Indirect RKKY interaction in any dimensionality

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We present an analytical method which enables one to find the exact spatial dependence of the indirect RKKY interaction between the localized moments via the conduction electrons for the arbitrary dimensionality n. The corresponding momentum dependence of the Lindhard function is exactly found for any n as well. Demonstrating the capability of the method we find the RKKY interaction in a system of metallic layers weakly hybridized to each other. Along with usual $2k_F$ in-plane oscillations, the RKKY interaction has the sign-reversal character in a direction perpendicular to layers, thus favoring the antiferromagnetic type of layers' stacking. [S0163-1829(97)05406-4]

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction was found to play an important role in various problems involving the interaction of the localized moments in a metal via polarization of conduction electrons. In this paper we provide the exact derivation of the spatial and momentum dependence of RKKY interaction for arbitrary dimensionality. In three dimensions the spatial dependence of this interaction was obtained in Ref. 1 about 40 years ago. It took some time to obtain the corresponding exact expression in two dimensions.[2] The primary goal of this paper is thus to present a promising analytical method for evaluation of the corresponding expressions.

The obtained expressions being the analytical function of dimensionality might prove to be useful for theoretical approaches dealing with the fractional and infinitely large dimensions. Closer to practical needs, we apply our method for an analysis of multilayer metal structure. We demonstrate here the sign-reversal character of the interaction in a direction perpendicular to layers. The period of these oscillations coincides with a double interlayer spacing thus favoring the antiferromagnetic ordering of layers. It is interesting to note that the above alternation of sign of the interaction coexists with the usual in-plane $2k_F$ oscillations.

We begin with conventional form of the exchange interaction between the localized moment $\mathbf{J}$ and electron spin density $\mathbf{s}(\mathbf{r})$:

$$V(\mathbf{r}) = -A\mathbf{J}(\mathbf{R})\mathbf{s}(\mathbf{r})\,\delta(\mathbf{R}-\mathbf{r}). \tag{1}$$

Here A is the exchange coupling constant. The RKKY interaction between two localized moments via the conducting electrons may then be written in the following form:

$$H_{\mathrm{RKKY}} = -\frac{1}{2}A^2\mathbf{J}_1\mathbf{J}_2\chi(\mathbf{R}_{12}), \tag{2}$$

where the R-dependent part of the interaction coincides with the Fourier transform of the nonuniform static susceptibility $\chi(q)$ (Lindhard function) and is given by

$$\chi(\mathbf{R}) = -T\sum_l G(i\omega_l,\mathbf{R})^2. \tag{3}$$

Here Matsubara frequency $\omega_l = \pi T(2l+1)$ and the electronic Green's function is

$$G(i\omega,\mathbf{R}) = \int \frac{d^n\mathbf{k}}{(2\pi)^n}\frac{\exp(i\mathbf{kR})}{i\omega-\varepsilon_k}. \tag{4}$$

We focus our attention below at the case of low temperatures and use the limiting relation $T\Sigma_l \to \int_{-\infty}^{\infty} d\omega/(2\pi)$.

The quadratic electron dispersion in n dimensions is explicitly assumed:

$$\varepsilon_{\mathbf{k}} = k^2/2m - \mu \tag{5}$$

with the Fermi energy $\mu = k_F^2/2m$. First we use the following representation of the Green's function:

$$G(i\omega,\mathbf{R}) = e^{-i\alpha}\int_0^\infty d\tau \int \frac{d^n\mathbf{k}}{(2\pi)^n}\exp\left[i\mathbf{kR} + \tau e^{i\alpha}\left(z - \frac{k^2}{2m}\right)\right], \tag{6}$$

where we introduced the value $z = \mu + i\omega$ and $\alpha = \mathrm{sgn}(\omega)\pi/2$. The Gaussian integration over $\mathbf{k}$ gives

$$G(i\omega,R) = \left(\frac{m}{2\pi}\right)^{n/2} e^{-i\alpha(1+n/2)}\int_0^\infty \frac{d\tau}{\tau^{n/2}}\exp\left(\tau z e^{i\alpha} - \frac{\rho}{2\tau}e^{-i\alpha}\right) \tag{7}$$

with $\rho = mR^2$. We notice that the last integral can be expressed via the modified Bessel (Mcdonald) function,[3] namely,

$$G(i\omega,R) = -2\left(\frac{m}{2\pi}\right)^{\nu+1}\left(\frac{\sqrt{-2z\rho}}{\rho}\right)^{\nu} K_\nu(\sqrt{-2z\rho}). \tag{8}$$

