Existence of a two-channel Kondo regime for tunneling impurities with resonant scattering

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Dynamical tunneling systems have been proposed earlier to display a two-channel Kondo effect, the orbital index of the particle playing the role of a pseudospin in the equivalent Kondo problem, and the spin being a silent channel index. However, as shown by Aleiner *et al.* [Phys. Rev. Lett. **86**, 2629 (2001)], the predicted two-channel Kondo behavior can never be observed in the weak coupling regime, where the tunneling induced splitting of the levels of the tunneling system always dominates the physics. Here we show that the above scenario changes completely in the strong coupling regime, where—as a nonperturbative analysis reveals—the two-channel Kondo regime can easily be reached. We show that tunneling systems end up quite naturally in this regime if the conduction electrons are scattered by *resonant scattering* off the tunneling impurity, and we also speculate about the possible origins of such a resonant scattering.

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I. INTRODUCTION

There are a number of somewhat mysterious low-temperature transport anomalies in disordered point contacts,[1–5] structurally disordered single crystals, and disordered alloys,[6–9] which have not been explained satisfactorily. In some cases, the observed anomalies display power law behavior[1,10] ($\sim T^{1/2}$ or $V^{1/2}$), sometimes they show universal scaling properties,[1] but they have the common feature that all of them seem to be related to the presence of some dynamical impurities. Although very attractive, electron-electron interactions fail to explain the absence of this zero bias anomaly in point contacts with strong static disorder,[11] and the complete absence of magnetic field dependence in some experiments.[2,7]

Much before the above-mentioned experimental results, Vladár and Zawadowski proposed that dynamical two-level systems—abundant in amorphous regions[12]—could lead to an orbital Kondo effect.[13,14] They considered the motion of an ion in an effective double well potential, depicted in Fig. 1, interacting with free conduction electrons. They assumed a simple potential scattering interaction between the atom and the conduction electrons and derived the following effective Hamiltonian for low temperatures, where the atom moves by tunneling between the two minima of the potential well:

$$H = -\frac{\Delta_0}{2}\tau_x - \frac{\Delta_z}{2}\tau_z + v_z \sum_\sigma \tau_z(\psi^\dagger_{e\sigma}\psi_{o\sigma} + \psi^\dagger_{o\sigma}\psi_{e\sigma}) + v_x \sum_\sigma \tau_x(\psi^\dagger_{e\sigma}\psi_{e\sigma} - \psi^\dagger_{o\sigma}\psi_{o\sigma}). \quad (1)$$

Here, the Pauli matrices τ_i describe the motion of the particle in the double well potential, with $\tau_z = \pm 1$ corresponding to the left and right potential wells, Δ_0 the tunneling, and Δ_z the asymmetry of the potential (see Fig. 1). The operators $\psi^\dagger_{e/o\sigma}$ create conduction electrons in some even and odd angular momentum channels (s and p, e.g.),[13] respectively, and are defined as

$$\psi^\dagger_{e/o\sigma} = \int_{-D_0}^{D_0} d\xi \psi^\dagger(\xi)_{e/o;\sigma}.$$

Here, D_0 is a high energy cutoff discussed later and the $\psi^\dagger(\xi)_{e/o\sigma}$'s satisfy canonical anticommutation relations

$$\{\psi^\dagger(\xi)_{\mu\sigma},\ \psi(\xi')_{\mu'\sigma'}\} = \delta(\xi - \xi')\delta_{\mu\mu'}\delta_{\sigma\sigma'}.$$

This corresponds to a normalization of the fields $\psi_{e/o,\sigma}$ in Eq. (1) such that the imaginary time propagators at $T=0$ temperature behave asymptotically as

$$\langle T_\tau \psi_{\mu,\sigma}(\tau)\psi^\dagger_{\mu',\sigma'}(0)\rangle = \frac{\delta_{\mu\mu'}}{\tau}. \quad (2)$$

The dimensionless couplings v_x and v_z in Eq. (1) and the splitting Δ_0 have also been estimated by Vladár and Zawadowski.[13] Assuming a simple s-wave scattering U off the tunneling impurity, they found

$$\Delta_0 \approx \hbar\omega_0 e^{-\lambda}, \quad (3)$$

$$v_x \approx U\varrho_0 \frac{(k_F d)^2}{24}\frac{\Delta_0}{V_B}, \quad (4)$$

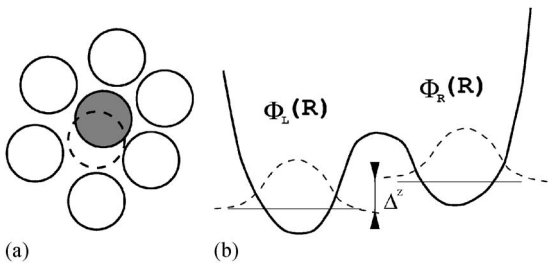

FIG. 1. Sketch of the tunneling system. The tunneling system is probably formed by a single atom in an amorphous region (a). The tunneling atom moves in an effective double well potential (b).

$$v_z \approx U\varrho_0 \frac{k_F d}{\sqrt{3}}, \tag{5}$$

where ϱ_0 denotes the density of states of the conduction electrons at the Fermi energy, d is the tunneling distance, k_F the Fermi momentum, V_B is the height of the tunnel barrier, and λ the Gamow factor. The attempt frequency ω_0 is typically somewhat less than the Debye temperature and is typically in the range $\omega_0 \sim 100$ K assuming a tunneling atom of mass $M \sim 50 m_p$, with m_p as the proton mass. Vladár and Zawadowski[13] also obtained the perturbative scaling equations for the model defined by Eq. (1) and showed that the couplings v_i and the dimensionless tunneling $\tilde{\Delta}_0 \equiv \Delta_0/D$ satisfy the following scaling equations:

$$\frac{dv_x}{dl} = 4v_y v_z - 8v_x(v_y^2 + v_z^2), \tag{6}$$

$$\frac{d\tilde{\Delta}_0}{dl} = [1 - 8(v_z^2 + v_y^2)]\tilde{\Delta}_0, \tag{7}$$

where $l = \ln(D_0/D)$ denotes the scaling variable with D the running cutoff (energy scale). The other equations are obtained by cyclic permutation from Eqs. (6) and (7). The coupling v_y is absent in the original Hamiltonian, it is, however, generated by the scaling procedure. Clearly, Eq. (6)—apart from a prefactor in the second term—is that of the anisotropic Kondo model[13] and generates a Kondo effect at the energy scale $\sim T_K$, the Kondo temperature, where the running coupling constants become of the order of unity. This Kondo effect is, however, strikingly different from the ordinary Kondo effect, where the low-temperature physics is that of a Fermi liquid below T_K. In the present case, spin is conserved in the course of the scattering, and the two spin channels give rise to a singular two-channel Kondo behavior below T_K, provided that the splitting of the two levels can be neglected.[15] The anomalous properties of this two-channel Kondo state (resistivity $\sim T^{1/2}$, V/T scaling, etc.) have been proposed to explain the experimentally observed anomalies.[1] However, the tunneling amplitude Δ_0 is always a relevant variable, and it ultimately kills orbital fluctuations (and thus the Kondo effect) of the tunneling system below a characteristic energy scale Δ_0^*. If this energy scale Δ_0^* is larger than T_K, then the anomalous properties of the two-channel Kondo fixed point cannot be observed. Vladár and Zawadowski[13] argued that—for a symmetrical tunneling system—there is a parameter range where $\Delta_0^* \ll T_K$, implying that there is a temperature window where the physics is dominated by the Kondo effect.

