Transmission Phase Shift of a Quantum Dot with Kondo Correlations

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We study the effects of Kondo correlations on the transmission phase shift of a quantum dot in an Aharonov-Bohm ring. We predict in detail how the development of a Kondo resonance should affect the dependence of the phase shift on transport voltage, gate voltage, and temperature. This system should allow the first direct observation of the well-known scattering phase shift of $\pi/2$ expected (but not directly measurable in bulk systems) at zero temperature for an electron scattering off a spin-$\frac{1}{2}$ impurity that is screened into a singlet.

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The Kondo effect for metallic electrons interacting with localized spins has been studied for more than three decades [1], yet one of its most fundamental properties has so far eluded direct experimental verification: at temperatures sufficiently low that a spin-$\frac{1}{2}$ impurity is screened into a singlet, a conduction electron scattering off the latter is predicted [2,3] to suffer a resonance phase shift of $\pi/2$ [4]. A direct observation of this phase shift, not possible in bulk systems, has now become feasible using quantum dots, due to two recent experimental breakthroughs: Kondo-type correlations were observed in dots strongly coupled to leads [5–9], and it was demonstrated that the transmission phase shift of a dot can be measured by Aharonov-Bohm (AB) interferometry [10,11].

In [5–9], a semiconductor quantum dot was coupled via tunnel junctions to leads and capacitively to a gate. Tuning the gate voltage V_g, which linearly shifts the dot's eigenenergies relative to the chemical potential of the leads, produced a Coulomb-blockade peak in the dot's conductance each time its electron number N changed by one. In valleys between two peaks in which N is odd and at sufficiently low temperatures T, the conductance showed anomalous features [5–9] in accord with earlier predictions [12–14]. These are due to "Kondo correlations," which arise when the dot's topmost (spin-degenerate) occupied energy level, henceforth called the d level, carries on average a *single* electron that can mimic a magnetic spin-$\frac{1}{2}$ impurity in a metal, leading to the well-known Kondo effect [1]. Quantum dots can thus be used as "tunable Kondo impurities." Embedding such a dot in one arm of an AB interferometer and measuring the *phase shift* of the transmission amplitude through the dot [10,11] would thus amount to measuring the scattering phase shift off a Kondo impurity [15]. In this Letter we predict in detail, within the framework of the Anderson model, how Kondo correlations influence the dot's transmission phase shift, and explain how the Kondo phase shift of $\pi/2$ should manifest itself.

AB interferometry.—Figure 1(a) depicts an AB interferometer [11]. A spin-σ electron injected from the source can reach the drain through both the upper and the lower arms, with transmission amplitudes $t_{u\sigma}$ or $t_{l\sigma}$. Their phase difference has the form $2\pi\Phi e/h + \delta\phi$, where Φ is the magnetic flux enclosed by the "ring" formed by the arms. Interference between $t_{u\sigma}$ and $t_{l\sigma}$ causes the differential conductance dI/dV measured at the drain to exhibit AB oscillations as functions of Φ, which are of the form [11]

$$G_{\mathrm{AB}} \propto \frac{e^2}{h} \sum_\sigma |t_{u\sigma}|\,|t_{l\sigma}| \cos(2\pi\Phi e/h + \delta\phi). \qquad (1)$$

The lower arm contains a quantum dot, hence $t_{l\sigma}$ is proportional to the transmission amplitude $t_{d\sigma}$ through the dot. By recording how the amplitude and phase of the AB oscillations change with gate voltage V_g, source-drain voltage V or temperature T, one can thus measure the dependence on these parameters of $|t_{d\sigma}|$ and the "transmission phase shift" $\phi_{d\sigma} = \arg(t_{d\sigma}) = \delta\phi + \text{const}$.

