Kondo effect in the presence of Rashba spin-orbit interaction

Rok Žitko and Janez Bonča
Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia, and Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia

(Received 31 August 2011; revised manuscript received 10 November 2011; published 28 November 2011)

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.

DOI: 10.1103/PhysRevB.84.193411 PACS number(s): 71.70.Ej, 72.10.Fk, 73.20.At

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. 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, and it is the bottom of the periodic system. The SO interaction plays a central role in many proposals for spintronic devices, and it is the bottom of the periodic system. The SO interaction plays a central role in many proposals for spintronic devices, and it is the bottom of the periodic system.
described using the single-orbital Anderson impurity model 
\(H_0\) with an additional Rashba interaction term \(H_{SO}\):

\[
H_0 = \epsilon(n_1 + n_j) + Un_1n_j \\
+ \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k\sigma} V_k (c_{k\sigma}^\dagger d_\sigma + H.c.),
\]

\(1\)

\[
H_{SO} = \alpha \sum_k \psi_k^\dagger (k, \sigma y - k, \sigma x) \psi_k \\
= \alpha \sum_k ke^{-i\phi_k} c_{k+}^\dagger c_{k-} + H.c.
\]

\(2\)

The operator \(d_\sigma^\dagger\) creates an electron in the impurity level, while \(c_{k\sigma}^\dagger\) correspond to the conduction-band electrons with the dispersion \(\epsilon_k = k^2/2m^* + E_0\), where \(k\) is the crystal momentum, \(m^*\) 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 \(n_\sigma = d_\sigma d_\sigma^\dagger\). The chemical potential is set to the energy zero, \(\mu = 0\). In \(H_{SO}\), \(\alpha\) parameterizes the strength of the Rashba interaction, \(\psi_k\) is a spinor field \((\psi_{k+}, \psi_{k-})^T\), while \(\sigma_{x,y}\) are Pauli matrices. \(k\) and \(\phi_k\) are the polar coordinates of the wave number \(k\), with the polar axis oriented along \(k_y\).

We switch to a continuum representation in a box of volume \(V = 1\). The sums are transformed in the standard way as \(\sum_k \rightarrow V/(2\pi)^2 \int dkd\phi\). The operators are transformed as \(c_{k\sigma} \rightarrow (2\pi/V)\psi_{k\sigma}\); they are normalized such that \(\{\psi_{k\sigma}, \psi_{k'\sigma'}\} = \delta(\sigma, \sigma')\delta(k, k')\). Noting that \(\delta; \kappa; \chi; \phi\) we switch to a polar representation using \(\psi_{k\sigma} \rightarrow 1/\sqrt{k} \xi_{k\sigma}\), with \(\{\xi_{k\sigma}, \xi_{k'\sigma'}\} = \delta(k, k')\delta(\sigma, \sigma')\). Finally, we switch to the angular momentum basis \(\xi_{m\sigma} = \frac{1}{\sqrt{\pi}} \sum_k e^{im\phi} c_{m\sigma}^\dagger\), where \(m\) is the orbital magnetic quantum number, \(|m| \leq \epsilon\), and the anticommutation relations take the form (\(c_{m\sigma}^\dagger, c_{m'\sigma'}^\dagger\)) = \(\delta(k, k')\delta(\sigma, \sigma')\). Collectively, these transformation steps can be written as

\[
c_{k\sigma} \rightarrow \sqrt{\frac{2\pi}{k}} \sum_{m=-\infty}^{\infty} e^{im\phi} c_{m\sigma}^\dagger.
\]

\(3\)

We introduce the linear combinations which diagonalize the band Hamiltonian, including the Rashba terms \(5, 17\):

\[
c_{kh}^{m+1/2} = \left(c_{kh}^m + h\epsilon_{kh}^{m+1}\right)\sqrt{2},
\]

\(4\)

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

\[
\epsilon_{kh} = \epsilon_k + akh = \frac{(k + kho)^2}{2m^*} + E_0 - E_R,
\]

\(5\)

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

\[
H = \sum_{kh} \int_0^\infty dk \epsilon_{kh} (\epsilon_{kh}^{m+1/2})^2 e^{i\epsilon_{kh}^{m+1/2}} \\
+ \epsilon(n_1 + n_j) + Un_1n_j
\]

\[+ \frac{1}{2\pi} \sum_k \int_0^\infty \sqrt{k} dV_k \sqrt{\frac{2\pi}{k}} \\
\times \left[c_{kh}^{1/2} d_1 + (-1)^{1/2} c_{kh}^{-1/2} d_1^\dagger + H.c.\right].
\]