Unfortunately, Vladár and Zawadowski[13] assumed in their analysis that the scaling equations above are valid at all energy scales below the Fermi energy E_F. However, as pointed out by Aleiner *et al.*,[16] this assumption is wrong: Electrons with energy $\xi \gg \omega_0$ follow the tunneling particle *adiabatically*[17] and do not give contribution to the vertex renormalization. As a consequence, Eqs. (6) and (7) become trivial for $\omega_0 < D < E_F$

$$\left.\begin{aligned} dv_i/dl &= 0 \\ d\tilde{\Delta}_i/dl &= 1 \end{aligned}\right\} \text{ for } \omega_0 < D < E_F. \tag{8}$$

Therefore, as pointed out by Aleiner *et al.*,[16] Eqs. (6) and (7) must be solved with the initial conditions $D = \omega_0$, $\tilde{\Delta}_0 \sim e^{-\lambda} > v_x \sim (\varrho_0 U)(k_F d)^2 e^{-\lambda}$. Since in the perturbative regime, $\tilde{\Delta}_0$ grows always faster than v_x, Δ_0^* is always larger than T_K, and the two-channel Kondo effect can never be observed for $v_z \ll 1$, in contrast to the original conclusions of Vladár and Zawadowski.[13]

In this paper, we first show that the arguments of Aleiner *et al.*[16] hold only in the weak coupling regime, $v_z \ll 1$. In the strong coupling regime, $v_z \sim 1$, one must treat the coupling v_z nonperturbatively and use the scaling equations originally derived by Vladár, Zimányi, and Zawadowski in Ref. 18 that treat v_z *exactly*, while handling the small coupling v_x and the tunneling only in leading order. The analysis based on these equations clearly shows that there exists a critical value, $v_z = v_{z,c} \equiv 1/\pi$. Above this so-called Emery-Kivelson line,[19] v_x *typically wins* over Δ_0, i.e., the renormalized splitting is smaller than the Kondo temperature, $T_K > \Delta_0^*$, and thus, there is usually a wide temperature range where the physics of the tunneling system is *dominated by the two-channel Kondo fixed point*.

Then, we show that a possible, and probably the most natural, way to get into this regime is to have a tunneling atom that also acts as a *resonant scatterer* at the Fermi energy.[20] Indeed, as was already observed in the original work of Vladár and Zawadowski,[13] it is known from experiments that the value of v_z can be *large*, suggestive of *resonant scattering* from the tunneling systems, whatever they are. As we shall see, in this case it is not enough to start from the simple potential scattering model studied in Refs. 13 and 16 and one must take into account the dynamical motion of the internal levels of the tunneling atom. As we show later, due to this resonant scattering, one easily gets outside the range of validity of the perturbative equations considered by Aleiner *et al.*,[16] Eqs. (6) and (7), and ends up in the strong coupling regime.

To show why resonant scattering is of primary importance, let us consider a simple toy model describing an atom with a single resonant level at the Fermi energy,

$$H = \sum_{\sigma,\mathbf{k}} \xi(\mathbf{k}) c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + V \sum_{\sigma,\mathbf{k}} (c^\dagger_{\mathbf{k},\sigma} d_\sigma + \text{H.c.}). \tag{9}$$

Here, d_σ is the annihilation operator describing the level, V is the hybridization, and $c^\dagger_{\mathbf{k},\sigma}$ creates a conduction electron with spin σ, momentum $\mathbf{k}$, and energy $\xi(\mathbf{k})$. This model can be trivially solved, and we can compute the spectral functions $\varrho_d(\omega)$ and $\varrho_\psi(\omega)$ of the d level and the fermionic field at the impurity site, $\psi_\sigma \equiv \Sigma_{\mathbf{k}} c_{\mathbf{k},\sigma}$,

$$\varrho_d(\omega) = \frac{1}{2\pi} \frac{\Gamma}{\omega^2 + \Gamma^2/4}, \tag{10}$$

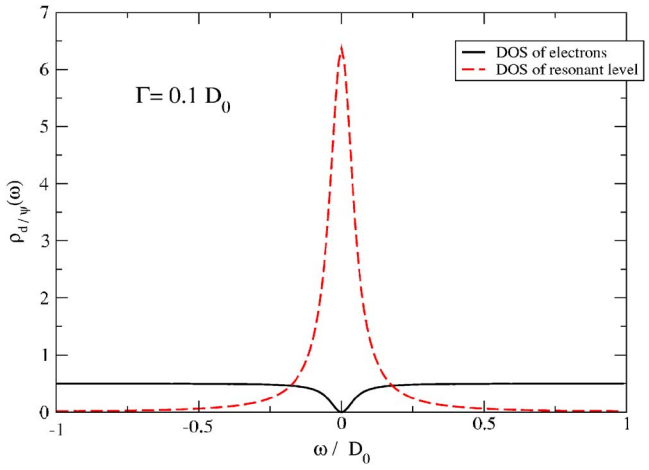

FIG. 2. (Color online) Density of states (spectral function) of a resonant level d and the conduction electron operator ψ hybridizing with it. The conduction electrons' spectral function is suppressed, while ϱ_d displays a huge resonance at the Fermi energy.

$$\varrho_\psi(\omega) = \varrho_0 \frac{\omega^2}{\omega^2 + \Gamma^2/4}. \tag{11}$$

Here, ϱ_0 is the density of states of the conduction electrons at the Fermi energy, and $\Gamma = 2\pi\varrho_0 V^2$ is the width of the resonance. Clearly, if we now try to move the atom, it will then couple to *its own resonant level d* the most strongly, which is centered at the atom, and not to the rest of the conduction electrons, which are sitting at neighboring ions in reality. Even for a not too narrow resonance with $\Gamma \sim 1$ eV, the density of states of the resonant level at the Fermi energy is large, $\sim 1/\Gamma$, while that of the conduction electrons hybridizing with the atom actually vanishes at the Fermi energy (see Fig. 2). This large increase in the density of states is what immediately pushes the system in the strong coupling regime, $v_z > v_{z,c}$, where the two-channel Kondo behavior prevails, provided that the resonance is narrow enough. For typical parameters, we obtain that the resonance should be narrower than about $0.1E_F - 0.01E_F \sim 1000 - 10\,000$ K.

