Kondo temperature for a quantum dot in an Aharonov–Bohm ring

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We study the Kondo temperature of a quantum dot embedded into one arm of an Aharonov–Bohm interferometer. The topology of a disordered or chaotic Aharonov–Bohm ring leads to a stochastic term in the scaling equation and in the renormalization procedure. As a result, the Kondo temperature displays significant fluctuations as a function of magnetic flux.

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Recently, the transmission phase of electrons passing through a quantum dot (QD) embedded in an Aharonov–Bohm (AB) interferometer has been measured\cite{1}. This was done in the Kondo regime and over an energy interval given by the width of the “odd” valley separating two conductance Coulomb–blockade peaks. The QD with half–integer spin plays the role of the Kondo impurity\cite{2}. Theory predicts the phase shift to be \( \pi \) at low temperature\cite{3}. The results are puzzling and do not follow this prediction. In the present Letter we show that the T–matrix \( \mathcal{T}_K \) of the Kondo problem acquires specific properties due to the topology of the AB ring. These have not been taken into account previously and profoundly affect the dependence of \( \mathcal{T}_K \) on the AB phase. They serve as one example for the role of finite–size effects\cite{4} and mesoscopic fluctuations\cite{5} which, together with experiments on semiconductor quantum dots\cite{6} and nanotubes\cite{7} have rekindled interest in the Kondo effect\cite{8} recently. Implications of our results for the experimental analysis are briefly discussed.

**Model.** We consider a QD carrying an odd number of electrons in the Kondo regime. The QD is embedded into one arm of an AB ring threaded by a weak magnetic flux \( \Phi \). We take account only of the AB phase \( \phi = 2 \pi \Phi / \Phi_0 \). Here \( \Phi_0 \) is the elementary flux quantum. The AB ring is attached to \( \Lambda \) leads labelled \( j = 1, \ldots, \Lambda \). Without counting spin degrees of freedom labelled \( s = \pm 1/2 \), lead \( j \) carries \( N_j \) channels (transverse modes with energies below the Fermi surface) labelled \( a = 1, \ldots, N_j \). The total number of channels is \( N = \sum_j N_j \).

The leads are separated from the interior of the AB ring by fictitious barriers, and the interior from the QD by real tunneling barriers caused by the gate potentials. With \( E \) the energy, the lead Hamiltonian is

\[
H_L = \sum_{j=1}^{\Lambda} H_j \quad \text{with} \quad H_j = \sum_j \sum_{s,s'} \int dE \, E \, c_{ja}^\dagger c_{ja'} \delta_{ss'} \delta(E - E'),
\]

where \( c_{ja}^\dagger \) creation and annihilations of quasiparticles in lead \( j \). The Hamiltonian \( H_{AB} \) of the AB ring has a discrete spectrum with eigenvalues \( \epsilon_{\mu} \) with \( \mu = 1, 2, \ldots \) and is given by

\[
H_{AB} = \sum_{\mu} \epsilon_{\mu} d_{\mu s}^\dagger d_{\mu s},
\]

where \( \{ d_{\mu s}^\dagger, d_{\nu s'} \} = \begin{cases} \delta_{ss'} & \text{if } \mu = \nu, \\ 0 & \text{otherwise}. \end{cases} \) Leads and AB ring are coupled by the tunneling Hamiltonian

\[
H_{AB-L} = \sum_j \sum_{\mu} \int dE \, W_{ja,}\mu(E) \left( c_{ja}^\dagger e_{\mu s} + \text{H.c.} \right).
\]

We assume that the real tunneling matrix elements \( W_{ja,}\mu(E) \) change little over an energy scale given by the width of the Kondo resonance. We also assume that the levels \( \epsilon_{\mu} \) lie so dense (and that their coupling to the leads is so large) that all scattering through the AB ring in the absence of the QD is smooth in energy on the same scale.

