

## RKKY interaction with diffused contact potential

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The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction is considered when the contact potential is replaced by an arbitrary distribution instead of the conventional Dirac's  $\delta$  function. The appropriate formulas for the RKKY exchange integrals, in the case of one-dimensional, two-dimensional, and three-dimensional systems, are derived. In order to exemplify the modification, the three distributions are used for numerical calculations of the interaction vs spin-spin distance, namely: Gaussian, uniform, and exponential. One of the results shows that "diffusion" of the contact potential removes an unphysical divergency of the RKKY integral at zero distance and the finite value obtained depends strongly on the distribution width.

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### I. INTRODUCTION

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction belongs to one of the most important and frequently discussed couplings between the localized magnetic moments in solids. Originally derived for the three-dimensional (3D) free-electron gas,<sup>1-3</sup> it has been extended to two-dimensional (2D) (Ref. 4) and one-dimensional (1D) situations,<sup>5-7</sup> and, recently, also for the case of ultrathin films.<sup>8,9</sup> Within the free-electron model a formula for the interaction in arbitrary dimensionality has been obtained.<sup>10</sup> Formerly, the derivation was generalized to include nonspherical Fermi surfaces.<sup>11</sup> The RKKY interaction has proven its usefulness in numerous cases:<sup>12</sup> for instance, providing explanation of the ordering of nuclear spins in metals as well as the magnetic properties of rare earths and diluted alloys. Another important application is connected with the description of magnetism in diluted magnetic semiconductors (see, for example, Ref. 13). Such a coupling between the distant magnetic moments can also be a source of decoherence.<sup>14</sup> Moreover, the RKKY interaction has been involved in constructing the interlayer coupling theory.<sup>15,16</sup>

It is known from the very beginning that the perturbative RKKY approach, developed for the pointlike contact potential (in form of Dirac's  $\delta$  function), leads to an unphysical result, predicting infinite magnetization of the charge carriers at the zero distance.<sup>3</sup> The principal factor behind this is the molecular field coming from the localized magnetic moment (perturbation), which is uniform in the wave-vector space, so the appropriate integral from the product of the field and susceptibility is divergent at  $r=0$ . The first to address this issue was Yosida,<sup>3</sup> who imposed some sharp cut-off condition on the molecular field together with simplifying the expression for magnetic susceptibility of the electron gas. However, in this way, the finite value of magnetization at  $r=0$  was achieved at the cost of changing the asymptotic behavior of the magnetization for large distances from perturbation (for instance, in the three-dimensional case, the magnetization is decreasing as  $1/r^2$  instead of  $1/r^3$ ).

Ruderman and Kittel discuss this problem for the interaction of electrons with the nuclear magnetic moments,<sup>1</sup> and have found that the divergency is completely unimportant in the physical situation they considered. They concluded that

the pointlike contact potential approximation is sufficient. Additionally, Kittel mentions the form of the molecular field in the case of the Gaussian interaction potential with finite width.<sup>6</sup>

Being negligible when the localized magnetic moment is of nuclear origin, the divergency of RKKY integral at zero distance is much more vivid for the cases when the localized moment arises from inner electronic orbitals. These orbitals possess a noticeable size (of the order of angströms), which is comparable to the nearest-neighbor distances in crystalline lattices. The model of a Mn impurity ion in GaAs is a good case in point<sup>17</sup> since it emphasizes the role of spatially extended interaction potential. On the other hand, it has also been found<sup>15</sup> that the point-type contact potential predicts incorrect phases for the interlayer couplings. Thus, it seems that the applicability of the contact potential approximation needs reconsideration.

The problem may be of particular importance in diluted magnetic semiconductors (DMS) where the  $p$ - $d$  coupling occurs between the electrons from  $d$  orbitals, forming the localized magnetic moments, and the charge carriers of  $p$  type.<sup>18</sup> As the situation stands now, the model, including the  $p$ - $d$  coupling potential with a nonzero spatial extension of the Gaussian type, has been applied to the studies of magnetic properties of the most known and popular DMS: GaMnAs.<sup>19,20</sup> On the other hand, the uniform distribution was used to model the exchange potential produced by a quantum dot containing magnetic moments in one dimension, in the studies of indirect interdot coupling.<sup>21</sup>

For the above reasons, it seems reasonable to undertake a more systematic study of the RKKY interaction mediated by the free-charge carriers with an arbitrarily "diffused" contact potential. The aim of this paper is to discuss the influence of such modification in the exchange Hamiltonian on the properties of RKKY exchange integral in 1D, 2D, and 3D systems. Special attention has been paid to the universal features that do not depend on the particular shape of the spatially distributed potential but rather on some of its general characteristics.

