

Orbital Kondo behavior from dynamical structural defectsL. Borda,^{1,2} A. Zawadowski,^{2,3} and G. Zaránd^{2,4}¹*Lehrstuhl für Theoretische Festkörperphysik and Center for Nanoscience, Sektion Physik der LMU München, Theresienstrasse 37, 80333 München, Germany*²*Department of Physics and Research Group of the Hungarian Academy of Sciences, Budapest University of Technology and Economics, Budafoki út 8, H-1521 Budapest, Hungary*³*Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, H-1525 Budapest, Hungary*⁴*Lyman Physics Laboratory, Harvard University, Cambridge, Massachusetts 02145, USA*

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The interaction between an atom moving in a model double-well potential and the conduction electrons is treated using renormalization-group methods in next-to-leading logarithmic order. A large number of excited states is taken into account and the Kondo temperature T_K is computed as a function of barrier parameters. We find that for special parameters T_K can be close to 1 K and it can be of the same order of magnitude as the renormalized splitting Δ . However, in the perturbative regime we always find that $T_K \lesssim \Delta$ with $T_K \lesssim 1$ K [I. L. Aleiner *et al.*, Phys. Rev. Lett. **86**, 2629 (2001)]. We also find that Δ remains unrenormalized at energies above the Debye frequency, ω_{Debye} .

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I. INTRODUCTION

There is a great number of experimental anomalies observed by point contact,^{1–3} dephasing,^{4,5} and transport^{6,7} measurements in metals at low temperature which have not been theoretically explained in a satisfactory way. Sensitivity on annealing,^{1,5} sample preparation,⁵ and electromigration² support that these anomalies may originate from some kind of dynamical defect.

The concept of two-level systems (TLS's), i.e., atoms or groups of atoms moving between two positions resulting in two almost degenerate levels, has been introduced to explain the low-temperature specific-heat anomalies in metallic glasses.⁸ In order to keep the level splitting very low, tunneling between the two positions has been assumed. The TLS model has later been generalized by incorporating dissipation effects⁹ and noncommutative couplings between the TLS and conduction electrons such as screening and assisted transition due to the metallic electrons,^{10,11} and a two-channel Kondo-like behavior has been conjectured.¹¹ The estimated Kondo temperature T_K , however, turned out to be too small. Taking a few of the higher levels of the atom into account increased T_K considerably,¹² however, this approximation has been shown recently to be incorrect.^{13,14} Most of the terms cancel out at energies above that of the few lowest levels if all excited states are included in the computation, and thus electron-assisted tunneling results only in a negligible T_K for TLS's.^{13,14} Similar results were obtained using the adiabatic approximation for an atom moving in a metallic host.¹⁵

The physical reason for the above cancellation is that the tunneling takes place on a typical time scale $\tau \sim 1/\omega_D$. Therefore electrons that are farther from the Fermi surface than ω_D follow the motion of the defect instantaneously, and can be ignored when considering complicated correlations between the TLS and the conduction electrons. In other words, the effective bandwidth of the conduction electrons is reduced from the Fermi energy E_F down to a value $\sim \omega_D$.

In the present paper we study a similar model but with smaller or negligible barriers, far from the tunneling regime, and keeping all excited states through our computations. We construct the perturbative scaling equations up to next-to-leading logarithmic order and show that the cancellation found in Ref. 13 also extends to the splitting of the TLS, which remains unrenormalized down to the scale ω_{Debye} , too. This supports again the picture of an “adiabatic conduction band,” proposed in Ref. 15.

In the most interesting cases the second level is just above or around the top of the barrier: In this regime we find a Kondo temperature in the range of $T_K \sim 0.1 - 1$ K using realistic parameters. For a special class of parameters the renormalized energy splitting between the lowest two levels is around T_K implying that such dynamical defects may give rise to some of the Kondo-like anomalies observed.^{1,3,6} Our calculations also indicate that to obtain a measurable T_K one needs *resonant scattering* on the defect.

In the present work we only study the perturbative region, and there we do not find convincing evidence of an observable two-channel Kondo behavior. However, one can show by performing analytical and numerical calculations using a more detailed model that there exists a regime *outside* the range of perturbative calculations where the two-channel Kondo behavior appears.¹⁶

II. MODEL

Our model consists of a particle (or collective coordinate z of the defect) with mass M ($M \sim 50m_p$; m_p is the proton mass) moving in some bare potential well, $V_{\text{bare}}(z)$. The potential $V_{\text{bare}}(z)$ can be thought of as the potential resulting from the interaction with the neighboring ionic charges. However, as we shall see later, V_{bare} is strongly renormalized due to the strong electron-defect interaction: In general, both $V_{\text{bare}}(z)$ and the electron-defect interaction are of the order of the Fermi energy (~ 10 eV), but their *sum*, the effective po-

tential, is only of the order of the Debye frequency. Therefore $V_{\text{bare}}(z)$ has very little physical meaning.

