

INDIRECT EXCHANGE OF LOCALIZED SPINS THROUGH "MAGNETIZED" ELECTRONS

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We consider the indirect exchange of magnetic ions through conduction electrons with separated Fermi spheres (a paramagnet or a ferromagnet in a magnetic field). We find new oscillations in the spin density of the conduction electrons with two periods depending on the magnitude of the magnetic induction or on the concentration of the magnetic impurities (in the case of an impurity ferromagnet). These oscillations may lead to long-wave magnetic structures in a system of localized spins.

1. INTRODUCTION

It is well known that magnetic ions lead by virtue of the exchange interaction

$$I(\mathbf{r} - \mathbf{R}_n) (S_n \sigma(\mathbf{r}))$$

to a shift in phase in the spatial distribution of electrons with different spin directions and lead thereby to a spin polarization of the system of conduction electrons. This polarization in turn affects the magnetic ions leading to an effective static interaction between them which is usually called an indirect exchange. Since the distribution of the conduction electrons has a discontinuity at $p = p_0$ (p_0 : the Fermi wave vector) the polarization oscillates with a period which is the reciprocal of the diameter of the Fermi sphere.^[1]

We consider here the indirect exchange between magnetic ions for the case when the conduction electrons with different spin directions have different radii of their Fermi spheres. This can occur in the case when the metal is in a magnetic field when the ions are ferromagnetically ordered^[1] or when both conditions occur. We write the energy of an electron in the general case in the form

$$\xi(p\alpha) = \xi(p) + \alpha\Delta - \xi_0, \quad \xi_0 = p_0^2/2m, \quad \alpha = (\pm), \quad \Delta = \text{const.} \quad (1)$$

In connection with the occurrence of a preferred direction (the moment of the sample) the exchange will be anisotropic. Moreover, in the exchange picture we must find reflected two peculiar features of the system under consideration: 1) the limiting momenta of electrons with different directions differ by

$$p_{0-} - p_{0+} = p_0\Delta/\xi_0 \equiv 2\kappa_1;$$

2) in spin-flip processes electrons (with spin z-component (-)) filling a sphere with radius p determined from the relation

$$\frac{p^2}{2m} = 2\Delta \equiv \frac{(2\kappa_2)^2}{2m}, \quad 2\kappa_2 = p_0 \left(\frac{2\Delta}{\xi_0} \right)^{1/2}$$

(i.e., $\kappa_2^2 = \kappa_1 p_0$) do not take part.

Finally, as was predicted by de Gennes^[2] and shown experimentally in^[3], if the magnetic ions are randomly distributed or if there are impurities or if both situa-

¹⁾The anisotropy of the exchange in this case originates in a natural way not through the exchange interaction but through the magnetic forces fixing the magnetic moment of the sample.

tions occur together, the pattern of a spin polarization generated by localized spins will "decay" according to the radioactive decay law

$$\sigma(r) = \sigma_0(r) \exp(-r/l),$$

where $l = v\tau$ is the mean free path. We shall take this fact into account also in what follows.

2. COORDINATE REPRESENTATION

We write down the Hamiltonian of the problem in the coordinate representation:

$$H = H_0 + H_1,$$

$$H_0 = \sum_{\alpha} \int \psi_{\alpha}^{+}(\mathbf{x}) \hat{T}(\mathbf{x}, \alpha) \psi_{\alpha}(\mathbf{x}) d\mathbf{x},$$

$$H_1 = \sum_{n\alpha\alpha'} \int \psi_{\alpha}^{+}(\mathbf{x}) I(\mathbf{x} - \mathbf{R}_n) (S_n \sigma_{\alpha\alpha'}) \psi_{\alpha'}(\mathbf{x}) d\mathbf{x}, \quad (2)$$