### II. THEORY

The interaction of  $z$  components of localized spin  $S_i^z$  (in  $i$ th lattice site) with conduction electron spin  $s^z$  is given by the Hamiltonian:

$$\mathcal{H}_i = -A_n p(\mathbf{r}, \sigma) s^z S_i^z. \quad (1)$$

The exchange constant  $A_n$  is connected with the contact potential in  $n$  dimensions ( $n=1, 2, 3$ ) and  $\mathbf{r}$  describes the relative position of both spins.  $A_n$  can be presented in the form  $A_n = 2JL^n/N$ , where  $J$  is the exchange integral,  $N$  is the number of lattice sites, and  $L$  stands for the linear size of the system. Thus,  $A_n$  constant is expressed in the units  $[A_n] = J \cdot \text{m}^n$ . Symbol  $p(\mathbf{r}, \sigma)$  denotes here the probability distribution describing diffusion of the localized spin around the point  $\mathbf{r}=0$  with the standard deviation  $\sigma$ . In the usual derivation of the RKKY interaction, one assumes that  $p(\mathbf{r}, \sigma)$  distribution has a form of Dirac's  $\delta$  function, i.e.,  $p(\mathbf{r}, 0) = \delta(\mathbf{r})$ , which in this paper is referred to as the pointlike contact potential.

In further considerations it is assumed that  $p(\mathbf{r}, \sigma)$  presents an arbitrary distribution with the only demand (made for the simplicity of calculations) that it is symmetric with respect to  $\mathbf{r}=0$ . In particular, this means that  $\langle \mathbf{r} \rangle = 0$  and, as a result, the variance of distribution can be expressed as the second-order moment:  $\sigma^2 = \langle \mathbf{r}^2 \rangle$ .

The characteristic function  $\varphi(\mathbf{q}, \sigma)$  is given by the Fourier transform of the original distribution  $p(\mathbf{r}, \sigma)$ ,

$$\varphi(\mathbf{q}, \sigma) = \int e^{i\mathbf{q}\mathbf{r}} p(\mathbf{r}, \sigma) d^n \mathbf{r}, \quad (2)$$

and

$$p(\mathbf{r}, \sigma) = \frac{1}{\Omega} \sum_{\mathbf{q}} e^{-i\mathbf{q}\mathbf{r}} \varphi(\mathbf{q}, \sigma), \quad (3)$$

where  $\Omega = L^n$  is the measure of integration area over  $\mathbf{r}$  in  $n$  dimensions and it serves as a normalization constant. Substituting Eq. (3) into Eq. (1), the initial Hamiltonian can be written in the form

$$\mathcal{H}_i = g_e \mu_B s^z H^z(\mathbf{r}, \sigma), \quad (4)$$

where  $g_e$  is the gyromagnetic factor of an electron,  $\mu_B$  denotes the Bohr magneton, and  $H^z(\mathbf{q}, \sigma)$  is the magnetic molecular field acting on the electron spin  $s^z$ . This field can be expressed by the Fourier transform as

$$H^z(\mathbf{r}, \sigma) = \sum_{\mathbf{q}} H^z(\mathbf{q}, \sigma) e^{-i\mathbf{q}\mathbf{r}}, \quad (5)$$

where

$$H^z(\mathbf{q}, \sigma) = -\frac{A_n}{\Omega g_e \mu_B} S_i^z \varphi(\mathbf{q}, \sigma). \quad (6)$$

The Fourier component of the molecular field,  $H^z(\mathbf{q}, \sigma)$ , enables calculations of the magnetization of electron gas at the point  $\mathbf{r}$ , arising from the localized spin  $S_i^z$ . Thus,

$$m^z(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{q}} \chi(\mathbf{q}) H(\mathbf{q}, \sigma) e^{-i\mathbf{q}\mathbf{r}}, \quad (7)$$

where  $\chi(\mathbf{q})$  is the static electronic paramagnetic susceptibility.

