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Suppression of Kondo-assisted co-tunneling in a spin-1 quantum dot with Spin-Orbit interaction

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Kondo-type zero-bias anomalies have been frequently observed in quantum dots occupied by two electrons and attributed to a spin-triplet configuration that may become stable under particular circumstances. Conversely, zero-bias anomalies have been so far quite elusive when quantum dots are occupied by an even number of electrons greater than two, even though a spin-triplet configuration is more likely to be stabilized there than for two electrons. We propose as an origin of this phenomenon the spin-orbit interaction, and we show how it profoundly alters the conventional Kondo screening scenario in the simple case of a laterally confined quantum dot with four electrons.

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A QD in the Coulomb blockade regime with an odd number of electrons acts as a localized magnetic moment and the spin degeneracy allows for Kondo effect to take place[1–5]. Conversely, a QD with an even number of electrons is usually in a non-degenerate spin-singlet configuration, hence the absence of any Kondo effect. For long time, the most direct signature of Kondo resonant tunneling was the so-called even-odd effect. In reality, the even-odd rule not always applies since also dots with an even number of electrons can become Kondo-active under an external field able to push a high spin configuration below the spin-singlet one.[6–12] This level crossing is called singlet-triplet (S-T) transition, since the high-spin state is usually a triplet, and is accompanied by several interesting phenomena. [11–14, 14–20] However the report of Kondo-like zero-bias anomalies in four or more electron dots [6, 12] is rare when compared with the wealth of data available for two-electron dots. In addition, even when these anomalies are indeed observed, like in the experiment by Granger *et al.*,[12] they are found to behave rather unconventionally as a function of temperature or magnetic field.

In this paper we propose that spin orbit interaction (SOI) may offer a natural explanation of the lack of Kondo-assisted co-tunneling in quantum dots with even number of electrons. When the number of electrons trapped in a QD increases, the separation between the single-particle orbitals lying closest to the chemical potential must diminish and eventually can be overwhelmed by the exchange splitting, thus stabilizing a magnetic ground state.[21, 22] This is certainly the case for an axially symmetric dot with four electrons. It is well known that SOI may affect significantly magnetic properties of QD's,[23] a feature that attracts great interest in the context of quantum computation through semiconducting dots.[24–27] By contrast, SOI is often not accounted

for when interpreting tunneling spectra across quantum dots. On the contrary, we will show that SOI may actually affect dramatically quantum dots with an integer spin, especially when coupled only to a single conducting channel from the leads. In particular, we shall consider a very simplified model of a four-electron laterally confined dot and show by Numerical Renormalization Group (NRG)[28] that the SOI totally suppresses zero-bias conductance even when the four-electron ground state is a spin triplet. We will show that the zero-bias conductance has a non monotonic behavior in temperature and magnetic field, which strongly resembles the experimental data of Ref.[12]

In a parabolic confining potential and in the absence of magnetic field, the single particle eigenstates are those of a two dimensional harmonic oscillator with eigenvalues $\epsilon_j = \hbar\omega_0(n_x + n_y + 1)$, where ω_0 is the confinement frequency and $j = (n_x, n_y)$ labels the states in a cartesian basis. Exact diagonalization calculations show that, in the case of four electrons, the largest weight configuration in the ground state has two electrons filling the lowest-lying level, $j = (0, 0)$, while the other two occupy the higher states, $j = (1, 0) \equiv a$ and $(0, 1) \equiv b$, in a spin-triplet configuration.[29] Therefore it is justified to consider the Hamiltonian of the isolated dot by including only the interaction within the $j = a, b$ shell

$$H_{dot} = \sum_{\sigma,j} \epsilon_j d_{j\sigma}^\dagger d_{j\sigma} + U \sum_{j=a,b} n_{j\uparrow} n_{j\downarrow} - \frac{J_H}{2} \mathbf{S} \cdot \mathbf{S}, \quad (1)$$

where $d_{j\sigma}^\dagger$ ($d_{j\sigma}$) are the fermionic creation (annihilation) operators on the QD, respectively, and $n_{j\sigma} = d_{j\sigma}^\dagger d_{j\sigma}$. Here \mathbf{S} is the total spin of the a - b shell and the Hund's term with $J_H \geq 0$ favors the triplet state. Spin-orbit coupling H_{SO} , involves, however, also the lowest lying levels $j = (0, 0)$. For a quantum dot defined in

