Nonlinear Conductance for the Two Channel Anderson Model

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Using the integral equations of the noncrossing approximation, the differential conductance is computed as a function of voltage for scattering from a two channel Kondo impurity in a point contact. The results compare well to experimental data on Cu point contacts by Ralph and Buhrman. They support a recently proposed scaling hypothesis, and also show finite temperature corrections to scaling in agreement with experiment.

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The two channel Kondo model [1], or equivalently the Kondo limit of the two channel Anderson model [2], has been applied to a wide variety of interesting physical systems: heavy fermion compounds [3,4], high-T_c superconductors [5], and two level systems (TLS) in metals [6–9]. Although this model contains many of the salient features of the experiments, e.g., marginal-Fermi-liquid behavior [5,10], the experimental proof for the physical existence of two channel Kondo impurities is far from certain.

One of the strongest experimental cases for the existence of two channel Kondo behavior is an experiment by Ralph and Buhrman [8] on clean Cu point contacts. At low temperatures T, the conductance of their samples shows the correct T, magnetic field, and voltage dependence for a two channel Kondo impurity such as a TLS with electron assisted tunneling. Recently [9], the data have also been shown to be consistent with a scaling ansatz motivated by the equilibrium conformal field theory (CFT) solution of the problem [11]. However, in order to verify the above hypothesis and to compare directly with experiment a nonequilibrium solution of the problem is required. In this paper we compute the differential conductance for a two channel Kondo impurity in a point contact for the experimental nonequilibrium situation. As seen below the good quantitative agreement with experiment lends strong evidence for the existence of two channel Kondo impurities in the samples of Ref. [8].

Generally, the M channel Kondo model consists of M kinds or channels of mutually noninteracting conduction electrons which are coupled to a system of $N = 2$ degenerate states via an exchange interaction [1]. In the case of interest here [8], the TLS presumably consists of the even and odd parity states of a defect atom bound in a symmetric double well potential; however, the actual physical realization of this TLS is inessential for the Kondo effect to occur. Parity plays the role of the *active* degree of freedom altered by the interaction, while the physical spin is a *spectator* degree of freedom, which is conserved by the interaction and which constitutes the $M = 2$ channels of the model [6].

It is convenient to represent this system by an Anderson Hamiltonian of a particle on an impurity level far below the Fermi surface hybridizing with the two channels of conduction electrons. Although the Anderson Hamiltonian does not explicitly represent the atomic tunneling system described above, both models belong to the same universality class and may be mapped onto each other in the Kondo limit by means of a Schrieffer-Wolff transformation, so that the model parameters may be identified. In slave boson representation [12], our Hamiltonian reads (we follow the notation of Ref. [13])

$$H = \sum_{p,\sigma,\tau,\alpha} (\epsilon_p - \mu_\alpha) c^{\alpha\dagger}_{p\sigma\tau} c^{\alpha}_{p\sigma\tau} + \epsilon_d \sum_{\tau} f^{\dagger}_{\tau} f_{\tau} + \sum_{p,\sigma,\tau,\alpha} U_\alpha (f^{\dagger}_{\tau} b_{\bar{\sigma}} c^{\alpha}_{p\sigma\tau} + \text{H.c.}), \quad (1)$$

where the first term describes the conduction electron bands labeled by their parity τ and their channel index, spin σ. In the presence of an external voltage V, the conduction electrons to the left and right of the junction also have different chemical potentials μ_α, $\alpha = L, R$. The second and third terms describe the core level ϵ_d and the hybridization terms, respectively, where f and b are the slave fermion and slave boson operators. The physical particle operator on the impurity is represented by $d^{\dagger}_{\tau} = \sum_\sigma f^{\dagger}_{\tau} b_{\bar{\sigma}}$, supplemented by the constraint $\sum_\tau f^{\dagger}_{\tau} f_{\tau} + \sum_{\bar{\sigma}} b^{\dagger}_{\bar{\sigma}} b_{\bar{\sigma}} = 1$.

We compute the differential conductance within the noncrossing approximation (NCA) for the infinite U Anderson model in the Kondo limit [14–16]. The NCA has been very successful in describing the one channel Kondo problem except for the appearance of spurious nonanalytic behavior at a temperature far below the Kondo temperature T_K. These spurious low-T properties are due to the fact that the NCA neglects vertex corrections responsible for restoring the low-T Fermi liquid behavior of the one channel model [17]. However, it has recently been shown [13] that for the two channel problem, where the complications of the appearance of a Fermi liquid fixed point are not present, the NCA does give the exact low-frequency power law behavior of the impurity spectral

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function $A_d(\omega)$ at zero T. Therefore, we expect to achieve a correct description for quantities involving A_d (like the conductance).

