Kondo effect in the presence of Rashba spin-orbit interaction

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We study the temperature scale of the Kondo screening of a magnetic impurity which hybridizes with a two-dimensional electron gas in the presence of the Rashba spin-orbit interaction. The problem is mapped to an effective single-band impurity model with a hybridization function having an inverse-square-root divergence at the bottom of the band. We study the effect of this divergence on the Kondo screening. The problem is solved numerically without further approximations using the numerical renormalization group technique. We find that the Rashba interaction leads to a small variation of the Kondo temperature (increase or decrease), which depends on the values of the impurity parameters.

The spin-orbit (SO) interaction is a relativistic effect due to the interdependence between electric and magnetic fields when considered from different reference frames. It leads to a coupling between an electron's spin and its (orbital) motion in real space.[1] The effect is stronger in heavy elements from the bottom of the periodic system. The SO interaction plays a central role in many proposals for spintronic devices,[2] and it is the physical origin of the recently discovered topological time-reversal-invariant insulator phases.[3–6] Since the SO interaction does not break the Kramers degeneracy, the Kondo screening of magnetic moments is possible[7–9] and should be observable in magnetic adatoms on topological insulator surfaces or on thin layers of heavy elements.[10]

The Kondo effect, due to magnetic impurities in bulk simple metals, was shown to be strongly suppressed by doping the host material with small amounts of Pt impurities which have large values of the SO coupling constant,[11] although these results have been questioned and the expected trend with the increasing strength of the the SO coupling has not been confirmed in later experiments.[12] An Anderson impurity model with SO scattering term for the conduction-band electrons was studied by performing a Schrieffer-Wolff transformation into an effective Kondo model,[13] and it captured some (but not all) of the observations of Ref. 11. Kondo screening has also been studied through weak-localization effects; the results indicate that adding SO scatterers does not change the magnetic scattering at all.[7,14] It was pointed out that the SO scatterers play the same role as elastic nonmagnetic impurities because they do not break the time-reversal symmetry,[7] and thus the Kondo temperature T_K is expected to remain unchanged, in agreement with the experiment. Because of time-reversal invariance (TRI), the Kondo screening of magnetic moments is expected to occur for magnetic impurities adsorbed on the surfaces of three-dimensional topological insulators,[8,9] unless the doping level is sufficiently high for the spontaneous breaking of the TRI due to magnetic ordering. The effect of the SO coupling in a two-dimensional (2D) electron gas with Rashba SO interaction[1] on the Kondo screening has been studied in Ref. 15. The work was based on a Kondo-impurity Hamiltonian, and after considering to which conduction-band angular modes the impurity spin couples to, a two-channel Kondo model was derived in which each channel has a different

dispersion relation. By expanding the dispersion relations to linear order, in which the Fermi velocity is the same in both helicity channels, and after some further manipulations, the model maps to a single-channel Kondo model with unchanged dimensionless Kondo coupling constant ρJ. In other words, it was predicted that turning on the Rashba coupling (all other parameters remaining the same) does not change T_K at all, except perhaps for some effective bandwidth effects.[15] The same problem has been considered starting from an Anderson impurity model and using the Varma-Yafet variational ansatz.[16] That work did not specifically address the question of T_K beyond noting that it remains constant in the limit of small Rashba coupling but focused instead on the spatial distribution of the spin correlations. Recently, a new study of this system used a Schrieffer-Wolff transformation to obtain an effective two-channel Kondo model with an additional Dzyaloshinsky-Moriya (DM) interaction.[17] Using a scaling renormalization group analysis, it was argued that the DM term renormalizes the Kondo coupling and produces an exponential enhancement of T_K. This effect has not been observed in the previous studies, although the role of the DM coupling has recently been also studied in a different setting where it arises due to spin-dependent hopping amplitudes.[18] Since the cited works are based on various mappings and approximations, it is unclear which result for the variation of T_K (or lack thereof) is correct and what approximations are responsible for the disagreement. For this reason, we re-examine the problem using an approach where all the approximations are well controlled. To wit, we integrate out the conduction-band degrees of freedom to obtain an impurity action with a hybridization function which has an inverse-square-root divergence at the bottom of the band. This step is exact. We then numerically study the effective impurity model using the numerical renormalization group (NRG) method.[19,20] While the NRG approach is not exact, the approximations involved are all well controlled. We find that T_K is only weakly affected by the Rashba interaction: It may weakly (approximately linearly) increase or decrease depending on the values of the impurity parameters.