We emphasize though that the above resonance does not have to be narrower than ω_0: As we discussed earlier, only electrons with energy $|\omega| < \omega_0$ are unable to follow the motion of the atom at a time scale $\sim 1/\omega_0$. These latter are exactly the electrons that are responsible for the Kondo effect. However, these electrons only need a time scale $\sim 1/\Gamma$ to notice the increased scattering strength at the Fermi energy, i.e., all these "slow" electrons see an increased scattering strength from the atom. This simple picture can be readily verified[21] through a path integral treatment similar to that of Ref. 22 as well as by the extension of the the diagrammatic approach of Refs. 16 and 23. For a resonance narrower than ω_0, our analysis must be slightly modified, and the vertex renormalization only occurs in the range $D < \Gamma$, since electrons with energy $\omega > \Gamma$ do not couple strongly to the atom.

As we show later, the increase in the coupling constant can simply be understood as a matrix element effect: The wave functions of the conduction electrons at the Fermi energy (where the resonance is located) have an *increased amplitude* at the tunneling atom's position, and therefore the motion of the atom couples more strongly to the conduction electrons.

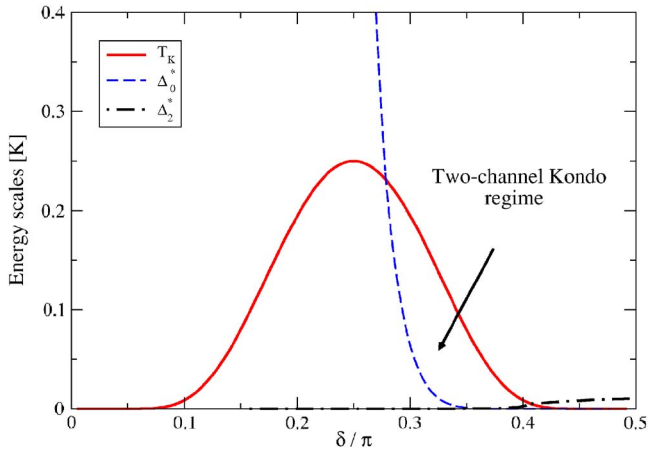

FIG. 3. (Color online) Phase diagram of the tunneling system as a function of the phase shift $\delta = \arctan(v_z \pi)$. The arrow indicates the two-channel Kondo regime. The symbol Δ_0^* denotes the energy scale where the tunneling becomes dominant, while Δ_2^* is the energy scale where a special two-electron scattering process becomes important. We have used $\omega_0 \approx 100$ K, $D_0 \sim 10^5$ K, $\Delta_0 = 10$ K, and $v_x \approx 0.1$ as bare parameters.

It is, thus, the structure of a resonant level itself which is ultimately responsible for the orbital Kondo effect in the above scenario, and this resonance cannot be replaced by a simple potential scatterer in a free electron gas.[24] The technical reason for this is that in a simple potential scattering model, there is always a term $\sim \Sigma_{\sigma,\mu=e,o} v_{0,\mu} \psi^\dagger_{\mu\sigma} \psi_{\mu\sigma}$, which is large, cannot be neglected, leads to a suppression of the conduction electron's density of states, and ultimately reduces the effective value of v_z. As we shall see, the effective Hamiltonian for this resonant level finally takes also the form, Eq. (1), however, the couplings will be related to some atomic orbitals, and no large term $\sim v_0 \Sigma_{\sigma,\mu} \psi^\dagger_{\mu\sigma} \psi_{\mu\sigma}$ appears. Therefore, we can use the nonperturbative scaling equations valid for all values of v_z, derived by Vladár, Zimányi, and Zawadowski in Ref. 18 to construct the phase diagram of our model. The summary of this analysis is shown in Fig. 3. The bell-shaped line in Fig. 3 shows the estimated value of the Kondo temperature T_K, while Δ_0^* is the renormalized tunneling amplitude. In Fig. 3, we also show another energy scale, Δ_2^*, associated with a two-electron scattering process.[25] Below this energy scale, the two-channel Kondo behavior is also suppressed. As one can see from Fig. 3, there is an extended regime dominated by the two-channel Kondo fixed point. The size of this region increases if we decrease the value of v_x and Δ_0, however, then T_K is also shifted toward smaller temperatures. As we discussed above, the tunneling system ends up immediately in this regime if there is a sufficiently narrow resonant scattering on the tunneling atom.

We would also like to mention that another possibility to get to the strong coupling regime is to *increase the tunneling distance* and have a broader resonance at the Fermi energy. This might be possible for very light tunneling impurities,

possibly by hydrogen: Hydrogen has typically resonant scattering in the *s* channel and it can possibly tunnel over a large distance in a metal. Zero bias anomalies have indeed been observed in hydrogen doped palladium point contacts where the anomaly is clearly related to the presence of hydrogen.[26]

The rest of the paper is structured as follows. In Sec. II, we shall construct a microscopic model that enables us to treat the resonance properly and map this problem to the original Vladár-Zawadowski model. We then analyze the scaling equations and construct the phase diagram of this model in Sec. III. Finally, in Sec. IV, we present our conclusions and speculate about possible candidates producing a resonant scattering at the Fermi energy.

II. MICROSCOPIC MODEL

As a first step in constructing a microscopic model for a tunneling system coupled to the electrons, we write the Hamiltonian in a first quantized form as

$$H = -\frac{1}{2M}\Delta_R - \sum_i \frac{1}{2m}\Delta_i + U(\mathbf{R}) + \sum_i V(\mathbf{r}_i - \mathbf{R}) + \sum_{j\neq 0}\sum_i V(\mathbf{r}_i - \mathbf{R}_j), \tag{12}$$

where $\mathbf{R}$ denotes the coordinate of the tunneling atom, and $\mathbf{r}_i$'s are the coordinates of the conduction electrons. We treat the motion of the tunneling atom quantum mechanically, however, we assume that all other atoms are immobile, and their position $\mathbf{R}_j$ ($j\neq 1$) is a constant classical variable. The tunneling atom has a mass M and moves in the double well potential $U(\mathbf{R})$ formed by the rest of the ions. In the Hamiltonian (12), we also assumed that electrons form a Fermi liquid and, thus, neglected the electron-electron interaction, which is supposed to be included in the effective electron-ion interaction potential $V(\mathbf{r}-\mathbf{R})$ at the Hartree or Hartree-Fock level.

