique, found no *qualitative difference* between the symmetric and asymmetric cases. Their calculation which is restricted to $T=0$ also considered electron spin-impurity spin-correlation functions. We will comment on this point later.

We have made a comprehensive study of the Kondo and Anderson models in gapped systems with and without particle-hole symmetry breaking using the numerical RG method. Our RG formulation is based on the numerical tridiagonalization technique developed by us,[6] which allows us to calculate various quantities in the entire temperature range. We report results for a zero-frequency response function, correlation functions, and the susceptibility: we emphasize the differences in their behaviors in the various regimes and clarify which of these are good probes of the nature of the low-temperature fixed-point behavior.

II. WILSON'S RG FORMULATION

We consider the Kondo and Anderson models with a conduction-electron Hamiltonian with the density of states $\rho(\epsilon)$; as a function of the energy ϵ, ρ is a constant for $D_0 > |\epsilon| > \Delta_0$, where the band edges lie at $\pm D_0$ from the Fermi level which is chosen to be in the middle of the gap. The width of the gap is thus $2\Delta_0$. The Hamiltonian for the spin $-\frac{1}{2}$ Kondo problem with the impurity spin denoted by $\vec{S}$ is given in standard notation by

$$H_K=\sum_{\mu}\int_{-D_0}^{D_0} d\epsilon\rho(\epsilon)\epsilon c^{+}_{\epsilon,\mu}c_{\epsilon,\mu}-J\sum_{\mu,\nu}\int_{-D_0}^{D_0} d\epsilon\sqrt{\rho(\epsilon)}\int_{-D_0}^{D_0} \times d\epsilon'\sqrt{\rho(\epsilon')}\vec{S}\cdot c^{+}_{\epsilon,\mu}\frac{1}{2}\vec{\sigma}_{\mu\nu}c_{\epsilon',\nu} +K\sum_{\mu}\int_{-D_0}^{D_0} d\epsilon\sqrt{\rho(\epsilon)}\int_{-D_0}^{D_0} d\epsilon'\sqrt{\rho(\epsilon')}c^{+}_{\epsilon,\mu}c_{\epsilon',\mu}, \quad (1)$$

where the K term describes potential (spin-independent) scattering of the conduction electrons at the impurity site and J is negative (antiferromagnetic coupling). $c^{+}_{\epsilon,\mu}$ refers to a conduction-electron s-wave state about the impurity of energy ϵ. In this truncation of the original Hamiltonian the low-energy states that determine the low-temperature properties are well sampled. For the Anderson model we have

$$H_A=\sum_{\mu}\int_{-D_0}^{D_0} d\epsilon\rho(\epsilon)\epsilon c^{+}_{\epsilon,\mu}c_{\epsilon,\mu}+\left(\epsilon_d+\frac{U}{2}\right)\sum_{\mu} c^{+}_{d\mu}c_{d\mu} +\frac{U}{2}\left(\sum_{\mu} c^{+}_{d\mu}c_{d\mu}-1\right)^2+\sum_{\mu}\int_{-D_0}^{D_0} d\epsilon\sqrt{\rho(\epsilon)}[Vc^{+}_{\epsilon,\mu}c_{d\mu} +V^{*}c^{+}_{d\mu}c_{\epsilon,\mu}], \quad (2)$$

where $c^{+}_{d\mu}$ creates an electron with spin μ at the impurity placed at the origin. The choice $K=0$ in the Kondo problem and $\epsilon_d+U/2=0$ in the Anderson model correspond to particle-hole symmetry.

Following Wilson we perform a *logarithmic* discretization of the energy variable; we rescale the energy by D_0 so that $\epsilon\in[-1,1]$, introduce a scale factor $\Lambda(>1)$, and define the nth interval for positive ϵ to lie between Λ^{-n-1} and Λ^{-n}. The band gap (in units of the bandwidth) is chosen to be

$$\Delta=\Lambda^{-M_0}. \quad (3)$$

Next we replace the continuous set of energy levels in the nth interval $[\Lambda^{-n-1},\Lambda^{-n}]$ and $[-\Lambda^{-n},-\Lambda^{-n-1}]$ by single levels at $(\Lambda^{-n-1}+\Lambda^{-n})/2$ and $-(\Lambda^{-n}+\Lambda^{-n-1})/2$, respectively, and denote the conduction-electron creation operators for the states with the corresponding energies $(\Lambda^{-n-1}+\Lambda^{-n})/2$ and $-(\Lambda^{-n-1}+\Lambda^{-n})/2$ by $a^{+}_{n\mu}$ and $b^{+}_{n\mu}$, respectively. After this discretization, the Anderson Hamiltonian can be rewritten in the following form[3] [a similar (RG) formulation can be written down for the Kondo Hamiltonian]

$$H_A=\frac{1+\Lambda^{-1}}{2}\sum_{m=0}^{M_0-1}\Lambda^{-m}(a^{+}_{m\mu}a_{m\mu}-b^{+}_{m\mu}b_{m\mu}) +\left(\epsilon_d+\frac{1}{2}U\right)c^{+}_{d\mu}c_{d\mu}+\left[\frac{2\Gamma}{\pi}\right]^{1/2}(f^{+}_{0\mu}c_{d\mu}+c^{+}_{d\mu}f_{0\mu}) +\frac{U}{2}(c^{+}_{d\mu}c_{d\mu}-1)^2, \quad (4)$$

where

$$f_{0\mu}=\sqrt{\frac{1-\Lambda^{-1}}{2(1-\Delta)}}\sum_{m=0}^{M_0-1}\Lambda^{-m/2}(a_{m\mu}+b_{m\mu})$$

is a normalized electron annihilation operator that corresponds to the most localized state that can be formed with the states which have been retained. The initial values of the couplings, the level width of the impurity orbital due to the mixing term denoted by $\Gamma\equiv\pi\rho|V|^2$, ϵ_d, and U, are now in units of D_0 (taken to be one); the gap in the density of states is between Δ and $-\Delta$.

We next re-express the Hamiltonian in terms of the Wilson basis set $\{f_n, n=0,1,\ldots\}$ that consists of a hierarchy of states from the most localized, high-energy state directly coupled to the impurity, f_0, defined above to progressively more spatially extended low-energy states that are orthogonal to each other and such that the free-electron part of the Hamiltonian has only nearest-neighbor coupling. We use the (numerical) tridiagonalization scheme devised by us earlier[6] to perform such a transformation of the Hamiltonian to the following tridiagonalized form:

$$H_A=\frac{1+\Lambda^{-1}}{2}\sum_{n=0}^{N_0-1}[\xi_n(f^{+}_{n\mu}f_{n+1\mu}+\text{H.c.})] +\left(\epsilon_d+\frac{1}{2}U\right)c^{+}_{d\mu}c_{d\mu}+\left[\frac{2\Gamma}{\pi}\right]^{1/2}(f^{+}_{0\mu}c_{d\mu}+c^{+}_{d\mu}f_{0\mu}) +\frac{U}{2}(c^{+}_{d\mu}c_{d\mu}-1)^2, \quad (5)$$

where $N_0=2M_0-1$. The coefficients $\{\xi_n\}$ are determined from the tridiagonalization procedure.

