Kondo Effect in Quantum Dots at High Voltage: Universality and Scaling

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We examine the properties of a dc-biased quantum dot in the Coulomb blockade regime. For voltages V that are large compared to the Kondo temperature T_K , the physics is governed by the scales V and γ , where $\gamma \sim V/\ln^2(V/T_K)$ is the nonequilibrium decoherence rate induced by the voltage-driven current. Based on scaling arguments, self-consistent perturbation theory, and perturbative renormalization group, we argue that due to the large γ the system can be described by renormalized perturbation theory in $1/\ln(V/T_K) \ll 1$. However, in certain variants of the Kondo problem, two-channel Kondo physics is induced by a large voltage V.

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In recent years, it became possible to observe the Kondo effect in quantum dots in the Coulomb blockade regime [1–4]. These systems allow one to investigate how nonequilibrium induced by external currents and bias voltages influences the Kondo physics. Similarly, the experimentally observed anomalies of the energy relaxation in strongly voltage-biased mesoscopic wires [5] have recently been shown [6] to be caused by scattering from magnetic impurities or two-level systems.

In equilibrium, almost all properties of the Kondo effect are well understood, and the Kondo model together with the methods used to solve it [e.g., renormalization group (RG), Bethe ansatz, conformal field theory, bosonization, density matrix RG, flow equations, or slave particle techniques] have become one of the central paradigms in condensed matter theory. However, in nonequilibrium many of the above-mentioned methods fail, and despite the experimental and theoretical relevance and a substantial body of theoretical work [7-16], several even qualitative questions about the Kondo effect in nonequilibrium have remained controversial. Recently, Coleman et al. [14] claimed that the Kondo model at high voltages $V \gg T_K$ cannot be described by (renormalized) perturbation theory (PT) but is characterized by a new two-channel Kondo fixed point (see also [13]). By contrast, Kaminski et al. [8] argue that the nonequilibrium decoherence rate γ destroys the Kondo effect. We will show in the following that the Kondo effect is indeed destroyed in the case of the usual Anderson model, but for certain variants of the Kondo model, where the current at high bias is suppressed, the scenario proposed in [14] appears to be recovered.

We model the quantum dot using the Anderson model

$$H_{A} = H_{0} + \varepsilon_{d} \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + \sum_{\alpha k \sigma} (t_{\alpha} c_{\alpha k \sigma}^{\dagger} d_{\sigma} + \text{H.c.}) + U n_{d\uparrow} n_{d\downarrow}, \qquad (1)$$

where $H_0 = \sum_{\alpha k\sigma} \varepsilon_{\alpha k} c^{\dagger}_{\alpha k\sigma} c_{\alpha k\sigma}$ is the Hamiltonian of the electrons in the left and right leads, $\alpha = L, R$, characterized by a dc bias voltage V, $\varepsilon_{L/Rk} = \varepsilon_k \pm V/2$, respectively. We will consider only symmetrical dots with

tunneling matrix elements $t_L = t_R \equiv t$. The negative ε_d with $|\varepsilon_d| \gg \Gamma = 2\pi N_0 t^2$, where N_0 is the electron density of states in the leads, and the large Coulomb repulsion $U \to \infty$ enforces the number of electrons $n_d = \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma}$ in the dot level to be approximately 1.

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In this regime, the local degree of freedom of the quantum dot is a spin $\vec{S} = \frac{1}{2} \sum_{\sigma,\sigma'} d_{\sigma}^{\dagger} \vec{\sigma}_{\sigma\sigma'} d_{\sigma'}$, where $\vec{\sigma}$ is the vector of Pauli matrices, and the low-energy properties of H_A are well described by the two-lead Kondo (or Coqblin-Schrieffer) model,

$$H_K = H_0 + V_0 \sum_{\sigma} (c_{L0\sigma}^{\dagger} + c_{R0\sigma}^{\dagger}) (c_{L0\sigma} + c_{R0\sigma})$$

$$+ \vec{S} \cdot \sum_{\sigma\sigma'} \left[J_L c_{L0\sigma}^{\dagger} \frac{\vec{\sigma}_{\sigma\sigma'}}{2} c_{L0\sigma'} + J_{LR} c_{L0\sigma}^{\dagger} \frac{\vec{\sigma}_{\sigma\sigma'}}{2} c_{R0\sigma'} \right] + (L \leftrightarrow R),$$
(2)

