Kondo effect in real quantum dots

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Exchange interaction within a quantum dot strongly affects the transport through it in the Kondo regime. In a striking difference with the results of the conventional model, where this interaction is neglected, here the temperature and magnetic field dependence of the conductance may become non-monotonic: its initial increase follows by a drop when temperature and magnetic field are lowered.

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The conventional theory of the Kondo effect in tunneling is based on the Anderson impurity model \[2\]. The use of this model for describing the electron transport through a conducting grain was first suggested in \[3\]. In these applications, the quantum dot is modeled by one singly occupied energy level. The model predicts a monotonically increasing tunneling conductance with lowering the temperature and magnetic field. The conductance dependence on the magnetic field is also non-monotonic. Making it narrower, one pinches the last propagating mode near its pinch-off. Coulomb blockade develops when the resistivity of a bulk metal, are equivalent \[6\]. Well below the Kondo temperature, the scattering cross-section reaches the unitary limit; accordingly, \( G \) saturates at the level \( G \approx e^2/\pi \hbar \).

In a real quantum dot, the truncation of the spectrum to a single level is not always possible. For example, dots with ground state spin \( S > 1/2 \) are not described by the Anderson impurity model \[2\]. In this paper we demonstrate that in general the problem of transport through a dot does not map onto the problem of resistivity in a bulk metal. In the most interesting case, the tunneling conductance first rises and than drops when temperature is lowered. The conductance dependence on the magnetic field is also non-monotonic.

The confining potential forming a lateral quantum dot is smooth. The dot-lead junction is essentially an electron waveguide \[8\]. Making it narrower, one pinches the propagating modes off. Coulomb blockade develops when the last propagating mode is near its pinch-off. Therefore, for lateral dots in the Coulomb blockade regime the number of channels per junction is one.

We start with a discussion of the dependence of the zero-temperature conductance on the magnetic field applied in the plane of the dot. The in-plane field results in the Zeeman splitting \( B \) of the spin states of the dot, but barely affects the orbital degrees of freedom. At a finite \( B \), the ground state of the system is not degenerate; therefore, at \( T = 0 \) an electron experiences only potential scattering. The amplitudes of scattering \( S_{s,\alpha \alpha'} \) of electrons with spin \( s \) from lead \( a \) to lead \( a' \) form the scattering matrix (here \( a, a' = R \) or \( L \) for the right or left lead, respectively). It can be diagonalized by rotation in the \( R-L \) space to the new basis of channels \( a \) and \( b \),

\[
U S U^\dagger = \text{diag} \{ e^{2i\delta_s}, \} , \quad \gamma = a, b , \quad s = \pm 1 .
\]

Here \( U = \exp(i\varphi \tau^z) \exp(i\vartheta \tau^x) \), and \( \tau^z \) are the Pauli matrices acting in the \( R-L \) space (\( \tau^x = \tau^x + i\tau^y \) transforms \( L \to R \)). The parameters \( \vartheta \) and \( \varphi \) depend on the microscopic properties of the dot-lead junctions. The \( T = 0 \) conductance is given by the Landauer formula,

\[
G(T = 0) = \frac{e^2}{2\pi \hbar} \sum_s |S_{s,RL}^2| ,
\]

and can be expressed now in terms of the scattering phase shifts \( \delta_s \) at the Fermi level:

\[
\frac{G}{G_0} = \frac{1}{2} \sum_s \sin^2(\delta_{as} - \delta_{bs}) , \quad G_0 = \frac{e^2}{\pi \hbar} \sin^2(2\vartheta) .
\]

(note that the conductance is independent of \( \varphi \)).

