

## Quantum Phase Transition in a Multilevel Dot

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We discuss electronic transport through a lateral quantum dot close to the singlet-triplet degeneracy in the case of a *single* conduction channel per lead. By applying the numerical renormalization group, we obtain rigorous results for the linear conductance and the density of states. A new *quantum phase transition* of the Kosterlitz-Thouless-type is found, with an exponentially small energy scale  $T^*$  close to the degeneracy point. Below  $T^*$ , the conductance is strongly suppressed, corresponding to a universal dip in the density of states. This explains recent transport measurements.

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**Introduction.**—In the past few years semiconductor quantum dots have gained considerable attention as tunable magnetic impurities [1]. Because of their small size electronic transport is strongly influenced by Coulomb blockade [2]. A well-known many-body phenomenon, the *Kondo effect*, was found in quantum dots [3] with an odd electron number, as predicted earlier [4]. In these systems, a single unpaired spin is screened at low temperatures, giving rise to an enhanced conductance at low bias.

Remarkably, a similar conductance enhancement was recently also observed for an *even* number of electrons both in vertical [5] and lateral [6] GaAs quantum dots. This can be understood by taking into account the strong intradot electronic exchange coupling [7] which is ferromagnetic, similar to Hund's rule in atomic physics. Tuning of the level spacing by an external magnetic field then induces a singlet-triplet transition in the ground state. This additional degeneracy leads to the enhanced conductance at low temperature [8–10].

Model calculations for the singlet-triplet transition, except [10], have so far mainly considered the case where the orbital quantum number characterizing the levels in the dot is also present in the leads. In particular, two conduction channels per lead have been taken into account. While this is appropriate for vertical devices [5], recent measurements on lateral quantum dots [11] suggest an interpretation in terms of a *single conduction channel per lead*, i.e., strong orbital mixing. In the following, we focus on this situation.

Our main tool of analysis is Wilson's numerical renormalization group (NRG) [12], a nonperturbative approach to quantum impurity systems. In contrast to mean-field or scaling calculations, this method does not rely on any assumptions regarding the ground state or leading divergent couplings. We find that this is crucial in the present analysis.

**The model.**—We consider a two-level Anderson impurity model as shown in Fig. 1. The Hamiltonian  $H = H_L + H_R + H_D + H_T$  contains two leads  $H_r = \sum_{kr} \epsilon_{kr} a_{k\sigma r}^\dagger a_{k\sigma r}$  with  $r = L/R$ . The isolated dot is described by

$$H_D = \sum_{n\sigma} \epsilon_{dn} d_{n\sigma}^\dagger d_{n\sigma} + JS_1 S_2 + E_C(N - \mathcal{N})^2, \quad (1)$$

where  $n = 1, 2$  denotes the two levels,  $N = \sum_{n\sigma} d_{n\sigma}^\dagger d_{n\sigma}$  is the total number of electrons occupying the dot, and  $S_n = (1/2) \sum_{\sigma\sigma'} d_{n\sigma}^\dagger \sigma_{\sigma\sigma'} d_{n\sigma'}$  are the spins of the two levels. Furthermore, we have introduced the *charging energy*  $E_C$  and an exchange coupling  $J$  which arises due to Hund's rule. We choose  $\mathcal{N} = 2$  in order to achieve double occupancy of the dot. Through the energies  $\epsilon_{dn}$  the level spacing  $\Delta\epsilon = \epsilon_{d1} - \epsilon_{d2}$  as well as the precise position in the Coulomb blockade valley can be tuned. Experimentally,  $\mathcal{N}$  depends on the gate voltage, while  $\Delta\epsilon$  is controlled by an external magnetic field. As a consequence of Hund's rule, the intradot exchange is ferromagnetic ( $J < 0$ ). Therefore, for  $\Delta\epsilon = -J/4$  the three triplet configurations  $|1, 1\rangle = d_{11}^\dagger d_{21}^\dagger |0\rangle$ ,  $|1, 0\rangle = (1/\sqrt{2}) \times (d_{11}^\dagger d_{21}^\dagger + d_{11}^\dagger d_{21}^\dagger) |0\rangle$ ,  $|1, -1\rangle = d_{11}^\dagger d_{21}^\dagger |0\rangle$ , and the singlet  $|0, 0\rangle = d_{21}^\dagger d_{21}^\dagger |0\rangle$  are degenerate. Motivated by the small  $g$ -factor in GaAs [5], we neglect the Zeeman splitting of the triplet states.

