Zero-bias anomalies and boson-assisted tunneling through quantum dots

Jürgen König1, Herbert Schoeller1,2 and Gerd Schön1
1 Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany
2 Department of Physics, Simon Fraser University, Burnaby, B.C., V5A 1S6, Canada

We study resonant tunneling through a quantum dot with one degenerate level in the presence of a strong Coulomb repulsion and a bosonic environment. Using a real-time approach we calculate the spectral density and the nonlinear response we calculate the spectral density and the nonlinear

pulsion and a bosonic environment. Using a real-time approach developed recently [12,13] to a quantum tunneling we apply a real-time, nonequilibrium many-bosonic fields. For the nonperturbative treatment of the nonperturbative treatment of the nonequilibrium situations and including coupling to nonequilibrium broadening of the resonant state in the dot). This

influence of external quantum-mechanical fields on transport phenomena through ultrasmall quantum dots at low temperatures and frequencies (compared to the intrinsic broadening of the resonant state in the dot). This requires a description of the Kondo effect, generalized to nonequilibrium situations and including coupling to bosonic fields. For the nonperturbative treatment of the tunneling we apply a real-time, nonequilibrium many-body approach developed recently [12,13] to a quantum dot with one level and spin degeneracy M. For M ≥ 2 and low lying dot level ε we obtain the usual Kondo peaks at the Fermi levels ϵα of the reservoirs. However, the emission of bosons causes additional Kondo singularities, for a one mode field at ϵα + nωB (n = ±1, ±2, . . .).

Furthermore, we will analyze the effect of the singularities in the spectral density on the differential conduc-
tance as function of the bias voltage. For a low lying level we obtain the well-known zero bias maximum [14], whereas for a level close to the chemical potentials of the reservoirs we find a zero bias minimum. The coupling to bosons gives rise to satellite anomalies, which can be traced back to the corresponding satellite peaks in the spectral density. In a certain range of gate voltages, for M = 2 and in the absence of bosons, we find that the temperature and bias voltage dependence of the conductance coincides with recent measurements of zero-bias minima in point-contacts [14]. Therefore, in addition to Refs. [15–17], we propose here another possible interpretation of this experiment.

We consider a dot containing only one energy level with degeneracy M connected via high tunnel barriers to reservoirs of noninteracting electrons. We, furthermore, include a coupling to bosonic modes representing phonons, photons or fluctuations of the electrodynamic environment. Our model Hamiltonian reads

\[ H = H_0 + H_T, \]

where \( H_0 \) describes the decoupled system and \( H_T \) the tunneling between leads and dot. We write \( H_0 = H_R + H_D \) where \( H_R = \sum_{kσα} ε_{kσα} d_{kσα}^\dagger d_{kσα} \) refers to the reservoirs (σ and α are spin and reservoir indices). Furthermore, \( (\hbar = k_B = 1) \)

\[ H_D = \epsilon_0 N + U_0 \sum_{σ<σ'} n_σ n_{σ'} + \sum_q n_σ d_q^\dagger d_q + N \sum_q g_q (d_q + d_q^\dagger) \]  

(1)

describes the isolated dot with M spin degenerate levels at position \( \epsilon_0 \), Coulomb repulsion \( U_0 \), bosonic modes \( ω_q \) and electron-boson coupling \( g_q \). The number of particles on the dot with spin \( σ \) is denoted by \( n_σ = c_σ^\dagger c_σ \), and \( N = \sum_σ n_σ \). Finally, the tunneling term is given by

\[ H_T = \sum_{kσα} (T_k^g a_{kσα}^\dagger c_σ + h.c.). \]

This Hamiltonian can be rewritten after a unitary transformation \([18]\) defined by \( V = \exp(-iNϕ) \) and \( ϕ = i \sum_q (g_q/ω_q) (d_q^\dagger - d_q) \). We get \( \hat{H} = VH V^{-1} = \hat{H}_0 + \hat{H}_T \), where \( \hat{H}_0 = H_R + H_D, \hat{H}_D = εN + U \sum_{σ<σ'} n_σ n_{σ'} + \sum_q ω_q d_q^\dagger d_q \) and \( \hat{H}_T = \sum_{kσα} (T_k^g a_{kσα}^\dagger c_σ e^{iϕ} + h.c.) \). Due to the electron-boson interaction the level position and the Coulomb repulsion are renormalized, \( ε = ε_0 - \sum_q g_q^2/ω_q \) and \( U = U_0 - 2 \sum_q g_q^2/ω_q \), and the tunneling part contains now phase factors \( e^{±iϕ} \).