We study a magnetic impurity embedded in the 2D electron gas with Rashba SO interaction.[1,15–17,21] The impurity is

described using the single-orbital Anderson impurity model H_0 with an additional Rashba interaction term H_{SO}:

$$H_0 = \epsilon(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$$
$$+ \sum_{\mathbf{k}\sigma} \epsilon_k c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} V_k(c_{\mathbf{k}\sigma}^\dagger d_\sigma + \text{H.c.}), \quad (1)$$

$$H_{SO} = \alpha \sum_{\mathbf{k}} \boldsymbol{\psi}_{\mathbf{k}}^\dagger (k_x \sigma_y - k_y \sigma_x) \boldsymbol{\psi}_{\mathbf{k}}$$
$$= \alpha \sum_{\mathbf{k}} k e^{-i\phi_{\mathbf{k}}} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow} + \text{H.c.} \quad (2)$$

The operator $d_\sigma^\dagger$ creates an electron in the impurity level, while $c_{\mathbf{k}\sigma}^\dagger$ correspond to the conduction-band electrons with the dispersion $\epsilon_k = k^2/2m^* + E_0$, where $\mathbf{k}$ is the crystal momentum, $k = |\mathbf{k}|$, m^* the effective electron mass, and E_0 the bottom of the band. Strictly speaking, such dispersion is only valid at the bottom of the band, but for reasons of simplicity we take it to hold up to some high-energy cutoff. The occupancy operator is $n_\sigma = d_\sigma^\dagger d_\sigma$. The chemical potential is set to the energy zero, $\mu = 0$. In H_{SO}, α parameterizes the strength of the Rashba interaction, $\boldsymbol{\psi}_{\mathbf{k}}$ is a spinor field $\{c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}\}^T$, while $\sigma_{x/y}$ are Pauli matrices. k and $\phi_{\mathbf{k}}$ are the polar coordinates of the wave number $\mathbf{k}$, with the polar axis oriented along k_y.

We switch to a continuum representation in a box of volume $\mathcal{V} \equiv 1$. The sums are transformed in the standard way as $\sum_{\mathbf{k}} \rightarrow \mathcal{V}/(2\pi)^2 \int k\,dk\,d\phi$. The operators are transformed as $c_{\mathbf{k}\sigma} \rightarrow (2\pi/\mathcal{V})\psi_{\mathbf{k}\sigma}^\dagger$; they are normalized such that $\{\psi_{\mathbf{k}\sigma}, \psi_{\mathbf{k}'\sigma'}^\dagger\} = \delta^{(2)}(\mathbf{k} - \mathbf{k}')\delta_{\sigma\sigma'}$. Noting that $\delta^{(2)}(\mathbf{k}) = \delta(k)\delta(\phi)/k$, we switch to a polar representation using $\psi_{\mathbf{k}\sigma} \rightarrow 1/\sqrt{k}\xi_{k\phi\sigma}$, with $\{\xi_{k\phi\sigma}, \xi_{k'\phi'\sigma'}^\dagger\} = \delta(k - k')\delta(\phi - \phi')\delta_{\sigma\sigma'}$. Finally, we switch to the angular momentum basis $\xi_{k\phi\sigma} = \frac{1}{\sqrt{2\pi}} \sum_m e^{im\phi} c_{k\sigma}^m$, where m is the orbital magnetic quantum number[8,15,17] and the anticommutation relations take the form $\{c_{k\sigma}^m, (c_{k'\sigma'}^{m'})^\dagger\} = \delta(k - k')\delta_{mm'}\delta_{\sigma\sigma'}$. Collectively, these transformation steps can be written as

$$c_{\mathbf{k}\sigma} \rightarrow \sqrt{\frac{2\pi}{k}} \sum_{m=-\infty}^{\infty} e^{im\phi} c_{k\sigma}^m. \quad (3)$$

We introduce the linear combinations which diagonalize the band Hamiltonian, including the Rashba terms[15,17]

$$c_{kh}^{m+1/2} = \left(c_{k\uparrow}^m + h c_{k\downarrow}^{m+1}\right)/\sqrt{2}, \quad (4)$$

where $h = \pm 1$ is the helicity quantum number. The corresponding band energies are

$$\epsilon_{kh} = \epsilon_k + \alpha k h = \frac{(k + hk_0)^2}{2m^*} + E_0 - E_R, \quad (5)$$

where $k_0 = m^*\alpha$ is the Rashba momentum and $E_R = k_0^2/2m^*$ is the Rashba energy. The bottom of the band thus shifts from E_0 to $E_0 - E_R$ upon switching on the SO interaction.