a two-dimensional electron layer, the SOI terms linear in momentum $\boldsymbol{\pi} = \mathbf{p} + e\mathbf{A}/c$ (\mathbf{A} is the vector potential) are dominant, provided the dot lateral size is much larger than the layer thickness. We shall parametrize the Rashba term[30] by α , and the Dresselhaus[31] one by β (ranging from tens to few hundreds of $meV\cdot\text{\AA}$). Thus

$$H_{SO} = -\frac{\alpha}{\hbar}(\pi_x\sigma_y - \pi_y\sigma_x) - \frac{\beta}{\hbar}(\pi_x\sigma_x - \pi_y\sigma_y),$$

where $\sigma_{x,y,z}$ are Pauli matrices. As the typical energy scale of the SO coupling is much smaller than the bare single-particle level spacing $\hbar\omega_0$ (α/\hbar and $\beta/\hbar \ll \sqrt{\hbar\omega_0/m_*}$), it is legitimate to treat H_{SO} perturbatively. This amounts to degenerate second-order perturbation theory in H_{SO} through intermediate excited states with holes in the $j = (n_x, n_y) = (0, 0)$ shell and/or electrons in the empty shell with $n_x + n_y = 2$. The calculation is straightforward (see Ref. [32] for details) and leads to

$$H_{SO}^{(2)} = -\lambda_s \sum_{\sigma,j=a,b} d_{j\sigma}^\dagger d_{j\sigma} + i\lambda \sum_{\sigma,j \neq j'} \sigma d_{j\sigma}^\dagger d_{j'\sigma}, \quad (2)$$

with $\lambda_s = m_*(\alpha^2 + \beta^2)/\hbar^2$ and $\lambda = m_*(\alpha^2 - \beta^2)/\hbar^2$. Here, m_* is the effective mass of the semiconducting two dimensional layer (e.g. GaAs or InAs). In the presence of a magnetic field, parametrized in what follows by the cyclotron frequency ω_c , ϵ_j as well as α and β become field-dependent and a Zeeman splitting must be added to H_{dot} , Eq.(1). The first term in Eq. (2) shifts the position of a, b with respect to the chemical potential, breaking particle-hole symmetry and can always be compensated by changing the gate voltage. The second term of Eq. (2) represents a spin dependent hopping between the two levels. Unlike the former, the latter it plays an important role that is more transparent at large U , as it provides an additional anisotropic contribution to the spin exchange besides the isotropic one $\propto J_H$. In this limit and at zero magnetic field, H_{dot} and H_{SO} can be mapped onto a simple spin-1 Hamiltonian:

$$H_{dot} + H_{SO} \longrightarrow -\frac{1}{2}(J_H + J_{SO}) \mathbf{S} \cdot \mathbf{S} + J_{SO} (S^z)^2. \quad (3)$$

Here $J_{SO} = 4\lambda^2/U$. The SOI thus generates a hard-axis single-ion anisotropy, which splits the spin-triplet into a lower state with $S^z = 0$ and a higher doubly-degenerate one with $S^z = \pm 1$. It follows that SOI competes against Kondo effect, which instead requires a QD degenerate ground state. We shall see that, in the specific geometry we consider, this competition is actually won by SOI.

We now supplement the Hamiltonian $H_{dot} + H_{SO}^{(2)}$ of Eqs.(1,2) with the Hamiltonian of the leads H_{lead} , assumed to be free, and a term $H_{hyb} = \sum_{\sigma k} V_k (c_{k\sigma}^\dagger d_{a\sigma} + H.c.)$ describing the hybridization to a suitable combination of states $|k\sigma\rangle$ from the two conducting leads. For sake of simplicity, we shall assume

that electrons from the leads can tunnel only into one level, e.g. a . Since Eq. (3) is invariant under any rotation in the space of the two orbitals a and b , the single screening channel could be coupled to a combination of both orbitals rather than to a single one, with no change of the physics. Our model hamiltonian is very similar to the two impurity single channel Kondo model studied in Refs.[33, 34]. However, in our case the two levels are coupled ferromagnetically and the interesting physics arises by the SOI rather than by an antiferromagnetic exchange between the impurities as in [33, 34].

