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Gate-controlled spin splitting in quantum dots with ferromagnetic leads in the Kondo regime

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The effect of a gate voltage (V_g) on the spin splitting of an electronic level in a quantum dot (QD) attached to ferromagnetic leads is studied in the Kondo regime using a generalized numerical renormalization group technique. We find that the V_g dependence of the QD level spin splitting strongly depends on the shape of the density of states (DOS). For one class of DOS shapes there is nearly no V_g dependence; for another, V_g can be used to control the magnitude and sign of the spin splitting, which can be interpreted as a local exchange magnetic field. We find that the spin splitting acquires a new type of logarithmic divergence. We give an analytical explanation for our numerical results and explain how they arise due to spin-dependent charge fluctuations.

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The manipulation of magnetization and spin is one of the fundamental processes in magnetoelectronics and spintronics, providing the possibility of writing information in a magnetic memory,[1] and also because of the possibility of classical or quantum computation using spin. In most situations this is realized by means of an externally applied, nonlocal magnetic field which is usually difficult to insert into an integrated circuit. Recently, it was proposed to control the magnetic properties, such as the Curie temperature of ferromagnetic semiconductors, by means of an electric field: In gated structures,[2] due to the modification of carrier-density-mediated magnetic interactions, such properties can be modified by a gate voltage. In this communication we propose to control the amplitude and sign of the spin splitting of a quantum dot (QD) induced by the presence of ferromagnetic leads, only by using a gate voltage without further assistance of a magnetic field. As a representative (but not the only) example of this effect we investigate its influence on the Kondo effect and its spin splitting, which acts as a very sensitive probe of the spin state of the dot and the effective local magnetic field in the QD generated by exchange interaction with the ferromagnetic leads.

Recently, the possibility of the Kondo effect in a QD attached to ferromagnetic electrodes was widely discussed,[3–9] and it was predicted that the Kondo resonance is split and suppressed in the presence of ferromagnetic leads.[7,8] This prediction has since been verified experimentally.[10] It was shown that this splitting can be compensated by an appropriately tuned external magnetic field, and the Kondo effect is thereby restored.[7,8] In all previous studies of QDs attached to ferromagnetic leads[3–9] an idealized, flat, spin-independent density of states (DOS) with spin-dependent tunneling amplitudes was considered. However, since the spin splitting arises from renormalization effects, i.e., is a many-body effect, it depends on the *full* DOS structure of the involved material, and not only on its value at the Fermi surface. In realistic ferromagnetic systems, the DOS shape is strongly asymmetric due to the Stoner splitting and the different hybridization between the electronic bands.[1]

In this communication we demonstrate that the gate voltage dependence of the spin splitting of a QD level, and the resulting splitting and suppression of the Kondo resonance, are determined by the DOS structure and can lead to crucially different behaviors. We apply the numerical renormalization group (NRG) technique extended to handle bands of arbitrary shape. For one class of DOS shapes, we find almost no V_g dependence of the spin splitting, while for another class the induced spin splitting, which can be interpreted as the effect of a local exchange field, can be controlled by V_g. The spin splitting can be fully compensated and its direction can even be reversed within this class. We explain the physical mechanism that leads to this behavior, which is related to the compensation of the renormalization of the spin-dependent QD levels induced by electronlike and holelike quantum charge fluctuations. Moreover, we find that for the QD level close to the Fermi surface, the amplitude of the spin splitting has a logarithmic divergence, indicating the many-body character of this phenomenon.

Model and method.—The Anderson model (AM) of a single level QD with energy ϵ_0 and Coulomb interaction U, coupled to parallel-oriented ferromagnetic leads, is given by

$$H = \sum_{rk\sigma} \epsilon_{rk\sigma} c^{\dagger}_{rk\sigma} c_{rk\sigma} + \epsilon_0 \sum_{\sigma} \hat{n}_{\sigma} + U \hat{n}_{\uparrow} \hat{n}_{\downarrow} + \sum_{rk\sigma} (V_{rk} d^{\dagger}_{\sigma} c_{rk\sigma} + \mathrm{h.c}) - B S_z. \quad (1)$$

Here $c_{rk\sigma}$ and $d_{\sigma}(\hat{n}_{\sigma}=d^{\dagger}_{\sigma}d_{\sigma})$ are Fermi operators for electrons with momentum k and spin σ in the leads $(r=L/R)$, and in the QD, V_{rk} is the tunneling amplitude, $S_z=(\hat{n}_\uparrow-\hat{n}_\downarrow)/2$, and the last term denotes the Zeeman energy of the dot. The energy ϵ_0 is experimentally controllable by V_g ($\epsilon_0 \simeq V_g$).