In order to carry out the RG calculation, we need to rescale the Hamiltonian at each iteration step. The rescaling is done by defining H_N as follows:

$$H_N=\frac{1}{\xi_{N-1}}\left[\sum_{n=0}^{N-1}[\xi_n(f_{n\mu}^{+}f_{n+1\mu}+\text{H.c.})]\right]$$
$$+\frac{1}{\xi_{N-1}}[(\tilde{\epsilon}_d+\tilde{U})c_{d\mu}^{+}c_{d\mu}+\tilde{\Gamma}^{1/2}(f_{0\mu}^{+}c_{d\mu}+c_{d\mu}^{+}f_{0\mu})$$
$$+\tilde{U}(c_{d\mu}^{+}c_{d\mu}-1)^2], \quad (6)$$

where $\tilde{\epsilon}=[2/(1+\Lambda^{-1})]\epsilon_d$, $\tilde{U}=U/(1+\Lambda^{-1})$, $\tilde{\Gamma}=[2/(1+\Lambda^{-1})]^2 2\Gamma/\pi$, and the rescaling factor is $S_N=2/(1+\Lambda^{-1})\xi_{N-1}$.

The recursion relation can be written in the following compact form:

$$H_{N+1}=\frac{\xi_{N-1}}{\xi_N}H_N+(f_{N\mu}^{+}f_{N+1\mu}+\text{H.c.}).$$

This recursion relation enables one to set up an iterative diagonalization scheme to calculate the energy levels of H_N and thus to determine thermodynamic properties; the recursion is implemented numerically and is stopped at $N=N_0$ corresponding to the edge of the gap below which there are no conduction-electron states. Recall that as we increase N, the system effectively evolves from high temperatures to low temperatures. At a given N, the thermodynamic quantities are calculated for $T_N=1/(\overline{\beta}S_N)$ for selected values of $\overline{\beta}$. By studying the evolution of the many-body energy level structures we also obtain information near the fixed points of the Hamiltonian.

For $N<N_0$, the thermodynamic quantities are calculated for $T_N=1/(\overline{\beta}S_N)$ for a selected value of $\overline{\beta}$; the accuracy of the numerical evaluations is enhanced by performing a second-order perturbation calculation by writing the Hamiltonian as

$$H_A=(H_N+H_I+H_B)/S_N,$$

where

$$H_I=\frac{\xi_N}{\xi_{N-1}}(f_{N\mu}^{+}f_{N+1\mu}+\text{H.c.}),$$

and

$$H_B=\frac{1}{\xi_{N-1}}\left\{\sum_{n=N+1}^{N_0-1}[\xi_n(f_{n\mu}^{+}f_{n+1\mu}+\text{H.c.})]\right\}.$$

For $N=N_0$, the thermodynamic quantities are calculated for a sequence of temperatures $\{T_l\}$. Since H_{N_0} is the full Hamiltonian (hence, no second-order perturbation is needed), we can calculate the quantities at temperatures much lower than typical energy scale at $N=N_0$, which is the bandgap Δ. We choose T_l to be a sequence of values from 0.175 of the maximum energy kept in the many-body states of H_{N0} to 0.000175 of the maximum energy. Thus the thermodynamic quantities at low temperatures are calculated with the ''effective Hamiltonian'' H_{N_0}.

III. RESULTS

We present the results obtained from our numerical calculations for the two models.

A. Kondo model

Our calculations were performed using a scale factor of $\Lambda=2$ and a band-gap energy $\Delta=1.22\times10^{-4}$ corresponding to $M_0=13$ [see Eq. (3)]. We denote the bare values of the Kondo coupling and the potential scattering in units of the bandwidth D_0 by J_0 and K_0, respectively. The first and obvious quantity to consider is the impurity susceptibility, χ, which we emphasize is defined as the total susceptibility of the system minus the susceptibility of the pure system. For *any* finite (>0) band gap in the Kondo problem without potential scattering $T\chi$ approaches the value 1/4 as $T\to0$. The ground state is a magnetic doublet, its quantum numbers are ($Q_T=0, S_T=1/2$) where Q_T is the total charge of the system defined at the Nth iteration as

$$Q_T=\sum_{n=0}^{N}\sum_{\mu}(f_{n\mu}^{+}f_{n\mu}-1).$$

This is in agreement with the results of Takegahara *et al.*[13] for the symmetric Anderson model. The susceptibility curves as a function of temperature are displayed in Fig. 1(a). Note that some data obtained at intermediate points have been suppressed for clarity in this figure as well as in other figures we are going to present in this paper. The calculation is done for initial values of the coupling, given by $J_0=-0.1,-0.2,-0.3,-0.4,-1.0$. Recall that for the Kondo impurity in a free-electron metal $k_BT\chi_{\text{imp}}$ (the ''effective'' moment of the impurity) is a universal function of T/T_K (for $k_BT\ll D_0$) that goes to zero as $T\to0$. Note that for large values of $|J|$, $k_BT\chi$ in the gapped case follows this universal shape of the ordinary Kondo problem at high temperatures as is evident in the figure, but below temperatures of the order of the gap $T\chi$ increases sharply reflecting the doublet ground state.

The effect of particle-hole symmetry breaking introduced by potential scattering is very important as has been noted before.[14,12] The results for $T\chi$ are displayed in Fig. 1(b). For $K_0=0.1$ and $J_0=-0.2$ ($T_K\approx7.4\times10^{-6}\ll\Delta$), $T\chi$ again goes to 1/4 as T goes to zero. For stronger Kondo coupling, $J_0=-0.4$ ($T_K\approx2.1\times10^{-3}\gg\Delta$), the impurity spin is quenched and $T\chi\to0$. There is a discontinuous (''first-order'') transition at Δ_c (which depends on T_K and K_0) due to a crossing of energy levels as Δ varies (or equivalently as Δ_c varies for fixed Δ). We will argue later using our effective Hamiltonian that Δ_c is of the order of K_0T_K; thus there is a transition for any nonzero potential scattering.

