It is shown that the rate limiting time constant for the formation of the Kondo state in a quantum dot can be extracted analytically from known perturbation theoretic results. The prediction obtained is verified via numerical simulations in the noncrossing approximation.

The basic time scale for equilibration processes in a Kondo system has eluded researchers for more than thirty five years. The Kondo effect has recently been unambiguously observed in quantum dots [1-3]. These are prototype Kondo systems, which are also important in their own right, and appropriate time dependent experiments should soon appear. The observation of Kondo resonance in the tunneling from an STM tip via a surface adsorbate atom [1-3] has further increased the excitement. Impurity models incorporating Kondo physics form one of the basic building blocks for theories of highly correlated systems. The recent success in incorporating such theories [5] into the basic apparatus used in electronic-structure calculations, means that exciting new progress in this area is close at hand. Here, we provide a surprisingly simple and elegant solution to the time-scale problem.

A half a century ago, the framework and starting point for discussion of the time scale $\tau$ for a localized spin in an electron sea was set by Korringa [6], whose contribution has been promulgated at the textbook level for decades [7]. In simple terms $1/\tau$ gives the fractional rate at which a component of spin $S$ representing a magnetic impurity (or a quantum dot) is changing due to the electrons in the conduction band (or in the leads of a quantum dot). It is given by an expression of the type

$$\frac{\hbar}{\tau} = \alpha k_B T,$$

where $\alpha$ is a dimensionless constant, $k_B$ is Boltzmann’s constant, and $T$ is the temperature.

The simplest model that contains the relevant physics is the Kondo model Hamiltonian $\sum_{i=1}^{n} (\epsilon_{k_i} - J s_i \cdot S)$, where $k_i$ is a generalized quantum number for the $i$th conduction (or lead) electron, $\epsilon_{k_i}$ is its energy, and $s_i$ is its spin operator. For a quantum dot, $k$ is assumed to include the information on which lead is referred to. The exchange coupling $J$ is taken to be independent of $k$, aside from the usual high-energy cutoff at energies further than $D$ above or below the Fermi level. The Kondo temperature $T_K$ is the single parameter characterizing the physics, and is of order $(D/k_B) \exp(-1/J \rho)$, where the density of states $\rho$ is assumed constant.

The factor of $k_B T$ in Eq. (1) arises because a change in $S$ involves the absorption of a spin one electron-hole pair of zero energy. The phase space for such an object is doubly restricted by the Pauli principle, and produces the factor $\int d\epsilon f(\epsilon)(1 - f(\epsilon)) = k_B T$ where $f(\epsilon)$ is the Fermi function. Although Korringa’s original derivation applied to a nuclear spin where the interaction with electrons is dipolar, it has been widely applied to impurity electron spins as well, using the Kondo model for the interaction. To lowest order in $J$, the quantity $\alpha$ in Eq. (1) is given by [8]

$$\alpha = \pi (J \rho)^2. \quad (2)$$

One should note that (2) represents a difference between rates and cannot be calculated directly by a second-order perturbation calculation. It rather involves the solution of a master equation, or, in many-body terminology, a sum of vertex corrections. For $S = \frac{1}{2}$, as would be appropriate for a quantum dot, the vertex corrections change the result only by a factor of order unity.

The application of these ideas to a biased quantum dot allows the phase space factor to be tuned in a continuous fashion by varying the bias $V$ across the two leads of the dot, which for simplicity we assume to be symmetric under lead interchange. The phase space restriction factor in this case is given by

$$\frac{\hbar}{\tau} = \alpha k_B T \frac{F(eV/k_B T)}{k_B T}, \quad (3)$$

where

$$F(x) = \frac{1}{4} \left( 1 + 1 + \frac{x}{1 - e^{-x}} + \frac{xe^{-x}}{1 - e^{-x}} \right). \quad (4)$$

In writing Eq. (4) we have sacrificed conciseness to facilitate clarification of the origin of the terms in parentheses, in terms of the wave function of the annihilated particle-hole pair. The first two terms arise when the two
components of this object are in the same lead; in this case the existence of $V$ has no effect on the result \[3\]; the phase space for these processes is still constricted, and the contribution to $1/\tau$ is still small. For the third term, the particle is on lead 1 and the hole on lead 2; here the phase space is opened wide by $V$. Finally for the fourth term, the particle is on lead 2 and the hole on lead 1; the phase space is, aside from an exponentially small tail, closed off entirely as $V$ is increased. So the essential physical feature deriving from Eq. (1) is that the factor of $k_B T$ in Eq. (1) is replaced at large $V$ by $1/eV$.

The notion of an expanded phase space is implicit in the Anderson model calculation of $\tau$ by Wingreen and Meir \[10\] and in a different context in the work of Kaminski et al. \[11\]. Here we have expanded the notion and expressed it more succinctly, because it is one of the cornerstones of what follows.

