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Spin-orbit scattering and the Kondo effect

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The effects of spin-orbit scattering of conduction electrons in the Kondo regime are investigated theoretically. It is shown that due to time-reversal symmetry, spin-orbit scattering does not suppress the Kondo effect, even though it breaks spin-rotational symmetry, in full agreement with experiment. An orbital magnetic field, which breaks time-reversal symmetry, leads to an effective Zeeman splitting, which can be probed in transport measurements. It is shown that, similar to weak localization, this effect has anomalous magnetic-field and temperature dependence.

The profusion of works on the Kondo effect in the last thirty years has led to a good understanding of the strongly correlated state,[1] with the possible exception of systems of reduced dimensionality.[2–4] As the temperature is lowered the electron gas screens the isolated impurity spin, leading to enhanced scattering on the Fermi surface. Elastic impurities do not change this picture, and their effect can be absorbed into renormalizing the Kondo temperature.[5,6] Spin scatterers, on the other hand, are expected to suppress the effect, as the electrons lose their spin memory after traveling the spin-scattering length.

Recently, Bergmann[7] has demonstrated in an elegant experiment that weak-localization effects can be used to study the effectiveness of the Kondo screening of magnetic impurities. By measuring the magnetoconductance for various systems and comparing to the theory of weak localization, he was able to identify the amount of magnetic scattering and, consequently, the screening of the magnetic impurities. Surprisingly, it was found that adding a large number of spin-orbit scatterers into the sample (such that the magnetoconductance changes sign due to the weak-antilocalization phenomenon) does not change the magnetic scattering at all. Accordingly, the spin-orbit scattering, even though it breaks the spin-rotational symmetry of the system, does not suppress the Kondo effect. Several other groups have also reported the observation of the Kondo effect in the presence of strong spin-orbit scattering.[8]

In this paper we discuss the effects of spin-orbit scattering in the Kondo regime. It is shown that because of time-reversal symmetry, the spin-orbit scatterers play the same role as elastic, nonmagnetic impurities. As the spin-orbit scattering rate is usually much smaller than the elastic scattering rate, we expect there will be no observable change in the Kondo temperature and hence in the Kondo screening of the magnetic impurities due to spin-orbit scattering, in full agreement with the experiment.[7] Interestingly, however, the application of a magnetic field leads to the breaking of time-reversal symmetry, and consequently, suppresses the Kondo effect. We calculate the effective Zeeman splitting resulting from this orbital magnetic field, and discuss its experimental implications.

The resonant scattering of the electrons near the Fermi energy can be traced back to the divergence of the self-energy in a perturbation expansion, either in the antiferromagnetic coupling between the local spin and the electronic spin in the Kondo s-d Hamiltonian, or in the hopping in the Anderson model. Both kinds of self-energies involve multiple scattering of the conduction electrons by the local impurity and accordingly involve those electrons only through the propagator $G(r,r;t)$, from the impurity position r back to the impurity position. If the electron spin is rotated randomly during that propagation, the correlations between consecutive scattering events are lost and the Kondo effect is suppressed. Here we prove that when time-reversal symmetry is obeyed, the propagator $G(r,r;t)$ is diagonal in spin space. Accordingly, even in the presence of spin-orbit scattering the Kondo effect persists. For example,

$$\begin{aligned}\langle c_\uparrow(r,t)c_\downarrow^\dagger(r,0)\rangle &= \frac{1}{Z}\sum_{n,m} e^{-\beta E_m + i(E_m-E_n)t}\langle\Psi_m|c_\uparrow(r,0)|\Psi_n\rangle\langle\Psi_n|c_\downarrow^\dagger(r,0)|\Psi_m\rangle \\ &= \frac{1}{Z}\sum_{n,m} e^{-\beta E_m + i(E_m-E_n)t}\langle\Psi_m|K^\dagger c_\uparrow(r,0)K|\Psi_n\rangle\langle\Psi_n|K^\dagger c_\downarrow^\dagger(r,0)K|\Psi_m\rangle \\ &= -\frac{1}{Z}\sum_{n,m} e^{-\beta E_m + i(E_m-E_n)t}\langle\Psi_n|c_\downarrow^\dagger(r,0)|\Psi_m\rangle\langle\Psi_m|c_\uparrow(r,0)|\Psi_n\rangle = -\langle c_\uparrow(r,t)c_\downarrow^\dagger(r,0)\rangle = 0, \qquad (1)\end{aligned}$$