We have also calculated the zero-frequency, (impurity-spin) response function $\langle\langle S_z;S_z\rangle\rangle$ defined by

$$\langle\langle S_z;S_z\rangle\rangle=\int_0^{\beta}\langle S_z(\tau)S_z(0)\rangle d\tau, \quad (7)$$

and $S_z(\tau)$ is the impurity-spin Heisenberg operator in imaginary time. Note that since S_z does not commute with the Hamiltonian (only the z component of the *total* spin does) this does not correspond to a simple correlation function. Recall that the susceptibility is given by

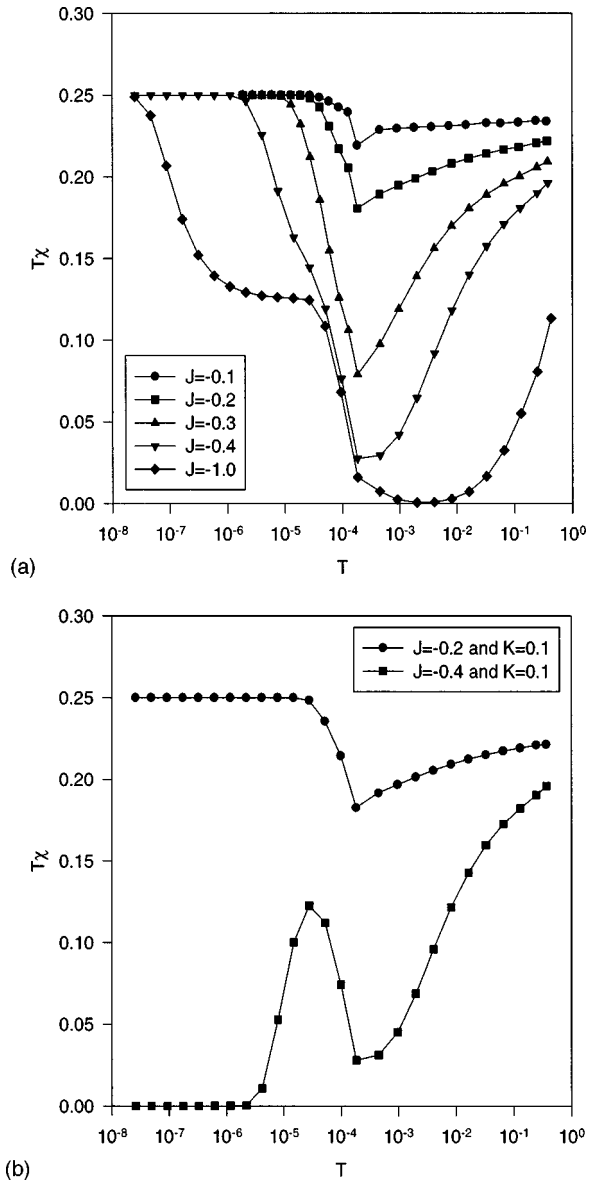


FIG. 1. $T\chi_{\rm imp}$ plotted as a function of T for the Kondo problem. The gap energy is $\Delta=1.22\times10^{-4}$. (a) The potential scattering is absent ($K=0.0$). The values of the coupling J used are -0.1, -0.2,-0.3,-0.4, and -1.0. Note that as $T\to0$, $T\chi$ approaches 1/4. (b) Particle-hole symmetry breaking is present ($K=0.1$). Note that for $J=-0.4$, $T\chi$ goes to zero, while for $J=-0.2$, it approaches 1/4.

$$T\chi=\langle\langle S_z^{\rm tot};S_z^{\rm tot}\rangle\rangle,$$

where $S_z^{\rm tot}$ is the z component of the total spin, the sum of the impurity, and the conduction-electron contributions. The techniques for calculating $\langle\langle S_z;S_z\rangle\rangle$ have been explained in an earlier paper for the ordinary Kondo problem.[7] We used $\Lambda=3.0$ in the calculation of the response function. For the ordinary Kondo problem with a constant density of states $\langle\langle S_z;S_z\rangle\rangle$ is essentially the same as the impurity susceptibility χ for small values of the initial coupling J_0.[7] However, for the density of states with a gap, $\langle\langle S_z;S_z\rangle\rangle$ and χ behave quite differently at low temperatures (when $T<\Delta$). In the absence of potential scattering, in contrast to $T\chi$ which approaches a fixed value of 1/4 as $T\to0$, $T\langle\langle S_z;S_z\rangle\rangle$ approaches a value C_0 which depends on the band gap; this persists also when the moment is not quenched in the presence of potential scattering. The results for C_0 are listed in Table I. For $K=0$ our results are consistent with the value C_0 being proportional to Δ^2 for $\Delta\ll T_K$. We will derive this result from our effective Hamiltonian description in the next section. This result agrees with the claim made by Takegahara *et al.* for the susceptibility;[12] we note that they appear to have identified $\langle\langle S_z;S_z\rangle\rangle$ with the impurity susceptibility. In the presence of potential scattering when Δ is increased for fixed T_K the ground state changes abruptly from a singlet $[(Q_T=-1,S_T=0)]$ to a doublet. The value of $T\chi$ jumps from 0 to 1/4 and correspondingly the value of C_0 also jumps discontinuously.

TABLE I. The values of $T\langle\langle S_z;S_z\rangle\rangle$ at zero temperature for a range of values of the band gap. The numbers enclosed in the parentheses are the total charge Q_T and spin S_T of the ground state.

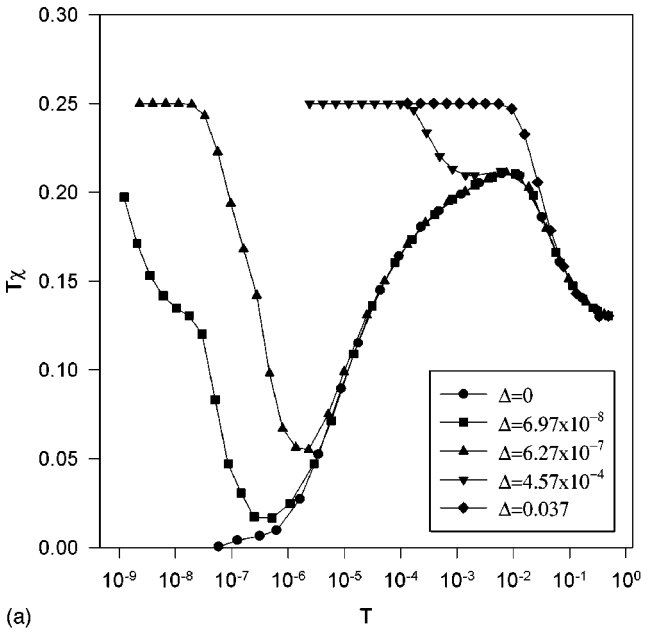
Δ	$J_0=-0.2,\ K=0.0$	$J_0=-0.2,\ K=0.1$
1.88×10^{-6}	0.0398 (0, 1/2)	0.0490 (0, 1/2)
6.27×10^{-7}	0.00797 (0, 1/2)	0.0110 (0, 1/2)
2.09×10^{-7}	0.00101 (0, 1/2)	$<1.2\times10^{-5}$ (−1, 0)
6.96×10^{-8}	0.000115 (0, 1/2)	$<4.0\times10^{-6}$ (−1, 0)

B. Anderson model

The calculations for the Anderson model were performed with the parameter $\Lambda=3$. A range of values was used for the band gap $\Delta=\Lambda^{-M_0}$: the value of M_0 was varied between 3 and 19.

For the symmetric Anderson model, with $U=0.1$, $\epsilon_d=-U/2=-0.05$, and $\Gamma=0.006$, $T\chi$ reaches the value of 1/4 as zero temperature is approached irrespective of the value of the band gap Δ, signaling a doublet ground state and an unquenched impurity moment. If $\Delta\ll T_K\approx5.12\times10^{-6}$, $T\chi$ first decreases toward zero along the universal Kondo curve; however, when $T<\Delta$, it rises to 1/4 as T goes to zero. If Δ is comparable or larger than T_K, on the other hand, $T\chi$ gradually increases to 1/4. Our results for $T\chi$ are displayed in Fig. 2(a).