We obtain the effective impurity model

$$H = \sum_{hm} \int_0^\infty dk\,\epsilon_{kh}\left(c_{kh}^{m+1/2}\right)^\dagger c_{kh}^{m+1/2}$$
$$+ \epsilon(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$$

$$+ \frac{1}{2\pi} \sum_h \int_0^\infty \sqrt{k}\,dk\,V_k \frac{\sqrt{2\pi}}{\sqrt{2}}$$
$$\times \left[\left(c_{kh}^{1/2}\right)^\dagger d_\uparrow + (-1)^{\frac{h-1}{2}}\left(c_{kh}^{-1/2}\right)^\dagger d_\downarrow + \text{H.c.}\right]. \quad (6)$$

We integrate out the conduction-band modes and obtain an effective impurity action of the following form:

$$S = \int_0^\beta d\tau \left[\sum_\sigma d_\sigma^\dagger \left(\frac{\partial}{\partial\tau} + \epsilon\right) d_\sigma + U n_\uparrow n_\downarrow\right]$$
$$+ \frac{1}{\pi} \sum_h \int_0^\beta d\tau \int_0^\beta d\tau' d_\sigma^\dagger \Delta_h(\tau - \tau') d_\sigma. \quad (7)$$

The hybridization function $\Delta_h(\tau)$ is the Fourier transform of

$$\Delta_h(i\omega_n) = \frac{1}{4\pi} \int_0^\infty k\,dk \frac{V_k^2}{i\omega_n - \epsilon_{kh}}. \quad (8)$$

For simplicity, the energy cutoff is here taken to infinity. While $\Delta_+(i\omega_n)$ and $\Delta_-(i\omega_n)$ are somewhat complicated functions, their sum $\Delta = \sum_h \Delta_h$ is simpler. We make the analytical continuation $i\omega_n \rightarrow E + i0^+$ and take the imaginary part, $\Gamma_h(E) = -1/(2\pi)\text{Im}\Delta_h(E + i0^+)$. Using the Sokhotski-Plemelj formula $\text{Im}[1/(x + i0^+)] = -\pi\delta(x)$ and assuming $V_k \equiv V$, we find

$$\Gamma_+(E) = \Gamma_0 \begin{cases} 0 & E < E_0 \\ 1/2 - \frac{\sqrt{E_R}}{2\sqrt{E - (E_0 - E_R)}} & E > E_0 \end{cases} \quad (9)$$

and

$$\Gamma_-(E) = \Gamma_0 \begin{cases} 0 & E < E_0 - E_R \\ \frac{\sqrt{E_R}}{\sqrt{E - (E_0 - E_R)}} & E_0 - E_R < E < E_0 \\ 1/2 + \frac{\sqrt{E_R}}{2\sqrt{E - (E_0 - E_R)}} & E > E_0 \end{cases} \quad (10)$$

where $\Gamma_0 = \pi \frac{m^*}{2\pi} V^2$. The imaginary part of the total hybridization function is found to be of the same functional form as the density of states (DOS) of the conduction band:

$$\Gamma(E) = \Gamma_0 \begin{cases} 0 & E < E_0 - E_R \\ \sqrt{\frac{E_R}{E - (E_0 - E_R)}} & E_0 - E_R < E < E_0 \\ 1 & E > E_0 \end{cases} \quad (11)$$

This result is remarkably simple and could have been guessed in advance, since the impurity is assumed to be pointlike and simply couples to the local DOS at its position. The only effect of the Rashba interaction as far as the local impurity properties are concerned is the emergence of an additional energy interval $[E_0 - E_R; E_0]$ with finite DOS, which diverges with an inverse-square-root divergence at the lower limit (see Fig. 1). The effect of this diverging DOS is difficult to evaluate analytically; therefore we resort to using a numerical technique.

