

Anomalous transmission phase of a Kondo-correlated quantum dot

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We study phase evolution of transmission through a quantum dot with Kondo correlations. By considering a model that includes nonresonant transmission as well as the Anderson impurity, we explain the unusually large phase evolution of about π across the resonant peak through the Kondo valley observed in recent experiments. We argue that this anomalous phase evolution is a universal property that can be found in the high-temperature Kondo phase in the presence of the time-reversal symmetry.

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I. INTRODUCTION

Recent measurements of transport through quantum dots have identified the Kondo effect in a very controllable way.¹⁻⁴ In particular, the scattering phase shift of the Kondo-assisted transmission has been measured experimentally.⁵⁻⁷ This measurement has attracted renewed interest in the Kondo effect since the phase shift cannot be accessed in bulk Kondo systems nor, even in mesoscopic systems, by means of conductance measurement. More importantly, the measured phase shift does not agree with the theoretical predictions. The Kondo scattering is expected to induce a phase shift of $\pi/2$.⁸ Indeed, theoretical study based on the impurity Anderson model predicts that the phase shift of transmission amplitude should have $\pi/2$ plateaus in the Kondo limit.⁹ However, Ji *et al.* observed various anomalous behavior of the phase evolution^{5,6} which cannot be explained in terms of the simple Anderson model. The experimental results indicate unusually large span of the phase, such as the plateaus of the phase shift about π in the presence of the Kondo correlation.⁵ Our aim here is to provide a theoretical explanation on such anomalous phase evolution.

We consider a model that incorporates a weak direct nonresonant transmission through a quantum dot (QD), as well as the Kondo-resonant transmission. The importance of including more than the simplest resonant transmission has been demonstrated in the experiment by Schuster *et al.*,¹⁰ which shows unexpected phase lapse by π in the Coulomb blockade (CB) limit. Fano-type interference between the resonant and the nonresonant transmission may provide a possible explanation for the anomalous phase drop accompanied by transmission zero,¹¹⁻¹³ in the presence of time-reversal symmetry (TRS).¹⁴ (Note that there have been other proposals based on the electron-electron interactions: see, e.g., Ref. 15). The role of the nonresonant transmission is expected to be even more important in the experiment of the Kondo limit^{5,6} because the QD should be more open to the leads in order to reach the Kondo limit, which has never been noticed before. It is also possible that QD has more than one level contributing to the transport.¹⁵⁻²⁰ In such a case, the off-resonant transmission plays a similar role as that of the direct transmission. Therefore, it is plausible to take into account the nonresonant transmission through a Kondo-

correlated QD, as a first correction to the problem.

In this paper, we show that some anomalous phase evolution observed in the experiment can be explained by considering a nonresonant transmission component interfering with the Kondo resonance. To be specific, we explain unusually large span of the phase (about π) across the resonance into the ‘‘Kondo’’ valley. Further we argue that this phenomenon is a universal property that can be observed in the presence of time-reversal symmetry.

II. MODEL AND FORMULATION

We begin with the model Hamiltonian $H = H_L + H_R + H_D + H_T$. The Hamiltonians for the left (L) and right (R) leads are given by

$$H_\alpha = \sum_{k\sigma} \varepsilon_{ak} c_{ak\sigma}^\dagger c_{ak\sigma} \quad (\alpha = L, R), \quad (1a)$$

where $c_{ak\sigma}$ ($c_{ak\sigma}^\dagger$) is a destruction (creation) operator of an electron with energy ε_k , momentum k , and spin σ on the lead α . The interacting QD is described by

$$H_D = \sum_{\sigma} \varepsilon_d d_{\sigma}^\dagger d_{\sigma} + U n_{\uparrow} n_{\downarrow}, \quad (1b)$$

where d_{σ} and d_{σ}^\dagger are dot electron operators, $n_{\sigma} = d_{\sigma}^\dagger d_{\sigma}$, and ε_d and U stand for the energy of the localized level and the on-site Coulomb interaction, respectively. The tunneling Hamiltonian H_T has the form

$$H_T = \sum_{\alpha=L,R} \sum_{k\sigma} (V_{\alpha} d_{\sigma}^\dagger c_{ak\sigma} + \text{H.c.}) + \sum_{kk',\sigma} (W c_{Lk\sigma}^\dagger c_{Rk'\sigma} + \text{H.c.}). \quad (1c)$$

Here the tunneling amplitude W is responsible for the direct transmission between the two leads, and V_{α} for the tunneling between the QD and the lead α , assumed to be independent of k and σ .

