Kondo screening suppression by spin-orbit interaction in quantum dots

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We study the transport properties of a quantum dot embedded in an Aharonov-Bohm ring in the presence of spin-orbit interactions. Using a numerical renormalization group analysis of the system in the Kondo regime, we find that the competition of Aharonov-Bohm and spin-orbit dynamical phases induces a strong suppression of the Kondo state singlet, somewhat akin to an effective intrinsic magnetic field in the system. This effective field breaks the spin degeneracy of the localized state and produces a finite magnetic moment in the dot. By introducing an in-plane Zeeman field we show that the Kondo resonance can be fully restored, reestablishing the spin singlet and a desired spin filtering behavior in the Kondo regime, which may result in full spin polarization of the current through the ring.

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Semiconductor quantum dot (QD) structures represent a promising platform on which to achieve charge and spin control, due to their discrete energy levels, sizable Coulomb interaction due to strong electron confinement, as well as precise level and size manipulation via gate voltages [1]. This flexibility allows probing fundamental aspects of spin systems and opens possibilities for devices with newly tailored properties [2]. Interestingly, coherent electron propagation at low temperatures and quantum interference may play a pivotal role in attaining the desired goal in these structures [3].

Control of electronic transport is now systematically achieved by exploiting interference in multiple-path geometries, such as those produced with one or multiple QDs embedded in a ring [4]. In these structures, a weak magnetic field through a ring (few mT for a submicron ring) produces significant changes in transport properties due to the Aharonov-Bohm (AB) effect [5]. The presence of Rashba spin-orbit (SO) interaction [6], which can be further modulated by applied gate voltages, provides additional dynamical control of charge and spin transport. The strong Coulomb interaction in these systems may also result in a Kondo state appearing below a characteristic Kondo temperature \( T_K \) [7], giving rise to strong antiferromagnetic correlations between localized and itinerant electrons in the leads. The Kondo state singlet produces an additional transport channel through the system at the Fermi level when the dot is in an otherwise Coulomb blocked configuration.

Several ring geometries have been proposed as spin polarizers and their behavior has been analyzed in different regimes and levels of approximation in models that include SO interactions [8, 9, 10]. The basic physics involved in the spin-filtering effect is the modification of the conductance for different spin species as a result of the AB flux and SO effects that introduce spin-dependent dynamical phases for the electrons in the multiply-connected geometry. The correct and complete inclusion of the Kondo physics is crucial in order to provide a proper description of the system, as we describe in this work, especially with respect to its spin transport behavior. One important element of this analysis is the full consideration of particle-hole (p-h) asymmetry, which has been ignored or included only approximately in previous works, and it is found to have dramatic effects in the correlations of the Kondo state for even the simplest geometry of a QD embedded in the ring. We present here a numerical renormalization group study of this system. This approach is capable of addressing the full spin-dependent character of the coupling to the leads and the p-h asymmetry in a non-perturbative fashion [11]. Our analysis demonstrates that the combination of AB and SO effects may strongly suppress the Kondo state, and in fact eliminate the desired spin filtering effect described previously in the literature [8]. Moreover, we demonstrate that this suppression can be fully compensated by the application of an in-plane Zeeman field. Under those conditions, the Kondo screening is restored and the spin filtering effect reestablished.