\(6\)

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

\[
S = \int_0^\beta dt \left(\sum_\sigma d_\sigma^\dagger \left[\frac{\partial}{\partial \tau} + \epsilon\right] d_\sigma + Un_1n_j \right) \\
+ \frac{1}{\pi} \sum_k \int_0^\beta dt' \int_0^\beta d\tau' \Delta_k(\tau - \tau')d_\sigma.
\]

\(7\)

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

\[
\Delta_k(\omega) = \frac{1}{4\pi} \int_0^\infty dk dV_k \sqrt{V_k^2 - V_0^2}.
\]

\(8\)

For simplicity, the energy cutoff is here taken to infinity. While \(\Delta_+ (\omega)\) and \(\Delta_- (\omega)\) are somewhat complicated functions, their sum \(\Delta = \sum_{\sigma} \Delta_k(\tau)\) is simpler. We make the analytical continuation \(i\omega_n \rightarrow E + i\delta\) and take the imaginary part, \(\Gamma_+(E) = -1/(2\pi) \Im\Delta_k(E + i\delta)\). Using the Sokhotski-Plemelj formula \(\Im[1/(\epsilon + i\delta)] = -\pi\delta(\epsilon)\) and assuming \(V_k = V\), we find

\[
\Gamma_+(E) = \Gamma_0 \left\{ \begin{array}{ll} 0 & E < E_R \\
1/2 - \sqrt{\frac{V_0}{\pi V}} & E > E_0 \end{array} \right.
\]

\(9\)

and

\[
\Gamma_- (E) = \Gamma_0 \left\{ \begin{array}{ll} 0 & E < E_R \\
\frac{\sqrt{V_0}}{\pi V} & E < E_0 \\
1/2 + \frac{\sqrt{V_0}}{\pi V} & E > E_0 \end{array} \right.
\]

\(10\)

where \(\Gamma_0 = \pi \frac{m^*}{\pi V^2}\). 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:

\[
\Gamma(E) = \Gamma_0 \left\{ \begin{array}{ll} 0 & E < E_R \\
\sqrt{\frac{E}{E_0 - E_R}} & E_0 - E_R < E < E_0 \\
E > E_0 \end{array} \right.
\]

\(11\)

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 \(22, 28\). 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
energy scales in the problem. NRG parameters were $\Lambda = 2$, twist-averaging over $N = 64$ discretization grids, and the truncation cutoff set at $10\omega_N$, where $\omega_N$ is the characteristic energy scale at the $N$th 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).

The width of atomic spectral peaks is approximately $2\Gamma(\omega)$, where $\omega$ is the peak position. 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 $\delta$ 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 $\epsilon$, $U$, and $\Gamma_0$, the Kondo temperature is either an increasing or decreasing function of $E_R$.

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

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

where $\rho J = 8\Gamma/\pi U$ is the dimensionless Kondo coupling constant and $\tilde{D}$ is the effective bandwidth. If the hybridization function $\Gamma$ 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.\textsuperscript{12,25} 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 $\sum_k V_k c_{k\sigma}^{\dagger}$) 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 $\mu$. We therefore do not expect any particular difference in the role of the Rashba interaction depending on whether $\epsilon + U/2$ is equal to $\mu$ or not,\textsuperscript{37} 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\textsuperscript{35–38} and couple it to a magnetic impurity.\textsuperscript{39}

Discussions with Anton Ramšak, Tomaž Rejec, Dirk Schuricht, and Mikhail Pletyukhov and the support of the Slovenian Research Agency (ARRS) under Program P1-0044 are acknowledged.

\begin{thebibliography}{50}
\bibitem{5} M. König et al., Science \textbf{318}, 766 (2007).
\bibitem{6} L. Fu and C. L. Kane, Phys. Rev. B \textbf{76}, 045302 (2007).
\bibitem{17} M. Zarea, S. E. Ulloa, and N. Sandler, e-print arXiv:1105.3522.
\bibitem{36} J. Dalibard, F. Gerbier, G. Juzeliunas, and P. Öhberg, e-print arXiv:1008.5378.
\end{thebibliography}