In the first part of the paper, we investigate in detail the Anderson model in the Kondo regime at high voltages using the so-called noncrossing approximation (NCA). In the second part we will use the insight gained from this analysis to study a heuristic version of "poor man's scaling" in nonequilibrium for a Kondo model with $J_{LR} < J_{L/R}$. To derive NCA, one first rewrites H_A in the limit $U \to \infty$

To derive NCA, one first rewrites H_A in the limit $U \to \infty$ using a so-called pseudofermion f_{σ} and a spinless slave

boson b with $d_{\sigma} = b^{\dagger}f_{\sigma}$, subject to the constraint $Q = \sum_{\sigma} f_{\sigma}^{\dagger}f_{\sigma} + b^{\dagger}b = 1$. The Anderson model then takes the form $H_A = H_0 + \varepsilon_d b^{\dagger}b + \sum_{\alpha,\sigma} (V_{\alpha}c_{\alpha\sigma0}^{\dagger}b^{\dagger}f_{\sigma} + \text{H.c.})$. In this language, the NCA is just the lowest-order self-consistent PT in t_{α} , where the constraint Q = 1 is taken into account exactly. While the NCA fails to describe the low-energy Fermi liquid fixed point in the Kondo regime correctly [17], it gives reliable results (with errors of the order of 10%) in equilibrium for temperatures down to a fraction of T_K . As a self-consistent and conserving approximation, it also displays the correct scaling behavior and reproduces the relevant energy scales.

While the NCA equations in nonequilibrium have been solved by many groups [15], we are not aware of any careful analysis of the relevant scales at high bias voltage, which is central for a qualitative understanding of the nonequilibrium Kondo effect. Generally, the NCA equations have to be solved numerically; however, in the limit of extremely high voltage, $\ln V/T_K \gg 1$ (but $V \ll D$), an analytical solution is possible: the problem is in the weak coupling regime. Finite V induces an inelastic spin relaxation or decoherence rate. Since in NCA the spin density is just a convolution of the pseudofermion propagators, this rate is given by $2 \operatorname{Im} \Sigma_f(0) = 2\gamma$, with Σ_f the pseudofermion self-energy. We start by calculating the retarded self-energy $\Sigma_b^r(\omega)$ of the boson, using the fact that (as shown below) the spectral function of the pseudofermion is a sharp peak of width $\gamma \ll V$. Throughout we consider the low temperature limit, T=0, and obtain $\text{Im}\Sigma_b^r(\omega)\approx$ $-\pi J N_0 |\varepsilon_d| [f_L^{\gamma}(-\omega) + f_R^{\gamma}(-\omega)],$ where $f_{R/L}^{\gamma}$ are the Fermi functions in the left and right leads, broadened by γ . The step function in $\mathrm{Im}\Sigma_b^r(\omega)$ leads to logarithmic contributions to $\text{Re}\Sigma_b^r(\omega)$, cut off by γ and the band width D. Using relations like $1 - 2N_0J \ln[D/|\omega|] =$ $2N_0J \ln[|\omega|/T_K]$ one obtains for the real part of the boson propagator $G_b^r(\omega)$, for $\ln V/T_K \gg 1$,

$$N_0 J_{\rm eff}^{\rm NCA}(\omega) \equiv 2N_0 t^2 \operatorname{Re} G_b^r(\omega)$$

$$\approx \frac{1}{\ln(\frac{|\omega - V/2|}{T_K} + \frac{\gamma}{T_K}) + \ln(\frac{|\omega + V/2|}{T_K} + \frac{\gamma}{T_K})}.$$
(3)

This combination plays the role of an effective (frequency dependent) exchange coupling $J_{\rm eff}$. Remarkably, the perturbative expression Eq. (3) would develop a pole close to $\omega=\pm V/2$ if $\gamma < T^*=\sqrt{T_K^2+(V/2)^2}-V/2\approx T_K^2/V$. The breakdown scale T^* of PT has also been discussed in the fourth reference listed in Ref. [6] and Ref. [14]. It indicates that Eq. (3) is valid only for $T^*<\gamma < V$. Indeed, this criterion is fulfilled (see Fig. 1), as one finds within NCA

$$\gamma^{\text{NCA}} \approx \frac{\pi}{8} \frac{V}{\ln^2 \frac{V}{T_r}} \left[1 + \frac{2}{\ln \frac{V}{T_r}} + O\left(\frac{\ln \frac{V}{\gamma}}{\ln^2 \frac{V}{T_r}}\right) \right].$$
 (4)