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where $c_\sigma(r,t)$ $[c_\sigma^\dagger(r,t)]$ annihilates (creates) a conduction electron of spin σ at position r and time t, and K is the time-reversal operator. In the above the propagator was expressed in terms of the exact many-body eigenfunctions of the system, Ψ_n, with energies E_n, and we have used the identities $\langle\Psi_m|K^\dagger c_\uparrow(r,0)K|\Psi_n\rangle=-\langle\Psi_n|c_\downarrow^\dagger(r,0)|\Psi_m\rangle$ and $\langle\Psi_n|K^\dagger c_\downarrow^\dagger(r,0)K|\Psi_m\rangle=\langle\Psi_m|c_\uparrow(r,0)|\Psi_n\rangle$. In (1) the chemical potential was taken as zero, for convenience. The same procedure can be applied to show that $\langle c_\downarrow^\dagger(r,0)c_\uparrow(r,t)\rangle$, and, consequently, the retarded Green function, $G_{\uparrow\downarrow}^r(r,r;t)\equiv-i\theta(t)\langle[c_\downarrow^\dagger(r,0)c_\uparrow(r,t)+c_\uparrow(r,t)c_\downarrow^\dagger(r,0)]\rangle$, are also identically zero, and that $G_{\uparrow\uparrow}^r(r,r;t)=G_{\downarrow\downarrow}^r(r,r;t)$. Note that the above results apply for any interacting system satisfying time-reversal symmetry, even including inelastic scattering.

Let us give another, more transparent argument why an electron always returns with the same spin. Consider a general closed path from point r to itself [e.g., the trajectory in Fig. 1(a)]. Such a path can be schematically represented by the left trajectory in Fig. 1(b). The electron spin is rotated due to spin-orbit scatterers along the path. Due to time-reversal symmetry the spin-scattering matrix along the path can be written as[9,10]

$$\mathbf{S}=\begin{pmatrix}\alpha & \beta\\ -\beta^* & \alpha^*\end{pmatrix}.$$

The electron can also follow the time-reversed trajectory [the right trajectory in Fig. 1(b)], where all the scatterers are met in opposite order, which gives rise to the rotation matrix $\mathbf{S}^\dagger$. Since both trajectories have exactly the same weight, one can add them up, leading to a matrix proportional to the unity matrix. Thus it is the destructive interference between time-reversed paths that leads to the vanishing of the off-diagonal terms.[11]

The above argument suggests that this picture will change dramatically in the presence of a magnetic field, which breaks time-reversal symmetry. In the absence of spin-orbit scattering a magnetic field suppresses the Kondo effect through the Zeeman splitting of the impurity state. The peak in the impurity density of states moves away from the Fermi energy by the Zeeman splitting.[12] Once the splitting is larger than the Kondo temperature, the ground state of the impurity is polarized, suppressing the resonant Kondo scattering at the Fermi surface. The split peaks can still be probed, though, via nonlinear transport measurements, where they produce split peaks in the differential I-V characteristics.[12–14]

In the presence of spin-orbit scattering an orbital magnetic field leads to similar effects, as it destroys the exact cancellation of the contributions of the time-reversed paths to the off-diagonal propagator. Thus an electron may return to the impurity position with a rotated spin, mixing the two spin directions and giving rise to an effective Zeeman splitting. Such a splitting appears in the Kondo Hamiltonian obtained via a Schrieffer-Wolff transformation[15] from the full Hamiltonian for the impurity and the conduction electrons. To calculate this effect we consider specifically an Anderson Hamiltonian in the presence of spin-orbit scattering and magnetic field,

$$\mathcal{H}=\epsilon_0\sum_\sigma d_\sigma^\dagger d_\sigma+Un_\uparrow n_\downarrow+\sum_\sigma\left[V_0c_\sigma^\dagger(0)d_\sigma+\text{H.c.}\right]+\mathcal{H}_{\text{el}}. \tag{2}$$

