Kondo Effect in the Presence of Itinerant-Electron Ferromagnetism Studied with the Numerical Renormalization Group Method

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The Kondo effect in quantum dots (QDs)—artificial magnetic impurities—attached to ferromagnetic leads is studied with the numerical renormalization group method. It is shown that the QD level is spin split due to the presence of ferromagnetic electrodes, leading to a suppression of the Kondo effect. We find that the Kondo effect can be restored by compensating this splitting with a magnetic field. Although the resulting Kondo resonance then has an unusual spin asymmetry with a reduced Kondo temperature, the ground state is still a locally screened state, describable by Fermi liquid theory and a generalized Friedel sum rule, and transport at zero temperature is spin independent.

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The prediction [1] and experimental observation of the Kondo effect in artificial magnetic impurities—semiconducting quantum dots (QDs) [2,3]—renewed interest in the Kondo effect and opened new opportunities of research. The successful observation of the Kondo effect in molecular QDs such as carbon nanotubes [4,5] and single molecules [6] attached to metallic electrodes opened the possibility to study the influence of many-body correlations in the leads (superconductivity [7] or ferromagnetism) on the Kondo effect. Recently, the question arose whether the Kondo effect in a QD attached to ferromagnetic leads can occur or not. Several authors have predicted [8–11] that the Kondo effect should occur. However, it was shown recently [12] that the QD level will be spin split due to the presence of ferromagnetic electrodes leading to a suppression of the Kondo effect, and that the Kondo resonance can be restored only by applying an external magnetic field. The analyses of Refs. [8–12] were all based on approximate methods.

In this Letter, we resolve the controversy by adapting the numerical renormalization group (NRG) technique [13,14], one of the most accurate methods available to study strongly correlated systems in the Kondo regime, to the case of a QD coupled to ferromagnetic leads with parallel magnetization directions. We find that, in general, the Kondo resonance is split, similar to the usual magnetic-field-induced splitting [15,16]. However, we find that, by appropriately tuning an external magnetic field, this splitting can be fully compensated and the Kondo effect can be restored [17](confirming Ref. [12]). We point out that precisely at this field the occupancy of the local level is the same for spin-up and -down, $n_\uparrow = n_\downarrow$, a fact that follows from the Friedel sum rule [19]. Moreover, we show that the Kondo effect then has unusual properties such as a strong spin polarization of the Kondo resonance and, just as for ferromagnetic materials, for the density of states (DOS). Nevertheless, despite the spin asymmetries in the DOS of the QD and the leads, the symmetry in the occupancy $n_\uparrow = n_\downarrow$ implies that the system's ground state can be tuned to have a fully compensated local spin, in which case the QD conductance is found to be the *same* for each spin channel, $G_\uparrow = G_\downarrow$.

The model.—For ferromagnetic leads, electron-electron interactions in the leads give rise to magnetic order and spin-dependent DOS $\rho_{r\uparrow}(\omega) \neq \rho_{r\downarrow}(\omega)$, ($r =$ L, R). Magnetic order of typical band ferromagnets such as Fe, Co, and Ni is mainly related to electron correlation effects in the relatively narrow $3d$ subbands, which only weakly hybridize with $4s$ and $4p$ bands [20]. We can assume that, due to a strong spatial confinement of d electron orbitals, the contribution of electrons from d subbands to transport across the tunnel barrier can be neglected [21]. In such a situation, the system can be modeled by noninteracting [22] s electrons, which are spin polarized due to the exchange interaction with uncompensated magnetic moments of the completely localized d electrons. In the mean-field approximation, one can model this exchange interaction as an effective molecular field, which removes spin degeneracy in the system of noninteracting conducting electrons, leading to a spin-dependent DOS. The Anderson model (AM) for a QD with a single energy level $\epsilon_{\rm d}$, which is coupled to ferromagnetic leads, is given by

$$\tilde{H} = \sum_{rk\sigma} \epsilon_{rk\sigma} c^\dagger_{rk\sigma} c_{rk\sigma} + \epsilon_{\rm d} \sum_{\sigma} \hat{n}_\sigma + U \hat{n}_\uparrow \hat{n}_\downarrow + \sum_{rk\sigma} (V_{r,k} d^\dagger_\sigma c_{r,k\sigma} + V^*_{r,k} c^\dagger_{r,k\sigma} d_\sigma) - g\mu_B B S_z. \quad (1)$$