Finally, tunneling between the dot and leads is modeled by  $H_T = \sum_{k\sigma nr} (V_{nr} a_{k\sigma r}^\dagger d_{n\sigma} + \text{H.c.})$  where we neglect the energy dependence of the tunneling matrix elements

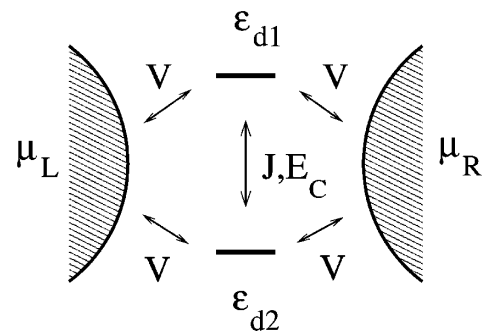


FIG. 1. Two-level quantum dot (1) with single-channel leads (chemical potentials  $\mu_L$  and  $\mu_R$ ).  $V$  denotes the tunneling matrix element between the dot levels and the leads.

$V_{nr}$  and in the following take them to be symmetric and identical for both levels; that is,  $V_{nr} = V$ . The intrinsic linewidth of the dot levels due to tunnel coupling to the leads is  $\Gamma = \Gamma_L + \Gamma_R$  with  $\Gamma_{L/R} = 2\pi|V|^2 N_{L/R}$ , where  $N_{L/R}$  is the density of states in the leads. This model has been studied before [13] without discovering the quantum phase transition we describe in this Letter.

*Transmission probability.*—We are interested in calculating electronic transport through the dot (1) close to the singlet-triplet transition. To this end, we use the generalized Landauer formula [14]

$$I = \frac{2e}{h} \int d\omega [f(\omega - \mu_L) - f(\omega - \mu_R)] T(\omega) \quad (2)$$

with the Fermi function  $f(\omega)$  and the transmission coefficient

$$T(\omega) = - \sum_{n,n',\sigma} \frac{\Gamma^L \Gamma^R}{\Gamma^L + \Gamma^R} \text{Im} G_{nn'\sigma}(\omega). \quad (3)$$

Here we have introduced the retarded dot Green's functions  $G_{nn'\sigma}(t) = -i\theta(t)\langle\{d_{n\sigma}(t), d_{n'\sigma}^\dagger\}\rangle$ . In the following we focus on the low bias regime, where  $T(\omega)$  can be evaluated in equilibrium, using the numerical renormalization group. For a detailed description of this technique, see Ref. [12]. Note that the equilibrium transmission  $T(\omega)$  also yields an approximation to the differential conductance  $dI/dV$  at finite bias.

In Fig. 2 we show results for the transmission as a function of the level spacing  $\Delta\epsilon$ , corresponding to a variation of the external magnetic field in the experiment. Our unit is the half bandwidth  $D$  of the conduction electrons. For  $\Delta\epsilon/D \lesssim 0.5$ , both orbitals are equally occupied and the dot is in a triplet state ( $S = 1$ ). Because of the hybridization with the leads, this local spin is partially screened,

giving rise to the Kondo resonance shown in Fig. 2 for  $\Delta\epsilon/D = 0.3$ . Note the unusual shape of this peak, which is due to the “underscreening” of the local moment—a free spin 1/2 remains present in the ground state [15] and leads to logarithmic corrections to Fermi-liquid behavior. Nevertheless, as for the spin 1/2 Kondo effect, the transmission reaches the unitary limit at low temperatures. Because of systematic numerical errors in the NRG calculation, this limit is underestimated by about 10%.

In the regime  $\Delta\epsilon/D \gtrsim 0.5$ , both electrons occupy the lower dot level and the ground state is a singlet. Remarkably, in this case a *pronounced dip* arises *within the Kondo peak*, leading to a strongly reduced transmission at low energy. The residual value  $T(0)$  is independent of  $\Delta\epsilon$  and is determined by the position in the Coulomb blockade valley. In particular, it vanishes in the center of the valley where  $\epsilon_{d1} = -\epsilon_{d2}$ .

In order to demonstrate clearly the importance of the number of conduction channels, we show results for the case of two transmission channels onto the dot (1) in the inset in Fig. 2. In this case, the local spin is always completely screened by the leads. One obtains a conventional Zeeman-type splitting of the conductance peak due to the energy difference between singlet and triplet. The sharp dip described above does not occur here and is thus *characteristic for the single channel situation*.