The operators $d_\sigma^\dagger$ create a local electron on the impurity; the second term describes the impurity on-site repulsion ($n_\sigma\equiv d_\sigma^\dagger d_\sigma$), while the third term describes the hopping between the impurity (positioned at $r=0$) and the electron gas. The conduction-electron Hamiltonian is given by

$$\mathcal{H}_{\text{el}}=\frac{1}{2m}\sum_{k,\sigma}\left(\hbar k-\frac{e\mathbf{A}}{c}\right)^2c_{k\sigma}^\dagger c_{k\sigma}+V\sum_{q,p}\rho_q c_{p+q\sigma}^\dagger c_{p\sigma}$$
$$+iV_{\text{SO}}\sum_{q,p}\rho_q^{(\text{SO})}\mathbf{q}\times\mathbf{p}\cdot(c_{p+q\sigma'}^\dagger\boldsymbol{\sigma}_{\sigma'\sigma}c_{p\sigma}), \tag{3}$$

where $c_{k\sigma}$ is the Fourier transform of $c_\sigma(r)$, $\mathbf{A}$ is the electromagnetic potential, and ρ_q and $\rho_q^{(\text{SO})}$ are the densities of the elastic scatterers and spin-orbit scatterers, respectively.

The presence of both spin-orbit scattering and magnetic field leads to anisotropy in spin space of the conduction-electron density of states. Through the hopping V, this anisotropy lifts the degeneracy between the spin states of the impurity. The resulting effective Zeeman splitting (for $U\to\infty$) is obtained by diagonalizing the impurity part of the Kondo Hamiltonian obtained via a Schrieffer-Wolff transformation,[15]

$$\mathcal{H}_{\text{imp}}=\vec{\Omega}\cdot\vec{S}=\frac{\hbar}{2}\vec{\Omega}\cdot\sum_{\sigma,\sigma'}d_\sigma^\dagger\vec{\boldsymbol{\sigma}}_{\sigma,\sigma'}d_{\sigma'}, \tag{4}$$

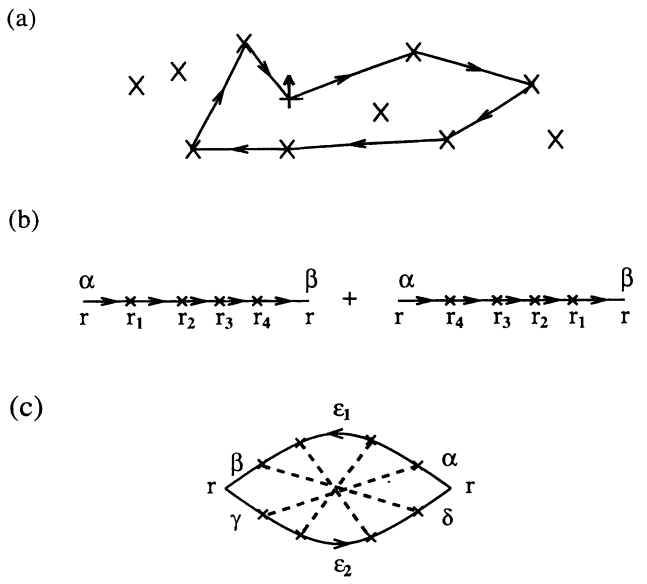

FIG. 1. (a) Schematic path contributing to the local density of states at a Kondo impurity. Even with spin-orbit scattering by impurities (the ×'s), the equal weighting of time-reversed paths (b) guarantees a diagonal single-particle propagator $G_{\beta\alpha}(r,r)$, which preserves the Kondo effect. (c) The cooperon contribution, $\langle G_{\delta\gamma}^a(r,r;\epsilon_2)G_{\beta\alpha}^r(r,r;\epsilon_1)\rangle$, to the disorder-averaged two-particle propagator, $\langle\Pi_{\alpha\beta\gamma\delta}(r,r;\epsilon_1,\epsilon_2)\rangle$.

where $\vec{\sigma}$ indicates the Pauli spin matrices. The energy splitting Δ between the eigendirections of spin is then given by

$$\Delta^2 \equiv (\epsilon_1-\epsilon_2)^2=(\delta\epsilon_{\uparrow\uparrow}-\delta\epsilon_{\downarrow\downarrow})^2+4|\delta\epsilon_{\uparrow\downarrow}|^2, \tag{5}$$

where

$$\frac{\hbar}{2}\vec{\Omega}\cdot\vec{\sigma}=\begin{pmatrix}\epsilon_0+\delta\epsilon_{\uparrow\uparrow} & \delta\epsilon_{\uparrow\downarrow}\\ \delta\epsilon_{\downarrow\uparrow} & \epsilon_0+\delta\epsilon_{\downarrow\downarrow}\end{pmatrix} \tag{6}$$

and

$$\delta\epsilon_{\sigma\sigma'}=\frac{iV_0^2}{2\pi}\int_{-\infty}^{\infty}d\epsilon\,\frac{1-f(\epsilon)}{\epsilon_0-\epsilon}\times[G^r_{\sigma\sigma'}(r,r,\epsilon)-G^a_{\sigma\sigma'}(r,r,\epsilon)]. \tag{7}$$

