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 unusually large phase evolution of about $\pi$ in 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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Recent measurements of transport through quantum dots have identified the Kondo effect in a very controllable way. In particular, the scattering phase shift of the Kondo-assisted transmission has been measured experimentally. 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 $\pi/2$. Indeed, theoretical study based on the impurity Anderson model predicts that the phase evolution of transmission amplitude should have $\pi/2$-plateaus in the Kondo limit. However, Y. Ji et al. observed various anomalous behavior of the phase evolution which cannot be explained in terms of the simple Anderson model. The experimental results indicate unusually large span of the phase evolution, such as the plateaus of the phase shift about $\pi$ in the presence of the Kondo correlation.

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., which shows unexpected phase lapse by $\pi$ in the Coulomb blockade (CB) limit. For a model, the resonant transmission provides a possible explanation for the anomalous phase drop accompanied by transmission zero, in the presence of time-reversal symmetry (TRS). The role of the nonresonant transmission is expected to be even more important in the experiment of the Kondo limit 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. 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 Letter, 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.

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

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

where $c_{\alpha k\sigma} (c_{\alpha k\sigma}^\dagger)$ is a destruction (creation) operator of an electron with energy $\varepsilon_k$, momentum $k$, and spin $\sigma$ on the lead $\alpha$. 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 $d_\sigma$ and $d_\sigma^\dagger$ are dot electron operators, $n_\sigma = d_\sigma^\dagger d_\sigma$, $\varepsilon_d$ and $U$ stand for the energy of the localized level and the on-site interaction, respectively. The tunneling Hamiltonian $H_T$ has the form

$$H_T = \sum_{\alpha=L,R} \sum_{\alpha k} (V_\alpha d_\sigma^\dagger c_{\alpha k\sigma} + h.c.)$$

$$+ \sum_{kk'\sigma} \left( W c_{Lk\sigma}^\dagger c_{Rk'\sigma} + h.c. \right). \quad (1c)$$

Here the tunneling amplitude $W$ is responsible for the direct transmission between the two leads, and $V_\alpha$ for the tunneling between the QD and the lead $\alpha$.

Formally, our model is equivalent to a two-terminal Aharonov-Bohm (AB) interferometer containing a QD, where the reference arm corresponds (formally) to the term in $W$ in Eq. (1c). However, the previous studies in Refs. were focused only on conductance, whereas our purpose in this work is to investigate the complex transmission amplitude that contains the phase information as well as the magnitude.
Even the magnitude of the nonresonant transmission is in a different range from the corresponding values for a typical reference arm in Refs. 13, 14. We also emphasize that the term in \( W \) in Eq. (1) 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., \( \epsilon_{LR} = \epsilon_{RK} = \epsilon_k \)) with the density of states \( \rho \) at the Fermi energy. The direct tunneling matrix element \( W \) is in general complex number, \( W = |W|e^{i\phi} \), while the hopping matrix elements \( V_\alpha \) can be kept as positive real numbers without loss of generality. Then \( \phi \) stands for the phase difference between the resonant and the nonresonant component. We assume the TRS so that the phase \( \phi \) takes either 0 or \( \pi \). (In fact, the external magnetic flux penetrating the QD is only a very small fraction of the flux quantum in the experiment of Ref. [5, 6], and hence the TRS is well preserved.)

Using the relation between the scattering matrix and the local Green’s function [3], one can write the transmission amplitude of the electrons with energy \( \varepsilon \) from the left to right lead as

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

Here \( |t_b| \equiv 2x/(1 + x^2) \) with \( x = \pi \rho W \) is 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 \( \Gamma_{\text{eff}} \) 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 rule [3] gives an exact expression for \( G_d^R(\varepsilon) \) in terms of the occupation number of the dot, \( n_d \), leading to the relation

\[
t_{LR} = \frac{ie^{i\phi}|t_b|}{e_d - i} (e_d + Q); \tag{3a}
\]

\[
e_d = \cot (\pi n_d/2); \tag{3b}
\]

\[
Q = -\frac{|r_b|}{|t_b|}\cos \varphi + \frac{i}{|t_b|}\sin \varphi . \tag{3c}
\]

Equation (3) already provides some important informations. First, transmission zero takes place at \( \cot (\pi n_d/2) = \pm |r_b|/|t_b| \) for \( \varphi = 0, \pi \), 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, \( n_d \simeq 0 \) or \( n_d \simeq 2 \), for \( \varphi = 0 \) or \( \varphi = \pi \), respectively. In the opposite limit \( (|t_b| \simeq 1) \), \( t_{LR} \) goes to zero in the Kondo limit \( (n_d \simeq 1) \). This limit was investigated previously for a ballistic quantum wire coupled to a QD [17].

