Enhancement of the Kondo Effect through Rashba Spin-Orbit Interactions

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We study a one-orbital Anderson impurity in a two-dimensional electron bath with Rashba spin-orbit interactions in the Kondo regime. The spin SU(2) symmetry-breaking term couples the impurity to a two-band electron gas. A Schrieffer-Wolff transformation shows the existence of the Dzyaloshinsky-Moriya interaction away from the particle-hole symmetric impurity state. A renormalization group analysis reveals a two-channel Kondo model with ferro- and antiferromagnetic couplings. The parity-breaking Dzyaloshinsky-Moriya term renormalizes the antiferromagnetic Kondo coupling with an exponential enhancement of the Kondo temperature.

The search for new materials and architectures appropriate for spintronic and quantum computing devices [1] has renewed the interest on the study of Rashba spin-orbit interactions (RSO) [2] in low-dimensional systems. For systems on surfaces, the natural lack of inversion symmetry makes RSO ubiquitous and particularly relevant for studies of surface-related magnetic properties [3]. Research on this area has been driven by rapid developments of STM techniques that have made possible the design and manipulation of atomic structures on surfaces and study charge and spin physics in two-dimensional (2d) systems. Among the many structures of interest, several groups have focused on the physics of isolated magnetic impurities on metallic substrates to investigate signatures of Kondo physics in two dimensions [4–14]. While these studies have unveiled new physics, they have not addressed the relevance of spin-orbit (SO) interactions possible on many metallic substrates serving as reservoirs for the magnetic impurity. The fact that these interactions can profoundly modify the spin structure on a surface was demonstrated in spin-polarized measurements of Mn impurities on W substrates [15]. Images and characterization of beautiful chiral spin-ordered structures are indeed understood in terms of the strong SO coupling on the surface. Moreover, recent investigations of magnetic impurities on graphene [16,17], the ultimate two-dimensional system, pose the question of the influence of the underlying graphene substrate on measured magnetic properties.

The role of SO interactions in the Kondo regime of magnetic impurities embedded in metallic hosts has been a topic of debate since the early measurements of electrical resistivity in CuMn compounds doped with Pt, carried out by Gainon and Heeger [18]. The reduced divergence in resistivity, interpreted as due to the presence of SO scatterers, was taken as evidence for the suppression of the Kondo effect. Much theoretical and experimental activity followed with rather inconclusive results [19]: while some

works supported the findings of Gainon and Heeger, others reached opposite conclusions. Noting that SO interactions preserve time-reversal symmetry, Meir and Wingreen [20] showed that the Kondo regime is unaffected by SO interactions in the infinite Hubbard-U limit. More recently, however, a solution for a two-dimensional Kondo model in the presence of SO interactions predicts that the Kondo temperature increases by a multiplicative factor proportional to the SO coupling constant [21]. Thus, the question: what is the role of SO interactions in the Kondo regime for two-dimensional systems? remains controversial. The purpose of this Letter is to provide a definitive answer by presenting a solution to the model of a one-orbital Anderson magnetic impurity [22] embedded in a two-dimensional metallic host with RSO interactions. We show that the presence of these interactions reduces the Anderson Hamiltonian to an effective two-band Anderson model coupled to the impurity. By an appropriate Schrieffer-Wolff transformation [23], the Hamiltonian reduces to an effective two-channel Kondo model plus a Dzyaloshinsky-Moriya (DM) [24] interaction term. The renormalization group analysis for this effective Hamiltonian reveals that the impurity couples to the bath with ferro- and antiferromagnetic couplings, with the one-channel Kondo model as the fixed point at low energies. More surprisingly, as we show below, the presence of DM interactions, which vanish at half-filling and at the infinite Hubbard-U limits, introduces an exponential increase in the value of the Kondo temperature.

