Probing the Kondo Resonance by Resonant Tunneling through an Anderson Impurity

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We compute the current as a function of voltage for resonant tunneling through an Anderson impurity in the low-temperature, Kondo, regime. The differential conductance curve has the same structure as the zero-bias spectral function, but is sharper because a finite voltage tends to destroy the Kondo resonance. This destruction of the Kondo resonance cannot be mapped onto an increase in the effective temperature at the impurity site. The calculation is performed in the symmetric Anderson model using perturbation theory in the Hubbard U repulsion.

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Mesoscopic systems allow us to study effects of interactions, such as the electron-electron interaction, in radically new situations. With improved microfabrication techniques it has become possible to reliably manufacture tunneling systems which exhibit suppression of tunneling due to charging effects. In a range of systems—from small metal-insulator-metal tunnel junctions connected in series [1,2], to quantum dots and narrow wires [3–5], to tunneling between localized states in an insulator [6] —the Coulomb interaction suppresses tunneling for certain ranges of applied voltages, leading to what is now commonly called the Coulomb blockade. As one continues to go to smaller samples and lower temperatures, one approaches the limiting case of tunneling through a single localized state with a Hubbard U repulsion. This is precisely the Anderson model [7]. It is well known that a new resonance, called the Kondo resonance, appears near the Fermi energy in the Anderson model at low temperatures. The tunneling spectrum of this system offers the possibility of seeing features of the Kondo effect not readily observable in bulk systems.

Earlier work on this model examined the conductance above the Kondo temperature [8,9] and the linear-response conductance for all temperatures [10,11]. The linear-response conductance is proportional to the impurity spectral function at the Fermi energy in equilibrium [11]. By varying the temperature, an external magnetic field, or the energy of the impurity state, one can enhance or destroy the Kondo resonance and hence change the linear-response conductance. While all of these are useful signatures of the Kondo effect, they are not powerful experimental probes of the Kondo resonance. For example, both bulk systems and this one-impurity system show a logarithmic temperature dependence in the resistance or conductance at high temperatures [8,9] followed by a rounding off at low temperatures [10,11]. In this paper we show that by measuring the nonlinear current-voltage characteristic and the differential conductance at low temperatures, one can see structure which is closely related to the spectral function of the impurity state. Also, the nonlinear IV characteristic probes the Kondo effect out of equilibrium while linear-response conductance only probes the equilibrium properties of the Kondo effect. Thus, the differential conductance not only provides a signature of the Kondo effect, but a valuable new probe of the Kondo resonance.

We consider a one-dimensional tight-binding model with a Hubbard U repulsion at the $n=0$ site [8–11]. The energy of the central site is ϵ_0, and the site energies in the right ($n \geq 1$) and left ($n \leq -1$) leads are U_R and U_L, respectively, with $U_L - U_R$ equal to the voltage drop, $e|V|$. All the hopping matrix elements are equal to W except those coupling the central site to the right (W_R) and left (W_L) leads. In addition to defining the Hamiltonian, it is necessary for a nonequilibrium problem to define how the system is perturbed from equilibrium. In our calculation we start initially at $t=-\infty$ with no Hubbard U repulsion at the central site, but with two different chemical potentials, $\mu_L = \mu + U_L$ and $\mu_R = \mu + U_R$, for electrons coming in from the left and right leads, respectively. The interaction is then turned on adiabatically using the perturbation theory of nonequilibrium quantum-statistical mechanics [12,13]. The same results are obtained by turning on both the hopping onto the central site and the interaction adiabatically.

Even though U may be large compared to the hopping rate onto the central site, perturbation in U yields qualitatively the correct results for the spectral function and other low-temperature properties of the Anderson model [14,15]. Indeed, Zlatic and Horvatic have shown that the exact solution of the symmetric Anderson model is analytic in U [16]. Recent quantum Monte Carlo calculations of the spectral function for the symmetric Anderson model show close agreement with the perturbation theory calculation when one keeps only the order-U^2 contribution to the self-energy [17].

