Low-Temperature Transport Through a Quantum Dot: The Anderson Model Out of Equilibrium

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The infinite-U Anderson model is applied to nonequilibrium transport through a quantum dot containing two spin levels weakly coupled to two leads. At low temperatures, the Kondo peak in the equilibrium density of states is split upon the application of a voltage bias. The split peaks, one at the chemical potential of each lead, are suppressed by nonequilibrium dissipation. In a magnetic field, the Kondo peaks shift away from the chemical potentials by the Zeeman energy, leading to an observable peak in the differential conductance when the nonequilibrium bias equals the Zeeman energy.

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The behavior of an atomic impurity coupled to conduction electrons has become one of the paradigms of condensed matter physics. Competition between on-site Coulomb repulsion and band hybridization produces the Kondo effect: a crossover from weak to strong coupling between the localized and band electrons below the Kondo temperature T_K. Since it is a daunting task to drive the host metal out of equilibrium, only the *equilibrium* properties of Kondo impurities have been explored so far [1].

In this paper we address a new Kondo system in which *nonequilibrium* is routinely achieved, namely, a quantum dot weakly coupled to leads. It is already evident that Anderson's model [2] for a Kondo impurity—discrete, interacting levels coupled to a band—also describes quantum dots. Experimentally, the discrete spectrum of a single dot has been probed by transport [3–5] and capacitance [6] spectroscopy, while the strong on-site Coulomb interaction is observed in Coulomb-blockade conductance oscillations [4,5,7]. Theoretically, Anderson's model has provided an excellent description of these experiments in both equilibrium [8,9] and nonequilibrium [10]. However, it is only the high-temperature regime that has been explored experimentally, while it is below T_K that the Kondo effect emerges.

Since the Anderson Hamiltonian describes the quantum dot, at low temperatures the dot must behave as a Kondo impurity. In fact, it was argued [11] that at zero-temperature equilibrium the Kondo resonance in the density of states of spin-degenerate levels will always lead to perfect transparency of the quantum dot at the Fermi energy. In contrast, above the Kondo temperature, resonant tunneling occurs only at a discrete set of Fermi energies. Furthermore, the leads coupled to the dot are easily biased to nonequilibrium and the dot potential can be swept continuously with a gate. Thus new physical questions which were not relevant to magnetic impurities can be raised. In particular, what happens to the Kondo effect out of equilibrium [12]? Since transport measurements on single quantum dots require significant applied bias, this question is of immediate importance.

In this Letter we combine several approaches [perturbation theory, noncrossing approximation (NCA) [13], equations of motion (EOM) [14], variational wavefunction calculation [15]] to present a consistent picture of low-temperature, nonequilibrium transport through a quantum dot. For spin-degenerate levels at equilibrium, the Kondo peak [16] in the density of states at the chemical potential [Fig. 1(a)] leads to resonant transmission through the dot [11]. A voltage bias between the left and right leads causes the Kondo peak to split, leaving a peak in the density of states at the chemical potential of each lead [Fig. 1(b)]. The split Kondo peaks are suppressed by a finite nonequilibrium lifetime, due to dissipative transitions in which electrons are transferred from the high chemical potential lead to the low chemical potential one. Upon application of a magnetic field, the Kondo peaks shift away from the chemical potentials by the Zeeman splitting, but in opposite directions for each spin [Figs. 1(c) and 1(d)]. Interestingly, therefore, when the chemical potential splitting equals the Zeeman splitting, a Kondo peak shifted away from one chemical potential crosses the other chemical potential. We predict an observable peak in the differential conductance at this crossing [17] [Fig. 2(b)].

We model the quantum dot and its leads by the Anderson Hamiltonian [2]

$$H=\sum_{\sigma;k\in L,R}\epsilon_{k\sigma}c_{k\sigma}^{\dagger}c_{k\sigma}+\sum_{\sigma}\epsilon_{\sigma}c_{\sigma}^{\dagger}c_{\sigma}+Un_{\uparrow}n_{\downarrow}+\sum_{\sigma;k\in L,R}(V_{k\sigma}c_{k\sigma}^{\dagger}c_{\sigma}+\text{H.c.}), \quad (1)$$

where $c_{k\sigma}^{\dagger}$ ($c_{k\sigma}$) creates (destroys) an electron with momentum k and spin σ in one of the two leads, and $c_{\sigma}^{\dagger}$ (c_{σ}) creates (destroys) a spin-σ electron on the quantum dot. Since we are interested in temperatures smaller than the orbital level spacing in the quantum dot, we consider only a single pair of levels on the dot with energies $\epsilon_{\uparrow}=\epsilon_0+\Delta\epsilon/2$ and $\epsilon_{\downarrow}=\epsilon_0-\Delta\epsilon/2$. The third term in (1)

