Zero-Bias Anomalies and Boson-Assisted Tunneling Through Quantum Dots

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We study resonant tunneling through a quantum dot with one degenerate level in the presence of strong Coulomb repulsion and a bosonic environment. Using a real-time diagrammatic formulation we calculate the spectral density and the nonlinear current. The former shows a multiplet of Kondo peaks split by the transport voltage and boson frequencies. This leads to zero-bias anomalies in the differential conductance, which shows a local maximum or minimum depending on the level position. We compare with recent experiments.

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Electron transport through discrete energy levels in quantum dots has been studied in perturbation theory [1,2] and beyond [3–5]. Resonant tunneling and nonequilibrium Kondo effects may play a role, as recently observed by Ralph and Buhrman [6]. Inelastic interactions in quantum dots with few levels have been studied only recently, e.g., the nondegenerate case [7,8] or Coulomb blockade effects in the presence of time-dependent fields [2,5]. Bosonic fields in the nonequilibrium Anderson model yield in the perturbative regime [9] resonant side peaks in the Coulomb oscillations.

The purpose of the present Letter is to investigate transport phenomena through ultrasmall quantum dots at low temperatures in the presence of external quantum-mechanical fields. Without bosonic modes this model has been studied extensively in recent years [3–5], motivated by experiments showing clearly the coexistence of Coulomb blockade phenomena and tunneling through zero-dimensional states [10]. For the nonperturbative treatment of the tunneling we generalize a real-time, nonequilibrium many-body approach developed recently [11,12] to a quantum dot with one level and spin degeneracy M. For $M \geq 2$ and low lying dot level ϵ we obtain the usual Kondo peaks at the Fermi levels μ_α of the reservoirs (with index α) [4]. The emission of bosons causes additional Kondo singularities, for a one-mode field at $\mu_\alpha + n\omega_B$ ($n = \pm 1, \pm 2, \ldots$).

Furthermore, we analyze the effect of a bias voltage on the singularities in the spectral density and the differential conductance. For a low lying dot level ϵ we obtain the well-known zero-bias *maximum* [4–6], 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. For a certain range of gate voltages, $M = 2$, and in the absence of bosons, the temperature and bias voltage dependence of the conductance coincides remarkably (up to an overall factor) with the zero-bias minima observed recently in point contacts [13] and with results derived in different models (Refs. [14–16]).

We consider a dot containing one energy level at position ϵ_0 with degeneracy M and Coulomb repulsion U_0. It is coupled to bosonic modes ω_q and electron-boson coupling g_q, $H_D = \epsilon_0 \hat{N} + U_0 \sum_{\sigma<\sigma'} n_\sigma n_{\sigma'} + \sum_q \omega_q d_q^\dagger d_q + \hat{N} \sum_q g_q (d_q + d_q^\dagger)$. The particle number on the dot with spin σ is $n_\sigma = c_\sigma^\dagger c_\sigma$, and $\hat{N} = \sum_\sigma n_\sigma$. The dot is coupled via tunnel barriers, described by $H_T = \sum_{k\sigma\alpha} (T_k^\alpha a_{k\sigma\alpha}^\dagger c_\sigma + \text{H.c.})$, to reservoirs of noninteracting electrons, $H_R = \sum_{k\sigma\alpha} \epsilon_{k\alpha} a_{k\sigma\alpha}^\dagger a_{k\sigma\alpha}$. Thus the model Hamiltonian is $H = H_0 + H_T$, where $H_0 = H_R + H_D$ describes the decoupled system.

The bosonic modes can represent interaction with phonons [7] or fluctuations of the electrodynamic environment [8] very similar to the Caldeira-Leggett model [17]. For our theory no assumption is needed for the specific kind of the modes ω_q and the couplings g_q. In this way we are able to present a general result for the current which shows the influence of inelastic interactions for an arbitrary environment.

A unitary transformation [18] with $V = \exp(-i\hat{N}\varphi)$ and $\varphi = i\sum_q (g_q/\omega_q)(d_q^\dagger - d_q)$ yields $\overline{H} = VHV^{-1} = \overline{H}_0 + \overline{H}_T$, where $\overline{H}_0 = H_R + \overline{H}_D$, $\overline{H}_D = \epsilon \hat{N} + U \sum_{\sigma<\sigma'} n_\sigma n_{\sigma'} + \sum_q \omega_q d_q^\dagger d_q$ and $\overline{H}_T = \sum_{k\sigma\alpha} (T_k^\alpha a_{k\sigma\alpha}^\dagger c_\sigma e^{i\varphi} + \text{H.c.})$. The electron-boson interaction renormalizes the level position and the Coulomb repulsion, $\epsilon = \epsilon_0 - \sum_q g_q^2/\omega_q$ and $U = U_0 - 2\sum_q g_q^2/\omega_q$, and the tunneling term acquires phase factors $e^{\pm i\varphi}$.