Suppose that another localized spin,  $S_j^z$ , is situated in the vicinity of the point  $\mathbf{r}$ . Then, the interaction Hamiltonian takes the form of

$$\mathcal{H}_{ij} = \frac{A_n}{g_e \mu_B} \langle m^z(\mathbf{r}) \rangle S_j^z, \quad (8)$$

where the configurational mean value of magnetization  $\langle m^z(\mathbf{r}) \rangle$  accounts for a diffusion of the localized spin position. In order to calculate this mean value, it is assumed that  $\mathbf{r}$  can be expressed as

$$\mathbf{r} = \mathbf{r}_{ij} + \mathbf{r}', \quad (9)$$

where  $\mathbf{r}_{ij}$  is a constant vector, describing relative mean position of the spins  $S_i^z$  and  $S_j^z$ , whereas the stochastic vector  $\mathbf{r}'$  takes into account spatial diffusion of the spin  $S_j^z$  according to the distribution  $p(\mathbf{r}', \sigma)$ . Substituting Eq. (7) into Eq. (8), one obtains

$$\mathcal{H}_{ij} = \frac{A_n}{\Omega g_e \mu_B} S_j^z \sum_{\mathbf{q}} \chi(\mathbf{q}) H^z(\mathbf{q}, \sigma) e^{-i\mathbf{q}\mathbf{r}_{ij}} \langle e^{-i\mathbf{q}\mathbf{r}'} \rangle. \quad (10)$$

According to Eq. (2),  $\langle \exp(-i\mathbf{q}\mathbf{r}') \rangle = \varphi(\mathbf{q}, \sigma)$ , which presents the characteristic function of the distribution. Also taking into account that  $H^z(\mathbf{q}, \sigma)$  is given by Eq. (6), the Hamiltonian [Eq. (10)] can be written in its final form as

$$\mathcal{H}_{ij} = -J_{ij}(\sigma) S_i^z S_j^z, \quad (11)$$

and it describes interaction of two localized spins,  $S_i^z$  and  $S_j^z$ , via effective exchange integral  $J_{ij}(\sigma)$ . This integral has a general form of

$$J_{ij}(\sigma) = \left( \frac{A_n}{\Omega g_e \mu_B} \right)^2 \sum_{\mathbf{q}} \chi(\mathbf{q}) e^{-i\mathbf{q}\mathbf{r}_{ij}} \varphi^2(\mathbf{q}, \sigma). \quad (12)$$

In particular, for the pointlike contact potential (where  $\sigma=0$ ), the characteristic function is equal to unity:  $\varphi(\mathbf{q}, 0) = 1$ . Then, formula (12) reproduces the conventional expression for the RKKY exchange integral in  $n$  dimensions.<sup>6</sup>

The static paramagnetic susceptibility  $\chi(\mathbf{q})$ , needed in Eq. (12), can be obtained from perturbation calculus and, for an arbitrary dimensionality of the system ( $n=1, 2, 3$ ), can be written in the form of<sup>12</sup>

$$\chi(\mathbf{q}) = \frac{m_e}{\hbar^2} (g_e \mu_B)^2 \sum_{\mathbf{k}}^{k_F} \left[ \frac{1}{(\mathbf{k} - \mathbf{q})^2 - \mathbf{k}^2} + \frac{1}{(\mathbf{k} + \mathbf{q})^2 - \mathbf{k}^2} \right], \quad (13)$$

where  $k_F$  is the Fermi wave vector in  $n$  dimensions. This susceptibility has been calculated in the literature for 1D, 2D, and 3D systems.<sup>6</sup> For instance, for 3D case the static paramagnetic susceptibility takes the form of<sup>6,12</sup>

$$\chi_{3D}(\mathbf{q}) = \chi_{3D}(0) \frac{1}{2} \left[ 1 + \frac{4k_F^2 - q^2}{4k_F q} \ln \left| \frac{2k_F + q}{2k_F - q} \right| \right], \quad (14)$$

where  $\chi_{3D}(0)$  is the Pauli paramagnetic susceptibility:

$$\chi_{3D}(0) = \frac{V}{4\pi^2} \frac{m_e}{\hbar^2} (g_e \mu_B)^2 k_F, \quad (15)$$

and  $\Omega=V$  is the volume. The Fermi wave vector for 3D case is given by  $k_F^3=3\pi^2 N_e/V$ , where  $N_e$  denotes the number of electrons in the system.

