Theoretical Analysis of the Transmission Phase Shift of a Quantum Dot in the Presence of Kondo Correlations

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We study the effects of Kondo correlations on the transmission phase shift of a quantum dot coupled to two leads in comparison with the experimental determinations made by Aharonov-Bohm (AB) quantum interferometry. We propose here a theoretical interpretation of these results based on scattering theory combined with Bethe ansatz calculations. We show that there is a factor of 2 difference between the phase of the *S*-matrix responsible for the shift in the AB oscillations and the one controlling the conductance. Quantitative agreement is obtained with experimental results for two different values of the coupling to the leads.

Quantum dots (QD), small puddles of electrons connected to leads, can be obtained in a controlled fashion because of recent progress in nanolithography. Under certain conditions a dot can be modeled as a localized spin coupled to Fermi baths (the leads). A Kondo effect takes place [1–3] when the temperature is lowered. A key ingredient of the Kondo effect is the phase shift δ an electron undergoes when it crosses the dot. While its direct measurement was out of scope in bulk systems, it became feasible recently in quantum dots via Aharonov-Bohm (AB) interferometry [4]. We mention here the experimental results obtained in two cases corresponding to a strong coupling to the leads [4,5]. In the unitary limit, the phase shift climbs almost linearly with V_G with a value at the middle of the Kondo enhanced valley which is almost π. At a smaller value of the coupling strength, the phase shift develops a wide plateau at almost π. We call the latter case the "Kondo regime." Early theoretical work on the phase shift for the bulk Kondo effect [6,7] predicts $\delta = \pi/2$. In the context of QD, Gerland *et al.* [8] had obtained, on the basis of numerical renormalization group and Bethe ansatz calculations, a variation of δ with the energy of the localized state leading to a value of $\pi/2$ in the symmetric limit, in disagreement with the recent experimental results quoted above [4,5]. In this Letter, we propose a new theoretical interpretation of the experimental results based on scattering theory and Bethe ansatz calculations. Our main prediction concerns a factor of 2 difference found between the phase of the *S* matrix observed by the phase shift measurements and the phase governing the conductance.

Let us consider a quantum dot coupled via tunnel barriers to two leads *L* and *R*, and capacitively to a gate maintained at the voltage V_G. The system can be described [9,10] by a one-dimensional Anderson model with two reservoirs *L* and *R*,

$$H = -t \sum_\sigma \left[\sum_{i \geq 1} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) + \sum_{i \leq -2} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) \right]$$
$$- V_R \sum_\sigma (c_{0,\sigma}^\dagger c_{1,\sigma} + \text{H.c.}) - V_L \sum_\sigma (c_{-1,\sigma}^\dagger c_{0,\sigma} + \text{H.c.})$$
$$+ \varepsilon_0 \sum_\sigma n_{0\sigma} + U n_{0\uparrow} n_{0\downarrow}, \qquad (1)$$

Consider the elastic component of the *S* matrix, $\hat{S}_{k\sigma}$, describing the scattering of a spin-σ electron with momentum *k* off the impurity. It is given by [6,10,11] $\hat{S}_{k\sigma} = C_\sigma(\hat{I} - i\hat{T}_{k\sigma}^{\text{res}})$, where C_σ is a multiplicative phase factor and $\hat{T}_{k\sigma}^{\text{res}}$ is the T matrix with matrix elements given by

$$T_{k\sigma}^{\text{res},\alpha\beta} = 2\pi V_\alpha V_\beta \rho_\sigma(\varepsilon_k) \mathcal{G}_\sigma(\varepsilon_k + i\eta), \qquad (2)$$

where $\alpha, \beta = L$ or *R*, $\rho_\sigma(\varepsilon_k)$ is the density of states of conduction electrons for σ and ε_k, and $\mathcal{G}_\sigma(\varepsilon_k + i\eta)$ is the exact localized electron retarded Green's function. Using exact results [6,12] on the self-energy at $T = 0$ in an interacting Fermi liquid, one can show that $n_{0\sigma} = \frac{1}{\pi} \text{Im} \ln \mathcal{G}_\sigma(\mu + i\eta)$. Friedel's sum rule [12,13] requires $n_{0\sigma}$ to be equal to the change in the number of conduction electrons with spin σ resulting from the addition of the impurity. Hence it is related to the transmission phase shift δ_σ at the Fermi level, $n_{0\sigma} = \frac{1}{\pi} \delta_\sigma$. Therefore δ_σ coincides with the phase of the Green's function at the Fermi level $\mathcal{G}_\sigma(\mu + i\eta)$. If we denote the associated self-energy by $\sum_\sigma(\mu + i\eta)$, one gets $\mathcal{G}_\sigma(\mu + i\eta) = \sin\delta_\sigma e^{i\delta_\sigma}/ \text{Im}\Sigma_\sigma(\mu + i\eta)$. with $\text{Im}\Sigma_\sigma(\mu + i\eta) = -\pi(V_L^2 + V_R^2) \times \rho_\sigma(\mu)$ [6,12] at $T = 0$ leading to

