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Ruderman-Kittel-Kasuya-Yosida interaction in disordered metals

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The spin polarization in the vicinity of a magnetic impurity [the origin of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between two spins] is calculated for small mean free paths of the conduction electrons in d dimensions in terms of a quantum-interference effect. It is found that at zero temperature the polarization depends on the distance as $1/r^d$. It is strongly enhanced in thin films. At finite temperature its range is limited to the thermal diffusion length. A magnetic or electric field changes the local polarization and may reverse the sign of the RKKY interaction.

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. Many magnetic systems (such as spin glasses where the RKKY interaction generates the interaction between spins) have a small electronic mean free path. It has been believed for more than two decades that the RKKY interaction is damped in disordered metals according to $\exp(-|r|/l)$ where l is the mean free path of the electrons.[1-3] This result has been obtained by impurity averaging. For further references, see, for example, Refs. 4 and 5. One has learned, however, during the last decade that impurity averaging of electron amplitudes can lead to wrong conclusions. Impurity averaging suggests, for example, that the phase coherence of a wave function in a disordered metal is damped according to $\exp(-|r|/l)$. In reality the phase coherence in disordered metals extends over much larger distances (see, for example, the effect of weak localization).[6-8]

A few years ago Chatel,[9] using a bonding-antibonding argument, and Wong and Poon,[10] who performed numerical tight-binding calculations (see also Samson[11]), did not find an exponential decay of the RKKY interaction. Recently Bulaevskii and Panyukov[12] and Zyuźin and Spivak[13] calculated the RKKY interaction in a free-electron system with impurities and found a $1/r^3$ dependence of the polarization of the electron system. In the present paper the author gives an independent derivation of the spin polarization in a disordered system using a very transparent physical description.

I shall interpret the RKKY oscillations as an interference of the (free) conduction-electron wave function scattered by the magnetic impurity. The argument proceeds in four steps: (i) a rederivation of the Friedel oscillation using an interference treatment; (ii) a generalization of the Friedel oscillations for a disordered metal; (iii) the application of the results to the spin polarization in a disordered metal in the presence of a magnetic impurity (at $r=0$ with the spin up) which interacts with the conduction electrons via $j(r)sS$; (iv) the inclusion of effects of finite temperature, magnetic and electrical fields, and thin films. This interference derivation makes it obvious that we may manipulate the RKKY oscillations by external parameters such as temperature and magnetic and electrical fields (and dimension of the system).

An impurity at the position $r=0$ is considered. It acts as a kind of internal boundary by which the conduction electrons are scattered. At a boundary, an electron wave is reflected and the interference causes a standing wave with a strong charge modulation. A similar approach may be undertaken at the impurity. We consider at the position r a free-electron wave function $\psi_n(r)$ with $|\psi_n(r)|^2=1/V$ where the point r acts according to the Huygens principle as a source for an electron wave,

$$\psi_n(r)\frac{1}{2i}\frac{1}{k|r-r'|}e^{ik|r-r'|} . \tag{1}$$

This Huygens wave reaches the impurity with the amplitude $\psi_n(r)A_1/2i$, where A_1 is given by

$$A_1=\frac{1}{kr}\exp(ik_Fr) . \tag{2}$$

At the impurity, the elementary wave is scattered and (for s scattering) the scattered wave has the form

$$\psi_n(r)\frac{1}{2i}A_1\delta_0\frac{1}{kr''}\exp(ik_Fr'')=\psi_n(r)\frac{1}{2i}A_1A_2\delta_0 , \tag{3}$$

where A_2 is the amplitude for the propagation from 0 to r'' (which is equal to A_1 at the position r). The total amplitude for the returning wave interferes at r with the original wave function and yields a modulation of the charge density

$$\Delta\rho_n(r)=|\psi_n(r)|^2\delta_0(A_1A_2/2i+\text{c.c.}) . \tag{4}$$

The phase shift along the whole path for an electron of Fermi energy is

$$\phi_0=k_F2r+\delta_0 . \tag{5a}$$

For an electron state with the frequency (energy) ε measured from the Fermi level the phase shift along the same path is $\phi=\phi_0+\Delta\phi$, where

$$\Delta\phi=\Delta k(2r)=\varepsilon(2r/v_F)=\varepsilon t , \tag{5b}$$

and where $t=2r/v_F$ is the time an electron wave packet would need to propagate from r to 0 and back. Now we sum over all occupied states (assuming zero temperature for the moment) and obtain for the total charge density