To discuss the gate voltage dependence of the QD level spin splitting, we consider a more realistic, both energy- and spin-dependent band structure [$\rho_{r\uparrow}(\omega) \neq \rho_{r\downarrow}(\omega)$], violating *p-h* symmetry $\rho_{r\sigma}(\omega) \neq \rho_{r\sigma}(-\omega)$. This leads to an energy-dependent hybridization function $\Gamma_{r\sigma}(\omega)=\pi\Sigma_k \delta(\omega-\epsilon_{k\sigma})V_{rk}^2 = \pi\rho_{r\sigma}(\omega)V_0^2$, where we take $V_{rk}=V_r$ to be constant. We apply the NRG method[11,12] extended to handle arbitrary DOS shapes and asymmetry. To this end, the standard logarithmic discretization of the conduction band is performed for *each* spin component separately, with the bandwidths, $D_\uparrow=D_\downarrow=D_0$.

Within each interval $[-\omega_n, -\omega_{n+1}]$ and $[\omega_{n+1}, \omega_n]$ (with $\omega_n=D_0\Lambda^{-n}$) of the logarithmically discretized conduction band (CB) the operators of the continuous CB are expressed in terms of a Fourier series. Even though we allow for a nonconstant conduction electron DOS, it is still possible to transform the Hamiltonian such that the impurity couples *only* to the zeroth-order component of the Fourier expansion of each interval.[13] Dropping the nonconstant Fourier components of each interval[11,12] then results in a discretized version of the Anderson model with the continous spectrum in each interval replaced by a single fermionic degree of freedom (independently for both spin directions). Since we allow for an arbitrary DOS for *each* spin component σ of the CB this mapping needs to be performed for each σ separately. This leads to the Hamiltonian

$$H = \sum_\sigma \epsilon_\sigma \hat{n}_\sigma + U\hat{n}_\uparrow\hat{n}_\downarrow + \sqrt{\xi_{0\sigma}/\pi}\sum_\sigma [d_\sigma^\dagger f_{0\sigma} + f_{0\sigma}^\dagger d_\sigma] + \sum_{\sigma n=0}^{\infty} [\varepsilon_{n\sigma} f_{n\sigma}^\dagger f_{n\sigma} + t_{n\sigma}(f_{n\sigma}^\dagger f_{n+1\sigma} + f_{n+1\sigma}^\dagger f_{n\sigma})], \quad (2)$$

where $f_{n\sigma}$ are fermionic operators at the nth site of the Wilson chain, $\xi_{0\sigma}=1/2\int_{-D_0}^{+D_0}\Gamma_\sigma(\omega)d\omega$ [$\Gamma_\sigma(\omega)=\Sigma_r\Gamma_{r\sigma}(\omega)$], $t_{n\sigma}$ denotes the hopping matrix elements, and $\epsilon_\sigma=\epsilon_0-BS_z$. The absence of particle-hole symmetry leads to the appearance of nonzero on-site energies, $\varepsilon_{n\sigma}$ along the chain. In this *general* case no closed expression for the matrix elements $t_{n\sigma}$ and $\varepsilon_{n\sigma}$, both depending on the particular structure of the DOS via $\Gamma_\sigma(\omega)$, is known; they have to be determined recursively.[14]

We calculate the level occupation $n_\sigma \equiv \langle \hat{n}_\sigma \rangle$ and the ϵ_0-dependent spin-resolved single-particle spectral density $A_\sigma(\omega)=-(1/\pi)\mathrm{Im}\,\mathcal{G}_\sigma^r(\omega)$, where $\mathcal{G}_\sigma^r(\omega)$ denotes a retarded Green's function, via Eq. (2). For symmetric coupling $\Gamma_{L\sigma}(\omega)=\Gamma_{R\sigma}(\omega)$ the spin-resolved conductance takes the form $G_\sigma=\pi(e^2/h)\int_{-\infty}^{+\infty}d\omega\Gamma_\sigma(\omega)A_\sigma(\omega)(-[\partial f(\omega)/\partial\omega])$, where $f(\omega)$ is the Fermi function.