$$T_{k_F\sigma}^{\text{res},\alpha\beta} = -2 \frac{V_\alpha V_\beta}{(V_L^2 + V_R^2)} \sin\delta_\sigma e^{i\delta_\sigma}. \qquad (3)$$

In the case of a symmetric QD with $V_L = V_R = V$, one has

$S_{k_F\sigma}^{LR} = S_{k_F\sigma}^{RL} = C_\sigma i \sin\delta_\sigma e^{i\delta_\sigma}$ and $S_{k_F\sigma}^{LL} = S_{k_F\sigma}^{RR} = C_\sigma \times \cos\delta_\sigma e^{i\delta_\sigma}$. The multiplicative phase factor C_σ contains additional information about the spectrum and the filling of the quantum dot. To determine it, we make use of Levinson's theorem [14,15]. In its original form, the theorem applies to the potential scattering of a particle in a given momentum l and relates the zero-energy phase shift δ_l to the number of bound states of the same l supported by the potential. It was generalized [16,17] later on to the case of the scattering of a particle by a neutral compound system as constituted, for instance, by an atom. In the present case of a QD, which can be viewed as an artificial atom, it follows that $\ln \det\hat{S}_{k_F\sigma}/(2i\pi)$ is equal to the total number of states, i.e., $\sum_\sigma n_{0\sigma} = n_0$. By applying generalized Levinson's theorem to $\hat{S}_{k_F\sigma}$, one finds $C_\sigma = e^{i\delta_{-\sigma}}$ and

$$\hat{S}_{k_F\sigma} = e^{i\delta}\begin{pmatrix} \cos\delta_\sigma & i\sin\delta_\sigma \\ i\sin\delta_\sigma & \cos\delta_\sigma \end{pmatrix}, \qquad (4)$$

where $\delta = \sum_\sigma \delta_\sigma$. One can easily check that, $\hat{S}_{k_F\sigma}$ being a unitary matrix, the optical theorem is fulfilled: $\hat{T}_{k_F\sigma}\hat{T}_{k_F\sigma}^\dagger = -2\,\mathrm{Im}\hat{T}_{k_F\sigma}$, where $\hat{T}_{k_F\sigma} = -i(\hat{I} - \hat{S}_{k_F\sigma})$.

In an open Aharonov-Bohm interferometry experiment [5], spin-σ electrons coming from the source through each of the two arms interfere coherently at the drain, leading to periodic oscillations of the differential conductance, the argument of which is given by $2\pi\Phi e/h + \delta_{QD}$. Φ is the magnetic flux and δ_{QD} is the transmission phase shift introduced by the QD, equal to $\delta = \pi n_0$ [cf. Eq. (4)]. In this Letter, we neglect the role of the reference arm on the phase shift considered by some authors [18] and concentrate on the contribution of the quantum dot to the interference pattern. The conductance through the QD is expressed by the Landauer formula [19,20], $G \propto \sum_\sigma |T_{k_F\sigma}^{LR}|^2$. Using Eq. (4), we get $G \propto \sum_\sigma \sin^2\delta_\sigma$. In the absence of magnetic field, $\delta_\uparrow = \delta_\downarrow = \delta/2$, one gets

$$G \propto \sum_\sigma \sin^2\delta/2. \qquad (5)$$

Because of recent developments in experimental techniques, one now disposes of simultaneous measurements of G and δ_{QD}. In this Letter we check the validity of the theoretical prediction of Eqs. (4) and (5) by reporting experimental results for G and δ_{QD} obtained in the unitary limit at different values of V_G. Before examining the experimental test, we make the following remarks: (i) in an interferometry experiment, only relative values of the transmission phase shifts can be measured. Hence we set $\delta = \pi$ at the location of the maximum of the visibility, evaluated to $V_G = 423$ mV. This implies a shift in the δ scale evaluated to $\Delta\delta = 0.29\pi$ with $\varphi = \delta + \Delta\delta$; (ii) typically the measurement of the conductance G is performed in a "one-arm" device (pinching off the reference arm with the barrier gate), whereas that of the visi-