In order to calculate the phase shifts, one needs to know the effective Hamiltonian \( \mathcal{H} \) of the system. Clearly, the term in it representing the interaction of itinerant electrons with the spin of the dot should obey the \( SU(2) \) symmetry,

\[
\mathcal{H} = \sum_{\gamma} \xi_k \psi^\dagger_{\gamma k} \psi \gamma_k + \sum_{\gamma} J_\gamma (\mathbf{s}_\gamma \cdot \mathbf{S}) - BS^2 ,
\]

where \( \mathbf{s}_\gamma = \sum_{kk' ss'} \psi^\dagger_{\gamma k} (\sigma_{ss'}/2) \psi_{\gamma k' s'} \) are local spin densities of itinerant electrons. The last term in \( \mathcal{H} \) describes the effect of the magnetic field. The Hamiltonian \[4\] does not include the potential scattering term; we defer the discussion of its role till later in the paper. The description by Eq. \[1\] is valid at energies below the energy gap \( \Delta \) for spin excitations in the dot, which is of the order of the single-particle level spacing in it. Note that the
symmetry allows for any signs of the exchange constants $J_a$. We will present a microscopic derivation of Eq. (4) towards the end of the paper.

Following [9], we remove the ambiguity in the definition of the phase shifts by fixing $\delta_{a} = 0$ at $J_a = 0$; then $|\delta_{a,b}| \leq \pi/2$ at any $J_a$. Furthermore, the invariance of the Hamiltonian [9] with respect to the particle-hole transformation, $\psi_{\gamma}^{\dagger} \rightarrow \psi_{\gamma-k}^{\dagger}$, yields the relation $S_a S_a = 1$ for the scattering matrix, which allows us to represent the phase shifts as

$$\delta_{a} = -s_\gamma, \quad 0 \leq \delta_a \leq \pi/2.$$  

(5)

Substitution into Eq. (3) then gives

$$G/G_0 = \sin^2(\delta_a - \delta_b).$$  

(6)

In order to find $\delta_a$ at $B = 0$, we need to invoke the properties of the ground state of the Kondo model. We start with $S > 1/2$ on the dot. In the case of an antiferromagnetic exchange in a channel, $J_a > 0$, the itinerant electrons participate in the screening of the localized spin, thus reducing its value by 1/2. By the Friedel sum rule, the corresponding phase shift $\delta_a = \pi/2$. The channels with the ferromagnetic coupling to the localized spin, $J_a < 0$, decouple at low energies, and $\delta_a = 0$. It is then clear from Eq. (4) that for $S > 1/2$ the conductance at $T = 0$ and $B = 0$ is enhanced due to the Kondo effect only if the two exchange constants have opposite signs.

At $S = 1/2$ the enhancement of the conductance occurs also if both exchange constants are positive. Indeed, the local spin is screened by the channel, say $a$, with the larger exchange constant, so that $\delta_a = \pi/2$. The other channel decouples [10] at low energies, and $\delta_b = 0$. Note that in the special case $J_a = J_b$ the conductance across the dot is zero, which is obvious from the rotational symmetry in the $R - L$ space, existing in this case.

There is no mapping between the Kondo problems for tunneling and for scattering in the bulk, except if one of the exchange constants in Eq. (4) is zero. However, if the constants are finite and have opposite signs (or both are positive at $S = 1/2$), the conductance behavior is qualitatively similar to the conventional [9] one: $G(T)$ and $G(B)$ increase monotonously when $T$ and $B$ are lowered, eventually saturating at the value $G \sim e^2/\pi h$. If both coupling constants are negative (fully ferromagnetic exchange interaction) there is no Kondo effect: $G$ decreases when $T$ and $B$ are lowered.

We concentrate now on the most interesting case of the antiferromagnetic coupling, $J_a \geq J_b > 0$, and spin $S \geq 1$. In this case, the Kondo effect manifests itself in a peculiar way: the field and temperature dependence of $G$ is not monotonic, which differs qualitatively from the conventional picture. Here we present a detailed analysis only of the dependence $G(B)$ at $T = 0$.

