

# Distinctive features of the electron-electron interaction in strongly anisotropic layered metals

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In layered metals, the anisotropic structure combines with the Coulomb and RKKY interactions to create unusual Friedel oscillations whose period exactly coincides with twice the spacing between layers. This results in a Coulomb-mediated mechanism for superconductive pairing of electrons and an RKKY interaction that leads to an antiferromagnetically-ordered magnetic structure with oppositely oriented magnetic layers.

## 1. INTRODUCTION

High-temperature superconductivity has been discovered in a number of families of compounds, specifically La–Ba–Cu–O, Y–Ba–Cu–O, Bi–Sr–Ca–Cu–O, and Tl–Ba(Ca)–Cu–O. Despite strenuous efforts directed at making sense of the experimental investigations, which are many and varied, at this time the microscopic mechanism for high-temperature superconductivity in these compounds remains obscure. Under these circumstances, we are well-advised to investigate the overall patterns imposed by experiment on the properties of high-temperature superconductors.

We will base our discussion on the well-known experimental fact<sup>1</sup> that all these compounds have a layered perovskite structure characterized by copper-oxygen layers in which the conduction electrons are concentrated. Measurements of the conductivity, upper critical field, penetration depth, and other physical quantities clearly indicate that all these systems are strongly anisotropic, which is a consequence of the different nature of the motion of conduction electrons along and transverse to the layers.

The unusual magnetic properties of these compounds are also noteworthy. The discovery of superconductivity in one of these systems—YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>—at temperatures above 90 K stimulated the fabrication and investigation of the series of rare-earth compounds RBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>. It was found that complete replacement of yttrium by rare-earth magnetic ions R had practically no effect on the superconducting transition temperature, which remains ≈90 K; the only exceptions to this rule are the compounds with R = Ce, Pr, and Tb, which are either normal metals or insulators. At lower temperatures (on the order of 1 K), three-dimensional magnetic ordering appears in the sublattice of rare-earth magnetic ions, which raises the question of how superconductivity and magnetism can coexist in these systems. This question has arisen before, and was intensely investigated,<sup>2</sup> with regard to the ternary magnetic superconductors RMo<sub>6</sub>S<sub>8</sub>, RMo<sub>6</sub>Se<sub>8</sub>, and RRh<sub>4</sub>B<sub>4</sub>.

The coexistence of superconductivity and magnetism is closely bound up with interactions between magnetic ions and the conduction electrons that are responsible for the superconducting properties. It is well-known<sup>3</sup> that when magnetic ions in a superconductor behave as expected they usually cause a very abrupt decrease in the superconducting transition temperature due to the exchange interaction between conduction electrons and ion spins. In this case the

magnitude of the drop in the superconductive transition temperature is comparable with the magnetic ordering temperature. In the ternary compounds the coexistence of magnetism and superconductivity is favored by the fact that the conduction electrons and the magnetic ions are spatially separated due to the peculiar crystal structure of these compounds.<sup>4</sup> The same phenomenon occurs in the high-temperature superconductors RBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>: the conduction electrons are located in the CuO<sub>2</sub> planes, while the rare-earth ions R are located between these planes, and this physical separation weakens the influence of the magnetic moments of the rare-earth ions on the superconducting pairing temperature.

In the high-temperature superconductors the conduction electrons are concentrated in narrow regions along the conducting planes. In this case the basic motion of the electrons has a marked two-dimensional character, with transitions between layers occurring only rarely. Under these circumstances, it is reasonable to suppose that within each conducting layer there is a well-defined dispersion law for electrons with the ordinary energy parameters  $\sim \epsilon_F$ , while the rare transitions between layers are characterized by a hopping integral  $t \ll \epsilon_F$ . Let us assume that the motion in the layer is isotropic and characterized by a longitudinal mass  $m$ , while the motion of electrons between layers can be described using the tight-binding approximation, and that these motions of the electrons are independent. Then the dispersion law for the electrons has the following form:

$$\xi(\mathbf{p}) = (p_x^2 + p_y^2)/2m + t \cos p_z d - p_0^2/2m, \quad t \ll p_0^2/2m, \quad (1)$$

where  $d$  is the interplanar spacing and  $p_0$  is the Fermi momentum.

For  $t = 0$  the Fermi surface is a cylinder; switching on the overlap  $t \neq 0$  creates corrugations on the cylinder (Fig. 1). In view of this, very general considerations based on the fact that the crystal structure is laminar and the motion of electrons is free in the conducting planes and restricted in the perpendicular directions imply that the coherent motion of conduction electrons is described by strongly anisotropic dispersion laws, and that the Fermi surface is open in the direction perpendicular to the layers (compare with Refs. 5–7). As we will see, this leads to marked peculiarities in the behavior both of the electron–electron interaction in layered metals and of the indirect exchange interaction of rare-earth magnetic ions via conduction electrons. These peculiarities

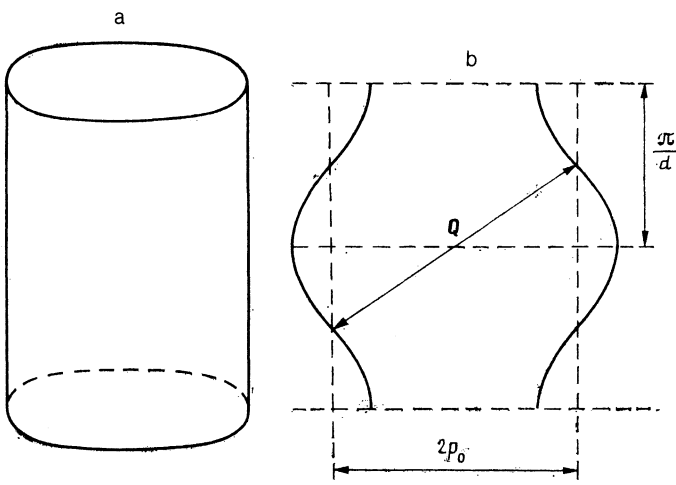


FIG. 1. Cylindrical Fermi surface in the absence ( $t = 0$ ) of interplanar hopping (a) and a cross section of the Fermi surface when interplanar hopping ( $t \neq 0$ ) is included (b)  $\mathbf{Q}$  is the distinctive vector which is associated with a corrugated cylinder.

will be discussed in both the normal and superconducting states.