In lowest order perturbation theory the rates for tunneling in and out of the dot to reservoir α are

\[ γ_α^\pm(E) = \int dE' γ_α^\pm(E') P^\pm(E - E'), \]

(2)
where \( \hat{\gamma}_\alpha^\pm(E) = 1/(2\pi) \Gamma_\alpha(E) f^\pm_\alpha(E) \) is the classical rate without bosons, \( \Gamma_\alpha(E) = 2\pi \sum_k |T^\alpha_k|^2 \delta(E - \epsilon_k) \), and \( f^\pm_\alpha(E) \) is the Fermi distribution of reservoir \( \alpha \) with chemical potential \( \mu_\alpha \) while \( f^\alpha_\alpha(E) = 1 - f^\alpha_\alpha(E) \). Furthermore, \( P^\pm(E) \) describes the probability for an electron to absorb (for \( P^+ \)) or emit (for \( P^- \)) the boson energy \( E \). It is given by

\[
P^\pm(E) = \frac{1}{2\pi^2} \int dt e^{iEt} \left< e^{i\varphi(0)} e^{-i\varphi(\pm t)} \right> >_0
\]  

where \(< ... >_0 \) denotes the expectation value with respect to the free boson Hamiltonian. The classical rates together with a master equation are sufficient in the perturbative regime \( \Gamma = \sum \alpha \gamma_\alpha \ll T \). In this letter we are interested in temperatures and frequencies which exceed in a conserving approximation, which takes into account non-diagonal matrix elements of the total density matrix up to the difference of one electron-hole pair excitation in the reservoirs. The difference in the case of a single level quantum dot is that we have now \( \gamma \) possibilities for the occupied state. The analytic resummation of the corresponding diagrams yields for the transitions between \( N = 0(1) \) and \( 1(0) \) the rates \( \Sigma^\pm = \lambda \int dE \gamma^\pm(E) |R(E)|^2 \). Here \( R(E) = [E - \epsilon - \sigma(E)]^{-1} \) defines a resolvent with broadening and energy renormalization given by the self-energy

\[
\sigma(E) = \int dE' \frac{M \gamma^+(E') + \gamma^-(E')}{E - E' + i0^+}
\]  

where \( \gamma^\pm = \sum \gamma^\pm_\alpha \) and \( \lambda = \int dE |R(E)|^2 \).

In the classical limit \( \Gamma \ll T \) we recover for \( \Sigma^\pm \) the classical rates \( \gamma^\pm \). The stationary probabilities \( P_0 \) and \( P_1 \) for an unoccupied or occupied dot state follow from the kinetic equation which uses the rates as input. The master equation which describes well the spectral density of the dot at resonance points. The reason is that position and value of the peaks of the spectral density are determined by a self-energy \( \sigma \) (see Eq. (4)) which is calculated here in lowest order perturbation theory in \( \Gamma \) including the bosons. Higher orders are small for high tunnel barriers.

Similar to the case of metallic islands \[12,13\] we proceed in a conserving approximation, which takes into account non-diagonal matrix elements of the total density matrix up to the difference of one electron-hole pair excitation in the reservoirs. The difference in the case of a single level quantum dot is that we have now \( M \) possibilities for the occupied state. The analytic resummation of the corresponding diagrams yields for the transitions between \( N = 0(1) \) and \( 1(0) \) the rates \( \Sigma^\pm = \lambda \int dE \gamma^\pm(E) |R(E)|^2 \). Here \( R(E) = [E - \epsilon - \sigma(E)]^{-1} \) defines a resolvent with broadening and energy renormalization given by the self-energy

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Our results satisfy all sum rules together with current conservation, and one can prove particle-hole symmetry in the case \( M = 1 \).

The difference to other approaches in the \( M = 1 \) case \cite{2} is clearly displayed by the effect of the self-energy \( \sigma(E) \) which determines via the resolvent \( R(E) \) the position of the maxima of the spectral density \( \Im \sigma \). In all previous works, \( \sigma(E) \) has been approximated by a constant. We find that the energy dependence of \( \sigma(E) \) cannot be neglected if the temperature \( T \) and the typical frequency \( \omega_B \) of the bosons are smaller than \( \Gamma \). To derive this analytically we consider from now on a one-mode environment (Einstein model) with boson frequency \( \omega_q = \omega_B \). Defining \( g = \sum_q g_q^2 / \omega_B^2 \) we obtain \( \Im \sigma \) is still important. They lead to an overall increase of the spectral density near zero energy with bias voltage. In the presence of bosons we obtain satellite steps at \( |eV| = m\omega_B \).