The model.—The Anderson Hamiltonian of a two-dimensional electron gas in the presence of RSO interactions is given by $H = H_0 + H_U + H_{\text{hyb}} + H_{\text{RSO}}$. Here, $H_0 = \sum_{ks} \varepsilon_k c_{ks}^{\dagger} c_{ks} + \sum_s \varepsilon_d c_{ds}^{\dagger} c_{ds}$ describes free electrons with momentum $\boldsymbol{k}$ and spin s and one spherically symmetric impurity level with energy ε_d. The Hubbard interaction term is given by $H_U = U n_{d\uparrow} n_{d\downarrow}$, with $n_{ds} = c_{ds}^{\dagger} c_{ds}$ as the impurity electron density. The hybridization term

$H_{\text{hyb}} = \sum_{ks} V_k c_{ks}^{\dagger} c_{ds} + \text{H.c.}$ describes the coupling between the impurity and bath electrons in the absence of the RSO interaction. We consider spin-1/2 electrons for the bath and the impurity site and (without loss of generality) V_k to be real and independent of the electron spin. The RSO interaction is described by

$$H_{\text{RSO}} = \sum_k \lambda_R (k_y + ik_x) c_{k\uparrow}^{\dagger} c_{k\downarrow} + \text{H.c.}$$
$$= \sum_k \lambda_R k e^{-i\theta_k} c_{k\uparrow}^{\dagger} c_{k\downarrow} + \text{H.c.}, \qquad (1)$$

with θ_k defined by $k_x = -k\sin\theta_k$, $k_y = k\cos\theta_k$, and $k = |\vec{k}|$. This model allows one to study the effect of the RSO with variable strength λ_R. Notice that the effect of local RSO interactions (acting only at the impurity atom) has been the topic of previous studies [25–31] but is not considered in the present model. An experimental setup where this model is realized consists, for example, of isolated magnetic impurities (Co, Mn, etc.) deposited on the surface of materials with high RSO interactions such as Au(111).

In the angular momentum basis, the electron operators are

$$c_{ks} = \sum_{m=-\infty}^{m=\infty} \frac{e^{im\theta_k}}{\sqrt{2\pi k}} c_{ks}^m; \qquad c_{ks}^m = \sqrt{\frac{k}{2\pi}} \int d\theta_k e^{-im\theta_k} c_{ks}. \quad (2)$$

The canonical transformation

$$c_{kh}^{m+1/2} = (c_k^m{}_{\uparrow} + h c_{k\downarrow}^{m+1})/\sqrt{2} \qquad (3)$$

diagonalizes the bath Hamiltonian in the presence of RSO. Here, $h = \pm 1$ and $j = m + h/2$ are the chirality and angular momentum quantum numbers, respectively. These operators satisfy standard anticommutation relations $\{(c_{kh}^{m+1/2})^{\dagger}, c_{k'h'}^{m'+1/2}\} = \delta_{k,k'} \delta_{h,h'} \delta_{m+1/2;m'+1/2}$.

The corresponding band energies are $\varepsilon_{kh} = \varepsilon_k + \lambda_R kh$. After the transformation, the total Hamiltonian is

$$H = \sum_{khm} \varepsilon_{kh} (c_{kh}^{m+1/2})^{\dagger} c_{kh}^{m+1/2} + H_{\text{imp}} + \sum_{khm} \frac{\tilde{V}_k \delta_{m,0}}{\sqrt{2}}$$
$$\times [(c_{kh}^{m+1/2})^{\dagger} c_{d\uparrow} + (-1)^{[(1-h)/2]} (c_{kh}^{m-1/2})^{\dagger} c_{d\downarrow} + \text{H.c.}], \qquad (4)$$

where $H_{\text{imp}} = \sum_s \varepsilon_d c_{ds}^{\dagger} c_{ds} + H_U$, c_{ds} is the operator for the local orbital in the angular momentum basis, and $\tilde{V}_k = V_k \sqrt{\frac{2\pi}{k}}$. Thus, the RSO term produces an effective two-band ($h = \pm 1$) Anderson problem with the impurity coupled to $j = \pm 1/2$ channels in each band.