We find that for small level spacing the dip has a *universal scaling form* which is completely determined by its width  $\omega^*$ . This can be seen more clearly in Fig. 3, where we focus on the singlet side close to the transition. The scaling curve is extracted in the inset.

*Linear conductance.*—Using the current formula (2), we now determine the behavior of the conductance as a function of temperature. Results are shown in Fig. 4. In

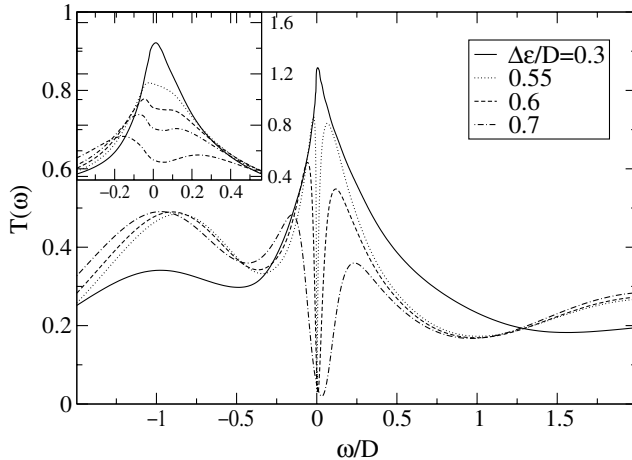


FIG. 2. Transmission coefficient at zero temperature for different level spacings  $\Delta\epsilon = \epsilon_{d1} - \epsilon_{d2}$  at  $\mathcal{N} = 2$ ,  $E_C/D = 1$ ,  $\epsilon_{d1}/D = 1$ ,  $\Gamma = 0.57D$ , and  $J/D = -2$ . The bandwidth is given by  $2D$ . Inset: For comparison, we show the transmission in the case of two conduction channels per lead, identical dot parameters,  $\Gamma = 0.28D$  and  $\Delta\epsilon/D = 0.4, 0.5, 0.55, 0.6, 0.7$  (from top to bottom).

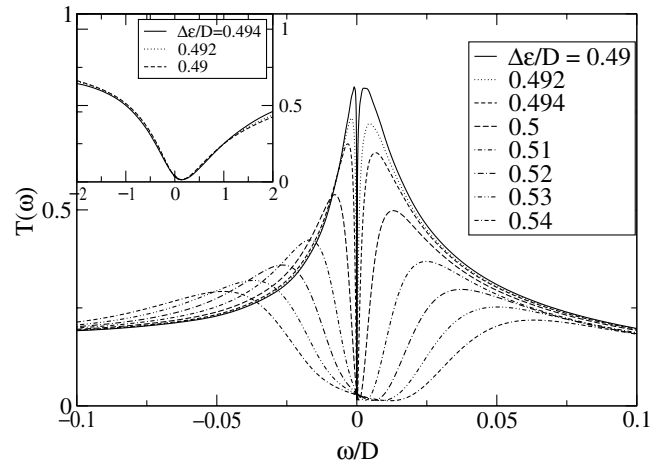


FIG. 3. Scaling of the dip at zero temperature. Parameters are chosen as in Fig. 2, but with a smaller broadening  $\Gamma = 0.25D$ . Note the “pinning” of the transmission at  $\omega = 0$ . Inset: Rescaled dip  $T(\omega/\omega^*)$  for parameter values close to the transition. The curves collapse onto a universal scaling function with a single parameter  $\omega^*$  (dip width).

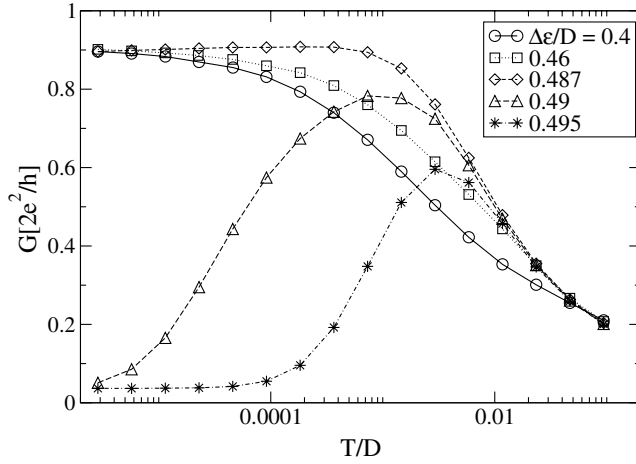


FIG. 4. Linear conductance for identical parameters as in Fig. 3 in three different regimes: on the triplet side ( $\Delta\epsilon/D = 0.4, 0.46$ ), at the transition ( $\Delta\epsilon/D = 0.487$ ), and on the singlet side ( $\Delta\epsilon/D = 0.49, 0.495$ ).

