Nonequilibrium electron transport through quantum dots in the Kondo regime

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Abstract. Electron transport at large bias voltage through quantum dots in the Kondo regime is described within the perturbative renormalization group extended to nonequilibrium. The conductance, local magnetization, dynamical spin susceptibility and local spectral function are calculated. We show how the Kondo effect is suppressed by nonequilibrium decoherence and how it is generated in excited states by a bias voltage.

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The transport of electrons through a quantum dot in the limit of weak coupling to the leads is governed by Coulomb interaction effects, forcing integral electron charge on the dot (Coulomb blockade) [1]. In the case that the total spin of the dot is nonzero, however, the antiferromagnetic exchange interaction of this local spin with the conduction electron spins in the leads gives rise to a Kondo resonance in the local density of states at the Fermi level. Electron transport may then take place via resonance tunneling, and the Coulomb blockade is removed. The enhancement of the linear conductance G as the Kondo resonance is formed for decreasing temperature, ideally up the unitarity limit $G = 1$ (in units of $2e^2/h$) has been seen in a number of experiments.

In the Kondo regime, the quantum dot may be represented by its local spin $\vec{S}$, exchange-coupled to the conduction electron spins in the leads $\alpha = L, R$

$$H = \sum_{k,\alpha,\sigma} (\varepsilon_k - \mu_\alpha) c^+_{k\alpha\sigma} c_{k\alpha\sigma} + \sum_{\alpha\alpha'} J_{\alpha\alpha'} \vec{s}_{\alpha\alpha'} \cdot \vec{S} - B S_z \quad , \tag{1}$$

where $\vec{s}_{\alpha\alpha'} = \frac{1}{2}\sum_{\vec{k}\sigma,\vec{k}'\sigma'} c^+_{k\alpha\sigma} \vec{\tau}_{\sigma\sigma'} c_{k'\alpha'\sigma'}$, $\vec{\tau}$ are the Pauli matrices, $J_{\alpha\alpha'}$ are coupling constants, and B is the Zeeman splitting of the local spin levels ($S = \frac{1}{2}$). We will consider the weak coupling regime $g_{\alpha\alpha'} = J_{\alpha\alpha'} N(0) << 1$, where $N(0)$ is the conduction electron density of states at the Fermi level.

The Kondo resonance is formed by successive, coherent, quasielastic spin-flip processes, generating a cloud of particle-hole excitations out of the conduction electron Fermi sea near the quantum dot. It is suppressed by finite temperature, $T \geq T_K$, washing out the sharp Fermi edge, or by a magnetic field causing a Zeeman splitting B, lifting the degeneracy of the local spin levels, at $B \geq T_K$. Here $T_K = D\exp(-\frac{1}{g})$ (D bandwidth, $g = N(0)J$) is the Kondo temperature. At finite bias voltage V the Kondo enhancement of the conductance is observed to be suppressed if $eV \geq T_K$ (zero bias anomaly).

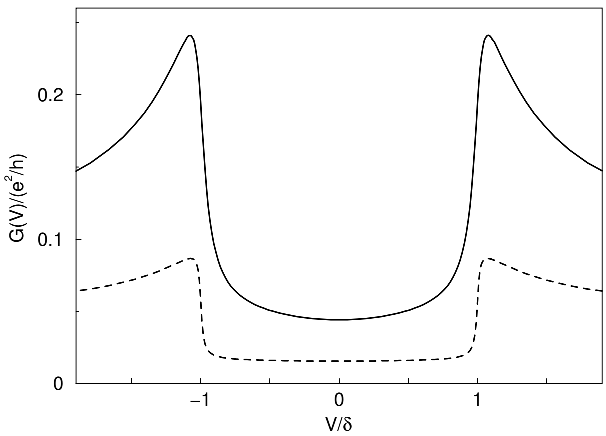

FIGURE 1. Differential conductance of a singlet-triplet quantum dot. Solid (broken) line: renormalized (second order) perturbation theory.

The reason for this suppression is an increase in decoherence caused by a sufficiently large finite current through the dot. As shown in [2], the decoherence rate Γ is given by the transverse or longitudinal spin relaxation rate $\frac{1}{T_2}$ or $\frac{1}{T_1}$, depending on the process considered. In equilibrium (i.e. linear response) one finds in the perturbative regime ($T >> T_K$), $\Gamma \sim \Sigma_{\alpha,\alpha'} g^2_{\alpha\alpha'} T$, the so-called Korringa law, and hence $\Gamma << T$ for $T >> T_K$ (this is correct even if the bare coupling constant g_o is replaced by the renormalized coupling $g = 1/\ell n(T/T_K)$). By contrast, for $eV >> T_K$,and $T << eV$, $\Gamma \sim g_{LR}^2 eV$ which can be much larger than T_K, for sufficiently large V. This means that the Kondo screening remains incomplete, the more so the larger V. Note that only the coupling constant g_{LR} enters, and roughly speaking Γ is proportional to the current through the dot.