The noninteracting part of the Hamiltonian is given by

$$H_0 = \sum_n \varepsilon_n b_n^\dagger b_n + \sum_{\mathbf{p}, \sigma} \varepsilon_{\mathbf{p}} a_{\mathbf{p}, \sigma}^\dagger a_{\mathbf{p}, \sigma}. \quad (1)$$

The first term describes the motion of the particle in the potential V_{bare} , and b_n^\dagger ($n=1, 2, \dots$; $\sum_n b_n^\dagger b_n \equiv 1$) denotes the creation operator corresponding to a state of the particle with energy ε_n and wave function $\varphi_n(z)$. The second term describes the conduction electrons, with $a_{\mathbf{p}, \sigma}^\dagger$ being the creation operator of an electron with momentum \mathbf{p} , spin σ , and energy $\varepsilon_{\mathbf{p}}$. In the following we use a simple free-electron approximation to describe the conduction band, and assume that the wave function corresponding to $a_{\mathbf{p}, \sigma}^\dagger$ is a simple plane wave $\sim e^{i\mathbf{k}\cdot\mathbf{r}}$. The density of states for the electrons is $\varrho(\varepsilon) \approx \varrho_0(1 + \alpha\varepsilon/D_0)$, where ϱ_0 is the value at the Fermi energy $\varepsilon=0$, D_0 is a symmetric bandwidth cutoff of the order of the Fermi energy, and $|\alpha| < 1$ accounts for possible electron-hole symmetry breaking due to band-structure effects.

We use a simple local interaction between the particle and the electrons as follows:

$$H_{\text{int}} = \sum_{\sigma} \int dz dz_p (\psi_{\sigma}^\dagger(z) \psi_{\sigma}(z) \Psi^\dagger(z_p) \Psi(z_p) \times \{U_0 \delta(z) + U[\delta(z-z_p) - \delta(z)]\}), \quad (2)$$

where $\psi_{\sigma}(z)$ is the electron field operator along the axis z of the defect motion ($x=y=0$), and $\Psi(z_p) = \sum_n b_n \varphi_n(z_p)$ is the particle field operator at the position of the heavy particle, z_p . U_0 describes a static scattering at the center while U describes the change in the scattering potential when the particle is displaced from the center.

In the following we shall simply take $U_0=0$. This simplification needs some explanation: In principle, the value of U should be precisely U_0 in Eq. (2). One can, however, argue that the electronic wave functions corresponding to the operators $a_{\mathbf{p}}^\dagger$ in Eq. (1) should be determined when the particle is at the origin, and should therefore already incorporate the effect of U_0 , which could therefore be ignored.

The previous argument is, however, not quite right. The consequences of the presence of U_0 would be quite important. The term $\sim U_0$ can be treated exactly for a single impurity.¹⁷ Since U_0 describes a static potential it can be incorporated in the electronic wave functions, which cannot be approximated by plane waves any more. Its most important effect is to *renormalize* the local density of states ϱ_0 in the s channel as $\varrho_0 \rightarrow \cos^2(\delta_0)\varrho_0$, where δ_0 denotes the scattering phase shift induced by the scattering potential $U_0 = U$. As we see below, experiments indicate that the value of U is rather large, and corresponds to almost resonant scattering. In other words, in this simple model with $U=U_0$ at resonant scattering $\delta_0 \approx \pi/2$, and the local density of states is strongly suppressed. As a result, the dimensionless couplings estimated below are reduced. This is a serious problem: One can show that for a potential scattering model with $U=U_0$

this suppression is so strong that one is always in the weak-coupling regime, and therefore one can never observe the two-channel Kondo behavior, while without the term U_0 one can go beyond the Emery-Kivelson line and prove even analytically the existence of a regime where a two-channel Kondo behavior appears.¹⁶

To resolve this problem, one has to go beyond approximating the particle by a simple potential scatterer and take into account the dynamics of the internal electronic degrees of freedom of the particle.¹⁶ This analysis turns out to justify our approximation of setting $U_0=0$ in Eq. (2).

To handle the interaction part of the Hamiltonian we follow Ref. 11 and introduce spherical coordinates. Assuming that the motion of the defect is restricted in space ($k_F z_p < 1$, with k_F the Fermi momentum), the dominant electron scattering occurs in the ($l=0, m=0$) and ($l=1, m=0$) angular momentum channels, and we can neglect scattering channels with $l > 1$.¹¹ H_{int} then becomes

$$H_{\text{int}} = \frac{1}{2\pi} \sum_{n', n} \int dk \int dk' V_{l'l}^{n'n} b_n^\dagger b_n a_{k'l'\sigma}^\dagger a_{kl\sigma}, \quad (3)$$

where $a_{kl\sigma}^\dagger$ creates an electron with angular momentum l ($m=0$), radial momentum k , and spin σ , and satisfies the anticommutation relation $\{a_{kl\sigma}^\dagger, a_{k'l'\sigma'}\} = 2\pi \delta(k-k') \delta_{\sigma\sigma'} \delta_{ll'}$. We evaluated the dimensionless interaction matrix elements $V_{l'l}^{n'n}$ using spherical wave functions with momentum $k \approx k_F$ for the electrons and the exact wave functions φ_n for the defect. The dynamics of the heavy particle is described in terms of the pseudofermions b_n^\dagger satisfying the constraint $\sum_n b_n^\dagger b_n = 1$.

III. RENORMALIZATION-GROUP ANALYSIS

To determine T_K we constructed the leading and next-to-leading logarithmic renormalization-group (RG) equations.¹² To this end one has to compute vertex and self-energy corrections to the pseudofermion propagator $\mathcal{G}_{nn'}(\tau) \equiv -\langle T_\tau b_n(\tau) b_n'(0) \rangle$ and the impurity-electron vertex function $\Gamma_{ll'}^{nn'}$, and then apply the relatively standard machinery of the multiplicative RG. The corresponding skeleton diagrams are shown in Fig. 2 below. [Note that the first-order self-energy diagram (not shown in Fig. 2 below) only generates a local nonlogarithmic and time-independent renormalization of the defect potential and can therefore be entirely ignored.] In the RG procedure the bandwidth cutoff is reduced, $D \rightarrow D + dD$, and the couplings are simultaneously changed to keep physical quantities invariant. In the present case a matrix version of the multiplicative RG must be employed.¹⁸

In this work we take also into account the energy dependence of the local density of states. This may also depend on the angular momentum channel l , $\varrho_l(\varepsilon)/\varrho_l(0) = 1 + \alpha_l \varepsilon/D_0$, where the slope α_l and value $\varrho_l(0)$ of the density of states is usually different for different values of l . The energy ε is measured from the Fermi energy and only the linear term has been kept in ϱ_l .