Applying nonequilibrium quantum-statistical mechanics to resonant tunneling through an Anderson impurity as described above, we find that the currents in the right and left leads, I_R and I_L, which are equal in steady state, may be expressed in terms of the density of occupied and empty states for one spin at the impurity, $n_{\rm occ}(\omega)$ and $n_{\rm emp}(\omega)$ [18]. No spin indices appear in $n_{\rm occ}(\omega)$ and $n_{\rm emp}(\omega)$ because the ground state is assumed to be a sing-

let [14]. The current entering the right lead is given by the product of the tunneling rate, $2\Gamma_R(\omega)$, the density of occupied states at the central site, $n_{\rm occ}(\omega)$, and the probability that a state in the right lead at energy ω is empty $[1-f^R(\omega)]$, where $f^R(\omega)=[1+e^{\beta(\omega-\mu_R)}]^{-1}$ [19]. Likewise, the current leaving the right lead is given by the product of $2\Gamma_R(\omega)$, $n_{\rm emp}(\omega)$, and the probability that a state at energy ω in the right lead is occupied, $f^R(\omega)$. The net current in the right lead is the difference of the current entering the right lead minus the current leaving it:

$$I_R=2\int d\omega\, 2\Gamma_R(\omega)\{n_{\rm occ}(\omega)[1-f^R(\omega)] - n_{\rm emp}(\omega)f^R(\omega)\}\,. \quad (1)$$

The current in the left lead is the negative of Eq. (1) with $R\rightarrow L$. Interactions enter I_R and I_L only through the density of occupied and empty states.

It will be useful to write the current in terms of the spectral function, $a(\omega)=n_{\rm occ}(\omega)+n_{\rm emp}(\omega)$, whose integrated intensity is 1. Let $\epsilon_0(\omega)$ be the energy of the central site renormalized by the coupling to the leads, $\Gamma(\omega)=\Gamma_L(\omega)+\Gamma_R(\omega)$, and $\sigma_r(\omega)$ be the retarded self-energy. Then $a(\omega)$ is given by

$$a(\omega)=-\frac{1}{\pi}\,{\rm Im}\frac{1}{\omega-\epsilon_0(\omega)+i\Gamma(\omega)-\sigma_r(\omega)}\,. \quad (2)$$

For a *noninteracting* system the ratio of $n_{\rm occ}(\omega)$ to $a(\omega)$ is an effective Fermi distribution function, $f^{\rm eff}(\omega)$, which is the weighted average of the Fermi functions in the two leads:

$$f^{\rm eff}(\omega)=\frac{\Gamma_L(\omega)f^L(\omega)+\Gamma_R(\omega)f^R(\omega)}{\Gamma_L(\omega)+\Gamma_R(\omega)}\,. \quad (3)$$

In the presence of interactions $f^{\rm eff}(\omega)$ is only *part* of $n_{\rm occ}(\omega)/a(\omega)$ because electrons can scatter inelastically in addition to entering from the two leads. Let the inelastic scattering rate at energy ω be $\Gamma_{\rm in}(\omega)=-2\,{\rm Im}\sigma_r(\omega)$ and the "scattering-in" self-energy be $\sigma_<(\omega)$ [12]. The general formula for $n_{\rm occ}(\omega)/a(\omega)$ is then

$$\frac{n_{\rm occ}(\omega)}{a(\omega)}=\frac{2\Gamma(\omega)f^{\rm eff}(\omega)+\sigma_<(\omega)}{2\Gamma(\omega)+\Gamma_{\rm in}(\omega)}\,. \quad (4)$$

A similar expression holds for $n_{\rm emp}(\omega)/a(\omega)$ with $f^{\rm eff}(\omega)$ replaced by $1-f^{\rm eff}(\omega)$ and $\sigma_<(\omega)$ replaced by the "scattering-out" self-energy, $\sigma_>(\omega)$.