The tunneling matrix elements \( v_{\mu}^j \) between the QD and state \( \mu \) of the AB ring carry an upper index \( P = L, R \) denoting tunneling through the left (right) barrier, respectively. The occurrence of two amplitudes for each state \( \mu \) of the AB ring reflects the topology of the ring. We choose the matrix elements \( v_{\mu}^j \) real and display the AB phase \( \phi \) explicitly in the Kondo Hamiltonian. Gauge invariance allows us to put the entire effect of the AB phase \( \phi \) onto the right barrier separating the QD from the AB ring. Whenever the electron leaves (enters) the QD through that barrier, it picks up the phase factor \( e^{i\phi} \) \((e^{-i\phi}, \text{respectively})\). We define \( v_{\mu}^j = v_{\mu}^j + e^{i\phi} v_{\mu}^R_j \).

We focus attention on the Coulomb blockade mid–valley region. Then it is justified to use the s–d model for the Kondo resonance\cite{9}. (We have convinced ourselves that our arguments hold likewise for the Anderson model\cite{10}. However, we have not yet performed a complete analysis of the latter model). In the s–d model, a spin \( \vec{S} \) (which represents the total spin of the electrons on the QD) is coupled to the spins of the electrons in the AB ring,

\[
H_K = \frac{2}{E_C} \sum_{\mu s} v_{\mu}^d \left( \vec{\sigma}_{ss'} \cdot \vec{S} \right) v_{\mu}^{d'*} d_{ss'}.
\]

Here \( E_C \) is the charging energy of the QD, and \( \vec{\sigma} \) stands for the vector of the three Pauli spin matrices. The total Hamiltonian is the sum of these terms,

\[
\mathcal{H} = H_L + H_{AB} + H_{AB-L} + H_K.
\]

Using standard techniques\cite{5} we obtain for the non–diagonal dimensionless conductance coefficients \( g_{jl} \) with \( j \neq l \) of the many–body Hamiltonian \( \mathcal{H} \)

\[
g_{jl} = \int dE \left( -\frac{df}{dE} \right) \text{Tr}_{\mu s} \left[ \Gamma_j(E) G^r(E) \Gamma_l(E) G^a(E) \right].
\]

Here \( f \) is the Fermi function, \( G^r \) and \( G^a \) are the ordinary retarded and advanced equilibrium many–body Green’s functions of \( \mathcal{H} \), and \( \left[ \Gamma_j \right]_{\mu \nu} = 2\pi \sum_{\alpha} W_{ja,}\mu W_{ja,}\nu \).
In the absence of the Kondo term, we deal with a pure single–particle problem, with a Green’s function $G_{\mu\nu}^{r,s}\left(\varepsilon,\ell\right)$ given by $G_{\mu\nu}^{-1} = \left(E-\epsilon_{\mu}\right)\delta_{\mu\nu}+(i/2)\sum_{j}\left[\Gamma_{j}\right]_{\mu\nu}$, and non–
diagonal elements of the spin–independent scattering matrix $S_{\mu\nu}(E) = -2i\pi\sum_{\mu\nu}W_{j,\mu\nu}\left[G_{\mu\nu}^{r}\left(E\right)\Gamma_{j}\right]_{\mu\nu}W_{l\nu\nu}$. Hence, as expected, the conductance is given by the
Landauer–Büttiker formula.

We return to the many–body case and expand $G_{\mu\nu}^{r}(E)$ in powers of $H_{K}$ to write $G_{\mu\nu}^{r}(E) = \left[G_{0}^{r}(E)\right]_{\mu\nu}$, where
\[
T_{K} = H_{K}\sum_{n=0}^{\infty}\left[G_{0}^{r}(E)H_{K}\right]^{n}
\]
defines the $T$–matrix for the Kondo effect. Using $T_{K}$ and the definition of $S(0)$, we write $g_{jl}$ as
\[
g_{jl} = \int dE \left( -\frac{df}{dE} \right) \sum_{ab} \left\{ 2 \left| S_{ja;lb}(E) \right|^{2} \right. + \left. \left( S_{ja;lb}^{(0)} \right)^{\ast} T_{K} \left[ -2i\pi \sum_{\mu\nu} W_{ja;\mu}(G_{0}^{r}\left(E\right)\Gamma_{j}\left[\Gamma_{j}\right]_{\mu\nu}W_{lb\nu} + \text{c.c.:} \right] + \text{Tr}_{\chi} \left[ -2i\pi \sum_{\mu\nu} W_{ja;\mu}(E)|G_{0}^{r}\left(E\right)\Gamma_{j}\left[\Gamma_{j}\right]_{\mu\nu}W_{lb\nu}|^{2} \right) \right\}. \tag{5}
\]

Three processes contribute to transport through the AB ring, each represented by one term on the r.h.s. of Eq. 5: Scattering of an electron through the AB ring without its passing through the QD, the interference term between the amplitude for that process and the amplitude for (multiple) visits of the QD, and the square of the latter amplitude. This structure differs fundamentally from that for a QD in the Kondo regime connected to two leads without the topology of the AB ring. Here only the interference term occurs 3. This is caused by the special form of the coupling between Kondo resonance and channels.