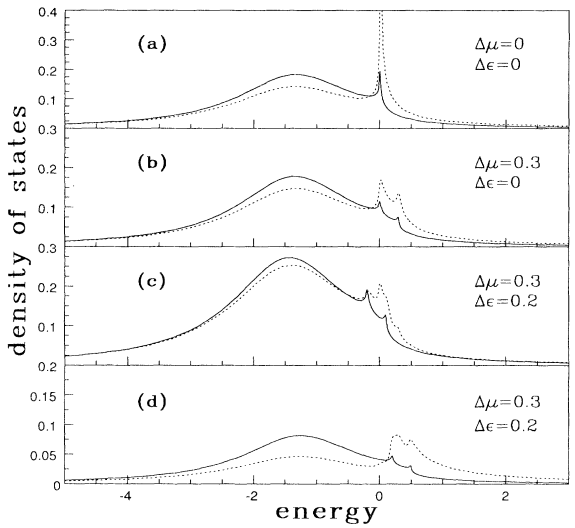

FIG. 1. Density of states for an Anderson impurity symmetrically coupled to two leads with chemical potentials μ_L and μ_R ($=0$) and Lorentzian bandwidth $2W$, from the equations-of-motion method (continuous line) and the noncrossing approximation (dashed line). The impurity has two spin states with energies $\epsilon_\uparrow$ and $\epsilon_\downarrow$ and an on-site interaction $U\rightarrow\infty$. All energies are in units of the total coupling to the leads, Γ. The bandwidth is $W=100$ and the temperature is $T=0.005$, roughly a factor of 2 lower than the magnetization Kondo temperature [13]. (a) The equilibrium ($\mu_L=0$) density of states at zero magnetic field $\epsilon_\uparrow=\epsilon_\downarrow=-2.0$, exhibiting a single peak at the Fermi level. (b) The nonequilibrium ($\mu_L=0.3$) density of states at zero magnetic field $\epsilon_\uparrow=\epsilon_\downarrow=-2.0$, with a suppressed Kondo peak at each chemical potential. (c) and (d) The nonequilibrium ($\mu_L=0.3$) density of states for spin up (c) and spin down (d) at finite magnetic field $\epsilon_\uparrow=-1.9$, $\epsilon_\downarrow=-2.1$. The Kondo peaks shift away from the chemical potentials by the Zeeman splitting $\Delta\epsilon=0.2$; the shift is up in energy for the up spin and down in energy for the down spin.

describes the Coulomb interaction between the two localized spins which we take to forbid double occupancy [18] ($U\rightarrow\infty$), while the fourth term describes the hopping between the leads and the dot.

Our aim is to calculate the current through the dot, J, which for the case of proportionate couplings to the leads, $\Gamma_\sigma^L(\omega)=\lambda\Gamma_\sigma^R(\omega)$, where $\Gamma_\sigma^{L(R)}(\omega)=2\pi\sum_{k\in L(R)}|V_{k\sigma}|^2\times\delta(\omega-\epsilon_{k\sigma})$, can be expressed [19] in terms of the density of states, $-(1/\pi)\mathrm{Im}G_\sigma^r(\omega)$, as

$$J=\frac{e}{\hbar}\sum_\sigma\int d\omega[f_L(\omega)-f_R(\omega)]\Gamma_\sigma(\omega)\left[-\frac{1}{\pi}\mathrm{Im}G_\sigma^r(\omega)\right]. \tag{2}$$

In Eq. (2), $\Gamma_\sigma(\omega)=\Gamma_\sigma^L(\omega)\Gamma_\sigma^R(\omega)/[\Gamma_\sigma^L(\omega)+\Gamma_\sigma^R(\omega)]$, and $G_\sigma^r(\omega)$ is the Fourier transform of the retarded Green function, $G_\sigma^r(t)=-i\Theta(t)\langle\{c_\sigma(t),c_\sigma^\dagger(0)\}\rangle$.

