Kondo spin screening cloud in two-dimensional electron gas with spin–orbit couplings

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Abstract
A spin-1/2 Anderson impurity in a semiconductor quantum well with Rashba and Dresselhaus spin–orbit couplings is studied by using a variational wavefunction method. The local magnetic moment is found to be quenched at low temperatures. The spin–spin correlations of the impurity and the conduction electron density show anisotropy in both spatial and spin spaces, which interpolates the Kondo spin screenings of a conventional metal and of a surface of three-dimensional topological insulators.

(Some figures in this article are in colour only in the electronic version)

A spin-1/2 impurity with large on-site repulsion and occupation energy well below the Fermi level of a conducting band will form a local magnetic moment [1]. At low temperatures, the impurity state hybridizes or couples with the conduction electron states and the local magnetic moment is completely screened by a conduction electron spin cloud surrounding the impurity, which is known as the Kondo effect [2]. To intuitively understand the Kondo effect, we may consider $N - 1$ conduction electrons and one impurity electron. In the absence of the hybridization, the impurity spin is free to form a local moment due to the on-site Coulomb repulsion at the impurity site. In the presence of a small hybridization, the virtual process of hopping between the conduction and impurity states favors a spin singlet state of the total $N$-electron system. More detailed Wilson’s renormalization group analysis shows that the energy gain is of the order of the Kondo temperature, which has an exponential dependence on the coupling [3]. After decades of intensive study, the Kondo effect as a quantum impurity problem is well understood [3]. The Kondo screening cloud has long been theoretically predicted. For more recent studies, see, for example, [4–6]. However, direct experimental observation of the Kondo screening cloud turns out to be more difficult. It was proposed that nuclear magnetic resonance could be used to measure the spin polarization of conduction electron spins of a proper metallic sample in dilute magnetic impurities (Fe for example) by applying a small magnetic field. The effect was later found to be too small to be detected [7], due to the small energy scale or the large Kondo spin cloud involved in the screening [8–11]. Recent developments in spin-resolved scanning tunneling microscopy may open a new possibility to detect the Kondo screening spin cloud in experiments by directly measuring the correlation between the impurity spin and the conduction electron spin density. This revives our interest in the study of the Kondo spin screening cloud.

In a metal or a semiconductor, the spin–orbit coupling breaks spin SU(2) symmetry. The spin of an electron feels an effective momentum-dependent magnetic field and is no longer conserved. A natural question is the effect of the spin–orbit coupling on the Kondo problem. Recently, the Kondo screening of an Anderson impurity in a helical metal has been studied [12, 13]. The problem is of interest in connection with the three-dimensional (3D) topological insulator, whose surface states are described by a helical metal with Dirac dispersion. The magnetic doping on the surface of the 3D topological insulator Bi$_2$Se$_3$ has recently been realized [14]. Similar to the Kondo problem in a conventional metal, the magnetic moment in a helical metal is found to be completely quenched at low temperatures. However, the texture of the spin correlations between the conduction electron and the impurity become more complex. Žitko [13] was able to map the Anderson impurity model in a helical metal to a conventional...
Kondo problem, in which the conduction electrons carry pseudo-spins. His work, however, does not provide direct information about the spin screening, since the pseudo-spin is a complicated combination of the real spins. The helical metal may be considered as a strong spin–orbit coupling limit of a 2D electron gas with Rashba spin–orbit coupling. In a Rashba model, the ratio of the spin–orbit coupling to the kinetic energy of the conduction electron is a tunable parameter. Therefore, the model allows us to study the Kondo spin screening continuously from a conventional to a helical metal.

In this paper, we consider an Anderson impurity in a 2D electron gas with Rashba and Dresselhaus spin–orbit couplings, which are common in narrow-gap semiconductor quantum wells [15, 16]. There has been a lot of activity recently on the Rashba systems in connection with semiconductor spintronics. The study of the Kondo screening in these systems may be of interest in the manipulation of the spins. We use a variational wavefunction to study the Kondo screening. Similar to the Anderson impurity models in conventional metal or in a helical metal, we find that the magnetic moment is also completely quenched in a semiconductor of Rashba coupling at low temperatures. The spin–spin correlations between the impurity and the conduction electrons through the Kondo screening. Similar to the Anderson impurity model, if the magnetic moment is also completely quenched in a semiconductor of Rashba coupling at low temperatures. The spin–spin correlations between the impurity and the conduction electrons through the Kondo screening. Similar to the Anderson impurity model, if the magnetic moment is also completely quenched in a semiconductor of Rashba coupling at low temperatures.

