

## Conduction through a Quantum Dot near a Singlet-Triplet Transition

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Kondo effect in the vicinity of a singlet-triplet transition in a vertical quantum dot is considered. This system is shown to map onto a special version of the two-impurity Kondo model. At any value of the control parameter, the system has a Fermi-liquid ground state. Explicit expressions for the linear conductance as a function of the control parameter and temperature  $T$  are obtained. At  $T = 0$ , the conductance reaches the unitary limit  $\sim 4e^2/h$  at the triplet side of the transition, and decreases with the increasing distance to the transition at the singlet side. At finite temperature, the conductance exhibits a peak near the transition point.

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The number of electrons  $N$  in a Coulomb-blockaded dot is a well-defined quantity at low temperatures. The existence of a finite energy gap for excited states carrying a different charge,  $e(N \pm 1)$ , normally results in a suppressed low-temperature conductance through the dot. However, the suppression may be largely lifted [1] if  $N$  is odd. This phenomenon is explained in terms of the Kondo effect [2]. In the case of tunneling through a spin-degenerate state, the conductance may reach the unit quantum  $2e^2/h$ , which corresponds to a perfect transmission [3] through the dot. The origin of the perfect transmission is in the formation of a ‘‘Kondo cloud’’ consisting of the itinerant electrons of the leads, which tends to screen the spin of the dot. The formation of such a collective state is accompanied by the appearance of the resonance for electrons right at the Fermi energy. Of course, this effect takes place only if the dot has a nonzero spin in the ground state. This is always the case for odd  $N$ . If  $N$  is even, then the spin of the dot is typically zero. However, if the spacing  $\delta$  between the last doubly occupied and the following empty one-electron states in the dot is anomalously small, then the exchange interaction, according to Hund’s rule, favors the triplet ground state of the dot [4]. For a quantum dot formed in a GaAs heterostructure,  $\delta$  can be tuned by means of a magnetic field. Indeed, because of a very small electron effective mass, magnetic field applied perpendicular to the plane of electron gas has a strong orbital effect. At a certain critical value of  $\delta$  the singlet-triplet transition occurs. Tuning through such a transition was demonstrated recently in the experiments on vertical quantum dots [5]. A similar effect also occurs in lateral devices [6]. The applied magnetic field causes also spin splitting. However the Zeeman energy, which lifts the spin degeneracy, may remain sufficiently small, even compared with the Kondo temperature, because of a small value of the effective  $g$ -factor. Therefore the Kondo effect persists throughout the entire domain of parameters corresponding to the triplet spin state.

The singlet-triplet transition was addressed in the recent paper [7], where a quite special model of the quantum dot was considered. As can be shown, the additional symmetries assumed in [7] may result in a non-Fermi-liquid behavior at the transition point.

As we show below, a generic model of a quantum dot undergoing the singlet-triplet transition allows for a mapping onto the two-impurity Kondo model. Using this mapping, we found that at finite temperature, the conductance  $G$  is a nonmonotonic function of the control parameter  $K$  with an asymmetric peak near the transition point  $K = K^*$ . The asymmetry becomes more pronounced at lower temperatures, and  $G(K)$  becomes constant ( $\sim 4e^2/h$ ) at  $T = 0$  at the triplet side of the transition ( $K < K^*$ ), but decreases monotonously with  $K$  at  $K > K^*$ . Despite the apparent nonanalyticity of  $G(K)$ , the system has a Fermi-liquid ground state for all  $K$ , including the transition point.