The Kondo regime.—To describe the Kondo regime, we perform a Schrieffer-Wolff transformation (SWT) [23]. As in the usual one-impurity Anderson model, the SWT is obtained by requiring the effective Hamiltonian $H_{\text{eff}} = e^S H e^{-S}$ not to contain an H_{hyb} term to first order. The

resulting H_{eff} contains $H_0 + H_U$ with renormalized parameters, plus an exchange Hamiltonian. Using Eqs. (3) and (4), we find S to be given by [32]

$$S = \sum_{kh} T_{kh} [(c_{kh}^{1/2})^{\dagger} c_{d\uparrow} + (c_{kh}^{-1/2})^{\dagger} c_{d\downarrow}] - \text{H.c.},$$
$$T_{kh} = V_k (n_{d\bar{h}} G_{kh} + g_{kh}),$$
$$G_{kh} = \frac{1}{\varepsilon_{kh} - \varepsilon_d - U} - \frac{1}{\varepsilon_{kh} - \varepsilon_d}, \qquad (5)$$
$$g_{kh} = \frac{1}{\varepsilon_{kh} - \varepsilon_d},$$

where we defined $n_{d\bar{h}} = n_{d\downarrow}(n_{d\uparrow})$, for $h = 1(h = -1)$, and $\bar{h} = -h$. As in the usual case, S involves the Green's functions of free particles moving in a bath that contains the localized impurity level. Notice that this transformation reduces to the standard form for the SWT, written in the chiral basis, when the RSO coupling is zero ($\lambda_R = 0$). The SWT reveals that the bath fermions relevant in the Kondo regime are

$$c_{k\pm}^{1/2} = (c_{k\uparrow}^0 \pm c_{k\downarrow}^1)/\sqrt{2}, \qquad c_{k\pm}^{-1/2} = (c_{k\uparrow}^{-1} \pm c_{k\downarrow}^0)/\sqrt{2}, \quad (6)$$

emphasizing the conservation of the total angular momentum in the z direction: a spin flip process is compensated by changes in the orbital angular momentum channels $m = 0, \pm 1$. Once the relevant modes are identified, it is more convenient to return to the original basis to describe band electrons and introduce standard spinor notation. The resulting effective Hamiltonian contains two different terms: $H_{\text{eff}} = \sum_{k,k'} (\mathcal{H}_K + \mathcal{H}_{\text{DM}})$. The first, equivalent to the standard Kondo Hamiltonian, is

$$\mathcal{H}_K = J_{kk'} (\mathbf{s}_{kk'} \cdot \mathbf{S} - \tfrac{1}{4} \rho_{kk'}^c \rho^d), \qquad (7)$$

where $\mathbf{s}_{kk'} = \frac{1}{2} c_{ks}^{\dagger} \boldsymbol{\tau}^{ss'} c_{k's'}$ and $\rho_{kk'}^c = c_{ks}^{\dagger} \tau_0^{ss'} c_{k's'}$. The corresponding definitions for the impurity operators are $\mathbf{S} = \frac{1}{2} c_{ds}^{\dagger} \boldsymbol{\tau}^{ss'} c_{ds'}$ and $\rho^d = c_{ds}^{\dagger} \tau_0^{ss'} c_{ds'}$. Here, $(\boldsymbol{\tau}, \tau_0)$ are the standard Pauli matrices. The Kondo coupling is given by $J_{kk'} = -V_k V_{k'} (G_{k+} + G_{k-} + G_{k'+} + G_{k'-})/2$, is averaged over the chirality quantum number h, and is spin-independent. One can verify that $\mathcal{H}_K$ reduces to the standard Kondo Hamiltonian when $\lambda_R = 0$. In the angular momentum basis (2), this Hamiltonian reads $\mathcal{H}_K \sim J_{kk'} \sqrt{kk'} (\mathbf{s}_{kk'}^0 \cdot \mathbf{S} - \frac{1}{4} \rho_{kk'}^0 \rho^d)$, with $\mathbf{s}_{kk'}^0 = \frac{1}{2} c_{ks}^{0\dagger} \boldsymbol{\tau}^{ss'} c_{k's'}^0$ and $\rho_{kk'}^0 = c_{ks}^{0\dagger} \tau_0^{ss'} c_{k's'}^0$, i.e., involving only the $m = 0$ mode. In this expression, the angular integration has already been carried out.