To simplify this Hamiltonian, as a first step, we rewrite Eq. (12) as $H=H_0+H_{\rm int}$ with

$$H_0 = -\frac{1}{2M}\Delta_R + U(\mathbf{R}) - \sum_i \frac{1}{2m}\Delta_i + \sum_{j\geqslant 0}\sum_i V(\mathbf{r}_i - \mathbf{R}_j), \tag{13}$$

$$H_{\rm int} = \sum_i [V(\mathbf{r}_i - \mathbf{R}) - V(\mathbf{r}_i - \mathbf{R}_0)], \tag{14}$$

where $\mathbf{R}_0$ is a somewhat arbitrary "reference position" of the ion, which is chosen to minimize the interaction part $H_{\rm int}$. A natural choice is, of course, to choose $\mathbf{R}_0$ to correspond to the maximum of the barrier in $U(\mathbf{R})$. Clearly, the noninteracting part H_0 can be diagonalized.

To make further progress, we shall adopt a tight-binding scheme for the atom. Though this approach is justified by the observation that the tunneling impurity moves in a small *cavity*, our analysis does not rely on it, and our conclusions are independent of this approximation. To arrive at a tight-binding Hamiltonian, we first solve the atomic Schrödinger equation

$$\left(-\frac{1}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}-\mathbf{R}_0)\right)\varphi_\mu(\mathbf{r}) = \epsilon_\mu \varphi_\mu(\mathbf{r}), \tag{15}$$

where ϵ_μ labels the atomic levels. The states φ_μ above are atomic eigenstates centered at the tunneling atom. As a next step, we solve the Schrödinger equation for the rest of the conduction electrons without making any approximation,

$$\left(-\frac{1}{2m}\Delta_{\mathbf{r}} + \sum_{j\neq 0} V(\mathbf{r}-\mathbf{R}_j)\right)\eta_n(\mathbf{r}) = \xi_n \eta_n(\mathbf{r}). \tag{16}$$

Then, using the wave functions φ_μ and η_n, we can compute the appropriate overlap matrix elements and construct the following tight-binding Hamiltonian for the conduction electrons:

$$H_0^{\rm el} = \sum_{\mu,\sigma} \epsilon_\mu d^\dagger_{\mu,\sigma} d_{\mu,\sigma} + \sum_{n,\sigma} \xi_n c^\dagger_{n,\sigma} c_{n,\sigma} + \sum_{\mu,n,\sigma} (t_{n,\mu} c^\dagger_{n,\sigma} d_{\mu,\sigma} + \text{H.c.}), \tag{17}$$

where $c^\dagger_{n,\sigma}$ denotes the creation operator of a conduction electron in the (extended) state n with spin σ, $d^\dagger_{\mu,\sigma}$ creates a conduction electron at the atomic orbital μ, and $t_{n,\mu}$ denotes the corresponding hopping matrix element. Since the interaction part $H_{\rm int}$ is large only at the position of the tunneling impurity, we can integrate out all electrons $c^\dagger_{n,\sigma}$ and arrive at the following imaginary time effective action for the d levels:

$$S^0_{\rm eff} = -\sum_{\mu,\mu',\sigma} \int_0^\beta d\tau \int_0^\beta d\tau' \bar{d}_{\mu\sigma}(\tau) \mathcal{G}^{-1}_{\mu\mu'}(\tau-\tau') d_{\mu'\sigma}(\tau'), \tag{18}$$

where $\mathcal{G}_{\mu\mu'}$ denotes the local propagator of the d levels, which can be expressed in Fourier space as

$$\mathcal{G}^{-1}_{\mu\mu'}(i\omega_n) = i\omega_n - \epsilon_\mu \delta_{\mu\mu'} - \sum_n t^*_{n,\mu} \frac{1}{i\omega_n - \xi_n} t_{n,\mu'}. \tag{19}$$

This Green's function can be written even more conveniently in a spectral representation as

$$\mathcal{G}_{\mu\mu'}(i\omega_n) = \int_{-\infty}^{\infty} d\omega \frac{\varrho_{\mu\mu'}(\omega)}{i\omega_n - \omega}. \tag{20}$$

It is this spectral function $\varrho_{\mu\mu'}(\omega)$ which contains the resonance discussed in Sec. I, and which solely determines the low-temperature properties of the tunneling system.

In the following, we shall consider the simplest case, where the tunneling system is fully symmetrical. We first diagonalize the Hamiltonian of the tunneling atom,

$$\left(-\frac{1}{2M}\Delta_R + U(\mathbf{R})\right)\Phi_\alpha(\mathbf{R}) = E_\alpha \Phi_\alpha(\mathbf{R}). \tag{21}$$

In principle, we could formulate our theory by keeping all levels of the tunneling particle,[27] However, at low enough temperatures, only the two lowest lying even and odd states, Φ_e and Φ_o, matter, and the role of all other eigenstates is to reduce the electronic cutoff to a value of the order of the Debye frequency, $D_0 \to \omega_0$.[16,23] Therefore, in the following,

we shall keep only these two states. To obtain the usual tunneling form that occurs in Eq. (1), we introduce the left and right states $\Phi_{\tau=\pm}$

$$\Phi_{\pm} \equiv \frac{1}{\sqrt{2}}(\Phi_e - \Phi_o), \tag{22}$$

which transform into each other under reflection, and rewrite the Hamiltonian, Eq. (21), in this restricted subspace as

$$H_0^{\text{tun}} = -\frac{\Delta_0}{2}\tau_x, \tag{23}$$

with τ_x as the Pauli matrix. The tunneling amplitude $\Delta_0 = E_o - E_e$ is approximately given by Eq. (3).[13]