The Green functions in (7) are for the conduction electrons in the absence of coupling to the impurity. The energy shift in Eq. (7) is due to processes in which the impurity electron hops to an unoccupied state in the conduction band, propagates as a conduction electron, and finally hops back to the impurity, possibly with a rotated spin. Combining Eqs. (5) and (7), we find that the effective Zeeman splitting Δ is given by[16]

$$\Delta^2=\frac{V_0^4}{(2\pi)^2}\int\int d\epsilon_1 d\epsilon_2\times\frac{[1-f(\epsilon_1)][1-f(\epsilon_2)]}{(\epsilon_1-\epsilon_0)(\epsilon_2-\epsilon_0)}\Pi_\Delta(\epsilon_1,\epsilon_2), \tag{8}$$

where

$$\Pi_\Delta(\epsilon_1,\epsilon_2)=\Pi_{\uparrow\uparrow\uparrow\uparrow}(r,r;\epsilon_1,\epsilon_2)+\Pi_{\downarrow\downarrow\downarrow\downarrow}(r,r;\epsilon_1,\epsilon_2)-2\Pi_{\downarrow\downarrow\uparrow\uparrow}(r,r;\epsilon_1,\epsilon_2)+4\Pi_{\downarrow\uparrow\uparrow\downarrow}(r,r;\epsilon_1,\epsilon_2) \tag{9}$$

and

$$\Pi_{\alpha\beta\gamma\delta}(r,r;\epsilon_1,\epsilon_2)=-[G^r_{\delta\gamma}(r,r;\epsilon_2)-G^a_{\delta\gamma}(r,r;\epsilon_2)]\times[G^r_{\beta\alpha}(r,r;\epsilon_1)-G^a_{\beta\alpha}(r,r;\epsilon_1)]. \tag{10}$$

In the absence of magnetic field, Π_Δ is explicitly zero and there is therefore no effective Zeeman splitting of the impurity.

The magnetic-field dependence of the splitting is determined by the magnetic-field dependence of Π_Δ, which, after averaging over disorder, is determined by the cooperon diagram [Fig. 1(c)]. The cooperon diagram has been calculated in the context of weak localization theory,[17–19] and the difference between Π_Δ at finite field and its zero field value is given in three dimensions by

$$\langle\Pi_\Delta^{(3D)}(\omega)\rangle=\frac{3\nu}{\hbar D(1-i\omega\tau)^2 l}\left\{F\left[\frac{l^2}{4\hbar D}\left(-i\omega+\frac{\hbar}{\tau_\phi}\right)\right]-F\left[\frac{l^2}{4\hbar D}\left(-i\omega+\frac{4\hbar}{3\tau_{SO}}+\frac{\hbar}{\tau_\phi}\right)\right]\right\}, \tag{11}$$

where $\omega=\epsilon_1-\epsilon_2$, and

$$F(\zeta)=\sum_{N=0}^{\infty}\left[2(\sqrt{N+1+\zeta}-\sqrt{N+\zeta})-\frac{1}{\sqrt{N+1/2+\zeta}}\right]. \tag{12}$$

In two dimensions, we find

$$\langle\Pi_\Delta^{(2D)}(\omega)\rangle=\frac{3\nu}{\hbar D(1-i\omega\tau)^2}\left\{\Psi\left[\frac{1}{2}+\frac{l^2}{4\hbar D}\left(-i\omega+\frac{\hbar}{\tau_\phi}\right)\right]-\Psi\left[\frac{1}{2}+\frac{l^2}{4\hbar D}\left(-i\omega+\frac{4\hbar}{3\tau_{SO}}+\frac{\hbar}{\tau_\phi}\right)\right]-\ln\left(\frac{-i\omega+\hbar/\tau_\phi}{-i\omega+4\hbar/3\tau_{SO}+\hbar/\tau_\phi}\right)\right\}. \tag{13}$$

In the above, ν is the single-spin conduction-electron density of states, l is the magnetic length $\sqrt{\hbar c/eH}$, D is the diffusion constant, τ_{SO} is the spin-orbit scattering time $(=\hbar/[2\pi\nu\rho^{(SO)}_{q=0}V^2_{SO}\overline{(p\times q)^2}])$, τ_ϕ is the phase-breaking time, and Ψ is the digamma function. In deriving those results it was assumed that $\tau\ll\tau_{SO},\tau_\phi$, where $\tau=\hbar/(2\pi\nu\rho_{q=0}V^2)$ is the elastic lifetime. By inspection, only the real parts of expressions (11) and (13) contribute to the effective Zeeman splitting given by Eq. (8).