The case of the the asymmetric Anderson model was studied using the parameter values $U=0.1$, $\epsilon_d=-0.0001$, and $\Gamma=0.00015$, and the results are displayed in Fig. 2(b). When $\Delta=0$, recall that the system can go through different regimes, the free-orbital regime, the mixed-valence regime, the local-moment regime, and the frozen moment regime[3] as a function of the temperature depending on the parameters: the free-orbital regime is characterized by the impurity degree of freedom being effectively decoupled from the conduction electrons; in the mixed-valence regime that occurs when $-\epsilon_d\ll U$ in the temperature range $U\gg k_BT\gg-\epsilon_d$, the doubly occupied state is thermally depopulated, while the $n_d=0$ and $n_d=1$ states are effectively degenerate and $\langle n_d\rangle$ is fractional; the behavior as the temperature is lowered in this case depends on the values of $-\epsilon_d$ and Γ; if $-\epsilon_d\gg\Gamma$ the $n_d=0$ state becomes depopulated thermally as the temperature drops below $-\epsilon_d$ and the impurity develops a local magnetic moment and this is referred to as the local-moment regime; now the Kondo coupling that arises due to the virtual



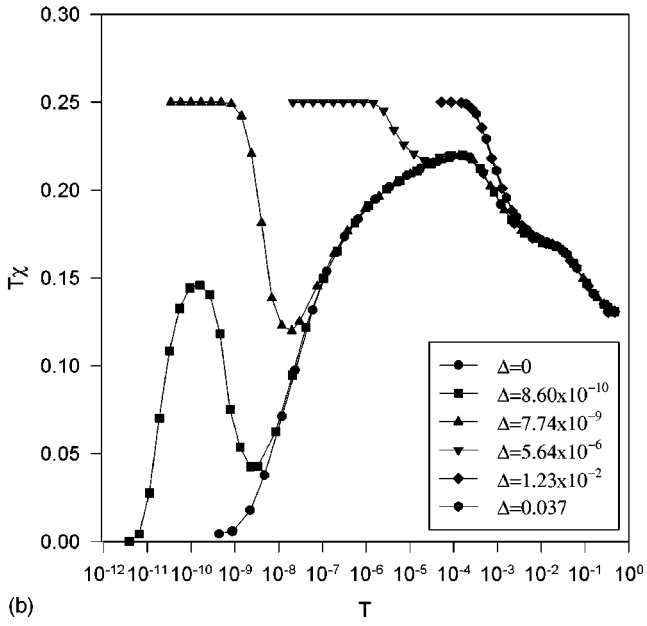


FIG. 2. $T\chi_{\rm imp}$ plotted as a function of T for the Anderson model. (a) Symmetric Anderson model with $U=0.1$, $\epsilon_d=-0.05$, and $\Gamma=0.006$. Note that as $T\rightarrow 0$, $T\chi$ approaches 1/4. (b) Asymmetric Anderson model with $U=0.1$, $\epsilon_d=-0.001$, and $\Gamma=0.00015$. Note that as $T\rightarrow 0$, $T\chi$ approaches 1/4 if $\Delta\gg T_K$ and 0 if $\Delta\ll T_K$. The values for the gap energy Δ used in the calculations are shown in the legends of the figures.

transitions from the $n_d=1$ subspace to the $n_d=0$ subspace leads eventually to the quenching of the magnetic moment by the Kondo effect below the Kondo temperature. The last regime is dubbed the frozen-impurity regime; note that this regime also includes the case when the ground state has no moment because ϵ_d is positive and no moment develops because the $n_d=0$ state is thermally favored. When $\Delta\neq 0$, for $T>\Delta$, the $T\chi$ curve initially follows the curve for $\Delta=0$ as the temperature is lowered. When T drops below Δ, $T\chi$ curves starts to rise. For $\Delta\gg T_K$, the curve continues to rise to 1/4 as T goes to zero. On the other hand, when $\Delta\ll T_K$,

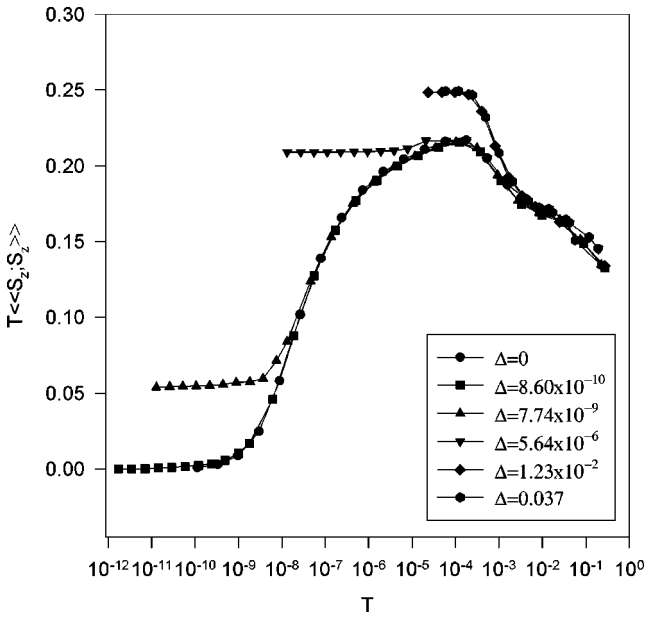


FIG. 3. The zero-frequency response function $T\langle\langle S_z;S_z\rangle\rangle$ plotted as a function of T for the asymmetric Anderson model with $U=0.1$, $\epsilon_d=-0.001$, and $\Gamma=0.00015$. Note the qualitative differences between $T\langle\langle S_z;S_z\rangle\rangle$ and $T\chi$ at low temperatures.

the curve stops rising, turns over and tends to zero as $T\rightarrow 0$, i.e., the moment is quenched. This behavior is clearly similar to that of the $K\neq 0$ case of the Kondo model.

In Fig. 3 we show the temperature dependences of the zero-frequency response function $T\langle\langle S_z;S_z\rangle\rangle$ for the asymmetric case. There is no qualitative difference in the behavior of the response function $T\langle\langle S_z;S_z\rangle\rangle$ between the Kondo and Anderson models. In the symmetric case where the ground state is characterized by $(Q_T=0,S_T=1/2)$, we again found that the zero-temperature value is proportional to Δ^2 when Δ decreases. Also for the asymmetric case C_0 jumps discontinuously as the ground state changes from a singlet to a doublet as Δ is increased.