The magnetic properties of a quantum dot can be understood from the following Hamiltonian:

$$H_{\text{dot}} = \sum_{ns} \epsilon_n d_{ns}^\dagger d_{ns} - E_s \mathbf{S}^2 + E_C (N - \mathcal{N})^2. \quad (1)$$

Here,  $N = \sum_{ns} d_{ns}^\dagger d_{ns}$  is the number of electrons in the dot,  $\mathbf{S} = \sum_{ns} d_{ns}^\dagger (\vec{\sigma}_{ss'}/2) d_{ns'}$  is the dot’s spin, and the parameters  $E_C$  and  $E_s$  are the charging and exchange energies [8]. We restrict our attention to the very middle of a Coulomb blockade valley with an even number of electrons in the dot (the dimensionless gate voltage  $\mathcal{N}$  is tuned to an even integer value). We assume that the spacing  $\delta$  between the last filled and first empty orbital states is of the order of  $E_s$ , and that  $\delta$  is tunable, e.g., by means of a magnetic field  $B$ . In order to model the singlet-triplet transition in the ground state of the dot, it is sufficient to consider these two states; we will assign indices  $n = \pm 1$  to them. The four low-energy states of the dot can be classified according to their spin  $S = 0, 1$  and its  $z$  projection  $S^z$ . Labeling the states by these two quantum numbers,

$|S, S^z\rangle$ , we find

$$\begin{aligned} |11\rangle &= d_{+1\uparrow}^\dagger d_{-1\uparrow}^\dagger |0\rangle, & |1-1\rangle &= d_{+1\downarrow}^\dagger d_{-1\downarrow}^\dagger |0\rangle, \\ |10\rangle &= \frac{1}{\sqrt{2}}(d_{+1\uparrow}^\dagger d_{-1\downarrow}^\dagger + d_{+1\downarrow}^\dagger d_{-1\uparrow}^\dagger) |0\rangle, & (2) \\ |00\rangle &= d_{-1\uparrow}^\dagger d_{-1\downarrow}^\dagger |0\rangle, \end{aligned}$$

where  $|0\rangle$  is the ground state of the dot with  $\mathcal{N} - 2$  electrons. Projected onto these states, the Hamiltonian of the dot becomes (up to a constant)

$$\mathcal{P}H_{\text{dot}}\mathcal{P} = \frac{K_0}{4} \sum_{S, S^z} |S, S^z\rangle (\delta_{S,1} - 3\delta_{S,0}) \langle S, S^z|, \quad (3)$$

where  $K_0 = \delta - 2E_s$  is the energy difference between the singlet and the triplet, and  $\mathcal{P}$  is the projection operator on the system of states (2).

Upon the variation of magnetic field  $B$ , the singlet-triplet transition occurs at  $K_0 = 0$ . Unlike the special case considered in Ref. [7], we are interested in the generic model with  $E_s \neq 0$  at the transition point.

In a vertical dot device, the potential creating lateral confinement of electrons most probably does not vary much over the thickness of the dot [5]. Therefore we assume that the electron orbital motion perpendicular to the axis of the device can be characterized by the same quantum number  $n$  inside the dot and in the leads; this quantum number is conserved in the process of tunneling. Thus, our model consists of the Hamiltonian of the dot, already discussed above, the Hamiltonian of the leads

$$H_l = \sum_{\alpha n k s} \xi_k c_{\alpha n k s}^\dagger c_{\alpha n k s}, \quad (4)$$

and the tunneling Hamiltonian:

$$H_T = \sum_{\alpha n k s} t_{\alpha n} c_{\alpha n k s}^\dagger d_{n s} + \text{H.c.} \quad (5)$$

Here  $\alpha = R, L$  for the right/left lead, and  $n = \pm 1$  for the two orbitals participating in the singlet-triplet transition;  $k$  labels states of the continuum spectrum in the leads, and  $s$  is the spin index. After a rotation in the R-L space,

$$\begin{pmatrix} \psi_{n k s} \\ \phi_{n k s} \end{pmatrix} = \frac{1}{t_n} \begin{pmatrix} t_{Rn} & t_{Ln} \\ -t_{Ln} & t_{Rn} \end{pmatrix} \begin{pmatrix} c_{Rn k s} \\ c_{Ln k s} \end{pmatrix},$$

the  $\phi$  field decouples:  $H_T = \sum_{n k s} t_n \psi_{n k s}^\dagger d_{n s} + \text{H.c.}$ ; here  $t_n^2 = t_{Ln}^2 + t_{Rn}^2$ . Next we integrate out the virtual transitions to the states with  $\mathcal{N} \pm 1$  electrons by means of the Schrieffer-Wolff transformation. The resulting effective low-energy Hamiltonian includes the operators

$$\mathbf{S}_{nn'} = \mathcal{P} \sum_{ss'} d_{ns}^\dagger \frac{\vec{\sigma}_{ss'}}{2} d_{n's'} \mathcal{P}.$$

