Perturbation treatment for transport through a quantum dot

Luis Craco and Kicheon Kang*
Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany

(Received 5 November 1998)

Resonant tunneling through an Anderson impurity is investigated by employing a perturbation scheme at nonequilibrium. This approach gives the correct weak and strong coupling limit in U by introducing adjustable parameters in the self-energy and imposing self-consistency of the occupation number of the impurity. We have found that the zero-temperature linear-response conductance agrees well with that obtained from the exact sum rule. At finite temperature the conductance shows a nonzero minimum at the Kondo valley, as shown in recent experiments. The effects of an applied bias voltage on the single-particle density of states and on the differential conductances are discussed for Kondo and non-Kondo systems. [S0163-1829(99)11519-4]

Electronic transport through an artificially fabricated quantum dot (QD) is of considerable current interest (for a review see, e.g., Ref. 1, and references therein). In addition to the Coulomb blockade and ordinary resonant tunneling through a discrete electronic level, a novel Kondo-assisted tunneling has been predicted.[2–6] This phenomenon has been verified in single-electron transistors[7,8] (SET) as well as in nanometer-sized metallic contacts.[9] In the SET structures several parameters can be controlled by external gates. This opens the possibility of studying a variety of electron correlation effects which are not available in the traditional Kondo problem of dilute magnetic impurities in a metal host. For example, the level position of the quantum dot and the coupling to reservoirs can be tuned in the single-electron transistor structure,[7,8] so that a *tunable Kondo effect* could be observed. Further, by applying an external voltage between two reservoirs, it is possible to study a new kind of Kondo effect out of equilibrium.

Transport through an Anderson impurity out of equilibrium has been studied theoretically by different methods including the perturbation treatment in Coulomb repulsion U (Refs. 4 and 6) and the noncrossing approximation (NCA).[5] The second order perturbation treatment gives reliable results for the symmetric case ($2\varepsilon_0+U=0$, ε_0 being the level position of the impurity). However, it is known that away from the symmetric case second order treatment does not reproduce the correct low- and high-energy limits.[6] For the limit of infinite U with weak hybridization, NCA provides quantitatively accurate results for the Kondo physics except for very small temperatures. Meanwhile, NCA has some drawbacks in the low-energy region: it fails to satisfy Fermi-liquid relations[10] and, as a consequence, overestimates the conductance due to the Kondo resonance[5] at low temperature. Although the qualitative physics of electron transport through the Anderson impurity is now well understood, a theory which can describe properly the wide range of parameters, including the physics of Kondo resonant transport, charge fluctuation, and the empty site limit, is still missing.

In this paper, we investigate the transport through an Anderson impurity by means of a new perturbation treatment which gives the correct weak and strong coupling limits in a self-consistent manner. Therefore, one can deal with an interpolation scheme between two limits. This treatment has been suggested by Kajueter and Kotliar[11] for an application to the Hubbard model in the high dimension limit. We extend this idea to study the transport through an Anderson impurity in a nonequilibrium regime. We have found that the zero-temperature linear-response conductance obtained from the density of states agrees well with those obtained from Langreth's exact relation.[14] Such good agreement has not been obtained before by the previous theories. Starting from this good agreement, we discuss the effects of finite temperature and of finite voltage on transport.

The resonant tunneling through a single quantum state can be described by the Anderson impurity model

$$\mathcal{H}=\sum_{k,\sigma,\alpha}\varepsilon_k^\alpha c_{k\sigma\alpha}^\dagger c_{k\sigma\alpha}+\sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma+U\hat{n}_\uparrow\hat{n}_\downarrow + \sum_{k,\sigma,\alpha}(t_k^\alpha c_{k\sigma\alpha}^\dagger d_\sigma+\text{H.c.}), \tag{1}$$

where ε_k^α represents the single-particle energy in the reservoir $\alpha(=L,R)$ with their chemical potential difference being the applied voltage, that is, $\mu_L-\mu_R=eV$. The parameters ε_0, U, and t_k^α denote the single-particle energy in the QD, the Coulomb repulsion, and the coupling between QD and reservoir states, respectively.