Finite field leads to deviations from the unitary limit $\delta_{a,b} = \pi/2$. The magnitude of the deviations is controlled by two parameters, $B/T_a$ and $B/T_b$, where $T_a \geq T_b$ are the Kondo temperatures corresponding to the two exchange constants. For $S = 1$ and $B = 0$ the dot’s spin is screened completely. If the Zeeman energy is small, $B \ll T_b$, then the phase shifts are calculated by a straightforward application of the Fermi-liquid technique [2][4], and we find from Eq. (3)

$$G = G_0 \left( \frac{B}{T_a} - \frac{B}{T_b} \right)^2.$$  

(7)

For $S > 1$ the screening is incomplete: at the fixed point $\delta_{a,b} = \pi/2$, and the remaining localized spin is $(S - 1)$. The fixed point is reached at $B = 0$, and the approach to it is governed by the ferromagnetic interaction of the remaining spin with itinerant electrons [9]. The corresponding corrections can be calculated with the logarithmic accuracy [1], yielding the asymptote of the conductance in the regime $B \ll T_b$,

$$G = \frac{\pi^2}{4} (S - 1)^2 \left[ \frac{1}{\ln(B/T_a)} - \frac{1}{\ln(B/T_b)} \right]^2.$$  

(8)

In the weak coupling regime, $B \gg T_a$, one readily obtains for arbitrary $S \neq 0$ (also with logarithmic accuracy)

$$G/G_0 = \frac{\pi^2}{4} S^2 \left[ \frac{1}{\ln(B/T_a)} - \frac{1}{\ln(B/T_b)} \right]^2.$$  

(9)

The asymptotes [6], [7] and [9] clearly demonstrate that the dependence of $G(B)$ is non-monotonous with a maximum at $B = T_0$ where $T_b \leq T_0 \leq T_a$. This maximum can be studied in detail if $T_b \ll T_a$. In this case, the intermediate ($T_b \ll B \ll T_a$) asymptote for $G(B)$ is

$$G = 1 - \frac{\pi^2}{4} (S - 1/2)^2 \left[ \frac{1}{\ln(B/T_a)} - \frac{1}{\ln(B/T_b)} \right]^2,$$  

(10)

and it displays maximum at $T_0 = \sqrt{T_a T_b}$. The conductance is expected to be featureless in the crossover regions ($B \sim T_a$ or $B \sim T_b$). The dependence of the conductance on the magnetic field is shown schematically in Fig. 1. It can be cast into the form

$$G = G_0 F_S (B/T_a, B/T_b).$$  

(11)

The asymptotes of $F_S$ are given in Eqs. [10]-[11].

The dependence of the conductance on temperature $G(T)$ is very similar to $G(B)$. The asymptotes for $G(T)$ in the leading logarithmic approximation can be obtained from Eqs. [7]-[10] by replacing $B \rightarrow T$ and, in addition to it, $(S - 1)^2 \rightarrow S(S - 1)$, $S^2 \rightarrow S(S + 1)$, and $(S - 1/2)^2 \rightarrow S^2 - 1/4$ in Eqs. [7], [8], and [9], respectively. The asymptote for $G(T)$ in the Fermi liquid regime ($S = 1$, $T \ll T_b$) follows from Eq. (9) after the substitution $B \rightarrow \pi T$. The derivation of these asymptotes is straightforward, but rather lengthy [9], since the conductance at a finite temperature is not expressed via elastic scattering phase shifts [cf. Eq. (8)].
For the model described by Eq. (4) conductance \( G \) vanishes in the limit \( J_\gamma \to 0 \). Yet, it is well-known that \( G \) may remain finite even in this limit due to the cotunneling processes, not involving the spin degrees of freedom [10]. These processes are described by adding to the Hamiltonian (4) a potential scattering term \( V_{\gamma} \). The combination of the Kondo and potential scattering yields

\[
G = G_0 F_S \left( B/T_a, B/T_b \right) + G_{el}, \tag{12}
\]

instead of Eq. (11). Here we sketch the derivation of Eq. (12) for a simplified model in which \( H_V \) is diagonal in the \( a - b \) basis,

\[
H_V = \sum_{\gamma} V_\gamma \sum_{kk',ss} \psi_\gamma^{k's} \psi_\gamma^{ks}, \tag{13}
\]