**Dependence upon the AB Phase.** We compare the dependence of $g_{jl}$ on the AB phase $\phi$ with that obtained for a simpler problem: An AB ring with a QD that carries a single level at energy $E_{0}$ and causes a Breit–Wigner resonance 4. The resulting expression for $g_{jl}$ (j ≠ l) has the form of our Eq. 5 except for the replacement 11 $-2i\pi W_{ja;\mu}(E)\left[\Gamma_{j}\left[\chi_{\mu}\right]_{\mu\nu}W_{lb\nu} \rightarrow -i(\gamma_{ja} + \eta_{ja}e^{i\phi}) \left( E - E_{0} + i\Gamma/2 \right)^{-1} (\gamma_{lb} + \eta_{lb}e^{-i\phi}) \right]$. The amplitudes $\gamma_{ja}$ and $\eta_{ja}$ are complex and independent of energy $E$ and AB phase $\phi$. The only dependence of the resulting expression on the phase $\phi$ is that given explicitly and that of the total width $\Gamma = \sum_{ja} \left| \gamma_{ja} + e^{i\phi}\eta_{ja} \right|^{2}$. Under the assumption that the electrons move chaotically and/or diffusively in the AB ring, the dependence of $\Gamma$ on $\phi$ is 11 of order 1/$\sqrt{N}$ and, thus, negligible whenever $N \gg 1$. The experimental determination of the transmission phase through the QD (defined as the phase of the Breit–Wigner term) is, thus, possible for $N \gg 1$.

In the case of Eq. 5, the $T$–matrix $T_{K}$ depends non–
trivially on $\phi$, see Eqs. 4 and 11. Thus, the central question is: How strong is this dependence of $T_{K}$ on $\phi$? The theoretical treatment of the Kondo resonance requires scaling and/or renormalization techniques. Our question can only be answered in this framework.

**Poor Man’s Scaling.** The essential aspects of poor man’s scaling emerge already when one considers the matrix element of the $T$–matrix to second order in $H_{K}$, given by $\langle \psi_{s}|H_{K}G_{0}^{r}(E)H_{K}|\psi_{t}\rangle$. We suppress the external factors $v_{\mu}$ and focus on the intermediate–state summation involving $G_{0}^{r}(E)$. Two processes contribute to this term: The scattering of an electron and that of a hole. Aside from spin–dependent factors, the first process yields
\[
\sum_{\tau_{\rho}}\langle \psi_{t}|G_{0}^{r}\left[E_{\tau} - E_{\rho} - \epsilon_{\tau} \right]|\psi_{s}\rangle = \sum_{\tau_{\rho}}\frac{|v_{\tau}|^{2}}{E_{\tau} - E_{\rho} - \epsilon_{\tau}}
\]
\[
+ \sum_{\tau_{\rho}}\frac{v_{\tau}^{*}G_{0}^{r}\left[E_{\tau} - E_{\rho} - \epsilon_{\tau} \right]v_{\rho}}{E_{\tau} - E_{\rho} - \epsilon_{\tau}}.
\tag{6}
\]

where $\delta_{jl} = \delta_{jl}ab + i\sum_{\mu\nu} W_{ja;\mu}(E_{\tau} - E_{\rho} - \epsilon_{\tau})^{-1} W_{lb\nu}$. A similar decomposition into a term involving only the states in the AB ring and a remainder applies to hole
scattering. Our problem differs from the standard Kondo situation of a magnetic impurity coupled to the conduction band 8 in three main respects, the last two being related to the topology of the AB ring: (i) The energies $\epsilon_{\tau} do not lie in the conduction band but are defined as the eigenvalues of electrons moving in the AB ring. Thus, the summation over $\tau_{\rho}$ extends to $+\infty$. (ii) $G_{0}^{r}(E)$ differs from the Green’s function for free electrons. This leads to the 2nd term on the r.h.s. of Eq. 5. (iii) The $v_{\mu}$’s involve the AB phase $\phi$. We address these in turn.