The effective Hamiltonian may be conveniently written in terms of two fictitious 1/2 spins  $\mathbf{S}_{1,2}$  which represent the same symmetries as the set of states (2). This one-to-one correspondence between the basis states allows us to represent operators  $\mathbf{S}_{nn'}$  in terms of  $\mathbf{S}_{1,2}$ . We find the following relations:

$$\mathbf{S}_{nn} = \frac{1}{2} (\mathbf{S}_1 + \mathbf{S}_2) = \frac{1}{2} \mathbf{S}_+,$$

$$\sum_n \mathbf{S}_{-n,n} = \frac{1}{\sqrt{2}} (\mathbf{S}_1 - \mathbf{S}_2) = \frac{1}{\sqrt{2}} \mathbf{S}_-, \quad (6)$$

$$\sum_n i n \mathbf{S}_{-n,n} = \sqrt{2} [\mathbf{S}_1 \times \mathbf{S}_2] = \sqrt{2} \mathbf{T}.$$

Using (6), the effective Hamiltonian is written in a form, resembling [9] the two-impurity Kondo model [10]:

$$H = \sum_{n k s} \xi_k \psi_{n k s}^\dagger \psi_{n k s} + K (\mathbf{S}_1 \cdot \mathbf{S}_2) + \sum_n H_n, \quad (7)$$

$$\begin{aligned} H_n &= J_n (\mathbf{s}_{nn} \cdot \mathbf{S}_+) + V n \rho_{nn} (\mathbf{S}_1 \cdot \mathbf{S}_2) \\ &+ \frac{I}{\sqrt{2}} [(\mathbf{s}_{-n,n} \cdot \mathbf{S}_-) + 2i n (\mathbf{s}_{-n,n} \cdot \mathbf{T})]. \end{aligned} \quad (8)$$

Here the particle and spin densities in the continuum are

$$\rho_{nn} = \sum_{k k' s} \psi_{k n s}^\dagger \psi_{k' n s}, \quad \mathbf{s}_{nn'} = \sum_{k k' s s'} \psi_{k n s}^\dagger \frac{\vec{\sigma}_{s s'}}{2} \psi_{k' n' s'},$$

and the bare values of the coupling constants are

$$J_n = \frac{2t_n^2}{E_C}, \quad I = \frac{2t_{+1}t_{-1}}{E_C}, \quad V = \frac{t_{+1}^2 + t_{-1}^2}{2E_C}. \quad (9)$$

We did not include in Eq. (7) the Hamiltonian of the  $\phi$  field, and other terms which are irrelevant for the low-energy renormalization. The Schrieffer-Wolff transformation also produces corrections to  $K_0$ , so  $K$  does not coincide with its bare value. This difference is not important, as it only affects the position of the singlet-triplet transition, but not its nature. A common factor  $I$  in the last two terms of Eq. (8) comes from the conservation of the orbital index  $n$ ; see Eq. (5).

