

Quantum phase transition in a gapped Anderson model: A numerical renormalization group study

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We use the numerical renormalization group method to investigate the spectral properties of a single-impurity Anderson model with a gap δ across the Fermi level in the conduction-electron spectrum. For any finite $\delta > 0$, at half filling the ground state of the system is always a doublet. Away from half filling a quantum phase transition (QPT) occurs as function of the gap value δ , and the system evolves from the strong-coupling (SC) Kondo-type state, corresponding to $\delta < \delta_C$ toward a localized moment (LM) regime for $\delta > \delta_C$. The opening of the gap leads to the formation of one (two) bound states when the system is in the SC (LM) regime. The evolution across the QPT of their positions and the corresponding weights together with the dynamic properties of the model are investigated.

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I. INTRODUCTION

One of the hallmarks of the Kondo effect¹ is the raise of a narrow resonance, at the Fermi level, in the spectral-density function of a magnetic impurity embedded into a metallic host. The width of the resonance is proportional to the so-called Kondo temperature T_K , which is the characteristic energy scale. Below T_K the impurity spin is completely screened into a singlet by the host material. Below the Kondo scale ($T < T_K$), the low-temperature properties, such as the resistivity, spin susceptibility, or specific heat are properly described in terms of Landau theory² of the Fermi liquid.

The simplest approach to capture the Kondo effect is through the Anderson model.³ It was used initially to describe the formation of the localized moments (LMs) in metallic hosts. The model has inspired a lot of theoretical work, and a multitude of analytical and numerical methods was developed.¹ One of them, the numerical renormalization group⁴⁻⁶ (NRG), originally proposed by Wilson, is known as one of the most reliable and accurate approach to capture the low temperature, low-energy physics of the model. Later, with the increase in the computing power, NRG was successfully extended to a broad range of more exotic quantum impurity models⁷ such as the two-channel Kondo problem,⁸ coupled magnetic moments,⁹ the coupling to a superconducting host,¹⁰ or the soft-gap model.¹¹

In the present work we address a slightly different problem. That of a magnetic impurity in a degenerate semiconductor host which presents a gap across the Fermi level in the conduction-electron spectrum. In the normal Anderson model the conduction band has a flat density of states (DOS) at the Fermi level and the Kondo temperature is the only energy scale of the problem. The opening of a gap δ in the conduction-band spectrum introduces a new energy scale. The first question that arises is whether the Kondo state will survive? The problem was originally addressed by using different techniques: the quantum Monte Carlo,¹² density-matrix renormalization group (DMRG),¹³ Poor Man's scaling, and $1/N$ expansion¹⁴ with no consensus reached. Later,

Chen and Jayaprakash¹⁵ have used NRG method for the same problem. It was found that at half filling, any gap $\delta > 0$ changes the ground state to a doublet. Away from half filling and for large enough gaps the Kondo state does not survive. More recently, the results obtained within the NRG framework were confirmed by using a local-moment approach.¹⁶

The main goal of the present work is to extend the analysis of the model and to investigate its dynamic properties and their evolution across the quantum phase transition (QPT). In Sec. II we present the theoretical model, then the results for the spectral properties are presented in Sec. III. We give the conclusions in Sec. IV.

II. MODEL AND NUMERICAL APPROACH

To describe a local, quantum impurity state, coupled to a conduction band we use the generic Anderson model

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \epsilon_d \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + U \sum_{\sigma} n_{d\uparrow} n_{d\downarrow} + V \sum_{\mathbf{k},\sigma} (c_{\mathbf{k},\sigma}^\dagger d_{\sigma} + d_{\sigma}^\dagger c_{\mathbf{k},\sigma}). \quad (1)$$