For strong Coulomb repulsion U we restrict ourselves to states with $N = 0, 1$. In perturbation theory the rates for tunneling in and out of the dot to reservoir α are

$$\gamma_\alpha^\pm(E) = \int dE' \overline{\gamma}_\alpha^\pm(E') P^\pm(E - E'), \qquad (1)$$

where $\overline{\gamma}_\alpha^\pm(E) = 1/(2\pi)\Gamma_\alpha(E) f_\alpha^\pm(E)$ is the classical rate without bosons, $\Gamma_\alpha(E) = 2\pi \sum_k |T_k^\alpha|^2 \delta(E - \epsilon_{k\alpha})$, and $f_\alpha^+(E)$ is the Fermi distribution of reservoir α with chemical potential μ_α, while $f_\alpha^-(E) = 1 - f_\alpha^+(E)$. Finally, $P^\pm(E) = 1/(2\pi) \int dt e^{iEt} \langle e^{i\varphi(0)} e^{-i\varphi(\pm t)} \rangle_0$ describes the probability that an electron absorbs (P^+) or emits (P^-) the boson energy E. The classical rates combined with a master equation are sufficient in the perturbative regime $\Gamma = \sum_\alpha \Gamma_\alpha \ll T$ [9].

Here we consider temperatures and frequencies of the order or smaller than Γ. This requires a nonperturbative treatment of the tunneling, where quantum fluctuations yield finite lifetime broadening and renormalization effects of the dot level. As an illustration we first assume that the broadening is given by the sum of the classical transition rates, Eq. (1). Using the Kramers-Kronig transformation we deduce the renormalization and obtain for the self-energy

$$\sigma(E) = \int dE' \, \frac{M\gamma^+(E') + \gamma^-(E')}{E - E' + i0^+}, \qquad (2)$$

where $\gamma^\pm = \sum_\alpha \gamma_\alpha^\pm$. The aim of the present Letter is to test and extend this simple physical picture within a systematic and conserving theory for all Green's functions and the current. To achieve this we use a real-time technique developed in [11,12] which provides a natural generalization of the classical and co-tunneling theory to the physics of resonant tunneling.

The nonequilibrium time evolution of the dot is described by its reduced density matrix, which we obtain in an expansion in $\overline{H}_T$. The reservoirs and boson bath are assumed to remain in thermal equilibrium and are traced out by using Wick's theorem. Matrix elements of the reduced density operator are visualized in Fig. 1. The forward and the backward propagator (Keldysh contour) are coupled by "tunneling lines" associated with the junctions to the reservoirs α. Each tunneling line with energy E represents the rate $\overline{\gamma}_\alpha^+(E)$ if the line is directed backward with respect to the closed time path and $\overline{\gamma}_\alpha^-(E)$ otherwise. The Fermi-Dirac statistics produce a factor -1 if two tunneling lines cross each other. The tunneling lines are associated with changes of the state of the dot, as indicated on the closed time path. The coupling to the bosons is introduced by connecting all vertices in all possible ways by boson lines with energy E. The rules for these contributions are the same as for the reservoir lines except that we have to replace $\overline{\gamma}_\alpha^\pm$ by $P^\pm$. Finally, we associate with each tunneling vertex at time t a factor $\exp(i\Delta E\, t)$, where ΔE is the difference of outgoing and incoming energies. If the vertex lies on the backward propagator it acquires a factor -1. Analogous graphical rules hold for the Green's functions of the dot, except that they contain external vertices.

In leading order, we include only boson lines between vertices which are already connected by tunneling lines,

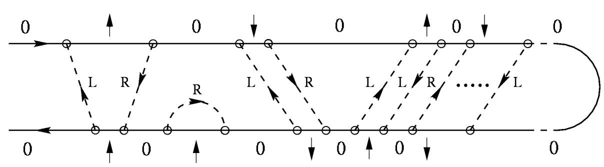

FIG. 1. A diagram showing sequential tunneling in the left and right junctions, a term preserving the norm, a co-tunneling process, and resonant tunneling.

which amounts to a dressing of the tunneling lines $\overline{\gamma} \to \gamma$. This approximation, while neglecting many diagrams, 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 σ [see Eq. (2)], which is calculated here in lowest order perturbation theory in Γ including the bosons. Higher orders are small for high tunnel barriers.