Formally, our model (1) is equivalent to a two-terminal Aharonov-Bohm (AB) interferometer containing a QD,^{21,22} where the reference arm corresponds (formally) to the term in W in Eq. (1c). However, the previous studies in Refs. 21 and 22 were focused only on conductance, whereas our pur-

pose in this work is to investigate the complex transmission amplitude that contains the phase information as well as the magnitude. We also emphasize that the term in W in Eq. (1c) describes the nonresonant direct transmission through the QD and has a completely different physical origin from the reference arm in an AB interferometer.

For simplicity, we assume symmetric junctions (i.e., $V_L = V_R = V$) and identical leads (i.e., $\varepsilon_{Lk} = \varepsilon_{Rk} = \varepsilon_k$) with the density of states ρ at the Fermi energy. The direct tunneling matrix element W is in general complex number $W = |W|e^{i\varphi}$, while the hopping matrix elements V_α can be kept as positive real numbers without loss of generality. Then φ stands for the phase difference between the resonant and the nonresonant component. We assume the TRS so that the phase φ takes either 0 or π . (In fact, the external magnetic flux penetrating the QD is only a very small fraction of the flux quantum in the experiment of Refs. 5 and 6, and hence the TRS is well preserved.)

Using the relation between the scattering matrix and the local Green's function,⁸ one can write the transmission amplitude of the electrons with energy ε from the left to right lead as

$$t_{LR}(\varepsilon) = ie^{i\varphi}|t_b| + ie^{i\varphi}\Gamma_{\text{eff}}G_d^R(\varepsilon)[|r_b|\cos\varphi - i(|t_b| + \sin\varphi)]. \quad (2)$$

Here $|t_b| \equiv 2x/(1+x^2)$ with $x = \pi\rho|W|$ being the magnitude of the direct transmission amplitude. $|r_b|$ is defined by the relation $|t_b|^2 + |r_b|^2 = 1$. The effective hybridization parameter Γ_{eff} in Eq. (2) is defined by $\Gamma_{\text{eff}} = \Gamma/(1+x^2)$ with $\Gamma = 2\pi\rho V^2$, and $G_d^R(\varepsilon)$ is the retarded Green's function for the dot electron.

At zero temperature, only the electrons at the Fermi energy contribute to the total transmission amplitude (t_{LR}), and the Friedel-Langreth sum rule⁸ gives an exact expression for G_d^R in terms of the occupation number of the dot, n_d , leading to the relation

$$t_{LR} = t_{LR}(0) = \frac{ie^{i\varphi}|t_b|}{e_d - i}(e_d + Q), \quad (3a)$$

$$e_d = \cot(\pi n_d/2), \quad (3b)$$

$$Q = -\frac{|r_b|}{|t_b|}\cos\varphi + \frac{i}{|t_b|}\sin\varphi. \quad (3c)$$

Equation (3) already provides some important informations. First, transmission zero takes place at $\cot(\pi n_d/2) = \pm|r_b|/|t_b|$ for $\varphi=0, \pi$, respectively, as a result of destructive interference between the two transmission components. For $|t_b| \ll 1$, transmission zero is located far from the Kondo limit, $n_d \approx 0$ or $n_d \approx 2$, for $\varphi=0$ or $\varphi=\pi$, respectively. In the opposite limit ($|t_b| \approx 1$), t_{LR} goes to zero in the Kondo limit ($n_d \approx 1$). This limit was investigated previously for a ballistic quantum wire coupled to a QD.²³

At finite temperatures, we need to take the thermal average of the transmission amplitude²⁴

$$t_{LR} = \int \left(-\frac{\partial f}{\partial \varepsilon} \right) t_{LR}(\varepsilon) d\varepsilon, \quad (4)$$

where f denotes the Fermi distribution function.