In the wide-band limit of the reservoirs, the current formula can be written in the form[12,13]

$$I=\frac{2e}{\hbar}\sum_\sigma\int d\omega\tilde{\Gamma}(\omega)\{f_L(\omega)-f_R(\omega)\}\rho_\sigma(\omega), \tag{2}$$

where $\tilde{\Gamma}(\omega)=\Gamma_L(\omega)\Gamma_R(\omega)/\Gamma(\omega)$ with $\Gamma_\alpha(\omega)=\pi\Sigma_k|t_k^\alpha|^2\delta(\omega-\varepsilon_{k\alpha})$ being the coupling strength between the QD level and the lead α, and $\Gamma(\omega)=\Gamma_L(\omega)+\Gamma_R(\omega)$. $f_\alpha(\omega)=1/(e^{\beta(\omega-\mu_\alpha)}+1)$ and $\rho_\sigma(\omega)=-(1/\pi)\text{Im}\,G_\sigma(\omega)$ are the Fermi function of lead α and the spectral density of states (DOS) of the electron in the QD, respectively.

In calculating the Green function

$$G_\sigma(\omega)=\frac{1}{\omega-\varepsilon_0-\sum_\alpha\Delta_\alpha(\omega)-\Sigma(\omega)}, \tag{3}$$

$\Delta_\alpha(\omega)=\Sigma_{k\in\alpha}|t_k^\alpha|^2/(\omega-\varepsilon_k^\alpha)$, we start with the ansatz for the self-energy

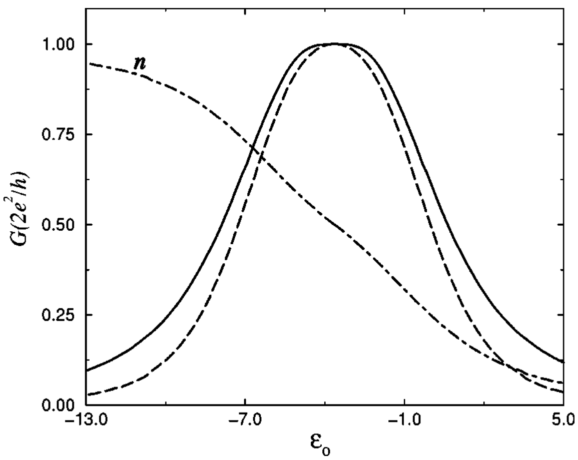

FIG. 1. Linear-response conductance at zero temperature as a function of the dot level position. The conductance is obtained from the DOS (solid line) and from Langreth's (exact) relation (dashed line). The dot-dashed line denotes the occupation number of the QD. $U=7.27\Gamma(0)$ and a parabolic form of $\Gamma(\omega)$ is used in this and all the other figures.

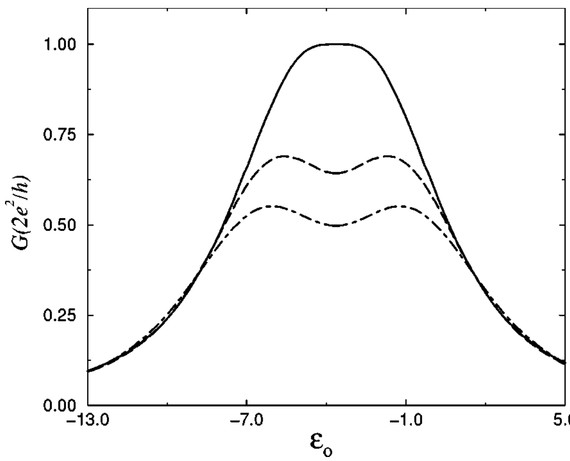

FIG. 2. Linear-response conductance at $T=0$ (solid line), $T=0.5\Gamma(0)$ (dashed line), and $T=\Gamma(0)$ (dot-dashed line). The conductance is symmetric around $\varepsilon_0=-U/2$ and it has minimum at this value for finite temperatures and a flat maximum at that point for $T=0$.

$$\Sigma(\omega)=Un+\frac{a\Sigma^{(2)}(\omega)}{1-b\Sigma^{(2)}(\omega)}, \tag{4}$$

where n is the occupation number of the QD level which should be determined self-consistently, and $\Sigma^{(2)}$ is the second order self-energy in U. Note that each Green's function line in the $\Sigma^{(2)}(\omega)$ diagram is given by

$$G_0(\omega)=\frac{1}{\omega-\varepsilon_0-Un-\sum_\alpha \Delta_\alpha(\omega)}. \tag{5}$$