We consider a single QD in contact with two leads \( L \) and \( R \). The leads are coupled to each other via the upper arm of the ring, as shown in the upper diagram in Fig. 1, while the lower arm contains the QD. The Hamiltonian of the system can be written as \( \hat{H} = \hat{H}_{QD} + \hat{H}_{leads} + \hat{H}_{T} \), where \( \hat{H}_{QD} = \sum_\sigma \epsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} \) describes interacting electrons confined in the QD with level energy \( \epsilon_d \) regulated by a local gate, and \( U \) is the local Coulomb repulsion in the dot; \( \hat{H}_{leads} = \sum_{\alpha R} [c_{d\alpha\sigma}^\dagger c_{d\alpha\sigma}^\dagger + H.c.] \), with \( \alpha = R, L \), describes the leads, and \( \hat{H}_{T} = \sum_{\alpha R} \sum_{i} V_{i} [c_{d\alpha\sigma}^\dagger c_{R\alpha\sigma}^\dagger + H.c.] + \sum_{\alpha} \sum_{i} [\tilde{V}_{i} c_{L\alpha\sigma}^\dagger c_{R\alpha\sigma} + H.c.] \), describes the connection between the leads through both arms of the ring, where \( c_{d\sigma}^\dagger \) creates an electron in the
dot, while $c_{\alpha k}^\dagger$ creates it in the $\alpha$-th lead with spin $\sigma$. The coupling $V_1$ is considered real and allows the QD electron to tunnel to/from the leads. The AB field is mapped, as usual, into a phase $\phi_{AB} (= 2\pi \Phi/\Phi_0$, where $\Phi$ is the magnetic flux through the plane of the ring, $\Phi_0 = hc/e$ is the flux quantum) accumulated when the electron undergoes a closed trajectory in the ring, so that $\tilde{V}_2 \rightarrow V_2 e^{i\phi_{AB}}$ is a complex number. In addition, a local SO interaction on a single-level QD can be mapped onto a spin-dependent phase $\sigma \phi_{SO}$, which is proportional to the strength of the SO interaction and accumulates along the ring (spin quantization axis of $\sigma$ is in the plane of the ring) [3]. The combined AB and SO effects can then be included by a spin-dependent phase of the tunneling coupling $V_2^\sigma = V_2 e^{i\phi_\sigma}$, where $V_2 = |V_2^\sigma|$ and $\phi_\sigma = \phi_{AB} + \sigma \phi_{SO}$. The appearance of $\phi_{SO}$ in the upper arm of the ring can also be thought to arise from a variable relative gate potential applied on that arm [3].

Non-interacting case. — To study the consequences of SO coupling and AB flux in the system, we consider first the non-interacting limit ($U = 0$). The exact Green’s functions of the system can be calculated; in particular the local GF at the QD is $G_{dd}^{(0)}(\omega) = (\omega - \epsilon_d + \Sigma_\sigma(\omega))^{-1}$, where the self-energy is

$$\Sigma_\sigma(\omega) = \frac{-2V_2^2}{1 - V_2^2 (\tilde{G}(\omega))^2} \left[ \tilde{G}(\omega) + V_2 (\tilde{G}(\omega))^2 \cos \phi_\sigma \right], \quad (1)$$

with $\tilde{G}(\omega) = \sum_k (\omega - \epsilon_k)^{-1}$. It is useful to write the self-energy in terms of its real and imaginary parts, $\Sigma_\sigma(\omega) = \Lambda_\sigma(\omega) + i \Delta_\sigma(\omega)$. All the information about SO and AB phases is contained in the second term of Eq. (1). The spin-dependent contribution to the self-energy is less important when the condition $V_2 \cos(\phi_\sigma) \ll 2D/\pi$ is fulfilled, where $D$ is the half-bandwidth of the leads [2]. In the non-interacting case, even when $V_2 \cos(\phi_\sigma) \approx 2D/\pi$, the spin dependent term in the self-energy is a relatively small correction. However, these changes are crucial in the interacting case, as we will discuss below.

Notice in Eq. (1) that for $\phi_{AB} = 0$, $\Sigma_\uparrow(\omega) = \Sigma_\downarrow(\omega)$ (since the cos is even) but the equality does not hold for arbitrary values of $\phi_{AB}$. As a consequence, one has in general $\Lambda_\uparrow(\omega) \neq \Lambda_\downarrow(\omega)$, which means that the local bare level acquires a spin dependent shift. This is similar to what happens when electrons are subject to a Zeeman field, although here the shifts are different in magnitude for each spin species, and the shift is $\omega$-dependent. Experiments where an intrinsic magnetic field is observed in the single-particle spectrum have been reported recently in an AB ring with strong Rashba SO interaction [3].