We compute the impurity spectral function using the numerical renormalization group (NRG) method[19,20] with extensions for arbitrary DOS.[22–29] NRG can handle diverging DOS both at the Fermi level[26,30] as well as away from the Fermi level.[31] The discretization has been performed using the scheme from Refs. [28] and [29], which easily handles inverse-square-root divergencies at finite frequencies. The conduction-band cutoff has been chosen larger than all the
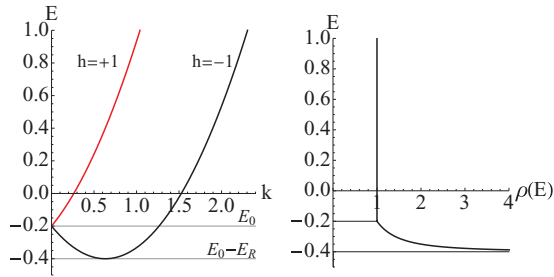
FIG. 1. (Color online) The dispersion and the density of states in the presence of the Rashba spin-orbit coupling. The label $h = \pm 1$ indicates the helicity of the band.

energy scales in the problem. NRG parameters were $\Lambda = 2$, twist-averaging over $N_z = 64$ discretization grids, and the truncation cutoff set at $10\omega_N$, where ω_N is the characteristic energy scale at the Nth NRG step. The broadening parameter was $\alpha = 0.1$.

The calculated spectral functions are shown in Fig. 2. Left panels show the spectral function over the full energy interval, while the right panels are a close-up of the Kondo resonance at the Fermi level. The hybridization function is shown as a gray curve (red online) in the left panels. The spectral function features two atomic resonances, one at $\omega = \epsilon$ (corresponding to the extraction of an electron) and one at $\omega = \epsilon + U$ (corresponding to the addition of an electron).
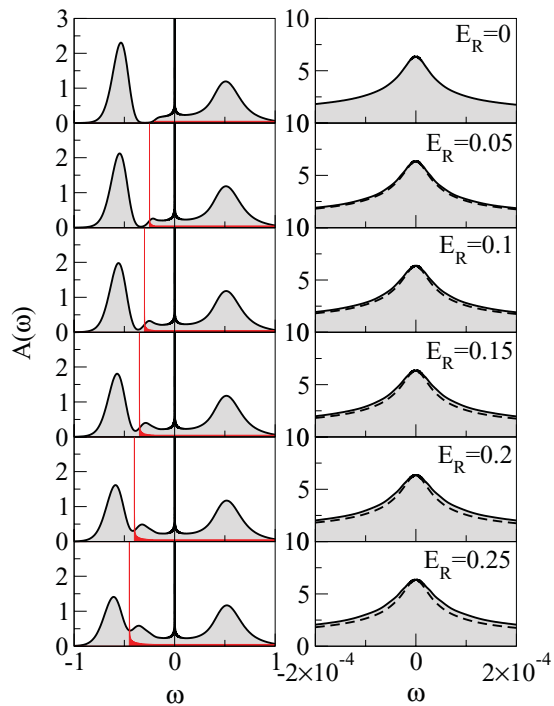

FIG. 2. (Color online) The impurity spectral functions for a range of the Rashba spin-orbit coupling strengths. The gray curve (red online) in the left panels is the effective hybridization function that the impurity state mixes with. The dashed line in the close-up plots on the right side is the Kondo resonance in the absence of the Rashba coupling, $E_R = 0$. The parameters are $U = 1$ and $\epsilon = -0.5$, and the hybridization strength at Fermi level for $E_R = 0$ has been set to $\Gamma_0 = 0.05$. The band bottom is $E_0 = -0.2$.
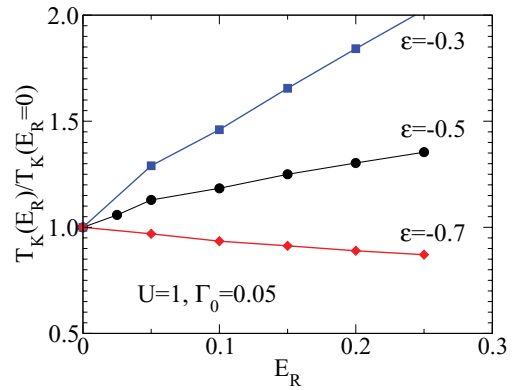

FIG. 3. (Color online) The Kondo temperature calculated using the NRG. The parameters are specified in the plot. The temperatures are rescaled by the Kondo temperature in the absence of the Rashba interaction.