\hat{T} is the operator of the energy (1). We perform a unitary transformation of the operator H in order to eliminate terms of first order in S_n :

$$\bar{H} = e^{iS} H e^{-iS} = H_0 + \frac{i}{2} [S, H_1] - \frac{1}{3} [S, [S, H_1]] + \dots, \quad (3)$$

where we have imposed the condition

$$i[H_0, S] = H_1. \quad (4)$$

Thus

$$\bar{H} = H_0 + H_2 + \dots,$$

where

$$H_2 = \frac{i}{2} [S, H_1].$$

We choose the transformation operator in the form

$$S = \sum_{m\beta\beta'} \int \hat{K}_{\beta\beta'}(\mathbf{y}, \mathbf{R}_m) (S_m \sigma_{\beta\beta'}) \psi_{\beta}^{+}(\mathbf{y}) \psi_{\beta'}(\mathbf{y}) d\mathbf{y}. \quad (6)$$

Using (4) we find

$$K_{\beta\beta'}(\mathbf{y}, \mathbf{R}_m) = iI(\mathbf{y} - \mathbf{R}_m) \{ \hat{T}(\mathbf{y}, \beta) - \hat{T}(\mathbf{y}, \beta') \}^{-1}. \quad (7)$$

Using then (5) we find

$$H_2 = -\frac{i}{2} \sum_{nm} \sum_{\alpha\alpha'\beta\beta'} \int d\mathbf{x} d\mathbf{y} (S_n \sigma_{\beta\beta'}) (S_n \sigma_{\alpha\alpha'}) \cdot \{ I(\mathbf{x} - \mathbf{R}_n) \hat{K}_{\beta\beta'}(\mathbf{y}, \mathbf{R}_m) - I(\mathbf{y} - \mathbf{R}_m) \hat{K}_{\alpha\alpha'}(\mathbf{x}, \mathbf{R}_n) \} \psi_{\beta}^{+}(\mathbf{y}) \psi_{\beta'}(\mathbf{y}) \psi_{\alpha}^{+}(\mathbf{x}) \psi_{\alpha'}(\mathbf{x}). \quad (8)$$

We take the average of (8) over the eigenstates of the

operator H . The average of the product of four Fermi operators is then written out as follows:

$$\langle \psi_{\beta}^{+}(\mathbf{y}) \psi_{\beta}(\mathbf{y}) \psi_{\alpha}^{+}(\mathbf{x}) \psi_{\alpha}(\mathbf{x}) \rangle \approx \langle \psi_{\beta}^{+}(\mathbf{y}) \psi_{\beta}(\mathbf{y}) \rangle \langle \psi_{\alpha}^{+}(\mathbf{x}) \psi_{\alpha}(\mathbf{x}) \rangle \delta_{\beta\gamma} \delta_{\alpha\alpha} \\ + \langle \psi_{\beta}^{+}(\mathbf{y}) \psi_{\beta}(\mathbf{x}) \rangle \langle \psi_{\alpha}(\mathbf{y}) \psi_{\alpha}^{+}(\mathbf{x}) \rangle \delta_{\alpha\beta} \delta_{\beta\alpha}. \quad (9)$$

The terms which are off-diagonal (in the spin indices) on the right-hand side of (9) vanish if the quantization axis is chosen along the moment of the sample, as we shall do. Moreover, the first term gives zero when substituted into (8). As is shown in^[4] each average can then be replaced here by an average over the eigenstates of the operator H_0 multiplying by $\exp(-|\mathbf{x} - \mathbf{y}|/2l)$. We can then rewrite the right-hand side of (9) as

$$\langle \psi_{\beta}^{+}(\mathbf{y}) \psi_{\beta}(\mathbf{x}) \rangle_0 \langle \psi_{\alpha}(\mathbf{y}) \psi_{\alpha}^{+}(\mathbf{x}) \rangle_0 \delta_{\alpha\beta} \delta_{\beta\alpha} \exp(-|\mathbf{x} - \mathbf{y}|/l).$$