Here $c_{rk\sigma}$ and d_σ ($\hat{n}_\sigma = d^\dagger_\sigma d_\sigma$) are the Fermi operators for electrons with momentum k and spin σ in the leads and, in the QD, V_{rk} is the tunneling amplitude, $S_z = (\hat{n}_\uparrow - \hat{n}_\downarrow)/2$, and the last term is the Zeeman energy of the dot. All information about spin asymmetry in the leads can be modeled by the spin-dependent hybridization function $\Gamma_{r\sigma}(\omega) = \pi\sum_k \delta(\omega - \epsilon_{k\sigma})V_{r,k}^2 = \pi\rho_{r\sigma}(\omega)V_r^2$, where $V_{r,k} \equiv V_r$ and $\rho_{r\sigma}(\omega)$ is the spin-dependent DOS.

In order to understand the Kondo physics of a QD attached to two identical ferromagnetic electrodes with parallel configurations, it suffices to study, instead of the above general model [Eq. (1)], a simpler one, which captures the same essential physics, namely, the fact that $\Gamma_{r\uparrow}(\omega) \neq \Gamma_{r\downarrow}(\omega)$ will generate an effective local magnetic field, which lifts the degeneracy of the local level (even for $B = 0$). A simple (but not unique) way of modeling this effect is to take the DOS in the leads to be constant and spin independent, $\rho_{r\sigma}(\omega) \equiv \rho$, the bandwidths to be equal $D_\uparrow = D_\downarrow$, and lump all spin dependence into the spin-dependent hybridization function, $\Gamma_{r\sigma}(\omega)$, which we take to be ω independent, $\Gamma_{r\sigma}(\omega) \equiv \Gamma_{r\sigma}$. By means of a unitary transformation [1], the AM [Eq. (1)] can be mapped onto a model in which the correlated QD level couples only to one electron reservoir described by Fermi operators $\alpha_{k\sigma}$ with strength $\Gamma_\sigma = \sum_r \Gamma_{r\sigma}$:

$$H = \sum_{k\sigma} \epsilon_k \alpha_{k\sigma}^\dagger \alpha_{k\sigma} + \epsilon_{\rm d} \sum_\sigma \hat{n}_\sigma + U\hat{n}_\uparrow \hat{n}_\downarrow + \sum_{k\sigma} \sqrt{\Gamma_\sigma/(\pi\rho)}(d_\sigma^\dagger \alpha_{k\sigma} + \alpha_{k\sigma}^\dagger d_\sigma) - g\mu_{\rm B} B S_z. \quad (2)$$

Finally, we parametrize the spin dependence of Γ_σ in terms of a spin-polarization parameter $P \equiv (\Gamma_\uparrow - \Gamma_\downarrow)/\Gamma$, by writing $\Gamma_{\uparrow(\downarrow)} \equiv \frac{1}{2}\Gamma(1 \pm P)$, where $\Gamma \equiv \Gamma_\uparrow + \Gamma_\downarrow$.

In the model of Eq. (2), we allowed for $\Gamma_\uparrow \neq \Gamma_\downarrow$ but not for $D_\uparrow \neq D_\downarrow$, as would be appropriate for real ferromagnets, whose spin-up and -down bands always have a Stoner splitting $\Delta D \equiv D_\uparrow - D_\downarrow$, with typical values $\Delta D/D_\uparrow \lesssim 20\%$ (for Ni, Co, and Fe). However, no essential physics is thereby lost, since the consequence of taking $D_\uparrow \neq D_\downarrow$ is the same as that of taking $\Gamma_\uparrow \neq \Gamma_\downarrow$, namely, to generate an effective local magnetic field [25].

