Ruderman-Kittel-Kasuya-Yosida interaction in thin wires

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The spin polarization in the vicinity of a magnetic impurity (the origin of the Ruderman-Kittel-Kasuya-Yosida interaction between two spins) is calculated for a quasi-one-dimensional wire. It is found that at zero temperature the polarization depends on the distance as $1/r$. It is strongly enhanced compared with a three-dimensional sample.

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between two spins in a metal plays an important role in solid-state physics and is actually the basis for the occurrence of spin glasses. In addition this interaction interferes with the occurrence of the Kondo effect because it is almost impossible to investigate a single Kondo impurity; the RKKY interaction always couples different Kondo impurities.

Because of the significant development of electron lithography during the past decade it is now possible to prepare metallic wires with a cross section of the order of a few nm^2. During the past year the first experiments have been performed which investigate the Kondo effect in such "quasi-one-dimensional wires."[1] It has been claimed that the Kondo effect is partially suppressed when the diameter of the wire (which generally has a rectangular shape) becomes smaller than the Kondo length $\hbar v_F/k_B T_K$. In this paper we want to demonstrate that for a thin wire the interaction between magnetic impurities should increase dramatically. Therefore the partial suppression of the Kondo effect could be caused by an enhancement of the impurity interaction.

The RKKY interaction has been calculated for the one-dimensional case by Kittel in the late 1960s (Ref. 2) and recently by Yafet.[3] They found a decay of the RKKY polarization as $1/z$ where z is the distance between the impurity and the observer. We consider here a wire with a mesoscopic cross section. Such a wire behaves as a quasi-one-dimensional system when the distance between the impurity and the observer is larger than the cross-sectional dimensions. The derivation of the RKKY interaction in a wire is then quite different than in a purely one-dimensional electron system although the results are quite similar.

In a recent paper one of the authors[4] expressed the polarization in the vicinity of a magnetic impurity in terms of Feynman paths. For this purpose we connect the magnetic impurity and the point r (where we want to determine the spin polarization) by all possible classical paths C. Now let $A(C_1)$ be the amplitude of an electron wave which propagates from P to O along the path C_1 and $A(C_2)$ be the amplitude for an electron wave propagating from O to P along the path C_2. The magnetic impurity interacts with the conduction electrons via the exchange potential $j(r)\mathbf{s}\cdot\mathbf{S}$. Let $\delta_0/2$ be the phase shift that an electron with spin up experiences when scattered by the impurity with spin S_z. The phase shift and the potential $j(r)$ are connected by the relation $\delta_0=\langle j\rangle S_z m k_F \Omega_0/(2\pi\hbar^2)$, where $\langle j\rangle$ is the averaged scattering potential and Ω_0 the atomic volume.

With these parameters the spin polarization at the point P (i.e., the position r) is given by the relation

$$\rho_p(r)=-\tfrac{1}{2}\delta_0 N_0 \hbar \sum_{C_1,C_2} \frac{1}{t}[A(C_1 A(C_2)+\text{c.c.}] . \quad (1)$$

Here t is the propagation time for the closed loop from P along C_1 to O and back along C_2 to P. $N_0=mk_F/(2\pi^2\hbar^2)$ is the (three-dimensional) density of states per spin.

In the calculation we consider a wire with rectangular cross section L_xL_y. This actually represents the experimental situation very well. The impurity is at $z=0$ somewhere in the x-y plane at the position $(x_0,y_0,0)$. In Fig. 1 we see that there is one path which connects O and P directly. However, in addition there are many other paths along which the electron is specularly reflected by the boundaries (dashed and dotted paths).

These other paths along which the electron wave is reflected at the boundaries $x=\pm L_x/2$ and $y=\pm L_y/2$ can be considered to connect the point P with the virtual point $O_{\nu\mu}$ whose position in the x-y plane is

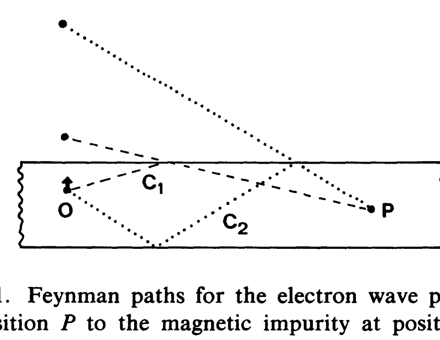

FIG. 1. Feynman paths for the electron wave propagating from position P to the magnetic impurity at position O and back. Along the dashed and dotted paths the electron experiences specular reflections. The paths can be replaced by straight lines connecting P with virtual impurity positions.

$$x_{2\nu}=x_0+2\nu L_x,\quad x_{2\nu-1}=(2\nu-1)L_x-x_0\ ,$$
$$y_{2\mu}=y_0+2\mu L_y,\quad y_{2\mu-1}=(2\mu-1)L_y-y_0\ . \tag{2}$$

The integer ν gives the number of reflections at the faces $x=\pm L_x/2$ and μ correspondingly at the faces $y=\pm L_y/2$. In addition each reflection introduces a phase shift of π in the amplitude of the electron wave. Therefore we obtain for the amplitude along the path $C_{\nu\mu}$

$$A(C_{\nu\mu})=A_{\nu\mu}=\frac{1}{k_F r_{\nu\mu}}\exp[ik_F r_{\nu\mu}+i(\nu+\mu)\pi] \tag{3}$$

with

$$r_{\nu\mu}=[z^2+\rho_{\mu\nu}^2]^{1/2},\quad \rho_{\nu\mu}=[x_\nu^2+y_\mu^2]^{1/2}\ .$$

This leads to the following expression for the polarization:

$$\rho_p(r)=-\tfrac{1}{2}\delta_0 N_0\hbar \sum_{\substack{\nu,\mu\\ \nu',\mu'}}\frac{1}{t}[A_{\nu\mu}A_{\nu'\mu'}+A^*_{\nu\mu}A^*_{\nu'\mu'}]\ . \tag{4}$$

The time t is given by $t=(r_{\nu\mu}+r_{\nu'\mu'})/v_F$.