The main features of the density of states can be determined via perturbation theory in the hopping matrix elements $V_{k\sigma}$. For each spin state at infinite U, we find, in addition to the single-particle resonance at ϵ_σ, logarithmic divergences, at $T=0$ and at order V^4, signaling Kondo peaks at $\mu_{L/R}-\Delta\epsilon$ for the low-lying spin and at $\mu_{L/R}+\Delta\epsilon$ for the high-lying spin. In order to calculate the full Green function $G_\sigma^r(\omega)$ we use both the NCA [13] and an EOM method [8,14]. The NCA is based on an exact mapping of the infinite-U Anderson Hamiltonian (1) onto a slave-boson Hamiltonian. If vertex corrections are neglected, the propagators for the empty site (a boson) and the singly occupied site (fermions) obey a set of coupled integral equations. Numerical solution of these equations has been very useful in obtaining quantitative results for the equilibrium system [13,20]. In this work we have generalized the NCA to nonequilibrium to produce densities of states, occupations, and the nonlinear current (2). However, as a large spin-degeneracy (large-N) technique, the NCA produces a Kondo peak even for the noninteracting system ($N=1$). Consequently, while quantitatively reliable at zero field, the NCA gives rise to spurious peaks in the density of states at the chemical potentials μ_L and μ_R at finite magnetic fields. Therefore, an EOM method was employed to complement the NCA. This method corresponds to a resummation of low-order hopping processes and is known [14] to give the right qualitative behavior at low temperatures. More importantly in the present context, being exact for $N=1$, the EOM method gives rise only to the proper Kondo peaks, even for finite magnetic fields (as identified by perturbation theory).

The EOM method consists of differentiating the Green function $G_\sigma^r(t)$ with respect to time, thereby generating higher-order Green functions which eventually have to be approximated to close the equation for $G_\sigma^r(t)$. The procedure employed here is the same as the one used in Ref. [8], which in the infinite-U limit leads to

$$G_\sigma^r(\omega)=\frac{1-\langle n_{\bar\sigma}\rangle}{\omega-\epsilon_\sigma-\Sigma_{0\sigma}(\omega)-\Sigma_{1\sigma}(\omega)}, \tag{3}$$

with $\Sigma_{0\sigma}(\omega)=\sum_{k\in L,R}|V_{k\sigma}|^2/(\omega-\epsilon_{k\sigma}+i\eta)$, and

$$\Sigma_{1\sigma}(\omega)=\sum_{k\in L,R}\frac{|V_{k\bar\sigma}|^2 f_{L/R}(\epsilon_{k\bar\sigma})}{\omega-\epsilon_\sigma+\epsilon_{\bar\sigma}-\epsilon_{k\bar\sigma}+i\hbar/2\tau_{\bar\sigma}}, \tag{4}$$

where $f_{L/R}(\epsilon)$ is the Fermi distribution in the left/right lead and $\tau_{\bar\sigma}$ is the intermediate-state lifetime. $G_\sigma^r(\omega)$ has an overall amplitude proportional to $1-\langle n_{\bar\sigma}\rangle$, where $\langle n_{\bar\sigma}\rangle$ is the occupation of the other spin state. Quantitative calculation of the occupations is beyond the scope of the EOM in the present approximation scheme. Accordingly, we use the occupations resulting from the NCA, which are known to be quantitatively reliable in equilibrium [20].

Within the EOM scheme, the Kondo peak for spin σ results from the self-energy, $\Sigma_{1\sigma}(\omega)$, due to virtual intermediate states in which the site is occupied by an electron of opposite spin, $\bar\sigma$. The remaining self-energy, $\Sigma_{0\sigma}(\omega)$, is the exact self-energy for the noninteracting case. Because of the sharp Fermi surfaces at low temperature,

$\mathrm{Re}\{\Sigma_{1\sigma}(\omega)\}$ grows logarithmically at $\omega=\mu_{L,R}\pm\Delta\epsilon$, giving rise to peaks in the density of states near those energies. The peaks for the high-lying spin (low-lying spin) appear near $\omega=\mu_{L,R}+\Delta\epsilon(\omega=\mu_{L,R}-\Delta\epsilon)$. At zero-field and zero-temperature equilibrium, the intermediate states giving rise to $\Sigma_{1\sigma}(\omega)$ have an infinite lifetime, and the true peak in the density of states has an amplitude corresponding to the unitarity limit [16]. Once either a voltage bias or a magnetic field is applied these intermediate states acquire a finite lifetime $\tau_{\bar{\sigma}}$, which cuts off the logarithmic divergence of $\mathrm{Re}\{\Sigma_{1\sigma}(\omega)\}$, resulting in a suppression of the peak amplitudes. The lifetime τ_σ of spin σ can be calculated using second-order perturbation theory. For a deep level at zero temperature and for constant Γ we find

$$\frac{1}{\tau_\sigma}=\frac{1}{2\pi\hbar}\sum_{\substack{A,B=L,R\\ \sigma'}}\Gamma_\sigma^A\Gamma_\sigma^B\Theta(\mu_B-\mu_A+\epsilon_\sigma-\epsilon_{\sigma'})\frac{\mu_B-\mu_A+\epsilon_\sigma-\epsilon_{\sigma'}}{(\mu_A-\epsilon_\sigma)(\mu_B-\epsilon_{\sigma'})}, \tag{5}$$

which explicitly shows that the lifetime is nonzero onl for finite bias or finite magnetic field.