We now turn to the calculation of $\alpha$ when there is a significant Kondo effect. The quantum dot model will also provide a framework for a precise definition of $\tau$. A primary feature of the Kondo effect is the appearance of a resonance in the imaginary part of the transition or $t$ matrix, which is centered at the Fermi level, and which extends logarithmically over many energy scales, the smallest of which is characterized by the Kondo energy $k_B T_K$. The transition matrix then determines the conductance $G \equiv I/V$, where here $I$ is the steady-state current induced by a constant bias voltage $V$. Thus a current measurement through a biased quantum dot provides a direct measurement of the changes in the Kondo resonance induced by a time dependent $J$ in the Kondo Hamiltonian. Specifically, we imagine that $J$, initially zero, is suddenly switched to its final value. The current $I(t)$ will increase, rapidly at first, but for large times $t$ should approach its final value of $G V$ exponentially with a constant rate. The exponent for this final decay should be independent of the method of excitation, and hence the true characteristic formation rate of the Kondo resonance.

Although the physics implicit in Eq. (2) and the order of magnitude it gives, has been used by several authors \[10,11\] to obtain time scales of the quantum dot, it is undoubtedly incorrect to expect that this expression, valid to order $J^2$ only, can capture the time scale for a phenomenon like the Kondo resonance, whose defining terms first appear in order $J^3$. Fortunately one can use previous analytic results \[12\] to extract this fundamental time. What was found there, was that the current response to a stepped turning on of $J$ would be the same as the equilibrium response to a time-dependent effective temperature $T_e$ given by $T_e = T \coth \pi T t / 2\hbar$. We start with the tautology $\delta I = [d\ln G] / d\ln T_e \delta T_e / T_e$. Defining the fraction $f$ as the finite difference

$$f \equiv \frac{I(\infty) - I(t)}{I(\infty)},$$

and

$$f_0 \equiv -2 \frac{d(\ln G)}{d(\ln T)};$$

we have approximately $f = f_0(\coth \pi T t / 2\hbar - 1)/2$. As $t$ becomes large, this approximation becomes exact, and we obtain

$$f \to f_0 \exp \left( -\frac{t}{\tau} \right),$$

where the value of $\alpha$ defining $\tau$ via Eq. (6) is given by

$$\alpha = \pi,$$

instead of by Eq. (2). When the phase space expansion factor \[3\] for finite $V$ is restored \[13\], then the predicted $\tau$ should be given by Eq. (3).

Our result for $\tau$, although analytically derived only in perturbation theory, contains no non-universal parameters like $J$ or $D$, and so might be expected to be valid in parameter ranges exceeding those implied in its derivation. However, the expressions do not contain $T_K$, so corrections may appear when $k_B T$ and $eV$ become much smaller than $k_B T_K$. For example, one could suspect that a particle-hole pair would require an energy of $\sim k_B T_K$ in order to excite the singlet ground Kondo state, so that $1/\tau$ would vanish exponentially as $\sim \exp(-T_K/T)$ for $eV \ll k_B T \ll k_B T_K$ instead of linearly with $T$.

![FIG. 1. Instantaneous current $I$ through the quantum dot versus the time $t$ after $J$ was turned on. The units $I_u = (e^2/\pi \hbar)V$ and $t_u = \hbar/k_B T_K$. The solid, dashed, dotted, and dash-dotted curves correspond to the respective $eV/k_B T_K$ values of 1, 5, 20, and 80. The temperature $T = 1.5 T_K$.](image_url)
We have made numerical simulations \[14\] to test the response of the current to sudden increases in $J$ at various biases and temperatures. The essential feature is that $J$ is suddenly increased from a negligible value to a substantial value, in this case given by $J\rho = 1/2\pi$. We found results for two temperatures: $T = 1.5T_K$ and $T = 15T_K$, where $T_K$ corresponds to the final value of $J$ above. A sampling of the data is shown in Fig. 1.

One sees clearly that the current versus time curves have the general features discussed above, with the time required for saturation decreasing with increasing bias $V$. For $eV$ somewhat greater than $k_B T_K$, small, damped oscillations occur \[15\] at the non-trivial frequency given by $\hbar \omega = eV$. They are caused by transitions between the split Kondo peaks (SKP), which occur \[15\] for $eV$ greater than several times $k_B T_K$. Such SKP oscillations should not occur at all for the completely symmetric mechanism of suddenly turning on $J$. However, as described below, in order to make our simulations numerically feasible, it was necessary to include a small (asymmetric) mixed valent admixture, which is responsible for the excitation of the SKP oscillations in this case.