## 2. DESCRIPTION OF THE SCREENED COULOMB INTERACTION IN LAYERED METALS

Let us consider a model of a layered metal in which the motion of conduction electrons follows an isotropic quadratic dispersion relation in the layer, while motion of conduction electrons between layers is treated in the tight-binding approximation; within the band picture we can use the dispersion law (1) to describe this motion. In order to analyze the screened Coulomb interaction in the high-density limit,<sup>8</sup> where  $p_0 a_B \gg 1$  [here  $a_B = (me^2)^{-1}$  is the Bohr radius], it is sufficient as usual to include only ring diagrams. Then the screened Coulomb interaction  $U$  can be found from the well-known equation

$$\begin{aligned} \bar{U}(\mathbf{r}\mathbf{r}', \omega) &= U(\mathbf{r}-\mathbf{r}') - 2T \sum_{\mathbf{e}} \int d\mathbf{r}_1 d\mathbf{r}_2 U(\mathbf{r}-\mathbf{r}_1) G(\mathbf{r}_1, \mathbf{r}_2, \varepsilon + \omega) \\ &\quad \times G(\mathbf{r}_2, \mathbf{r}_1, \varepsilon) \bar{U}(\mathbf{r}_2, \mathbf{r}', \omega). \end{aligned} \quad (2)$$

Here  $U(r)$  is the unscreened Coulomb interaction, which equals  $e^2/r$ , while  $G(\mathbf{r}\mathbf{r}', \omega)$  is the temperature Green's function for electrons with the dispersion law (1).

The electron density is concentrated primarily in a narrow region along the layers. Therefore we will neglect the regions outside the layers where the electron density is small. This description corresponds to transforming from the continuous coordinate representation ( $\rho, z$ ) to a discrete Wannier representation with respect to the coordinate  $z$  perpendicular to the layers, i.e., ( $\rho, n$ ), where the variable  $n$  labels the layer. The screened Coulomb interaction in the Wannier representation has the form

$$\bar{U}_{nm}^{n'm'}(\rho\omega) = \iint dz dz' \bar{U}(zz', \rho\omega) w_n(z) w_m^*(z) w_{n'}(z') w_{m'}^*(z'),$$

where  $w_n(z)$  is the Wannier function for layer  $n$ . In the same way, the Green's function also can be expressed by using Wannier functions:

$$G(zz', \kappa\omega) = \sum_{mn} w_n(z) w_m^*(z') G_{nm}(\kappa\omega), \quad (3)$$

here the vector  $\kappa = (p_x, p_y)$  denotes the momentum of an electron moving in the conducting layer. The Green's func-

tion  $G_{nm}$  depends only on the difference between the arguments  $m$  and  $n$ , which is a consequence of the invariance of the system with respect to translations with period  $d$ , and is given by the relation

$$G_{m-n}(\kappa, \omega) = d \int_{-\pi/d}^{\pi/d} \frac{dq}{2\pi} \frac{\exp[i(n-m)qd]}{i\omega - \xi(\kappa, q)}$$

Substituting Eq. (3) into Eq. (2) and going to a Fourier representation with respect to the coordinate  $\rho$ , we obtain an integral equation with interchange of momentum along the conducting layer. Then, by using Wannier functions to project this equation onto the plane of the conducting layer, we obtain an equation for the quantities  $\bar{U}_{nm}^{n'm'}(\kappa, \omega)$ . Since the overlap of electronic layers is small, i.e., the Wannier function  $w_n(z)$  is localized near the  $n$ th layer, we need only retain those terms that do not contain any small quantities connected with integration with respect to Wannier functions from different layers. In this approximation

$$\bar{U}_{nm}^{n'm'} = \bar{U}_{nn'} \delta_{nm} \delta_{n'm'}.$$

This results in the following equation for the screened Coulomb interaction:

$$\begin{aligned} \bar{U}_{nn'}(\kappa, \omega) &= U_{nn'}(\kappa) \\ &\quad - 2T \sum_{\mathbf{e}} \int \frac{d^2\kappa_1}{(2\pi)^2} \sum_{kl} U_{nk}(\kappa) G_{kl}(\kappa_1 + \kappa, \varepsilon + \omega) \\ &\quad \times G_{lk}(\kappa_1, \varepsilon) \bar{U}_{ln'}(\kappa, \omega). \end{aligned} \quad (4)$$

Let us first consider the unscreened Coulomb interaction:

$$\begin{aligned} U_{nn'}(\kappa) &= \int dz dz' U(z-z', \kappa) |w_n(z)|^2 |w_{n'}(z')|^2 \\ &= \int dz dz' U(z-z') |w_{n-n'}(z)|^2 |w_0(z')|^2. \end{aligned} \quad (5)$$

Here we have used the property  $w_n(z) = w_0(z - nd)$  of the Wannier functions. As we see, (5) depends only on the difference  $n - n'$ , and Eq. (4) is found to be an integral equation with a difference kernel in the variable  $n$ :

$$\bar{U}_{nn'} = U_{n-n'} - \sum_{kl} U_{n-k} \Pi_{k-l} \bar{U}_{ln'}. \quad (6)$$

The polarization operator is a simple loop:

$$\Pi_k(\kappa, \omega) = 2T \sum_{\epsilon} \int \frac{d^2 \kappa_1}{(2\pi)^2} G_k(\kappa_1 + \kappa, \epsilon + \omega) G_{-k}(\kappa_1, \epsilon).$$

Equation (6) is easily solved by a Fourier transform:

$$\tilde{U}(\kappa q, \omega) = U(\kappa q) / [1 + U(\kappa q) \Pi(\kappa q, \omega)]. \quad (7)$$

The denominator in (7) is the momentum- and frequency-dependent dielectric permittivity of the conduction electrons calculated within the random phase approximation. After summation over the frequency the polarization operator takes the usual form:<sup>8</sup>

$$\Pi(\kappa q, \omega) = 2 \sum_p \frac{n(\xi_{p+k}) - n(\xi_p)}{\xi_p - \xi_{p+k} + i\omega}, \quad (8)$$

where  $n(\xi_p)$  is the Fermi distribution.