In Fig. 1, we plot the density of states for two spins symmetrically coupled to two leads, consisting of Lorentzian bands of width $2W$, so that $\Gamma_\sigma^L(\omega)=\Gamma_\sigma^R(\omega)=\Gamma W^2/2(\omega^2+W^2)$, with $\Gamma\equiv 1$ and $W=100$. Results are shown for the NCA (dashed lines), which is reliable for zero magnetic field, and for the EOM method (continuous lines), which has the correct Kondo peak energies for all magnetic fields. In equilibrium and zero magnetic field, the density of states exhibits a single peak at the Fermi level as expected [16] [Fig. 1(a)]. As the chemical potentials split, the Kondo peak also splits, giving rise to a suppressed Kondo peak at each chemical potential [Fig. 1(b)]. Upon the application of a magnetic field, the densities of states for the two spins become different and the Kondo peaks shift away from the chemical potentials by the Zeeman splitting [$\Delta\epsilon=0.2$ in Figs. 1(c) and 1(d)]. The peaks move up in energy for the high-lying spin [Fig. 1(c)] and down in energy for the low-lying one [Fig. 1(d)].

The main conclusion of Fig. 1 is the emergence of new energy scales not present in equilibrium. The Kondo peak in the equilibrium density of states splits out of equilibrium to two peaks spaced by the chemical potential difference $\Delta\mu$ and suppressed from equilibrium by the finite dissipative lifetime τ_σ. In Fig. 1(b), the lifetime broadening $\hbar/\tau_\sigma$ is about the same as the temperature. To understand the shift of the Kondo peaks with magnetic field, it is helpful to recall how the peaks in the density of states derive from the eigenstates of the system. At $T=0$, $G_\sigma^r(t)$ involves transitions from the N-particle ground state to all possible $N+1$ or $N-1$ states. At $B=0$ the correlated ground state has a finite amplitude to have an empty site, and thus $c_\sigma^\dagger$ (c_σ) can generate transitions from the N-particle ground state to the ground state with one more (one less) electron. Since, by definition, the ground state energies differ by the chemical potential, the density of states includes a Kondo peak at the chemical potential. Within a variational calculation [15], we find that at finite magnetic field the ground state is polarized, and adding or removing an electron produces no overlap with the new ground state. However, there is a correlated excited state of opposite polarization which gives rise to a peak in the density of states, shifted by the difference in energy between polarization states, i.e., the Zeeman energy.

The current follows immediately from the densities of states (2). In particular, the zero-temperature current is the integrated density of states between the two chemical potentials, weighted by the coupling to the leads $\Gamma_\sigma(\omega)$. At zero magnetic field, therefore, the Kondo peak at the Fermi energy gives rise to a linear-response conductance of $2e^2/h$ for symmetric barriers, corresponding to perfect resonant transmission through the quantum dot [11]. As the bias is increased the differential conductance falls rapidly [Fig. 2(a)] [12]. This occurs first because the differential conductance due to a peak in the density of states must fall off once $\Delta\mu$ exceeds the peak width, and second because the decreasing dissipative lifetime suppresses the peak amplitudes. Since the peaks in the density of states persist until the temperature is roughly one-tenth the coupling to the leads, Γ, the peak in the differential conductance is observable well above the Kondo temperature T_K [Fig. 2(a), continuous line].

In a finite magnetic field the Kondo peaks are shifted away from the chemical potential so they contribute very little to the conductance in linear response. As the bias is increased, however, the current-carrying region between the chemical potentials grows until, at $\Delta\mu=\Delta\epsilon$, it reaches one Kondo peak in the density of states of each spin [see inset of Fig. 2(b)]. Accordingly, in Fig. 2(b), where the EOM density of states has been used, one sees peaks in the differential conductance at $\Delta\mu=\Delta\epsilon$ (continuous line). In fact, by comparison with the NCA (Fig. 1), we expect the EOM to underestimate the full strength of these peaks. Experimentally, observation of peaks in the differential conductance at $\Delta\mu=\Delta\epsilon$ would provide a "smoking gun" for the presence of Kondo physics in transport through a quantum dot.