(the general case will be discussed elsewhere [11]). Potential scattering results in finite phase shifts, \( \delta_{\gamma,s} = \delta_{\gamma}^s \), at \( J_\gamma = 0 \); the corresponding elastic cotunneling conductance is \( G_{el} = G_0 \sin^2(\delta_{\gamma}^0 - \delta_{\gamma}^0) \), see Eq. (10). In order to consider now \( J_\gamma \neq 0 \), one can rewrite the Hamiltonian \( H + H_V \) in the new basis [12], which accounts for the phase shifts \( \delta_{\gamma}^s \). In this basis, the Hamiltonian again assumes the form of Eq. (10), but with the modified exchange constants \( \tilde{J}_\gamma = J_\gamma \cos^2 \gamma_s^0 \), which define new Kondo temperatures \( \tilde{T}_\gamma \). The phase shifts with respect to the new basis are \( \tilde{\delta}_{\gamma}^s = -s\tilde{\delta}_{\gamma}^s \) [cf. Eq. (10)]. The phase shifts \( \delta_{\gamma}^s \) depend on the magnetic field \( B \) via two parameters, \( B/T_a \) and \( B/T_b \). Returning to the original basis, one finds \( \tilde{J}_\gamma \) for the phase shifts \( \delta_{\gamma,s} = \delta_{\gamma}^0 - s\tilde{\delta}_{\gamma}^s \). Substitution of \( \delta_{\gamma,s} \) into Eq. (10) then yields Eq. (12) with \( \tilde{G}_0 = G_0 - 2G_{el} \). Microscopic calculation [12] performed for two specific models, the Anderson model and the model of almost open dot-lead junctions [13], gives \( \tilde{G}_0 \geq 0 \).

So far, we assumed that both exchange constants \( J_\gamma \) in the Hamiltonian (4) differ from zero. Such an assumption was made in a number of papers, see, e.g., Ref. [14]. However, if a quantum dot is modelled by the Anderson impurity [15], then the corresponding effective Hamiltonian (4) inevitably has only one non-zero exchange constant [15]. We will demonstrate now that in fact both exchange constants are finite, if Eq. (4) is derived directly from a generic model of a quantum dot. The microscopic Hamiltonian of the system consists of the part describing the free electrons in the leads:

\[
H_l = \sum_{\alpha k s} \xi_{\alpha k} \bar{c}^{\dagger}_{\alpha k s} c_{\alpha k s}, \quad \alpha = R, L, \tag{14}
\]

the tunneling part:

\[
H_t = \sum_{\alpha n k s} \left( t_{\alpha n} c^{\dagger}_{\alpha k s} d_{n s} + t^{*}_{\alpha n} d^{\dagger}_{n s} c_{\alpha k s} \right), \tag{15}
\]

and the Hamiltonian of the dot:

\[
H_d = \sum_{n s} \epsilon_n d^{\dagger}_{n s} d_{n s} + H_{int}. \tag{16}
\]

The first term in the r.h.s. of Eq. (14) is the single-particle part of \( H_d \). The second term, \( H_{int} \), represents the electron-electron interaction within the dot. Extensive numerical renormalization group calculations based on such a model were performed in Ref. [16], where a non-monotonic temperature dependence of the conductance was found for a special choice of \( H_{int} \) and \( t_{\alpha n} \). However, the study [13] did not reveal the two-stage character of the Kondo screening, which shows that the non-monotonic behavior is a general feature, rather than a result of model assumptions.