Let us first focus on the case of $\varrho_{l=0} = \varrho_{l=1} = \varrho_0$ and $\alpha_0 = \alpha_1 = \alpha$. Then the second-order self-energy correction of the pseudofermion propagator, e.g., contains both logarithmic and nonlogarithmic corrections, and is given by the following expression:

$$\Sigma_{nm}(\omega) = -2 \sum_{\epsilon_n < D_0} \text{tr} \left\{ \underline{\underline{V}}^{nn} \underline{\underline{V}}^{\tilde{m}m} \right\} \left\{ D_0 f(\alpha) + (\omega - \epsilon_n^-) \right. \\ \left. \times \left[\ln \frac{D_0}{|\omega - \epsilon_n^-|} + g(\alpha) \right] \right\}, \quad (4)$$

where we introduced a matrix notation, $V_{ll'}^{nn'} \rightarrow \underline{\underline{V}}^{nn'}$, $\text{tr}\{\dots\}$ denotes the trace in the electronic angular momentum indices, and the constants $f(\alpha)$ and $g(\alpha)$ are given by

$$f(\alpha) = \frac{2}{3} \alpha^2 (\ln 2 - 1) + 2 \ln 2, \quad (5)$$

$$g(\alpha) = 1 - \ln 2 + \alpha^2 \left(\frac{1}{2} - \ln 2 \right). \quad (6)$$

The factor 2 in Eq. (4) is due to the spin degeneracy of the electrons. The effect of the nonlogarithmic terms proportional to f and g is to strongly renormalize the eigenstates and eigenfunctions of the double-well potential by replacing the heavy particle Hamiltonian by

$$\sum_n \epsilon_n b_n^\dagger b_n \rightarrow \sum_{n,m} \Delta_{nm} b_n^\dagger b_m, \quad (7)$$

where the matrix Δ_{nm} is given by

$$\Delta_{nm} = \epsilon_n \delta_{nm} - 2 \sum_{\tilde{n}} \text{tr} \left\{ \underline{\underline{V}}^{n\tilde{n}} \underline{\underline{V}}^{\tilde{m}m} \right\} [D_0 f(\alpha) - \epsilon_n^- g(\alpha)]. \quad (8)$$

The effect of the static (ω -independent) nonlogarithmic terms in Eq. (4) can be taken into account by diagonalizing Δ_{nm} through a *unitary transformation*

$$(U \Delta U^\dagger)^{nm} = \tilde{\epsilon}_m \delta_{nm}, \quad (9)$$

$$\underline{\underline{V}}^{nm} \rightarrow (\underline{\underline{U}} \underline{\underline{V}} \underline{\underline{U}}^\dagger)^{nm}, \quad (10)$$

where the $\tilde{\epsilon}_n$'s denote the renormalized values of the heavy particle energies. The effective Hamiltonian corresponding to Δ_{nm} generally contains nonlocal terms, too, but the largest terms actually turn out to be simple local corrections to V_{bare} . Therefore, in the rest of the paper we drop these nonlogarithmic self-energy corrections, and assume instead that we can model the entire effective Hamiltonian by a simple local quasi-one-dimensional symmetrical square potential with a barrier in the middle and infinite walls (see Fig. 1). We determine the corresponding wave functions by solving simple transcendental equations and then use these wave functions to compute the interaction matrix elements $\underline{\underline{V}}^{nm}$.

Note that it is only the renormalized Hamiltonian that can be measured and has therefore physical meaning. Note also,

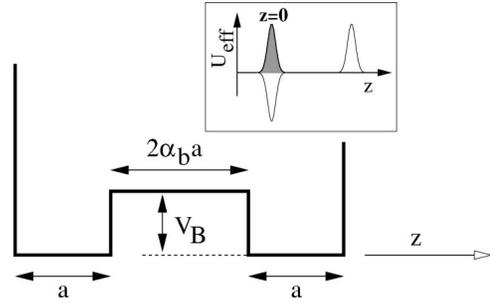


FIG. 1. The simple square-shaped double-well potential used: V_B is the height of the barrier, $a \sim 0.1 \text{ \AA}$ is the width of the wells, and $2\alpha_b a \sim 0.4 - 0.5 \text{ \AA}$ is the barrier width. Inset: Effective scattering potential for the electrons. The shaded potential corresponds to the defect sitting at the center. The white potential is due to the displacement of the defect.

that both V_{bare} and the corrections are usually of the order of the Fermi energy, however, their *sum* is usually of the order of the Debye energy only.