In order to calculate the conductance at finite bias, the NCA must be generalized using nonequilibrium Green functions [18]. One solves for both the retarded Green functions for these operators, G_r^f and G_r^b, and for the "lesser" Green functions $G_<^f$ and $G_<^b$, which contain information about the nonequilibrium distribution function. The derivation of the integral equations for these four functions follows the work of Meir, Wingreen, and Lee [19].

In a point contact the Kondo effect is governed by the couplings of the impurity to left and right moving electrons Γ_L and Γ_R, normalized to the width $\Gamma = \pi[(U_L + U_R)/2]^2 N(0)$ of the bare Anderson impurity level [15] ($\Gamma_L + \Gamma_R = 1$). Motivated by the symmetry of the experimental conductance-voltage curves we conclude that the system is symmetric under the total parity operation $V \rightarrow -V$, $\Gamma_L \leftrightarrow \Gamma_R$, i.e., $\Gamma_L = \Gamma_R$ [20]. Letting $F_{\rm eff}(\omega) = \Gamma_L F(\omega + eV/2) + \Gamma_R F(\omega - eV/2)$, where $F(\omega) = 1/(1 + e^{\beta\omega})$, and using the conventions of Müller-Hartmann [15] for the spectral functions, $A(\omega) = -{\rm Im}G_r^f(\omega)/\pi$, $B(\omega) = -{\rm Im}G_r^b(\omega)/\pi$, and the lesser Green functions, $a(\omega) = {\rm Im}G_<^f(\omega)/2\pi$ and $b(\omega) = {\rm Im}G_<^b(\omega)/2\pi$, the nonequilibrium NCA equations for the $N = 2$, $M = 2$ Anderson model are [21]

$$\frac{B(\omega)}{|G_r^b(\omega)|^2} = \Gamma N \int \frac{d\epsilon}{\pi} A(\omega + \epsilon) F_{\rm eff}(\epsilon), \quad (2)$$

$$\frac{A(\omega)}{|G_r^f(\omega)|^2} = \Gamma M \int \frac{d\epsilon}{\pi} B(\omega - \epsilon)[1 - F_{\rm eff}(\epsilon)], \quad (3)$$

$$\frac{b(\omega)}{|G_r^b(\omega)|^2} = \Gamma N \int \frac{d\epsilon}{\pi} a(\omega + \epsilon)[1 - F_{\rm eff}(\epsilon)], \quad (4)$$

$$\frac{a(\omega)}{|G_r^f(\omega)|^2} = \Gamma M \int \frac{d\epsilon}{\pi} b(\omega - \epsilon) F_{\rm eff}(\epsilon), \quad (5)$$

where the real and imaginary parts of G_r^f and G_r^b are related to each other by a Kramers-Kronig relation. We have solved Eqs. (2)–(5) numerically by iteration. Optimizing the computational speed at the cost of computer memory, we can substantially increase the number of iterations per time and, subsequently, are able to go more than 2 orders of magnitude lower in T [22] than shown in Ref. [19], deep into the low T scaling regime described below. The true impurity spectral function, A_d, is computed from the slave Green functions via the convolution

$$A_d(\omega) = \int \frac{d\epsilon}{\pi}[a(\epsilon)B(\epsilon - \omega) + A(\epsilon)b(\epsilon - \omega)]. \quad (6)$$

A point contact consists of two leads joined by a small constriction. Any additional scattering in the vicinity of the constriction should cause a decrease in the conductance because it impedes the flow of electrons. On the other hand, in a tunnel junction, tunneling may be assisted by electrons hopping on impurities in the junction, increasing the conductance. Thus, it is not surprising that when we generalize earlier calculations for the nonlinear current through a tunnel junction [23,24] to the case of a point contact, we find a similar expression for the current, except for an overall minus sign:

$$I - I_0 \propto -\int d\omega\, A_d(\omega)[F(\omega - V/2) - F(\omega + V/2)], \quad (7)$$

where I and I_0 are the currents with and without the impurity. In deriving Eq. (7) we have assumed that the point contact is clean, namely the transmission coefficients are close to unity, and that all hopping matrix elements are slowly varying on the scale of T_K. The conductance $G(V,T)$ is computed by taking a numerical derivative, dI/dV. We will assume that the background conductance dI_0/dV is Ohmic.