Similar to the case of metallic islands [11,12] we proceed in a conserving approximation, taking into account nondiagonal matrix elements of the total density matrix up to the difference of one electron-hole pair excitation in the reservoirs. The analytic resummation of the corresponding diagrams yields for the transitions between $N = 0$ and 1 the rates $\Sigma^\pm = \lambda \int dE\, \gamma^\pm(E)|R(E)|^2$, where $\lambda^{-1} = \int dE|R(E)|^2$. The resolvent $R(E) = [E - \epsilon - \sigma(E)]^{-1}$ accounts for broadening and energy renormalization contained in the self-energy $\sigma(E)$, Eq. (2). In the classical limit $\Gamma \ll T$ the rates $\Sigma^\pm$ reduce to the classical rates $\gamma^\pm$.

Summing equivalent diagrams for the real-time Green's functions of the dot, we obtain the spectral density $\rho \equiv (G^< - G^>)/(2\pi i)$,

$$\rho(E) = \int dE' \sum_{r=\pm} \gamma^r(E') P^{-r}(E' - E)|R(E')|^2, \quad (3)$$

and the current I_α flowing into reservoir α

$$I_\alpha = e2\pi M \sum_{\alpha'} \int dE' \sum_{r=\pm} r\gamma_\alpha^{-r}(E')\gamma_{\alpha'}^r(E') \times |R(E')|^2. \quad (4)$$

For the special case of two reservoirs $\alpha = L/R$ and constant level broadening $\Gamma = \Gamma_L = \Gamma_R$ the current $I = I_L = -I_R$ can be written as $I = eM\Gamma/2 \int dE \rho(E)[f_R^+(E) - f_L^+(E)]$. 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 case $M = 1$ [7,8] 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 (3). In 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 ω_B of the bosons are smaller than Γ. To show this analytically we consider from now on a one-mode environment (Einstein model) with boson frequency $\omega_q = \omega_B$. Experimentally, this can be realized by optical phonons [7] or by fluctuations of an external LC circuit with frequency $\omega_B = (LC)^{-1/2}$ [8]. The results for a general environment can be anticipated approximately from the one-mode case by a superposition. Defining $g = \sum_q g_q^2/\omega_B^2$ we obtain $P^\pm(E) = \sum_n p_n \delta(E \pm n\omega_B)$, where $p_n = e^{-g[1+2N_0(\omega_B)]} e^{n\omega_B/2T_B} I_n[2gN_0(\omega_B)e^{\omega_B/2T_B}]$ is the probability for the emission of n bosons with frequency ω_B. Here, $N_0(\omega_B)$ is the Bose function and I_n the modified Bessel function. The temperature of the boson bath T_B may differ in real experiments from the electron temperature T. Using (1) and (2) we obtain $\mathrm{Re}\sigma(E) = \sum_{n,\alpha}(Mp_n - p_{-n})(\Gamma/2\pi)\{\ln(E_C/2\pi T) - \mathrm{Re}\Psi[1/2 + i(E + n\omega_B - \mu_\alpha)/2\pi T]\}$. Here Ψ denotes the digamma function, and we have chosen in the energy integrals a Lorentzian cutoff at E_C. The real part of σ depends logarithmically on energy, temperature, voltage, and frequency. These logarithmic terms are typical for the occurrence of Kondo peaks and do not cancel for $M \geq 2$ or $p_n \neq p_{-n}$. Hence we anticipate logarithmic singularities not only for the degenerate case but also for a single dot level without spin since the probabilities for absorption and emission of bosons are different. This is an important difference from the case of classical time-dependent fields [5] where both probabilities are equal. At low temperatures we obtain logarithmic peaks in $\sigma(E)$ at $E = \mu_\alpha + n\omega_B$ ($n \neq 0$ for $M = 1$). They lead to the maxima of the resolvent $R(E)$ at $E = n\omega_B$ ($n > 0$ for $M = 1$, $n \geq 0$ for $M > 1$) for $\epsilon < 0$ and at $E = n\omega_B$ ($n < 0$) for $\epsilon > 0$. The spectral density (3) shows resonances at the same points but, due to the additional $P^{\pm}$ functions in the numerator, they are shifted by multiples of ω_B. This boson-assisted tunneling is completely independent of the influence of the bosons on the self-energy $\sigma(E)$.