The parameter a in Eq. (4) is determined from the condition that the self-energy has the exact behavior at high frequencies, and b is determined from the atomic limit.[11] Both conditions lead to the expressions

$$a=\frac{n(1-n)}{n_0(1-n_0)} \tag{6}$$

and

$$b=\frac{(1-2n)}{n_0(1-n_0)U}, \tag{7}$$

where n_0 is a fictitious particle number obtained from $G_0(\omega)$. Hence, these two parameters give the correct weak and strong coupling limits in any region, including Kondo, charge fluctuation, and even-number site limit.

The linear-response conductance $G=dI/dV|_{V=0}$ can be obtained from the spectral density of states according to the current formula Eq. (2). At zero temperature, it reduces to

$$G=\frac{2e^2}{h}4\pi\tilde{\Gamma}(0)\rho_\sigma(0). \tag{8}$$

In Fig. 1 we show the zero-temperature linear-response conductance as a function of the dot level for symmetric coupling $\Gamma_L(0)=\Gamma_R(0)$. For this and all the other figures we have chosen $U=7.27\Gamma(0)$. A parabolic form of $\Gamma(\omega)$ centered at $\omega=0$ with bandwidth $W=16.62\Gamma(0)$ is used and the energy scale in the x axis is normalized to $\Gamma(0)$. According to our results (see Fig. 1), $G\lesssim 2e^2/h$ in the Kondo limit, which implies the Kondo-assisted transmission. At zero temperature, the linear-response conductance may also be deduced from the Friedel-Langreth[14] sum rule, which leads to the relation[3]

$$G=\frac{2e^2}{h}\frac{4\Gamma_L(0)\Gamma_R(0)}{[\Gamma_L(0)+\Gamma_R(0)]^2}\sin^2\pi n. \tag{9}$$

In Fig. 1 one can see that the conductance obtained from the density of states presents good agreement with those obtained from the sum rule. It is important to note that such agreement could not be achieved by other treatments such as the ordinary second order perturbation theory or by the NCA.[15]

The linear-response conductance at finite temperatures is displayed in Fig. 2. The conductance shows a strong temperature dependence in the Kondo limit, while it is almost temperature independent for $\varepsilon_0>0$ and $\varepsilon_0+U<0$. The suppression of the conductance in the Kondo limit at finite temperatures is related with the reduction of the density of states near the Fermi level. As a result, the conductance has two maxima at certain points in $-U<\varepsilon_0<0$, and a minimum at $\varepsilon_0=-U/2$. Note that the conductance is symmetric around $\varepsilon_0=-U/2$ because of electron-hole symmetry of the model and has a minimum value at this energy for $T\neq 0$. To our knowledge, this is the first quantitative result which shows the nonzero conductance minimum due to the Kondo effect. Due to the Kondo resonance at finite temperature, the peak spacing for an odd-number QD is smaller than that of an even-number QD. The peak spacing between two conductance maxima is reduced as the temperature decreases, which can be attributed to the quantum fluctuation of the number of electrons in the QD. These effects have been observed in recent experiments for the SET.[7,8] The asymmetry comes from a transition between Kondo and non-Kondo system and is reproduced in our calculation. The Kondo effect shows up as a nonzero conductance between the conductance peaks for

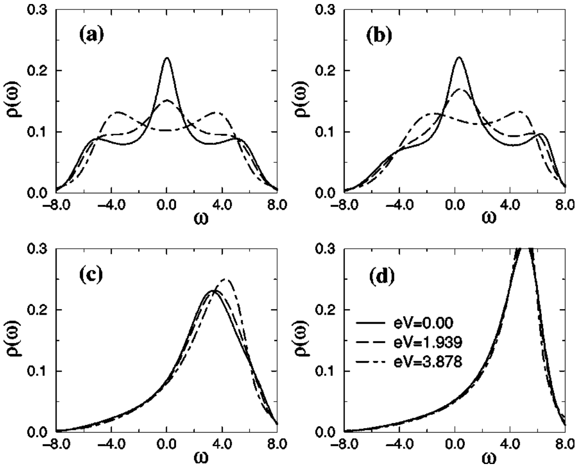

FIG. 3. Zero-temperature single-particle DOS of the QD level in the presence of the applied voltage. For (a) $\varepsilon_0 = -U/2$ and (b) $\varepsilon_0 = -0.286U$ the Kondo peaks are suppressed by applying the voltage, while the shape of the spectral DOS remains almost unchanged for non-Kondo systems, (c) $\varepsilon_0 = 0.19U$ and (d) $\varepsilon_0 = 0.38U$.