At finite temperatures, we need to take the thermal average of the transmission amplitude [18]:

\[
t_{LR}(\varepsilon) = \int \frac{\partial f}{\partial \varepsilon} t_{LR}(\varepsilon) d\varepsilon , \tag{4}
\]

where \( f \) denotes the Fermi distribution function.

For a quantitative study, we will adopt the slave-boson mean field theory (SBMFT) assuming \( U = \infty \) [19]. We will also do the numerical renormalization group (NRG) calculations to confirm the results from the SBMFT. The SBMFT satisfies the unitarity of the scattering matrix [17], which cannot be preserved in some other approaches based on the 1/Ns expansion (with \( N_s \) being the degeneracy of the level). After some algebra, we obtain the relation

\[
t_{LR}(\varepsilon) = \frac{ie^{i\phi}|t_b|}{e_d - i} (\tilde{e}_d + Q) , \tag{5a}
\]

\[
\tilde{e}_d \equiv \frac{\tilde{e}_d - \varepsilon}{(1 - n_d)\Gamma_{\text{eff}}} , \tag{5b}
\]

The renormalized energy level \( \tilde{e}_d \) 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 \( \varphi = 0 \) [20]. 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 Fig. 1(c) and (d). One can see clearly that while the magnitude

![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).]
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 sub-regions: the “unitary Kondo regime” ($T < T_0$), and the so-called “Fano-Kondo regime” ($T > T_0$) [21], see below 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 [22, 23], $|t_{LR}|$ ($|\Delta \gamma|$) changes from 0 to 1 ($\pi/2$) as $\varepsilon_d$ varies from the empty dot limit ($\varepsilon_d \gg \Gamma_{eff}$) to the singly occupied limit ($\varepsilon_d \ll -\Gamma_{eff}$).

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 $|t_b|^2$. There occurs an interference between the nonresonant transmission and the transmission through the Kondo resonance. 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 important; compare Figs. 1 (a) and (c). However, the phase shift ($\Delta \gamma$) is affected significantly by even a small value of $|t_b|$. As shown in Fig. 1 (b), the plateau of $\Delta \gamma$ as a function of $\varepsilon_d$ is lifted significantly from $\pi/2$ to a value close to $\pi$. This behavior is consistent with the experimental observation [4], but is in a 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 the nonresonant transmission can be a natural explanation observed in the experiment [4], that is, the phase evolution of about $\pi$ in the Kondo valley [21].

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 $\varepsilon_d$ varies from $\varepsilon_d \gg \Gamma_{eff}$ to $\varepsilon_d \ll -\Gamma_{eff}$ 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 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 $\pi$, since $t_b$ has pure imaginary value in the presence of TRS (i.e., $t_b = ie^{i\varphi}|t_b|$ and $\varphi = 0, \pi$).

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.

**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 like a Fermi liquid, we substitute

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

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

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

where

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

The integral in Eq. (3) can be calculated exactly with the help of contour integration [25], which leads in the limit of $T \gg T_K$ to the form

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

Inserting this expression into Eq. (4), one can find that the crossover from $\Delta \gamma = \pi/2$ to $\Delta \gamma = \pi$ takes place at $T \sim T_0$ such that

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

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

Equation (10) 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 (10) then estimates $T_0$. One has only to compare $\Delta \gamma$ as a function of $\varepsilon_d$ at $T \ll T_0$ and $T > T_0$. We add that $T_0$ is slightly overestimated in Eq. (10) since the Fermi liquid form has been used for estimation even at finite temperatures. The $\pi$-plateaus in the Fano-Kondo regime were observed experimentally [2, 4], 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.

In conclusion, we have theoretically explained 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 $\pi$, as long as the nonresonant transmission is small but finite.

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[20] In this work we mainly focus on the case of $\varphi = 0$. One can show that the Hamiltonian is invariant under the electron-hole transformation together with the change $\varphi = \pi \to 0$; i.e., the results for $\varphi = \pi$ can be deduced...
from those for $\varphi = 0$.

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