Random phase approximation. For the evaluation of this expression we note first that the width and thickness of the wire are mesoscopic, i.e., they are much larger than the Fermi wavelength λ_F. For $z\lambda_F<L_x^2,L_y^2$ the phases $k_F r_{\nu\mu}$ for different $(\nu\mu)$ differ by values large compared to 2π. Therefore (as long as x_0 and y_0 are nonzero) we make the approximation of random phases, i.e., we assume that the amplitudes for different $C_{\nu\mu}$ are uncorrelated.

In the case of random phases for different paths the polarization oscillates randomly in space. However, we can calculate the envelope of the oscillation. It is essentially given by the average of the square of the polarization $\rho_p^2(r)$ (over a distance of the order of the Fermi wavelength).

$$\langle|\rho_p(z)|^2\rangle=[\delta_0 N_0\hbar/2]^2\sum_{\nu,\mu,\nu',\mu'}4\frac{v_F^2}{(r_{\nu\mu}+r_{\nu'\mu'})^2}\times|A_{\nu\mu}|^2|A_{\nu'\mu'}|^2\ . \tag{5}$$

This result contains a coherence factor of 2. It results from the effect that propagation along the path $C_{\nu\mu}\rightarrow C_{\nu'\mu'}$ yields the same phase shift as the time-reversed propagation along the path $C_{\nu'\mu'}\rightarrow C_{\nu\mu}$. (For $c_{\nu'\mu'}$ identical to $C_{\nu\mu}$ the factor 2 does not occur, but this yields only corrections of higher order in $1/z$.) Therefore the two contributions have to be first summed and then squared. (In disordered systems this contribution is often called the weak-localization part.)

We substitute the amplitudes from Eq. (3) and perform the sum. When the distance z from the impurity (along the wire) is much larger than L_x and L_y then the sum can be replaced by an integral. This yields

$$\left[\overline{\langle|\rho_p(z)|^2\rangle}\right]^{1/2}=\frac{1}{L_xL_y}\frac{\delta_0}{\pi}\frac{1}{z}I_0^{1/2}\ , \tag{6}$$

where I_0 represents the integral

$$I_0=\int_1^\infty\int_1^\infty\frac{du\,dv}{uv(u+v)^2}=\ln(2)-\tfrac{1}{2}\simeq 0.193\ . \tag{6'}$$

Polarization in high-symmetry positions. If we assume an ideal wire with perfectly parallel sides then there are positions of high symmetry where some of the contributions of different paths C_1 and C_2 are coherent so that we have to add the amplitudes of these paths before we square the polarization. For example, when both the magnetic impurity and the observer are at $x_0=0$ then we may replace x by $-x$ in the path C_1, arriving at a path C_1' which has the same amplitude as the path C_1. Therefore one first has to add the amplitudes of these coherent paths before one squares the amplitudes to add the "incoherent" contributions. This yields essentially a factor of 2 for each of the paths C_1 and C_2 (the additional terms are of higher power in $1/z$). The total contribution to $\langle|\rho_p(z)|^2\rangle$ is therefore increased by a factor of 4. This coherence factor increases again by another factor of 4 when both impurity and observer lie in the center of the wire at $x_0=y_0=0$.

At very large distance z between impurity and observer. If the distance between the impurity and observer is very large so that $L_x^2,L_y^2<z\lambda_F/2$, then the different paths may have a phase difference which is less than $\pi/2$. In that case one has to add the amplitudes of the polarization for different paths instead of the square. At this point the boundary conditions for the reflection of the electron wave become important. At each reflection from the surface of the wire the phase changes by π. This case is rather academic since the boundaries of a realistic wire are not perfectly parallel. Then the contributions from the different paths are again incoherent and the result of Eq. (6) applies.

By the way, this coherence of neighboring paths is also the reason that the polarization caused by a ferromagnetic layer in a pure metal depends on the distance as $1/z^2$.[5,3] The polarization of a single magnetic moment goes as $1/z^3$ and the number of paths from the ferromagnetic layer which have a difference in path length less than $\lambda_F/2$ is essentially $\pi z\lambda_F/a^2$ (a is the lattice parameter). Therefore the total polarization goes as $1/z^2$.

Small mean free path. In a former paper one of the authors calculated the square of the polarization in the d-dimensional case for very short mean free path. In this case the paths C_1 and C_2 are diffusion paths and for the calculation of the square of the polarization one can use the classical diffusion density. For the quasi-one-dimensional case the result is (after evaluating the integral in Ref. 4)

$$\left[\overline{\langle|\rho_p(z)|^2\rangle}\right]^{1/2}=0.706\frac{1}{L_xL_y}\frac{\delta_0}{\pi}\frac{1}{z}\ . \tag{7}$$

The ratio of the square of the polarization for the dirty and clean cases is about 2.59, i.e., the RKKY interaction is considerably larger in the highly disordered wire.

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