$\rho_p(r)$ of the pure metal in the first Born approximation (see, for example, Ref. 14),

$$\rho_p(r) = \delta_0 N_0 \hbar \left[\frac{1}{2i} A_1 A_2 \int d\varepsilon f(\varepsilon) e^{i\varepsilon t} + \text{c.c.} \right]$$
$$= -\tfrac{1}{2} \delta_0 N_0 \hbar \left[\frac{1}{t} A_1 A_2 + \text{c.c.} \right]$$
$$= -\frac{\delta_0}{4\pi^2 r^3} \cos(2k_F r + \delta_0) \tag{6a}$$

or

$$\rho_p(r) = \frac{6\pi z}{\Omega_0} \rho \langle w \rangle \frac{1}{(2k_F r)^3} \cos(2k_F r + \delta_0) \ , \tag{6b}$$

where $N_0 = mk_F/(2\pi^2 \hbar^2)$ is the (three-dimensional) density of states per spin, z is the valence, $\langle w \rangle$ the scattering potential, and ρ the density of states per atomic volume Ω_0 and spin.

The integral $\int d\varepsilon f(\varepsilon) e^{i\varepsilon t}$ over all occupied states yields at zero temperature $1/it$ while at finite temperature one has essentially an exponential cutoff after the time $2\tau_T$ where $\tau_T = \hbar / 2\pi k_B T$. This cutoff yields in pure systems a finite although rather large range of the Friedel oscillation which is given by $v_F \hbar / \pi k_B T$. In disordered systems we will find at finite temperature a much shorter range of the Friedel oscillation.

This calculation can be easily transferred to the RKKY interaction. For the latter one has a magnetic impurity with the spin component S_z at the origin. Its (diagonal) interaction with the conduction electrons (i.e., without spin flip) is given by

$$H' = j(r) S_z s_z \ . \tag{7}$$

This interaction has opposite sign for spin-up and spin-down electrons and yields for each spin direction a charge-density variation as a function of r. Since both spin-up and spin-down electrons feel an opposite potential, $\pm j(r) S_z / 2$, at the magnetic impurity their Friedel oscillations have opposite sign. This means they compensate their charge but not their spin polarization. The spin densities add up and yield a spin polarization of the same amplitude as in Eq. (6b) if one interprets δ_0 as the phase shift of the potential $j(r) S_z$ (see, for example, Ref. 15 and references therein).

Our scattering treatment yields the Friedel and RKKY oscillations. Its advantage is that it can be generalized to the case of many impurities. In the following $\rho_i(r)$ can be interpreted either as an oscillation of the electrical or the magnetic polarization.

For the generalization of this consideration to a disordered metal we recall that the charge modulation is due to the interference between the free-electron wave function at the position r and the returning Huygens wave. The elementary Huygens wave starts at the time $t < 0$ from the point r, reaches the impurity at the origin 0 at the time t' with $t < t' < 0$, and returns to the position r at the time 0. In the pure metal $|t'| = |t|/2 = r/v_F$. One has to integrate the amplitude over all occupied energy states. $|A_1|^2$ can be considered as the density of an outgoing spherical electron wave. It corresponds to a radial flow of $2/\pi\hbar N_0$ electrons per time and spin (the flow of the Huygens wave is $|\psi_n|^2 / 2\pi\hbar N_0$).

In a disordered metal the propagation of the Huygens wave is diffusive. In Fig. 1, the path of a conduction electron is drawn. It starts at the position r and scatters from impurity to impurity, eventually reaching the magnetic impurity at the position $r = 0$ where it experiences the exchange interaction and continues afterwards on its scattering path until it returns to the position r. Here it interferes with the original wave function $\psi_n(r)$ and forms an interference pattern. Only those scattering paths which have a closed loop and visit the magnetic impurity contribute finally to the polarization.

This pattern is essentially identical with the generalized Friedel oscillations in a disordered metal. The author[16] recently interpreted the Hartree part of the Coulomb anomaly in disordered electron systems in terms of such a generalized Friedel oscillation.