The occurrence of the Kondo effect requires spin fluctuations in the dot as well as zero-energy spin-flip excitations in the leads. Indeed, a Stoner ferromagnet without full spin polarization $-1 < P < 1$ provides zero-energy Stoner excitations [26], even in the presence of an external magnetic field.

Method.—The model [Eq. (2)] can be treated by Wilson's NRG method. This method, with recent improvements related to high-energy features and finite magnetic field [15,16], is a well-established method to study the Kondo impurity (QD) physics. It allows one to calculate the level occupation $n_\sigma \equiv \langle \hat{n}_\sigma \rangle$ (a static property), the QD spin spectral function, $\mathrm{Im}\,\chi_s^z(\omega) = \mathcal{F}\{i\Theta(t)\langle[S_z(t), S_z(0)]\rangle\}$, where $\mathcal{F}$ denotes the Fourier transform, and the spin-resolved single-particle spectral density $A_\sigma(\omega, T, B, P) = -\frac{1}{\pi}\mathrm{Im}\,\mathcal{G}_{{\rm d},\sigma}^{\rm R}(\omega)$ for arbitrary temperature T, magnetic field B, and polarization P [where $\mathcal{G}_{{\rm d},\sigma}^{\rm R}(\omega)$ denotes a retarded Green function]. From this we can find the spin-resolved conductance $G_\sigma = (e^2/\hbar)(2\lambda)/(\lambda+1)^2\Gamma_\sigma \int_{-\infty}^{\infty} d\omega\, A_\sigma(\omega) \times \{-\partial f(\omega)/\partial\omega\}$, where $f(\omega)$ is the Fermi function and $\lambda = \Gamma_{{\rm L}\sigma}/\Gamma_{{\rm R}\sigma}$ denotes the coupling asymmetry. We choose $\lambda = 1$ below.

Generation and restoration of spin splitting.—In this Letter, we focus exclusively on the properties of the system at $T = 0$ in the local moment regime, where the total occupancy of the QD, $n = \sum_\sigma n_\sigma \approx 1$. The occurrence of charge fluctuations broadens and shifts the position of the QD levels (for both spin-up and -down), and, hence, changes their occupation. For $P \neq 0$, the charge fluctuations and, hence, level shifts and level occupations become *spin dependent*, causing the QD level to split [12] and the dot magnetization $n_\uparrow - n_\downarrow$ to be finite (Fig. 1). As a result, the Kondo resonance is also spin split [28,29] and weakened (Fig. 2), similarly to the effect of an applied magnetic field [15,16]. This means that Kondo correlations are reduced or even suppressed in the presence of ferromagnetic leads. However, for any fixed P, it is possible to compensate the splitting of the Kondo resonance [Figs. 2(c) and 3(c)] by fine-tuning the magnetic field to an appropriate value, $B_{\rm comp}(P)$, defined as the field which maximizes the height of the Kondo resonance. This field is found to depend linearly [27] on P [Fig. 1(c)] (as predicted in [12] for $U \to \infty$). Remarkably, we also find (throughout the local moment regime) that at $B_{\rm comp}$ the local occupancies satisfy $n_\uparrow = n_\downarrow$ [Fig. 1(b)]. The fact that this occurs simultaneously with the disappearance of the Kondo resonance splitting suggests that the local spin is fully screened at $B_{\rm comp}$.