Here $\epsilon_{\mathbf{k}}$ is the host band dispersion, which is treated as a noninteracting one, ϵ_d is the impurity-level energy, U is the on-site Coulomb energy at the impurity site, and V is the hybridization-matrix element of the local impurity orbitals with the band states, which, in the present approach, is considered momentum and spin independent. The number operator $n_{d\sigma} = d_{\sigma}^\dagger d_{\sigma}$, describes the occupation of the impurity level for spin- σ electrons. The mixing of impurity level with the host states is generically described by the hybridization function $\Delta(\omega) = \Delta_R(\omega) + i\Delta_I(\omega) = V^2 \sum_{\mathbf{k}} [\omega - \epsilon_{\mathbf{k}} + i\eta \operatorname{sgn}(\omega)]^{-1}$. In general $\Delta_I(\omega)$ can be related to the density of states of the host band: $\Delta_I(\omega) = \pi V^2 \varrho(\omega)$. In our model, a gap $\delta > 0$ is present in the density of states. Then, $\Delta_I(\omega)$ has the form

$$\Delta_I(\omega) = \Gamma \Theta(|\omega| - \delta) \Theta(D - |\omega|) \quad (2)$$

with $2D$ the bandwidth of the host band. The normal Anderson model with a flat density of states is recovered in the

limit of zero gap $\delta \rightarrow 0$, in which case the properly normalized density of states is $\varrho(\omega) = 1/2D$ for $\omega \in [-D, D]$ and the broadening function becomes $\Gamma = \pi V^2/2D$. In the followings we will consider D as the energy unit. The real part of the hybridization function is obtained through the Hilbert transform as

$$\begin{aligned} \Delta_R(\omega) &= -\frac{\Gamma}{\pi} \left[\ln \left| \frac{\omega - D}{\omega - \delta} \right| - \ln \left| \frac{\omega + D}{\omega + \delta} \right| \right] \\ &\simeq -\frac{\Gamma}{\pi} \ln \left| \frac{\omega + \delta}{\omega - \delta} \right|, \quad |\omega| \ll D. \end{aligned} \quad (3)$$

The region of relevance corresponds to small gap values, of the order of Kondo temperature (we use the Haldane's expression for the Kondo temperature,¹⁷ so it is properly defined only in the limit of zero gap, $\delta=0$). We are mostly interested in the dynamical properties of the model. These are best described by the single-particle, retarded Green's function of the impurity site: $G_{ret}(t-t') = -i\langle\{d_\sigma(t), d_\sigma^\dagger(t')\}\rangle\Theta(t-t')$. In general, the time-ordered Green's function of the interacting problem is given by the Dyson equation: $G(\omega) = [G_0(\omega) - \Sigma(\omega)]^{-1}$, in terms of the noninteracting, ($U=0$), Green's function $G_0(\omega) = [\omega - \epsilon_d - \Delta(\omega)]^{-1}$ and of the self-energy $\Sigma(\omega)$. Then, the spectral representation $\mathcal{A}(\omega) = -1/\pi \Im G_{ret}(\omega)$ can be readily obtained.

Away from the half filling it can be readily shown,¹⁸ by the simple perturbation theory at the Hartree-Fock level, that outside the gap, ($|\omega| > \delta$) both real and imaginary parts of the self-energy are nonzero, so the spectrum is continuum. On the other hand inside the gap, ($|\omega| < \delta$) the imaginary part of the self-energy vanishes. Because of that, the d -level Green's function has a *single* pole inside the gap. This pole corresponds to a resonant state with a lifetime inverse proportional with the imaginary part of the self-energy. Therefore, it corresponds to a *real bound state* with infinite lifetime. The position of the bound state (E_b) can be obtained by solving the equation $G_{ret}^{-1}(E_b) = 0$ for E_b . At the noninteracting level, (neglecting the self-energy corrections) the bound-state energy is determined from

$$E_b - \epsilon_d = \Delta_R(E_b). \quad (4)$$

Away from the half filling this equation has always only *one* solution. When the self-energy corrections are included, it only leads to a renormalization of the local energy $\tilde{\epsilon}_d = \epsilon_d + \Re \Sigma(E_b)$, otherwise, the same scenario holds, and still a single bound state is formed in the gap, but with the position slightly shifted.

At half filling a more careful analysis is necessary. At the noninteracting level we do expect a single bound state to appear exactly at zero energy. However, the same perturbative analysis gives for the imaginary part of the self-energy inside the gap: $\Im \Sigma(\omega) \propto \delta(\omega)$ and by the Hilbert transform the real part becomes $\Re \Sigma(\omega) \propto 1/\omega$. Using now Eq. (4), but with the self-energy correction included, it can be shown that at half filling, a pair of two, particle-hole symmetric poles are formed inside the gap.