For 2D systems the paramagnetic susceptibility can be presented in the form of Lindhard function<sup>4,6</sup>

$$\chi_{2D}(\mathbf{q}) = \chi_{2D}(0) \left[ 1 - \sqrt{1 - \left(\frac{2k_F}{q}\right)^2} \Theta\left(1 - \frac{2k_F}{q}\right) \right]. \quad (16)$$

In Eq. (16), by  $\Theta$ , we denote the Heaviside step function, whereas the Pauli paramagnetic susceptibility is then expressed by

$$\chi_{2D}(0) = \frac{S}{4\pi} \frac{m_e}{\hbar^2} (g_e \mu_B)^2, \quad (17)$$

where  $\Omega=S$  is the surface. The Fermi wave vector for 2D systems is given by the expression  $k_F^2=2\pi N_e/S$ .

In turn, for 1D systems, the static paramagnetic susceptibility can be presented as<sup>7</sup>

$$\chi_{1D}(\mathbf{q}) = \chi_{1D}(0) \frac{k_F}{q} \ln \left| \frac{2k_F + q}{2k_F - q} \right|, \quad (18)$$

where  $\chi_{1D}(0)$  is the Pauli paramagnetic susceptibility,

$$\chi_{1D}(0) = \frac{L}{2\pi} \frac{m_e}{\hbar^2} (g_e \mu_B)^2 \frac{1}{k_F}, \quad (19)$$

and  $\Omega=L$  is the length. The Fermi wave vector for 1D systems takes the form of  $k_F=(\pi/2)(N_e/L)$ .

A common feature characterizing the susceptibilities [Eqs. (14), (16), and (18)] is their sole dependence on the modulus  $q=|\mathbf{q}|$ , not on the direction of  $\mathbf{q}$ . Taking into account that for spatially symmetric distributions  $p(\mathbf{r}, \sigma)$ , the characteristic function also depends on  $q$  (more precisely, on the product  $q\sigma$ ), we can easily integrate the angular dependence in Eq. (12), occurring only in the exponential term  $\exp(-i\mathbf{q}\mathbf{r}_{ij})$ . Namely, by turning in Eq. (12) from summation to integration over  $\mathbf{q}$  according to the prescription,

$$\sum_{\mathbf{q}} \rightarrow \frac{\Omega}{(2\pi)^n} \int d^n \mathbf{q}$$

(where  $n$  is dimensionality), we are able to obtain formulas for the RKKY interaction dependent on the modulus  $r=|\mathbf{r}_{ij}|$  and the diffusion parameter  $\sigma$ . By introducing the notation  $J_{nD}(\mathbf{r}, \sigma) \equiv J_{ij}(\sigma)$ , the final result for 3D systems can be written in the form of

$$J_{3D}(r, \sigma) = C_3 \frac{(ak_F)^4}{\pi(2k_F r)} \int_0^\infty \left[ dx \left( x + \frac{1-x^2}{2} \ln \left| \frac{1+x}{1-x} \right| \right) \times \sin(2k_F r x) \varphi^2(x, \sigma) \right], \quad (20)$$

where the energetic constant  $C_3$  is given by the expression

$$C_3 = \frac{2A_3^2 m_e}{\pi \hbar^2 a^4}, \quad (21)$$

and  $a$  is the lattice constant. For the sake of numerical convenience, we have introduced the dimensionless parameter  $x=q/(2k_F)$ .