The polarization density $\rho_i(r)$ is essentially given by an expression similar ro Eq. (6a):

$$\rho_i(r) = -\tfrac{1}{2} \delta_0 N_0 \hbar \sum_{C_1, C_2} \frac{1}{t} [A(C_1) A(C_2) + \text{c.c.}] \ . \tag{8}$$

Here we have to take the sum over all closed loops C which connect the points r with 0 by the path C_1 and 0 with r by the path C_2. The time t is the total diffusion time from r to r along the closed loop. There are of course many closed loops in which the electron visits the magnetic impurity more than one time. However, these paths are ignored here because we are only interested in contributions to the polarization which are linear in $\langle j \rangle$. Higher power in $\langle j \rangle$ have to include the Kondo effect.

The disordered metal shows a few important differences compared with the pure one.

(i) There are many paths in the disordered metal leading from r to 0 and from 0 to r. One has to sum the amplitudes $A(C_1)$ and $A(C_2)$ over all possible paths. The resulting polarization $\rho_i(r)$ depends on the arbitrary position of the impurities and varies from sample to sample. If one averages over the impurity position then $\rho_i(r)$ van-

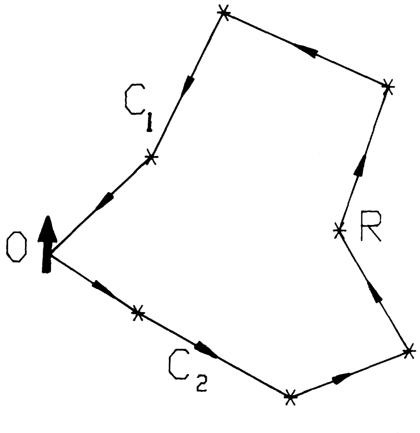

FIG. 1. The diffusion path of a Huygens wave from a position r to the magnetic impurity and back where it interferes with the original wave function.

ishes. However, for each impurity distribution there is a finite polarization $\rho_i(r)$ which oscillates as a function of position r and its amplitude varies only slowly with position. Therefore it is more useful to consider the square of the charge or polarization density. Because the phases of different loops are independent $\langle \rho_i(r)^2 \rangle$ is essentially given by squared amplitudes summed over all loops C_1, C_2. The square of the amplitudes can be identified with a well known physical quantity, the diffusion density. In the pure case $|A_i|^2$ is just the density of a constant radial electron flow with the source rate $2/\pi\hbar N_0$. In the disordered metal one has the same source rate but a diffusive motion and $|A_i|^2$ is given by the diffusion of the electron flow, i.e., the integrated diffusion density $p(r,t)$,

$$\tfrac{1}{2}\pi\hbar N_0 |A_1|^2 = \int_{-\infty}^{0} dt''\, p(|r|, -t'') \,, \tag{9}$$

where $p(r,t)$ is given in a disordered d-dimensional metal by

$$p(r,t) = \frac{1}{(4\pi D t)^{d/2}} \exp\left(-\frac{r^2}{4Dt}\right) . \tag{10}$$

(ii) The path from r to 0 can be very different than the path from 0 to r. The amplitude A_2 fulfills a similar relation as in Eq. (9).

(iii) The Huygens wave can propagate along the closed loop in both directions. This causes quantum interferences (as in weak localization) and the square of the polarization exhibits an additional factor of 2.

The final expression for the polarization is then

$$|\rho_i(r)|^2 = \left(\frac{2\delta_0}{\pi}\right)^2 \int_{-\infty}^{0} dt \int_{t}^{0} dt' \frac{1}{t^2} p(|r|, t'-t) \times p(|r|, -t') . \tag{11}$$

The integral in Eq. (11) can be evaluated and yields for the polarization in the presence of impurities in d dimensions

$$|\rho_i(r)|^2 = \left(\frac{2\delta_0}{\pi}\right)^2 \frac{1}{\pi^d} \frac{1}{r^{2d}} I_d(0) \,, \tag{12a}$$

where

$$I_d(z) = \int_0^{1/z} dx \int_0^{x} dx' \frac{1}{x^2} [(x-x')x']^{-d/2} \times \exp\left(-\frac{1}{x-x'} - \frac{1}{x'}\right) \tag{12b}$$

with $I_3(0) \approx 0.147$ in three dimensions.