In Fig. 1 we show the zero bias conductance, $G(0,T)$, computed in this manner ($\Gamma_L = \Gamma_R$). As expected [11], the conductance shows a $T^{1/2}$ dependence at low T with deviations starting at about $\frac{1}{4}T_K$. T_K is determined by the width at half maximum of the zero bias impurity spectral function A_d at the lowest calculated T (see inset). The slope of the $T^{1/2}$ behavior defines the constant B_Σ:

$$G(0,T) - G(0,0) = B_\Sigma T^{1/2}. \quad (8)$$

The experimental data also show a $T^{1/2}$ dependence, but it is difficult to deduce an accurate estimate of T_K by

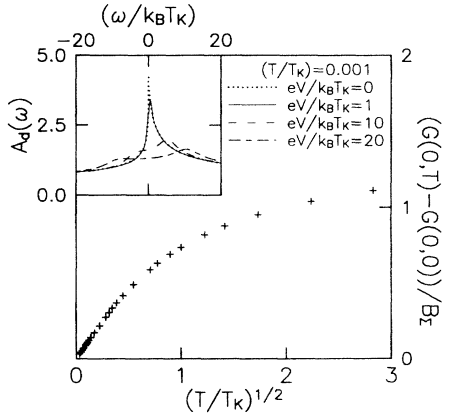

FIG. 1. T dependence of the zero bias conductance ($\Gamma_L = \Gamma_R$). The zero bias conductance has $T^{1/2}$ dependence for $T < T_K/4$. This can be used to roughly extract T_K from the experimental data. Inset: The impurity spectral function $A_d(\omega)$ for several voltages. The width at half maximum of the zero bias spectral function (dotted curve) determines T_K. As the voltage is increased to $eV = k_B T_K$ the Kondo resonance is reduced (solid curve). At very large bias the resonance shows a shoulder and eventually two peaks. In this paper we compare theory and experiment in the scaling regime, $T \ll T_K$.

looking at the deviations from $T^{1/2}$ behavior (assuming that they would occur at $\frac{1}{4}T_K$). An educated guess gives $T_K \simeq 8$ K for samples 1 and 2 and significantly less for sample 3 of Ref. [9].

Recently, it has been proposed from a CFT solution of the problem in equilibrium that the experimental data show scaling of the conductance G as a function of voltage bias V and T of the form [9]

$$G(V,T) - G(0,T) = B_\Sigma T^{1/2} H\left(A\frac{eV}{k_B T}\right), \qquad (9)$$

where H is a universal scaling function [$H(0) = 0$ and $H(x) \sim x^{1/2}$ for $x \gg 1$] and B_Σ and A are nonuniversal constants. In order to examine whether this ansatz is correct, in Fig. 2 the rescaled conductance is plotted as a function of $(eV/k_BT)^{1/2}$ for the numerical data (a) and the experimental data [(b), for the best sample (1)]. Considering that after fixing B_Σ using Eq. (7) there are no adjustable parameters, the agreement is quite good. The collapse of the various T curves at low bias and the linear behavior for the low T curves in the range of $2 < (eV/k_BT)^{1/2} < 4$ is in agreement with the proposed scaling ansatz Eq. (9). However, the slope of the linear part shows T dependence for both the experimental and the numerical data. This is not contradictory to the scaling ansatz, but it does show that there are significant T dependent corrections to scaling.

To analyze the scaling plots in more detail, the low bias portion is replotted in Fig. 3(a). The conductance follows an approximate $(eV/k_BT)^2$ behavior even for $eV/k_BT > 1$ before it levels off and enters the $(eV/k_BT)^{1/2}$ region at higher bias. The prefactor of the quadratic dependence shows no observable T dependence until approximately $0.1T_K$ and consequently obeys the scaling ansatz.

In Fig. 3(b) the slopes of the straight line fits of the linear regions in Fig. 2 are plotted as a function of T. Both the numerical data and the experiment show clear T dependence. Although B_Σ may be determined directly from the zero bias conductance, T_K is more difficult to determine experimentally. In Fig. 3(b) we have chosen values for T_K which are consistent with the estimates from the deviation of the zero bias conductance from $T^{1/2}$ behavior. The resulting curves are in good quantitative agreement. In order to show that the experimental and numerical curves indeed coincide (for a given T/T_K) we also compare the intercepts of the straight line fits for the same T_K's [inset Fig. 3(b)]. The numerical data do fall