In addition, we have also computed the following correlation functions: $\langle\vec{S}\cdot\vec{\sigma}(0)\rangle$, $\langle n_d\rangle$, and $\langle n_d(2-n_d)\rangle$. Representative figures are shown in Figs. 4(a) and 4(b). Here the main point to be emphasized is that once there are no charge fluctuations (for example, when the system approaches the local-moment regime, or when $T<\Delta$) the correlation functions do not change and approach constant values. In particular, when the local-moment regime is reached (Δ is less than the temperature for the local-moment formation), the correlation functions tend to the same constants as $T\rightarrow 0$ independent of the band gap. While the mixed-valence regime is still reflected in the temperature dependence of the correlation functions, the Kondo effect does not show up in the correlation functions. This point is not very well appreciated. One simply *cannot* investigate the Kondo effect using *local* correlation functions, such as the impurity-spin conduction-electron spin density at the origin, since they do not contain information about the system on the energy scale of T_K: the main contributions to the local correlations come from the high-energy degrees of freedom, and the contribution from many-body effects at the low-energy scale T_K to the correlation functions is small as has been shown in our earlier

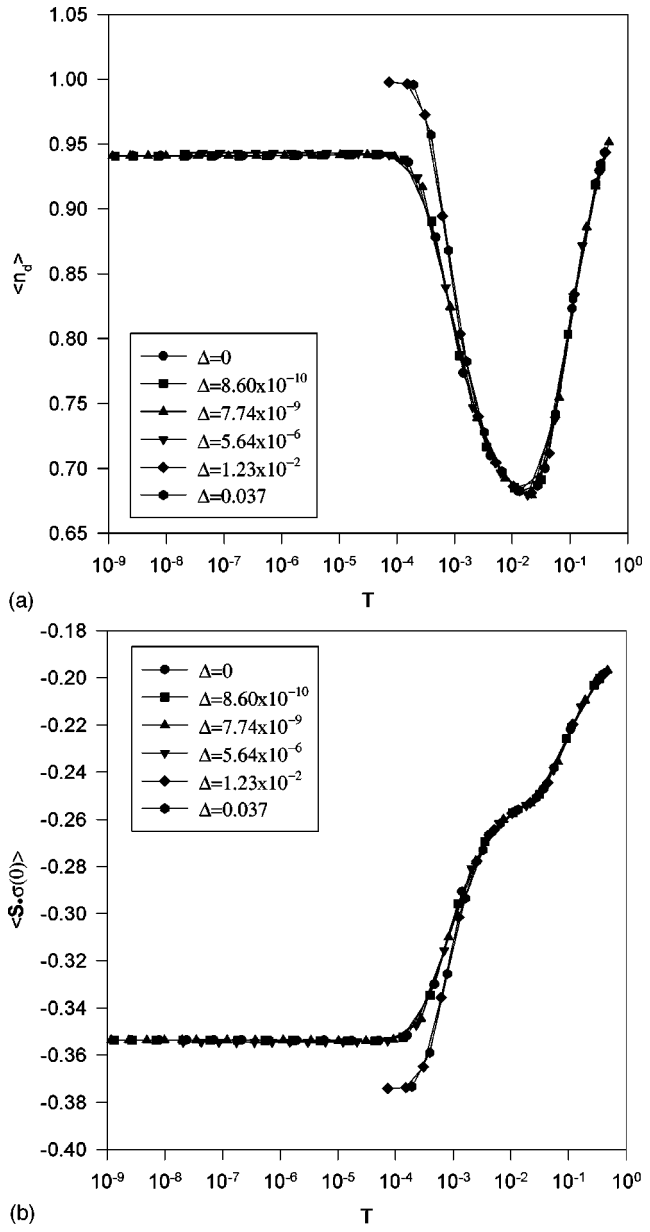


FIG. 4. The local correlation functions: (a) $\langle n_d \rangle$ and (b) $\langle \vec{S} \cdot \vec{\sigma}(0) \rangle$, plotted as a function of T for the asymmetric Anderson model with $U=0.1$, $\epsilon_d=-0.001$, and $\Gamma=0.00015$. Note that when $\Delta \ll T_K$, the correlation functions approach constant values independent of Δ as $T \to 0$.

paper in Ref. 7. Our calculation of the correlation functions and the average electron number at the impurity orbital $\langle n_d \rangle$ show general trends in agreement with Yu and Guerrero. However, we find that the local spin-spin correlation functions and $\langle n_d \rangle$ are not sensitive to the breaking of particle-hole symmetry (for fixed T_K and Δ) and behave similarly even though the nature of the ground state is different.

We point out that there is a difference between our ground state and the ground state obtained in Yu and Guerrero for the symmetric case. We obtained a doublet, as did Ogura and Saso and Takegahara *et al.*, while Yu and Guerrero obtained a singlet. This may be due to differences in the Hamiltonian, in particular, to the fact that the impurity does not correspond to an additional degree of freedom in Yu and Guerrero.[15]

Finally, we present our results for the mixed-valence regime. We considered the asymmetric Anderson model, with $U=0.1$, $\epsilon_d=-0.025$, and $\Gamma=0.01$. When $\Delta=0$, the system goes from the free-orbital regime through the mixed-valence regime directly to the frozen moment regime, without going through the local-moment regime. The results for the susceptibility, $\langle n_d \rangle$, and $T\langle\langle S_z;S_z \rangle\rangle$ are shown in Figs. 5(a)–5(c). Again, depending on the value of the band gap, $T\chi$ can go to zero or 1/4 (there is a sharp transition). For the cases that $T\chi$ goes to zero, $T\langle\langle S_z;S_z \rangle\rangle$ also goes to zero, and all correlation functions approach constants, which are independent of the band gap. But for the cases that $T\chi$ goes to 1/4, both $T\langle\langle S_z;S_z \rangle\rangle$ and the correlation functions approach values which are band-gap dependent.

IV. EFFECTIVE HAMILTONIAN DESCRIPTION

In this section we provide a simple interpretation of the low-temperature behavior of the models in the various regimes on the basis of a simple effective Hamiltonian. Let us consider first the Kondo model with the gap in the conduction-electron density of states between $-\Delta$ to Δ. The initial couplings are J_0 and K_0 in units of the bandwidth D_0, which is taken to be unity. In our RG calculation, the band gap is taken to be $\Delta=\Lambda^{-M_0}$, where M_0 is an integer; this corresponds to the maximum N being $N_0=2M_0-1$—there are an even number of conduction-electron levels in the discretized system.

Imagine that we have successively integrated out the high-energy degrees of freedom and arrived at the effective Hamiltonian at the energy scale $\Delta \equiv \Lambda^{-(N_0+1)/2}$; as we pointed out earlier the iterative RG procedure cannot be carried beyond this energy scale corresponding to the maximum iteration number N_0 since there are no conduction-electron states left. The low-temperature properties (i.e, for $T \ll \Delta$) can be calculated with this effective Hamiltonian.