The width of atomic spectral peaks is approximately $2\Gamma(\omega)$, where ω is the peak position.[32,33] The peak at $\omega = \epsilon$ is outside the band for all values of E_R considered, and thus it should have zero width (i.e., it is a δ peak). The finite width in the presented spectral functions is due to the spectral broadening in the NRG. In addition to the atomic peaks, the spectral function features the many-body Kondo resonance, which peaks near the Fermi level. The long logarithmic tails of the Kondo resonance are asymmetric due to the particular energy dependence of the hybridization function. At the bottom of the band, at $\omega = E_0 - E_R$, the spectral function has a maximum, then it drops to zero at frequencies below the band (this drop is overbroadened due to technical reasons). The maximum near the band edge is a hybridization self-energy effect which is a direct consequence of a discontinuous (and diverging) hybridization function.

The results for the Kondo temperature (defined as in Ref. 34) for several different choices of the impurity parameters are shown in Fig. 3. We have included parameter sets both with $\epsilon + U/2 = \mu$ and with $\epsilon + U/2 \neq \mu$. We find that the Kondo temperature exhibits some variation as a function of E_R; however, the variation is not exponential, but rather linear in the large-E_R limit with more complex variation for small values of E_R, which can be attributed to the emergence of the inverse-square-root divergence in $\Gamma(E)$. Depending on the values of ϵ, U, and Γ_0, the Kondo temperature is either an increasing or decreasing function of E_R.

In "flat band" systems with constant hybridization function Γ and neglecting the potential scattering, T_K is given by

$$T_K = \tilde{D}\sqrt{\rho J}\exp\left(-\frac{1}{\rho J}\right),\qquad(12)$$

where $\rho J = 8\Gamma/\pi U$ is the dimensionless Kondo coupling constant and $\tilde{D}$ is the effective bandwidth. If the hybridization function Γ is energy dependent, we have to use its value at the Fermi level in the expression above. In the presence of the Rashba interaction, if the bottom of the band is initially below the Fermi level (i.e., $E_0 < 0$), $\Gamma(0)$ will remain unchanged when the Rashba coupling is increased. This explains the absence of an exponential renormalization of T_K and is in agreement with Ref. 15. Nevertheless, the Kondo temperature

does depend on the details of the hybridization function; thus some variation of T_K is in fact expected and indeed observed, as shown in Fig. 3.

We emphasize that the impurity action S, Eq. (7), has the form of a single-band (single-channel) problem. In fact, the single-orbital Anderson impurity model is always effectively a single-channel problem, no matter what kind of the conduction band it couples to.[8,25] The reduced conduction band (channel) can always be constructed by taking the combination of states which couples to the impurity orbital (here a state proportional to the linear combination $\sum_{\mathbf{k}} V_k c_{\mathbf{k}\sigma}^{\dagger}$) as an initial state in the Gram-Schmidt orthogonalization procedure applied to the band Hamiltonian. Consequently, one obtains a single tight-binding chain Hamiltonian, while all other band states are fully decoupled from the impurity. This argument holds universally. A multichannel Kondo model can be in some cases obtained from the single-orbital Anderson model by using a nonoptimal basis for the band modes that also includes states which are in reality fully decoupled from the impurity. These redundant states should not in any way affect the impurity properties. Unfortunately, the complete irrelevance of these states can only be observed if the problem is solved exactly. However, if the problem is approached with an approximate method, there exists a potential pitfall: The presence of the redundant states can affect the impurity properties in some spurious way.

The problem of an impurity in the ideal 2D electron gas can never be truly particle-hole symmetric, because the conduction band itself is not particle-hole symmetric with respect to the chemical potential μ. We therefore do not expect any particular difference in the role of the Rashba interaction depending on whether $\epsilon + U/2$ is equal to μ or not,[17] even if the DM interaction is generated in some basis, but we do expect effects due to the potential scattering on the impurity.

The predictions of this work could be experimentally tested in a system with tunable SO interaction, such as 2D electron systems in semiconductors with metal gates. Furthermore, the rapid advances in the field of ultracold atom systems suggest that it might become possible to build a 2D fermionic gas with tunable SO interaction[35–38] and couple it to a magnetic impurity.[39]

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