For the conductance in units of the conductance quantum

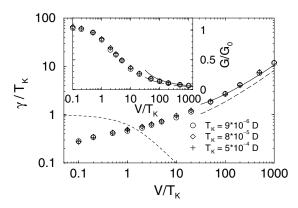


FIG. 1. Nonequilibrium decoherence rate $\gamma = \mathrm{Im}\Sigma_f(0)$ calculated within NCA compared to the strong coupling scale $T^* = \sqrt{T_K^2 + (V/2)^2} - V/2$ (dashed line). For $\gamma \gg T^*$ one stays in the weak coupling regime. The symbols correspond to three different values of T_K , $T_K/D = 9 \times 10^{-6}$, 8×10^{-5} , 5×10^{-4} . Inset: conductance G in units of $G_0 = 2e^2/(2\pi\hbar)$. Long-dashed and solid lines: asymptotic analytical results, Eqs. (4) and (5), in leading and next-to-leading order, respectively.

 $G_0 = 2e^2/(2\pi\hbar)$ we obtain for $\ln V/T_K \gg 1$

$$\frac{G^{\text{NCA}}}{G_0} \approx \frac{\pi^2}{4} \frac{1}{\ln^2 \frac{V}{T_K}} \left[1 + \frac{2}{\ln \frac{V}{T_K}} + O\left(\frac{\ln \frac{V}{\gamma}}{\ln^2 \frac{V}{T_K}}\right) \right]. \quad (5)$$

Numerical results for smaller voltages down to $V < T_K$ are shown in Fig. 1 and display universal behavior over the complete range of voltages and over several orders of magnitude in T_K . Despite the fact that for high voltages, $\ln V/T_K \gg 1$, one stays in the weak coupling regime, the prefactors of $\gamma^{\rm NCA}$ and $G^{\rm NCA}$ are not exact, since the NCA for the Anderson model treats the potential scattering V_0 and the Kondo coupling J incorrectly on equal footing. It is not difficult to obtain the correct asymptotic prefactors [8] by calculating γ and G in leading order PT in J for the Kondo model Eq. (2) (with $V_0 = 0$) and by replacing J by $1/(2 \ln V/T_K)$. This corrects the leading term of the NCA results Eqs. (4) and (5) by a prefactor 3/4. It is, however, important to stress that the asymptotic result in the limit $\ln V/T_K \rightarrow \infty$ is almost useless as, due to the logarithmic dependence [Eq. (4)], subleading corrections are very large (e.g., still 10% for $V/T_K = 10^6$).

In the limit of large V, the scale γ influences quantities like the conductance, where all electrons in an energy window V contribute only slightly. The situation is different for the spectral function $A_d(\omega)$ of the electron on the quantum dot. $A_d(\omega)$ calculated numerically within NCA is shown in Fig. 2. Like many groups before, we obtain two well defined peaks at voltages $\pm V/2$. In the limit $\ln V/T_K \to \infty$ we find approximately $A_d^{\rm NCA}(\omega) \approx (\pi^2/\Gamma) \left[N_0 J_{\rm eff}^{\rm NCA}(\omega)\right]^2$, with large but universal subleading corrections and a nonuniversal, (almost) constant potential scattering background of $O(\Gamma/\varepsilon_d^2)$. NCA incorrectly treats potential and spin flip scattering on equal footing and, thus, overestimates the asymmetry of the peaks with respect to

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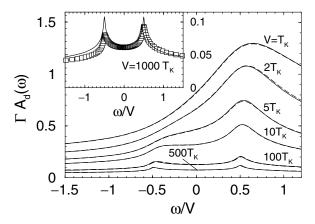


FIG. 2. Spectral function $A_d^{\rm NCA}(\omega)$ for various voltages V, each calculated in NCA at two values of T_K (solid and dashed lines) differing by a factor of 10. The NCA systematically overestimates the asymmetry of the peaks. Inset: Asymptotic behavior of $A_d^{\rm NCA}(\omega)$ in the Kondo scaling limit. Squares: numerical NCA result; solid line: asymptotic expression for $\ln(V/T_K) \to \infty$.