bility is done in a "two-arm" device. As a result, while the evolution of the visibility with V_G mimics that of the conductance, the value of the former is shifted with respect to that of the latter, by $\Delta V_G = 15$ mV. Therefore we take the values of G at $(V_G - \Delta V_G)$, and of δ at V_G; (iii) the conductance is normalized by its maximum value at $V_G = 423$ mV. Taking all these points into account, the graph reported in Fig. 1 shows that the experimental dependence of $\sin^2\varphi/2$ with V_G reproduces that of the "shifted" conductance $G_{\exp}$ in a quite remarkable way, providing further support to the validity of Eqs. (4) and (5) [21].

We now want to evaluate n_0 in order to derive $\delta = \pi n_0$. Starting from Eq. (1), one can show [9] that only the symmetric linear combination of electrons couples to the localized state. Therefore if we are interested only in n_0, it is sufficient to study a single reservoir Anderson model with a hybridization potential $\tilde{V} = \sqrt{V_L^2 + V_R^2}$. We have solved the equations of the Bethe ansatz (BA) numerically at $T = 0$ [22–24]. This allows us to determine the value of n_0 as a function of the parameters of the Anderson model ε_0, V, and U. The three parameters enter through their ratios ε_0/U and Γ/U, where $\Gamma = \pi V^2\rho_0$. Denote by $n_0(\varepsilon_0, \Gamma/U)$ the value of n_0 for the corresponding values of the parameters. The following relation holds due to the particle-hole symmetry of the model [23]: $n_0(-(\varepsilon_0 + U), \Gamma/U) = 2 - n_0(\varepsilon_0, \Gamma/U)$. This automatically ensures $n_0(-U/2, \Gamma/U) = 1$ in the symmetric limit $\varepsilon_0 = -U/2$ whatever Γ/U is. Furthermore, it follows from the preceding relation that the study can be restricted to $-U/2 \leq \varepsilon_0 \leq U/2$ and the remaining part can be deduced from it. The results of the calculations are reported in Fig. 2(a). For strong coupling strengths $\Gamma/U \geq 0.25$, n_0 is found to climb almost linearly with $-(\varepsilon_0/U + 1/2)$, whereas for weak coupling strengths $\Gamma/U \leq 0.25$, the energy dependence of n_0 develops a plateau around $\varepsilon_0 = -U/2$. This
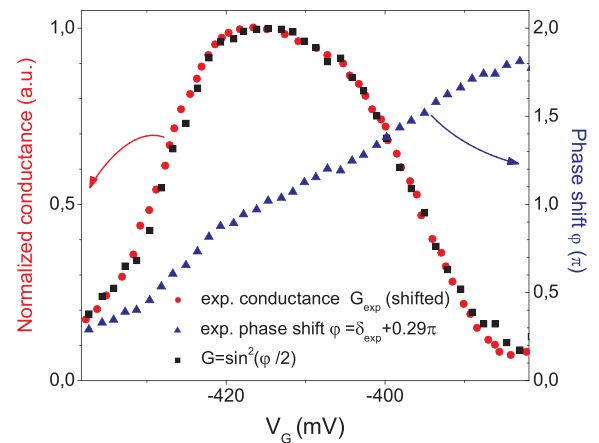