Having diagonalized the noninteracting part (13) of the Hamiltonian, we now turn to the analysis of the interaction part. First, we shall simplify our treatment by keeping only those two even and odd electronic states d_μ ($\mu = e, o$), which couple the most strongly to the tunneling particle. In a real system, these correspond to the most strongly coupled d and p states or s and p states. In case of a p state, e.g., it is clear that the p state aligned along the tunneling axis couples the most strongly to the motion of the atom. Due to the assumed spatial symmetry of the Hamiltonian, the corresponding spectral function is diagonal in the index μ, $\varrho_{\mu\mu'} = \delta_{\mu\mu'}\varrho_\mu$. We shall assume, furthermore, that at least one of the spectral densities, say ϱ_o contains a *resonance* of width Γ, while the other one is approximately constant, $\varrho_e \approx \varrho_0 \sim 1/E_F$,

$$\varrho_o(\omega) = \frac{1}{2\pi}\frac{\Gamma}{\omega^2 + \Gamma^2/4}, \tag{24}$$

$$\varrho_e(\omega) = \varrho_0. \tag{25}$$

To construct the interaction part of the Hamiltonian in this restricted basis, we have to compute matrix elements of H_{int} given by Eq. (14). Assuming that the tunneling distance is small, we can approximate H_{int} as

$$H_{\text{int}} \approx -\sum_{q=x,y,z} R_q \frac{\partial V}{\partial r_q} + \frac{1}{2}\sum_{p,q=x,y,z} R_p R_q \frac{\partial^2 V}{\partial r_p \partial r_q} + \cdots, \tag{26}$$

and then compute the appropriate matrix elements to obtain the effective Hamiltonian as

$$H_{\text{int}} \approx A(|\Phi_e\rangle\langle\Phi_o| + |\Phi_o\rangle\langle\Phi_e|)(d_{e\sigma}^\dagger d_{o\sigma} + d_{o\sigma}^\dagger d_{e\sigma}) + (B_e|\Phi_e\rangle \times\langle\Phi_e| + B_o|\Phi_o\rangle\langle\Phi_o|)(C_e d_{e\sigma}^\dagger d_{e\sigma} + C_o d_{o\sigma}^\dagger d_{o\sigma}),$$

where summation is assumed over repeated spin indices, and the constants A, $B_{e/o}$ and $C_{e/o}$ are given by the following integrals:

$$A = -\langle\Phi_e|R_z|\Phi_o\rangle\langle\varphi_e|\frac{\partial V(\mathbf{r})}{\partial r_z}|\varphi_o\rangle, \tag{27}$$

$$B_{e/o} = \frac{1}{2}\langle\Phi_{e/o}|R_z^2|\Phi_{e/o}\rangle, \tag{28}$$

$$C_{e/o} = \langle\varphi_{e/o}|\frac{\partial^2 V(\mathbf{r})}{(\partial r_z)^2}|\varphi_{e/o}\rangle. \tag{29}$$

This Hamiltonian can easily brought to the form, Eq. (1), if we notice that only electronic excitations with energies $< \omega_0$ contribute to the orbital Kondo correlations.[16] Therefore, if the width of the resonance is broader than the attempt frequency, $\Gamma > \omega_0 \sim 100$ K ~ 0.01 eV, then we can introduce the new fermionic fields normalized according to Eq. (2)

$$d_{e\sigma} \to \psi_{e\sigma} \equiv d_{e\sigma}/\sqrt{\varrho_e}, \quad d_{o\sigma} \to \psi_{o\sigma} \equiv d_{o\sigma}/\sqrt{\varrho_o}, \tag{30}$$

where ϱ_e and ϱ_o denote the density of states at the Fermi energy in the even and odd channels, respectively. In terms of these fields, the interaction Hamiltonian takes on the form Eq. (1), with the couplings v_x and v_z given by

$$v_z = A\sqrt{\varrho_e \varrho_o},$$

$$v_x = \frac{1}{4}(B_e - B_o)(C_e\varrho_e - C_o\varrho_o). \tag{31}$$

There are two more terms that appear in addition to these two terms, both of which are small: One is a simple potential scattering term, $\sim(\psi_e^\dagger\psi_e - \psi_o^\dagger\psi_o)$, that only renormalizes the spectral densities ϱ_o and ϱ_e and can be eliminated by a simple counterterm procedure. The other term is proportional to $\sim\tau_x(\psi_e^\dagger\psi_e + \psi_o^\dagger\psi_o)$ and gives a small renormalization of the double well potential $U(\mathbf{R})$.[23] This term can be taken into account at the Hartree level and is of no importance. In the following, we shall, therefore, keep only the two couplings v_x and v_z in Eq. (31).

Note that the above procedure of integrating out the electrons $c_{n,\sigma}$ and then rescaling the couplings is just a technical trick to extract the dimensionless couplings and to derive quickly the scaling equations. However, one can proceed in the usual way and obtain the dimensionless couplings by analysis of the structure of the dimensionless vertex functions, as in Refs. 23 and 28.

The couplings v_z and v_x can be estimated along similar lines as in Refs. 13 and 15, and one obtains

$$v_z \approx \sqrt{\varrho_e\varrho_o}\langle\varphi_e|d\frac{\partial V(\mathbf{r})}{\partial r_z}|\varphi_o\rangle, \tag{32}$$

$$v_x \approx -\Delta_0\frac{\lambda}{16}\frac{1}{V_B}\varrho_o\langle\varphi_o|d^2\frac{\partial^2 V(\mathbf{r})}{(\partial r_z)^2}|\varphi_o\rangle, \tag{33}$$

where in the second equation, we assumed a quartic double well potential with barrier height V_B and displayed only the contribution of the odd channel. The constant d in Eqs. (32) and (33) denotes the tunneling distance. A similar but smaller contribution is given by the nonresonant even channel. Remarkably, the matrix elements above are expressed in terms of the atomic (tight-binding) orbitals of the tunneling atom. They can be easily estimated assuming a simple Coulomb interaction, $V(\mathbf{r}) = -e^2/r$, and hydrogen-like wave functions. Taking the $1s$ and $2p$ orbitals, e.g., we find

$$\langle 2p|\frac{\partial V(\mathbf{r})}{\partial r_z}|1s\rangle = \frac{e^2}{a_0}\frac{4}{27\sqrt{2}a_0} \approx 5.4\frac{\text{eV}}{\text{Å}}, \tag{34}$$

$$\langle 2p|\frac{\partial^2 V(\mathbf{r})}{(\partial r_z)^2}|2p\rangle = -\frac{e^2}{a_0}\frac{1}{40a_0^2} \approx -2.43\frac{\text{eV}}{\text{Å}^2}, \tag{35}$$

where a_0 is the Bohr radius.

It is not difficult to show that even for a wide resonance with $\Gamma \sim 1000-10\,000$ K and $d \sim 0.3$ Å, v_x is about the same as the dimensionless tunneling Δ_0/ω_0. More importantly, however, v_z is proportional to $1/\sqrt{\Gamma}$. Therefore, if the conduction electrons scatter resonantly off the tunneling atom, then the value of v_z can become large, and eventually become larger than the critical value corresponding to the Emery-Kivelson line mentioned in the Introduction, $v_{z,c} = 1/\pi$. For typical parameters, this transition takes place where the width of the resonance is around $\Gamma \sim 1000-10\,000$ K.