In this work, we addressed the nonequilibrium behavior of Anderson's model for a magnetic impurity. Experimentally, the model describes low-temperature transport through a quantum dot, where nonequilibrium is readily accessible. We have shown that new energy scales emerge in nonequilibrium. Specifically, the difference in chemical potentials $\Delta\mu$ and the inverse dissipation time $\hbar/\tau_\sigma$ lead, respectively, to splitting and suppression of the Kondo resonances in the density of states. Our finding via several methods of two Kondo peaks in the nonequilibrium density of states, one for each chemical potential,

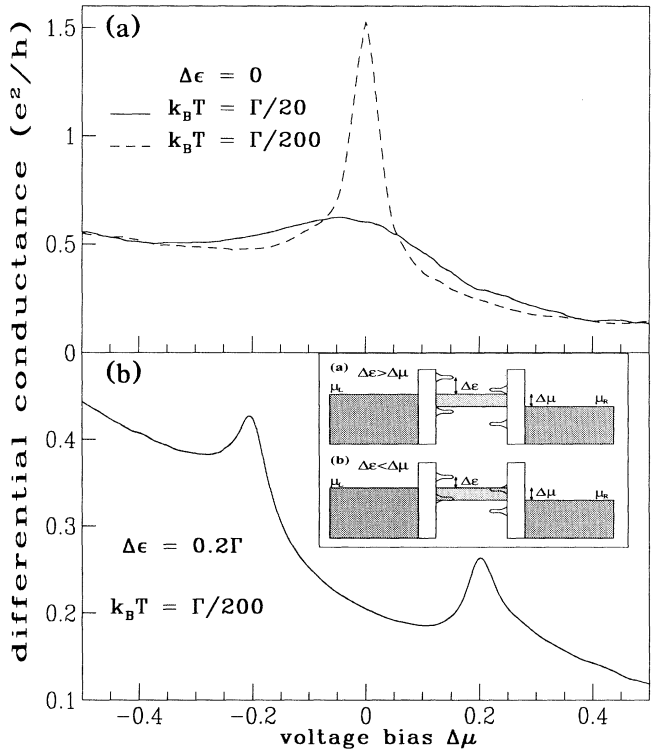

FIG. 2. Differential conductance, $e\,dJ/d\Delta\mu$, with $\mu_R=0$ vs applied bias. (a) Zero magnetic field differential conductance via the noncrossing approximation. (b) Differential conductance at the finite magnetic field, $\Delta\epsilon=0.2$, used in Figs. 1(c) and 1(d), via equations of motion. As shown in the inset, when the chemical potential difference $\Delta\mu$ reaches the Zeeman splitting $\Delta\epsilon$, the Kondo peaks in the density of states enter the region between the chemical potentials, giving rise to a peak in the differential conductance.

contrasts with the results of Hershfield, Davies, and Wilkins [12]. They used a small-U expansion to study the symmetric Anderson model in zero magnetic field and found a single peak in the density of states which is destroyed with increasing chemical potential difference. However, the Hartree solution about which they expand has intrinsically only a single Kondo peak, at $\epsilon_\sigma+U\langle n_{\bar\sigma}\rangle$, and so is an inadequate starting point for nonequilibrium.

Our results have led to a novel experimental prediction—when the Zeeman splitting of the spins, $\Delta\epsilon$, equals the applied bias $\Delta\mu$, there will be a peak in the differential conductance, provided these energies are smaller than the coupling to the leads, Γ, and smaller than the depth of the levels, $\mu_{L,R}-\epsilon_\sigma$. Importantly, this signature of the Kondo effect persists for a wide range of parameters to temperatures $\sim\Gamma/20$. The observation of resonance widths $\Gamma\sim 40$ μeV by Foxman *et al.* [4] in electrostatically defined quantum dots indicates a Kondo peak in the differential conductance at $T\sim 20$ mK. In contrast, the Kondo contribution to the linear-response conductance [11] is only apparent at temperatures below the magnetization Kondo temperature [13] $T_K\sim(W\Gamma/\pi)^{1/2}\exp(-\pi|\mu-\epsilon_\sigma|/\Gamma)$. Even for $\mu-\epsilon_\sigma=2\Gamma$ [Fig. 1(a)], this exponential falloff leads to $T_K\sim\Gamma/100$, a prohibitive temperature for existing quantum dots. We hope that this work will encourage further efforts, both experimental and theoretical, to probe the nonequilibrium physics of interacting quantum systems.

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