The perturbative approach described above provides us with helpful information relative to the formation of the

bound states. Regardless of its simplicity it has its own limitations. Computing the self-energy in the second-order perturbation theory in U , the spectral function of the impurity site can be resolved only at a qualitative level. More than that, in the large- U limit the perturbation theory is supposed to fail. The previous analysis indicates that there is a fundamental difference between symmetric and asymmetric cases, but we can only speculate that the particle-symmetric case cannot be perturbatively connected to the noninteracting limit while the asymmetric model does. At the same time no information relative to the nature of the ground state can be extracted.

A much more rigorous analysis of the problem is possible by using the NRG method,²⁰ which is a reliable approach to study a variety of quantum impurity models. It consists of a logarithmic discretization of the host band into intervals of the form $[\Lambda^{-(n+1)}, \Lambda^{-n}]$ with Λ some positive number larger than 1, (usually $\Lambda \simeq 2$) and a mapping of the original Hamiltonian (1) into a one-dimensional tight-binding chain (Wilson chain) such that the hopping couplings between nearest neighbors acquire a Λ dependence of the form $\propto \Lambda^{-n/2}$, followed by an iterative diagonalization of the chain with one extra site added at each iteration step. In general the on-site energies in the Wilson chain are also nonzero, but it can be analytically shown that for a host density of states with electron-hole symmetry they do vanish. The continuous limit corresponds to $\Lambda \rightarrow 1$ and for any $\Lambda > 1$ the NRG is an approximation. Keeping Λ small ($\simeq 1.5$) the computing time increases a lot while having a large Λ (~ 3.0) the accuracy of the calculation is compromised, especially for spectral properties at large energies. Therefore, in the present work, we present results for $\Lambda = 2$. There is major difference in the way the NRG is used when a gap is opened in the density of states. For example, at $T=0$, in the normal Anderson model it is, in principle, possible to increase the number of iterations to any value, but usually an upper limit is chosen such that, once the fixed point is reached, the NRG stops after a few iterations. In principle, the more iterations we use, the better the spectral functions at the Fermi level are resolved. On the other hand, for a gapped Anderson model the threshold δ fixes somehow the maximum number of iterations. Because there are no longer states in the host band below δ , we need to stop the NRG procedure at a given iteration N_{max} which is gap dependent: $N_{max} = N(\delta)$ such that the typical energy scale $\Lambda^{-(N_{max}-1)/2}$ is *not much smaller* than the gap δ . As a technical detail, we can take advantage of the symmetries of the model and classify the eigenstates of the Hamiltonian into multiplets. Here, we have used two quantum numbers to label the multiplets: (i) Q —the number of particle measured relative to the one particle per site; (ii) S —the total spin. In the normal Anderson model the relevant energy scale is the Kondo temperature. It can be defined through the Haldane's expression:¹⁷ $T_K^0 = \sqrt{U\Gamma}/2e^{\pi\epsilon_d(\epsilon_d+U)/2U\Gamma}$. The gap δ introduces a new energy scale. As we will see next, the relevant, dimensionless parameter that characterizes the QPT is δ/T_K^0 .

III. SPECTRAL FUNCTIONS AND THE PHASE DIAGRAM

We will start with a qualitative description of the renormalization group flow diagrams. These are displayed in Fig.

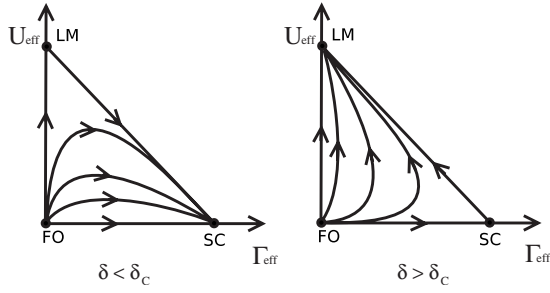


FIG. 1. Renormalization group flow diagram at $T=0$ for the gapped Anderson model, when the system is away from half filling. When $\delta < \delta_c$ the SC fixed point is stable while for $\delta > \delta_c$ the LM becomes the stable fixed point. At half filling $\delta_c=0$ so LM is stable irrespective of the value $\delta > 0$.