The interaction vertex also contains a nonlogarithmic part. Up to second order in V the dimensionless vertex function can be calculated as

$$\underline{\underline{\gamma}}^{nm}(\omega) = \underline{\underline{V}}^{nm} - \alpha \sum_{\epsilon_k < D_0} \left\{ \underline{\underline{V}}^{nk} \underline{\underline{V}}^{km} + \underline{\underline{V}}^{km} \underline{\underline{V}}^{nk} \right\} \\ - \sum_{\epsilon_k < D_0} \ln \frac{D_0}{|\omega - \epsilon_k^-|} [\underline{\underline{V}}^{nk}, \underline{\underline{V}}^{km}]. \quad (11)$$

The effect of the nonlogarithmic terms in Eq. (11) can be taken into account by renormalizing the bare vertex as

$$\underline{\underline{V}}^{nm} \rightarrow \tilde{\underline{\underline{V}}}^{nm} \equiv \underline{\underline{V}}^{nm} - \alpha \sum_k \left\{ \underline{\underline{V}}^{nk} \underline{\underline{V}}^{km} + \underline{\underline{V}}^{km} \underline{\underline{V}}^{nk} \right\}. \quad (12)$$

This transformation must be constructed order by order, and it sums up systematically all higher-order nonlogarithmic vertex contributions.

After performing the transformations above, the expressions of \mathcal{G}^{-1} and $\underline{\underline{\gamma}}$ simplify considerably, and contain only logarithmic terms in D_0 :

$$[\mathcal{G}^{-1}]_{nm}(\omega) \\ = \omega - \delta_{nm} \tilde{\epsilon}_n + 2 \sum_{\epsilon_k < D_0} \text{tr} \left\{ \tilde{\underline{\underline{V}}}^{nk} \tilde{\underline{\underline{V}}}^{km} \right\} (\omega - \tilde{\epsilon}_k) \ln \frac{D_0}{|\omega - \tilde{\epsilon}_k^-|}, \quad (13)$$

$$\underline{\underline{\gamma}}^{nm}(\omega) = \tilde{\underline{\underline{V}}}^{nm} - \sum_{\epsilon_n < D_0} \ln \frac{D_0}{|\omega - \epsilon_n^-|} [\tilde{\underline{\underline{V}}}^{n\tilde{n}}, \tilde{\underline{\underline{V}}}^{\tilde{m}m}]. \quad (14)$$

The remaining logarithmic terms in Eqs. (13) and (14) can be summed up using a generalized version of the multiplicative RG,¹⁸ leading to the following RG equations:

$$\frac{d\tilde{V}^{ij}}{dx} = - \sum_{\tilde{\epsilon}_k < D} [\tilde{V}^{ik}, \tilde{V}^{kj}] + \sum_{\tilde{\epsilon}_k, \tilde{\epsilon}_l < D} 2 \left(\tilde{V}^{kl} \text{tr}[\tilde{V}^{ik} \tilde{V}^{lj}] - \frac{1}{2} \tilde{V}^{ik} \text{tr}[\tilde{V}^{kl} \tilde{V}^{lj}] - \frac{1}{2} \text{tr}[\tilde{V}^{ik} \tilde{V}^{kl}] \tilde{V}^{lj} \right). \quad (15)$$

Here $x = \ln(D_0/D)$ is the scaling variable, and D_0 denotes the initial value of the cutoff. Since the Hamiltonian is diagonal in the spin, each closed electron loop results in a multiplicative factor of 2 corresponding to $\mathcal{N}_f = 2$ conduction-electron channels.

The renormalization-group equations for the energies $\tilde{\epsilon}_n$ are somewhat more complicated. In particular, the RG generates off-diagonal terms to the heavy particle Hamiltonian:

$$\delta_{nm} \tilde{\epsilon}_n \rightarrow \delta_{nm} \tilde{\epsilon}_n + dx \sum_{\tilde{\epsilon}_k < D} \{ 2 \tilde{\epsilon}_k \text{tr}[\tilde{V}^{nk} \tilde{V}^{km}] - \tilde{\epsilon}_n \text{tr}[\tilde{V}^{nk} \tilde{V}^{km}] - \text{tr}[\tilde{V}^{nk} \tilde{V}^{km}] \tilde{\epsilon}_m \}, \quad (16)$$

where $\tilde{\epsilon}_n, \tilde{\epsilon}_m < D$, and $dx = \ln[D/D']$. Therefore, in each RG step we diagonalize the self-energy by constructing a new set of defect states with renormalized energy eigenvalues, and express all couplings in this new basis: $\tilde{\varphi}_n = \sum_m U_{mn} \varphi_m$. Note that Eq. (15) is invariant under this unitary transformation.

When the reduced cutoff reaches the renormalized energy eigenvalue of some defect level, the dynamics of that level is frozen out, and we therefore drop it in the following RG steps. Usually only a few levels remain active in the region where the relatively weak initial couplings become comparable to the stronger ones. In many cases only one level remains by this time, meaning that no Kondo effect occurs at all.

In the original tunneling model¹¹ only the states $n=1,2$ were kept, giving rise to two initial dimensionless coupling constants, v^x and v^z , corresponding to the diagonal and off-diagonal terms in indices n and n' :

$$v^z = \frac{1}{4} (V_{01}^{21} + V_{10}^{21} + V_{01}^{12} + V_{10}^{12}), \quad (17)$$

$$v^x = \frac{1}{4} (V_{00}^{11} - V_{11}^{11} - V_{00}^{22} + V_{11}^{22}). \quad (18)$$

We identify Kondo temperature T_K with the energy scale at which the initially small dimensionless coupling v^x reaches about half of its fixed-point value, $v_x \sim 0.1$,¹⁹ and we keep the last two levels active even if their separation is larger than the running cutoff D . Below the Kondo temperature the perturbative RG breaks down and more efficient methods are needed. If only two levels are kept then Bethe-ansatz²⁰ results for the two-channel Kondo problem could be applied.