We defined $\nu = n/2-1$ here. In this equation the branch of root $\sqrt{-2z\rho}$ should be chosen from the condition of its positive real part. In particular, this latter condition means that the argument of Mcdonald function $K_\nu(\sqrt{-2z\rho})$ has a discontinuity at $\omega = 0$:

$$K_\nu(\sqrt{-2z\rho}) = \begin{cases} \dfrac{\pi i}{2} e^{\nu\pi i/2} H_\nu^{(1)}(k_F R), & \omega \to +0, \\[2ex] -\dfrac{\pi i}{2} e^{-\nu\pi i/2} H_\nu^{(2)}(k_F R), & \omega \to -0, \end{cases}$$

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where $H_\nu^{(1,2)}(x)$ are Hankel functions.[3]

Next we observe that one can change the variable $\omega \rightarrow Z = \sqrt{-2z\rho}$ in Eq. (3) and integrate over complex Z using the exact form for the Green's function (8). Note that the limits of integration by Z are $(1 \pm i)\infty$. Without the above discontinuity at $Z = \pm i\sqrt{2\mu\rho}$ one could shift the integration contour to $Z \rightarrow +\infty$ and obtain zero for Eq. (3) in view of the property $K_\nu(Z) \propto e^{-Z}$. Due to the discontinuity, the function χ has a finite value. After some calculations we get[4]

$$\chi(R) = \frac{m\pi}{1-n}\left(\frac{k_F}{2\pi R}\right)^n R^2 \Phi_n(k_F R), \tag{9a}$$

$$\Phi_n(x) = J_{n/2-1}(x) Y_{n/2-1}(x) + J_{n/2}(x) Y_{n/2}(x). \tag{9b}$$

This expression is the main finding of this section. Let us take a closer look at this result. First we note that Eq. (9) is the continuous function of both distance R and the dimensionality n.

At large distances $k_F R \gg 1$ the leading terms of the asymptotes of Bessel functions appearing in Eq. (9) cancel each other. The next terms produce the following expression:[5]

$$\chi(R) \simeq \frac{m}{k_F^2}\left(\frac{k_F}{2\pi R}\right)^n \sin(2k_F R + \pi n/2). \tag{10}$$

In particular cases of physical interest the general expression (9) immediately provides the exact form of the RKKY interaction in three and two dimensions.[1,2] For $n=3$ one has

$$\chi(R) = -\frac{mk_F}{8\pi^3 R^3}\left(\cos 2k_F R - \frac{\sin 2k_F R}{2k_F R}\right), \tag{11}$$

and for $n=2$

$$\chi(R) = -\frac{mk_F^2}{4\pi}[J_0(k_F R) Y_0(k_F R) + J_1(k_F R) Y_1(k_F R)]. \tag{12}$$

The one-dimensional case can be obtained either by the continuation[4] of Bessel functions in Eq. (9) upon the index n or by the direct evaluation of the integral with a Green's function (8) at $n=1$. The result is[6]

$$\chi(R) = \frac{m}{\pi}\mathrm{si}(2k_F R) \quad (n=1) \tag{13}$$

with the sine integral

$$\mathrm{si}(x) = \int_x^\infty \frac{dt}{t}\sin t.$$

It is useful to define here the density of states at the Fermi level $N(E_F) = \int d^n\mathbf{k}/(2\pi)^n \delta(\varepsilon_k) = -\pi^{-1}\mathrm{Im}G(i\omega \rightarrow +i0, R \rightarrow 0)$. From Eq. (8) one immediately finds

$$N(E_F) = \frac{m}{2\pi\Gamma[n/2]}\left(\frac{k_F^2}{4\pi}\right)^{n/2-1}. \tag{14}$$