To derive an explicit expression for $t_{l\sigma}$, we calculated [16] G_{AB} using the general theory for AB interferometers

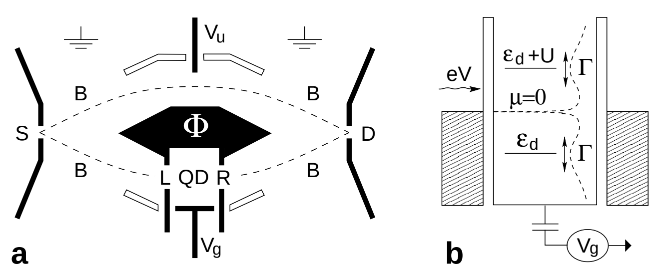

FIG. 1. (a) An AB interferometer: The source S, base region B, and drain D have chemical potentials $\mu_S = eV$, $\mu = 0$, and $\mu_D = 0$, respectively. In the base region four reflectors (shown in white) and a central barrier (black) define an upper and a lower arm forming a "ring" (dotted lines) threaded by an applied magnetic flux Φ. The lower arm contains a quantum dot (QD), coupled to the base region via tunable left and right tunnel barriers (L, R). The gate voltages V_g or V_u can be used to sweep the dot's energy levels relative to μ, or to change the transmission amplitude of the upper arm, respectively. (b) Energy diagram of a QD whose density of states (dashed line) has a Kondo resonance with width of order T_K at energy $E = \mu = 0$, and two broad single-particle resonances, with widths Γ, at $\varepsilon_d < 0$ and $\varepsilon_d + U > 0$. Electrons incident from the source have average energy eV relative to μ.

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of Ref. [17], which assumes (i) that transport through the ring is fully coherent [18]. We further assumed that (ii) the dot level spacing Δ is so large that only the d-level influences transport through the dot [5–9]; (iii) the slits of the source and the drain are so small that only one conducting mode carries current between them [11]; (iv) multiple traversals of the ring can be neglected due to the open nature of the base region [11]; and (v) the source and the drain do not drive the dot out of equilibrium [19].

The result for G_{AB} is of the form (1), with $t_{l\sigma} = (\mathcal{N}_0 t_{0\sigma}|t_L t_R|/\Gamma) t_{d\sigma}$, where $\mathcal{N}_0$ is the density of states per mode in the base region (assumed constant), $t_{0\sigma}$ is a geometrical factor of order unity depending on the amplitudes to reach the dot from the source or the drain, t_L (t_R) is the amplitude per mode for tunneling between the dot and the base region through the left (right) tunnel barrier, and Γ is the width acquired by the d level due to this coupling. All V_g, V, and T dependencies reside in the remaining factor (a $V \neq 0$ generalization of Ref. [20]),

$$t_{d\sigma}(V_g, V, T) = \Gamma \int dE \, \frac{\partial f(E - eV)}{\partial E} \, \mathcal{G}_{d\sigma}(E) \,, \qquad (2)$$

the "thermally averaged transmission amplitude" through the dot for electrons incident with mean energy eV. Here $f(E)$ is the Fermi function and $\mathcal{G}_{d\sigma}(E)$ the retarded Green's function for a spin-σ electron on the d level. $\mathcal{G}_{d\sigma}$ depends on V_g (via ε_d) and on T (due to Kondo correlations), but not on V [by assumption (v), the dot is in equilibrium with the base region]. Since AB oscillations can be produced already with a magnetic field H much too weak to lift the spin degeneracy of the d level, we for the most part shall take $\mathcal{G}_{d\sigma}$ to be H independent, so that $\mathcal{G}_{d\uparrow} = \mathcal{G}_{d\downarrow}$. If the upper arm of the ring is closed off (by adjusting V_u), the conductance G_l through the lower arm is proportional to [21] $|t_L t_R|^2/(|t_L|^2 + |t_R|^2) \sum_\sigma \mathrm{Im}(t_{d\sigma})$. Hence the amplitude of the oscillations in G_{AB}, normalized to G_l, should be proportional to $|t_{d\sigma}|/\mathrm{Im}(t_{d\sigma}) = 1/\sin(\phi_{d\sigma})$, which can be used as a consistency check on assumptions (i) to (v).

Measurements of $\phi_{d\sigma}$ have so far been performed only for dots without Kondo correlations, but even so the V_g dependence was interesting: $\phi_{d\sigma}$ increased by π whenever the dot was tuned through a Coulomb-blockade peak, as expected for a Breit-Wigner–type resonance. It also suffered a "phase lapse" (a drop by $-\pi$) between consecutive peaks [11], which can be explained by taking Coulomb interactions (at a mean-field level) on the dot into account [20,22]. More puzzling is the fact that the lapses persisted over many consecutive valleys, but we do not wish to address this matter here [23].