For 2D systems,

$$J_{2D}(r, \sigma) = C_2 (ak_F)^2 \int_0^\infty dx \left[ x - \sqrt{x^2 - 1} \Theta\left(1 - \frac{1}{x}\right) \right] \times \pi J_0(2k_F r x) \varphi^2(x, \sigma), \quad (22)$$

where the Bessel function of the first kind,  $J_0(z)$ , is given by the formula:

$$\pi J_0(z) = \int_0^\pi dt \cos(z \cos t). \quad (23)$$

The energetic constant  $C_2$  for 2D systems takes the form of

$$C_2 = \frac{2A_2^2 m_e}{\pi \hbar^2 a^2}. \quad (24)$$

In turn, for 1D system, the RKKY interaction can be presented as

$$J_{1D}(r, \sigma) = C_1 \pi \int_0^\infty dx \frac{1}{x} \ln \left| \frac{1+x}{1-x} \right| \cos(2k_F r x) \varphi^2(x, \sigma), \quad (25)$$

and the energetic constant  $C_1$  has a form of

$$C_1 = \frac{2A_1^2 m_e}{\pi \hbar^2}. \quad (26)$$

The obtained formulas [Eqs. (20), (22), and (25)] can be simplified in a particular case of the pointlike contact potential. Then, the distribution  $p(\mathbf{r}, \sigma)$  evolves into Dirac's  $\delta$  distribution with the characteristic function  $\varphi(x, 2k_F \sigma) \xrightarrow{\sigma \rightarrow 0} 1$ . In such a case, the integration over  $x$  in Eq. (20) can be carried out by parts and the well-known result for 3D systems is retrieved:<sup>6,12</sup>

$$J_{3D}(r, \sigma=0) = C_3 (ak_F)^4 \frac{\sin(2k_F r) - 2k_F r \cos(2k_F r)}{(2k_F r)^4}. \quad (27)$$

In turn, for 2D and 1D cases, the integrals over  $x$  with  $\varphi(x, 0)=1$  can be presented by special functions. For instance, for 2D systems, one obtains<sup>4</sup>

$$J_{2D}(r, \sigma=0) = -C_2 \frac{\pi^2}{4} (ak_F)^2 \times [J_0(k_F r) N_0(k_F r) + J_1(k_F r) N_1(k_F r)], \quad (28)$$

where  $J_n$  are the Bessel functions of the first kind and  $N_n$  are the Bessel functions of the second kind (Neumann functions).

Finally, the 1D case has been considered in Refs. 5–7 and the result is

TABLE I. Probability distributions and their characteristic functions used in the numerical calculations in one, two, and three dimensions.

	Gaussian		Exponential		Uniform	
$n$	$p(r, \sigma)$	$\varphi(q, \sigma)$	$p(r, \sigma)$	$\varphi(q, \sigma)$	$p(r, \sigma)$	$\varphi(q, \sigma)$
1	$\frac{1}{\sigma(2\pi)^{1/2}} e^{-r^2/2\sigma^2}$	$e^{-q^2\sigma^2/2}$	$\frac{1}{\sqrt{2}\sigma} e^{-r\sqrt{2}/\sigma}$	$\frac{1}{1 + \frac{1}{2}(q\sigma)^2}$	$\frac{1}{2\sqrt{3}\sigma} \theta(\sigma\sqrt{3}-r)$	$\frac{\sin(\sqrt{3}q\sigma)}{\sqrt{3}q\sigma}$
2	$\frac{1}{\sigma^2 2\pi} e^{-r^2/2\sigma^2}$	$e^{-q^2\sigma^2/2}$	$\frac{3}{2\pi\sigma^2} e^{-r\sqrt{3}/\sigma}$	$\frac{1}{\left[1 + \frac{1}{3}(q\sigma)^2\right]^{3/2}}$	$\frac{1}{4\pi\sigma^2} \theta(2\sigma-r)$	$\frac{J_1(2q\sigma)}{2q\sigma}$
3	$\frac{1}{\sigma^3(2\pi)^{3/2}} e^{-r^2/2\sigma^2}$	$e^{-q^2\sigma^2/2}$	$\frac{1}{\pi\sigma^3} e^{-2r/\sigma}$	$\frac{1}{\left[1 + \frac{1}{4}(q\sigma)^2\right]^2}$	$\frac{3}{20\sqrt{5}\pi\sigma^3} \theta(\sigma\sqrt{5}-r)$	$\frac{3}{(\sqrt{5}q\sigma)^3} \frac{\sin(\sqrt{5}q\sigma) - (\sqrt{5}q\sigma)\cos(\sqrt{5}q\sigma)}{(\sqrt{5}q\sigma)^3}$

$$J_{1D}(r, \sigma=0) = C_1 \pi^2 \left[ \frac{\pi}{2} - \text{Si}(2k_F r) \right], \quad (29)$$

where  $\text{Si}(x)$  is the sine integral ( $\text{Si}(x) = \int_0^x \frac{\sin t}{t} dt$ ).