The bare values of v^z can be estimated from ultrasound data¹¹ and for alloys with stronger couplings they correspond to $v^z \sim 0.2$ and thus $U\rho_0 \sim 3$ for typical parameters. This rather large value of $U\rho_0$ implies *resonant scattering* on the atom.²¹ Nonetheless, even $U\rho_0 \sim 3$ turns out to be small

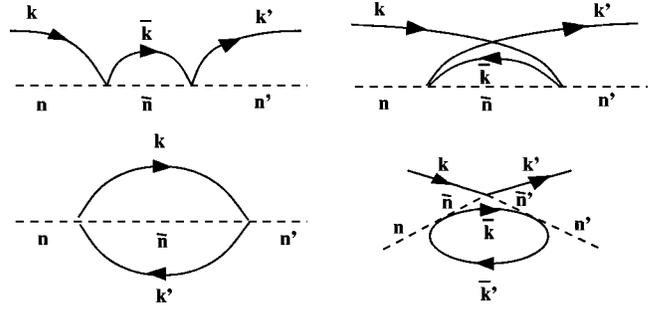


FIG. 2. Diagrams used to construct the renormalization-group equations. Dashed lines correspond to the defect atom, solid lines to the electrons.

enough so that the couplings $V^{nn'}$ corresponding to it are still in the perturbative regime: Restricting our discussion to $n=1,2$, the largest matrix elements are those where both the electron and defect parities are changed and are about $v^z \sim 0.2$. The reduction from $U\rho_0 \sim 3$ is due to a factor $v^z \sim k_F d U\rho_0$, with $d = 2a(1 + \alpha_b) \sim 0.4 \text{ \AA}$ the width of the potential well, and $k_F^{-1} \sim 1 \text{ \AA}$ the Fermi momentum. Couplings with conserved parities such as v_x are even smaller, and are further reduced by the Gamow factor in the case of a large barrier in the tunneling regime.¹¹

IV. RESULTS

In this work we used the following procedure: We first diagonalized the effective heavy particle Hamiltonian to obtain the renormalized defect energies $\tilde{\epsilon}_n$ and the renormalized couplings \tilde{V} numerically. Then we summed up logarithmic terms by performing the RG steps described in the previous section.

First, to determine the fixed-point structure of the flow equations and to determine the Kondo temperature we continued the RG even after reaching the first excited state (where the dynamics of the defect must be entirely frozen due to the energy splitting) and verified that then the couplings indeed flow to the two-channel Kondo fixed point as expected.

The leading logarithmic scaling equations for many levels were investigated by Aleiner *et al.* in the tunneling regime.¹³ They correspond to the first two diagrams in Fig. 2 and to the second-order terms in Eq. (15). Aleiner *et al.* have shown that in leading logarithmic order the logarithmic contribution of the excited states cancels out due to a sum rule, related to the approximate completeness of the defect wave functions. This reduces the effective cutoff to the order of the Debye temperature and thus the essential renormalization of the couplings occurs in the region where only few excited states remain active.

We find that this is also true for the renormalization of the tunneling rate. Figure 3 shows the renormalization of the couplings, v_x , and the tunneling rate, $\Delta_{12} \equiv \tilde{\epsilon}_2 - \tilde{\epsilon}_1$, computed by solving leading and next-to-leading logarithmic scaling equations numerically. Though we could not find a simple sum rule similar to that of Ref. 13, we found that both

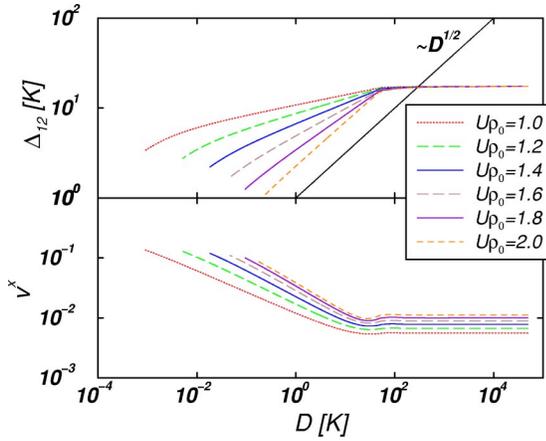


FIG. 3. (Color online) The RG flow of Δ_{12} and v_x in next-to-leading logarithmic order for $\alpha=0.4$, $d=0.5$ Å, and $V_B=100$ K. Only curves corresponding to $\rho_0 U \leq 2.0$ are shown, since for larger $\rho_0 U$ the weak-coupling approximation is not valid.

v_x and Δ_{12} remain unrenormalized throughout a large energy region, down to an energy scale of the order of the Debye temperature $\sim \omega_D$. This is in agreement with the “adiabatic conduction band” picture of Kagan and Prokof’ev,¹⁵ who argued that, since the tunneling takes place during a time scale $\sim 1/\omega_D$, electrons with energies larger than ω_D follow the defect instantaneously and therefore do not contribute to the logarithmic singularities summed up by the renormalization group. Therefore the drastic changes in the effective couplings appear only when a few levels remain.

For typical bare values of the splitting $\Delta \equiv \Delta_{21} \equiv E_2 - E_1 \geq 1$ K, the renormalization of Δ turned out to be less than about 25%. This must be opposed to the case where only two levels are kept from the beginning, and therefore a strong power-law renormalization occurs even at high energies.¹¹ Our results agree with those obtained by means of an adiabatic approximation where the renormalization occurs only when the cutoff is already in the range of the few lowest-energy levels.¹⁵

It is very instructive to see how T_K depends on the number of defect states (see Fig. 4). Such a calculation was performed by Aleiner *et al.*¹³ The first few states result in a strong increase in T_K , but then T_K suddenly drops, and the states $n \geq 6$ practically do not produce any further changes. In the following only the “saturation values” of T_K that we obtained by eventually continuing the RG flows below the first excited state if $\Delta_{21} > T_K$ are reported.