To explore how this effect depends on system parameters, we define $\delta \Lambda_\sigma(\omega) = \Lambda_\sigma(\omega, \phi_{SO}) - \Lambda_\sigma(\omega, 0)$: this quantity plays the role of the $\sigma$-dependent magnetic field producing the spin splitting. Figure 1h shows typical curves $\delta \Lambda_\sigma(\omega)$ for $V_1 = 0.1414D$, $\phi_{AB} = \phi_{SO} = \pi/4$ and different values of $V_2$. Figure 1h shows $\delta \Lambda_\sigma(0)$ as a function of the coupling $V_2$. The maximum absolute value of $\delta \Lambda_\sigma(0)$ is obtained for $V_2 = 2D/\pi$. Notice that $|\delta \Lambda_\uparrow(0)| \neq |\delta \Lambda_\downarrow(0)|$ highlights the p-h asymmetry and makes this phenomenon very different from that of an external Zeeman field. Figure 4a-d show the effective coupling $\Delta_\sigma$ that the localized electrons in the QD have with the conducting leads. The SO interaction and AB effect result in drastically different couplings $\Delta_\uparrow(\omega)$ and $\Delta_\downarrow(\omega)$ [although identical at the Fermi energy, $\Delta_\uparrow(0) = \Delta_\downarrow(0)$]. This has an important effect on the interacting case, especially when the system enters the Kondo regime. We emphasize that larger $V_2$ values correspond to better connectivity of the upper arm in the ring, while larger $\phi_{SO}$ arises from larger SO coupling [3].

Interacting case. — In the following, we take $U = 0.5D$ and $\epsilon_d = -U/2$. In the NRG approach, the system is mapped into an Anderson impurity coupled to an effective non-constant conduction band given by the effective spin-dependent coupling $\Delta_\sigma(\omega) = \Im[\Sigma_\sigma(\omega)]$. A generalization of the NRG discretization for a non-constant conduction band [12] is used to calculate the local interacting Green’s function [13]. The latter is written as $[G_{dd}^\sigma(\omega)]^{-1} = \omega - \epsilon_d + \Sigma_\sigma(\omega)$, where $\Sigma_\sigma(\omega)$ is the proper self-energy, from which we obtain the normalized local density of states (LDOS), defined as $\tilde{\rho}_\sigma = -\Delta_\sigma(0) \Im[G_{dd}^\sigma(\omega)]$.

Figure 3 shows the LDOS for $V_1 = 0.1414D$, $\phi_{AB} =$
\[\pi/4 \text{ and different } V_2 \text{ and } \phi_{\text{SO}}.\] Starting with \(V_2 = 2D/\pi\) and \(\phi_{\text{SO}} = \pi/16\) in Fig. 2, one can see a small spin-resolved shift in the Kondo peak, in addition to a clear \(\phi\) asymmetry in resolved shift in the Kondo peak, in addition to a clear \(\phi\) and \(\pi/2\) for \(V_2 = 2D/\pi\) vs \(\phi_{\text{SO}}\). Central inset shows QD effective free moment \(\mu^2\) for \(V_2 = 2D/\pi\) vs \(\phi_{\text{SO}}\).

We calculate the conductance in the zero-bias regime, which can be written as \(G_{\sigma} = G_0 \cdot T_0 - 2\Delta_0 \sqrt{T_0 R_0 \cos(\phi_{\sigma})} \Re \{G_{4d}^\sigma(0)\} - \Delta_0 \{1 - T_0[1 + \cos^2(\phi_{\sigma})]\} \Im \{G_{4d}^\sigma(0)\},\)

where \(G_0 = e^2/h, T_0 = 4r/(1 + r)^2\) is the transmission through the upper arm of the ring, \(R_0 = 1 - T_0, \Delta_0 = \Delta_0/(1 + r),\) with \(r = \pi^2 V_2^2/4 D^2,\) and \(\Delta_0 = 2\pi V_2^2/D.\)