III. SLAVE BOSON MEAN-FIELD THEORY ON THE TRANSMISSION AMPLITUDES

For a quantitative study, we adopt the slave-boson mean-field theory (SBMFT) assuming $U = \infty$.²⁵ We will also report results from the numerical renormalization group (NRG) calculations to confirm the results from the SBMFT. The SBMFT satisfies the unitarity of the scattering matrix,²³ which cannot be preserved in some other approaches based on the $1/N_s$ expansion (with N_s being the degeneracy of the level). After some algebra, we obtain the relation

$$t_{LR}(\varepsilon) = \frac{ie^{i\varphi}|t_b|}{\tilde{\varepsilon}_d - i}(\tilde{\varepsilon}_d + Q), \quad (5a)$$

$$\tilde{\varepsilon}_d \equiv \frac{\tilde{\varepsilon}_d - \varepsilon}{(1 - n_d)\Gamma_{\text{eff}}}. \quad (5b)$$

The renormalized energy level $\tilde{\varepsilon}_d$ in Eq. (5) will be determined self-consistently together with n_d . We note that at $T = 0$, the expression in Eq. (5) based on the SBMFT reduces to the exact form of Eq. (3).

The results from the SBMFT are summarized in Fig. 1 for $\varphi=0$.²⁶ Figure 1 shows (a) the magnitude $|t_{LR}|$ and (b) the phase shift $\Delta\gamma$ of the total transmission amplitude t_{LR} at several temperatures in the presence of a small direct transmission ($|t_b|=0.08$). For a comparison, the results for $t_b=0$ are also shown in Figs. 1(c) and 1(d). One can see clearly that while the magnitude is affected very little, a small $|t_b|$ can lead to completely different behavior of the phase at finite temperatures, as we discuss in detail now.

According to the behaviors of the transmission phase in the presence of direct transmission, the low-temperature region can be divided into two subregions: the ‘‘unitary Kondo regime’’ ($T < T_0$), and the so-called ‘‘Fano-Kondo regime’’ ($T > T_0$):²⁷ see Sec. V for an estimate of the crossover temperature T_0 . In the unitary Kondo regime, the Kondo resonance provides a transmission channel with a transmission probability larger than the direct transmission $|t_b|^2$. Therefore, neither the magnitude nor the phase of t_{LR} is affected by the small $|t_b|$. Namely, as well understood by the studies based on the Anderson impurity model,^{28,29} $|t_{LR}|(\Delta\gamma)$ changes from 0 to 1 ($\pi/2$) as ε_d varies from the empty dot limit ($\varepsilon_d \gg \Gamma_{\text{eff}}$) to the singly occupied limit ($\varepsilon_d \ll -\Gamma_{\text{eff}}$).

In the Fano-Kondo regime, on the other hand, one can observe much richer behaviors. As the temperature increases, the Kondo effect is partially suppressed and the transmission probability through the Kondo resonance becomes comparable to the nonresonant transmission $|t_b|^2$. An interference between the nonresonant transmission and the transmission through the Kondo resonance occurs. Such a Fano-type interference affects $|t_{LR}|$ very little, since the nonresonant transmission and the transmission through the Kondo resonance are both already small in the region where the interference is