The system we study is described by a 2D Hamiltonian in the $x$–$y$ plane. In Nambo’s spinor representation, it is

$$H = H_c + H_h + H_d$$

$$H_c = \sum_{\kappa} c_{\kappa}^d (\frac{\hbar^2 k^2}{2m^*} - \mu) c_{\kappa}$$

$$+ c_{\kappa}^\dagger [\alpha(\sigma_x k_y - \sigma_y k_x) + \beta(\sigma_x k_x + \sigma_y k_y)] c_{\kappa}$$

$$H_h = \sum_{\kappa} V_k c_{\kappa}^d c_{\kappa}^d + \text{h.c.}$$

$$H_d = (\epsilon_d - \mu) d^\dagger d + Ud^\dagger d^\dagger d^\dagger d^\dagger.$$  \hspace{1cm} (1)

In the above expressions, $\kappa = (k_x, k_y)$ and $H_c$ is the Hamiltonian for the conduction electrons of effective mass $m^*$. $\alpha$ and $\beta$ describe the strengths of the Rashba-and Dresselhaus-type spin–orbit couplings, respectively. $\mu$ is the chemical potential. $c_{\kappa}^d = (c_{\kappa}^d, c_{\kappa}^\dagger)$ is the creation operator in spinor representation. $\sigma_x$ and $\sigma_y$ are the Pauli matrices. $H_d$ is the Hamiltonian for the impurity states. The impurity is placed at the origin of the $x$–$y$ plane, and the energy level of the impurity state is $\epsilon_d$ and $d^\dagger = (d^\dagger, d^\dagger)$. The impurity state hybridizes with the conduction electrons through $H_h$.

Let us first focus on the conduction electrons. The strength of the Dresselhaus spin–orbit coupling is determined by the asymmetric atomic field of the crystal lattice and it is absent in the crystal with structural inversion symmetry. The strength of the Rashba spin–orbit coupling in a quantum well structure is allowed to be tuned by an external gate voltage and it is usually one order in magnitude smaller than the kinetic energy of the electron gas.

After diagonalizing $H_c$, we obtain the single-electron energy eigenvalue $\epsilon_{\kappa s}$ and the corresponding quasiparticle operators $\gamma_{\kappa}$:

$$\epsilon_{\kappa s} = \frac{\hbar^2 k^2}{2m^*} - \mu + s \sqrt{(\alpha^2 + \beta^2)k^2 + 4\alpha \beta k_x k_y}$$

$$\gamma_{\kappa s} = \frac{1}{\sqrt{2}} \left( e^{ik_y/\hbar} c_{\kappa t}^\dagger + e^{-ik_y/\hbar} c_{\kappa b}^\dagger \right)$$  \hspace{1cm} (2)

where $s = \pm$ is the index of the energy band, $k = (k_x^2 + k_y^2)^{1/2}$ and $\theta_\kappa$ is the angle of the vector $(\alpha k_x + \beta k_y, \alpha k_y - \beta k_x)$ with the $k_x$ axis. The ground state of the many-electron system $H_c$ in the absence of $H_d$ is then simply given by $|\Psi_0\rangle = \prod_{\kappa \in \Omega} \gamma_{\kappa s}^\dagger |0\rangle$, where $|0\rangle$ is the vacuum, and $\Omega$ denotes the Fermi sea.