Spectral functions.—We henceforth fix the magnetic field at $B = B_{\rm comp}(P)$. To learn more about the properties of the corresponding ground state, we computed the spin spectral function $\mathrm{Im}\{\chi_s^z(\omega)\}$ for several values of P at $T = 0$ (Fig. 3). Its behavior is characteristic for the formation of a local Kondo singlet: As a function of decreasing frequency, the spin spectral function shows a

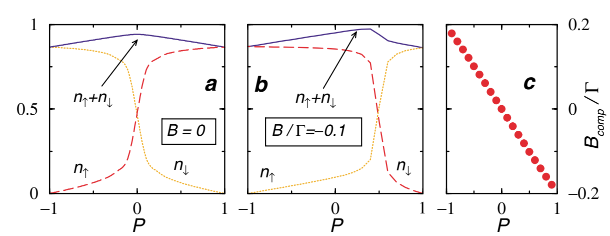

FIG. 1 (color online). Spin-dependent occupation of the dot level at (a) $B = 0$ and (b) $B = -0.1\Gamma$, as a function of spin polarization P. (a) For $B = 0$, the condition $n_\uparrow = n_\downarrow$ holds only at $P = 0$. (b) For finite P, it can be satisfied if a finite, fine-tuned magnetic field, $B_{\rm comp}(P)$, is applied, whose dependence on P is shown in (c). As expected, it is approximately linear [12,27]. Here $U = 0.12D$, $\epsilon_{\rm d} = -U/3$, $\Gamma = U/6$, and $T = 0$.

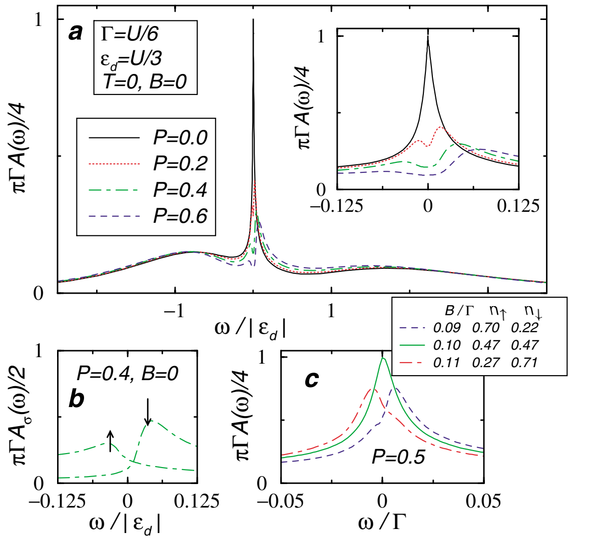

FIG. 2 (color online). (a) QD spectral function $A(\omega) = \sum_\sigma A_\sigma(\omega)$ for several values of spin polarization P; inset: expanded scale of $A(\omega)$ around ϵ_F. (b) The spin-resolved spectral function for fixed P. For $P \to -P$, we have $A_\sigma \to A_{-\sigma}$. (c) Compensation of the spin splitting by fine-tuning an external magnetic field. Parameters U, ϵ_d, Γ, and T as in Fig. 1.