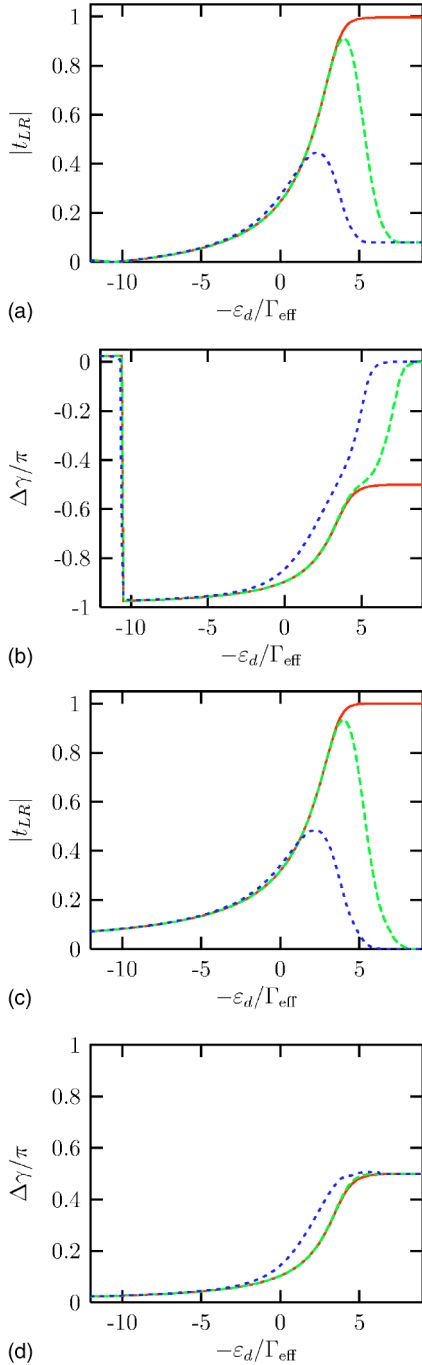


FIG. 1. (a) The magnitude and (b) the phase of the transmission amplitude t_{LR} for $\varphi=0$ and $|t_b|=0.08$ with the temperatures $T=0$ (solid lines), $0.02\Gamma_{\text{eff}}$ (dashed lines), $0.5\Gamma_{\text{eff}}$ (dotted lines). (c) The magnitude and (d) the phase for $t_b=0$ with the temperatures $T=0$ (solid lines), $0.02\Gamma_{\text{eff}}$ (dashed lines), $0.5\Gamma_{\text{eff}}$ (dotted lines).

important; compare Figs. 1(a) and 1(c). However, the phase shift ($\Delta\gamma$) is affected significantly even by a small value of $|t_b|$. As shown in Fig. 1(b), the plateau of $\Delta\gamma$ as a function of ε_d is lifted significantly from $\pi/2$ to a value close to π . This behavior is consistent with the experimental observation,⁵ but is in strong contrast with the almost temperature-independent Kondo plateaus at $\pi/2$ for $t_b=0$ [Fig. 1(d)]. We believe that this anomalous phase behavior in the presence of

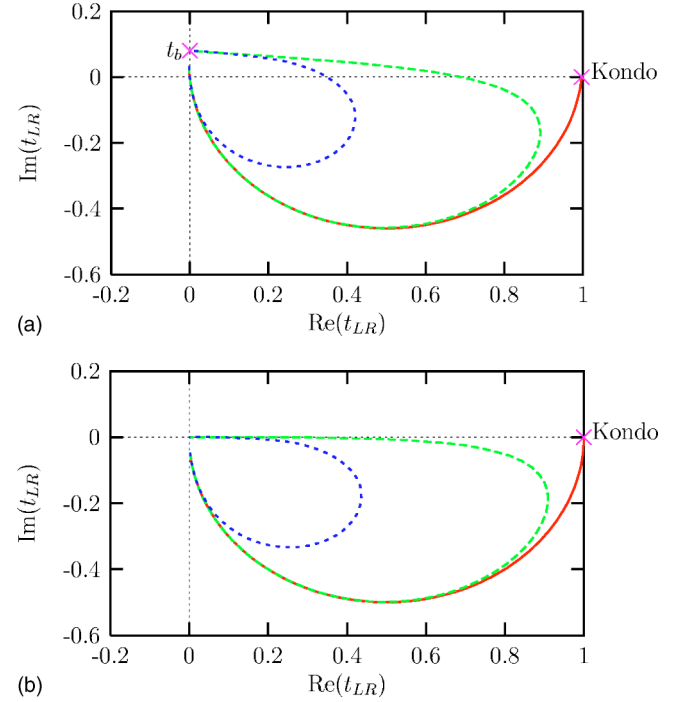


FIG. 2. Trajectories in the complex plane for the numerically obtained transmission amplitudes in Fig. 1 for (a) $|t_b|=0.08$, $\varphi=0$, and for (b) $t_b=0$.