Throughout this paper, we shall assume that $\Gamma > \omega_0$, i.e., that the resonance is relatively broad compared to typical frequencies related to atomic motion. Under these conditions, the cutoff energy is given by ω_0 and the couplings between the tunneling system and the electrons can be safely approximated by their values at the Fermi energy.

The above large increase in the effective couplings can be understood as a simple matrix element effect and is related to the well-known structure of scattering states: To clarify this point, let us consider the textbook example of scattering states in the s channel of a simple spherically symmetric potential scatterer, $U(r)=V\delta(r-r_0)$. The scattering wave functions in this simple case take the form $\sin(kr+\delta)/r$ and $b\sin(kr)/r$ for $r>r_0$ and $r<r_0$, respectively, with k as the radial momentum of the electrons and δ as the scattering phase shift. The amplitude b^2 of the wave function inside the sphere is given by the expression,

$$b^2 = \frac{k^2}{k^2 + V^2\sin^2(k) + 2kV\sin(2k)}, \tag{36}$$

where we used units of $r_0=2m=\hbar=1$. For $V\equiv 0$, the amplitude of the wave function is simply 1. However, for larger values of V, a resonance appears, and b^2 displays a sharp peak as a function of energy (Fig. 4). It is a trivial matter to show that the amplitude b of the resonance is simply related to the width Γ of the resonance, $b \sim 1/\sqrt{\Gamma}$, and becomes larger and larger for sharper and sharper resonances. This large factor b shows up in the local density of states and also any matrix element computed in terms of the appropriately normalized scattering states and results in an increase of all couplings, provided that the resonance appears at the Fermi energy.

III. NONPERTURBATIVE SCALING ANALYSIS

We have seen in Sec. II that for resonant scattering from the tunneling impurity the coupling, v_z can be very large. In this case, the perturbative scaling equations, Eqs. (6) and (7), are insufficient and a new approach is needed. Fortunately, for $\tilde{\Delta}_0$, $v_x \ll 1$, one can construct scaling equations which are *nonperturbative* in the coupling v_z by generalizing the computations of Yuval and Anderson.[18,29] In this limit, one obtains the following scaling equations:[18]

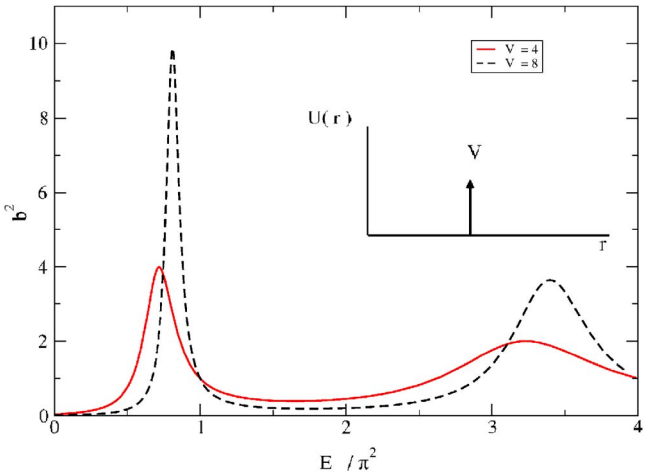

FIG. 4. (Color online) Amplitude b^2 of the scattering state of the conduction electrons at the origin in a simple scattering state model. The amplitude of the scattering state at the origin increases as the resonance gets sharper and sharper. The inset shows the potential producing the resonance.

$$\frac{d\tilde{\Delta}_0}{dl} = \left[1 - 8\left(\frac{\delta}{\pi}\right)^2\right]\tilde{\Delta}_0, \tag{37}$$

$$\frac{dv_x}{dl} = 4\frac{\delta}{\pi}v_y - 8\left(\frac{\delta}{\pi}\right)^2 v_x, \tag{38}$$

$$\frac{dv_y}{dl} = 4\frac{\delta}{\pi}v_x - 8\left(\frac{\delta}{\pi}\right)^2 v_y, \tag{39}$$

with the phase shift δ defined as $\delta=\arctan(\pi v_z)$. Here we neglected terms of order $O(v_x^2, v_y^2, \tilde{\Delta}_0^2)$. These terms give rise to a renormalization of δ in the strong coupling regime and slightly change the numerical values of the various energy scales we estimate, but do not affect their overall scale and the picture obtained using the above equations. Equations (38) and (39) can be rewritten in terms of the average coupling, $v_\perp \equiv (v_x+v_y)/2$, and the asymmetry, $v_- \equiv (v_x-v_y)/2$, as

$$\frac{dv_\perp}{dl} = \left[4\frac{\delta}{\pi} - 8\left(\frac{\delta}{\pi}\right)^2\right]v_\perp, \tag{40}$$

$$\frac{dv_-}{dl} = -\left[4\frac{\delta}{\pi} + 8\left(\frac{\delta}{\pi}\right)^2\right]v_-. \tag{41}$$

In other words, the anisotropy $v_x \neq v_y$ is *irrelevant*, while the average coupling $v_\perp$ is relevant. Therefore, the two couplings v_x and v_y become rapidly equal in the initial stage of the scaling. Equations (40) and (41) are only valid below the scale $D \approx \omega_0$; above this energy scale, the couplings v_x, v_y remain unrenormalized, while $\tilde{\Delta}_0$ transforms according to its engineering dimension and satisfies Eq. (8). Therefore, Eqs. (40) and (41) must be solved with the initial conditions $D=\omega_0$, $\tilde{\Delta}_0(\omega_0)=\Delta_0/\omega_0 \sim e^{-\lambda}$, $v_y(\omega_0)=0$, and $v_x(\omega_0)$ given by Eq. (33).

From Eqs. (37) and (38), we see that the value $v_z = 1/\pi$ corresponding to $\delta = \pi/4$ is very special: For $\delta < \pi/4$, the scaling dimension of $\tilde{\Delta}_0$ is always larger than that of v_x, and therefore, tunneling is always more relevant than assisted tunneling. As a result, the motion of the tunneling system freezes out at an energy scale $\Delta_0^* \ll \Delta_0$

$$\Delta_0^* = \Delta_{0,>}^* \equiv \Delta_0 \left(\frac{\Delta_0}{\omega_c}\right)^{\alpha}, \quad \alpha = \frac{8\left(\frac{\delta}{\pi}\right)^2}{1 - 8\left(\frac{\delta}{\pi}\right)^2}, \tag{42}$$

where the assisted tunneling is still small compared to unity, and thus, the system is far from the two-channel Kondo fixed point.