This result is almost identical to the result for the pure metal. We find the same power $1/r^3$ in three dimensions for the r dependence of the amplitude. In the case of spin polarization one has to replace δ_0 by $\langle j \rangle S_z m k_F \Omega_0 / 2\pi\hbar^2$. It is, however, sufficient to perform the ratio between the disordered and the pure case for the averaged squared polarizations because then the prefactors like δ_0, i.e., $\langle j \rangle S_z$, cancel. Taking $|\rho_p(r)|^2 = \frac{1}{2}(\delta_0/4\pi^2)^2/r^6$ from Eq. (6a) for the pure case one obtains

$$\langle |\rho_i(r)|^2 \rangle / \langle |\rho_d(r)|^2 \rangle \approx 6 \,. \tag{13}$$

Until now we have essentially evaluated the RKKY oscillation at zero temperature and in zero field. Finite temperature and magnetic and electrical fields modify the oscillation. We discuss their influence on the RKKY oscillations.

(1) Finite temperature. The effect of finite temperature is exactly described in Eq. (6a) where one sums over all occupied states $\int d\varepsilon f(\varepsilon) e^{i\varepsilon t}$ which can be expressed as a sum of Matsubara frequencies. It introduces essentially an exponential cutoff of the amplitude A at the time $2\tau_T$, where $\tau_T = \hbar/(2\pi k_B T)$, and manifests the fact that at finite temperature the coherence of the Huygens wave lasts only for the time τ_T. Afterwards it is thermally smeared. This means that at finite temperature the integral $I_d(0)$ in Eq. (12a) has to be replaced with $I_d(x_T)$ where $x_T = (r^2 \pi k_B T)/4D\hbar)$. This limits the range of the RKKY oscillations to a distance $(D\hbar/\pi k_B T)^{1/2}$.

(2) Magnetic field. A finite magnetic field has the effect that the loop C encloses a magnetic flux and changes the phase of the interfering waves. The enclosed flux is about $\pi D t H$ where D is the diffusion constant and t the total diffusion time as defined above. This has two different effects. (a) The coherence of the two time-reversed partial waves, propagating along C in opposite directions, is destroyed when the phase difference $4DtHe/\hbar$ is of the order of one. This means that in a magnetic field the polarization reduces to half the value of Eq. (13) for distances from the magnetic impurity larger than $[\hbar/(eH)]^{1/2}$. (b) The second effect is that the magnetic field changes the phase relation between the Huygens wave and the original wave and therefore the interference pattern. When the enclosed flux takes the value $\pi\hbar/e$ then the polarization changes sign. This has no influence on the (averaged) value of $|\rho(r)|^2$ but the potential energy between two spins separated by more than $[\hbar/(eH)]^{1/2}$ changes its "phase" randomly. This means that a finite magnetic field applied to a spin glass can change the frustration of individual spins.

(3) Electric field. In the case of an applied magnetic field one cannot avoid an additional effect of the magnetic field on the moment of the spins. This is much more favorable in the case of an applied electric field. When the Huygens wave diffuses in the direction of the electric field it gains the energy eEr and its phase oscillates therefore faster than in the absence of the field. This causes an electrical phase shift (not present in weak localization) which is roughly $eErt/2$. When the resulting phase shift reaches the value $\pi/2$ the polarization changes sign, i.e., for $r^3 \approx 2\pi Dd/eE$ (in this first-order consideration r points parallel or antiparallel to the field).

Of particular interest is the effect of reduced dimensions on the RKKY oscillations. For a thin film of thickness W the diffusion density $p(r,t)$ is given by the two-dimensional expression of Eq. (10) but normalized with $1/W$. One easily derives the ratio $\langle |\rho_f|^2 \rangle / \langle |\rho_p|^2 \rangle = 128 I_2(0) r^2/W^2$ for distances from the magnetic impurity larger than the film thickness ($r \gg W$). Here

$I_2(0) \approx 0.164$ is the value of the integral (12b) in two dimensions. This means that one has in thin films at low temperature only a decay of the RKKY amplitude as $1/r^2$. As a consequence the interaction plays a much stronger role in thin films than in bulk samples.

These modifications should cause substantial changes in theory and experiment of disordered spin glasses and offer a rather valuable possibility of manipulation of the forces and frustrations which act on the individual spin.

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