Kondo correlations.—Instead, we consider here a *single* odd valley and study how $t_{d\sigma}$ is influenced by Kondo correlations of the kind observed recently [5–9]. These were predicted [12,13] and interpreted [7] by using a standard model describing a localized state (the d level) coupled to a band of conduction electrons [both the left and the right sides of the base region; by assumption (v) we henceforth neglect the influence of the source and the drain], namely, the much-studied and well-understood Anderson model [1,24,25]. The parameters of this model, illustrated in Fig. 1(b), are the energy ε_d of the d level (measured relative to the chemical potential of the base region, $\mu = 0$); the additional Coulomb energy cost U for having the d level doubly occupied; the width of the conduction band, which we take $\gg U$; and the width [12(a)] $\Gamma = \pi \mathcal{N}_0^{\mathrm{tot}}(|t_L|^2 + |t_R|^2)$ of the d level, where $\mathcal{N}_0^{\mathrm{tot}}$ is the combined density of states of all modes in the base region which are coupled to the dot.

Sweeping the gate voltage V_g into and through an "odd valley" in this model corresponds to sweeping the dot level ε_d from above Γ to below $-(U + \Gamma)$, in the course of which the total average occupation of the d level, $\bar{n}_d$ ($= 2\bar{n}_{d\sigma}$), smoothly changes from 0 to 2. The valley center is at $\varepsilon_d = -U/2$, and its two halves are related by particle-hole symmetry, with $\varepsilon_d + U/2 \to -(\varepsilon_d + U/2)$ implying $\bar{n}_d \to 2 - \bar{n}_d$. As ε_d is lowered through a half-valley towards $-U/2$, three different regimes can be distinguished: (i) the "empty-orbital" regime $\varepsilon_d \gtrsim \Gamma$, in which $\bar{n}_d \simeq 0$; (ii) the "mixed-valence" regime $|\varepsilon_d| \lesssim \Gamma$, in which $\bar{n}_d$ begins to increase due to strong charge fluctuations; and (iii) the "local-moment" regime $-U/2 \leq \varepsilon_d \lesssim -\Gamma$, in which $\bar{n}_d$ approaches 1, so that the d level acts like a localized spin. The latter can give rise to Kondo correlations: as the temperature is lowered below the Kondo temperature, a crossover scale given by $T_K = (U\Gamma/2)^{1/2} e^{\pi\varepsilon_d(\varepsilon_d + U)/2\Gamma U}$ [25], the d-level density of states $\rho_{d\sigma}(E)$ begins to develop a sharp peak near $E = 0$ [dotted line in Fig. 1(b)], whose width is of the order of T_K when $T \ll T_K$. This so-called Kondo resonance arises due to coherent virtual transitions between the d level and the conduction band, which "screen" the spin of the d level in such a way that the ground state is a spin singlet. The resonance strongly enhances the magnitude $|t_{d\sigma}|$ of the transmission amplitude of electrons incident on the dot with energies $E \simeq 0$, causing the dot's conductance in the local-moment regime of an odd valley to be anomalously large at low T and V, as seen in [5–9]. Typical dot parameters [5–7] were $\Delta \simeq 0.1–0.5$ meV for the level spacing, and $\Delta/\Gamma \simeq 1–3$, $U/\Gamma \simeq 1–10$, resulting in T_K's between 45 mK and 2 K.

Methods.—To study how Kondo correlations affect $\phi_{d\sigma}$, we calculated $t_{d\sigma}$ via (2) by three standard methods:

(a) For $T \gtrsim \Gamma(\gg T_K)$, where Kondo correlations are weak, we used the *equations of motion* (EOM) method; it decouples higher into lower order Green's functions to yield an analytical expression for $\mathcal{G}_{d\sigma}(E)$ [Eq. (8) of [13(a)], in which we calculated $\bar{n}_d$ self-consistently].