From the formal point of view, Eqs. (7) and (8) establish the equivalence between perpendicular and parallel directions with respect to the conducting layers. At first glance this is unexpected, since no such equivalence is apparent in coordinate space. The inequivalence between transverse and longitudinal directions is manifest only in the dispersion law for electrons and the explicit form of the unscreened Coulomb interaction. Because the Wannier function  $w_n(z)$  is localized around the  $n$ -th layer, its contribution to  $U_n(\rho)$  is concentrated near the points  $z = nd$ :

$$U_n(\mathbf{r}) = U(\rho, nd) \int dz dz' |w_n(z)|^2 |w_n(z')|^2 = e^2 / [\rho^2 + (nd)^2]^{1/2}.$$

In the momentum representation the unscreened interaction has the form

$$U(\kappa, q) = \frac{2\pi e^2}{\kappa} \frac{\text{sh } \kappa d}{\text{ch } \kappa d - \cos qd}. \quad (9)$$

For small momentum transfer the bare Coulomb interaction (9) is three-dimensional in character:  $4\pi e^2 / (q^2 + \kappa^2)d$ , and all components of momentum are equivalent. The situation changes in a fundamental way for momentum transfers  $\kappa > d^{-1}$ , for which the unscreened Coulomb interaction becomes two-dimensional in character and equal to  $2\pi e^2 / \kappa$ , and ceases altogether to depend on the transverse momentum component  $q$ .

### 3. DISTINCTIVE PROPERTIES OF COULOMB REPULSION AND FRIEDEL OSCILLATIONS IN A LAYERED METAL

The behavior of the screened Coulomb interaction is determined by the form of the polarization operator in (8). Its form is simplest for a pure two-dimensional dispersion law,<sup>9</sup> i.e., when the transfer integral between conducting layers satisfies  $t = 0$ . The static polarization operator equals a constant which coincides with the two-dimensional density of states for momenta less than twice the Fermi momentum  $2p_0$ :

$$\Pi(\kappa) = m/\pi, \quad \kappa \leq 2p_0,$$

and then decreases with increasing  $\kappa$ :

$$\Pi(\kappa) = \Pi(0) \{1 - [1 - (2p_0/\kappa)^2]^{1/2}\}^{1/2}, \quad \kappa > 2p_0. \quad (10)$$

Note that the screening is absolutely independent of the electron density for  $\kappa < 2p_0$ ; we emphasize that this is specific to the two-dimensional problem.

In the quasi-two-dimensional case, i.e., for arbitrary

transfer integral  $t \neq 0$ , the polarization operator can be written in the form

$$\begin{aligned} \Pi(\mathbf{p}) / \Pi(0) = & 1 - \pi^{-1} \kappa^{-2} \int_0^\pi d\varphi \theta \left( \kappa^2 - 4m \left| t \sin \frac{qd}{2} \right| \sin \varphi \right) \\ & \times F^{1/2}(\varphi) \theta(F(\varphi)), \end{aligned} \quad (11)$$

$$\begin{aligned} F(\varphi) = & \kappa^2 (\kappa^2 - 4p_0^2) + 8\kappa^2 m t \cos \frac{qd}{2} \cos \varphi \\ & + 16m^2 t^2 \sin^2 \frac{qd}{2} \sin^2 \varphi, \end{aligned}$$

where  $\Pi(0) = m/\pi$  is the two-dimensional density of states. It is apparent from (11) that in the quasi-two-dimensional case the static polarization operator for momenta  $\kappa$  smaller than  $2p_0$  remains constant to accuracy  $t/\epsilon_F$ , and equals the two-dimensional density of states. Equation (11) allows us to study the screened Coulomb interaction as a function of the spacing between layers.

When there is no hopping between layers ( $t = 0$ ) the dependence of the screened Coulomb interaction on the transverse momentum is determined by the bare Coulomb interaction  $U(\mathbf{p})$  which enters into (9). Therefore the screened Coulomb interaction can be written in the form

$$\tilde{U}(\kappa, q) = \frac{2\pi e^2}{\kappa} \frac{\text{sh } \kappa d}{A(\kappa) - \cos qd},$$

$$A(\kappa) = \text{ch } \kappa d + (2\pi e^2/\kappa) \Pi(\kappa) \Big|_{t=0} \text{sh } \kappa d.$$

From  $\Pi(0) > 0$  it follows that  $A(\kappa) > 1$ . In particular, for  $\kappa = 0$  we have  $A(0) = 1 + 2d/a_B$ . Since the interplanar spacing  $d$  is much larger than the Bohr radius  $a_B$  in real metals, we find that  $A(0) \gg 1$ . As  $\kappa$  increases  $A(\kappa)$  increases monotonically as well, and so we have  $A(\kappa) \gg 1$  for all  $\kappa$ . The parameter which measures the extent to which this inequality is fulfilled is the ratio of the interplanar spacing to the Bohr radius,  $d \gg a_B$ . Let us expand the screened Coulomb interaction in a Fourier series:

$$\tilde{U}(\mathbf{p}) = \sum_n \tilde{U}_n(\kappa) \exp(-inqd).$$

The Fourier component  $\tilde{U}_n(\kappa)$  is determined by the simple expression

$$\tilde{U}_n(\kappa) = \frac{2\pi e^2}{\kappa} \text{sh } \kappa d \{A(\kappa) - [A^2(\kappa) - 1]^{1/2}\}^{|n|} / [A^2(\kappa) - 1]^{1/2}. \quad (12)$$

Since  $A(\kappa) \gg 1$  holds for all  $\kappa$ , we find that  $U_n(\kappa)$  decreases rapidly as the label  $n$  increases, and that  $U_n(\kappa) \propto (2A)^{-n-1}$ . Although the Coulomb interaction is important for  $n = 0$ , it decreases exponentially with  $n$ ; moreover, the exponent involved has a factor  $2 \ln(2d/a_B) \gg 1$ . For  $n = 1$ , this weakening of the Coulomb

interaction implies that screening which involves the interaction of electrons located in adjacent layers is mediated not by single electrons with charges of magnitude  $e$  but rather by dipoles of size  $\sim a_B$  and distance between dipoles  $\sim d$ . The interaction of charges from more distant planes corresponds to increasing multipolarity.

This exponential decrease of the Coulomb repulsion in directions perpendicular to the conducting layers takes place only for a cylindrical Fermi surface, i.e., for  $t = 0$ . For  $t \neq 0$  the Fermi surface becomes a corrugated cylinder, in which case a special vector is singled out with  $k_z = \pi/d$  (Fig. 1b) corresponding to a new singularity of the polarization operator (11). This singularity of the polarization operator leads to the appearance of a new period in the Friedel oscillations, which equals twice the spacing  $2d$  between conducting layers. The period of the oscillations coincides with twice the spacing between layers because the Fermi surface is open in the direction parallel to the  $k_z$  axis. As the width of the band increases, the overlap integral increases as well until  $t \gtrsim p_0^2/2m$  is satisfied, at which point the Fermi surface becomes closed. From here on, the period of the Friedel oscillations ceases to equal twice the period of the lattice.