the nonresonant transmission can be a natural explanation observed in the experiment,⁵ that is, the phase evolution of about π across the resonant peak to the Kondo valley.³⁰

In fact, this unexpected behavior of transmission phase is better understood by investigating the trajectories of the transmission amplitude t_{LR} in the complex plane as ε_d varies from $\varepsilon_d \gg \Gamma_{\text{eff}}$ to $\varepsilon_d \ll -\Gamma_{\text{eff}}$ at different temperatures for $t_b \neq 0$ (and also for $t_b=0$); see Fig. 2. Notice that the following argument is quite universal that relies only on the existence of nonresonant transmission and the TRS. The most important change due to the the direct transmission is that the transmission coefficient has a finite value $t_{LR}=t_b$, even when the resonant transmission component is suppressed. This put a negligible effect on t_{LR} at $T < T_0$, where the resonant transmission component is not suppressed and larger in magnitude than the direct transmission component. But it plays a significant role in the Fano-Kondo regime, where the Kondo-assisted transport is partially suppressed. The suppression of the Kondo-assisted transmission leads to $\Delta\gamma$ significantly larger than $\pi/2$, even close to π , since t_b has pure imaginary value in the presence of TRS (i.e., $t_b = ie^{i\varphi}|t_b|$) and $\varphi=0, \pi$).

We would like to stress that our findings about this unusual phase evolution are quite universal, which does not depend on the approximation scheme adopted here. To be precise, the phase evolution at $T \neq 0$ with $t_b \neq 0$ is close to $\pi/2$, but not exactly π . It will be natural to define the phase evolution $\Delta\gamma$ by the phase difference between the high temperature Kondo plateau [denoted as t_b in Fig. 2(a)] and the point near the transmission zero. Then one finds that for not very large value of $|t_b|$,

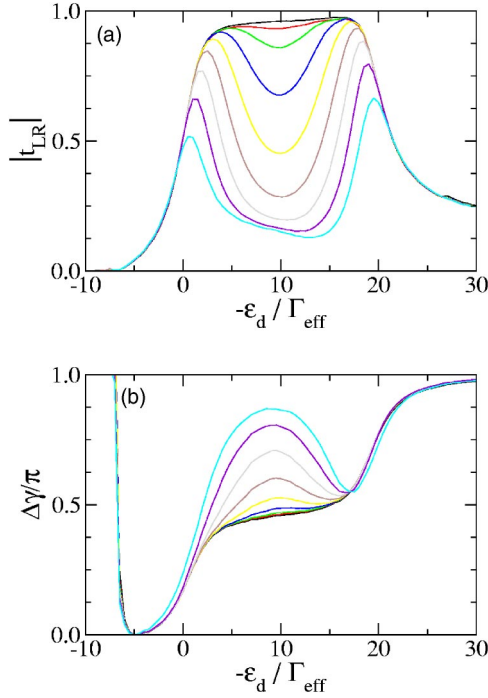


FIG. 3. The same as Figs. 1(a) and 1(b), except that the results are from the NRG calculations and for finite U . $U=20\Gamma_{\text{eff}}$, $W=0.065D$ ($|t_b|=0.2$), $V=0.2D$, and $T/\Gamma_{\text{eff}}=0, 10^{-4}, 10^{-3.5}, 10^{-3}, \dots, 10^{-0.5}$ from top to bottom in (a) and bottom to top in (b).

$$\Delta\gamma = \frac{\pi}{2} - \arctan\left(-\frac{|r_b|}{|t_b|}\right). \quad (6)$$

From this relation, we can conclude that the phase evolution of π takes place for very small $|t_b|$. For larger value of $|t_b|$, $\Delta\gamma$ becomes smaller than π . As stated above, Eq. (6) is exact which does not rely on the approximation scheme adopted. It is because of the fact that $t_{LR} \rightarrow t_b$ in the high-temperature Kondo phase ($T > T_0$).