Spectral function and conductance.—Here, we focus our attention on $T=0$ properties. We have analyzed several types of DOS shapes and found three typical classes of the V_g dependence of the Kondo resonance splitting, which smoothly cross over into another. Since our method enables us to perform NRG calculations for arbitrary band shapes, we decide to choose an example which turns out to encompass all three classes, namely $\rho_\sigma(\omega) = \frac{1}{2}(3\sqrt{2}/8)D^{-3/2}(1+\sigma Q)\sqrt{\omega+D+\sigma\Delta}$, where $\omega\in[-D-\sigma\Delta, D-\sigma\Delta]$, $D_0=D+\Delta$, [$\sigma\equiv 1(-1)$ for $\uparrow(\downarrow)$], a square-root shape DOS equivalent to a parabolic band (as for free electrons) with Stoner splitting Δ (Ref. 15), and some additional spin and *p-h* asymmetry Q, which modifies the amplitude of the DOS [see Fig. 1 (insets)].

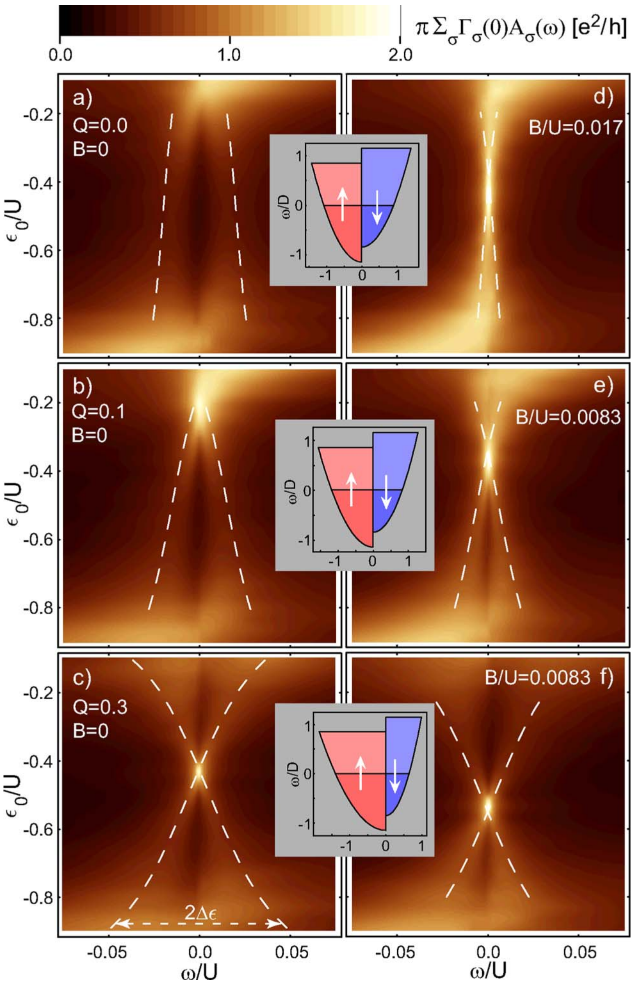

FIG. 1. (Color online) V_g dependence of the spin splitting: Normalized spectral function $\pi\Sigma_\sigma\Gamma_\sigma(0)A_\sigma(\omega)$ as a function of energy ω and gate voltage ϵ_0, for the three different parabolic DOS shapes [insets: corresponding DOS for spin ↑ (red) and ↓ (blue)] characterized by a different Q, which modifies both the spin and *p-h* asymmetry: (a-c) for magnetic field $B=0$, (d) $B/U=0.017$, (e) and (f) $B/U=0.0083$. The white dashed lines are obtained using Eq. (3). Here $U=0.12D_0$, $\pi V_0^2=UD/6$, $\Delta=0.15D$, and $T=0$.