the triplet regime, upon lowering of the temperature, the conductance rises monotonously up to the unitary limit due to the partial screening of the local spin  $S = 1$ . Note that the associated Kondo temperature  $T_K$  is extremely low. This may be the reason why the triplet Kondo effect has so far not been observed experimentally, though some indications have been seen in Ref. [5]. Close to the singlet-triplet transition,  $T_K$  is strongly enhanced. On the singlet side, we find a “bump”-type behavior of the conductance when  $T$  is lowered: After an initial rise due to the Kondo effect,  $G(T)$  decreases strongly at  $T \lesssim T^*$ , with a small residual value for  $T \rightarrow 0$  determined by the position in the Coulomb blockade valley. Note that, as the increase, the decrease of  $G(T)$  is logarithmic, indicating a *two-stage Kondo effect*. In particular, the  $T \rightarrow 0$  behavior of  $G(T)$  is again universal and can be characterized by a single fit parameter  $T^* \sim \omega^*$ .

*Quantum phase transition.*—Here we present a physical explanation of the above results. It had been suggested earlier [16] that the singlet-triplet degeneracy of the dot can be parametrized in terms of a two-spin  $S = 1/2$  Kondo model. Formally, this is achieved by performing a Schrieffer-Wolff projection [17] of our two-level Anderson Hamiltonian on the (almost) degenerate subspace spanned by the four states  $|0, 0\rangle$ ,  $|1, 1\rangle$ ,  $|1, 0\rangle$ , and  $|1, -1\rangle$ . One obtains an effective Hamiltonian of the following form:

$$H_{\text{eff}} = H_L + H_R + J_1 \tilde{S}_1 s + J_2 \tilde{S}_2 s + I \tilde{S}_1 \tilde{S}_2, \quad (4)$$

where both Kondo spins are coupled to the same conduction channel  $s \equiv (1/2N) \sum_{kk'} a_{k\sigma}^\dagger \sigma_{\sigma\sigma'} a_{k'\sigma}$ . Here,  $N$  is the number of  $k$  states in the leads and we have already taken a symmetric combination of left and right leads according to  $a_{k\sigma} = (a_{k\sigma L} + a_{k\sigma R})/\sqrt{2}$ . Additional potential scattering terms have been neglected. Note that the  $\tilde{S}_1$ ,  $\tilde{S}_2$  introduced above are fictitious spins, different from the original levels.

To leading order, the parameters in (4) are given by the following expressions (note that  $V \sim 1/\sqrt{N}$ ):

$$J_{1(2)} = 2NV^2 \left( \frac{1 \mp \sqrt{2}}{\epsilon_{d1} + E_C - J/4} + \frac{1}{\epsilon_{d2} + E_C - J/4} - \frac{1}{\epsilon_{d1} - E_C + J/4} - \frac{1 \mp \sqrt{2}}{\epsilon_{d2} - E_C + J/4} \right) \quad (5)$$

$$I = 2NV^2 \left( \frac{1}{\epsilon_{d1} - E_C + J/4} + \frac{1}{\epsilon_{d2} - E_C + J/4} - \frac{2}{\epsilon_{d2} - E_C} \right) + \Delta\epsilon + \frac{J}{4}. \quad (6)$$

In particular, we find  $J_1 \neq J_2$ . The effective direct exchange  $I$  will be a function of the level splitting  $\Delta\epsilon$  in the original model.

The Hamiltonian (4) has been analyzed recently [18]. Depending on the strength of  $I$ , the ground state of the two spins is either an interimpurity singlet or a triplet. The associated transition at  $I = I_{\text{crit}}$  is of the *Kosterlitz-Thouless*-type. The triplet side corresponds to an under-screened  $S = 1$  Kondo model, while on the singlet side, a *two-stage screening* process of the two impurities has been found for small  $\Delta I \equiv I - I_{\text{crit}} > 0$ . First, the larger one of the two couplings (e.g.,  $J_1$ ) leads to a screening of the corresponding spin  $\tilde{S}_1$  by the Kondo effect, thus decoupling  $\tilde{S}_2$  from the conduction band for  $T < T_K$ . The effective interimpurity exchange  $\Delta I$  then leads to a second Kondo effect for  $\tilde{S}_2$ . At low temperatures, the two spins form a singlet with a binding energy