IV. RESULTS FROM NUMERICAL RENORMALIZATION GROUP CALCULATION

So far we have discussed the results based on the SBMFT for $U=\infty$. We stress that our findings about the unusual phase evolution are quite universal, which do not depend on the approximations adopted here nor on the constraint of $U=\infty$. To confirm this, we also provide the results from the NRG calculations in Fig. 3, which are in good agreement with those from the SBMFT except that now there is a region where the dot is doubly occupied ($\varepsilon_d < -U$). Further, the results show clearly the crossover from the unitary to the Fano-Kondo region as temperature increases.

For $T > T_0$, the phase evolution shows a plateau with $\Delta\gamma \approx \pi$. This agrees with the experimental results of Ref. 5. Nevertheless, it should be noted that the experimental results show more complicated behavior than ours. For example, the overall phase shift through the two resonant peaks exceeds π , which depends on the parameters. We have carefully ex-

amined the trajectory of the experimental transmission amplitude (not shown here) as in Fig. 2. From this, we conclude that the disagreement may be related some nonuniversal effects in real devices.

V. ESTIMATION OF THE CROSSOVER TEMPERATURE T_0

We now estimate the crossover temperature T_0 . T_0 can be determined by comparing $|t_b|$ and the magnitude of the resonant component. That is, crossover from the unitary to the Fano-Kondo phase takes place at the temperature where the magnitude of the resonant transmission is comparable to $|t_b|$. Since the Kondo-correlated state behaves similar to a Fermi liquid, we substitute

$$G_d^R(\varepsilon) \approx \frac{T_K/\Gamma_{\text{eff}}}{\varepsilon + iT_K} \quad (7)$$

into Eqs. (2) and (4), and find that (for $\varphi=0$)

$$t_{LR} = i|t_b| + i(|r_b| - i|t_b|)\mathcal{F}(T_K), \quad (8)$$

where

$$\mathcal{F}(T_K) = \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{T_K}{\varepsilon + iT_K}. \quad (9)$$

The integral in Eq. (9) can be calculated exactly with the help of contour integration,³¹ which leads in the limit of $T \gg T_K$ to the form

$$\mathcal{F}(T_K) \approx -i \frac{T_K}{T_K + \pi T}. \quad (10)$$

Inserting this expression into Eq. (8), one can find that the crossover from $\Delta\gamma = \pi/2$ to $\Delta\gamma = \pi$ takes place at $T \sim T_0$ such that

$$T_0 = \frac{|r_b|}{\pi|t_b|} \min(T_K), \quad (11)$$

where $\min(T_K) = T_K(\varepsilon_d = -U/2)$.

Equation (11) is useful to test our claims. We recall that T_K can be extracted from the temperature dependence of the conductance, and $|t_b|$ from the Fano-resonance shape of the conductance at higher temperatures. Equation (11) then estimates T_0 . One has only to compare $\Delta\gamma$ as a function of ε_d at $T \ll T_0$ and $T > T_0$. We add that T_0 is slightly overestimated in Eq. (11) since the Fermi-liquid form has been used for estimation even at finite temperatures. The π plateaus in the Fano-Kondo regime were observed experimentally,^{5,6} according to our interpretation. In the same experiments, however, the $\pi/2$ plateaus in the unitary Kondo limit were not observed. We point out that in those experiments, the dot was too open and in the mixed valence regime (instead of the unitary Kondo limit) for strong coupling between the leads and the QD.

VI. CONCLUSION

In conclusion, we have theoretically explained the unusually large value of the transmission phase ($\sim\pi$) found in a recent experiment for the Kondo regime of a quantum dot. For the Anderson impurity as well as the nonresonant transmission between the two leads, we found that time-reversal symmetry at high-temperature Kondo phase results in the

plateaus of about π , as long as the nonresonant transmission is small but finite.

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- ²⁴We have in mind an experiment on an AB interferometer with our system put in one of the two arms. Equation (4) actually accounts only for the interference term when multiple backscatterings are negligible (see Ref. 10).
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- ²⁷At even higher temperatures (the CB region), phase lapses by π were observed experimentally. While this effect is partially understood for noninteracting models, there is no theoretical explanation for strongly correlated systems in question. In this work we are only confined in the region where the temperature is much lower than such a crossover region.
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