The formulas (27)–(29) are in agreement with the paper of Aristov<sup>10</sup> (for  $n=3, 2, 1$ , respectively) when, in our normalization constants ( $C_3$ ,  $C_2$  and  $C_1$ ), the atomic units with  $\hbar=1$  are used. These results are also in agreement with the paper of Diel *et al.*<sup>13</sup> when the ground-state envelope function of the carriers, introduced in Ref. 13 for 1D and 2D systems, is replaced by unity. However, it should be emphasized that the exchange constant  $A_n$  must be expressed in different physical units for various dimensionalities  $n$ , according to the formula:  $A_n = 2J\Omega/N$  (where  $\Omega=L, S$ , or  $V$  for  $n=1, 2$ , or  $3$ , respectively). It seems that this fact has not been discussed in both the papers (Refs. 10 and 13) where, for all dimensions, the same constant  $A$  has been considered.

The numerical results, which will be presented in the next section, concern calculations of the RKKY exchange integral for different types of the diffused contact potential (with  $\sigma > 0$ ). These calculations are based on our integral formulas (20), (22), and (25), corresponding to the dimensions  $n=3, 2$ , and  $1$ , respectively.

### III. NUMERICAL RESULTS AND DISCUSSION

In order to illustrate an influence of the diffused contact potential on the RKKY exchange integral, the numerical calculations have been performed for the three discussed dimensionalities: 1D, 2D, and 3D. For each dimensionality, the three representative isotropic distributions  $p(\mathbf{r}, \sigma)$  have been chosen, namely Gaussian, uniform, and exponential. In Table I the formulas for all distributions have been listed together with their characteristic functions  $\varphi(\mathbf{q}, \sigma)$ . The distributions are normalized in each corresponding dimension, so that  $\int_0^\infty p(\mathbf{r}, \sigma) d^n \mathbf{r} = 1$ . It can be easily checked that for  $\sigma \rightarrow 0$ , all the characteristic functions are equal to unity,  $\varphi(\mathbf{q}, 0) = 1$ , and as a result,  $p(\mathbf{r}, 0) = \delta(\mathbf{r})$ . Thus, for  $\sigma \rightarrow 0$ , it is possible to obtain the results that are valid for the pointlike contact potential. For all numerical calculations, the convention in which the positive values of  $J_{nD}(r, \sigma)$  correspond to ferromagnetic interactions is assumed.

In Fig. 1 the exchange integral  $J_{1D}(r, \sigma)$  for one-dimensional system is presented vs dimensionless distance  $2k_F r$ . The calculations are based on formula (25). The three figure parts: (a), (b), and (c), correspond to different distributions: Gaussian, uniform, and exponential, respectively. In each part, the solid lines denote the standard result for the