(b) For $T = V = 0$, we have $t_{d\sigma} = -\mathcal{G}_{d\sigma}$; using well-known Fermi-liquid results for the latter [Eqs. (5.47) and (5.50) of Ref. [1]], one finds

$$|t_{d\sigma}| = \sin(\bar{n}_{d\sigma}\pi), \qquad \phi_{d\sigma} = \bar{n}_{d\sigma}\pi \,. \qquad (3)$$

The second relation is the Friedel sum rule [2,3]. Thus, $t_{d\sigma}(V_g)$ (for $V = T = 0$) is completely determined by $\bar{n}_{d\sigma}(T = 0)$, which for all Γ, U, ε_d is known exactly from the *Bethe ansatz* [Eqs. (8.2.47–48) of [25]].

(c) For arbitrary temperatures ($\lesssim\Gamma$), the only approach which gives reliable results for $\mathcal{G}_{d\sigma}(E)$ for all Γ, U, ε_d is the *numerical renormalization group* (NRG) [1,26]. It is designed to calculate the density of states $\rho_{d\sigma}(E) \equiv -\mathrm{Im}\mathcal{G}_{d\sigma}(E)/\pi$, but this is sufficient to determine $\mathrm{Re}\,\mathcal{G}_{d\sigma}(E)$ too, via a Kramers-Kronig relation.

We calculated $t_{d\sigma}$ for two types of situations:

(1) *V dependence.*—Sweeping the source-drain voltage V, with V_g fixed in an odd valley (Fig. 2), is the most direct way of "imaging" the Kondo resonance, since by Eq. (2) the V dependence of the transmission amplitude $t_{d\sigma}(V_g^{\mathrm{fixed}}, V, T)$ reflects the (thermally smeared) E dependence of $\mathcal{G}_{d\sigma}(E)$ [but only if assumptions (i) and (v) hold [18,19]]. For an asymmetric choice $\varepsilon_d = -3\Gamma$ in the local-moment regime [Figs. 2(a) and 2(b)] and large temperatures, $|t_{d\sigma}|$ shows two broad peaks near ε_d and $\varepsilon_d + U$, and $\phi_{d\sigma}$ a weak phase lapse in between, as expected for two not-very-well-separated single-particle resonances. As T is lowered, a strong Kondo resonance in $|t_{d\sigma}|$ develops, as seen in [5–9]. Simultaneously, $\phi_{d\sigma}$ develops a novel sharp "Kondo double phase lapse," because, intuitively speaking, it tends to lapse between every two resonances, and now there are three, two broad and one sharp. These features become more pronounced the deeper ε_d lies in the local-moment regime, so much so that in the symmetric case $\varepsilon_d = -U/2$ [Figs. 2(c) and 2(d)] the Kondo peak in $|t_{d\sigma}|$ and the double phase lapse in $\phi_{d\sigma}$ are still faintly noticeable even for the highest temperature shown ($T = 33T_K$). Encouragingly, these features might thus be observable even at the center of an odd valley, where T_K is smallest and $T \lesssim T_K$ is hardest to achieve. If ε_d is shifted from the local-moment into the empty-orbital regime, the Kondo resonance merges with the lower broad single-particle resonance and the double phase lapse for $\phi_{d\sigma}$ disappears.

(2) *V_g dependence.*—Sweeping V_g through an odd valley, with $V = 0$ (Figs. 3 and 4) probes the low-energy window $|E| \lesssim T$ within which the Kondo resonance shoots up for $T \lesssim T_K$; the magnitude of $t_{d\sigma}(V_g, V = 0, T)$ thus reflects the weight of the Kondo resonance. For large T (say $\simeq \Gamma$, i.e., negligible Kondo correlations) and a small Γ/U, $t_{d\sigma}$ shows the familiar behavior [Figs. 3(a) and 3(b)] experimentally observed in Ref. [11]: its magnitude $|t_{d\sigma}|$ has well-resolved Coulomb-blockade peaks near 0 and $-U$, at each of which its phase $\phi_{d\sigma}$ rises (by almost π), with a significant phase lapse in the valley in between. The larger Γ/U, the less sharp these features, since the peaks increasingly overlap. As T is lowered, the Kondo resonance develops throughout the local-moment regime, leading to a dramatically different picture at $T = 0$ [Figs. 3(c) and 3(d)]: $|t_{d\sigma}|$ has just one, much higher peak, and $\phi_{d\sigma}$ increases *monotonically* from 0 to π; by Eq. (3), both reflect the monotonic change in the occupation $\bar{n}_d$ of the d level as ε_d is swept. If Γ/U decreases, the extent (in units of Γ) of the $\bar{n}_d \simeq 1$ local-moment regime increases, so that both $|t_{d\sigma}|$ and $\phi_{d\sigma}$ develop flat plateaus around $\varepsilon_d = -U/2$.