Since the magnetic-field dependence of the cooperon diagram also determines the magnetoconductance in the weakly localized regime, we can deduce the magnetic-field dependence of the splitting from the weak-localization magnetoconductance. Thus we expect the splitting to be linear in small magnetic fields, crossing over at high fields to $\sqrt{\ln(H)}$ in two dimensions and to $H^{1/4}$ in three dimensions. To see the amplitude of the effect we expand the Π's in small magnetic field and find

$$\langle\Delta^2\rangle=\begin{cases}2\pi\left[\dfrac{m}{m^*}\dfrac{\mu_B H}{4\ln(W/k_BT_K)}\right]^2\dfrac{\sigma_0}{e^2/h}\dfrac{1}{k_F^2 l_{SO}} & \text{for 3D}\\ \dfrac{2}{\pi}\left[\dfrac{m}{m^*}\dfrac{\mu_B H}{4\ln(W/k_BT_K)}\right]^2\dfrac{\sigma_0}{e^2/h}\ln\left(\dfrac{3\tau_\phi}{4\tau_{SO}}\right) & \text{for 2D,}\end{cases} \tag{14}$$

where $\mu_B=e\hbar/2mc$ is the Bohr magneton, W is the bandwidth of the conduction electrons, m^* is their effective mass, σ_0 is the conductivity (conductance in two dimensions), and $l_{SO}=\sqrt{D\tau_{SO}}$ is the spin-orbit length. For quasi-two-dimensional systems (where the thickness of the sample d is larger than one-half the Fermi wavelength) the two-dimensional result has to be divided by the square of the number of subbands k_Fd/π. To obtain Eq. (14) it was assumed that the depth of the impurity level, $\mu-\epsilon_0$, is much larger than the energy broadening due to elastic scattering $\hbar/\tau$ and that $\tau_\phi\gg\tau_{SO}$. The result indicates that the splitting in a finite magnetic field increases the more conductive the sample is. In two dimensions it is also predicted that the splitting depends on the temperature logarithmically through the inelastic lifetime. We thus predict that nonlinear measurements will reveal a temperature-dependent splitting, with anomalous magnetic-field dependence at high fields. In typical metallic samples, three dimensional or quasi-two-dimensional, the amplitude of the effect is only a small fraction of the usual Zeeman splitting for typical experimental values.[8] This explains why the Kondo effect has been observed in experiments with strong spin-orbit scattering even in the presence of a magnetic field.[7,8] On the other hand, the effect is expected to be much larger in two-dimensional semiconductor systems, because of the reduced dimensional-

ity and because of the higher mobility. The Kondo effect has indeed been observed in dilute magnetic semiconductors,[20,21] while spin-orbit scattering in the weakly localized regime has been systematically investigated in several semiconductor compounds.[22] In fact, spin-orbit scattering in the weakly localized regime has been recently reported in a dilute magnetic semiconductor.[23] With the experimentally measured parameters for a two-dimensional electron gas in $Hg_{0.79}Cd_{0.19}Mn_{0.02}Te$ reported by Dietl, Grabecki, and Jaroszyński,[23] where both spin-orbit and magnetic scattering have been observed, the impurity splitting due to the orbital magnetic field is an order of magnitude larger than the usual Zeeman splitting. In addition, with the progress in building heterostructures involving diluted magnetic semiconductors,[24] it should be feasible to systematically check the predictions of our theory.

To conclude, we have studied in detail spin-orbit scattering in the Kondo regime. It was shown that due to time-reversal symmetry, spin-orbit scattering, even though it breaks spin-rotation symmetry, does not suppress the Kondo effect. This explains the surprising results of Bergmann[7] on thin films containing both Kondo impurities and spin-orbit scatterers. We find that in a finite magnetic field, which breaks time-reversal symmetry, spin-orbit scattering leads to an effective Zeeman splitting, with anomalous magnetic field and temperature dependence, similar to the magnetoconductance in the weakly localized regime. It is hoped that this work will stimulate further experiments to explore these effects.

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