1. We will consider first the symmetrical model. For a normal Anderson model the strong-coupling (SC) fixed point is the only stable one, and the ground state is always a degenerate Kondo singlet characterized by the quantum numbers $(Q, S)=(\pm 1, 0)$. When a gap is opened in the density of states, the flow diagram completely changes. The SC fixed point becomes unstable and the flow is toward the LM fixed point. At the same time the ground state changes to a doublet $-(0, \frac{1}{2})$, irrespective of the value of the gap, so for the symmetric model the critical gap that describes the transition is $\delta_c=0$.

Away from the half filling, and for the normal Anderson model ($\delta=0$), probably the most interesting limit corresponds to the case when $\Gamma \ll -\epsilon_d \ll U$. Correspondingly, the flow is toward the frozen impurity (FI) fixed point, which on the other hand can be identified with the SC fixed point.⁵ When a gap starts to open in the density of states the FI remains stable as long as the gap is smaller than a critical value δ_c . For gap values larger than δ_c (δ_c depends on the asymmetry of the problem, see Fig. 4) the FI becomes unstable and the flow is toward the LM regime. At the same time the ground state changes accordingly as in the case of symmetrical model from a singlet to a doublet.

In the following we will present results for the impurity spectral function, in these regimes. In general, within the NRG framework, the spectral function is given as a weighted sum⁷ of δ functions of the form

$$A(\omega) = \sum_i W_i \delta(\omega - \omega_i), \quad (5)$$

where the weights W_i can be computed directly with the NRG. To get a smooth spectral function the δ functions need to be replaced by some smooth kernels such that the spectral sum rule $\int d\omega A(\omega)=1$ remains valid. When investigating the spectral properties of the gapped model we have used a slightly modified broadening procedure such that only the delta peaks which correspond to energies outside the gap ($|\omega| > \delta$) are broadened while for energies inside the gap ($|\omega| < \delta$) the weights W_b and the corresponding bound-state energies E_b are extracted directly from the excitation spectrum, so the spectral function becomes

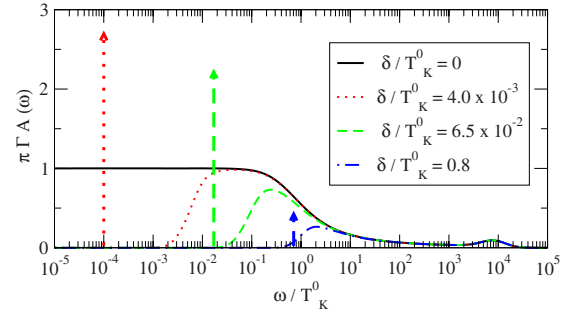


FIG. 2. (Color online) Spectral function for the symmetrical model for different gap values. The parameters used are $-\epsilon_d = \frac{U}{2} = 0.2$, $\Gamma=0.04$. T_K^0 is the Kondo temperature in the absence of the gap. The up arrows indicate the positions of the bound states in each case, their magnitude being proportional to the corresponding weight rescaled with the gap value, i.e., $\pi\Gamma W_b/\delta$. Only the positive frequency is plotted, the spectrum for negative energies being symmetric.

$$A(\omega) = A_{cont}(\omega)|_{|\omega|>\delta} + \sum_b W_b \delta(\omega - E_b)|_{|\omega|<\delta}. \quad (6)$$

We will discuss separately the results for the cases when the system is at/away from half filling. In Fig. 2 we present typical results for the spectral function of the d level of a symmetrical model. The presence of the gap in DOS preserves the electron-hole symmetry, so the spectrum remains symmetric. The black solid line is the spectral function for the normal Anderson model which develops the usual Kondo resonance below T_K^0 . Below the Kondo temperature the localized spin is screened by the conduction electrons, and the ground state is a singlet corresponding to $S=0$. The opening of a gap in the density of states changes the physics dramatically. First of all, because no states are longer available at the Fermi level below the gap edge δ , the localized spin is no longer Kondo quenched into a singlet, and the ground state changes to a doublet $(0, \frac{1}{2})$.