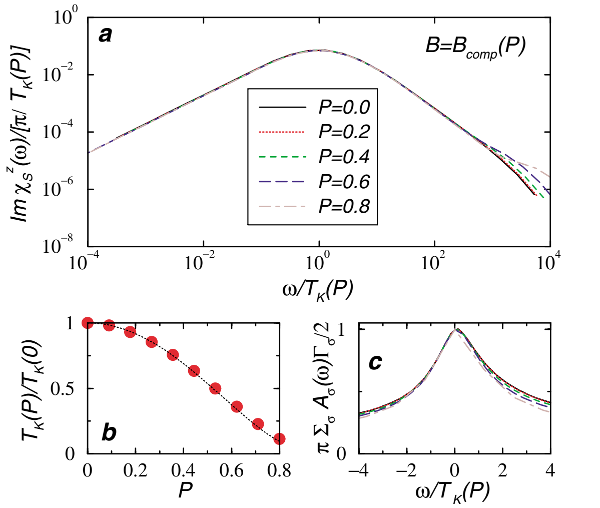

FIG. 3 (color online). (a) The spin spectral function $\mathrm{Im}\{\chi_s^z(\omega)\}$. (b) Dependence of T_K on spin polarization P. The dotted line shows the prediction from Ref. [12]—namely, $T_K(P)/T_K(0) = \exp[C \operatorname{arctanh}(P)/P]$, where the best fit is obtained for $C = -5.98$. Equation (6) from Ref. [12] with $(\rho_\uparrow + \rho_\downarrow)J_0 = (\Gamma/\pi)U/[|\epsilon_d|(U + \epsilon_d)]$ would lead to $C = -4.19$. (c) QD spectral function for several values of P. Parameters U, ϵ_d, Γ, and T are as in Fig. 1, $B = B_{\mathrm{comp}}(P)$.

maximum at a frequency $\omega_{\max}$ which we associate with the Kondo temperature [i.e., $k_B T_K \equiv \hbar\omega_{\max}$ at $B = B_{\mathrm{comp}}(P)$], and then decreases linearly with ω, indicating the formation of the Fermi liquid state [14]. By determining $T_K(P)$ (from $\omega_{\max}$) for different P values, we find that T_K decreases with increasing P [Fig. 3(b)]. For metals such as Ni, Co, and Fe, where $P = 0.24$, 0.35, and 0.40, respectively, the decrease of T_K is weak, so the Kondo effect should be experimentally accessible. Remarkably, both $\mathrm{Im}\{\chi_s^z(\omega)\}$ and the $A_\sigma(\omega)$ collapse rather well onto a universal curve if plotted in appropriate units [Figs. 3(a) and 3(c)]. This indicates that an applied magnetic field B_{comp} restores the universal behavior characteristic for the isotropic Kondo effect, in spite of the presence of spin-dependent coupling to the leads. Figure 4(a) shows that the amplitude of the Kondo resonance is now strongly spin dependent, which is unusual and unique. The nature of this asymmetry is related to the asymmetry of the DOS in the leads, and its value is exactly proportional to $\sim 1/\Gamma_\sigma$. As a result, the total conductance G_σ is not spin dependent [Fig. 4(b)]. This indicates the robustness of the Kondo effect in this system: If the external magnetic field has been tuned appropriately, it is able to compensate the presence of a spin asymmetry in the leads by creating a proper spin asymmetry in the dot spectral density, thereby conserving a fully compensated local spin and achieving perfect transmission.

Friedel sum rule.—Further insights can be gained from the Friedel sum rule, an exact $T = 0$ relation [19] that holds for arbitrary values of P and B [30]. The interacting Green's function can be expressed as [14] $\mathcal{G}^R_{d,\sigma}(\omega) = [\omega - \epsilon_{d\sigma} + i\Gamma_\sigma - \Sigma_\sigma(\omega)]^{-1}$, with spin dependent $\epsilon_{d\sigma}$ and Γ_σ; the former due to Zeeman splitting ($\epsilon_{d\sigma} = \epsilon_d - 1/2\, \sigma g \mu_B B$) and the latter due to the ferromagnetic leads. Here $\Sigma_\sigma(\omega)$ denotes the spin-dependent self-energy. Now, the Friedel sum rule [19] implies that, at $T = 0$, the following relations hold:

$$n_\sigma = \phi_\sigma/\pi = \frac{1}{2} - \frac{1}{\pi}\tan^{-1}\left(\frac{\epsilon_{d\sigma} - \epsilon_F + \Sigma^R_\sigma(\epsilon_F)}{\Gamma_\sigma}\right), \quad (3)$$

$$A_\sigma(\epsilon_F) = \frac{\sin^2(\pi n_\sigma)}{\pi\Gamma_\sigma}, \quad (4)$$