The $\phi_{d\sigma} = \pi/2$ plateau is the manifestation of the famous $\pi/2$ Kondo phase shift mentioned earlier. It arises because the local spin is screened into a singlet at $T = 0$. Since *no* spin-flip scattering occurs, a Fermi-liquid description of the system is possible [4]: to low-energy Fermi-liquid quasiparticles scattering off the singlet Kondo resonance, it looks like a *static* (as opposed to dynamical) impurity, which scatters them without randomizing their phase, and which is strongly repulsive, causing a resonance phase shift [2,3] of $\pi/2$.

T dependence.—Figures 4(a) and 4(b) show the crossover from Figs. 3(a) and 3(b) to 3(c) and 3(d) as the temperature is lowered from Γ to 0, for $\varepsilon_d \geq -U/2$ and $\Gamma = U/4\pi$ (this value was also used in [26], whose Figs. 5–10 show how the Kondo peak changes correspondingly).

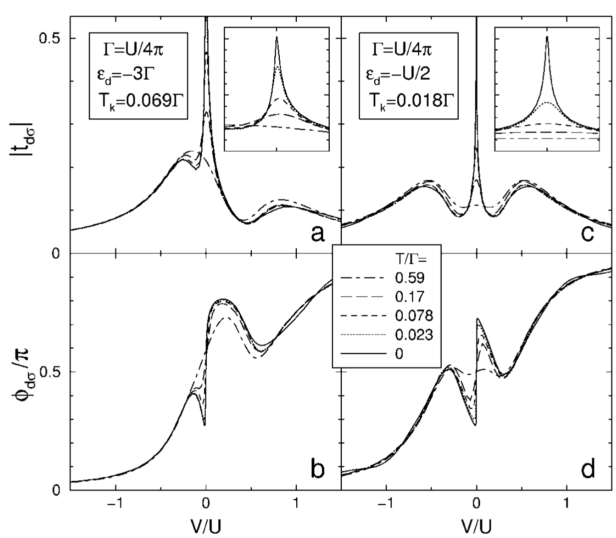

FIG. 2. Magnitude and phase of $t_{d\sigma}(V_g^{\mathrm{fixed}}, V, T)$ (from NRG) as functions of V/U and T/Γ, for $\Gamma = U/4\pi$ and fixed $\varepsilon_d = -3\Gamma$ (a),(b) or $\varepsilon_d = -U/2$ (c),(d). Insets show the range $|V| \leq 20T_K$; the $T = 0$ peak heights are within 2% of Eq. (3).

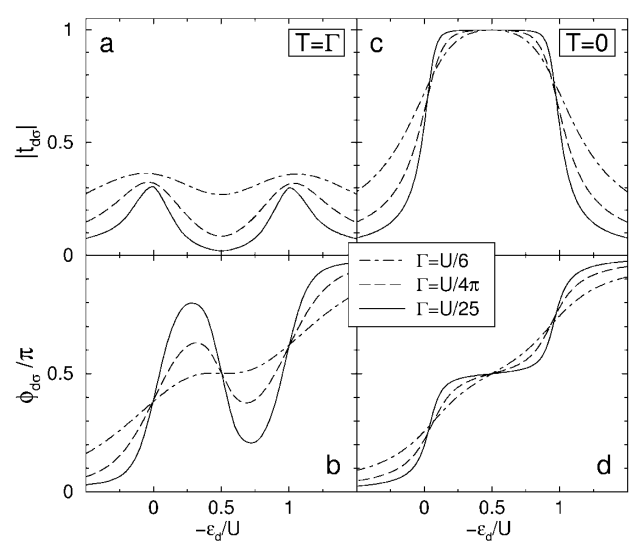

FIG. 3. Magnitude and phase of $t_{d\sigma}(V_g, 0, T)$ as a function of $-\varepsilon_d/U$, for three values of U/Γ, with (a),(b) $T = \Gamma$ (from EOM); and (c),(d) $T = 0$ (from Bethe ansatz).