Changing to the momentum representation we get as a result

$$\langle \psi_{\beta}^{+}(\mathbf{y}) \psi_{\beta}(\mathbf{x}) \rangle_0 = \int \frac{d\mathbf{p}}{(2\pi)^3} n_{\mathbf{p}\beta}^0 e^{i\mathbf{p}(\mathbf{y}-\mathbf{x})}, \\ H_{\text{eff}} = \frac{1}{N^2} \sum_{nn'} \sum_{\alpha\beta} (S_n S_{\alpha\beta}) (S_{n'} S_{\beta\alpha}) \exp\left(-\frac{|\mathbf{R}_n - \mathbf{R}_{n'}|}{l}\right) \\ \times \int \frac{d\mathbf{p} d\mathbf{p}'}{(2\pi)^6} |I(\mathbf{p}' - \mathbf{p})|^2 \frac{n_{\mathbf{p}\beta}^0 (1 - n_{\mathbf{p}\alpha}^0)}{\xi(\mathbf{p}'/\beta) - \xi(\mathbf{p}/\alpha)} \exp[-i(\mathbf{p}' - \mathbf{p})(\mathbf{R}_n - \mathbf{R}_{n'})] \quad (10)$$

We rewrite (10) in a form convenient for calculations:

$$H_{\text{eff}} = \frac{I^2}{N^2} \sum_{nn'} \exp\left(-\frac{R_{nn'}}{l}\right) \int \frac{d\mathbf{p} d\mathbf{p}'}{(2\pi)^6} \exp[-i(\mathbf{p}' - \mathbf{p})\mathbf{R}_{nn'}] \\ \times \left\{ S_n^z S_{n'}^z \frac{n^0(\xi_{\alpha}) - n^0(\xi'_{\alpha})}{\xi_{\alpha} - \xi'_{\alpha}} + (S_n^x S_{n'}^x + S_n^y S_{n'}^y) \frac{n^0(\xi_{\alpha}) - n^0(\xi'_{\alpha})}{\xi_{\alpha} - \xi'_{\alpha}} \right\} \quad (11)$$

where (we consider in the following the zero-temperature case)

$$n_0^0(\xi_{\alpha}) = \begin{cases} 1, & \xi_{\alpha} < 0 \\ 0, & \xi_{\alpha} > 0 \end{cases} \quad \xi'_{\alpha} \equiv \xi(\mathbf{p}', \alpha),$$

and we assume that $|\mathbf{I}(\mathbf{p}' - \mathbf{p})| = I = \text{const}$, $\mathbf{R}_{nn'} = \mathbf{R}_n - \mathbf{R}_{n'}$.

Expressions such as (11) have often been evaluated (see, e.g.,^[5]). We give therefore at once the final result:

$$H_{\text{eff}} = -\frac{\pi}{2} \frac{I^2 \rho^2(0) \xi_0}{N^2} \sum_{nn'} \frac{\exp(-R_{nn'}/l)}{p_0^4 R_{nn'}^4} \{ (\Phi^+ + \Phi^-) S_n^z S_{n'}^z \\ + 2\Phi (S_n^x S_{n'}^x + S_n^y S_{n'}^y) \}, \quad (12)$$

where

$$\rho(0) = mp_0/2\pi^2, \quad R = R_{nn'}, \\ \Phi^{\pm} = \sin(2p_0 R) - 2p_0 R \cos(2p_0 R), \\ \Phi = \sin(2p_0 R) - 2p_0 R \cos(2p_0 R) \\ + 8\kappa_2^4 R^4 \left[\frac{\sin(2p_0 R)}{(2p_0 R)^2} + \frac{\cos(2p_0 R)}{2p_0 R} + \text{Si}(2p_0 R) \right] \\ - \left\{ \sin(2\kappa_2 R) - 2\kappa_2 R \cos(2\kappa_2 R) \right. \\ \left. + 8\kappa_2^4 R^4 \left[\frac{\sin(2\kappa_2 R)}{(2\kappa_2 R)^2} + \frac{\cos(2\kappa_2 R)}{2\kappa_2 R} + \text{Si}(2\kappa_2 R) \right] \right\}, \quad (14)$$

Si is the sine integral.

Assuming that always $\Delta/\xi_0 \ll 1$ we rewrite the expression for $\Phi^+ + \Phi^-$ in the form

$$\Phi^+ + \Phi^- \approx 2[\sin(2p_0 R) - 2p_0 R \cos(2p_0 R)] \cos(2\kappa_1 R) \\ + 2(2\kappa_1 R) \sin(2\kappa_1 R) \sin(2p_0 R). \quad (15)$$

Let us discuss the results.