Now we consider the system with an impurity. For an isolated impurity, if $\epsilon_d < \mu < \epsilon_d + U$, the impurity is singly occupied and a local magnetic moment is formed. Due to the presence of $H_h$, the conduction electron hybridizes the impurity state and tends to screen the impurity moment at low temperature. To study the ground state properties of the system, we adopt the trial wavefunction method, which was first introduced by Varma and Yafet in 1976 [17]. The trial wavefunction captures many of the important aspects in the Kondo problem and has been widely used in the literature. We believe the method should at least qualitatively or semi-quantitatively accurately study the Kondo spin screening cloud for our purpose. The trial wavefunction is given by [12]

$$|\Psi\rangle = \left( a_0 + \sum_{\kappa} a_{\kappa s} d_{\kappa s}^\dagger \right) |\Psi_0\rangle$$  \hspace{1cm} (3)

where $\kappa = \{k, s\}$ and $d_{\kappa s} = \frac{1}{\sqrt{2}} (e^{ik_y/\hbar} d_{\kappa t} + e^{-ik_y/\hbar} d_{\kappa b})$. The large $U$ limit is taken so that the double occupation of the impurity electrons is completely excluded. The parameters $a_0$ and $a_{\kappa s}$ are to be determined using the variational method which optimizes the ground state energy $E = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$. Note that the variational parameter $\kappa$ depends on both momentum and spin. The spin dependence is via the band index $s$ contained in $\kappa$, which is a function of the momentum.

The construction of the trial wavefunction (3) is similar to that in [17] for a helical metal. In the limit $\alpha = \beta = 0$, the trial wavefunction is reduced to that for an Anderson impurity in conventional metal. The wavefunction contains the lowest energy sector of the single-particle components and is expected to grasp the essential physics of the Kondo problem. If all kinds of particle–hole excitations of the conduction electrons are included, the wavefunction would be the exact eigenstate of the system.

The variational procedure leads to the expression for $a_{\kappa s}$:

$$a_{\kappa s} = \frac{V_k}{\epsilon_{\kappa s} - \Delta_p} a_0.$$  \hspace{1cm} (4)

This will be used in the calculation of the spin correlations between impurity and conduction electrons. The equation to determine the binding energy, defined by the energy difference between the state without the hybridization term $H_h$ and the...
The central physical quantity we shall study is the Kondo effect, we examine the magnetic properties of the magnetic moment is quenched.

To investigate the role of the spin–orbit couplings to the system, we plot the spatial distribution of all the spin correlations between the impurity and the conduction electrons. We see that the SU(2) symmetry in space and it has no contribution to the spin part of the Kondo screening in the present systems. The total spin of the conduction electrons and the impurity spin is no longer appropriate here. A proper quantity to measure the spin correlation is given by

$$ J_{zz}(r) = -\frac{1}{4} |B(r)|^2 + \frac{1}{4} |A(r)|^2 $$

$$ J_{xx}(r) = -\frac{1}{8} |B(r)|^2 - \frac{1}{8} \text{Re} A^2(r) $$

$$ J_{yy}(r) = -\frac{1}{8} |B(r)|^2 + \frac{1}{8} \text{Re} A^2(r) $$

$$ J_{xy}(r) = J_{yx} = -\frac{1}{4} \text{Im} A^2(r) $$

$$ J_{xz}(r) = -J_{zx} = -\frac{1}{4} \text{Re}(A(r))B(r) $$

$$ J_{yz}(r) = -J_{zy} = -\frac{1}{4} \text{Re}(A(r))B(r) $$

The above equations

$$ A(r) = N^{-\frac{1}{2}} \sum_{k \in \Omega} e^{i(kr + ik_0)} \Delta_k, $$

$$ B(r) = N^{-\frac{1}{2}} \sum_{k \in \Omega} e^{ikr} \Delta_k. $$

Firstly, we study the system with a pure Rashba coupling ($\alpha \neq 0, \beta = 0$). From the expression for $A$ and equation (4), it is easy to check that $A(r) = 0$ in the limit $\alpha = 0$. In figure 1, we plot the spatial distribution of all the spin correlations between the impurity and the conduction electrons. We see that the $J_{zz}$ is always isotropic about the origin point while its density around this point decreases as $\alpha$ increases. For $\alpha \neq 0$, $J_{xx}$ and $J_{yy}$ are anisotropic and the anisotropy becomes stronger at larger $\alpha$, as we can see from figure 2. In sharp contrast with the system without spin–orbit coupling, all of the off-diagonal spin correlations $J_{uv}$, where $u \neq v$, are nonzero and they become larger for larger $\alpha$. These results are closely related to the broken spin $SU(2)$ symmetry.