Although the Friedel oscillations of the Coulomb interaction decay, their decrease is governed by a power law, i.e., considerably slower than exponential. This implies that the oscillatory part of the interaction will dominate over its monotonic repulsive part starting with a certain layer label  $n_r$ . Because the Friedel part of the interaction changes sign as we go from one layer to another, electrons in different conducting layers attract one another beginning with labels  $n > n_r$ . This latter effect mediates a superconducting transition in the system of conduction electrons, which we will discuss below.

The fact that the period of the Friedel oscillations equals twice the distance between layers can also lead to a structural phase transition with a period twice that of the crystal lattice in the  $z$ -axis direction. This structural transition is one possible channel by which the Fermi surface can change its topology, as was discussed in Refs. 10 and 11; see Fig. 2.

#### 4. THE ELIASHBERG EQUATION AND THE SUPERCONDUCTING TRANSITION TEMPERATURE

In order to determine the superconducting transition temperature  $T_c$  we write the Eliashberg equation for the gap in the following form:

$$\Delta(x, x') = \int d^3y d^3z G(x, y) G(x', z) \Delta(y, z) \Gamma(y, z), \quad (13)$$

where the kernel  $\Gamma$  includes both the electron-phonon and the Coulomb interaction:  $\Gamma(\mathbf{p}, \omega) = D(\mathbf{p}, \omega) + \tilde{U}(\mathbf{p}, \omega)$ . It is convenient to introduce the momentum and Wannier representations in the Eliashberg equation, as we did above in analyzing the screened Coulomb interaction (see also Refs. 5 and 6). After a Fourier transform with respect to the longitudinal coordinates  $x, y$  we can expand the gap in Wannier functions:

$$\Delta(zz', \kappa\omega) = \sum_{nn'} w_n(z) w_{n'}(z') \Delta_{nn'}(\kappa\omega).$$

This leads to the equation

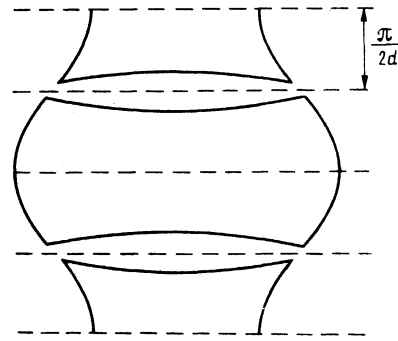


FIG. 2. Splitting of the Fermi surface when the period of the crystal lattice is doubled.

$$\Delta_{nn'}(\kappa\omega) = -T \sum_{\kappa_1\omega_1} \Gamma_{m'l'}^{m'l'}(\kappa - \kappa_1, \omega - \omega_1) G_{nl}(\kappa\omega) \times G_{n'l'}(-\kappa, -\omega) \Delta_{mm'}(\kappa_1\omega_1).$$

In obtaining this equation we have used the following property of the kernel of Eq. (14) in the Wannier function representation:

$$\Gamma_{m'l'}^{m'l'} = \Gamma_{mm'} \delta_{m_l} \delta_{m'l'},$$

which is connected with the localization of the Wannier functions in narrow regions around the conducting layers. Carrying out the Fourier transform with respect to the layer index and introducing the new function  $\Delta \rightarrow \Delta/(\omega^2 + \xi^2)$ , we obtain the Eliashberg equation in the momentum representation:

$$\Delta(\mathbf{p}, \omega) = -T \sum_{\mathbf{p}_1\omega_1} \Gamma(\mathbf{p} - \mathbf{p}_1, \omega - \omega_1) \Delta(\mathbf{p}_1, \omega_1) / (\omega_1^2 + \xi_1^2). \quad (14)$$

All the projections of the momentum enter into (14) in an identical way. This is analogous to the symmetry between components mentioned earlier which emerged in the course of our description of the screened Coulomb interaction. The lack of equivalence of the longitudinal and transverse motion is manifest only in the form of the kernel  $\Gamma$  and the dispersion law  $\xi(\mathbf{p})$ . In this analysis we will ignore both Coulomb- and phonon-induced renormalization of the electron Green's function, since these refinements do not change our results qualitatively.

The solution of Eq. (14) is conveniently expanded in Fourier harmonics, resulting in a corresponding equation for each harmonic whose nontrivial solution  $\Delta_n \neq 0$  leads to a transition temperature  $T_n$ :

$$T_n = (2\gamma/\pi) \omega_0 \exp[-1/(\lambda_n - \mu_n^*)], \quad (15)$$

$$\mu_n^* = \frac{\mu_n}{1 + \mu_n \ln(\epsilon_F/\omega_0)}.$$

Here  $\lambda_n$  is the  $n$ th harmonic of the electron-phonon interaction constant and  $\mu_n$  is the angular average of the screened Coulomb interaction  $\tilde{U}(\kappa, q)$ :

$$\mu_n = \frac{md}{\pi^2} \int_{-\pi/d}^{\pi/d} \frac{dp_z}{2\pi} \exp(inqd) \int_0^{2p_0} \frac{d\kappa}{(4p_0^2 - \kappa^2)^{1/2}} \mathcal{U}(\kappa, q).$$

The transition temperature is obviously determined by the maximum  $T_n$ .

Let us investigate the Coulomb pseudopotential  $\mu_n$ , which can be written in the form of a sum of two terms:

$$\mu_n = \mu_n^{(1)} + \mu_n^{(2)}. \quad (16)$$

The first (repulsive) term in this interaction is short-range and is determined by the polarization operator (11) for  $t = 0$ :

$$\begin{aligned} \mu_0^{(1)} &= (\alpha/\pi) \ln(1/\alpha), \quad \alpha = e^2/\hbar v, \\ v &= p_0/m, \quad \mu_n^{(1)} = \mu_0^{(1)} (a_B/2d)^{n+1}. \end{aligned} \quad (17a)$$

Thus, in layered metals the Coulomb repulsion is weakened within all the layers except the layer with  $n = 0$  by a small factor of order  $a_B/2d \ll 1$ .