Let us first consider the case when $\Delta \gg T_K$. Recall that in this case the nonperturbative, numerical RG calculations showed that the ground state was a doublet both in the presence and absence of potential scattering. The effective Hamiltonian is close to that of the $J=0$ fixed point (the increase in the magnitude of the marginal variable $\tilde{J}=J/\Delta$ is small as the scaling is performed only down to $\Delta \gg T_K$) and can be written, keeping the leading-order terms, as

$$H_{\text{eff}}=-J\vec{S}\cdot\vec{\sigma}(0)+Kf_\mu^+ f_\mu+\Delta(a_\mu^+ a_\mu-b_\mu^+ b_\mu).$$

Here $\vec{\sigma}(0)=\frac{1}{2}f_\mu^+\vec{\sigma}_{\mu\nu}f_\nu$ and $f_\mu=1/\sqrt{2}(a_\mu+b_\mu)$. In the above effective Hamiltonian we have only kept the lowest single electron/hole levels of the conduction-electron Hamiltonian; these are represented by the creation operators a_μ^+ and b_μ^+ and we have neglected the irrelevant operators. Since f_0 is proportional to $\Lambda^{-N_0/4}$, we have[1]

$$f_{0\mu}=\alpha_0\Lambda^{-N_0/4}(a_\mu+b_\mu)+\cdots.$$

Thus the first two terms of H_{eff} are marginal, and J and K must scale as $J=J_0\Delta$ and $K=K_0\Delta$. This can also be understood in the perturbative RG language as follows. The effective Hamiltonian $\mathcal{H}(D)$ at the energy scale $D \gg T_K$, with renormalized couplings J and K, is obtained by integrating

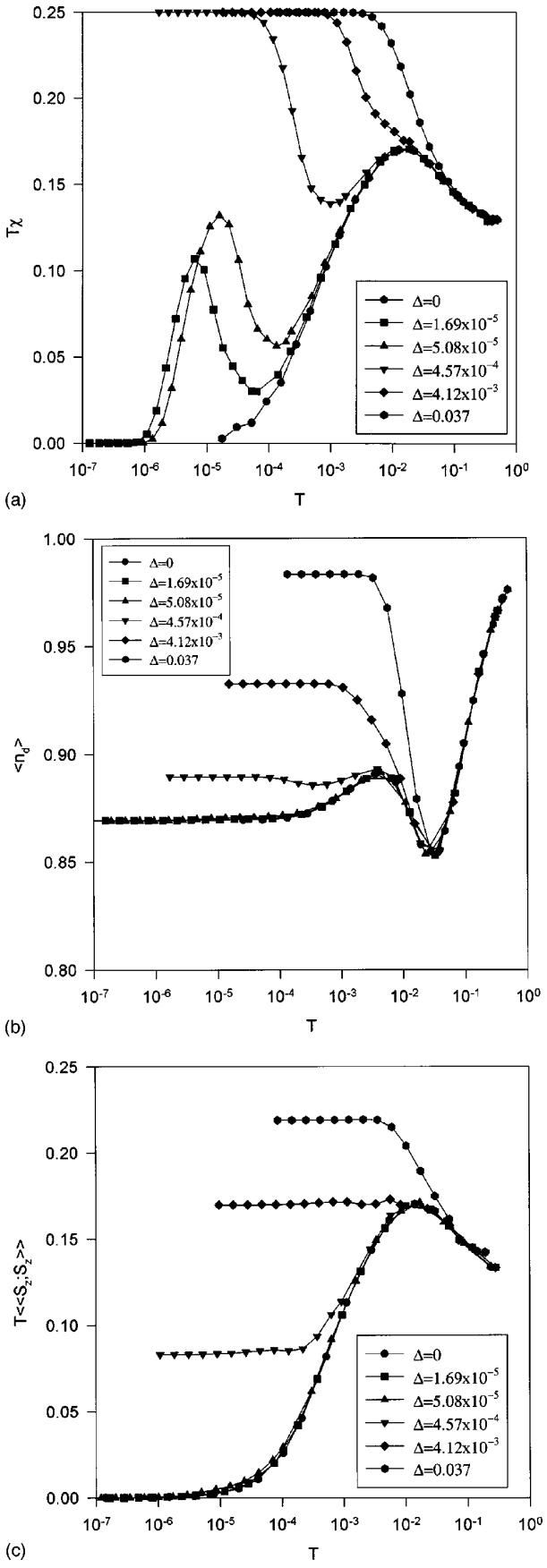


FIG. 5. The impurity susceptibility (a), $\langle n_d \rangle$ (b), and $T\langle\langle S_z ; S_z \rangle\rangle$ (c), plotted as a function of T for the asymmetric Anderson model with $U=0.1$, $\epsilon_d=-0.025$, and $\Gamma=0.01$.

out the degrees of freedom between the initial band edge $D_0=1$ and the cutoff D. When the cutoff is rescaled back to unity, the thermodynamics is determined by $\mathcal{H}(D)/D$, and to the leading order the rescaled J and K will be the same as the original coupling constants (because they are coupling constants for the marginal terms). Thus we have $J/D=J_0$ and $K/D=K_0$ to the leading order. Now for the above effective Hamiltonian at the energy scale $D\approx\Delta$, we have $J=J_0\Delta$ and $K=K_0\Delta$. It is clear that when $|J_0|\ll 1$ and $|K_0|\ll 1$, the last term of the Hamiltonian dominates, and the ground state is a doublet. This agrees with the nonperturbative results.

Next we consider the case $\Delta\ll T_K$. In this case, we clearly move away from the $J=0$ fixed point and the situation is more complicated. As we lower the energy scale to Δ, the operator f_0 or f is frozen out,[1] but f_1 is proportional to $\Lambda^{-N_0/4}$:

$$f_{1\mu}=\hat{\alpha}_0\Lambda^{-N_0/4}g_\mu+\cdots.$$

The operator g represents the single electron level at zero energy (the number of electron levels is odd, since f_0 is frozen). Now the effective Hamiltonian (at the energy scale Δ) can be written as

$$H_{\rm eff}=-J\vec{S}\cdot\vec{\sigma}(0)+Kf_\mu^+f_\mu+w(f^+g+\text{H.c.}). \tag{8}$$

The operators f and g arise when we express f_0 and f_1 in terms of the lowest single electron/hole levels of the conduction-electron Hamiltonian. In the effective Hamiltonian given above J and K are renormalized coupling constants. According to the RG analysis of the Kondo problem, the rescaled coupling constant $J(D)/D$ will increase in magnitude as the cutoff D is reduced and will be of the order 1 at the energy scale $D\approx T_K$; on the other hand, $K(D)/D$ is essentially unchanged up to the energy scale of T_K. Thus we have, at the energy scale of the Kondo temperature T_K, $J\approx T_K$ and $K\approx K_0T_K$. Due to the fact that the operator f is frozen at the energy scale of T_K, the values of J and K are not altered when the energy scale is further reduced from T_K (the rescaled coupling constants J/D and K/D are now coupling constants for the relevant terms around the strong-coupling fixed point, and they increase linearly with $1/D$). The coupling constant w, on the other hand, will continue to scale as $w\propto\Lambda^{-N_0/4}$ when N_0 increases (or as Δ decreases), we expect $w\propto\sqrt{\Delta}$. Since w should be of the order of T_K when $\Delta=T_K$, we can rewrite $w=\alpha T_K\sqrt{\Delta/T_K)}$. Note that in writing down the above Hamiltonian we have neglected all irrelevant terms, the inclusion of which will not change the results qualitatively.