To simplify the analysis of Eqs. (7)–(9), we further restrict our attention to the symmetric case  $t_{\alpha n} = t_\alpha$ , for which the definition (9) reduces to

$$J_n \equiv J = I = 2V = 2(t_L^2 + t_R^2)/E_C. \quad (10)$$

This simplification is adequate to the experimentally relevant case of very thin barriers separating the dot from the leads, and, more importantly, only insignificantly affects the low-energy properties of the model. To calculate the differential conductance in the leading logarithmic approximation, we apply the ‘‘poor man’s’’ scaling technique [11]. The procedure consists of a successive integration out of the high-energy degrees of freedom, and yields the set of scaling equations

$$\begin{aligned} \frac{dJ}{d\mathcal{L}} &= \nu(J^2 + I^2), & \frac{dI}{d\mathcal{L}} &= 2\nu I(J + V), \\ \frac{dV}{d\mathcal{L}} &= 2\nu I^2, \end{aligned} \quad (11)$$

with the initial conditions (10). Here  $\mathcal{L} = \ln E_C/D$ , and  $\nu$  is the density of states in the leads; the initial value

of the energy cutoff  $D$  is  $D = E_C$ . This procedure also generates nonlogarithmic corrections to  $K$ . In the following we absorb these corrections in the redefined value of  $K$ . Equations (11) are valid for  $D \gg |K|, T$ .

At certain value of  $\mathcal{L} = \mathcal{L}_0$ , the inverse coupling constants simultaneously reach zero:

$$1/J(\mathcal{L}_0) = 1/I(\mathcal{L}_0) = 1/V(\mathcal{L}_0) = 0.$$

This defines, through the equation  $\mathcal{L}_0 = \ln E_C/T_0$ , the characteristic energy scale of the problem:

$$T_0 = E_c \exp[-\tau_0/\nu J(0)].$$

Here  $\tau_0$  is a parameter that depends on the initial conditions and should be found numerically. We obtained  $\tau_0 = 0.36$  (see Fig. 1). Thus, the strong coupling regime is reached at much higher temperatures than in the usual Kondo model (for which the Kondo temperature would be given by the same expression as  $T_0$ , but with  $\tau_0 = 1$ ).

The solution of the renormalization group (RG) equations (11) can now be expanded near  $\mathcal{L} = \mathcal{L}_0$ . To the first order in  $\mathcal{L}_0 - \mathcal{L} = \ln D/T_0$ , we obtain

$$\frac{1}{\nu J} = \frac{\sqrt{\lambda}}{\nu I} = \frac{\lambda - 1}{2\nu V} = (\lambda + 1) \ln D/T_0, \quad (12)$$

where  $\lambda = 2 + \sqrt{5} \approx 4.2$  is a model-independent constant, i.e., it does not change if the restriction  $t_{\alpha n} = t_\alpha$  is lifted.

The solution (12) can be used to calculate the differential conductance at high temperature  $T \gg (K), T_0$ . In this regime, the coupling constants are still small, and the conductance is obtained by applying a perturbation theory to the Hamiltonian (7)–(8) with renormalized parameters. This yields

$$G/G_0 = A \ln^{-2} T/T_0, \quad (13)$$

where

$$A = (3\pi^2/8)(\lambda + 1)^{-2}[1 + \lambda + (\lambda - 1)^2/8] \approx 0.9$$

is a numerical constant, and

$$G_0 = \frac{4e^2}{h} \left( \frac{2t_L t_R}{t_L^2 + t_R^2} \right)^2. \quad (14)$$

Note that (13) includes contributions from both the processes conserving the orbital index [the first two terms

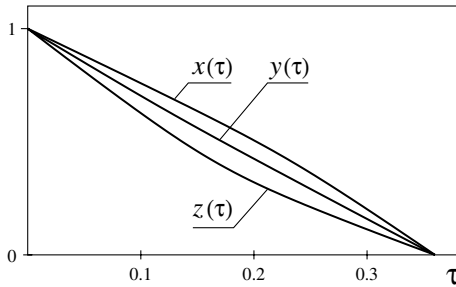


FIG. 1. Numerical solution of the scaling equations. The RG equations (11) are rewritten in terms of the new variable  $\tau = \nu J(0) \ln E_C/D$  and the new functions  $x(\tau) = J(0)/J(\tau)$ ,  $y(\tau) = I(0)/I(\tau)$ , and  $z(\tau) = V(0)/V(\tau)$ . The three functions reach zero simultaneously at  $\tau = \tau_0 = 0.36$ .

in Eq. (8)], and the processes involving an interorbital scattering.