The occurrence of zero-bias minima is well known for Kondo scattering from magnetic impurities \cite{14}. Here we have shown that zero-bias minima can also occur by resonant tunneling via local impurities if the level position is high enough to enter the mixed valence regime. We have also compared the scaling behavior of the conductance as function of temperature and bias voltage with recent experiments of Ralph & Buhrman \cite{14} (see insets of Fig. \( \delta \)). The coincidence is quite remarkable. The explanation of this experiment, either interpreting it as 2-channel Kondo scattering from atomic tunneling systems \cite{15,16} or by tunneling into a disordered metal \cite{17}, is still controversial. The mechanism described in this work offers another possibility although the magnetic field dependence of the experiments remains unexplained.

Finally, we also investigate the differential conductance at fixed bias voltage as function of the position of the dot level, which experimentally can be varied by changing the gate voltage coupled capacitively to the dot. Fig. \( \sigma \) shows the classically expected pair of peaks at \( |eV| = eV/2 \) together with satellites between the main peaks (due to emission and absorption) and peaks for \( |e| > eV/2 \) (only due to absorption of bosons). The imaginary part of \( \sigma(E) \) gives rise to a classically unexpected asymmetry of the peak heights. The peak at \( e = eV/2 \) is larger than the one at \( e = -eV/2 \) since \( \Im \sigma(E) = \pi |M \sigma(E) + \gamma^{-}(E)| \) is always smaller for higher energies (except for the \( M = 1 \) case where particle-hole symmetry holds). This demonstrates a significant effect due to the broadening of the spectral density by quantum fluctuations.

In conclusion, we have studied for the first time low-energy transport in the nonequilibrium Anderson model with bosonic interactions. A one-mode environment yields new Kondo resonances in the spectral density which can be probed by the measurement of the nonlinear differential conductance. We have shown that both the gate and bias voltage dependence is important. Quantum fluctuations due to resonant tunneling yield zero-bias anomalies as function of the bias voltage, which can...
be changed from maxima to minima by varying the gate voltage. We found similarities to recent experiments.

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FIG. 1. A diagram showing various tunneling processes: sequential tunneling in the left and right junctions, a term preserving the norm, a cotunneling process, and resonant tunneling.

FIG. 2. The spectral density for $T = T_B = 0.01\Gamma$, $\epsilon = -4\Gamma$, $g = 0.2$, $\omega_B = 0.5\Gamma$ and $E_C = 100\Gamma$ at different voltages. For $V = 0$ there are resonances at multiples of $\omega_B$, which split for finite bias voltage.

FIG. 3. The differential conductance vs. bias voltage for $T = T_B = 0.01\Gamma$, $\epsilon = -4\Gamma$, $\omega_B = 0.5\Gamma$ and $E_C = 100\Gamma$. The curves show a maximum at zero bias and satellite maxima at multiples of $\omega_B$ for a finite electron-boson coupling. Inset ($g = 0$): increasing voltage leads to an overall decrease of the spectral density in the range $|E| < eV$, which explains the zero-bias maximum.

FIG. 4. The differential conductance vs. bias voltage for $T = T_B = 0.01\Gamma$, $\epsilon = 0$, $\omega_B = 0.5\Gamma$ and $E_C = 100\Gamma$. The curves show a minimum at zero bias and steps at multiples of $\omega_B$ for a finite electron-boson coupling. Left inset: the rescaled curves for $g = 0$ at different temperatures collapse onto one curve. Right inset: The temperature dependence of the linear conductance (solid line) coincides with experimental data from [7] (triangles).

FIG. 5. The differential conductance as a function of $\epsilon$ for $T = 0.25\Gamma$, $eV = 30\Gamma$, $g = 0.3$, $\omega_B = 5\Gamma$ and $E_C = 500\Gamma$.

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\[ G(V,T) - G(0,T) = \frac{G(V=0,T) - G(0,0)}{(k_B T/E_C)^{1/2}} \times \left( \frac{e^2}{h} \right) \times \left( \frac{\ln(E_C^2/2 \pi T)}{\Gamma} \right)^{-2} \]
$G[e^2/h]$

- $T_B = 0.05 \omega_B$
- $T_B = \omega_B$