It is very important to determine the range of validity of the perturbative scaling analysis we use. Fortunately, there is a few non-perturbative results available for the TLS model that can be used to achieve this goal. In the limit of small Δ_{12} and v_x the scaling equations take a simple form:²²

$$\frac{dt}{dx} = y_t t, \quad (19)$$

$$\frac{dv_x}{dx} = y_x v_x, \quad (20)$$

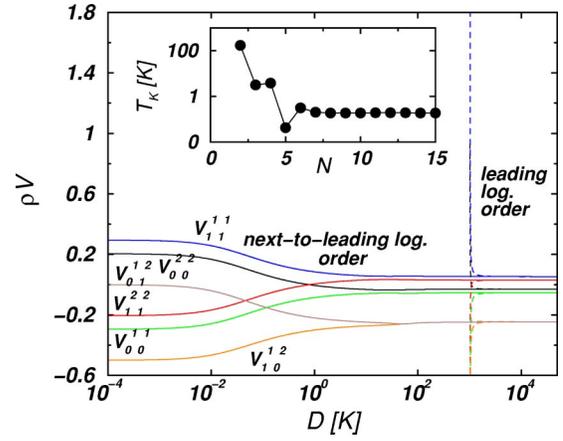


FIG. 4. (Color online) The RG flow of the couplings in leading logarithmic order and in next-to-leading logarithmic order. Inset: Kondo temperature as a function of the number of defect states, for $U\rho_0=2.1$, $d=0.5$ Å, and $V_B=100$ K.

where the scaling exponents y_t and y_x of the dimensionless tunneling (splitting) $t \equiv \Delta_{12}/D$, and assisted tunneling v_x only depend on the coupling v_z in Eq. (17):

$$y_t = 1 - 8 \left(\frac{\delta}{\pi} \right)^2, \quad (21)$$

$$y_x = 4 \left(\frac{\delta}{\pi} \right) - 8 \left(\frac{\delta}{\pi} \right)^2, \quad (22)$$

$$\delta = \arctan(\pi v_z). \quad (23)$$

In the multiplicative RG scheme these nonperturbative exponents are replaced by the following approximate exponents:

$$y_t^{RG} = 1 - 8v_z^2, \quad (24)$$

$$y_x^{RG} = 4v_z - 8v_z^2. \quad (25)$$

These approximate exponents are compared to the exact ones in Fig. 5. The exponent y_x of the assisted tunneling is surprisingly well approximated by y_x^{RG} in the range $v_z < 0.25$, and therefore we expect that the estimate of the Kondo temperature is reliable in the range $v_z \leq 0.25 - 0.3$. However,

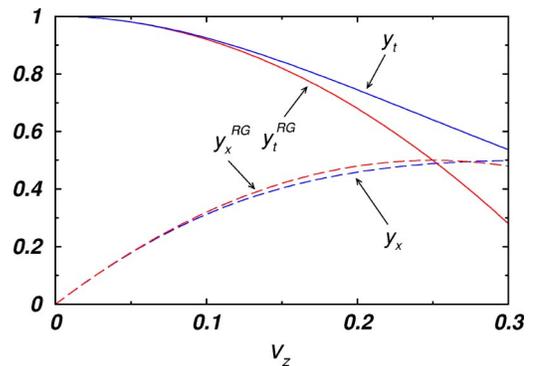


FIG. 5. (Color online) Comparison of the exact scaling exponents y_t and y_x with their approximate values y_t^{RG} and y_x^{RG} .

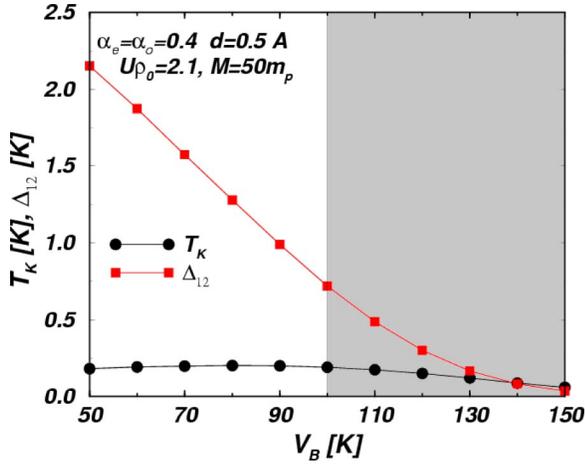


FIG. 6. (Color online) The Kondo temperature as a function of the height of the central barrier, for $\alpha=0.4$ and $M=50m_p$. The renormalized level splittings are plotted as well. The shaded part of the figure indicates the region in which the estimate of the renormalized Δ_{12} is unreliable.

y_i^{RG} underestimates the value of y_i^{RG} and therefore overestimates the renormalization of Δ_{12} , for which the RG results should be trusted only in the range $v_z \leq 0.22$. Considering that essentially no renormalization of the splitting takes place above the energy scale of the third level, one comes to the conclusion that the renormalized splitting Δ^* is underestimated by a factor of

$$\left(\frac{\Delta}{E_3}\right)^{1/y_i - 1/y_i^{RG}}, \quad (26)$$

which is a factor of 3–10 for the most extreme cases (of course, in the tunneling regime this overestimate can be much larger for small y_i 's).