In Fig. 1 we present the weighted spectral function $\widetilde{A}(\omega)\equiv \pi e^2/h\Sigma_\sigma\Gamma_\sigma(0)A_\sigma(\omega)$, normalized such that for $\omega=0$ it corresponds to the linear conductance $G=\widetilde{A}(0)$, as a function of energy ω and ϵ_0. We focus on a narrow energy window around the Fermi surface where the Kondo resonance appears; charge resonances are visible when ϵ_0 or $U+\epsilon_0$ approach the Fermi surface, namely at energies $\epsilon_0/U \gtrsim -0.1$ or $\lesssim -0.9$. Although the NRG method is designed to calculate equilibrium transport, one can still roughly deduce, from the spin splitting of the Kondo resonance of the equilibrium spectral function $\widetilde{A}(\omega)$, the splitting of the zero-bias anomaly ΔV in the nonequilibrium conductance $G(V)$, since $e\Delta V \sim 2\Delta\epsilon$ (Ref. 7) ($\Delta\epsilon \equiv \widetilde{\epsilon}_\uparrow - \widetilde{\epsilon}_\downarrow$ is the splitting of the renormalized levels).

We present $\widetilde{A}(\omega)$ for three DOS shapes depicted in the insets of Fig. 1: (i) $Q=0$ (a,d), (ii) $Q=0.1$ (b,e), and (iii) $Q=0.3$ (c,f), with $2\Delta=0.3D$ (Ref. 16). Changing the parameter Q, which tunes the spin and p-h asymmetry [see the definition of $\rho_\sigma(\omega)$], causes the ϵ_0 dependence of the Kondo resonance splitting to display three different classes of behavior, which smoothly cross over into another [and whose origin is explained after Eq. (3) below]. For (i) we hardly find any ϵ_0 dependence of the spin splitting; for (ii) a strong ϵ_0 dependence without compensation of the spin splitting in the local-moment regime, and for (iii) a strong ϵ_0 dependence with a compensation (i.e., a crossing) and a change of the direction of the QD magnetization. The compensation (crossing) corresponds to the very peculiar situation where the Kondo effect (strong coupling fixed point) can be recovered in the presence of ferromagnetic leads without any external magnetic field. A behavior as presented in Figs. 1(a) and 1(b) was recently observed experimentally,[17] where indeed a variation of the gate voltage results in two split conduction lines $G(V,V_g)$ which are parallel for one case and converging for the other case, similar to our findings.

Effect of a magnetic field.—In Figs. 1(d)–1(f) we show how a magnetic field B modifies the results of Figs. 1(a)–1(c): in (i) the spin splitting can be compensated at a particular magnetic field $B_{\rm comp}$ ($B_{\rm comp}/U=0.017$) and the Kondo effect is visible in a wide range of ϵ_0; for (ii), at $B/U=0.0083$, the Kondo effect is recovered only at one particular ϵ_0 value, which depends on the applied magnetic field; case (iii) shows that the crossing point shifts with B. Since $B_{\rm comp}$ can be viewed as a measure of the zero-field splitting, $\Delta\epsilon(B=0,\epsilon_0) \simeq -B_{\rm comp}(\epsilon_0)$, the ϵ_0 dependence of $\Delta\epsilon$ can be measured by studying that of $B_{\rm comp}$, for which one needs to measure the linear conductance $G(\epsilon_0,B)$ as a function of both B and ϵ_0. In Figs. 2(a)–2(c) we plot $G(\epsilon_0,B)$ for the three bands of Fig. 1. The two horizontal ridges (resonances) in Figs. 2(a)–2(c) correspond to quantum charge fluctuations (broadened QD level) of width $\sim\Gamma$. The bright lines with finite slope in Figs. 2(a)–2(c) reflect the restored Kondo resonance and hence map out the ϵ_0 dependence of $B_{\rm comp}(\epsilon_0) \simeq -\Delta\epsilon(\epsilon_0)$ when the magnetic field compensates the spin splitting. Interestingly, the spin splitting and the corresponding $B_{\rm comp}$ tend to diverge ($|\Delta\epsilon| \to \infty$) when approaching the charging resonance, as is best visible in Fig. 2(c). From Fig. 2(a)–2(c), it is clear that even for $B=0$, compensation can always be achieved (the bright lines always cross $B=0$); the main difference between the three classes is whether this occurs in the local-moment regime (c) or in the mixed-valence regime (a,b).