FIG. 1 (color online).   Experimental conductance $G_{\exp}(V_G)$ and phase shift $\varphi(V_G)$ as a function of V_G (values taken from Ref. [4]; cf. text). Comparison is made with the curve $G(V_G) = \sin^2[\varphi(V_G)/2]$.
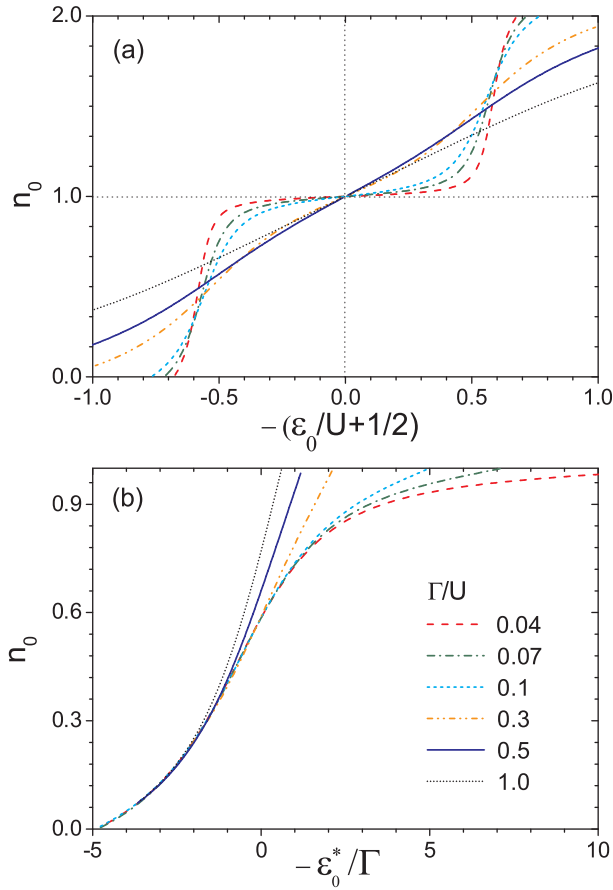
FIG. 2 (color online). (a) Theoretical results from the BA calculations for the occupation number n_0 as a function of the normalized energy $(-\varepsilon_0/U + 1/2)$ at different values of Γ/U. Note that $n_0 = 1$ at the symmetric limit $\varepsilon_0 = -U/2$ and the existence of a plateau in its vicinity when $\Gamma/U \leq 0.25$. (b) The same quantity as a function of the renormalized energy ε^*/Γ at different values of Γ/U.

change of behavior is due to the fact that the extent of the local moment regime (centered around $\epsilon_0 = -U/2$ with $n_0 \simeq 1$) increases when Γ/U decreases. As the temperature is lowered, the Kondo resonance develops through this local moment regime. This plateaulike structure can be viewed as the beginnings of the "staircase" variation of n_0 with ε_0 obtained in the localized regime $\Gamma/U \to 0$.

The experimental data can be fitted then with two parameters, Γ/U and ε_0/U. The value of ε_0 is governed by the strength of the gate voltage. Fitting the experimental data from results presented in Fig. 2(a) is a difficult task since one needs to fix the correspondence between ε_0/U and V_G on the one hand (we take it linear as usual, independent of the regime considered), and to find the best fitting value for Γ/U in the different regimes on the other hand. A valuable help for doing this is provided by taking advantage of some special properties of the Anderson model. These properties can easily be recognized when physical quantities such as n_0 are plotted as a

function of some renormalized energy defined as $\varepsilon^*/\Gamma = \varepsilon_0/\Gamma + g(U/\Gamma)$. In the asymmetric regime [24] when $(U + 2\varepsilon_0) \gg \sqrt{\Gamma U}$ and $|\varepsilon_0| \ll U$, $g[U/\Gamma]$ equals $\frac{1}{\pi} \times \ln(\pi e U/(4\Gamma))$ and the behavior of n_0 as a function of $-\varepsilon_0^*/\Gamma$ is universal [24,25]. This property is illustrated in Fig. 2(b). The universality is reached when $\Gamma/U \leq 0.25$ and the range of energy over which universal behavior extends is given by $|\varepsilon_0^*/\Gamma - 1/\pi \ln(\alpha U/\Gamma)| \ll U/\Gamma$. One can also see from Fig. 2(b) that in the empty level regime ($n_0 \to 0$), the curves $n_0 = f(\varepsilon_0^*/\Gamma, \Gamma/U)$ at various values of Γ/U merge, displaying an asymptotic behavior [26]. The existence of both these universal and asymptotic behaviors is of valuable help in fitting the experimental data. Figure 3 reports the results of the fit in the unitary limit and Kondo regimes. The experimental results incorporate a shift in the δ scale, $\varphi = \delta + \Delta\delta$ in order to get $\varphi = \pi$ at the symmetric limit. We establish the correspondence between V_G and ε_0/U by fitting the experimental data to the theoretical results in the empty level regime when all the curves merge. One finds $\Delta V_G/\Delta(\varepsilon_0/U)$ of the order of 30 mV in both of the regimes considered. The best fit is obtained for $\Gamma/U = 0.5$ in the unitary limit both below and above the symmetric limit, and for $\Gamma/U = 0.04$ or 0.07 in the Kondo regime (below or above the symmetric limit, respectively). Finally, by keeping the same correspondence between V_G and ε_0/U and using $\delta = \pi n_0$, we derive the dependence of the phase shift with V_G from results obtained in Fig. 2(a). As can been
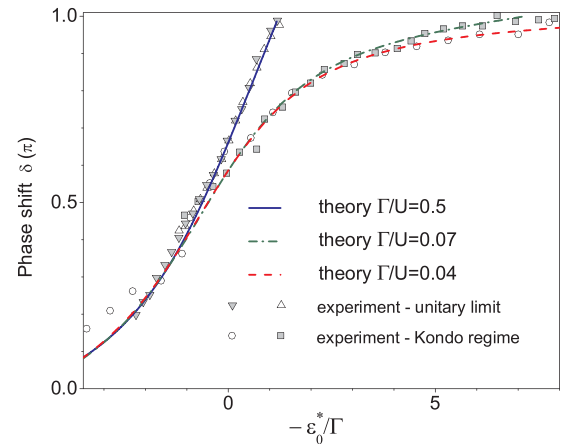