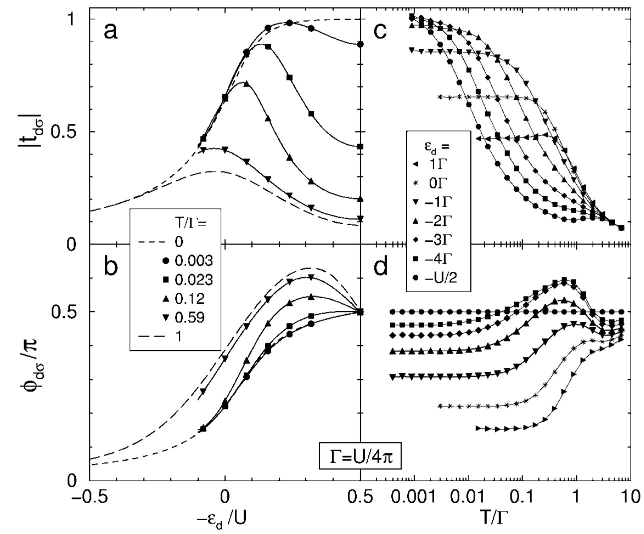

FIG. 4. Magnitude and phase of $t_{d\sigma}(V_g, 0, T)$, for $\Gamma = U/4\pi$: (a),(b) as functions of $-\varepsilon_d/U$, for $T = \Gamma$ (long-dashed line, from EOM), $T = 0$ (short-dashed line, from Bethe ansatz), and four intermediate values of T/Γ; (c),(d) as functions of T/Γ, for various ε_d. The symbols represent points calculated using the NRG; they are connected by spline fits.

Figures 4(c) and 4(d) show the same crossover, but now with T/Γ on the horizontal axis. As T approaches Γ from above, $\phi_{d\sigma}$ initially rises if $\varepsilon_d \lesssim 0$ and drops if $\varepsilon_d > 0$, because the phase rise in Fig. 3(b) sharpens. As T is decreased further, $\phi_{d\sigma}$ decreases for *all* ε_d, reflecting the Kondo suppression, shown in Fig. 4(b), of the phase lapse. Thus, a maximum (instead of a low-T saturation) in $\phi_{d\sigma}(T)$ for $-U/2 < \varepsilon_d \lesssim 0$ would signify the onset of Kondo correlations.

H dependence.—A strong magnetic field that lifts the spin degeneracy of the local level by $\varepsilon_\uparrow - \varepsilon_\downarrow = \Delta_h$ will split the Kondo resonance into two subresonances, separated by $\simeq \Delta_h$ [6,13], while strongly reducing their combined weight, and thereby also the spectral weight at $E \simeq 0$. Thus, with increasing Δ_h, type (2) measurements should behave similarly as for increasing T, which also reduces the spectral weight at $E \simeq 0$; and type (1) measurements should show two Kondo peaks (of reduced height) in $|t_{d\sigma}|$ and a Kondo triple phase lapse in $\phi_{d\sigma}$ [16].

To summarize, we studied phase-coherent transport of electrons traversing a strongly interacting environment (the dot-lead system) that is tunable from being weakly correlated at high temperatures through a strongly correlated crossover regime to a Fermi liquid [4] at sufficiently low temperatures. We identified three "smoking guns" for Kondo correlations in the behavior of $\phi_{d\sigma}$: the Kondo double phase lapse in Figs. 2(b) and 2(d), the $\pi/2$ plateau in Fig. 3(d), and the maxima in Fig. 4(d). The experimental observation of the $\pi/2$ plateau would constitute the first direct measurement of the $\pi/2$ Kondo phase shift predicted more than 30 years ago.

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