 $\omega \leftrightarrow -\omega$ in the small J limit. This can be seen from an analysis of the Schrieffer-Wolff transformation which shows that this asymmetry is nonuniversal and of $O(N_0V_0)$. Since the antisymmetrical in ω contributions to $A_d(\omega)$ cancel in the integral for the conductance, nonuniversal corrections to G are much smaller. Note that the logarithmic cusps of $A_d(\omega)$ have an additional, small rounding of $O(\gamma)$ compared to Eq. (3), but for large voltage, the half width at half-maximum Δ of the peaks is not given by γ but by $\Delta \approx \sqrt{\gamma V}/2 \approx 0.3 V / \ln(V/T_K) > \gamma$ (see Fig. 2).

Our analysis of the Kondo model suggests that qualitatively different behavior can be expected if the nonequilibrium relaxation rate γ is sufficiently small, $\gamma < T_K^2/V$. Since a nonzero γ requires finite current, e.g., within bare PT $\gamma \propto N_0 J_{LR}^2 V$, it is therefore interesting to study the Kondo model Eq. (2) for $J_{LR} \ll J_L, J_R$, using ideas from perturbative RG. Such a model cannot be derived from a simple Anderson model but may arise in more complicated situations. It was also considered in [16]. Not much is known about how the concepts of fixed points and renormalization group can be applied to a nonequilibrium situation (see, however, Ref. [11]). The problem is that in the presence of a finite bias voltage, many physical quantities like the conductance are *not* determined by low-energy excitations even at T=0, since all states with energies of order of the applied voltage V contribute. Therefore, a controlled perturbative RG must probably be formulated for the full frequency-dependent vertices in Keldysh space. We will not try to develop such a method here but propose to use a heuristic version of poor-man's scaling adapted to the present situation. As usual, we investigate how coupling constants change when the cutoff Λ of the theory is modified. As long as the cutoff is large compared to the voltage, we expect that the usual poor-man's scaling equations hold. For the model with $N_0J_L = N_0J_R = g_d$, $N_0 J_{LR} = g_{LR}$, and $V \ll \Lambda$, one obtains [8,14]

$$\frac{dg_d}{d\ln\Lambda} = -(g_d^2 + g_{LR}^2), \qquad \frac{dg_{LR}}{d\ln\Lambda} = -2g_d g_{LR}. \quad (6)$$

These are the RG equations of a channel-asymmetric twochannel Kondo model, where the even and odd channels couple to the spin with coupling constants $g_e = g_d + g_{LR}$ and $g_o = g_d - g_{LR} \le g_e$. Note that for the Anderson model, the odd channel decouples and $g_o = 0$. Two parameters, T_K and α , determine the physics of the channelasymmetric two-channel Kondo model,

$$T_K = De^{-1/(g_d + g_{LR})}, \qquad \alpha = \frac{(g_d - g_{LR})(g_d + g_{LR})}{2g_{LR}},$$
(7)

where T_K is defined by $g_e(T_K) = 1$. The dimensionless number α is the natural parameter to characterize the channel anisotropy, since it is invariant under the perturbative RG flow Eq. (6), i.e., $\alpha(\Lambda) = \alpha_0 = \text{const for } \Lambda > V$. If higher orders of g are included in Eqs. (6), the prefactor of T_K , Eq. (7), changes and the definition of the RG invariant α has to be slightly adjusted (a dimensionless invariant characterizing the flow will exist even in higher orders). For the usual one-channel Kondo effect or the Anderson model Eq. (1), $\alpha_0 = 0$, while for $\alpha_0 \to \infty$ the model is just the well-known channel-symmetric twochannel Kondo model. We will therefore investigate how α will change for $\Lambda < V$ in order to determine if the system flows towards the two-channel fixed point proposed by Wen [13] and Coleman et al. [14]. For $V \gg T_K$, Eq. (6) is valid down to $\Lambda = V$ and we obtain

$$g_d(V) = \frac{1}{2} \left(\left[\ln \frac{V}{T_K} \right]^{-1} + \left[\frac{1}{\alpha_0} + \ln \frac{V}{T_K} \right]^{-1} \right), \quad (8)$$

$$g_{LR}(V) = \frac{1}{2} \left(\left[\ln \frac{V}{T_K} \right]^{-1} - \left[\frac{1}{\alpha_0} + \ln \frac{V}{T_K} \right]^{-1} \right).$$
 (9)