Since the total spin of the conduction electrons is not a good quantum number, the description of the spin singlet of the total spin of the conduction electrons and the impurity spin is no longer appropriate here. A proper quantity to measure the spin part of the Kondo screening in the present systems is then the correlation between the impurity spin and the total spin of the conduction electrons, namely $I_0 = \sum_u I_u$, where $u = x, y, z$ and $I_u = \oint d\vec{r} j_{uu}(r)$. Re $A^2(r)$ has a d-wave symmetry in space and it has no contribution to $I_z$ and $I_y$. 

\[ \Delta_{\text{h}} = 0.02 \text{ and } \mu = 1. \text{ The length unit is } k_0^{-1} = 10^{-3} \text{ m, the energy unit is } \hbar^2/2m = 3.6 \times 10^{-2} \text{ eV and } \alpha \text{ is in units of } \frac{\hbar^2}{m}.\]
The spatial distribution of the spin correlations for systems with both Rashba and Dresselhaus spin–orbit couplings. (a1)–(f1) are for Figure 3.

We have \( I_x = I_y \) and usually they are not equal to \( I_z \). Note that there is also the orbital part of the Kondo screening, which contributes to the screening of the impurity spin. In the limit the Rashba coupling (assumed to be positive without loss of generality) is small, we have analytic expressions below for these correlations (hereafter we use the units given in the caption of figure 1 for brevity):

\[
\begin{align*}
I_z &\approx -\frac{1}{4} \left( 1 - \frac{\alpha \sqrt{\mu}}{2 \Delta_b} \right), \\
I_x = I_y &\approx -\frac{1}{4} \left[ 1 - \frac{\alpha \sqrt{\mu}}{2 \Delta_b} \right], \\
I_0 &\approx -\frac{3}{4} \left( 1 - \frac{2\alpha \sqrt{\mu}}{3 \Delta_b} \right).
\end{align*}
\]

(9)

From the above equations, at \( \alpha = 0 \), we have \( I_x = I_y = I_z = -\frac{1}{4} \) and \( I_0 = -\frac{3}{4} \), which is the limiting case for the Kondo screening in conventional metal. For more general values of the spin–orbit coupling, we show our numerical results of the correlations in figure 2. As we can see, \( I_x, I_y \) or \( I_z \) increases from \(-1/4\), initially linearly at small \( \alpha \), then to a saturated value of \( I_z = 0 \) or \( I_x = I_y = -1/8 \) at large \( \alpha \). Note that the value of \( \alpha \) may be tunable in experiments by applying a gate voltage. We remark that a small increase of \( \alpha \) may suppress the spin correlation significantly and this behavior is enhanced with smaller \( \Delta_b \), as indicated in equations (9). Note that \( I_z = 0 \) implies that the \( z \) component of the impurity spin is unscreened globally by the spins of the conduction electrons. (As discussed in [12], the \( z \) component of the impurity spin is actually completely screened by the \( z \) component of the orbital angular momentum of the conduction electron.) The large \( \alpha \) limit of \( I_0 \) is \(-\frac{3}{4}\), which is exactly the value for the Anderson impurity in the helical metal with the chemical potential potential below the Dirac point. Here we connect the Rashba system with the helical metal. The helical metal exists on the surface of a 3D topological insulator [19, 20]. It is the large \( \alpha \) (or large \( m^* \)) limit of the Rashba system. For the helical metal, we have to take an ultraviolet cutoff which is usually taken as half the bulk gap, while for the Rashba system, to choose an energy cutoff is not severe, the dispersion is bound below and the width of the conduction band is a natural energy cutoff.

Now we study the spin–spin correlation functions in the presence of a pure Dresselhaus coupling. The problem can be mapped onto the pure Rashba coupling case by a unitary transformation as examined by Shen et al [21]. Under the unitary transformation \( UT = \frac{\sqrt{\pi}}{2}(\sigma_x - \sigma_y) \), the Pauli matrices are transformed as \( \sigma_x \rightarrow -\sigma_y, \sigma_y \rightarrow -\sigma_x \), and \( \sigma_z \rightarrow -\sigma_z \). Therefore under such a transformation the Rashba and Dresselhaus couplings in the Hamiltonian (1) are interchanged [21]. If the system possesses pure Dresselhaus coupling, it can be mapped onto the system with pure Rashba coupling under the action of \( UT \). Denote the spin correlations of the Dresselhaus systems as \( J'_{\alpha \beta}(r) \), then they are related to the ones of the Rashba system as \( J_{\alpha \beta}(r) = J'_{\alpha \beta}(r) \), \( J'_{xx}(r) = J_{xx}(r), J'_{xy}(r) = J_{xy}(r), J'_{yz}(r) = J_{yz}(r) \), and \( J'_{zz}(r) = J_{zz}(r) \).