1. Equation (15) shows that the Ruderman-Kittel-Kasuya-Yosida (RKKY)^[1] oscillations of the spin den-

sity of the conduction electrons are modulated in our case by long-wave oscillations with period $1/2\kappa_1$. These "beats" of the spin density can lead to a corresponding magnetic structure in the system of localized spins. We estimate the temperature T_{C1} of such a magnetic transition (see also the interesting paper by Liu^[6]). Let the RKKY interaction lead to ferromagnetism with a Curie point T_C . T_{C1} will then be of the order

$$T_{C1} \sim T_C \frac{\kappa_1^3}{\rho_0^3} \exp\left(-\frac{\xi_0}{\Delta} \frac{1}{\rho_0 l}\right) \sim T_C \left(\frac{\Delta}{\xi_0}\right)^3.$$

We see that for an impurity ferromagnet ($\Delta = c\langle S_{\Omega}^z \rangle I$, c is the concentration of the magnetic impurities) $T_{C1} = 10^{-6} T_C$. If $T_C \sim 10^2$ K, $T_{C1} \sim 10^{-4}$ K. In the case of a strong ferromagnet (from the iron group) $T_{C1} \sim 10^{-3}$ K. In these estimates we took the ratio of the Fermi energy to the sd-exchange integral to be equal to 100. In the case of a metal with magnetic impurity ions in achievable magnetic fields ($\Delta = \mu B$, $\mu =$ Bohr magneton, $B =$ magnetic induction) $T_{C1} \lesssim 10^{-7}$ K.

2. Equation (14) shows the occurrence of additional oscillations with a period $1/2\kappa_2$ in the transverse part of the exchange. Such a structure can be observed in the absorption of electromagnetic waves with wavelengths $1/2\kappa_2$ at temperatures below T_{C2} :

$$T_{C2} \sim T_C \left(\frac{\kappa_2}{\rho_0}\right)^4 \sim T_C \left(\frac{\Delta}{\xi_0}\right)^2,$$

i.e., T_{C2} is larger than T_{C1} by a factor ξ_0/Δ . For instance, in the case of a ferromagnet $T_{C2} \sim 10^{-1}$ K.

The predicted magnetic structures in a system of localized spins lie thus in general in an achievable range of temperatures. We note the characteristic dependence of the periods of the structures on the concentration of magnetic impurities in the case of an impurity ferromagnet (see also^[7]).

3. MOMENTUM REPRESENTATION

We calculate now the spin susceptibility as function of the momentum transfer $\mathbf{p}' - \mathbf{p} = \mathbf{q}$. To do this it is necessary to stop halfway in the transition from Eq. (11) to (12). For the longitudinal part of the exchange we get

$$H_{\text{eff}}^{(0)} = -\frac{1}{2} \int \frac{d\mathbf{q}}{(2\pi)^3} |I(\mathbf{q})|^2 [S^z(\mathbf{q})]^2 [\mathfrak{M}_{1-}(\mathbf{q}) + \mathfrak{M}_{1+}(\mathbf{q})], \quad (16)$$

where we have written as usual

$$[S^z(\mathbf{q})]^2 = \frac{1}{N^2} \sum_{nn'} S_n^z S_{n'}^z \exp\{i\mathbf{q}(\mathbf{R}_n - \mathbf{R}_{n'})\} \exp\left\{-\frac{|\mathbf{R}_n - \mathbf{R}_{n'}|}{l}\right\}. \quad (17)$$

As $l \rightarrow \infty$, (17) changes to

$$|S^z(\mathbf{q})|^2, \quad S^z(\mathbf{q}) = \frac{1}{N} \sum_n S_n^z e^{i\mathbf{q}\mathbf{R}_n}, \quad (18)$$

$$\mathfrak{M}_{1\mp}(q) = \frac{1}{4} \rho_{\mp}(0) \left[\frac{4p_{0\mp}^2 - q^2}{4p_{0\mp} q} \ln \frac{2p_{0\mp} + q}{2p_{0\mp} - q} + 1 \right].$$