(i) The coupling matrix elements $v_{\mu}^{ja}$ and $v_{\mu}^{lb}$ reflect the dynamics of the coupling of the QD to the AB ring. The $v_{\mu}$’s are overlap integrals involving the wave function $\chi$ of the electron on the QD and that of states $\tau_{\rho}$ with mean level spacing $\Delta$ in the AB ring. Two tendencies characterize the behavior of the $v_{\mu}$’s. (a) As the number of nodes of the state $\tau_{\rho}$ in the overlap region becomes much bigger or smaller than that of $\chi$, the overlap is strongly reduced. (b) In a diffusive and/or chaotic AB ring, the states $\tau_{\rho}$ within an energy interval given by the Thouless energy $E_{T}$, are strongly mixed. We take account of both features in terms of a cutoff model. Within an energy window of bandwidth $D \leq E_{T}$ around the energy of the state $\chi$, the $v_{\mu}$’s are 11 uncorrelated Gaussian distributed random variables with mean value zero and a common constant variance $\nu^{2}$ while the $v_{\mu}$’s for states $\tau$ outside of this window vanish. For both ballistic and diffusive rings $E_{T}$ is large compared to the mean level spacing $\Delta$ of the states in the AB ring but small in comparison to the Fermi energy. The cutoff then applies likewise to the summation over particles and to that over holes. The cutoff restricts the summation over $\tau_{\rho}$ to a finite number $g \approx E_{T}/\Delta$ states, with $g \gg 1$. To identify
the influence of the large contributions to Eq. (3) and to resum them, we let $g \to \infty$ and use scaling.

(ii) Scaling needs to be applied only to the first term on the right–hand side of Eq. (5) since only this term produces a logarithmic singularity at the upper band edge. As for the second term, the expression in brackets is obviously finite. There are two contributions to the summations over $\tau$ and $\rho$. For $\tau = \rho$, we sum squares of amplitudes $v_\tau$ but also of the propagator. The result is inversely proportional to $D$ and vanishes for $D \to \infty$. For $\tau \neq \rho$, we use that the $v_\tau$’s are Gaussian random variables with mean value zero. Their random signs quench the intermediate–state summations and ensure that the result is convergent even as $g \to \infty$. Thus, the singular contributions to the second–order particle matrix element are obtained by replacing $G_0(E)$ by $[E^+ - H_{AB}]^{-1}$. Corresponding statements apply to the terms of higher order in $H_K$. These arguments apply likewise to hole scattering. Thus we have reduced our problem to one which is quite similar in appearance to the standard Kondo case: Singular terms arise only from the coupling of the QD to the states in the AB ring, i.e., from the Hamiltonian $H_{AB} + H_K$. The terms $H_L$ and $H_{AB-L}$ in $H$ of Eq. (2) are irrelevant for scaling.

(iii) We turn to the AB phase appearing in the intermediate–state summation. The first term on the right–hand side of Eq. (5) contains the phase through $|v_\tau|^2 = (v_L^\tau)^2 + (v_R^\tau)^2 + 2 \cos \phi \ v_L^\tau v_R^\tau$. To define the scaling variable, we write this expression in the form $[(v_L^\tau)^2 + (v_R^\tau)^2][1 + \cos \phi \cos \psi_\tau]$ where

$$\cos \psi_\tau = \frac{2v_L^\tau v_R^\tau}{(v_L^\tau)^2 + (v_R^\tau)^2}. \quad (7)$$

Since the $v_\tau$’s are uncorrelated Gaussian variables, $\psi_\tau$ is also a random variable which is uniformly distributed in the interval $0 \leq \psi_\tau \leq \pi$. Moreover, the $\psi_\tau$’s with different indices $\rho$ are uncorrelated. We replace the positive quantity $[(v_L^\tau)^2 + (v_R^\tau)^2]$ by its average $2\bar{v}^2$. An equivalent assumption (independence of the coupling strength on the index $\tau$ characterizing states in the conduction band) is usually made in the standard Kondo case. We checked that this assumption does not affect the generic features of our results.