Figure 6 shows the barrier height dependence of the Kondo temperature. T_K increases with increasing barrier height up to a certain value of V_B and then it drops suddenly, while the splitting Δ_{21} decreases continuously. Initially, increasing the barrier height concentrates the wave functions of the first two states more and more around the potential minima and this results in an increase of the coupling v_z , and thus a gradual increase in T_K . This tendency is, however, suddenly reversed once the barrier reaches the first level, and one enters the tunneling regime ($V_B \geq 150$ K for the parameters of Fig. 6). There the assisted tunneling v_x , responsible for the generation of the Kondo effect, decreases exponentially, and both Δ_{12} and T_K decrease dramatically.

T_K is also very sensitive to the width of the entire potential well d . In Fig. 7 we show the d dependence of T_K for a defect that has a relatively low barrier height and is not in the tunneling regime. As d is decreased from $d=0.5 \text{ \AA}$, the energy levels are shifted to higher values and also the initial values of the coupling v_z decrease while v_x does not change dramatically. Thus the width of the well is a fundamental parameter and the Kondo effect can only occur if the room for the particle considered is anomalously large in one direction. For defects in the tunneling range T_K decreases with

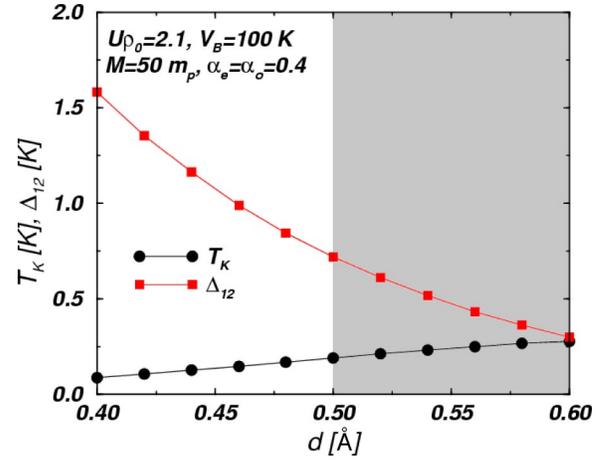


FIG. 7. (Color online) The Kondo temperature and the renormalized level splittings as a function of the total width d of the potential well for $\alpha=0.4$ and $M=50m_p$. The shaded part of the figure indicates the region in which the estimate of the renormalized Δ_{12} is unreliable.

increasing d since the bare value of v_z only slightly increases while the assisted tunneling v_x is exponentially suppressed in the tunneling regime.

In Fig. 8 we show the dependence on the strength of the defect-electron interaction U . Again, T_K increases continuously with increasing U , since all couplings generating the Kondo effect increase. On the other hand, the renormalized Δ decreases continuously since the scaling exponent y_i^{RG} also decreases with increasing U .

Finally, let us discuss the electron-hole asymmetry dependence of T_K . For $U_0=0$, $\varrho_{l=0}=\varrho_{l=1}$, and $\alpha=\alpha_0=\alpha_1$ we find no significant α dependence of the renormalized splitting and T_K . In general, however, the local density of states is different for the $l=0$ and $l=1$ channels and thus both ϱ_0 and α depend on l . A nonzero potential scattering term $U_0 \neq 0$ in Eq. (2), e.g., would have a twofold effect: (i) It would

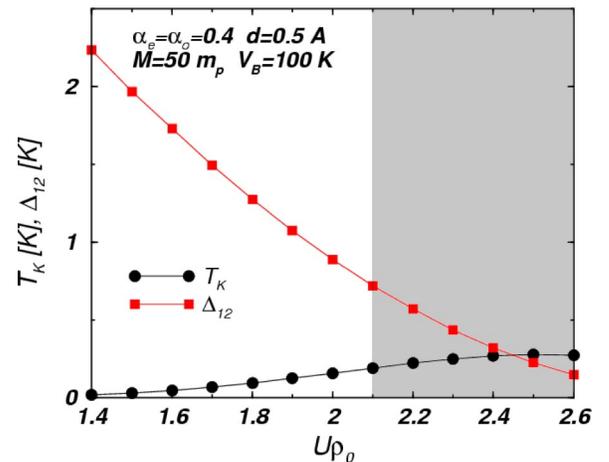


FIG. 8. (Color online) The Kondo temperature and renormalized level splittings as a function of the scattering strength U . The shaded part of the figure indicates the region in which the RG estimate of the renormalized Δ_{12} is unreliable.

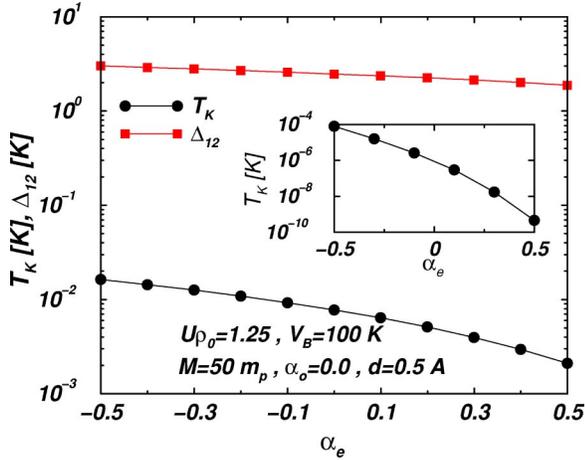


FIG. 9. (Color online) Electron-hole asymmetry dependence of T_K and the splitting Δ_{12} . Inset: The effect is more dramatic for very small T_K 's.