Using Eqs. (1)–(4) the average current, $I=(I_R+I_L)/2$, and current-conservation condition, $I_R-I_L=0$, are given by the exact expressions

$$I=\int d\omega\,\frac{4\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}a(f^L-f^R) + \int d\omega\,\frac{\Gamma_R-\Gamma_L}{\Gamma_R+\Gamma_L}(n_{\rm emp}\sigma_<-n_{\rm occ}\sigma_>)\,, \quad (5)$$

$$0=2\int d\omega\,(n_{\rm emp}\sigma_<-n_{\rm occ}\sigma_>)\,, \quad (6)$$

where the energy dependence of the integrands is to be understood. The first line in Eq. (5) is the noninteracting expression for the current with the full spectral function replacing the noninteracting spectral function. The second line is new and shows that the nonlinear current is *not* a simple generalization of the noninteracting result. However, in the case of wide bands in the leads, where we can neglect the energy dependence of the Γ's, the second term in Eq. (5) is zero because of the current-conservation condition, Eq. (6). In the following we will be taking this wide-band limit so only the first line in Eq. (5) contributes.

We have calculated the current and spectral functions using the second-order self-energy of Refs. [14,15]. In general these self-energies do not lead to a current-conserving approximation, i.e., Eq. (6) is not zero; however, in the symmetric Anderson model ($\epsilon_0=-U/2$) with the extra symmetry $\Gamma_L=\Gamma_R$ this approximation for the spectral function does conserve current. We thus examine only this case. In Fig. 1(a) we have plotted the current as a function of voltage for three different temperatures. The zero-temperature current shows a sharp rise at zero voltage, which rounds off and becomes almost linear. This feature disappears with increasing temperature.

To bring out the structure in the current-voltage characteristic, the differential conductance, dI/dV, is shown in Figs. 1(b) and 1(c). From Eq. (5) the derivative $dI/de|V|$ at zero temperature would be equal to $\Gamma a(\omega)$ evaluated at $\omega=e|V|/2$ if the spectral function did not

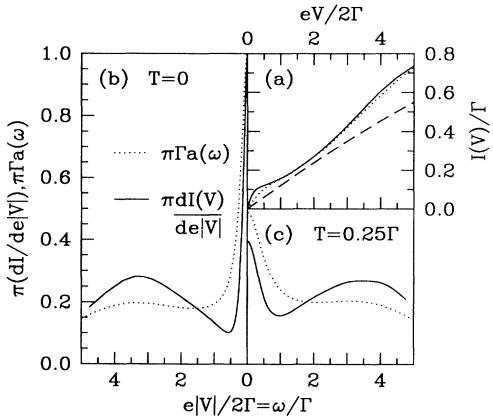

FIG. 1. Current-voltage and differential conductance curves for a tunnel junction consisting of single symmetric Anderson impurity equally coupled to two leads. (a) The current at $T=0$ (solid curve), 0.25Γ (dotted curve), and 2.5Γ (dashed curve). As the temperature is increased the low-voltage structure disappears. (b),(c) Comparison of the differential conductance (solid curves) to the zero-bias spectral function (dotted curves). At both $T=0$ and $T=0.25\Gamma$ the differential conductance has the same shape as the zero-bias spectral function but it is sharper. The Kondo temperature is $T_K=0.05\Gamma$ ($U/\pi\Gamma\approx 2.39$).

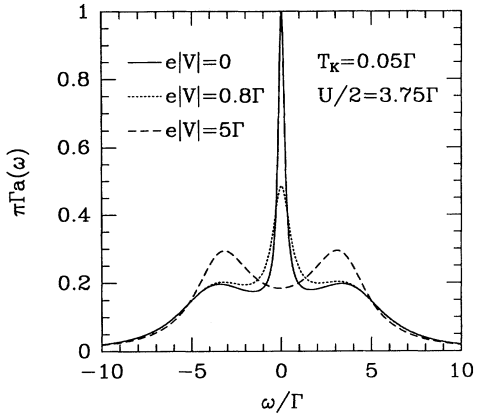

FIG. 2. Destruction of the Kondo resonance by an applied bias. As the voltage is increased the spectral weight is shifted away from the Kondo resonance towards the two side peaks. Eventually, for large voltages, there is no remnant of the Kondo resonance.