We want to investigate the nature of the ground states of the above Hamiltonian, $H_{\rm eff}$, for the case $\Delta\ll T_K$ both when $K=0$ and $K\neq 0$, by diagonalizing $H_{\rm eff}$. This is mildly tedious but can be carried out in a straightforward fashion. The main results are as follows: For $K\neq 0$ (and $|K|$ larger than Δ), the ground state is a singlet [when $K>0$, the ground state is in the subspace $(Q_T=-1,S_T=0)$; for $K<0$, it is in the subspace $(1,0)$]. The first excited state is in the subspace $(0,1/2)$ and has a gap relative to the ground state proportional to Δ. For $K=0$, the ground state is in the subspace $(0,1/2)$, which is a doublet with the energy gap to the first excited state proportional to Δ^2. For the case that K is also very

small ($|K|$ smaller than Δ), the ground is also a doublet. Thus for $K\neq 0$, there is transition from singlet to doublet as Δ varies, but the transition is absent when $K=0$. These results are in agreement with our numerical RG computations. For the benefit of the reader a derivation of these results is presented below.

A. Diagonalizing the effective Hamiltonian

We diagonalize $H_{\rm eff}$ in Eq. (8) in two steps. Diagonalizing the first two terms of the Hamiltonian $H_{\rm eff}$ in the subspace of the f states gives rise to four eigenstates given below:

State A $(-1,1/2)$: $E=0$, State B $(0,0)$: $E=\frac{3}{4}J+K$, State C $(0,1)$: $E=-\frac{1}{4}J+K$, State D $(1,1/2)$: $E=2K$,

Here the numbers in the parentheses denote the charge and spin of the energy states.

Now we add the g states. The Hamiltonian can be written in the basis consisting of A, B, C, D, and g states using a procedure similar to what was employed in the iteration scheme of Wilson's RG iteration [see, for example, Eq. (B2) in Appendix B of the paper by Krishnamurthy *et al.*[3]). Let A1, A2, A3, A4 denote the basis states obtained by combining A with zero, one, and two g states, etc. The Hamiltonian matrix in each charge-spin subspace can be written down as

State A1 $(2,1/2)$: $H_{2,1/2}=0$, State A3+B1 $(-1,0)$:

$$H_{-1,0}=\begin{pmatrix} 0 & w \\ w & \frac{3}{4}J+K \end{pmatrix},$$

State A2+C1 $(-1,1)$:

$$H_{-1,1}=\begin{pmatrix} 0 & w \\ w & -\frac{1}{4}J+K \end{pmatrix},$$

State A4+B2+C3+D1 $(0,1/2)$:

$$H_{0,1/2}=\begin{pmatrix} 0 & \frac{w}{\sqrt{2}} & -\sqrt{\frac{3}{2}}w & 0 \\ \frac{w}{\sqrt{2}} & \frac{3}{4}J+K & 0 & \frac{w}{\sqrt{2}} \\ -\sqrt{\frac{3}{2}}w & 0 & -\frac{1}{4}J+K & -\sqrt{\frac{3}{2}}w \\ 0 & \frac{w}{\sqrt{2}} & -\sqrt{\frac{3}{2}}w & 2K \end{pmatrix},$$

State C2 $(0,3/2)$

$$H_{0,3/2}=-\frac{1}{4}J+K,$$

State B4+D3 $(1,0)$:

$$H_{1,0}=\begin{pmatrix} \frac{3}{4}J+K & -w \\ -w & 2K \end{pmatrix},$$

State C4+D2 $(1,1)$:

$$H_{1,0}=\begin{pmatrix} -\frac{1}{4}J+K & -w \\ -w & 2K \end{pmatrix},$$

State D4 $(2,1/2)$:

$$H_{2,1/2}=2K.$$

Whether the ground state is a singlet or doublet depends on the relative energies of the lowest energy levels in subspaces $(-1,0)$, $(1,0)$, and $(0,1/2)$. If the lowest energy level in the subspaces $(-1,0)$ and $(1,0)$ is lower than the lowest energy level in the subspace $(0,1/2)$, then we have a singlet ($T\chi$ will approach zero); otherwise, we have a doublet and $T\chi$ approaches 1/4.

Let us first consider the case $K\neq 0$ and the magnitude of K is much greater than Δ. Since the off-diagonal matrix elements are small compared to the diagonal ones ($|w/J|$ is of order $\sqrt{\Delta/T_K}$) one can use perturbation theory to determine the ground state. We perform a second-order perturbation calculation of the energy of the eigenstate with the eigenvalue near $\frac{3}{4}J+K$:

For the subspace $(-1,0)$, we have

$$E_0=\frac{3}{4}J+K+\frac{w^2}{\frac{3}{4}J+K},$$

For the subspace $(1,0)$, we have

$$E_0=\frac{3}{4}J+K+\frac{w^2}{\frac{3}{4}J-K},$$

For the subspace $(0,1/2)$, we have

$$E_0=\frac{3}{4}J+K+\frac{1}{2}\frac{w^2}{\frac{3}{4}J+K}+\frac{1}{2}\frac{w^2}{\frac{3}{4}J-K}.$$

It is clear that the ground state is always a singlet: when $K>0$, the ground state is in the subspace $(-1,0)$, whereas for $K<0$, the ground state is in the subspace $(1,0)$. The energy level of the first excited state [in subspace $(0,1/2)$] relative to the ground state is (assuming $K_0>0$)

$$E_1=\frac{1}{2}\frac{w^2}{\frac{3}{4}J-K}-\frac{1}{2}\frac{w^2}{\frac{3}{4}J+K}, \tag{9}$$

which is proportional to Δ. The energy level of the second excited state (in subspace $[Q_T=1,S_T=0]$) is $E_2=2E_1$ (this result was also found in our numerical results for the energy levels).

How about $K=0$? The issue cannot be resolved at the level of second-order perturbation theory. A fourth-order perturbation calculation for the lowest energy in the subspace $(0,1/2)$ yields

$$E_0\approx\frac{3}{4}J+\frac{4}{3}\frac{w^2}{J}+\frac{80}{27}J\left(\frac{w}{J}\right)^4.$$

For the subspaces $(-1,0)$ and $(1,0)$, the lowest energy is given by

$$E_0=\frac{3}{4}J-\sqrt{\left(\frac{3}{4}J\right)^2+w^2}\approx\frac{3}{4}J+\frac{4}{3}\frac{w^2}{J}-\frac{1}{2}J\left(\frac{w}{J}\right)^4.$$

It is clear that the ground state is in the subspace $(0,1/2)$, which is a doublet. This agrees with our numerical results. The energy gap of the first excited state is proportional to w^4 or Δ^2.

Now for the case that $|K|$ is of the order of Δ or smaller, it is a bit difficult to analyze. However, it is easy to see that the crossover of the energy levels [of states $(0,1/2)$ and $(\pm1,0)$] should occur when $w^2|K|/J^2$ is of the order of w^4/J^3, or when Δ is of the order $|K|\approx(K_0T_K)$. Thus for a finite K, there is transition from a singlet state to a doublet state when Δ increases and cross Δ_c which is of the order K_0T_K.