In a quantitative description the bare coupling constants get renormalized. The degree of renormalization depends on the energy of the conduction electrons involved in the interaction process. Therefore, the renormalization group (RG) equations describing how the couplings change when high energy states are projected out have to be formulated for energy dependent coupling functions [3] rather than only the coupling constants at the Fermi energy as in the usual equilibrium RG. This is because at finite bias voltage excitations are possible within an energy window of finite width eV even at zero temperature. For a given energy ω, e.g. above the Fermi energy, the RG flow stops when the running cutoff D moves below $\omega, D <| \omega |$. As a consequence, the coupling functions form peaks at the resonance frequencies corresponding to the different Fermi energies at $\omega = \pm eV/2 \pm B$. At or near resonance the RG flow is stopped by the decoherence rate Γ.

These coupling functions may be inserted into the low order expressions for the current, the decoherence rate Γ or any other quantity one wishes to calculate [4]. In addition, the energy levels of the states involved are broadened by an amount given by the decoherence rate Γ [3].

In the presence of a magnetic field the local spin will be partially polarized, $< S_z > \neq 0$. The degree of polarization is determined by the current flowing through the dot, provided $eV >> T$, rather than by the thermal equilibrium occupation [3]. Since $< S_z >$ enters most of the observable quantities, in particular the current, and the decoherence rate Γ, it is evaluated simultaneously with the coupling functions in the RG process.

While a finite current through the dot generates decoherence and tends to suppress the Kondo effect, a finite bias voltage can help to promote the Kondo effect in a situation where it is suppressed at zero bias. Such a situation arises when a magnetic field is applied, splitting the degenerate levels of the local spin and suppressing the Kondo effect if $B >> T_K$. A finite bias voltage such that $eV = B$ provides the energy necessary for a spin flip-down tunneling process followed by a spin flip-up process in reverse and thus restores the Kondo effect to some extent. The differential conductance is then seen to develop "Kondo peaks" at $eV = \pm B$ [5].

A more direct example of the Kondo effect generated by nonequilibrium is provided by a quantum dot with a spin singlet ground state and a low-lying spin triplet excited state with low-energy exchange Hamiltonian expressable in terms of the spin operator $\vec{S}$ (now $S = 1$) and the singlet-triplet transition operators $\vec{P}_{ij}$ ($i, j = 1,2$ denotes the two levels):

$$H_{exch} = \sum_{\alpha\alpha'} \sum_{ij} J^{ij}_{\alpha\alpha'} \left[\delta_{ij} \vec{S} + \tau^1_{ij} \vec{P}_{ij} \right] \cdot \vec{s}_{\alpha\alpha'} \tag{2}$$

where $P^z_{21} = (P^z_{12})^+ = - \mid 0 >< s \mid$, $P^+_{21} = (P^-_{12})^+ = \sqrt{2} \mid 1 >< s \mid$ and $P^-_{21} = (P^+_{12})^+ = -\sqrt{2} \mid -1 >< s \mid$, where $\mid s >$ and $\mid m >$, $m = \pm 1, 0$ denote the singlet ground state and the triplet excited states of the dot. A finite bias voltage $eV = \delta$, where δ is the singlet-triplet level splitting, allows to populate the triplet state, in which coherent spin flip processes may take place, leading to a Kondo effect. A Kondo enhancement of this type has been seen in a recent experiment on a short piece of carbon nanotube serving as the quantum dot [6].

We have calculated the differential conductance G of a singlet-triplet two-level quantum dot [7]: As seen in Fig. 1, G is enhanced by Kondo correlations (solid line) in comparison to lowest order perturbation theory (dashed line).

The perturbative renormalization group method extended to nonequilibrium systems allows for a controlled calculation of the properties of quantum dots in the Kondo regime, provided any one of the relevant energy scales, eV, B, level splitting δ, or T is sufficiently large compared to T_K. The small parameter of the theory is $1/\ell n(X/T_K)$, where $X = \max(\mathrm{eV}, \mathrm{B}, \delta, \mathrm{T})$. For a "usual" (Anderson-type) quantum dot, the decoherence generated by the current stops the RG flow of the couplings in the weak coupling regime. Only for special situations (not yet realized in experiment), when the coupling J_{LR} responsible for the current is much smaller than the couplings $J_{\alpha\alpha}$ may the RG flow extend into the strong coupling regime, requiring new methods.

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REFERENCES

1. I. Aleiner, P. Brouwer, and L. Glazman, *Phys. Rep*, **3**58, 309 (2002).
2. J. Paaske, et al., *Phys. Rev. B*, **70**, 155301 (2004).
3. A. Rosch, et al., *Phys. Rev. Lett.*, **90**, 076804 (2004).
4. J. Paaske, et al., *Phys. Rev. B*, **69**, 155330 (2004).
5. A. Rosch et al., *J. Phys. Soc. Jap.*, **74**, 118 (2005).
6. N. Mason, C.M. Marcus, J. Nygaard, unpublished.
7. J. Paaske, et al., unpublished.