After some algebra [32], the expression for the second term, $\mathcal{H}_{\text{DM}}$, is

$$\mathcal{H}_{\text{DM}} = i\lambda_R k_F C(\mathbf{k} - \mathbf{k}') \cdot (\mathbf{s}_{kk'} \times \mathbf{S}), \qquad (8)$$

which corresponds to the DM interaction [24]. Here, $\mathbf{k} - \mathbf{k}'$ is a vector in the 2d plane and $\mathbf{s}_{kk'}$ and $\mathbf{S}$ are the bath and impurity spin vectors, respectively. The expression has

been evaluated for scattering processes near the Fermi surface where $\varepsilon_{kh} \approx 0$ and $k \approx k' = k_F$ up to first order in λ_R, with $C = C(\varepsilon_d, U)$. It is important to remark that C vanishes in the limit of $U \to \infty$ and when the impurity state is particle-hole symmetric, i.e., $\varepsilon_d = -U/2$, in agreement with general time-reversal symmetry arguments [20,32]. Similar terms were found in previous works [33], when the hybridization coupling V_k is made to be spin-dependent, i.e., V_{ks}. However, in these models, the DM term does not vanish at the particle-hole symmetric point as expected.

It is also instructive to write the DM term in the angular momentum basis [using Eq. (2) and carrying out the angular integration part], where it reads $\mathcal{H}_{\mathrm{DM}} = \lambda_R k_F C(s_{kk'}^\lambda \cdot S - \frac{1}{4}\rho_{kk'}^\lambda \rho_d)$, where $s_{kk'}^\lambda = \frac{1}{2}(c_{ks}^{0\dagger} \tau^{ss'} c_{k'-s'}^{2s'} + c_{k-s}^{2s\dagger} \tau^{ss'} c_{k's'}^0)$ and $\rho_{kk'}^\lambda = (c_{ks}^{0\dagger} \tau_0^{ss'} c_{k'-s'}^{2s'} + c_{k-s}^{2s\dagger} \tau_0^{ss'} c_{k's'}^0)$. It is clear that this interaction couples the $m = 0$ and $m = \pm 1$ modes of band electrons (as $c_{k-s}^{2s} = c_{k\downarrow}^1$ for $s = \frac{1}{2}$, etc.).

Renormalization group analysis.—To understand the effect of the DM terms in the Kondo regime, we perform a renormalization group (RG) analysis, assuming that $V_k \approx V_{k_F}$ and $J_{kk'} \approx J_{k_F}$. The RG flow reveals the existence of an additional term involving higher energy bands $H_\gamma = \gamma(s_{kk'}^\gamma \cdot S - \frac{1}{4}\rho_{kk'}^\gamma \rho_d)$, introducing a new coupling constant γ. In the angular momentum basis (after angular integration), the expression for $s_{kk'}^\gamma$ reads $s_{kk'}^\gamma = c_{k-s}^{2s\dagger} \tau^{ss'} c_{k'-s'}^{2s'}$ and $\rho_{kk'}^\gamma = c_{k-s}^{2s\dagger} \tau_0^{ss'} c_{k'-s'}^{2s'}$. The resulting coupled equations are

$$\dot{J} = J^2 + \lambda_F^2/4, \qquad \dot{\gamma} = \gamma^2 + \lambda_F^2/4,$$
$$\dot{\lambda}_F = (J + \gamma)\lambda_F, \tag{9}$$

where $\lambda_F = 2C\lambda_R k_F$. These equations become

$$\dot{J}_1 = J_1^2, \qquad \dot{J}_2 = J_2^2, \tag{10}$$

where $J_1 = \frac{1}{2}(J_+ + \sqrt{J_-^2 + \lambda_F^2})$, $J_2 = \frac{1}{2}(J_+ - \sqrt{J_-^2 + \lambda_F^2})$, $J_\pm = J \pm \gamma$, and the ratio $\lambda_F/J_- = \mathrm{constant}$. Equation (10) describes the RG flow of two decoupled Kondo Hamiltonians with couplings J_1 and J_2. Considering an initial condition with $\gamma = 0$ and an antiferromagnetic Kondo coupling $J > 0$, the equations render $J_1 > 0$ and $J_2 < 0$. Therefore, as temperature is lowered, J_1 grows to the strong coupling regime while J_2 goes to zero, hence reducing to the standard one-channel Kondo problem. There is also another possible initial condition that has $J < 0$ (ferromagnetic Kondo Hamiltonian). In this seemingly unfavorable case for the development of a Kondo regime, however, (10) predicts the appearance of an antiferromagnetic coupling at low energies for J_1 while J_2 remains < 0, becoming eventually zero. Note that, in both cases, the final Kondo state is formed by the impurity coupled to a combination of $m = 0$ and ± 1 modes from the bath.