The conductance \(G_{\sigma}\) is shown in Fig. 4 as function of the LDOS for different values of the in-plane magnetic field \(B\) for the case with \(V_1 = 0.1414D, V_2 = 2D/\pi,\) and \(\phi_{\text{SO}} = \phi_{AB} = \pi/4\) (same as in Fig. 2). Notice that by increasing the Zeeman field the Kondo peaks are progressively restored and reach their maximum height for \(B = 0.0049\) (notice this field is measured in energy units, and would correspond to several tesla in GaAs—of course, the compensating field depends on the parameters of the system, especially \(V_2\) and \(\phi_{\text{SO}}\)). Increasing \(B\) further, rapidly suppresses the Kondo peak, as seen in Fig. 4, overcompensating the intrinsic magnetic field. The inset of Fig. 4 depicts \(\mu^2\) vs \(B\), showing that \(\mu^2 \to 0\) as \(B \to 0.0049\), and the complete screening of the local magnetic moment is restored. Notice that the amplitude of the Kondo peak, although restored by the Zeeman field, is somewhat different for spin \(\uparrow\) and \(\downarrow\). This asymmetry in spins arises not only from differences in \(\Delta_\sigma\), especially as \(\Delta_\uparrow(0) = \Delta_\downarrow(0),\) but rather from the fact that \(|\delta\Lambda_\downarrow(0)| > |\delta\Lambda_\uparrow(0)|\), as seen in Fig. 4b. This demonstrates the non-trivial effect of the p-h asymmetry and the importance of considering it fully when evaluating the role of electronic interactions. Moreover, as we will now describe, this asymmetry has dramatic effects on the conductance of the system and on its spin filtering properties.
the Zeeman field, for the same parameters of Fig. 3. Notice that while \( G_1 \) remains in the unitary limit, \( G_1 \) drops sharply near \( B \approx 0.0049 \). This behavior can be understood in terms of the contribution to the conductance in Eq. (2). For \( V_2 = 2D/\pi, r = T_0 = 1 \) and \( R_0 = 0 \); in this case the second term gives no contribution and the third term becomes \( \Delta_0 \cos^2(\phi_0) \text{Im}[G_{dd}(0)] \). For \( \phi_{SO} \approx \phi_{AB} = \pi/4 \), \( G_1/G_0 \approx 1 \) and \( G_1/G_0 = 1 - \Delta_0 \pi \phi_0 \approx 0 \) [17], which gives the spin filtering condition (other values of the phases result in smaller contrast for the two spins). In Fig. 4, we fix \( \phi_{AB} = \pi/4 \) and \( B = 0.0049 \) and plot the conductance as function of \( \phi_{SO} \). We see that \( G_1 \) remains close to the unitary limit in the interval \( 0 < \phi_{SO} < \pi/2 \) while \( G_1 \) vanishes for \( \phi_{SO} = \pi/4 \); the opposite occurs in the complementary interval. The spin polarization of the conductance, \( \eta = (G_1 - G_{1'})/(G_1 + G_{1'}) \), as function of \( \phi_{SO} \) is shown in Fig. 4. Notice that for \( \phi_{SO} = \pi/4 \) and \( \phi_{SO} = 3\pi/4 \) the system exhibits almost perfect spin polarized conductance.

In conclusion, we have shown that the combination of SO interaction and AB effect results in an effective magnetic field that strongly suppresses the Kondo resonance. As a consequence, the transport behavior and the possibility of producing spin polarized conductance is greatly affected. However, we show it is possible to fully restore the Kondo state screening and spin polarized transport by applying an in-plane Zeeman field. Apart from its importance in spin polarized transport, this effect emphasizes the subtle interplay of many body correlations and their control via external fields. It would be interesting to explore this effect by measuring spin polarized currents in this geometry.

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FIG. 4: (color online) (a) Conductance vs Zeeman field for Fig. 3 parameters. (b) \( G_1 \) vs SO phase for \( V_2 = 0.1414D \), \( V_2 = 2D/\pi, \phi_{AB} = \pi/4 \) and \( B = 0.0049 \). (c) Conductance polarization \( \eta \) (see text) vs \( \phi_{SO} \) for conductances of panel (b).