Now knowing the exact expression (9) for the RKKY interaction in R space one can find its correspondence in q space as follows:

$$\chi(q) = \int d^n\mathbf{R}\, e^{i\mathbf{qR}}\chi(R) = \frac{m}{2(1-n)}\left(\frac{k_F^3}{2\pi q}\right)^\nu \int_0^\infty dx\, x^{1-\nu} J_\nu\left(\frac{q}{k_f}x\right)\Phi_n(x). \tag{15}$$

We see that $\chi(q)$ is reduced to the Mellin convolution of $J_\nu(x)$ and $\Phi_n(x)$. A straightforward calculation then gives the answer expressed via the Gauss hypergeometric function ${}_2F_1[a,b,c;z]$:

$$\chi(q) = N(E_F)\phi_n\left(\frac{q}{2k_F}\right), \tag{16a}$$

$$\phi_n(x) = \begin{cases} \dfrac{x^{-2}}{n} F\left[1, \dfrac{1}{2}; 1+\dfrac{n}{2}; \dfrac{1}{x^2}\right], & x \geq 1, \\ F\left[1, 1-\dfrac{n}{2}; \dfrac{3}{2}; x^2\right], & x \leq 1. \end{cases} \tag{16b}$$

Again, the result is the continuous function both in q and n. From the general properties of hypergeometric function, one has $\phi_n(0) = 1$, $\phi_n(x \gg 1) \sim 1/(nx^2)$, and $\phi_n(1) = 1/(n-1)$. At last, one can easily verify[7] that the expressions known previously[1,2,6] are reproduced in particular cases $n = 1,2,3$.

It is interesting to note that both exact (9) and asymptotic (10) expressions for $\chi(R)$ let one mimic the ''switching on'' the extra dimensionality of a metal by simple change of the index n. Thus at first sight one could tackle the case of a system of weakly hybridized metallic planes by ascribing the dimensionality $2+\epsilon$ to it. Actually the situation is more complicated as we discuss below.

Let us consider the (infinite) set of metallic layers, weakly connected to each other. By this we assume the following dispersion:

$$\varepsilon_{\mathbf{k}} = (k_x^2 + k_y^2)/2m - \mu - \zeta \quad \cos k_z \tag{17}$$

with $\zeta \ll \mu$ and $|k_z| < \pi$. The Fermi surface has a cylinder-like shape with maximum and minimum in-plane radii defined by $k_F^\pm = \sqrt{2m(\mu \pm \zeta)}$. We write $\mathbf{kR} = \mathbf{k}_\parallel \mathbf{R}_\parallel + k_z l$ where l is the integer number of layers. Below we retain the definitions of $\rho = mR_\parallel^2$ and $k_F = \sqrt{2m\mu}$ for the simplicity of writing.

Using Eqs. (4) and (7) we come to expression

$$G(R) = -\frac{m}{2\pi}e^{-i\alpha l}\int_0^\infty \frac{d\tau}{\tau} J_l(\tau\zeta)\exp\left(\tau z e^{i\alpha} - \frac{\rho}{2\tau}e^{-i\alpha}\right). \tag{18}$$

The latter integral can be evaluated (for large in-plane distances) by the steepest descent method. We note that when $\sqrt{2z\rho} \simeq k_F R_\parallel \gg 1$, the principal contribution to the integral comes from the vicinity of the point $\tau_0 = \sqrt{\rho/2z} \simeq k_F R_\parallel/2\mu$, more rigorously, at $\tau = \tau_0[1 + (k_F R_\parallel)^{-1/2} O(1)]$. It follows then that at $k_F R_\parallel \lesssim (\mu/\zeta)^2$ one can replace τ by τ_0 in an argument of the Bessel function in Eq. (18). As a result the quasi-two-dimensional RKKY interaction is

$$\chi(R) = \chi_{2\mathrm{D}}(R_\parallel) J_l^2(R_\parallel/R_0)(-1)^l, \quad R_\parallel \lesssim k_F R_0^2, \tag{19}$$

where $k_F R_0 = 2\mu/\zeta \gg 1$ and $\chi_{2D}(R)$ is given by Eq. (12). Analyzing this expression we first note the appearance of the length scale R_0 inversely proportional to the strength of hybridization of layers. Since $J_l(x) \simeq (x/2)^l/l!$ for $x < 1$, at moderate in-plane distances $R_\| < R_0$ the interaction (19) rapidly decays as a function of l.