According to Eq.(3), the physics of the model Hamiltonian H for large U is controlled by three energy scales: the Kondo screening temperature T_{1K} of the level a in the absence of any coupling to b , i.e. for $J_H = J_{SO} = 0$, the Coulomb exchange, J_H , and finally the spin-orbit anisotropic exchange, J_{SO} . When $J_{SO} \gg T_{1K}$, the spin degeneracy is lost much before Kondo effect could start playing any role and the conductance must be small and structureless at low bias. A richer behavior instead emerges in the opposite limit of $J_{SO} \ll T_{1K}$. Here we can adopt a two-cutoff scaling approach and imagine to initially follow the system from high temperature/energy ($\gg J_{SO}$) as if SOI is absent. When the temperature/energy becomes of order J_{SO} , SOI fully comes into play. In this approximate scheme, on a scale T_{1K} a first underscreened Kondo effect sets in, where only half of the dot-spin gets screened by the single conducting channel.[35] The quasiparticles[36] that are coupled to the residual spin-1/2 acquire a local density-of-states (DOS) $\sim 1/T_{1K}$. The spin-1/2 that is left aside has a weak residual ferromagnetic exchange with the conduction bath whose effective strength $-J_* < 0$ vanishes at low temperature/energy.[35] At an energy scale $\sim J_{SO}$, SOI modifies the effective exchange with the conduction bath into a spin-anisotropic one, see Eq.(3), with the coupling in the x - y plane, $\sim -J_* - J_{SO}$, being larger in magnitude than that along z , $\sim -J_* + J_{SO}$. This case is known to lead to a further Kondo effect controlled by the Kondo temperature[37]

$$T_{2K} \sim T_{1K} \exp \left[-\frac{T_{1K}}{A} \left(\frac{\pi}{2} - \tan^{-1} \frac{J_z}{A} \right) \right], \quad (4)$$

where $A = 2\sqrt{J_* J_{SO}}$. This looks like if a kind of two-stage Kondo effect takes place with well separated energy scales $T_{1K} \gg T_{2K}$, whose low temperature phase is strongly driven by the spin dependent hopping due to the SOI. The resemblance with recent findings on the role of magnetic anisotropies in models for magnetic impurities on surfaces [38, 39] (where single-ion anisotropies like in Eq. (3) emerge as well) is striking.

The above expectations that we drew from very qualitative arguments are nicely confirmed by the full NRG calculation.

The zero-bias conductance G as function of the temperature is shown in Fig. 1a for different λ 's. At very

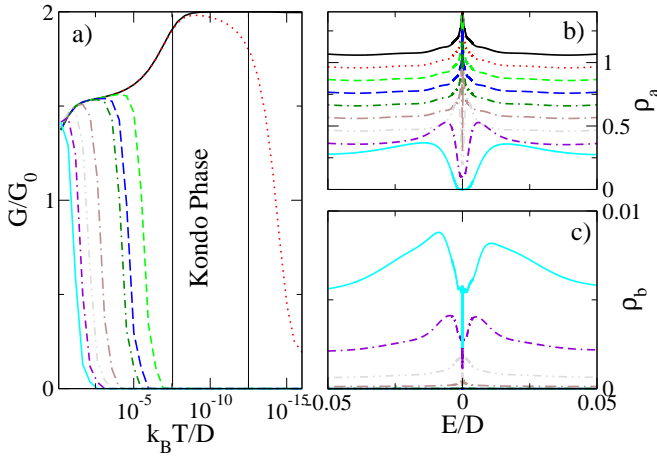


FIG. 1: (Color online) a): Zero bias conductance as a function of temperature for different values of $\lambda/\hbar\omega_0 = 0.0001, 0.0025, 0.0064, 0.01, 0.04, 0.09, 0.16, 0.25$, increasing from the rightmost curve towards the leftmost one. Hamiltonian parameters are: $\epsilon_a = \epsilon_b = -1\text{meV}$, $U = 2\text{meV}$, $\Gamma = \pi\rho_0|V_k|^2 = 0.1\text{meV}$, $D = 1\text{meV}$, $J_H = 0.1\text{meV}$, $\omega_c = 0$ and $\lambda_s = 0$. The reference value $G_0 = e^2/h$. b): Spectral function at the impurity site a . By increasing the spin orbit coupling the Kondo peak is suppressed and the central resonance turns into an antiresonance. Curves have been shifted from clarity by a uniform amount and the scale on the y axis refers to the bottom curve. From bottom to top λ decreases. c): Spectral function at the impurity site b non directly connected to the contact leads.