where $\Sigma^R_\sigma(\omega) \equiv \mathrm{Re}\,\Sigma_\sigma(\omega)$, and $\phi_\sigma(\omega)$ is the phase of $\mathcal{G}^R_{d,\sigma}(\omega)$. Since $\Sigma^R_\uparrow(\epsilon_F) \neq \Sigma^R_\downarrow(\epsilon_F)$, an equal spin occupation, $n_\uparrow = n_\downarrow$, is possible only for $(\epsilon_{d\uparrow} - \epsilon_F + \Sigma^R_\uparrow(\epsilon_F))/\Gamma_\uparrow = (\epsilon_{d\downarrow} - \epsilon_F + \Sigma^R_\downarrow(\epsilon_F))/\Gamma_\downarrow$, which can be obtained only for an appropriate external magnetic field $B = B_{\mathrm{comp}}$. For the latter, in the local moment regime ($n \approx 1$), we have $n_\uparrow = n_\downarrow \approx 0.5$, so that $\phi_\uparrow = \phi_\downarrow \approx \pi/2$, which implies that the peaks of $A_\uparrow$ and $A_\downarrow$ are aligned. Thus, the Friedel sum rule clarifies why the magnetic field B_{comp}, at which the splitting of the Kondo resonance disappears, coincides with that for which $n_\uparrow = n_\downarrow$. For $B = B_{\mathrm{comp}}$, the spin-dependent amplitude $A_\sigma(\epsilon_F)$ of Eq. (4) and the conductance $G_\sigma \sim \Gamma_\sigma A_\sigma(\epsilon_F)$ agree well with the above-mentioned NRG results [Figs. 4(a) and 4(b)].

In conclusion, we showed that the Kondo effect in a QD attached to ferromagnetic leads is in general suppressed, because the latter induce a spin splitting of the QD level, which leads to an asymmetry in the occupancy $n_\uparrow \neq n_\downarrow$. Remarkably, the Kondo effect may nevertheless be restored by applying an external magnetic field B_{comp}, tuned

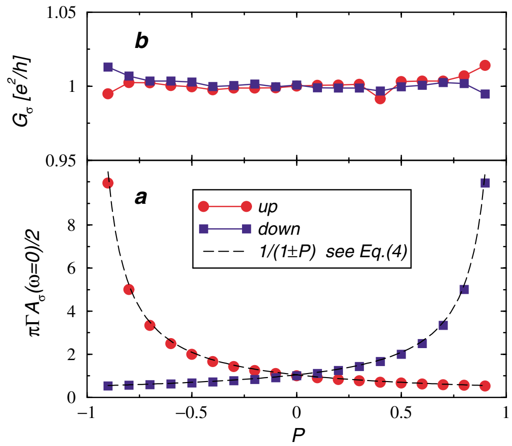

FIG. 4 (color online). (a) Spin resolved QD spectral function amplitude $A_\sigma(\omega = 0)$ at the Fermi level, and (b) the QD conductance G_σ, as functions of the spin polarization P, for $B = B_{comp}(P)$ and symmetric couplings ($\Gamma_{L\sigma} = \Gamma_{R\sigma}$), with U, ϵ_d, Γ, and T as in Fig. 1, implying $n_\sigma \approx 0.5$. The dashed line in (a) is $1/(1 \pm P)$ [Eq. (4) with $n_\sigma = 0.5$]. As expected, we find $G_\sigma = e^2/h$, with a numerical error less than 1%.

such that the splitting of the Kondo resonance is compensated and the condition $n_\uparrow = n_\downarrow$ is fulfilled. Although the Kondo resonance is strongly spin polarized, it then features a locally screened state, a spin-independent conductance, and a Kondo temperature which decreases with increasing spin asymmetry.

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Note added.—After submission of our paper, a preprint [31] studying a similar problem using the NRG technique appeared, with conclusions consistent with ours.

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[29] For certain special (nongeneric) cases, the spin-up and -down level positions and, hence, also the Kondo resonance do not split up in two, even for $P \neq 0$: This occurs, for example, at the symmetry point $\epsilon_d = -U/2$ of the Anderson model, provided the bands are also symmetric around ε_F (but this is unrealistic for ferromagnets).
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