At the same time, the spectral function $A(\omega)$ develops a

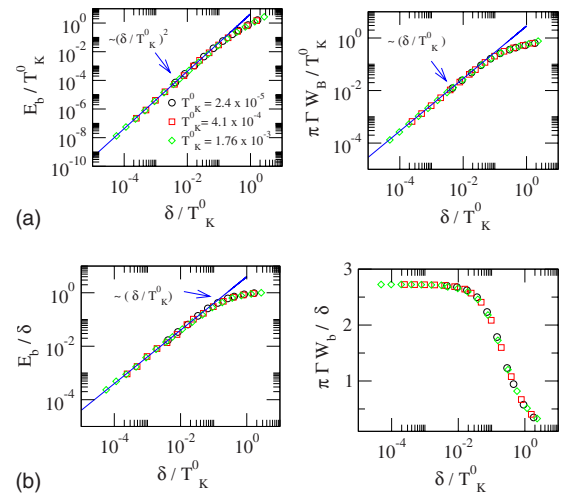


FIG. 3. (Color online) The positions of the bound states and the corresponding spectral weights rescaled with the Kondo temperature T_K^0 (top layer) and with the gap value δ (bottom layer).

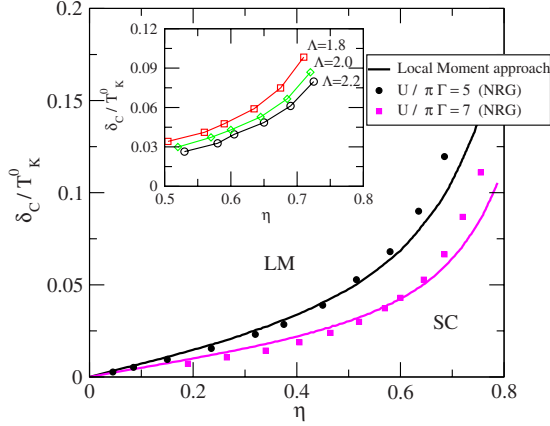


FIG. 4. (Color online) Phase diagram indicating the separation between SC and LM regimes. The parameter $\eta=1+2\epsilon_d/U$ describes the asymmetry of the system. At half filling, the critical gap is $\delta_C=0$, and the system is always in the LM regime. The solid lines correspond to the analytical results obtained within the local-moment approach (see Ref. 16) with similar rescaled coupling $\tilde{U}=U/\pi\Gamma$. The inset displays the shift of the phase boundary line as function of Λ for $0.5 < \eta < 0.75$.

gap and vanishes for energies $|\omega| < \delta$ while *two symmetric bound states* at $\pm E_b$ with exactly the same weights develop inside the gap ($E_b < \delta$). Although the ground state changes from a singlet to a doublet for any $\delta \ll T_K^0$ there are some reminiscence features of the Kondo peak and the behavior at energies $|\omega| > \delta$ resembles that of the normal Anderson model. For small enough gap values the bound states are deep inside the gap. Increasing δ , the E_b moves toward the band edge. At the same time there is some transfer of spectral weight from the bound states to the continuum states. In the limit of $\delta \gg T_K^0$ the bound states merge with the continuum, their spectral weights becoming vanishingly small and it cannot be resolved any more. In Fig. 2 the positions of the bound states are indicated by up arrows while their magnitudes are rescaled with the gap value: $\pi\Gamma W_b/\delta$. In Fig. 3 the evolution of the rescaled bound-state energy and weights as

function of the gap is plotted in two different ways: (i) rescaled with T_K^0 —the Kondo temperature; (ii) rescaled with δ —the value of the gap. We have found that the energies E_b and the corresponding rescaled weights $w_b = \pi\Gamma W_b$ satisfy the following scaling equations in the limit $\delta \ll T_K^0$:

$$\frac{E_b}{T_K^0} \propto \left(\frac{\delta}{T_K^0}\right)^2$$

$$\frac{w_b}{T_K^0} \propto \left(\frac{\delta}{T_K^0}\right). \quad (7)$$

This scaling behavior can be understood in terms of an effective Hamiltonian. First the Anderson Hamiltonian (1) is mapped by the help of the Schrieffer-Wolff transformations¹⁹ into a Kondo problem and then a low-energy, effective Hamiltonian (at the energy scale δ) is constructed, in which the impurity spin is coupled to the lowest electron/hole levels. The Hamiltonian is described in terms of an effective exchange coupling $J_{eff} \propto T_K^0$ and a potential-like scattering term $K_{eff} \propto K_0 T_K^0$. In the presence of electron-hole symmetry, and in the LM regime, the scattering term vanishes: $K_{eff}=0$, while only the exchange term survives. For a finite gap δ the system is always in a LM state with a ground state in the $(0, \frac{1}{2})$ sector while the first excited state is in the $(\pm 1, 0)$ sector. The energy E_b of the bound state¹⁵ corresponds to the transition between the lowest energies within these sectors $[(0, \frac{1}{2}) \leftrightarrow (\pm 1, 0)]$ and this energy difference scales as $E_b \simeq E_{(\pm 1, 0)} - E_{(0, 1/2)} \propto \delta^2/T_K^0$.

Next, we will describe the quantum phase transition when the system is away from the half filling. Here the SC regime is much robust as compared to the symmetric case and the transition occurs always at a finite critical gap, δ_C , such that for $\delta < \delta_C$ the system is in the SC regime and for $\delta > \delta_C$ the flow is toward the LM fixed point. The critical gap δ_C depends on the asymmetry parameter $\eta=1+2\epsilon_d/U$. In Fig. 4 we present the separation between these two regimes in the parameter space $(\eta, \delta_C/T_K^0)$. We represent our numerical results for the critical values (symbols) together with the ones

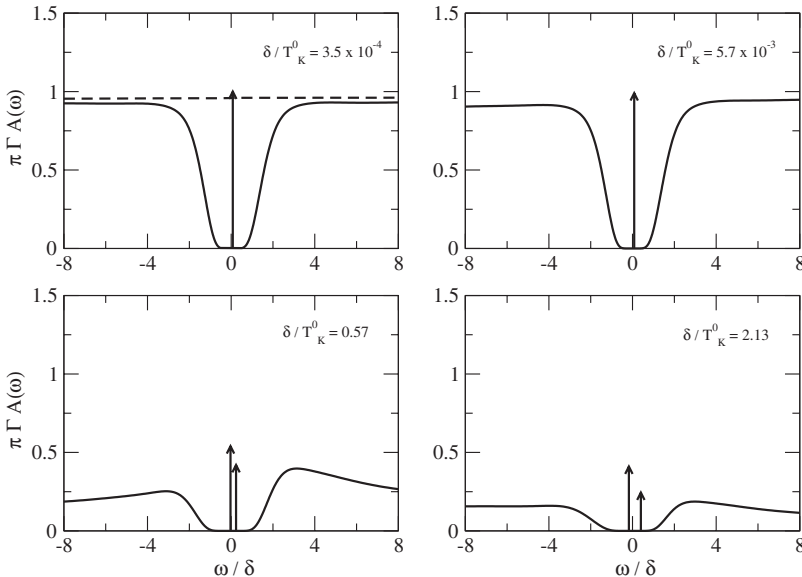


FIG. 5. Spectral functions for the asymmetrical case, close to the Fermi energy. In the upper panel the system is in the strong-coupling regime, characterized by $\delta \ll T_K^0$. In the lower panel the system is in the local-moment regime with the gap δ of the order of T_K^0 or larger. The arrows indicate the positions of the bound states and their amplitude is rescaled to $\pi\Gamma W_b/\delta$. In the SC regime a single resonance develops while in the LM regime there are two. The dotted line in the left upper panel is the spectral function for the normal Anderson model.