Figure 2 shows the spectral density at different voltages for a low lying level $\epsilon < 0$. For $M = 2$, without applied bias we obtain the usual Kondo peak near the Fermi level (which we choose as zero energy). The emission of bosons leads to additional resonances at multiples of ω_B. For $M = 1$ and $\epsilon < 0$ ($\epsilon > 0$), resonances occur at negative (positive) energies. In these cases, the effects are less pronounced and are only visible for very low temperatures. At finite bias voltages all peaks split and decrease in magnitude.

The resonances in the spectral density have pronounced effects on the nonlinear differential conductance as a function of the bias voltage V, as shown in Fig. 3 for the case $\epsilon < 0$. We recover the zero-bias maximum [4–6] since the splitting of the Kondo peak leads to an overall decrease of the spectral density in the energy range $|E| < eV$ (see inset of Fig. 3). The emission of bosons produces a set of symmetric satellite maxima. They can be traced back to the fact that pairs of Kondo peaks can merge if the bias voltage is a multiple of the boson frequency (see Fig. 2). This gives rise to pronounced Kondo peaks at $E = \pm eV/2$ and thus to an increase of the spectral density with bias voltage near these points.

The differential conductance for $\epsilon \geq 0$ is shown in Fig. 4 with and without bosons. A striking result is that the whole structure is inverted compared to the case $\epsilon < 0$, and we find a zero-bias anomaly although the Kondo peak at zero energy is absent. The bosons yield satellite steps at $|eV| = m\omega_B$. The contributions of sequential and co-tunneling lead, compared to resonant tunneling, only to a weak bias voltage dependence of the differential conductance. This shows clearly that the influence of the logarithmic terms in $\sigma(E)$ are still important. They lead to an overall increase of the spectral density near zero energy with bias voltage (see left inset of Fig. 4). The reason is that the logarithmic peaks in $\mathrm{Re}\sigma(E)$ decrease with increasing bias voltage and approach the value of $E - \epsilon$ if ϵ is large enough. Thus the value of $E - \epsilon - \mathrm{Re}\sigma(E)$ decreases, which in turn increases the resolvent $R(E)$ and the spectral density $\rho(E)$.

Zero-bias minima are known from Kondo scattering from magnetic impurities [19]. They have been observed in recent experiments [13] and have been interpreted

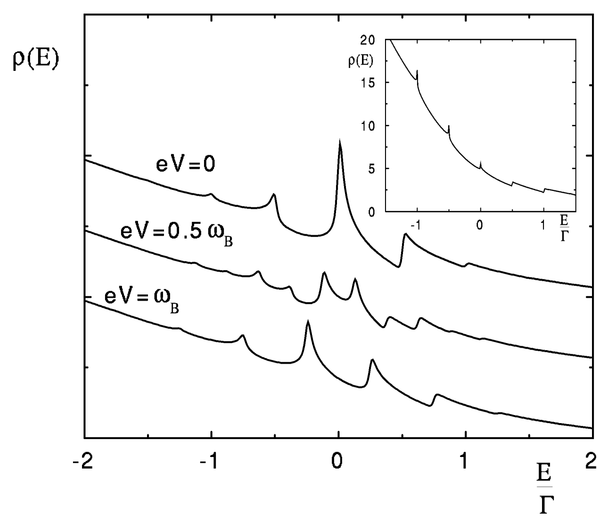

FIG. 2. The spectral density for $M = 2$, $T = T_B = 0.01\Gamma$, $\epsilon = -4\Gamma$, $g = 0.2$, $\omega_B = 0.5\Gamma$, and $E_C = 100\Gamma$ at different voltages. Inset: spectral density for $M = 1$, $T = 0.0001\Gamma$, $T_B = \Gamma$, $\epsilon = -2\Gamma$, $V = 0$, $g = 0.5$, $\omega_B = 0.5\Gamma$, and $E_C = 100\Gamma$.