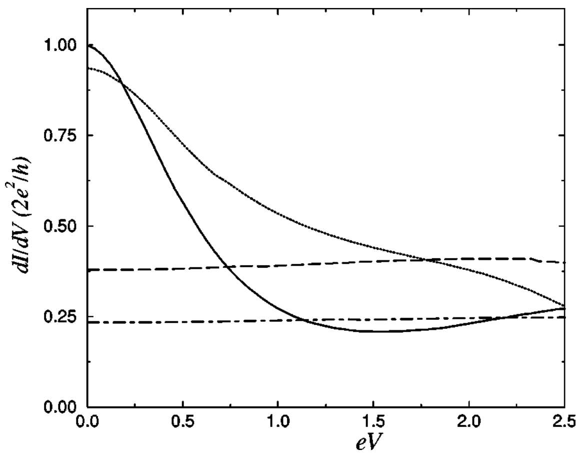

FIG. 4. Zero-temperature differential conductance as a function of the external voltage. Pronounced zero-bias maxima are shown in the Kondo limit [$\varepsilon_0 = -U/2$ (solid line), $-0.286U$ (dotted line)], while flat minima can be shown in the empty site limit [$\varepsilon_0 = 0.19U$ (dashed line), $0.38U$ (dot-dashed line)].

the QD with odd number of electrons. As the temperature increases, the minimum conductance at $\varepsilon_0 = -U/2$ decreases and the positions of the maximum conductance approach the bare levels, which implies that the transport properties are similar to the ordinary resonant tunneling at high temperature.

Let us now turn our attention to the nonequilibrium situation. For simplicity, we assume a symmetric voltage drop, that is, $\mu_L = -\mu_R = eV/2$. Figure 3 shows the spectral DOS of the QD at nonequilibrium for different values of ε_0. As one can easily find, the effects of the applied voltage are very different for the Kondo systems [(a) and (b)] and for the non-Kondo systems [(c) and (d)]. In Figs. 3(a) and 3(b) one can see that the resonance in the Fermi level is suppressed by applying the voltage, because the external voltage produces inelastic scattering of quasiparticles located between the two different chemical potentials. For the symmetric case $(2\varepsilon_0 + U = 0)$, the spectral weight in the Fermi level is transferred to the satellite peaks. In Fig. 3(b), we investigate the asymmetric case. Here, the reduction of the Kondo peak is less pronounced than in the symmetric case.

The DOS for $\varepsilon_0 > 0$, Figs. 3(c) and 3(d), is insensitive to the external voltage. This is very different from the behavior of the Kondo system. In this limit, the transport properties are similar to the noninteracting system and the differential conductance has a weak dependence on the temperature and on the external voltage, as we discuss below.

The differential conductance dI/dV as a function of V is displayed in Fig. 4 for several values of ε_0. The conductance is symmetric under bias reversal, since we considered a symmetric voltage drop as well as symmetric coupling for two tunnel barriers. The conductance has a maximum at zero bias in the Kondo system, because the Kondo resonance is reduced by the external voltage. This reduction is most pronounced in the symmetric case. This zero-bias maximum has been well known from previous calculations[4–6] and observed in experiments.[7–9] The conductance for the symmetric case increases at larger voltage, which is related to the ordinary resonance of the QD level with the leads. In contrast, the conductance shows very weak zero-bias minimum for the non-Kondo system $(\varepsilon_0 > 0)$. This can be understood from the behavior of the spectral DOS in the presence of applied voltage in Figs. 3(c) and 3(d). If the voltage dependence of the spectral DOS is neglected, the conductance at zero temperature is given by

$$\frac{dI}{dV} = \frac{2e^2}{\hbar}[\tilde{\Gamma}(eV/2)\rho_\sigma(eV/2) + \tilde{\Gamma}(-eV/2)\rho_\sigma(-eV/2)]. \tag{10}$$