The second term in (16) appears as soon as we allow hopping from one layer to the next, and is analogous to the ordinary Friedel oscillations that accompany the screening of a charge placed in a quasi-isotropic metal.<sup>12</sup> This part of the interaction is oscillatory and decreases at large distances as

$$\mu_n^{(2)} = \frac{(-1)^{n+1}}{4\pi^2} \frac{\alpha^2}{(1+\alpha)^2} \frac{m|t|}{p_0^2} \frac{1}{n^2 - 1/4}. \quad (17b)$$

We emphasize that  $\mu_n^{(2)}$  is negative for all even  $n$  and is positive for all odd  $n$ . For the even- $n$  layers there is a competition between the attractive and repulsive parts of the Coulomb interaction. Beginning with a certain critical label  $n_t$ , which can always be found for a given bandwidth, the attractive part of the interaction dominates over the repulsive. This situation is realized even for  $n = 2$  if  $t > t_2$ , where

$$t_2 = (p_0^2/2m) (a_B/\alpha d)^3 \ln(2/\alpha).$$

In this case, the width of the band transverse to the layer is much smaller than it is along the layer, i.e.,  $t_2 \ll p_0^2/2m$ . Thus, even in the absence of the electron-phonon interaction this leads to a Coulomb mechanism for superconducting pairing with a transition temperature

$$T_c = \epsilon_F \exp(-15\pi^2 v^3 p_0 / |t| e^4). \quad (18)$$

This mechanism for superconductivity is analogous to the Kohn-Luttinger mechanism,<sup>13</sup> in which superconducting pairing involving nonzero orbital angular momentum can take place for an isotropic Fermi surface.

## 5. DESCRIPTION OF MAGNETIC INTERACTIONS IN LAYERED METALS

Let us consider the interaction of magnetic moments in a layered metal which also form a layered crystalline sublattice. In general, the layers of magnetic moments need not coincide with the conducting layers, and can be spatially displaced with respect to them.

The dipole interaction of a spin  $S_a$  located at a point  $R_a$  has the form

$$V_a = -\mu S_a B(R_a), \quad (19)$$

where  $\mu$  is the effective Bohr magneton. The interaction between the magnetic moment of an ion and the magnetic field induced by the magnetic moments of its neighbors has an additional contribution in the superconducting state compared to a normal metal due to the nonattenuating conduction electron currents which occur in superconductors.

The magnetic field can be found from the Maxwell equations including the supercurrents. The exchange interaction between the conduction electrons and the magnetic moment of the spin  $S_a$  has the usual form

$$U(\mathbf{r}) = - \int d^3 r' J(\mathbf{r}-\mathbf{R}_a) \psi_{\alpha}^+(\mathbf{r}) \sigma_{\alpha\beta} S_a \psi_{\beta}(\mathbf{r}), \quad (20)$$

where  $J$  is the exchange integral. Indirect exchange between two spins is expressed in terms of the magnetic susceptibility<sup>14</sup> in the following way:

$$U(\mathbf{R}_b, \mathbf{R}_a) = - (S_b S_a) \int d^3 r d^3 r' J(\mathbf{r}-\mathbf{R}_b) \chi(\mathbf{r}, \mathbf{r}') J(\mathbf{r}'-\mathbf{R}_a), \quad (21)$$

where  $\chi(\mathbf{r}, \mathbf{r}')$  is the nonlocal spin susceptibility, which can be written as a correlator:

$$\begin{aligned} \chi(\mathbf{r}, \mathbf{r}') &= - \int_0^{1/T} d\tau_2 \sigma_{\alpha\beta}^2 < T_{\tau} \psi_{\beta}(x_1) \psi_{\gamma}^+(x_2) \sigma_{\gamma\delta}^2 \psi_{\delta}(x_2) \\ &\times \psi_{\alpha}(x_1') > |_{\tau_1'=\tau_1, \tau_1'=\tau_1+\tau_2}. \end{aligned} \quad (22)$$

In a pure superconductor the susceptibility (22) is immediately given in terms of the temperature Green's function:

$$\begin{aligned} \chi(\mathbf{r}, \mathbf{r}') &= -2T \sum_{\omega} G_{\omega}(\mathbf{r}', \mathbf{r}) G_{\omega}(\mathbf{r}, \mathbf{r}') + F_{\omega}(\mathbf{r}, \mathbf{r}') F_{\omega}^+(\mathbf{r}', \mathbf{r}), \\ \omega &= \pi T (2n+1). \end{aligned} \quad (23)$$

Since the electron density is negligibly small outside the conducting layers, it is convenient to carry out a transformation from the continuous coordinate representation  $(\mathbf{p}, z)$  to the discrete Wannier representation  $(\mathbf{p}, n)$  perpendicular to the planes of the layers along the  $z$ -axis. This representation corresponds to the tight-binding approximation and agrees with the dispersion law (1). The variable  $n$  labels the layers. Using the relation between Bloch functions and Wannier functions, we write the Green's function of the electrons in the following form:

$$\begin{aligned} G_{\omega}(\mathbf{r}, \mathbf{r}') &= \sum_{kl} w_k(z) w_l^*(z') G_{kl}, \\ F_{\omega}(\mathbf{r}, \mathbf{r}') &= \sum_{kl} w_k(z) w_l(z') F_{kl}. \end{aligned} \quad (24)$$

Relation (21) in this case takes the form

$$\begin{aligned} U(\mathbf{R}_b, \mathbf{R}_a) &= - (S_b S_a) \int d^3 r d^3 r' \sum_{klmn} J(\mathbf{r}-\mathbf{R}_b) J(\mathbf{r}'-\mathbf{R}_a) w_k(z) w_l^*(z') \\ &\times w_m(z') w_n^*(z) \chi_{mk}^{ln}(\mathbf{p}, \mathbf{p}'), \end{aligned} \quad (25)$$

where the spin susceptibility can be written

$$\begin{aligned} \chi_{km}^{ln}(\mathbf{p}, \mathbf{p}') &= -2T \sum_{\omega} G_{kl}(\mathbf{p}, \mathbf{p}') G_{mn}(\mathbf{p}', \mathbf{p}) \\ &+ F_{km}(\mathbf{p}, \mathbf{p}') F_{ln}^+(\mathbf{p}', \mathbf{p}). \end{aligned} \quad (26)$$

Further simplification is possible only if we use certain assumptions regarding the behavior of the exchange integral

$J(\mathbf{r})$  and the Wannier functions  $w_n(z)$ . In the compounds under discussion the magnetic moments are associated with rare-earth ions which have unfilled  $4f$  shells of electrons. These shells are more localized than the external shells of copper and oxygen from the conduction layers. Because the thickness of the latter determines the characteristic scale of decay of the Wannier functions, we can assume that the spatial size of the exchange integral  $J(\mathbf{r})$  is much smaller than the width of the Wannier functions. This implies that it is possible to replace  $J(\mathbf{r})$  by  $J\delta(\mathbf{r})$ , where  $J$  is the zero Fourier component. For indirect exchange we obtain from (25)

$$U(\mathbf{R}_b, \mathbf{R}_a)$$

$$= -J^2(\mathbf{S}_b \mathbf{S}_a) \sum_{klmn} w_k(z_a) w_l^*(z_b) w_m(z_b) w_n^*(z_a) \chi_{klmn}^{in}(\rho_a, \rho_b). \quad (27)$$

In what follows we limit ourselves to discussing the following two cases for the positions of the magnetic ions.