low temperatures $T \ll T_{2K}$, G is indeed extremely small, practically zero. However, at intermediate temperatures $T_{2K} \ll T \ll T_{1K}$, the conductance can reach (or be very close to) its unitary value of an underscreened Kondo-like plateau. The local spectral properties are shown in Fig. 1b for the same values of λ of Fig. 1a. The density of states (DOS) $\rho_a(\epsilon)$ of the level a that is coupled to the leads develops a conventional Abrikosov-Suhl resonance of width T_{1K} , signaling the underscreened Kondo effect. At lower energies, a deep pseudogap of width T_{2K} is digged inside the former resonance. Conversely, the DOS $\rho_b(\epsilon)$ of the level b , which hosts most of the residual spin-1/2, is quite low on the scale $\sim T_{1K}$ (note that it is two orders of magnitude smaller than ρ_a in the figure) and develops a narrow antiresonance below T_{2K} . Since the zero-bias conductance G is proportional to $\rho_a(0)$, G has an inverted zero-bias anomaly, being small at zero temperature and increasing on increasing T . As long as only a single channel of conduction electrons is coupled to the dot, this behavior must hold whatever is the value of $\alpha^2 - \beta^2 \neq 0$, even if the space symmetry of the device is weakly perturbed. In fact, the ultimate cause of the ineffectiveness of the Kondo co-tunneling can be traced back to the spin-exchange (3), which is invariant under any unitary transformation in the a - b space. We note that, if the two orbitals are split or hybridized

among each other because of an asymmetric shape of the confining potential, which is more likely the rule, the situation would not change provided the splitting and/or hybridization are small enough compared with J_H , so that the lowest energy state has still $S = 1$. However, should the splitting and/or hybridization be so large to stabilize a spin-singlet state of the dot, still Kondo co-tunneling would be ineffective.[33, 34] Therefore, in the most general case of non-degenerate levels, we predict that, whatever is the magnitude of the Coulomb exchange J_H , Kondo-like zero-bias anomalies in four electron dots should be absent at low temperatures, provided a single conducting channel tunnels into the dot. If J_H is small, this occurs because the dot electrons prefer to lock into a Kondo-inactive spin-singlet configuration.[33, 34] If J_H is large, it is the unavoidably present SOI that stabilizes a non-degenerate state, i.e. the $S_z = 0$ component of the spin-triplet.

The suppression of the Kondo effect due to the SOI is quite different from that caused by a magnetic field. The magnetic field affects the whole low-energy ($\leq T_{1K}$) spectrum[37]; it splits the Abrikosov-Shul resonance and leads to a tiny zero-bias conductance that keeps decreasing on increasing temperature, see e.g. Refs. [40, 41]. By contrast, the SO coupling is gentler on the high energy scales $\sim T_{1K}$, but much more dramatic at low energy $\leq T_{2K}$. The Abrikosov-Shul resonance develops as usual, but in the end, the SOI digs a narrow but very deep pseudogap at the chemical potential. Thus the conductance shows a Kondo plateau at intermediate temperatures, unlike what happens in the presence of a magnetic field, but falls down rapidly below T_{2K} to much lower values than those at finite magnetic field.

The combined action of SOI and magnetic field is presented in Figs. 2 and 3. The intermediate underscreened Kondo phase disappears, no matter how small the magnetic field is (see Fig. 2a). Very weak magnetic fields give rise to a sudden drop of the conductance. In the absence of magnetic field the same result could be achieved only by means of unphysically large SOI. The Kondo peak splits and a wide gap opens in the whole low energy region $\sim T_{1K}$ (see Fig. 2b), very similar to what found in the absence of SOI.[40, 41] The magnetoconductance is shown in Fig. 3 for increasing values of λ 's. The conductance first rises to a maximum at $\omega_c = \omega_c^*$ and then drops for large fields as $\sim 1/\omega_c^2$. By increasing λ also ω_c^* increases. The sharp rise of the conductance at $\omega_c = \omega_c^*$ is an artifact of our simplified model and likely it will be rounded off in real devices.