We define the scaling variable $J = 4\bar{v}^2/E_C$ and apply the standard algebra of poor man’s scaling to write

$$\frac{\delta J}{\delta D} = -2\rho_0 J^2/D(1 + \cos \phi \cos \psi). \quad (8)$$

Here $\rho_0 = \Delta^{-1}$ is the density of states $|\mu\rangle$ in the AB interferometer. We assume that $\rho_0$ is constant. Because of the appearance of the random variable $\psi$, Eq. (5) is a stochastic differential equation. To solve it, we first consider the case without stochastic term and define the “standard scaling trajectory” by choosing a Kondo temperature $T_K$ and initial values $\rho_0 D_0$ (where $D_0 \approx E_T$) for the bandwidth and $\rho_0 J_0$ for the coupling strength such that the relation $T_K = D_0 \exp(-1/2\rho_0 J_0)$ holds. We then solve Eq. (3) by reducing $\rho_0 D$ in unit steps drawing $\psi$ from a random–number generator. We thereby eliminate the states of the AB ring one by one. In the $p^{th}$ step, the coupling constant $\rho_0 J$ is “kicked” out of one scaling trajectory and into another by the term proportional to $\cos \phi \cos \psi_\rho$. The effect becomes larger as $\rho_0 D$ is decreased and $\delta J/\delta D$ increases. As a result, every realization $\{\psi_\rho\}$ of the sequence $\psi$–values determines a different scaling trajectory given by a discrete sequence of points $\{D_\rho, J_\rho\}$. The scaling process has necessarily to end when all ring states are reduced to a single remaining one that absorbs all interaction effects, giving a lower energy cutoff $\Delta$. The lower cutoff is modified for two reasons: (i) The AB ring is open, and the states $\mu$ have finite widths with mean value $\Gamma = \Delta N/(2\pi)$. We have neglected $\Gamma$ by omitting the second term on the r.h.s. of Eq. (5). This is justified only as long as $D \gg \Gamma$. (ii) The electrons which screen the QD spin, form a Kondo cloud of size $\xi$ in the AB ring. The energy scale $E_\xi$ which is required to attain a state of correlation length $\xi$, can be estimated using the uncertainty relation. Hence, the lower cutoff is $\lambda = \max(\Delta, \Gamma, E_\xi)$.

We have solved the discretized version of Eq. (3) for a choice of parameters which resembles the weak Kondo coupling experiment in Ref. [1]: (i) $\Gamma/\Delta \approx 10 (\Lambda = 6, N_j \approx 10)$; $E_\xi/\Delta \approx 1$ (since $\xi \approx 1\mu m$ is about the size $L$ of the ring). (ii) $E_T/\Delta = 4\pi N_e$, where $N_e$ is the number of electrons on the ring. This formula follows for ballistic system $E_T \approx h/L$ and the Weyl formula. The same formula yields $N_e \approx 1000$. (iii) $T_K/\Delta \approx 5$.

Our results are shown in Figure 1. The insert shows five representative trajectories for $\cos \phi = 1$ (where the stochastic effect is largest). The deviations from the standard scaling trajectory increase with decreasing bandwidth, as expected. Averaging over the stochastic trajectories, we recover the standard scaling trajectory (straight line in the insert). In the main part of the figure, we show the distributions $P(T_K)$ of Kondo temperatures $T_K$ for $\cos \phi = 1/2$ and $\cos \phi = 1$. These are obtained from $10^4$ realizations of $\{\psi_\rho\}$. For each realization, the final value of $T_K$ is found by a best–fit procedure. Mean value $(T_K)$ and dispersion $\delta T_K$ are deduced from $P(T_K)$. The average value $(T_K)$ is very close to the standard scaling value and does not show a significant dependence on $\cos \phi$. The fluctuations are large, however, and $\delta T_K$ increases with $\cos \phi$, reaching a maximum value of $\delta T_K/(T_K) \approx 0.25$ at $\cos \phi = 1$.