1. The layers of magnetic ions exactly coincide with the conducting layers, i.e., they are located at the points  $z_a = ad$  and  $z_b = bd$ . Since the Wannier functions are localized near  $z = nd$  and fall off rapidly outside the layers, terms in the sum with  $k = n = a$  and  $l = m = b$  in (27) are dominant in the nearest-neighbor approximation, which leads to the following expression:

$$U(\mathbf{R}_b, \mathbf{R}_a) = -J_{eff}^2(\mathbf{S}_b \mathbf{S}_a) \chi_{ab}^{ba}(\rho_a, \rho_b), \quad (28)$$

where  $J_{eff}^2 = J^2 |w_0(0)|^4$ .

2. The magnetic-ion layers are located exactly midway between the conducting layers, i.e., for  $z_a = ad + d/2$ ,  $z_b = bd + d/2$ . In contrast to the previous case, in the same approximation we must retain more terms in the sum (28):

$$U(\mathbf{R}_b, \mathbf{R}_a) = -J_{eff}^2(\mathbf{S}_b, \mathbf{S}_a) \sum_{h,n=a}^{a+1} \sum_{l,m=b}^{b+1} \chi_{hlmn}^{in}(\rho_a, \rho_b), \quad (29)$$

where  $J_{eff}^2 = J^2 |w_0(d/2)|^4$ . Naturally the quantity  $J_{eff}^2$  is much smaller in this case than in (28).

The Green's functions  $G_\omega(\rho, n, n')$  and  $F_\omega(\rho, n, n')$  can be written in the following form:

$$G_\omega(\rho, n, n') = d \int_{-\pi/d}^{\pi/d} \frac{dp_z}{2\pi} \int \frac{d^2\kappa}{(2\pi)^2} \left( -\frac{i\omega + \xi(\kappa, p_z)}{\omega^2 + \xi^2 + \Delta^2} \right) \times \exp[i\kappa\rho + ip_z d(n - n')],$$

$$F_\omega(\rho, n, n') = d \int_{-\pi/d}^{\pi/d} \frac{dp_z}{2\pi} \int \frac{d^2\kappa}{(2\pi)^2} \left( \frac{\Delta(\kappa, p_z)}{\omega^2 + \xi^2 + \Delta^2} \right) \times \exp[i\kappa\rho + ip_z d(n - n')].$$

These Green's functions depend on the difference between  $n$  and  $n'$  due to invariance of the system with respect to translation by the lattice period  $d$ . The isotropy in the conducting layer implies that the superconducting gap is uniform and does not depend on the value of momentum along the layer. This allows us to integrate over the momentum  $\kappa$  in the layer

and over angle. As a result we obtain the coordinate representation of the Green's function in a layered superconductor:

$$G_\omega(\rho, n) = -\frac{m}{2\pi} \int_{-\pi}^{\pi} \frac{dp}{2\pi} \left( \frac{\omega}{(\omega^2 + \Delta^2)^{1/2}} (K_0^* - K_0) + (K_0^* + K_0) \right) \times \exp(inp_z), \quad (30)$$

$$F_\omega(\rho, n) = -\frac{m}{2\pi} \int_{-\pi}^{\pi} \frac{dp}{2\pi} \frac{i\Delta}{(\omega^2 + \Delta^2)^{1/2}} (K_0^* - K_0) \times \exp(inp_z),$$

where  $K_0(x)$  is a zero-order Bessel function of the second kind with imaginary argument:

$$K_0 = K_0(y_\omega \rho), \quad K_0^* = K_0(y_\omega^* \rho),$$

$$y_\omega^2 = -(p_0^2 - 2mt \cos p) + 2im(\omega^2 + \Delta^2)^{1/2}.$$

Here it is assumed that  $\text{Re } y_\omega > 0$  and  $\text{Re } y_\omega^* > 0$ . In regions that satisfy the inequality  $2p_0\rho \gg 1$  Eq. (30) can be written in a simpler form. Because the sum over frequencies in (26) converges for  $|\omega| \sim v/\rho \ll p_0^2/2m$ , we can expand  $y_\omega$  for  $|\omega| \ll p_0^2/2m$ :

$$y_\omega = ip_0 \left( 1 - \frac{t}{vp_0} \cos p \right) + \frac{(\omega^2 + \Delta^2)^{1/2}}{v} \left( 1 + \frac{t}{vp_0} \cos p \right).$$

From here on we will use the asymptotic form of the Bessel function for large arguments. The behavior of the coordinate dependence of the Green's function (30) depends on the character of the dependence of the superconducting gap on the momentum component  $p_z$ . For simplicity we neglect the anisotropy of the gap and assume that

$$\Delta(p_z) = \text{const.}$$

This assumption will be quite accurate if the pairing takes place within a conducting layer, and if the pairing between layers can be neglected. As a result, for distances  $2p_0\rho \gg 1$  the Green's function is determined in the following way:

$$G_\omega(n, \rho) = -\frac{m}{(2\pi p_0 \rho)^{1/2}} J_n \left( \frac{t\rho}{v} \right) \exp \left[ -\frac{\rho(\omega^2 + \Delta^2)^{1/2}}{v} \right] \times \left[ \cos \Phi_n + \frac{i\omega}{(\omega^2 + \Delta^2)^{1/2}} \sin \Phi_n \right], \quad (31)$$

$$F_\omega(n, \rho) = \frac{m}{(2\pi p_0 \rho)^{1/2}} \frac{\Delta}{(\omega^2 + \Delta^2)^{1/2}} J_n \left( \frac{t\rho}{v} \right) \times \exp \left[ -\frac{\rho(\omega^2 + \Delta^2)^{1/2}}{v} \right] \sin \Phi_n,$$

where  $\Phi_n = p_0\rho + \pi/4 + n\pi/2$  and  $J_n(x)$  is a Bessel function. In the region  $\rho < p_0^{-1}$ , Eq. (31) is incorrect. An analytic expression for the Green's functions can be obtained for  $\rho = 0$ . For an arbitrary layer  $n \neq 0$  we obtain from (30)

$$G_\omega(n, 0) = -\frac{m}{4\pi n} \left[ z^n + z^{*n} + \frac{\omega}{(\omega^2 + \Delta^2)^{1/2}} (z^{*n} - z^n) \right], \quad (32)$$

$$F_\omega(n, 0) = -\frac{m}{4\pi n} \frac{i\Delta}{(\omega^2 + \Delta^2)^{1/2}} (z^{*n} - z^n),$$

where  $z = mt / [p_0^2 - 2im(\omega^2 + \Delta^2)^{1/2}]$ . Equations (31) and (32) can be used to calculate the exchange interaction.