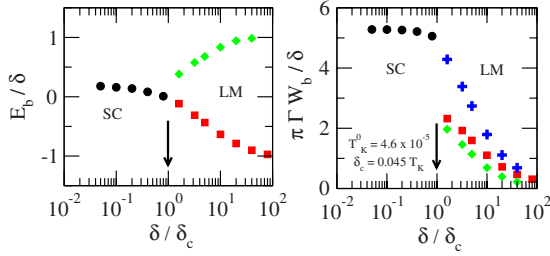


FIG. 6. (Color online) Typical evolution of the bound-state energies (left panel) and the corresponding weights (right panel) across the SC-LM quantum phase transition. In the left panel, the circles (squares) represent the positions of the bound states in the SC(LM) regime. The crosses in the right panel indicate the sum of the weights of two bound states formed in the LM regime. The arrows point to the critical gap δ_c where transition occurs.

obtained by using the local-moment approach¹⁶ (solid lines). Close to the half filling the agreement between the methods is almost perfect, and only for $\eta > 0.6-0.7$ deviations start to appear. The method of extracting the critical gap in the present approach is to some extent different from the one used in the soft-gap Anderson model¹¹ where the phase transition boundaries can be extracted directly from the NRG flow diagram. This kind of analysis is not possible in our approach since the NRG gets truncated at the gap edge. In our approach the phase boundary was obtained by changing the asymmetry parameter for a fixed gap and counting the number of bound states in the gap. We believe that there is no other more efficient procedure for constructing the phase diagram for this model. More exactly, we have fixed the gap value δ as well as the Coulomb interaction U , and we have changed the asymmetry parameter $\eta = 1 + 2\epsilon_d / U$. When the system is in the SC regime, away from the half filling, there is always one bound state in the gap, but decreasing the asymmetry, at some point we cross the phase boundary and the system evolves toward the LM fixed point with two bound states in the gap. To give a quantitative description of the transition, in terms of the spectral properties, when the gap is changed smoothly from $\delta = 0$ to some large, $\delta \gg T_K^0$, value, we have focused on the regime with $U = 0.4$, $\epsilon_d = -0.05$, and $\Gamma = 0.01$. For this set of parameters the Kondo temperature is $T_K^0 = 4.6 \times 10^{-5}$ and the critical gap is found numerically to be $\delta_c = 0.045 T_K^0$. In this particular regime (corresponding to $\Gamma \ll -\epsilon_d \ll U$) and for the normal Anderson model, below the Kondo temperature, the flow is always toward the SC fixed point, and the ground state is a nonde-

generate singlet within the $(-1, 0)$ channel. If we steadily increase δ , when $\delta \ll T_K^0$, the ground state remains a singlet. At the same time a gap is opening in the spectral function $\mathcal{A}(\omega)$ below energies $|\omega| < \delta$. In the high-energy region, $|\omega| > \delta$, $\mathcal{A}(\omega)$ has a similar structure with that corresponding to the normal Anderson model. The Kondo resonance forms below T_K^0 while the Hubbard side peaks develop at similar energies. In this SC regime only one bound state develops inside the gap (top layer in Fig. 5) in agreement with the perturbation theory. As approaching the transition $\delta \rightarrow \delta_c$ the energy of the bound state is shifted slowly toward the Fermi energy ($E_b \rightarrow 0$) (see Fig. 6). When δ becomes larger than δ_c the SC is no longer the fixed point, and the flow is toward the LM regime. The ground state changes to a doublet: $(0, \frac{1}{2})$ while two nonsymmetrical bound states develop in the gap. In Fig. 6 we present the evolution of the bound-states energy together with their characteristic weights across the transition point. On the LM side of the transition the localized states start to loose their weights as the gap is increased and their energy slowly merges into the continuum.

IV. CONCLUSIONS

Numerical renormalization group is by now a well-established method for studying correlation effects in quantum impurity models. We have applied it here to investigate the Anderson model with a gap in the conduction band. By using a slightly modified version we were able to capture the modifications in the spectral properties of the local operators across the quantum phase transition and the positions of the bound states formed inside the gap. In this way we were able to construct the phase diagram of the model. The NRG provides one of the most accurate tools for investigating the dynamical quantities of quantum impurity models. When DM-NRG is used (such as in our case) the sum rules for the spectral properties are satisfied up to the numerical precision. Therefore, the NRG results for the spectral functions are net superior to those obtained within other approaches such as the local moment approach (see Ref. 16) which do capture correctly only the positions of the bound states while the spectral properties suffer because of the approximations made.

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