Although the presence of RSO results on known physics in the Kondo regime, its effect on the Kondo temperature is quite dramatic. Away from particle-hole symmetry conditions at the impurity, the DM term increases the Kondo coupling, producing an exponential increase in the Kondo temperature, given by

$$\frac{T_K}{T_0} = \left(\frac{T_0}{D}\right)^{1-J_1/J}, \tag{11}$$

where T_0 is the Kondo temperature in the absence of RSO and D is the bandwidth cutoff [32]. We should note that the change in the coupling J produced by RSO interactions is not compensated by changes in the effective density of states $\rho(\epsilon_F)$ at the Fermi level. One can show that terms in the SWT that can renormalize $\rho(\epsilon_F)$ are of two types: (i) those that are independent of λ_R and as such cannot eliminate the effect of the DM term in J or (ii) those that depend on λ_R via the renormalized value of this coupling. As this last renormalization is mainly due to the presence of the Hubbard term U and the DM corrections depend on both U and ε_d, the correction on $\rho(\epsilon_F)$ can not generically compensate the change in J. These effects can be substantial and significantly enhance T_K. Figure 1 illustrates T_K as a function of the RSO parameter λ_F, changing in a clearly superlinear fashion, unlike the linear increase expected from density-of-state effects [21]. For a Co atom adsorbed on graphene with SiO_2 as a substrate [16], for example, T_0 has been measured to be ≈ 14 K; changing the substrate to Au/Ni has been shown to enhance the RSO strength to $\lambda_R \simeq 0.2$ eV [34]. We estimate $\lambda_F/J \approx 0.3$, which would result in a 20% increase for $T_K \approx 17$ K. We emphasize that this strong enhancement holds in the generic situation away from particle-hole symmetry at the impurity, suggesting that it should be observed in quite general situations.

Conclusion.—In summary, we have analyzed the Kondo regime of an Anderson impurity model with RSO interactions in a 2d electron gas. Because of the broken SU(2) spin symmetry in the presence of RSO, the coupling
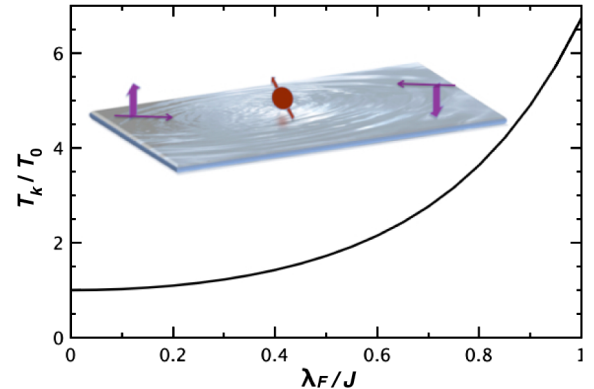

FIG. 1 (color online). The Kondo temperature enhancement due to RSO grows exponentially with λ_F. The inset shows the schematics of the magnetic adatom on the 2d electron gas system with the RSO coupling, where the states for a given momentum have a definite spin.

between impurity and band electrons occurs via a combination of different angular momentum modes in the bath. The resulting two-band model produces a two-channel Kondo regime with ferro- and antiferromagnetic coupling constants, having a standard one-channel Kondo physics as a fixed point. We have shown, in agreement with previous studies, that the effects of the RSO interactions vanish for an impurity in the particle-hole symmetry point. Away from this point, however, RSO interactions introduce dramatic modifications to the Kondo regime by generating a DM term that has been missed in previous studies. The DM term is responsible for an exponential increase in the Kondo temperature. It is reasonable to expect that these effects can be observed in experiments carried on with magnetic atoms placed on the surfaces of different metals [4,35,36] or 2d semiconductor systems [37,38], where the strength of the RSO coupling can be varied. Other interesting candidate systems are those with magnetic adatoms on graphene [16,17], when supported by substrates that enhance the RSO interactions [34,39], or on top of topological insulators [40]. Work along these lines will be reported elsewhere.

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