FIG. 3 (color online). Fit of the experimental data for the V_G dependence of the phase shift with the BA results for $\delta = \pi n_0$ as a function of $-\varepsilon_0^*/\Gamma$. Making use of the electron-hole symmetry, experimental results both below and above the symmetric limit are reported using the same scales. They are represented by triangles pointing down and up, respectively, in the unitary limit, and by circles and squares, respectively, in the Kondo regime (incorporating a shift in the δ scale; cf. text). The best fit is obtained for $\Gamma/U = 0.5$ in the unitary limit (both below and above the symmetric limit), and for $\Gamma/U = 0.07$ or 0.05 in the Kondo regime (below or above the symmetric limit, respectively).
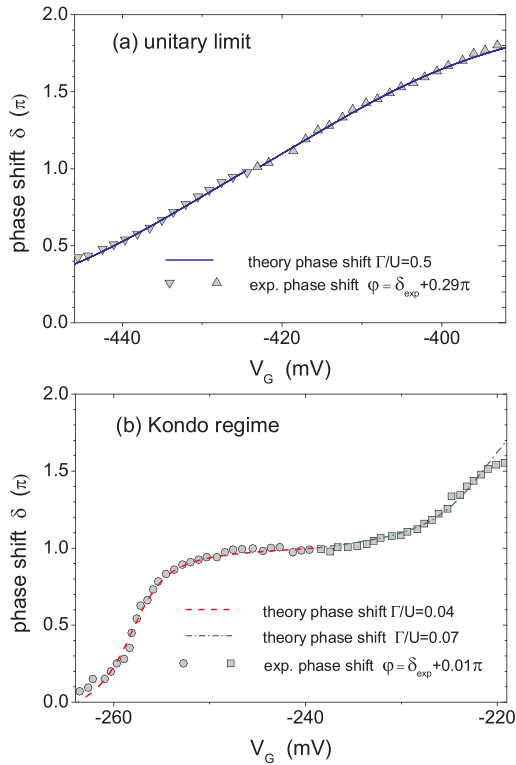
FIG. 4 (color online). Phase shift as a function of the gate voltage V_G. (a) Unitary limit. Theoretical results from Bethe ansatz calculations at $\Gamma/U = 0.5$ compared to the experimental data for $\varphi/\pi = \delta_{\exp}/\pi + 0.29$ (triangles pointing down and up). (b) Kondo regime. Same thing with $\Gamma/U = 0.04$ and 0.07, $\varphi/\pi = \delta_{\exp}/\pi + 0.01$ (circles and squares).

seen from Fig. 4, our theoretical predictions are in quantitative agreement with the experimental data. The fit is all the more remarkable that it is performed in the presence of a single fitting parameter Γ/U only.

In conclusion, we have proposed a theoretical analysis of the transmission phase shift of a quantum dot in the presence of Kondo correlations and confronted our results with the Aharonov-Bohm interferometry and conductance measurements. We have explained the presence of a factor of 2 difference between the total phase of the S-matrix (responsible for the shift in the AB oscillations), and the one appearing in the expression of the conductance $G \sim \sin^2(\delta/2)$. Our calculations based on Bethe ansatz lead to a remarkable quantitative agreement with experimental results. The whole discussion so far has been restricted to the low temperature regime. One of the next goals will be to include finite temperature effects as well as to study the role of a magnetic field and consider the out-of-equilibrium situation.

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