B. Response function

Let us consider the calculation of $T\langle\langle S_z;S_z\rangle\rangle$ in the ground state when $\Delta\ll T_K$. By definition

$$\langle\langle S_z;S_z\rangle\rangle=\int_0^\beta\langle S_z(\tau)S_z\rangle d\tau.$$

Close to zero temperature, we can write

$$\langle\langle S_z;S_z\rangle\rangle=\sum_{|I\rangle}\frac{|\langle G|S_z|I\rangle|^2[1-\exp(-\beta(E_I-E_G))]}{E_I-E_G},$$

where $|I\rangle$ represents many-body states of the system and $|G\rangle$ denotes the ground state. For temperatures much smaller than the energy gap between the first excited state and the ground state, we have (separating out the contribution of the ground state from the summation)

$$\langle\langle S_z;S_z\rangle\rangle=\beta|\langle G|S_z|G\rangle|^2+\sum_{|I\rangle\neq|G\rangle}\frac{\langle G|S_z|I\rangle|^2}{E_I-E_G}.$$

Since the second term in the above expression is finite, we obtain in the limit as $T\to0$, $T\langle\langle S_z;S_z\rangle\rangle=|\langle G|S_z|G\rangle|^2$. For the case $K_0\neq0$ and $\Delta<\Delta_c$, the ground state is at the subspace $(\pm1,0)$ and it is easy to verify that $T\langle\langle S_z;S_z\rangle\rangle$ is zero.

For the case that $K_0=0$, we find that

$$\langle G|S_z|G\rangle=\pm\frac{4w^2}{3J^2}.$$

Thus $T\langle\langle S_z;S_z\rangle\rangle$ in this case is proportional to w^4 or Δ^2 in agreement with the numerical results.

C. Anderson model

We now discuss the Anderson model briefly since the results are similar to those of the Kondo problem discussed above. We consider the limit that U is very large and Γ is very small. The effective Hamiltonian is of the form

$$H_{\rm eff}=\tilde{\epsilon}_d d_\mu^+ d_\mu+\tilde{V}(d_\mu^+ f_{0\mu}+\text{H.c.})+\Delta(a_\mu^+ a_\mu-b_\mu^+ b_\mu).$$

Here $\tilde{\epsilon}_d$ is the effective impurity level at the energy scale Δ and $\tilde{V}$ is the effective coupling to the conduction-electron states. As pointed out by Haldane[16] within perturbative scaling the impurity level energy is renormalized when the high-energy degrees of freedom are integrated out:

$$\tilde{\epsilon}_d\approx\epsilon_d+\frac{\Gamma}{\pi}\ln\left(\frac{D_0}{\Delta}\right).$$

Since we have assumed that U is large the impurity level cannot be doubly occupied: $n_d\leqslant1$. The behavior depends on the magnitude of $\tilde{\epsilon}_d$. For the case that $-\tilde{\epsilon}_d>\Delta$, then the local moment regime will be reached as the temperature is lowered, and the effective Hamiltonian can be converted to the Kondo Hamiltonian; this has been considered above. Here we focus on the case that $|\tilde{\epsilon}_d|\ll\Delta$, so that the effective impurity level lies in the gap.

Consider the case when V is very small; to leading order, the ground state depends on the sign of $\tilde{\epsilon}_d$. If $\tilde{\epsilon}_d>0$, then the ground state corresponds to two electrons occupying the conduction-electron level at $-\Delta$, and thus it is a *singlet*. This situation arises, for example, when the initial ϵ_d is greater than zero; this has been checked by the nonperturbative RG calculation. On the other hand, when $\tilde{\epsilon}_d<0$, then the ground state corresponds to two electrons occupying the conduction-electron level at $-\Delta$ and one electron occupying the impurity level. So the ground state is a *doublet*.

We now discuss the different physics underlying the doublet ground state that occurs when (a) $-\tilde{\epsilon}_d>\Delta$ and the local moment regime is reached as the temperature decreases with $k_BT_K>\Delta$ and (b) $-\tilde{\epsilon}_d\ll\Delta$ when the mixed-valence regime is reached. In the first case, the system develops a local moment and as the temperature is further lowered, the moment begins to be quenched by the Kondo effect due to large effective $|J|$. The existence of the gap is not yet apparent and the system appears to be driven toward a singlet ground state. However, as the temperature drops below Δ, the finite gap energy causes the doublet to be lower in energy than the singlet with a small splitting given by Eq. (9). In case (b), on the other hand, the local moment is not formed at the energy scale Δ. However, as the temperature is lowered to the energy scale of $-\tilde{\epsilon}_d$, charge fluctuations are suppressed and they eventually cease to occur, and the system becomes a doublet without any intervening Kondo-like effects.

V. CONCLUSIONS

We have performed a Wilson renormalization-group calculation of the Kondo and Anderson models with a gap in the conduction-electron density of states. The impurity sus-

ceptibility, correlation functions, and a zero-frequency response function have been calculated as functions of temperatures in various regimes. Our calculations confirm earlier results on the qualitative differences in the low-temperature behaviors between the cases with and without particle-hole symmetry when the gap is much smaller than the Kondo temperature. We have shown that the numerical results at low temperatures can be understood in terms of simple low-temperature effective Hamiltonians.

ACKNOWLEDGMENT

C.J. would like to thank the Ohio Supercomputer Center for granting computer time on the Cray.

[1] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[2] P. Nozières, J. Low Temp. Phys. **17**, 31 (1974).
[3] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980); **21**, 1044 (1980).
[4] L. Cruz, P. Phillips, and A. H. Castro Neto, Europhys. Lett. **29**, 389 (1995).
[5] H. Takayama, Y. R. Lin-Liu, and K. Maki, Phys. Rev. B **21**, 2388 (1980).
[6] Kan Chen and C. Jayaprakash, Phys. Rev. B **52**, 14 436 (1995).
[7] Kan Chen, C. Jayaprakash, and H. R. Krishnamurthy, Phys. Rev. B **45**, 5368 (1992).
[8] Kan Chen and C. Jayaprakash, J. Phys.: Condens. Matter **7**, L491 (1995).
[9] T. Saso, J. Phys. Soc. Jpn. **61**, 3439 (1992).
[10] T. Saso and J. Ogura, Physica B **186-188**, 372 (1993).
[11] J. Ogura and T. Saso, J. Phys. Soc. Jpn. **62**, 4364 (1993).
[12] K. Takegahara, Y. Shimizu, and O. Sakai, J. Phys. Soc. Jpn. **61**, 3443 (1992).
[13] K. Takegahara, Y. Shimizu, N. Goto, and O. Sakai, Physica B **186-188**, 381 (1993).
[14] K. Ingersent, Phys. Rev. B **54**, 11 936 (1996).
[15] C. C. Yu and M. Guerrero, Phys. Rev. B **54**, 8556 (1996).
[16] F. D. M. Haldane, Phys. Rev. Lett. **40**, 416 (1978).