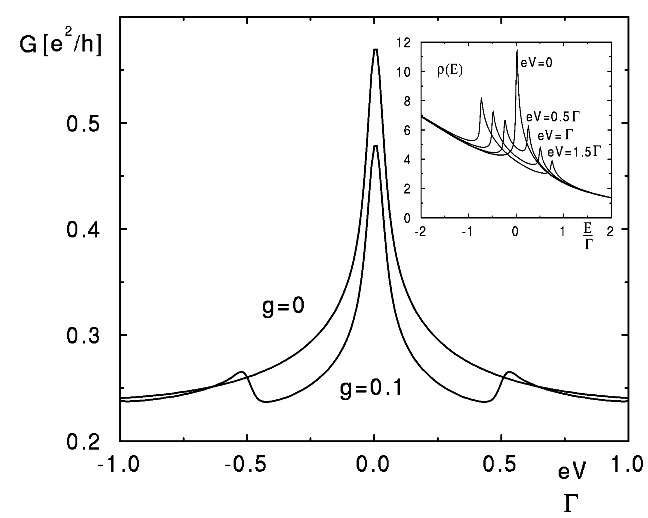

FIG. 3. The differential conductance vs bias voltage for $T = T_B = 0.01\Gamma$, $\epsilon = -4\Gamma$, $\omega_B = 0.5\Gamma$, and $E_C = 100\Gamma$. Inset: spectral density for various voltages and $g = 0$.

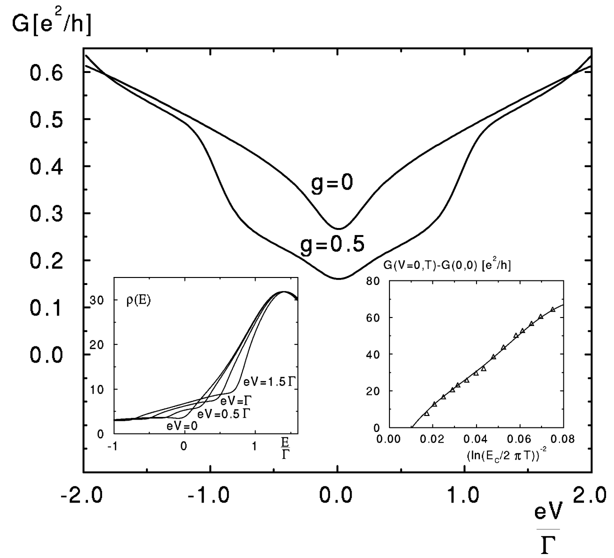

FIG. 4. The differential conductance vs bias voltage for $T = T_B = 0.05\Gamma$, $\epsilon = 0$, $\omega_B = \Gamma$, and $E_C = 100\Gamma$. Left inset: spectral density for various voltages and $g = 0$. Right inset: The temperature dependence of the linear conductance (solid line) coincides with experimental data from [13] (triangles).

as two-channel Kondo scattering from atomic tunneling systems [14,15] or by tunneling into a disordered metal [16]. Here we have shown that zero-bias minima can also arise due to resonant tunneling via local impurities if the level position is high enough such that we are in the mixed valence regime. We have also compared the temperature dependence of the linear conductance (see right inset of Fig. 4) as well as the scaling behavior of the nonlinear conductance with experiments [13] and find a remarkable coincidence. In order to explain the signal strength, however, one would need a large number of quantum dots in the sample of [13], for which there seems to be no experimental indication.

Finally, we have investigated the differential conductance at fixed bias voltage as a function of the position of the dot level, which experimentally can be varied by a gate voltage coupled capacitively to the dot. We obtain a (classical) pair of peaks at $|\epsilon| = eV/2$ together with satellites (due to emission and absorption of bosons) and peaks for $|\epsilon| > eV/2$ (only due to absorption). The imaginary part of $\sigma(E)$ gives rise to a (nonclassical) asymmetry of the peak heights. The peak at $\epsilon = eV/2$ is higher than the one at $\epsilon = -eV/2$ since $|\mathrm{Im}\sigma(E)| = \pi|M\gamma^+(E) + \gamma^-(E)|$ is smaller for higher energies (except for $M = 1$ when particle-hole symmetry holds). This significant effect is due to the broadening of the spectral density by quantum fluctuations.

In conclusion, we have studied low-temperature transport in the nonequilibrium Anderson model with bosonic interactions. The latter yield new Kondo resonances in the spectral density which can be probed by the measurement of the nonlinear differential conductance. Quantum fluctuations due to resonant tunneling yield zero-bias anomalies, *which can be changed from maxima to minima by varying the gate voltage*. We discussed similarities to recent experiments.

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