In the presence of both the Rashba and Dresselhaus couplings, the energy dispersion is no longer isotropic in momentum space as in the Rashba system and so does the \( a_k \). However, they still possess reflection symmetries in momentum space about the lines \( k_x \pm k_y = 0 \). An immediate result is that \( J_{\alpha \beta}(r) \) loses its isotropy and is symmetric about \( x \pm y = 0 \) in real space. As shown in figure 3, for systems with

Figure 3. Spatial distribution of the spin correlations for systems with both Rashba and Dresselhaus spin–orbit couplings. (a1)–(f1) are for \( J_{xx}, J_{xy}, J_{yy}, J_{xz}, J_{yx}, J_{zy} \), with \( \alpha = 0.3 \) and \( \beta = 0.1 \); (a2)–(f2) are for the corresponding correlations with \( \alpha = \beta = 0.3 \). The other parameters are \( \Delta_b = 0.02 \) and \( \mu = 1 \). The energy and length units are the same as in figure 1.
the Dresselhaus coupling, the patterns of $J_{xx}$, $J_{yy}$, $J_{xz}$ and $J_{yz}$ are rotated and $J_{xy}$ is remarkably redistributed. At $\alpha = \beta$, the model has an interchange symmetry between $x$ and $y$. In this case, $J_{xx} = J_{yy}$ and $J_{xz} = J_{yz}$.

In summary, we have examined a spin-1/2 Anderson impurity in a 2D electron system with spin–orbit couplings. The binding energy and the spin correlation functions are calculated using a trial wavefunction method, which is widely used to study the Kondo problem. Being consistent with former studies [22, 23], the magnetic moment of the impurity is found to be fully quenched at low temperatures, the same as in the conventional Anderson impurity problem. However, because of the spin–orbit couplings, the spin correlations between the impurity and the conduction electrons are different from the ones in conventional metal. The diagonal components $J_{xx}$ and $J_{yy}$ are anisotropic in space. The off-diagonal components are nonzero and have particular spatial distributions. The introduction of the Dresselhaus coupling changes the patterns of the correlation functions dramatically.

Our theory is variational in nature. The variational wavefunction method has been widely used to study the Kondo impurity problem and the basic results are consistent with more accurate methods such as the numerical renormalization group technique. We note that spatial extension of the Kondo cloud in the Anderson impurity model in conventional metal was recently studied by Bergmann [24] by using the Friedel artificially inserted resonance method, where the screening length is quantitatively calculated. Our focus in the present paper is on the anisotropic spin correlation functions due to the Rashba-type spin–orbit coupling. We expect that the spatial spin screening length in our variational calculation is also associated with the Kondo temperature, similar to [24]. In the parameter region we study, the screening decay is rather rapid as we showed in the case of the Anderson impurity in a helical metal [12]. We believe that our results presented here on the anisotropic screening are qualitatively or semi-quantitatively correct. Although more sophisticated methods may be needed to provide precisely quantitative results of the Kondo spin cloud, this may be left for future work. Our study may be of interest in semiconductor spintronics, where the Rashba system has played important roles. The impurity spin may be used to control or to manipulate the conduction electrons and the physics of Kondo screening in these systems should be interesting. Direct experimental observation remains a major challenge. Nuclear magnetic resonance does not seem to be promising for the tiny signal in a large Kondo spin cloud. Recently developed spin-resolved scanning tunnelling microscopy (STM) may offer a new route. By adding a small magnetic field around the impurity site, the STM may, in principle, measure the spin-dependent local density of states to probe both diagonal and off-diagonal spin correlations. However, it may still be challenging to probe the electrons in the quantum well structure, which may require long wave optical probes. Nevertheless, the modern technique is developing very rapidly and the interesting phenomenon of the Kondo spin cloud, and the anisotropic spin screening examined in the present paper, will be observed in the near future.

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