Hamiltonian \( H_d \) commutes with the total number of electrons in the dot, \( N = \sum_{n s} d^{\dagger}_{n s} d_{n s} \), and with its total spin, \( \mathbf{S}_{\text{tot}} = \sum_{n s} d^{\dagger}_{n s} c_{n s} \sigma_{n s} \) (we neglect the weak spin-orbit interaction here). The ground state of \( H_d \) is characterized by the number of electrons \( N \) and by spin \( S \). In the absence of the magnetic field, the ground state is \( (2S + 1) \)-fold degenerate and SU(2)-symmetric. This can be represented by introduction of the operator of spin of the dot in the ground state [cf. Eq. (10)],

\[
\mathbf{S} = \mathcal{P} \hat{\mathbf{S}}_{\text{tot}} \mathcal{P}, \tag{17}
\]

where \( \mathcal{P} \) is the projector onto the ground state manifold.

Tunneling Hamiltonian \( H_t \) mixes the ground state with the states having \( N = 1 \) electrons on the dot. For brevity we assume that the dot is tuned to the middle of the Coulomb blockade valley, i.e., its energy is increasing by the same amount \( E_C \) if the number of electrons is changed by \( \pm 1 \). The energy deficit \( E \sim E_C \) for the corresponding transitions is high, which allows us to apply the second-order perturbation theory in \( H_t \) (Schrieffer-Wolff transformation). The resulting effective Hamiltonian, which is valid at energies less than the gap for intra-dot spin excitations \( \Delta \ll E_C \), has the form

\[
H = H_l + \frac{4}{E_C} \sum_{\alpha \alpha' m n} t_{\alpha m}^{*} t_{\alpha' n} (s_{\alpha \alpha'} \cdot \mathcal{P} \hat{\mathbf{S}}_{mn} \mathcal{P}), \tag{18}
\]

where

\[
s_{\alpha \alpha'} = \sum_{k k' s s'} \bar{c}_{\alpha k s}^{\dagger} \sigma_{s s'} c_{\alpha' k' s'}, \quad \mathbf{S}_{mn} = \sum_{s s'} d^{\dagger}_{m s} \sigma_{s s'} d_{n s'}. \]
In the derivation of (18) we have neglected the potential scattering terms associated with the elastic cotunneling.

By SU(2) symmetry, the operators $\mathcal{P}S_{m'n'}\mathcal{P}$ for any $m$ and $n$ should be proportional to $S$ given by Eq. (17):

$$\mathcal{P}S_{m'n'}\mathcal{P} = \Lambda_{mn}S.$$  

This allows us to rewrite Eq. (18) as

$$H = H_{1} + \sum_{\alpha\alpha'} J_{\alpha\alpha'}(s_{\alpha} \cdot s_{\alpha'}),$$

where the matrix of the exchange constants is

$$J_{\alpha\alpha'} = \frac{4}{E_{C}} \sum_{m'n'} t_{\alpha m}^{*} t_{\alpha'n} \Lambda_{mn}.$$  

Note that the factors $t_{\alpha m}$ here depend on the properties of the tunneling junctions, whereas $\Lambda_{mn}$ characterize the ground state of the isolated dot, and depend on the electron-electron interaction term $H_{\text{int}}$ in Eq. (14).

We can diagonalize matrix $J_{\alpha\alpha'}$, and thereby bring the Hamiltonian (21) to the form of Eq. (1). To do that, we perform the unitary transformation $\psi' = \sum_{\alpha} U_{\alpha\alpha'} \psi_{\alpha}$, where $U_{\alpha\alpha'}$ is the same unitary matrix as in Eq. (1). The eigenvalues of the matrix $J_{\alpha\alpha'}$ are $J_{a}$ and $J_{b}$ of Eq. (1).

The matrix $\Lambda_{mn}$ of Eq. (19) obviously satisfies the relations $\Lambda = \Lambda^{\dagger}$ and $\text{Tr} \Lambda = 1$. For a generic choice of the tunneling amplitudes $t_{\alpha m}$ these conditions alone fix neither the signs nor the magnitudes of the exchange amplitudes $J_{\gamma}$. To make further progress one has to rely upon assumptions regarding the form of $H_{\text{int}}$ in (16).