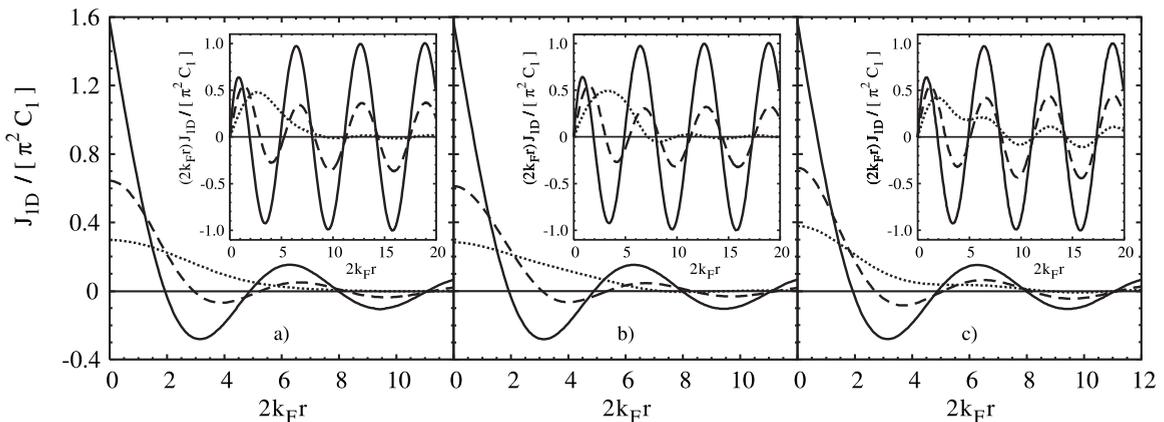


FIG. 1. The dependence of RKKY exchange integral on dimensionless distance  $2k_F r$  in one dimension for Gaussian (a), uniform (b), and exponential (c) probability distributions. Solid line is for standard deviation  $2k_F \sigma = 0$ , dashed for  $2k_F \sigma = 1$ , and dotted for  $2k_F \sigma = 2$ .

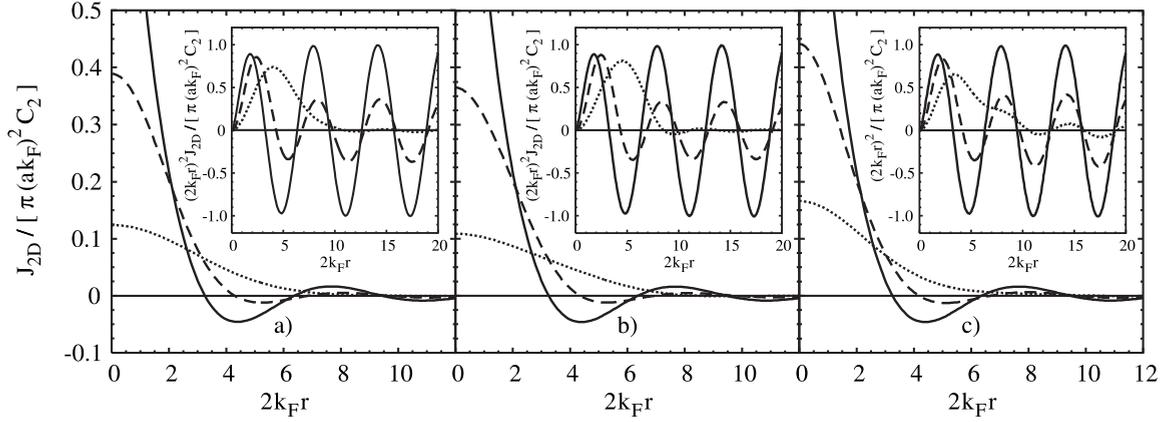


FIG. 2. The dependence of RKKY exchange integral on dimensionless distance  $2k_F r$  in two dimensions for Gaussian (a), uniform (b), and exponential (c) probability distributions. Solid line is for standard deviation  $2k_F \sigma = 0$ , dashed for  $2k_F \sigma = 1$ , and dotted for  $2k_F \sigma = 2$ .

exchange integral, i.e., when the contact potential is point-like, with  $\sigma = 0$ . The dashed lines correspond to the choice of dispersion  $2k_F \sigma = 1$ , whereas the dotted lines are for  $2k_F \sigma = 2$ .

The characteristic feature of the RKKY exchange integral for 1D system with  $\sigma = 0$  is its finite value for  $r = 0$ . This is not the case for 2D and 3D systems where for  $r = 0$ , the exchange integral tends to  $+\infty$ . According to formula (29), the finite value of  $J_{1D}/[\pi^2 C_1]$  obtained for  $r = 0$  (and  $\sigma = 0$ ) is  $\pi/2$ .

It is seen from Fig. 1 that the diffusion of the contact potential diminishes the RKKY integral at  $r = 0$ , and, at the same time, the first minimum becomes shallow and is shifted toward higher distances  $r$ . It can be noted that for high dispersion ( $2k_F \sigma = 2$ ), the first minimum has even disappeared. These effects are similar for both the Gaussian and uniform distributions [parts (a) and (b) of Fig. 1] but seem to be weaker for the exponential one [part (c)]. For small values of  $r$ , the amplitude of oscillations diminishes which is accompanied by remarkable phase shifts.