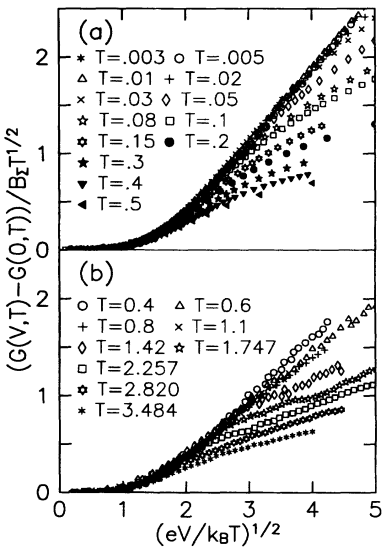

FIG. 2. Scaling plots of the conductance for (a) theory and (b) experiment [9]. With $\Gamma_L = \Gamma_R$ and B_Σ determined from the zero bias conductance (see Fig. 1), there are no adjustable parameters. There are roughly two regimes in these plots. For $(eV/k_BT)^{1/2} < 1.5$ the curves collapse onto a single curve and the rescaled conductance is proportional to $(eV/k_BT)^2$. For $2 < (eV/k_BT)^{1/2} < 4$ the rescaled conductance is linear on these plots. There are substantial corrections to scaling even at T small compared to T_K [see Fig. 3(b)]. At even larger biases this linear behavior rounds off, indicating the breakdown of scaling. The temperatures in the theory and experimental plots are in units of T_K and kelvin, respectively.

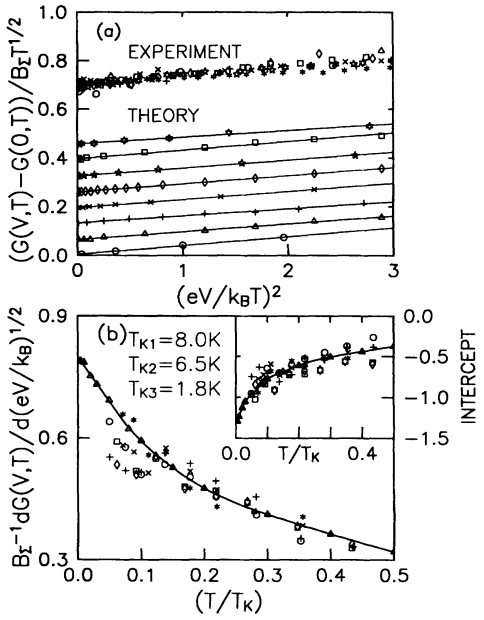

FIG. 3. Quantitative analysis of the scaling plots at (a) low bias and (b) high bias. (a) The low bias rescaled conductance as a function of $(eV/k_BT)^2$ (curves are offset). Both theory and experiment (sample 1 of Ref. [9]) show quadratic behavior at low bias. The symbols correspond to the temperatures shown in Fig. 2. (b) The slope of the straight line fits of the linear region in Fig. 2 as a function of T for sample 1 (∘,+), sample 2 ($\diamond$,□), sample 3 (×,*) (for $V > 0$, $V < 0$), and the numerical data (△). The T_K for the experimental curves is consistent with the deviation of the zero bias conductance from $T^{1/2}$ behavior. All curves drop with increasing T even at T small compared to the T_K. The inset shows the behavior of the intercepts of the fits.

right in the middle of the scatter from the three different samples. Note that our theory does not have the additional parameter, A, of Eq. (9), but adjusting T_K has some of the same effect as adjusting A.

In determining the origin of the scaling behavior displayed in Eq. (9) it should not be overlooked that *the same* scaling form could also arise from a quantum interference effect between Coulomb interaction and scattering off defects in a nanojunction [25]. If this were the case, the characteristic temperature for scaling to set in would be given by the impurity scattering rate. The experimental value for the characteristic temperature of ≤ 8 K would then correspond to a mean free path of $\simeq 10^3$ lattice constants, far more than the size of the junctions of Ref. [8], to which any defects in their clean samples would be confined. Therefore, the above interference effect is ruled out as a possible origin of the scaling behavior Eq. (9).

In conclusion, we have performed numerical evaluations of the NCA integral equations for the two channel Anderson model out of equilibrium. We find very good agreement with data from an experiment on Cu point contacts [9]. Scaling of the conductance at low bias ($eV < k_BT$) and T is verified. As V and T are increased, the calculation exhibits finite-T corrections to scaling, again in agreement with experiment. Quantum interference between Coulomb and impurity scattering is ruled out as a possible origin of the scaling behavior. Thus, this work lends strong support to the existence of two channel Kondo impurities in the Cu point contacts of Ralph and Buhrman.

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