## 6. INDIRECT EXCHANGE IN LAYERED SUPERCONDUCTORS

1. Let us consider the simplest case, where the magnetic moments are located in the conducting layer. The indirect exchange between spins  $S_1$  and  $S_2$  that are separated from one another by  $n$  layers and by a distance  $\rho$  along the layers is determined by Eq. (28). Substituting (31) into (28) we obtain the RKKY interaction which is correct at distances  $2p_0\rho \gg 1$ :

$$U_n(\rho) = J_{eff}^2 N(0) (S_1 S_2) J_n^2 \left( \frac{t\rho}{v} \right) \times [ (-1)^{n+1} \Phi_1(\rho) \sin 2p_0\rho + \Phi_2(\rho) ]. \quad (33)$$

Here  $N(0) = m/\pi$  is the two-dimensional density of states at the Fermi level with a fixed projection of spin, and  $v$  is the Fermi velocity. The functions  $\Phi_1(\rho)$  and  $\Phi_2(\rho)$  are determined by the expressions

$$\begin{aligned} \Phi_1(\rho) &= \frac{2T}{v\rho} \sum_{\omega} \frac{\omega^2}{\omega^2 + \Delta^2} \exp \left[ -\frac{2\rho(\omega^2 + \Delta^2)^{1/2}}{v} \right], \\ \Phi_2(\rho) &= \frac{2T}{v\rho} \sum_{\omega} \frac{\Delta^2}{\omega^2 + \Delta^2} \exp \left[ -\frac{2\rho(\omega^2 + \Delta^2)^{1/2}}{v} \right]. \end{aligned} \quad (34)$$

The following asymptotic expressions can be obtained for the functions  $\Phi_1(\rho)$  and  $\Phi_2(\rho)$  at  $T = 0$ :

$$\begin{aligned} \Phi_1(\rho) &= \begin{cases} 1/\pi\rho^2, & \rho \ll \xi_0, \\ \xi_0^{-2} (2\pi)^{-1/2} (\xi_0/\rho)^{1/2} \exp(-\rho/\xi_0), & \rho \gg \xi_0, \end{cases} \\ \Phi_2(\rho) &= \begin{cases} (2\xi_0\rho)^{-1}, & \rho \ll \xi_0, \\ \xi_0^{-2} (2\pi)^{-1/2} (\xi_0/\rho)^{1/2} \exp(-\rho/\xi_0), & \rho \gg \xi_0. \end{cases} \end{aligned} \quad (35)$$

Here  $\xi_0 = v/2\Delta$  is the superconducting coherence length. For distances  $\rho \leq p_0^{-1}$  it is not possible to obtain an analytic expression except at  $\rho = 0$ . In the approximation used here the indirect exchange reduces to zero for spins located on different layers.

$$U_n(0) = 0, \quad n \neq 0. \quad (36)$$

For spins located within the same layer we can expect the interaction  $U_0(\rho)$  to diverge as  $\rho^{-2} \ln^2(2p_0\rho)$  for  $\rho \rightarrow 0$ . In the absence of either hopping from one layer to the next ( $t = 0$ ) or a gap ( $\Delta = 0$ ) the interaction (33) wholly coincides with the RKKY interaction in a normal isotropic 2D-metal.<sup>9</sup>

2. We now turn to the second case, where the magnetic moments are located midway between adjacent conducting layers. The indirect exchange between spins  $S_1$  and  $S_2$  separated by  $n$  layers and a distance  $\rho$  along the layers is determined by Eq. (29). Analogous calculations allow us to obtain the following expression for the RKKY interaction, which is valid for  $2p_0\rho \gg 1$ :

$$\begin{aligned} U_n(\rho) &= J_{eff}^2 N(0) (S_1 S_2) \{ [4J_n^2 - (J_{n-1} - J_{n+1})^2] \\ &\quad \times (-1)^{n+1} \Phi_1(\rho) \sin 2p_0\rho \\ &\quad + 4J_n (J_{n-1} - J_{n+1}) (-1)^{n+1} \Phi_1(\rho) \cos 2p_0\rho \\ &\quad + [4J_n^2 + (J_{n-1} - J_{n+1})^2] \Phi_2(\rho) \}. \end{aligned} \quad (37)$$

The functions  $\Phi_1$  and  $\Phi_2$  were determined above, and  $J_n = J_n(t\rho/v)$  is a Bessel function. As before, the approximations we have used imply that the indirect exchange reduces to zero for spins at the same  $\rho$ :

$$U_n(0) = 0, \quad n \neq 0, 1. \quad (38)$$

For spins in nearest-neighbor layers ( $n = 0, 1$ ) the interaction  $U_n(\rho)$  diverges as  $\rho^{-2} \ln^2(2p_0\rho)$  for  $\rho \rightarrow 0$ . Note that in contrast to the previous case the interaction between spins separated by only a single layer is only slightly weaker than the interaction of spins from the same layer:

$$U_1(\rho)/U_0(\rho) = 1/4, \quad \rho < v/t. \quad (39)$$

## 7. CONCLUSION

Recently a number of experimental papers have appeared which have considerably advanced our understanding of the possible mechanism for high-temperature superconductivity.<sup>15,16</sup> In these papers the systems  $(YBa_2Cu_3O_7)_m (PrBa_2Cu_3O_7)_n$  were investigated, i.e., superlattices in which  $m$  layers of the yttrium-based 1-2-3 system alternate with  $n$  layers in which the yttrium is replaced by praseodymium. Since the crystal structure of the layers with praseodymium differs only slightly from that of the yttrium layers, the former produce almost no mechanical perturbations in the yttrium subsystem. However, there is a great difference with respect to conductivity, as the layers with praseodymium are very poor conductors. Therefore, this system is an ideal model for investigating superconductivity of the 1-2-3 yttrium system. At this time the ultimate reason for the difference in conductivity between the praseodymium and yttrium systems is unclear. There are suggestions<sup>15-17</sup> that it is connected with the valence instability of Pr.