Away from the singlet-triplet degeneracy point,  $|K| \geq T_0$ , the RG flow yielding Eq. (13) terminates at energy  $D \sim |K|$ . At the triplet side of the transition ( $K < 0$ ), the two spins  $\mathbf{S}_{1,2}$  are locked into a triplet state. The system is described by the effective two-channel Kondo model with  $S = 1$  impurity, obtained from Eqs. (7) and (8) by projecting out the singlet state:

$$H_{\text{triplet}} = \sum_{nks} \xi_k \psi_{nks}^\dagger \psi_{nks} + J_t \sum_n (\mathbf{s}_{nn} \cdot \mathbf{S}) + V_t \sum_n n \rho_{nn},$$

where  $J_t = J(|K|)$ , and  $V_t = V(|K|)/4$ . As  $D$  is further lowered,  $J_t$  is governed by the standard Kondo RG equation

$$dJ_t/d\mathcal{L} = \nu J_t^2, \quad \mathcal{L} = \ln D/(K).$$

The solution of this equation,  $1/\nu J_t(D) = \ln D/T_k$ , is expressed through the  $K$ -dependent Kondo temperature  $T_k(K) = (K) \exp(-1/\nu J_t)$ , which, using (12), is in turn expressed through  $T_0$  as

$$T_k/T_0 = (T_0/|K|)^\lambda. \quad (15)$$

Recall that the exponent here,  $\lambda \approx 4.2$ , is universal. Equation (15) was obtained also in [7], but with a rather different value of the exponent  $\lambda$  (according to [7],  $\lambda \leq 1$  and appears to be nonuniversal).

Since  $V_t$  is not renormalized, the differential conductance at  $T \ll -K$  is dominated by the exchange (the second term in  $H_{\text{triplet}}$ ) and is given by

$$G/G_0 = f(T/T_k) = f\left[\frac{T}{T_0} \left(\frac{|K|}{T_0}\right)^\lambda\right], \quad (16)$$

where  $f(x)$  is a smooth function that interpolates between  $f(x \gg 1) = (\pi^2/2) \ln^{-2} x$  and  $f(0) = 1$ . It coincides with the scaled resistivity  $f(T/T_K) = \rho(T/T_K)/\rho(0)$  for the symmetric two-channel  $S = 1$  Kondo model. The conductance at  $T = 0$  (the unitary limit value),  $G_0$ , is given above in Eq. (14); see also Fig. 2.

On the singlet side of the transition,  $K \geq T_0$ , the scaling terminates at  $D \sim K$ , and the low-energy effective Hamiltonian is

$$H_{\text{singlet}} = \sum_{nks} \xi_k \psi_{nks}^\dagger \psi_{nks} + V_s \sum_n n \rho_{nn},$$

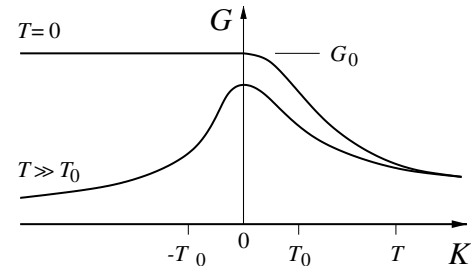


FIG. 2.  $K$  dependence of the differential conductance at two different temperatures. The two asymptotes merge at  $K \gg T, T_0$ .

where  $V_s = -3V(K)/4$ . The conductance at temperatures  $T \ll K$  is given by

$$G/G_0 = B \ln^{-2} K/T_0, \quad B = \left( \frac{3\pi}{8} \frac{\lambda - 1}{\lambda + 1} \right)^2 \approx 0.5. \quad (17)$$