Although model realizations yielding any desired sign of $J_{\gamma}$ can be easily constructed [13], here we consider only the simplest example,

$$H_{\text{int}} = E_{C}(\hat{N} - N)^{2} - E_{S}S_{\text{tot}}^{2},$$

which nevertheless results in the most interesting case $J_{\gamma} > 0$, $S \geq 1$. The parameter $E_{S}$ characterizes the strength of the intradot exchange interaction; $E_{S}$ is of the order of the single-particle level spacing in the dot. In the middle of the Coulomb blockade valley, the dimensionless gate voltage $\hat{V}$ is an integer, so the dot in the ground state has $N = \hat{N}$ electrons. The model (23) is fully justified [14] only for large dots with chaotic single-particle states; the relative magnitude of terms which are not included in Eq. (22), is $\sim N^{-1/4} \ll 1$ (we assume here ballistic motion of electrons within the dot).

For the Hamiltonian (14), (22), occupations of the single-particle energy levels are good quantum numbers. In the ground state with spin $S$, there are $2S$ singly occupied energy levels, while all other levels are either empty or are occupied by a pair of electrons with opposite spins. The matrix $\Lambda$ is diagonal, and its only non-zero elements are the ones corresponding to the singly occupied levels, $\Lambda_{mn} = (1/2S)\delta_{mn}$. Using Eq. (21), it is easy to calculate the determinant of the matrix $J_{\alpha\alpha'}$:

$$J_{a}J_{b} = \frac{2}{E_{C}S^{2}} \sum_{m,n=1}^{2S} \left| (t_{Lm} t_{Rn} - t_{Rm} t_{Ln})^{2} \right|. \quad (23)$$

For $S > 1/2$ the sum in the r.h.s. here contains terms with $m \neq n$. For a generic choice of tunneling amplitudes, these terms are positive, and $J_{a}J_{b} > 0$. The trace of $J_{\alpha\alpha'}$,

$$J_{a} + J_{b} = \frac{2}{E_{C}S} \sum_{\alpha} \sum_{m=1}^{2S} |t_{\alpha m}|^{2}, \quad (24)$$

is also positive. Therefore, eigenvalues $J_{a,b}$ are positive, and at $S > 1/2$ both channels are coupled to the dot via antiferromagnetic exchange interaction.

In the case of model interaction (23) and the dot spin $S = 1/2$, only one discrete level is singly occupied. Then Eqs. (23) and (24) yield $J_{a} > 0$ and $J_{b} = 0$, just like in the Anderson model. Accounting for corrections to the Hamiltonian (23) results in finite values of both constants, $|J_{b}| \sim J_{a}N^{-1/4}$.

The two characteristic temperatures, $T_{a}$ and $T_{b}$, should be of the same order to allow for an observation of the predicted here non-monotonic temperature dependence $G(T)$. Because of the exponential dependence of $T_{a,b}$ on the corresponding exchange constants, the two temperatures are very sensitive to the values of the tunneling amplitudes for specific discrete levels, see Eqs. (23), (24), and (26); these values hardly can be predicted in advance. However, one can tune the amplitudes by applying a weak magnetic field perpendicular to the plane of the dot. (It is sufficient to thread about one flux quantum through the area of the dot [17]; in the case of GaAs, such a field has a negligible Zeeman effect.) The continuous tuning should allow one to go from a conventional manifestation [18] of the Kondo effect at $T_{b} \ll T_{a}$, to a non-monotonic $G(T)$ at $T_{b} \lesssim T_{a}$, to a total suppression of the Kondo contribution to the conductance at some value of the field, where $T_{b} = T_{a}$ [15].

To conclude, in this paper we considered electron transport through lateral quantum dots. We predict that if the spin of the dot $S > 1/2$, then the dependence of conductance on temperature and in-plane magnetic field is non-monotonic. This work was supported by NSF Grant DMR-9731756.

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[18] Tunneling amplitudes can be controlled without the use of a magnetic field in quantum dot systems of special geometry, such as two quantum dots connected in series.