For $\Lambda < V$, the calculation of the RG flow is less obvious. Some of the logarithmically diverging vertex corrections of J are cut off by the voltage V, changing the RG flow to

$$\frac{dg_d}{d\ln\Lambda} = -g_d^2, \qquad \frac{dg_{LR}}{d\ln\Lambda} = 0, \tag{10}$$

in complete agreement with the analysis of Coleman *et al.* [14]. However, all remaining logarithmic contributions are cut off by the decoherence rate γ as it is evident, e.g., from our analysis of NCA. Thus, Eqs. (10) are valid only for $\gamma \ll \Lambda \ll V$.

Since in the perturbative regime of the RG the bare coupling constant N_0J_{LR} is replaced by the renormalized one, g_{LR} , we find

$$\gamma \sim V g_{LR}^2(V), \tag{11}$$

which is $V/[2\ln(V/T_K)]^2$ for $\alpha_0 \ll 1/\ln(V/T_K)$ and $V/[4\alpha_0^2\ln^4(V/T_K)]$ for $\alpha_0 \gg 1/\ln[V/T_K]$. (The precise

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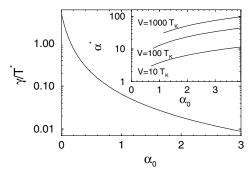


FIG. 3. γ/T^* as a function of α_0 at $V=10T_K$. Inset: α^* as a function of α_0 for various voltages. For $\gamma/T^*\ll 1$, the system displays strong coupling behavior for $T< T^*$. $\alpha^*\gg 1$ indicates that this regime is dominated by two-channel physics.

prefactor is irrelevant for our discussion.) If we assume for the moment that γ is small, we find that g_d flows to strong coupling at a scale T^* defined by $g_d(T^*) = 1$,

$$T^* \approx T_K \left(\frac{T_K}{V}\right)^{1/[1+2\alpha_0 \ln(V/T_K)]}.$$
 (12)

For $\alpha_0 = 0$ this scale coincides with the one introduced in [14], where the effects of γ have been neglected. The system will, however, flow to strong coupling only if $\gamma < T^*$, while it remains in the weak coupling regime for $\gamma \gg T^*$. For the usual Kondo or Anderson model with $\alpha_0 = 0$, γ is always larger than T^* for $V \gg T_K$ (as $V/T_K > \ln V/T_K$), and we therefore conclude in contradiction to Ref. [14] that in the symmetrical Kondo model there is no strong coupling regime for $V \gg T_K$. The situation is, however, different in the asymmetric model with $\alpha_0 \gtrsim 1/2$ (Fig. 3). Here $\gamma/T^* \approx (V/T_K)/(4\alpha_0^2 \ln^4 [V/T_K])$ is much less than 1 for $V \ll V^* \approx T_K(4\alpha_0^2 \ln^4[4\alpha_0^2 \ln^4[4\alpha_0^2 \ln^4[\cdots]]))$, e.g., $V^* \approx 6 \times 10^4 T_K$ for $\alpha_0 = 1$. What is the nature of this strong coupling regime which is reached for $T_K \ll V \ll$ V^* and $\alpha_0 > 1/2$? Insight into this question can be gained from a calculation of $\alpha(\Lambda = T^*)$, defined in Eq. (7). Note that in the regime $\gamma \ll \Lambda \ll V$, α is not invariant under the RG flow Eqs. (10). We obtain

$$\alpha^* \equiv \alpha(T^*) \approx \ln \frac{V}{T_K} \left(1 + \alpha_0 \ln \frac{V}{T_K} \right) \approx \alpha_0 \ln^2 \frac{V}{T_K}.$$
(13)

Obviously, α is strongly enhanced by the voltage (e.g., $\ln^2[10^3] \approx 50$). Since for $\alpha \to \infty$ the system maps to a two-channel Kondo problem, we conclude that for $\alpha_0 > 1/2$ and $T_K \ll V \ll V^*$ the system will likely be dominated by two-channel physics over a large regime.