$$T^* \sim \exp(-T_K/\Delta I) \quad (7)$$

that is indeed exponentially small in the distance  $\Delta I \approx \Delta\epsilon - \Delta\epsilon_{\text{crit}}$  from the critical point. This argument holds only as long as  $\Delta I < T_K$ . For larger values of the effective exchange,  $\Delta I$  provides a cutoff on the “first” Kondo effect and the singlet binding energy is then linear,  $T^* \approx \Delta I$ , as a function of the level splitting. In both cases, transport at  $T < T^*$  is strongly suppressed due to the singlet formation which leads to the dip in the density of states.

In order to demonstrate that this is the correct low-temperature scenario of the two-level quantum dot, we have calculated the characteristic energy scale  $T^*$  determined by the width of the dip. This calculation has been performed for the full dot Hamiltonian (1). In Fig. 5, we give  $T^*$  as a function of the distance from the critical point. Clearly, for large  $|\Delta\epsilon - \Delta\epsilon_{\text{crit}}|$  the dip scales linearly, while close to the critical point a crossover to an exponential dependence occurs. Note that different level broadenings lead to largely different Kondo temperatures; in particular, for  $\Gamma/D = 0.063$  only the linear behavior of  $T^*$  is seen because  $T_K$  is extremely small.

At this point we point out the robustness of our results with respect to parameter changes in the model. We

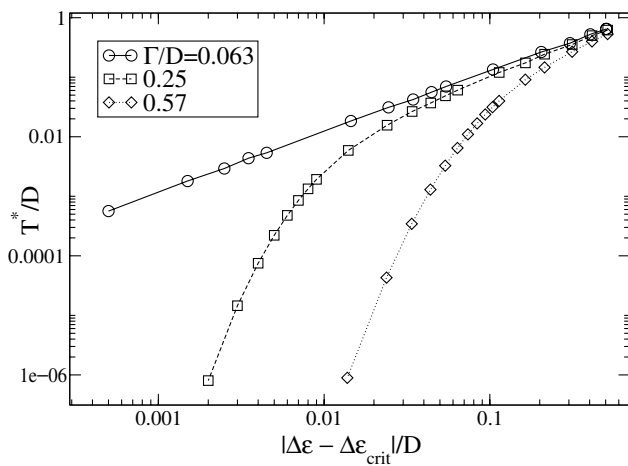


FIG. 5. Scaling of the characteristic temperature scale  $T^*$  (width of the dip) versus the distance from the transition point for  $E_C/D = 1$ ,  $\epsilon_{d1}/D = 1$ , and  $J/D = -2$ .

have chosen our quantum dot to be at a generic position in the Coulomb blockade valley, thus demonstrating that the quantum phase transition and the suppression of low-temperature transport discussed here are not restricted to special situations like particle-hole symmetry. The dip is also found when the broadening of the two levels is tuned to different values and/or when an asymmetry between the coupling to the right and the left lead is introduced.

*Conclusion and experimental relevance.*—Motivated by recent experiments [11] we have studied transport through a lateral quantum dot modeled by two levels close to the Fermi surface coupled to a single conduction channel in the leads. Correlations between different electrons in the dot are taken into account via the charging energy and a ferromagnetic exchange coupling due to Hund’s rule.

At the associated singlet-triplet degeneracy, we find a *quantum phase transition* of the Kosterlitz-Thouless-type, as in the two-impurity model [18]. On the triplet side of the transition the conductance simply increases up to the unitary limit upon lowering of  $T$ . On the singlet side, we find a nonmonotonic behavior of the conductance as a function of temperature (bump) corresponding to a characteristic “dip” in the transmission, which is also expected to be seen in the differential conductance. In particular, the width of the dip represents a new low-energy scale—the singlet binding energy—which becomes exponentially small close to the transition. For two conduction channels, none of the two effects is observed.

These findings are in good agreement with recent conductance measurements for a lateral quantum dot [11] close to the singlet-triplet transition. In this system, orbital symmetry is not conserved during tunneling. Both the nonmonotonic behavior of  $G(T)$  and the sharp dip in  $dI/dV$

have been observed, in contrast to previous studies of vertical quantum dots [5].

We therefore conclude that the number of conduction channels plays a crucial role for low-energy transport properties of a quantum dot. Symmetry and physical behavior of such a device are thus strongly related.

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