More interesting however is the fact of *sign-reversal character of interaction* in a direction perpendicular to layers. This modulation of interaction has a period *exactly coinciding* with a double lattice parameter and should obviously lead to the preferential antiferromagnetic stacking of layers. This phenomenon is accompanied by the usual $2k_F$ oscillations of the in-plane term $\chi_{2D}(R_\|)$.

We can further clarify this point by performing the Fourier transform with the result[3]

$$\chi(\mathbf{k}) = \int d^2\mathbf{R}_\| e^{i\mathbf{k}_\|\mathbf{R}_\|} \chi_{2D}(R_\|) J_0\left(2\frac{R_\|}{R_0}\cos\frac{k_z}{2}\right)$$

$$\simeq \int \frac{d\varphi}{2\pi} \chi_{2D}(\mathbf{k}_\| + \mathbf{k}_*), \tag{20}$$

with $k_* = (2/R_0)\cos k_z/2 \ll 1$. The last integration is over the angle φ of $\mathbf{k}_*$ in the plane, i.e., the points $\mathbf{k}_\| + \mathbf{k}_*$ lie on the circle of radius k_* and with center at $\mathbf{k}_\|$.

According to Eq. (2) a maximum of $\chi_{2D}(\mathbf{k}_\|)$ at some $\mathbf{k}_0$ corresponds to the possible in-plane magnetic ordering, characterized by this wave vector. We see from Eq. (20) that the inclusion of weak interplane hopping leads to the position of a true maximum at $k_z = \pi$, when $k_* = 0$. The other values of k_z cause the loss in the magnetic energy of order of the value $\chi(\mathbf{k}_0) k_*^2/k_F^2$.

It is worth noting that the weak interplane hopping ζ and large effective in-plane Fermi momentum k_F are obviously realized in the high-T_c cuprates. It is known that the 2D Fermi surface has a complicated form in these substances.[8] We believe however that the RKKY interaction in this case preserves the general form (19) and (20) with the anisotropic in-plane form of interaction $\chi_{2D}(\mathbf{k}_\|)$ and R_0 defined by some effective $k_F \sim 1$. It is also known that in the compounds $R\mathrm{Ba}_2\mathrm{Cu}_3\mathrm{O}_{7-\delta}$ the subsystem of rare-earth ions undergoes a magnetic ordering transition at low temperatures;[9] generally the type of ordering depends on a particular ion R^{3+}. A remarkable fact is however that *for all* substances the antiferromagnetic stacking of magnetic R^{3+} layers was reported in accordance with our finding (19).

Concluding this section, we wish to stress the following point. It was previously shown[5,10] for the case of a complicated Fermi surface (FS) that the period of oscillations (and general power-law behavior) of the RKKY interaction is determined by the calipering pairs of points on the FS. These are the points where the direction of normal to the FS is (anti)parallel to the direction of **R**. One can see that the very notion of calipering points implies the closeness of the Fermi surface at a given direction of **R**. In contrast, the FS is obviously open in our case at the z direction and the oscillations exist, albeit the roughly exponential law of their decay.

In conclusion, we found the exact form of the spatial dependence of the RKKY interaction for arbitrary dimensionality. Its counterpart in momentum space is also found. Applying our method to the system of weakly hybridized metallic layers, we demonstrate the existence of spatial oscillations of indirect RKKY exchange in the direction perpendicular to layers. The period of oscillations equals exactly double interlayer spacing, which indicates the preferential antiferromagnetic ordering of layers.

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