Such a finite slope in $G(\epsilon_0,B)$ was observed for a singlet-triplet transition Kondo effect in a two level QD [Fig. 2(d) in Ref. 18]. The corresponding transition leads to a characteristic maximum in the valley between two charging resonances [Fig. 3(c) in Ref. 18], similarly as in our Fig. 2(e). In that system the effective spin asymmetry (assumed by our model) is realized by the asymmetry in the coupling of two QD levels.[19]

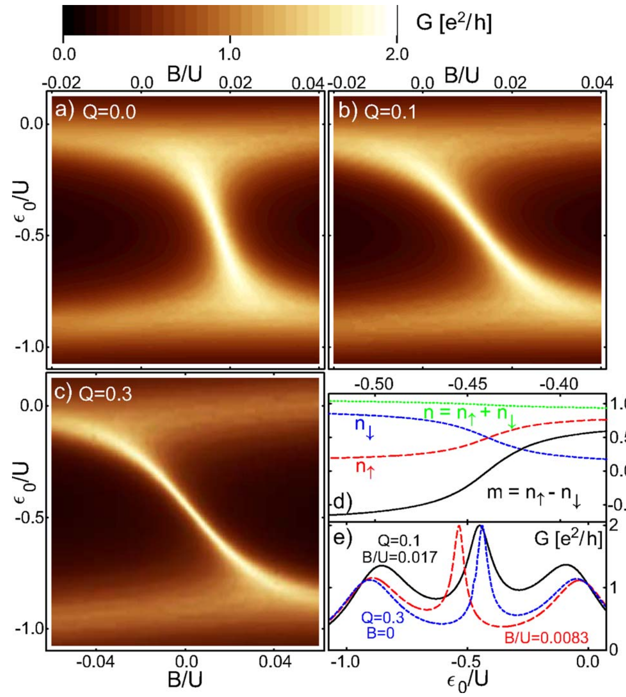

FIG. 2. (Color online) The QD's linear conductance G as a function of gate voltage ϵ_0 and external magnetic field B for the DOS shapes (a) (c) as for Figs. 1(a) and 1(c), respectively. (d) Spin-dependent occupancy n_σ of the dot level as a function of gate voltage ϵ_0 for the DOS shape as in Fig. 1(c) and $B=0$. (d) The ϵ_0 dependence of the total occupancy of the dot n and magnetization m for the situation from Fig. 1(c). (e) The conductance G for the situations from Figs. 1(c) (dashed); 1(d) (solid); and 1(f) (long dashed). Parameters U,Γ, and T as in Fig. 1.

In Fig. 2(d) we show how the occupation n_σ and the magnetic moment (spin) of the QD $m=n_\uparrow - n_\downarrow = 2\langle S_z \rangle$ change as a function of ϵ_0 for the situation of Fig. 1(c). One finds that even though $B=0$, it is possible to control the level spin splitting of the QD and thereby change the average spin direction of the QD from the parallel to antiparallel alignment with respect to the lead's magnetization. This opens the possibility (also for $T \gg T_{\rm K}$, and $T \lesssim \Gamma_\sigma$) of controlling the QD's spin splitting by a gate voltage without further need of an external magnetic field.

Perturbative analysis.—One can understand the behavior presented in Figs. 1(a)–1(c) by using Haldane's scaling method,[20] where charge fluctuations are integrated out. This leads to a spin-dependent renormalization of the QD's level position $\widetilde{\epsilon}_\sigma$ and a level broadening Γ_σ. In contrast to Ref. 7 we consider here the case of finite Coulomb interactions $U<\infty$, which means that also the doubly occupied state $|2\rangle$ is of importance. The spin splitting is then given by $\Delta\epsilon \equiv \delta\epsilon_\uparrow - \delta\epsilon_\downarrow + B$, where[21]

$$\delta\epsilon_\sigma \simeq -\frac{1}{\pi}\int d\omega \left\{ \frac{\Gamma_\sigma(\omega)[1-f(\omega)]}{\omega-\epsilon_\sigma} + \frac{\Gamma_{-\sigma}(\omega)f(\omega)}{\epsilon_{-\sigma}+U-\omega} \right\}. \quad (3)$$