![Graph](image)

**FIG. 2.** Comparison of Eq. (3) with the simulation results. The ordinate shows the rate $1/t_{1/10}$ as defined in the text in units of $1/t_K = k_B T_K/\hbar$. For $T = 1.5T_K$, the dashed and solid lines show the theoretical curves for $\alpha_{1/10}$ values of 1.6 and 2.0 respectively, while the squares show the simulation results. The dotted and dash-dotted lines and circles respectively show the corresponding results for $T = 15T_K$.

The scheme we adopted for analyzing the data of Fig. 1, comprised first of determining the time, which we call $t_f$, corresponding to the current fraction $f$ defined earlier. We choose this fraction to be $1/10$, an amplitude that is sufficiently large that the SKP oscillations do not spoil the analysis, and sufficiently small that the ultimate time scale has been reached approximately. One finds, by solving Eq. (6) for $t$, that $t_f$ is given simply by replacing $\tau$ by $t_f$ in Eq. (6), provided that $\alpha$ is replaced by $\alpha_f = \alpha/\ln(f_0/f)$. The amplitude $f_0$ was calculated directly both from the large-time asymptotes of the simulations and from Eq. (6), with similar results; it was found to be remarkably slowly varying with temperature in the temperature range of the simulations. \[10\] Assuming that $\alpha = \pi$, we found taking $f = 1/10$ that $\alpha_f = 1.6$ for both $T = 1.5T_K$ and $T = 15T_K$. In Fig. 2 we show our simulation results along with the theoretical prediction from Eq. (3) with $\alpha_{1/10} = 1.6$. Better fits to the simulation can be obtained by taking $\alpha_{1/10} = 1.8$ (not shown) or $\alpha_{1/10} = 2.0$; these correspond to $\alpha$ values of $1.1\pi$ and $1.2\pi$ respectively. Such a 10–20% difference from the prediction of Eq. (4) is consistent with the expected accuracy of the simulation method, exacerbated by the fact that the simulations contained a small mixed valent contribution not present in the Kondo Hamiltonian. The perturbative value of $\alpha = 0.03\pi$ predicted by Eq. (4) is definitely ruled out. The substantial agreement gives added support to our time scale predictions of Eqs. (3) through (6). The challenge of extending our results to the range $k_B T, eV \ll k_B T_K$ still remains.

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*Note added on 27 September 2001.* Since this work was originally posted, we became aware of work by A. Rosch, J. Kroha, and P. Wölfle, Phys. Rev. Lett. **87**, 156802 (2001). These authors calculate the imaginary part of the pseudo-fermion self-energy in time-independent NCA. If this quantity is closely related to the time-dependent definition, Eq. (7), of the Kondo state’s formation rate, then their work would include corrections that go beyond the simple argument that led to Eq. (3), but which would automatically be included in our NCA simulations. It is possible that the small deviation of the squares in Fig. 2 above the solid line for the highest three points could be due to this. However, the accuracy achievable by our data analysis is limited in this region and drawing any physical conclusion from this deviation might be straining these limits. Because the relative effect of the mixed valent contribution increases with increasing $V$, we are unable approach the asymptotic limit exemplified by Eq. (4) of the work of Rosch et al. We thank Achim Rosch for correspondence.
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[14] The simulations used the noncrossing approximation, a reliable calculational scheme, whose time-dependent version we have adequately described and referenced previously in Refs. [4,5]. It is valid in the temperature range of our simulations, but breaks down for $T \ll T_K$. In the same notation as we used previously in Ref. [3], we took Anderson model parameters $\epsilon_{\text{dot}} = -2\Gamma_{\text{dot}}$, with a parabolic band of width $9\Gamma_{\text{dot}}$. These give an equivalent Kondo model $Jp = 1/2\pi$ and $k_B T_K = 10^{-3}\Gamma_{\text{dot}}$. The equivalence between the models is good, but not perfect, because for computational-resource reasons, the small mixed valent overlap could not be reduced to zero by choosing a much larger $|\epsilon_{\text{dot}}|$. For times $t < 0$, the coupling $J$ was for practical purposes turned off by taking $\epsilon_{\text{dot}} = -5\Gamma_{\text{dot}}$.
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[19] Interestingly, $f_0$ can be evaluated analytically for the high-temperature region $\ln T/T_K \gg 1$, although such temperatures would be way out of the range used in our simulations. If we note that very early work [A. A. Abrikosov, Physics 2, 5 (1965)], valid in the high T range defined above, implies that $(h/2e^2)G \to 3\pi^2/16\ln^2(T/T_K)$, then we find from Eq. (1) that $f_0 \to 4/\ln(T/T_K)$. More recent work [A. Kaminski, Y. V. Nazarov, and L. I. Glazman, Phys. Rev. B 62, 8154 (2000)] suggests that $V$ dependence might also be important for comparably large values of $V$. 

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