The only regime of parameters left beyond the range of the validity of Eqs. (13), (16), and (17) is that of the very vicinity of the singlet-triplet transition  $K = 0$  at low temperature  $T \lesssim T_0$ . Understanding of this regime requires knowledge of the properties of the system's ground state. This can be inferred from the following simple symmetry-based argument, devised originally for the two-impurity Kondo model [10]. The Hamiltonian (7), (8) in the symmetric case  $J_n = J$  is invariant with respect to the particle-hole transformation

$$\psi_{n,k,s} \rightarrow s\psi_{-n,-k,-s}^\dagger. \quad (18)$$

Consider now the scattering problem at the Fermi energy:

$$\Phi_{ns}^{\text{out}} = S_{ns,n's'} \Phi_{n's'}^{\text{in}}. \quad (19)$$

Particle-hole symmetry (18) implies that for any  $\Phi^{\text{in(out)}}$  which solves Eq. (19),  $\Phi^{\text{in(out)}} = i\Sigma\Phi^{\text{out(in)}}$  will be a solution as well (here  $\Sigma_{ns,n's'} = \sigma_{ss'}^y \sigma_{nn'}^x$ , and  $\sigma^i$  are the Pauli matrices). Substituting this into (19) one finds a relation for the  $S$  matrix:  $(\Sigma S)^2 = 1$ . Among the diagonal  $S$ , this is satisfied by  $S_{ns,n's'} = \delta_{nn'} \delta_{ss'} e^{-2in\theta}$  with arbitrary  $\theta$ . In other words, the particle-hole symmetry imposes a restriction on the scattering phase shifts at the Fermi energy:  $\theta_{ns} = n\theta$ . The phase  $\theta$  and therefore scattering phases  $\theta_{ns}$  vary *continuously* from  $\pm\pi/2$  to 0 as  $K$  is varied from  $K = -\infty$  to  $K = +\infty$ . At the triplet side of the transition,  $-K \gg T_0$ , the low-temperature physics is described by the effective two-channel  $S = 1$  Kondo model, as discussed above. In that model, the zero-energy phase shift  $\theta \equiv \pi/2$ . This means that there exists  $K^* \geq -T_0$  such that  $\theta(K) = \pi/2$  for all  $K < K^*$ . On the other hand, at the singlet side of the transition,  $\theta(K)$  decreases with  $K$  logarithmically at large positive  $K \gg T_0$ , but approaches  $\pi/2$  at smaller  $K$  because of larger values of  $V_s$  in  $H_{\text{singlet}}$ . We expect therefore that  $\theta(K)$  is a continuous, though a nonanalytical, function. The singlet-triplet transition may be associated with the point of the non-analyticity  $K = K^*$ . According to these arguments, it is natural to conjecture that the Fermi-liquid description [12] is applicable at all  $K$  and thus the conductance at  $T = 0$  is  $G = G_0 \sin^2\theta(K)$ . The interorbital scattering processes make no contribution to  $G$  in this regime, unlike at high temperature  $T \gg |K|, T_0$ .

It should be noticed that the problem under consideration is quite different from what one faces if the Zeeman

splitting is the leading effect of the magnetic field [13] (which may happen if the magnetic field is applied in the plane of the lateral dot). In this case, the twofold degeneracy of the ground state of an isolated dot appears only at one special value of magnetic field, such that the Zeeman energy equals  $\delta$ . Accordingly,  $G(T, B)$  exhibits a Kondo peak at this strength of the field at all temperatures.

To conclude, we considered the linear conductance  $G(T, K)$  of a vertical quantum dot near the singlet-triplet transition. The transition occurs due to the strong orbital effect of an external magnetic field. At high temperature  $G$  exhibits a peak near the transition point, in agreement with the experiments [5]. At low temperature  $G$  reaches the unitary limit value at the triplet side of the transition, and decreases monotonously at the singlet side (see Fig. 2). The characteristic energy scale of the effect is much larger than that for the usual Kondo effect with the similar system parameters.

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