For the transverse part of the exchange we find

$$H_{\text{eff}}^{(2)} = -\frac{1}{2} \int \frac{d\mathbf{q}}{(2\pi)^3} |I(\mathbf{q})|^2 ([S^x(\mathbf{q})]^2 + [S^y(\mathbf{q})]^2) [\mathfrak{M}_{2-}(\mathbf{q}) + \mathfrak{M}_{2+}(\mathbf{q})], \quad (19)$$

$$\mathfrak{M}_{2\mp}(q) = \pm \frac{m}{4\pi^2 q} \left[\frac{1}{2} (p_{0\mp}^2 - w_{\mp}^2) \ln \frac{p_{0\mp} + w_{\mp}}{p_{0\mp} - w_{\mp}} + w_{\mp} p_{0\mp} \right], \\ w_{\mp} = (4\kappa_2^2 \pm q^2) / 2q. \quad (20)$$

Equations (18) and (20) generalize the Yosida formula (see also the interesting paper^[8] by Anderson and Suhl) to the case of exchange through electrons with separated Fermi spheres.

Let us discuss these results.

1) For small q

$$\chi_{1-} + \chi_{1+} \approx \frac{1}{2} [\rho_{-}(0) + \rho_{+}(0)] - \frac{m}{12(2\pi)^2} \left(\frac{1}{p_{0-}} + \frac{1}{p_{0+}} \right) q^2. \quad (21)$$

The minimum momentum transfer connected with a conduction electron spin flip is equal to $q = p_{0-} - p_{0+} = 2\kappa_1$. For this minimum value of q a maximum is reached in the effective exchange integral, as can be seen from (21); this can, as we showed above, lead to a magnetic structure with a period $1/2\kappa_1$ in a system of localized spins.

2) The part χ_{2+} of the transverse susceptibility causing absorption of electromagnetic waves vanishes for $q = 2\kappa_2$ and increases on the positive side when $q > 2\kappa_2$. Then $(d\chi_{2+}/dq)_{q=2\kappa_2} \rightarrow \infty$ as $1/2\kappa_2$ as $2\kappa_2 \rightarrow 0$, i.e., the absorption has a resonance character. We must thus expect resonance absorption of electromagnetic waves with wavelength $1/2\kappa_2$ as was noted earlier.

4. CONCLUSION

1. In principle one can observe oscillations of the conduction electron spin density with period $1/2\kappa_1$ at room temperatures in paramagnets in a magnetic field, using the Knight shift. Oscillations of the conduction electron spin density with period $1/2\kappa_2$ can also be observed in paramagnetics in a magnetic field at normal temperatures and in ferromagnets in (very weak) absorption of electromagnetic waves.

2. It is necessary to generalize the results obtained for the case of non-spherical Fermi surfaces, unquenched orbital angular momenta, and so on. There may then appear interesting details (especially in the case of the rare earths). The calculations must take into account quantum orbits for the case of very pure metals.

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¹M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954); T. Kasuya, Progr. Theor. Phys. **16**, 45 (1956); K. Yosida, Phys. Rev., **893** (1957).

²P. G. de Gennes, J. Phys. Radium **23**, 630 (1962).

³A. J. Heeger, A. P. Klein, and P. Tu, Phys. Rev. Letters **17**, 803 (1966).

⁴A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, *Metody kvantovoi teorii polya v statisticheskoi fizike* (Quantum Field Theoretical Methods in Statistical Physics) Fizmatgiz, 1962 [English translation published by Pergamon Press].

⁵J. H. Van Vleck, Revs. Modern Phys. **34**, 681 (1962).

⁶S. H. Liu, J. Phys. Chem. Solids **24**, 475 (1963).

⁷A. A. Berdyshev and O. S. Akhtyamov, Fiz. Met. Metallov. **23**, 220 (1967) [English translation in Phys. Metals Metallogr.].

⁸P. W. Anderson and H. Suhl, Phys. Rev. **116**, 898 (1959).

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