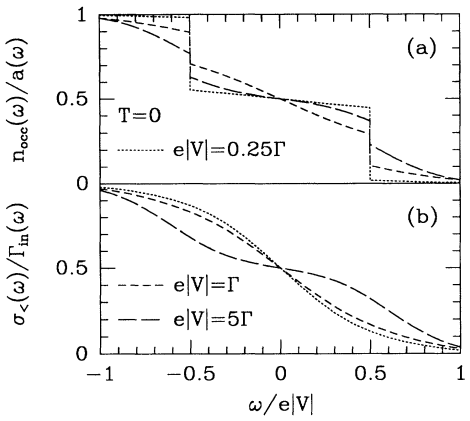

FIG. 3. Search for an effective temperature. In equilibrium the ratios $n_{\rm occ}(\omega)/a(\omega)$ and $\sigma_<(\omega)/\Gamma_{\rm in}(\omega)$ are Fermi functions. If applying a voltage is the same as raising the temperature, then for a nonzero bias these ratios should also be Fermi functions. (a) $n_{\rm occ}(\omega)/a(\omega)$, which involves electrons which come from the leads without scattering inelastically, has a discontinuity and is not a Fermi function. (b) $\sigma_<(\omega)/\Gamma_{\rm in}(\omega)$, which involves electrons which have scattered inelastically, is qualitatively similar, but *not* quantitatively equal, to a Fermi function.

change as a function of the applied voltage. Both the $T=0$ and $T=0.25\Gamma\approx 5T_K$ differential conductance curves show the resonance near the Fermi energy ($\omega=0$) and the side peak at $U/2$ of the zero-bias spectral function. At these temperatures the differential conductance is actually *sharper* than the zero-bias spectral function, indicating that the spectral function is changing substantially as the voltage is increased. Thermal smearing dominates at high temperatures and the differential conductance is smoother than the zero-bias spectral function.

To see how the spectral function changes we have plotted it in Fig. 2 for three different applied voltages at zero temperature. As the voltage is increased to $e|V|=0.8\Gamma$ the Kondo resonance becomes smaller and the spectral weight is shifted to the two side peaks. This shifting of spectral weight to the side peaks is what causes the differential conductance to be sharper than the zero-bias spectral function. At large voltages there is no remnant of the Kondo resonance.

Raising the temperature has an effect similar on the spectral function to applying a voltage. Is there a correspondence between temperature and voltage? The inelastic scattering rate for small voltage, temperature, and energy is proportional to $\omega^2+(\pi T)^2+\frac{3}{4}(e|V|)^2$, suggesting that there is such a correspondence. However, the ratio $n_{\rm occ}(\omega)/a(\omega)$, which is a Fermi function in equilibrium, has steps for a finite voltage at zero temperature [Fig. 3(a)]. These steps are due to electrons which come from the leads without scattering inelastically. In Eq. (4) they are contained in $f^{\rm eff}(\omega)$ and have magnitude $\Gamma/(2\Gamma+\Gamma_{\rm in})$ evaluated at $\omega=e|V|/2$. The part of $n_{\rm occ}(\omega)/a(\omega)$ which involves electrons which have scattered inelastically, $\sigma_<(\omega)/\Gamma_{\rm in}(\omega)$, is a smooth function, although it is not quantitatively equal to a Fermi function [Fig. 3(b)].

In this paper we have seen that the differential conductance for tunneling through an Anderson impurity allows one to "see" directly the Kondo resonance. In the symmetric Anderson model the fact that Kondo resonance is destroyed by increasing the voltage does not wash out the structure in the differential conductance, but actually enhances it. Although applying a voltage and raising the temperature do have similar effects on the Kondo resonance, a finite voltage cannot be mapped simply onto a temperature increase.

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[18] $n_{\rm occ}(\omega)$ and $n_{\rm emp}(\omega)$ are the Fourier transforms of $\langle c^{\dagger}_{0,s}(t')c_{0,s}(t)\rangle/2\pi$ and $\langle c_{0,s}(t)c^{\dagger}_{0,s}(t')\rangle/2\pi$, where $c^{\dagger}_{0,s}$ and $c_{0,s}$ are creation and destruction operators in the Heisenberg representation for an electron with spin s at the central site.
[19] $2\Gamma_R(\omega)$ is $2\pi W_R^2$ times the single spin density of states in the right lead, $(\pi W)^{-1}\{1-[(\omega-U_R)/2W]^2\}^{1/2}$.