Equation (42) only makes sense if $\Delta_0^* > T_K$. This is always the case for $\delta < \pi/4$. If, however, $\delta > \pi/4$, then the physics can become very different. In this case, v_x grows *faster* than $\tilde{\Delta}_0$, so $v_x \sim 1$ can be satisfied first. The condition $v_x \sim 1$ defines the so-called Kondo temperature

$$T_K \approx \omega_o \left(\frac{v_x}{2}\right)^{\gamma}, \quad \gamma^{-1} = 4\frac{\delta}{\pi} - 8\left(\frac{\delta}{\pi}\right)^2, \tag{43}$$

where the renormalized tunneling satisfies

$$\Delta_0(T_K) \approx T_K \frac{2\Delta_0}{\omega_0 v_x}\left(\frac{v_x}{2}\right)^{\beta}, \quad \beta = \frac{4\frac{\delta}{\pi} - 1}{4\frac{\delta}{\pi}\left(1 - 2\frac{\delta}{\pi}\right)}. \tag{44}$$

From this equation, it is obvious that for $\delta > \pi/4$ the effective tunneling amplitude is usually still small at the energy scale $T \sim T_K$ compared to the temperature itself. Below the Kondo energy T_K the scaling equations are governed by the two-channel Kondo fixed point. There the tunneling is still relevant and has a scaling dimension 1/2 and, therefore, its scaling equation must be replaced by[15]

$$\frac{d\tilde{\Delta}_0}{dl} = \frac{1}{2}\tilde{\Delta}_0, \quad (D < T_K). \tag{45}$$

Integrating this equation, we obtain for the renormalized tunneling amplitude for the case $\Delta_0^* < T_K$,

$$\Delta_{0,<}^* \approx T_K \left(\frac{2\tilde{\Delta}_0}{v_x}\right)^2 \left(\frac{v_x}{2}\right)^{2\beta} \ll T_K, \tag{46}$$

From our discussions, it immediately follows that in the tunneling regime for a symmetrical tunneling center with $v_z > v_{z,c}$ there is typically *a large temperature window*, $\Delta_0^* < T < T_K$, where the two-channel Kondo fixed point rules and the non-Fermi liquid properties such as the $\sim\sqrt{T}$ resistivity anomaly associated with the two-channel Kondo fixed point should be manifest. We have to emphasize, however, that below the scale Δ_0^*, the physics becomes again that of a boring Fermi liquid. The corresponding crossover lines were sketched in Fig. 3 for typical parameters of the tunneling system. As one can see in the figure, there is a large region in the parameter space, which is governed by the two-channel Kondo behavior. This region increases even further for smaller values of $\tilde{\Delta}_0 \sim v_x$, however, it also shifts toward smaller values of T_K.

Before we conclude this section, let us discuss another important issue, raised by Moustakas and Fisher.[25] Moustakas and Fisher observed that at the two-channel Kondo fixed point, a special two-electron scattering of the form

$$H_2 = \frac{\tilde{\Delta}_2}{D_0}\tau_x(\psi_{+\uparrow}^\dagger \psi_{+\downarrow}^\dagger \psi_{-\downarrow}\psi_{-\uparrow} + \text{H.c.}) \tag{47}$$

is also relevant, and that for $\delta > \pi/4$ this operator is *more relevant* than the tunneling $\tilde{\Delta}_0$ discussed above. The coupling $\tilde{\Delta}_2$ above denotes a dimensionless coupling constant, and its bare value can be estimated to be around v_x, while the energy scale D_0 is of the order of the Fermi energy E_F. Below the energy scale $D = \omega_0$, this operator satisfies the scaling equation

$$\frac{d\tilde{\Delta}_2}{dl} = \left[-1 + 8\frac{\delta}{\pi} - 8\left(\frac{\delta}{\pi}\right)^2\right]\tilde{\Delta}_2. \tag{48}$$

Fortunately, this operator is *irrelevant* at high energies, $\omega_0 < D$, where its scaling dimension is simply -1,

$$\frac{d\tilde{\Delta}_2}{dl} = -\tilde{\Delta}_2, \quad (D > \omega_0). \tag{49}$$

As a result, by the time we get into the regime $D < \omega_0$, this two-electron process is reduced by a factor $\omega_0/D_0 \sim 10^{-3}$ compared to v_x.

Below ω_0, this process becomes relevant and generates a crossover to a Fermi liquid at an energy scale Δ_2^*. Similar to Δ_0^*, we have to distinguish two possibilities. For larger values of δ, $T_K < \Delta_2^*$, and Δ_2^* is given by the following expression:

$$\Delta_2^* \approx \Delta_{2,>}^* \equiv \omega_0 \left(\frac{\omega_0}{E_F}\tilde{\Delta}_2\right)^{\kappa}, \tag{50}$$

$$\kappa^{-1} = 8\frac{\delta}{\pi} - 8\left(\frac{\delta}{\pi}\right)^2 - 1. \tag{51}$$

However, this formula is not correct if $T_K > \Delta_2^*$, since $\tilde{\Delta}_2$ has scaling dimension 1/2 below the Kondo temperature.[25] Carrying out an analysis similar to the case of $\Delta_0^* < T_K$, we find in this regime that

$$\Delta_2^* \approx \Delta_{2,<}^* \equiv \omega_0 \left(\frac{\omega_0}{E_F}\tilde{\Delta}_2\right)^2 \left(\frac{v_x}{2}\right)^{\rho},$$

$$\rho = \frac{3 + 16\left(\frac{\delta}{\pi}\right)^2 - 16\frac{\delta}{\pi}}{4\frac{\delta}{\pi} - 8\left(\frac{\delta}{\pi}\right)^2}. \tag{52}$$

The corresponding crossover line is also shown in Fig. 3. As one can see, Δ_2 does not play a significant role in the regime where T_K is the largest, however, for larger values of δ it is indeed Δ_2 that provides an infrared cutoff for the two-channel Kondo behavior.

IV. CONCLUSION

In the present paper, we constructed a theory which describes the low-temperature behavior of a tunneling particle with resonant scattering. We have shown that the resonance plays a crucial role in the physics of the tunneling center. While the local density of states of the resonant atomic state has a huge peak inversely proportional to the width of the resonance, $\varrho_d \sim 1/\Gamma$, the density of states of the corresponding conduction electrons is strongly suppressed, and thus, the tunneling atom couples the most efficiently to its own electronic state. Despite this complication, after a proper treatment of the electron-tunneling particle interaction, we arrive at the original model of Vladár and Zawadowski. However, our treatment does not rely on the free electron approximation, the various coupling constants can be large and they are determined by atomic integrals.