The non-monotonic behavior of G both in temperature and in magnetic field has been observed experimentally in a four electron QD by Granger *et al.*[12] The explanation given by the authors invoked the two-stage Kondo effect proposed in Refs. [19] and [18]. In that scenario, it is assumed that both the symmetric and the antisymmetric combination of the tunneling channels of

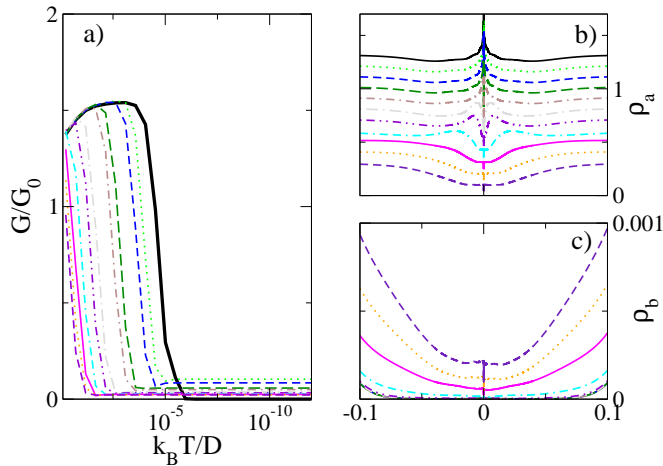


FIG. 2: (Color online) a): Zero bias conductance as a function of temperature for different values of $\omega_c/\omega_0 = 0.00005, 0.0001, 0.001, 0.005, 0.01, 0.025, 0.05, 0.075, 0.1$ (from right to left), where ω_c is the cyclotron frequency, at fixed spin orbit coupling $\lambda/\hbar\omega_0 = 0.01$. All other parameters are the same as in Fig. 1. b): Spectral function of the a -level. We note that by increasing the magnetic field the Kondo peak is suppressed and the central resonance turns into a wide antiresonance. Curves have been shifted from clarity by a uniform amount and the scale on the y axis refers to the bottom curve. From bottom to top ω_c/ω_0 decreases. c): Spectral function of the b -level.

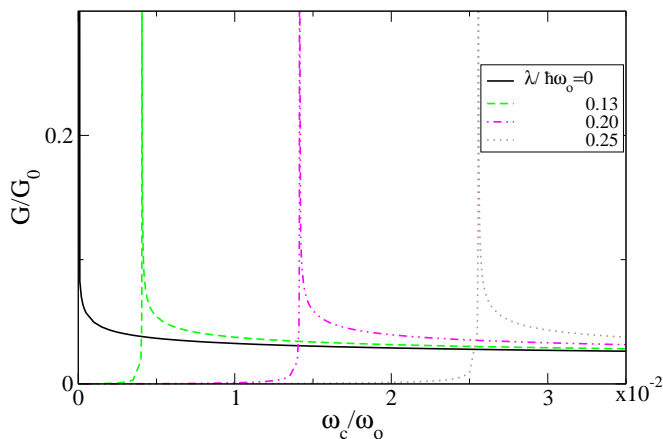


FIG. 3: (Color online) Zero bias conductance at zero temperature as a function of the magnetic field ω_c/ω_0 for increasing values of the SOI $\lambda/\hbar\omega_0 = 0.0, 0.12, 0.2, 0.25$ (from left to right).

each lead is coupled to the spin $S = 1$ of the dot, so that eventually this spin gets fully screened although on two different temperature scales. The zero-bias conductance $G = G_0 \sin^2 \delta$, where δ is the difference between the phase shifts of the symmetric and antisymmetric combinations, vanishes in that case since both channels acquire a $\pi/2$ phase shift. G as function of magnetic field or temper-

ature turns out to be non-monotonous just like in our model. In spite of this, the two-stage Kondo effect and our scenario are very different. Indeed, in the two-stage Kondo effect of Ref[18, 19] both levels will have a Kondo peak at the Fermi level, larger in a than in b , while we do not find any in b . Since the zero-bias conductance behaves similarly in both scenarios, it could be worth exploiting the tunability of the SOI to get further experimental insights. In the presence of SOI, the lowest lying state above the $S^z = 0$ component of the spin-triplet should be the $S^z = \pm 1$ doublet, followed at higher energy by the singlet, a feature that could be uncovered by a detailed analysis of the inelastic tunneling spectrum in the absence and presence of a magnetic field.

In conclusion, zero-bias anomalies have been so far quite elusive when quantum dots are occupied by an even number of electrons greater than two, even though a spin-triplet configuration is more likely to be stabilized here than for two electrons (e.g. at zero magnetic field). Here we have proposed that a possible explanation of the suppression of the Kondo conductance in an even electron quantum dot can be traced back to the role of the SOI, which has been often disregarded in interpreting experiments. We have shown that SOI, in an underscreened four-electron dot hybridized with one single channel, gives rise to a conductance behavior in the presence of a magnetic field, very close to what has been recently observed experimentally.[12]

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After the submission of the paper we became aware of Ref.[42] stressing the importance of SOI in molecular transport.

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