The first term in the brackets corresponds to electronlike processes, namely charge fluctuations between a single occupied state $|\sigma\rangle$ and the empty $|0\rangle$ one, and the second term to holelike processes, namely charge fluctuations between the states $|\sigma\rangle$ and $|2\rangle$. The amplitude of the charge fluctuations is proportional to Γ, which for $\Gamma \gg T$ determines the width of QD levels. Equation (3) shows that $\Delta\epsilon$ depends on the shape of $\Gamma_\sigma(\omega)$ for all ω, not only on its value at the Fermi surface. The same is true for the slope of the bright lines in Figs. 2(a)–2(c), $\partial B_{\mathrm{comp}}/\partial\epsilon_0$. The dashed lines in Figs. 1(a)–1(c) show $\pm\Delta\epsilon$ as a function of ϵ_0 [from Eq. (3)] for the same set of parameters as in the NRG calculation, and are in good agreement with the position of the (split) Kondo resonances observed in the latter. Equation (3) shows that the dramatic changes observed in Fig. 1 upon changing Q are due to the modification of both the *p-h* and spin asymmetry.

Equation (3) predicts that even for systems with spin-asymmetric bands $\Gamma_\uparrow(\omega) \neq \Gamma_\downarrow(\omega)$, the integral can give $\Delta\epsilon = 0$, which corresponds to a situation where the renormalization of ϵ_σ due to electronlike processes are compensated by holelike processes. An example is a system consisting of *p-h* symmetric bands, $\Gamma_\sigma(\omega) = \Gamma_\sigma(-\omega)$, where no splitting of the Kondo resonance ($\Delta\epsilon = 0$) for the symmetric point, $\epsilon_0 = -U/2$, appears. For real systems *p-h* symmetric bands cannot be assumed, however, the compensation $\Delta\epsilon = 0$ is still possible, as shown in Fig. 1(c). Equation (3) also shows that the characteristic energy scale of the spin splitting is given by Γ rather than by the Stoner splitting $\Delta(\Delta \gg \Gamma)$, since the states far from the Fermi surface enter Eq. (3) only with a logarithmic weight. However, the Stoner splitting introduces a strong *p-h* asymmetry, so it can influence the character of gate voltage dependence significantly.

For a flatband $\Gamma_\sigma(\omega) = \Gamma_\sigma$, Eq. (3) can be integrated analytically. For $D_0 \gg U, |\varepsilon_0|$ one finds: $\Delta\epsilon \simeq (P\,\Gamma/\pi)\,\mathrm{Re}[\phi(\epsilon_0) - \phi(U+\epsilon_0)]$, where $P \equiv (\Gamma_\uparrow - \Gamma_\downarrow)/\Gamma$, $\phi(x) \equiv \Psi[\frac{1}{2} + i(x/2\pi T)]$, and $\Psi(x)$ denotes the digamma function. For $T=0$, the spin splitting is given by

$$\Delta\epsilon \simeq (P\,\Gamma/\pi)\ln(|\epsilon_0|/|U+\epsilon_0|), \tag{4}$$

showing a logarithmic divergence for $\epsilon_0 \to 0$ or $U+\epsilon_0 \to 0$. Since any sufficiently smooth DOS can be linearized around the Fermi surface, this logarithmic divergence occurs quite universally, as can be observed in log-linear versions (not shown) of Figs. 2(a) and 2(c). For finite temperature ($T>0$) the logarithmic divergence for $\epsilon_0 \to 0$ or $\epsilon_0 \to -U$ is cut off, $\Delta\epsilon \simeq -(1/\pi)P\Gamma[\Psi(\frac{1}{2}) + \ln(2\pi T/U)]$, which is also important for temperatures $T \ll T_{\mathrm{K}}$.

In conclusion, we used an extended NRG technique for general band shapes to demonstrate the possibility of controlling the local exchange field, and thereby the spin splitting, of a QD attached to ferromagnetic leads by means of the gate voltage. This can be tested experimentally by measuring the linear and nonlinear conductance as a function of gate voltage and magnetic field.

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