The numerical simulations show that the fluctuations become larger (smaller) as either $\rho_0 T_K$ or the lower cutoff $\lambda$ are decreased (increased). The reason is that the stochastic “kicks” become more effective for smaller values of $T_K$ and/or $D$, see Eq. (5). Our results are less sensitive to $E_T$. As $E_T$ is increased, the slopes of the scaling trajectories become dominated by the upper band edge,
were the stochastic kicks have little effect. However, this happens very slowly: We observe only small quantitative changes as we increase $E_T$ by an order of magnitude.

For the physical interpretation of our result, we say that an electron is on the QD when it interacts with the fixed spin $\vec{S}$ of the Kondo Hamiltonian $H_K$. Each term of the perturbation expansion describes a process or a sequence of processes where an electron leaves the QD moves in the AB ring, and re-enters the QD. Whenever the electron leaves and enters the QD through the same barrier, the result is a factor $(v^R)^2$ or $(v^L)^2$, as the case may be. Processes of this type are not different from the ones that are taken into account in the standard approach and lead to the standard form of the scaling equation. The fact that the QD is coupled to the AB ring via two barriers only contributes a factor two and is otherwise irrelevant. There are, however, additional processes where the electron leaves the QD through the left barrier and re-enters it through the right one, or vice versa. Such processes correspond to a complete loop through the AB ring, carry the factor $v^R v^L$ and the AB phase, and are absent in the standard approach. Loops in either direction are equally likely, hence the dependence of the relevant term on $\cos \phi$, $v^R v^L$. The AB ring is assumed to be chaotic or diffusive. This makes the loop terms in the scaling equation stochastic.

Renormalization. Poor man’s scaling breaks down for temperatures below the Kondo temperature $T_K$. We discuss this temperature regime only qualitatively in order to demonstrate the existence and action of the stochastic term. We use renormalization group arguments without actually performing the calculation. Following standard procedure [8], one would construct a new basis of orthonormal states $|n\rangle$ where $n = 0, 1, 2, \ldots$. With $|\text{vac}\rangle$ denoting the vacuum, the state $|0\rangle$ is defined as $|0\rangle = (\sum_\mu |v_\mu|^2)^{-1} \sum_\mu v_\mu^* d_\mu^\dagger |\text{vac}\rangle$. For $n \geq 1$, the states $|n\rangle$ would be obtained with the help of Schmidt’s orthogonalization procedure from the sequence $H_{AB}|0\rangle$, $H_{AB}^2|0\rangle$, $\ldots$. (We have shown that it is again justified to approximate the Hamiltonian $H - H_K$ by $H_{AB}$.) The terms in the resulting tridiagonal Hamiltonian depend upon the matrix elements $v_\mu$ via expressions of the type $\sum_\mu v_\mu^2 (\epsilon_\mu)^m$, with $m = 0, 1, 2, \ldots$. Just as for poor man’s scaling, the averages (fluctuations) of such expressions are independent of (dependent on) the AB phase. The fluctuations are maximal for $\cos \phi = 1$ and vanish for $\cos \phi = 0$. Again, the stochastic part is expected to cause a spread in the renormalization group trajectories. The trend of the spread with temperature $T$ can be ascertained as follows. The Kondo temperature $T_K$ defines a marginal fixed point of the problem, while $T = 0$ is a stable fixed point. All trajectories converge to that point. Therefore, as the sample is cooled down, the stochastic spread of the trajectories first increases monotonically to reach its maximum at $T = T_K$. Thereafter, the spread decreases monotonically and vanishes at $T = 0$.

Discussion. Because of the topology of the AB ring, the Kondo temperature $T_K$ of a QD embedded into the ring depends stochastically on the AB phase $\phi$. The resulting spread in Kondo temperature versus AB phase is significant, amounting to 20 or even 40 percent. The influence of stochasticity is expected to decrease as the temperature is lowered below $T_K$, and to vanish at $T = 0$. The precise form of the dependence of $T_K$ on $\phi$ cannot be predicted for an individual experimental sample. We expect that for $T \approx T_K$, this stochastic dependence seriously limits attempts to determine the transmission phase through the QD experimentally, although quantitative predictions will have to be based upon a study of the Anderson model. Such work is now in progress.

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