According to the behavior observed in Figs. 3(c) and 3(d) as well as Eq. (10) one can conclude that the differential conductance has a weak zero-bias minimum for a non-Kondo system. The experimental results for the non-Kondo valley do not show a universal behavior.[8] That is, both zero-bias minima and maxima have been shown in the nonlinear conductance. This issue seems to be still open, while a pronounced zero-bias minimum in the mixed valence limit has been predicted in a previous study.[16]

In conclusion, we have studied resonant tunneling through a quantum dot by means of a new perturbation treatment which correctly takes into account the weak and strong coupling limits. In our study, we have found that the zero-temperature linear-response conductance agrees well with that obtained from the exact sum rule. At finite temperature the conductance has been shown to have a nonzero minimum at the Kondo valley and the minimum conductance decreases with increasing temperature. We have shown that the Kondo resonance is reduced by applying a small voltage. This leads to a pronounced zero-bias maximum of the differential conductance as a function of the voltage. On the other hand, the density of states is insensitive to the voltage in a non-Kondo system, and accordingly weak zero-bias minima occur in the differential conductance.

The authors wish to acknowledge P. Fulde for his hospitality during their stay at the Max-Planck-Institut für Physik Komplexer Systeme (MPI-PKS). This work has been supported by the MPI-PKS. One of us (K.K.) has also been supported in part by the KOSEF.

*Electronic address: kckang@mpipks-dresden.mpg.de

[1] L. P. Kouwenhoven *et al.*, in *Mesoscopic Electron Transport, Vol. 345 of NATO Advanced Study Institute*, edited by L. L. Sohn, L. P. Kouwenhoven, and G. Schön (Kluwer, Dordrecht, 1997).

[2] L. I. Glazman and M. E. Raikh, Pis'ma Zh. Éksp. Teor. Fiz. **47**, 378 (1988) [JETP Lett. **47**, 452 (1988)].

[3] T. K. Ng and P. A. Lee, Phys. Rev. Lett. **61**, 1768 (1988).

[4] S. Hershfield, J. H. Davies, and J. W. Wilkins, Phys. Rev. Lett. **67**, 3720 (1991); Phys. Rev. B **46**, 7046 (1992).

[5] Y. Meir, N. S. Wingreen, and P. A. Lee, Phys. Rev. Lett. **70**, 2601 (1993); N. S. Wingreen and Y. Meir, Phys. Rev. B **49**, 11 040 (1994).

[6] A. L. Yeyati, A. Martín-Rodero, and F. Flores, Phys. Rev. Lett. **71**, 2991 (1993).

[7] D. Goldhaber-Gordon, H. Shtrikman, D. Abush-Magder, U. Meirav, and M. A. Kastner, Nature (London) **391**, 156 (1998); D. Goldhaber-Gordon *et al.*, Phys. Rev. Lett. **81**, 5225 (1998).

[8] S. M. Cronenwett, T. H. Oosterkamp, and L. P. Kouwenhoven, Science **281**, 540 (1998).

[9] D. C. Ralph and R. A. Buhrman, Phys. Rev. Lett. **72**, 3401 (1994).

[10] Y. Kuramoto and H. Kojima, Z. Phys. B **57**, 95 (1984); E. Müller-Hartmann, *ibid.* **57**, 281 (1984).

[11] H. Kajueter and G. Kotliar, Phys. Rev. Lett. **77**, 131 (1996).

[12] Y. Meir and N. S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).

[13] This formula can be equally applied to the case of superconducting electrodes if the Andreev reflections are negligible due to large charging energy of the confined region. See K. Kang, Phys. Rev. B **57**, 11 891 (1998).

[14] D. C. Langreth, Phys. Rev. **150**, 516 (1966).

[15] The NCA is known to overestimate the Kondo resonance. See Ref. 5.

[16] J. König, H. Schoeller, and G. Schön, Phys. Rev. Lett. **76**, 1715 (1996); J. König, J. Schmid, H. Schoeller, and G. Schön, Phys. Rev. B **54**, 16 820 (1996).