As we have shown, the resonant scattering can completely change the physics of the tunneling impurity and push it in the nonperturbative regime. While in the weak coupling regime, the tunneling always intervenes before we enter the two-channel Kondo regime, in this nonperturbative regime, the two-channel Kondo behavior usually dominates over the spontaneous tunneling over a wide temperature range of possibly several decades for physically relevant parameters. We emphasize again that a model where the tunneling center interacts with some local interaction with a free electron gas is unable to capture this behavior.[24,29] The physical reason for this is simply that electrons are *not free*. Even if we do not move the tunneling atom, the electron's wave function is adjusted to the atomic potential of the tunneling impurity. This effect has been heuristically taken into account in Ref. 23, where only the *change* in the scattering potential has been considered as a perturbation, without justifying this approach. Also, the simple potential scattering model is unable to take into account the dynamics (retardation effects) of the electronic states at the tunneling impurity itself, which one actually tries to eliminate from the theory.

It is not quite clear what the origin of such a resonant level could be in practice. In the point contact measurements, one natural candidate would be hydrogen. Hydrogen is small enough, can diffuse into the substrate, and is known to have a phase shift $\pi/2$ in the s channel.[30] [This phase shift, which just characterizes the atomic scattering off a hydrogen ion is not to be confused with the phase shift δ corresponding to v_z.] Moreover, hydrogen is light: This implies that the cutoff ω_0 can be in the range of $\omega_0 \sim 1000$ K. As a result, all temperature scales can be about an order of magnitude larger for hydrogen than the ones in Fig. 3, and T_K can be easily in the range of a few Kelvins. Being light, hydrogen can tunnel over relatively large distances, $d \sim 1$ Å, implying that v_z is presumably large even if the resonance is very broad. In fact, in the point contact experiments, it is very difficult to exclude the presence of hydrogen in the course of sample preparation,[31] and recent experiments on hydrogen doped palladium point contacts indeed exhibit zero bias anomalies associated with the presence of hydrogen.[26] However, more detailed calculations would be needed to estimate the size of the coupling v_z for tunneling hydrogen.

Tunneling systems with small effective masses can be formed by dislocations too.[32] In this case, however, the spatial extent of the defect can be large, and it is not quite clear how the two orbital scattering channels driving the two-channel Kondo effect could be selected.

Other natural candidates would be impurities with strong magnetic correlations, i.e., Kondo-type impurities. In this scenario, two types of Kondo effect take place: (i) a *magnetic* Kondo effect with a large Kondo temperature, T_K^{magn}, and (ii) the *orbital* Kondo effect discussed so far at a much smaller energy scale, $T_K^{\mathrm{orb}} \ll T_K^{\mathrm{magn}}$. The magnetic Kondo resonance would provide the resonance needed for the orbital Kondo effect, and the magnetic correlations serve only to boost up the couplings of the tunneling system and generate an *orbital Kondo effect* at lower temperatures. Above the magnetic Kondo temperature, $T > T_K^{\mathrm{magn}}$, magnetic scattering provides also a strong inelastic scattering. Correspondingly, there is a temperature-dependent time scale, $\tau_{\mathrm{spin}}(T)$ at which the spin of a conduction electron is flipped. These spin-flip processes could, in principle, destroy the two-channel Kondo behavior. To be able to neglect these spin-flip processes, one needs to satisfy the criterion $1/\tau_{\mathrm{flip}}(T) < T$ at all temperatures. Luckily enough, the rate $1/\tau_{\mathrm{flip}}(T)$ is suppressed below the Kondo scale. Unfortunately, however, to our knowledge, this spin-flip rate has never been determined so far reliably. However, one can obtain a simple estimate for it using the knowledge about the inelastic scattering cross section.[33] From these considerations, one concludes that well below T_K, in the Fermi liquid range, the spin-flip rate must scale as $\sim T^2/T_K$, while in the vicinity of T_K, it must be of the order of $1/\tau_{\mathrm{spin}}(T) \sim T$. Above T_K, this rate must scale to zero logarithmically. From these considerations, it appears that the criterion $1/\tau_{\mathrm{flip}}(T) < T$ is always satisfied, and one can, therefore, probably safely neglect spin-flip scattering processes. We have to emphasize though that these impurities do not need to be Kondo impurities in the usual sense, since the width of the magnetic "Kondo resonance" can be in the range of thousands of Kelvins or even larger. For such a correlated impurity, the local density of states remains unrenormalized.[34] However, there is a strong *field renormalization* proportional to the Z factor, $Z \sim T_K^{\mathrm{magn}}/E_F$, which ultimately rescales v_z as $v_z \to v_z/\sqrt{Z}$. We emphasize again that even an extremely large (magnetic) Kondo temperature in the range $\sim 1000-10\,000$ K could give rise to the phenomena discussed in this paper, and therefore, the usual transport and specific heat anomalies associated with the magnetic Kondo effect may be hardly observed in this case.

In the case of a tunneling system with strong magnetic correlations, the zero bias anomaly may be very sensitive to the external field too. The reason is that, in this case, the density of states and thus the couplings in the two spin channels may depend rather sensitively on the applied magnetic field. This translates to a channel anisotropy in the effective two-channel Kondo model and drives the system to a Fermi liquid. This may possibly explain the strong magnetic field dependence in some experiments.[1]

Strongly coupled electron-phonon systems have also been proposed as possible candidates to produce an orbital Kondo effect.[35] In this case, the two-level systems form dynamically. It is, however, not clear how the regime of extremely strong electron-phonon coupling needed can be reached. Fur-

thermore, in these studies, only a few vibrational modes could be considered, which has been shown to be insufficient to produce the correct low-temperature behavior.[16,23]

Finally, let us comment on the presence of the splitting Δ_z. In our previous analysis, we completely neglected the asymmetry of the tunneling centers. In lattice structures such as in Refs. 7–9, Δ_z can be rather small. However, in a disordered point contact, Δ_z has a random distribution and should provide a low energy cutoff for the non-Fermi liquid properties similar to the spontaneous tunneling. Therefore, a breakdown of universal scaling is expected due to the presence of Δ_z. Such a breakdown of universal scaling has indeed been observed in Ti point contacts,[2] where the zero bias anomaly did not depend on the presence of an external magnetic field, was sensitive to electromigration, and had an amplitude consistent with the presence of just a few tunneling centers. These experiments seem to be in perfect agreement with all predictions of the two-level system model. However, it is much harder to explain the origin of the zero bias anomaly in Cu samples.[1] While the sensitivity to the magnetic field could be explained assuming that the tunneling impurities have a sharp resonance, the zero bias anomaly in these experiments has a very large amplitude, and as pointed out by Smolyarenko and Wingreen,[36] the observed anomalous resistivity exponent close to $1/2$ can hardly be understood assuming a completely random distribution of Δ_z.

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