In summary, the usual Kondo model at high voltages, $T_K \ll V \ll D$, is a weak coupling problem because non-equilibrium relaxation processes allowed even at T=0 destroy the Kondo effect, as their rate $\gamma \gg T^* \approx T_K^2/V$ is large. Nevertheless, bare perturbation theory cannot be

applied and even the leading order of renormalized perturbation theory does not give precise results in the experimentally accessible regime due to large subleading corrections. We find two well-defined peaks of width Δ in the local spectral function. In the asymptotic regime $\Delta \approx \sqrt{\gamma V}/2$. In variants of the Kondo model with $J_{LR} < J_L, J_R$, a large voltage can, however, induce qualitatively new behavior reminiscent of two-channel Kondo physics.

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- [1] D. Goldhaber-Gordon *et al.*, Nature (London) **391**, 156 (1998).
- [2] S. M. Cronenwett, T. H. Oosterkamp, and L. P. Kouwenhoven, Science **281**, 540 (1998).
- [3] J. Schmid, J. Weis, K. Eberl, and K. von Klitzing, Physica (Amsterdam) 256-258B, 182 (1998).
- [4] W. G. van der Wiel et al., Science 289, 2105 (2000).
- [5] H. Pothier *et al.*, Phys. Rev. Lett. **79**, 3490 (1997); F. Pierre *et al.*, cond-mat/0012038.
- [6] J. Kroha, Adv. Solid State Phys. 40, 216 (2000); A. Kaminski and L. I. Glazman, Phys. Rev. Lett. 86, 2400 (2001);
 G. Göppert and H. Grabert, Phys. Rev. B 64, 033301 (2001); J. Kroha and A. Zawadowski, cond-mat/0104151.
- [7] L. I. Glazman and M. E. Raikh, Pis'ma Zh. Eksp. Teor. Fiz.
 47, 378 (1988) [JETP Lett. 47, 452 (1988)]; T. K. Ng and P. A. Lee, Phys. Rev. Lett. 61, 1768 (1988).
- [8] A. Kaminski, Yu. V. Nazarov, and L. I. Glazman, Phys. Rev. Lett. 83, 384 (1999); Phys. Rev. B 62, 8154 (2000).
- [9] S. Hershfield, J. H. Davies, and J. W. Wilkins, Phys. Rev. Lett. 67, 3720 (1991); Y. Goldin and Y. Avishai, Phys. Rev. Lett. 81, 5394 (1998).
- [10] J. König, J. Schmid, H. Schoeller, and G. Schön, Phys. Rev. B 54, 16 820 (1996).
- [11] H. Schoeller and J. König, Phys. Rev. Lett. **84**, 3686 (2000); H. Schoeller, Lect. Notes Phys. **544**, 137 (2000).
- [12] A. Schiller and S. Hershfield, Phys. Rev. B 58, 14978 (1998).
- [13] X.-G. Wen, cond-mat/9812431.
- [14] P. Coleman, C. Hooley, and O. Parcollet, Phys. Rev. Lett. 86, 4088 (2001).
- [15] Y. Meir, N. S. Wingreen, and P. A. Lee, Phys. Rev. Lett. 70, 2601 (1993); M. H. Hettler, J. Kroha, and S. Hershfield, Phys. Rev. Lett. 73, 1967 (1994); Phys. Rev. B 58, 5649 (1998); N. S. Wingreen and Y. Meir, Phys. Rev. B 49, 11 040 (1994); P. Nordlander et al., Phys. Rev. Lett. 83, 808 (1999); M. Plihal, D. C. Langreth, and P. Nordlander, Phys. Rev. B 61, R13 341 (2000).
- [16] P. Coleman et al., cond-mat/0108001.
- [17] A theory to correct this deficiency is developed in J. Kroha,
 P. Wölfle, and T. A. Costi, Phys. Rev. Lett. 79, 261 (1997);
 J. Kroha and P. Wölfle, Adv. Solid State Phys. 39, 271 (1999).

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