These experiments have shown that even individual isolated layers of the Y system 1-2-3 are superconducting with a transition temperature of  $\sim 10$ – $20$  K. Therefore, superconductivity in this system has an essentially two-dimensional character, and the question of the possible existence of high-temperature superconductivity in an individual isolated layer with a thickness on the order of the unit cell has been answered from a fundamental-physics point of view. Furthermore, the role of correlations involving electrons in different layers has been clarified: these experiments show that the superconducting transition temperature increases with increasing number of yttrium layers up to  $\approx 90$  K, the value of  $T_c$  in bulk. At this point it is clear that correlations between electrons from different conducting layers have made the superconductivity quasi-three-dimensional, and that electron correlations between different conducting layers are now roughly the same order of magnitude as the correlations within a layer.

One possible source of correlations which is unavoidable in a layered metallic structure comes from the Friedel oscillations we have discussed here, whose features are especially pronounced in layered quasi-two-dimensional systems.

We view layered metals as systems of parallel conducting layers with a conduction electron density concentrated primarily in narrow regions along the layers. Although the motion of an electron from one conducting layer to another

is coherent, the width of the electron band along the layers is considerably larger than the width of the band transverse to the layers. In this case the dispersion law for electrons is strongly anisotropic, and the Fermi surface is found to be open in the direction transverse to the layers. As a result, screening of the Coulomb interaction in the system is strongly anisotropic.

To lowest-order approximation, neglect of hopping between conducting layers causes the screening along the layer to have a two-dimensional character. In the transverse direction the Coulomb interaction between electrons is strongly overscreened with a radius  $d/\ln(2d/a_B)$  that is much smaller than the interplanar spacing  $d$ . Due to this strong screening, even relatively small contributions to the interaction become important if they fall off more slowly with distance. For example, there is a contribution associated with the singularity of the polarization operator for transverse momentum directions. These special transverse projections appear immediately as soon as we take into account the overlap between conducting layers, which deforms the cylindrical Fermi surface into a corrugated cylinder. The new singularity of the polarization operator leads to a contribution to the Coulomb interaction that falls off slowly, which corresponds to the Friedel oscillations of the layered metal.

The unusual feature of these Friedel oscillations is the fact that their period exactly coincides with twice the distance between the layers. These oscillations lead to a Coulomb-based mechanism for superconducting pairing between electrons and to an enhancement, e.g., of the electron-phonon pairing. This tendency can be enhanced in cases where the electronic spectrum has considerable anisotropy not only in the direction transverse to the layer but also along the layer, which in fact converts it to a quasi-one-dimensional spectrum. This situation is encountered when the conducting layers have square crystalline unit cells, and when the Brillouin zone is close to half-occupied by conduction electrons. Here the increase in the critical superconducting transition temperature is due to the large amplitude of the Friedel oscillations, whose size is due first of all to the large density of states and secondly to the stronger singularity of the polarization operator. The increase in the critical temperature is limited in this case by an instability with respect to a transition to an insulating state near half-occupation by electrons. The instability first arises at an (incommensurate) momentum equal to the diameter of the Fermi surface, where the polarization operator reaches its maximum; an analysis of this instability for the case of exact nesting was carried out in Ref. 18. In addition to its influence on the superconducting pairing, the fact that the period of the Friedel oscillations is exactly twice the distance between conducting layers can also induce a type of structural phase transition in the system which leads to doubling of the number of conducting layers in an elementary cell and correspondingly to a doubling of the period of the crystal structure in this direction. This also leads to a change in the topology of the Fermi surface, which amounts to splitting it into two parts (see Fig. 2).

The new singularity of the polarization operator affects not only the Friedel oscillations but the exchange interaction in layered metals as well. The indirect exchange interaction has an anisotropic character and falls off slowly with dis-

tance. It is convenient to represent it as a sum of two terms. The first term oscillates with period  $2p_0\rho$  as we pass from layer to layer and falls off with distance as  $\rho^{-2}$  only for the first layer. For layers with labels  $n \geq 1$  the interaction first increases according to the law  $\rho^{2(n-1)}$  and then decays as  $\rho^{-3}$  for distances  $\rho > v/t$ ; this dependence is characteristic of quasi-isotropic 3D-metals.

An important feature of these oscillations in the direction perpendicular to the layers is that, like the Friedel oscillations, their period coincides with twice the spacing between the layers. Furthermore, the interaction of an individual magnetic moment in a layer with moments from the nearest-neighbor layers is opposite in sign to its interaction with magnetic moments in the same layer. This property rather quickly leads us to the conclusion that in the presence of indirect exchange alone the three-dimensional magnetic ordering consists of alternation of oppositely oriented layers, and is always antiferromagnetic.

The second term, which is determined by  $\Phi_2$ , reduces to zero for  $\Delta = 0$ . It does not oscillate, has antiferromagnetic character and decreases slowly with distance. Both terms are cut off at distances  $\sim \xi_0$ , as in the case of a quasi-isotropic three-dimensional superconductor.<sup>19</sup> At distances  $\rho > v/t \gg p_0^{-1}$  there is a transition to the types of dependences which occur in quasi-isotropic metals. This behavior of the exchange integral leads to the following model for describing magnetic ordering. Neighboring momenta located in the same layer interact with a large exchange constant  $J_1$ , leading to anti- or ferromagnetic ordering in an isolated layer. In addition, it is necessary to take into account the exchange interaction  $J_2$  between moments which are not nearest neighbors but are located in neighboring layers. For nearest neighbors from different layers the interaction reduces to zero. The constant  $J_2$  is much smaller than  $J_1$  in order of magnitude and opposite to it in sign. For a constant  $J_1$  that is ferromagnetic this interaction as a whole leads to an antiferromagnetic structure consisting of alternating ferromagnetic layers with opposite orientations. For a sign of  $J_1$  corresponding to antiferromagnetic order in an individual layer, the magnetic structure consists of repeating antiferromagnetically ordered layers which are displaced one with respect to another by half the magnetic period in the layer.

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