change the local density of states in the $l=0$ scattering channel, and (ii) would generate a different electron-hole symmetry breaking for the $l=0$ and $l=1$ channels.¹⁷ (Note that in Ref. 23 U_0 has not been set to zero and has been treated inappropriately. Instead of incorporating it in the parameters ϱ_0 and α_0 we included it in the RG equations as a coupling constant. Though the results obtained are qualitatively similar to the ones we obtained below, this procedure is wrong, since mass terms such as U_0 have to be treated always differently from the coupling constants in the multiplicative RG.¹⁷)

It is easy to generalize our previous calculations to the cases $\alpha_0 \neq \alpha_1$ and $\varrho_{l=0} \neq \varrho_{l=1}$. The l -dependent densities of state can be treated by defining the fermion fields slightly differently. However, for $\alpha_0 \neq \alpha_1$ the electron-hole symmetry breaking generates strong nonlogarithmic corrections to the bare coupling constants. In Fig. 9 we plotted the dependence of T_K on α_0 while keeping α_1 zero and $\varrho_{l=0} = \varrho_{l=1}$. We find that for typical parameters we used earlier T_K can change by about an order of magnitude. This renormalization can have even more dramatic effects for very small T_K 's where T_K can change by several orders of magnitude due to changes in the value of the electron-hole asymmetry (see inset of Fig. 9).

Let us conclude this section with a general observation. Increasing the mass (the M/m_p ratio), the energies of the levels are scaled down. If the central barrier is similarly reduced then T_K becomes smaller by the same ratio and thus Δ/T_K is not affected, since the dependence on the high-energy cutoff D is weak.

V. CONCLUSIONS

In this paper we performed a thorough scaling analysis of a dynamical defect coupled to the conduction electrons, by taking into account all the excited states of the defect, and constructing the next-to-leading logarithmic scaling equations. We also discussed how to take into account large nonlogarithmic terms that renormalize the bare parameters of the theory. In the perturbative regime our calculations confirmed

the results of Ref. 13. The electron-defect couplings remain unrenormalized down to an energy scale of the order of the Debye temperature $D \sim \omega_{\text{Debye}}$ due to a cancellation pointed out in Ref. 13.

In the leading logarithmic approach of Ref. 13 the energy levels of the impurity are unrenormalized, and the above next-to-leading logarithmic analysis is needed to compute the renormalization of the defect states. We found that, similar to the defect-electron coupling, the splitting of the first two defect states remains unrenormalized down to ω_{Debye} . In contrast to the expectations of Ref. 24, where the generation of a large splitting has been predicted, we found that the renormalization of the defect states remains small if one takes into account all defect states.

Our results perfectly agree with the adiabatic picture of Kagan and Prokof'ev.¹⁵ Electrons with excitation energies $|\epsilon| > \omega_{\text{Debye}}$ follow the defect instantaneously, and therefore the role of the excited states is only to reduce the effective electronic cutoff from the order of the Fermi energy down to the energy scale ω_{Debye} .

We also analyzed the range of validity of our approach by using some analytical results in the strong-coupling regime. We found that the perturbative RG predicts the Kondo temperature correctly for surprisingly large couplings, however, it tends to overestimate the renormalization of the splitting Δ .

We solved the RG equations for initial couplings obtained by changing various parameters of the double-well potential. We always found a region where T_K and the renormalized Δ_{12} were comparable and therefore one should be able to observe the Kondo anomaly in various measurements. Our calculations show that to have $T_K \sim \Delta_{12}$ in the measurable range one needs a defect that (i) has anomalously large room to move in one direction, (ii) is close to but not yet in the tunneling regime, and (iii) has a large scattering strength, $U\varrho_0 \geq 2.5$, implying resonant scattering on the particle. The best candidates are therefore atoms with resonant d or f scattering at the Fermi energy or possibly small groups of atoms.²⁵ Thus dynamical local defects with special realistic model parameters can explain the Kondo-like anomalies observed in some experiments for $T > T_K$.^{1,3,6} Note that in amorphous materials the positions of the defect f or d orbitals usually have a distribution, and therefore many of the defects may have resonant scattering at the Fermi energy.

However, to explain the two-channel Kondo scaling reported in Ref. 26, one would need a renormalized Δ_{12} that is less than T_K at the energy scale $D \sim T_K$. Unfortunately, our calculations are only of logarithmic accuracy, and therefore we cannot decide if the ratio Δ_{12}/T_K is small enough to display a clear two-channel Kondo scaling. In the perturbative regime (i.e., the regime where our perturbative RG works), our results seem to indicate that T_K can be comparable to, but somewhat smaller than, Δ_{12} , and is thus too small to result in an observable two-channel Kondo behavior. However, one can prove both analytically and with numerical RG calculations the existence of a regime *outside* the range of the perturbative RG,¹⁶ where T_K can be larger than Δ_{12} . This is also indicated by our perturbative results.

We have to emphasize that for a defect with resonant

scattering in a disordered environment many of our approximations (free-electron model, simple delta scattering on the defect, usage of a local effective potential, etc.) are questionable, and the estimates of the various couplings are therefore inadequate. Also, in reality, the dynamical defect is not formed by a single atom, but it is probably rather a group of atoms (e.g., dislocation) that is responsible for the defect dynamics. Though our general conclusions probably do not depend on these approximations, T_K , e.g., depends exponentially on the coupling constants and more sophisticated models/calculations would be needed to give a quantitative estimate of T_K and the ratio Δ_{12}/T_K . It remains an open question as to whether for larger couplings (i.e., defects with resonant scattering at the Fermi energy) a larger $T_K \sim 5$

–10 K can be reached, as required to explain the experiments for Refs. 1–3.

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