For large distances  $r$ , the analysis of the results needs a separate comment and the situation is illustrated in the insets included in each part of the figure. The normalization of the vertical axes in the insets has been chosen in such a way that for  $\sigma = 0$ , the reference results remain within  $[-1; 1]$  range. The asymptotic form for the 1D exchange integral is<sup>7</sup>  $J_{1D}(r, \sigma = 0) = C_1 \pi^2 \cos(2k_F r)/(2k_F r)$ . This asymptotic character remains conserved (with accuracy to the scale) independently on the  $\sigma$  values, as can be seen from the  $(2k_F r)J_{1D}/[\pi^2 C_1]$  curves. The only effect of the diffusion  $\sigma$  for large  $r$  is a decrease in the exchange integral amplitude, whereas the period of oscillations remains unchanged and no phase shift occurs. It has also been found that some damping of the exchange integral upon  $\sigma$  for large distances becomes independent of  $r$ , which will be analyzed further in Fig. 5.

In Fig. 2 the analogous calculations are presented for 2D system. In this case the numerical results are based on formula (22). The (a), (b), and (c) parts of Fig. 2 correspond to the Gaussian, uniform, and exponential distributions, respectively. As previously explained, the solid, dashed, and dotted lines correspond to  $2k_F \sigma = 0, 1$ , and  $2$ , respectively, for each part of the figure. In agreement with literature, the exchange

integral for  $\sigma = 0$  and  $r = 0$  has a pole. As shown in the Fig. 2, this divergency is radically removed when  $\sigma > 0$ .

The influence of  $\sigma$  on the  $J_{2D}$  exchange integral for 2D case is similar to that mentioned above (for 1D systems). Again, for small distances  $r \rightarrow 0$ , the value of  $J_{2D}(r, \sigma)$  is reduced when  $\sigma$  increases and, at the same time, the first minimum vanishes. On the other hand, for large distances, the behavior of  $J_{2D}$  can be analyzed from the insets of the figure. Since the asymptotic behavior of  $J_{2D}$  for large distances  $r$  (and  $\sigma = 0$ ) is<sup>4</sup>  $J_{2D} = C_2 \pi (ak_F)^2 \sin(2k_F r)/(2k_F r)^2$ , the convenient normalization of the vertical axes in the insets should be  $(2k_F r)^2 J_{2D}/[\pi(ak_F)^2 C_2]$ . Then the values of the reference function for  $\sigma = 0$  are within the range  $[-1, 1]$ . In this representation, the graphs for large  $r$  and various  $\sigma$  parameters show neither change in the period of oscillations nor the phase shift. When  $\sigma$  increases (and  $r \rightarrow \infty$ ), the only change observed in the insets is the damped amplitude of oscillations, which does not depend on  $r$ .

In Fig. 3 an influence of the diffused contact potential on the exchange integral is illustrated for 3D case. The numerical results have been obtained on the basis of formula (20). As in previous figures, the parts (a), (b), and (c) correspond to the Gaussian, uniform, and exponential distributions, respectively. Again, the three curves: solid, dashed, and dotted correspond to  $2k_F \sigma = 0, 1$ , and  $2$ , respectively, showing the influence of the standard deviation  $\sigma$  on the range function. This influence turns out to be similar to that described for 2D and 1D cases. In particular, the unphysical divergency, which occurs for  $J_{3D}(r \rightarrow 0, \sigma = 0)$ , is definitely removed when  $\sigma > 0$ . Again, the first minimum, which, for 3D case, is most shallow and situated at larger distances than for 2D and 1D systems, disappears as  $\sigma$  increases.

In the insets of Fig. 3, the dependency of the exchange integral on  $r$  for large distances is illustrated. According to the asymptotic behavior<sup>6</sup> for  $r \rightarrow \infty$  and  $\sigma = 0$ ,  $J_{3D} = -C_3 (ak_F)^4 \cos(2k_F r)/(2k_F r)^3$ , the ordinate is conveniently expressed by  $(2k_F r)^3 J_{3D}/[(ak_F)^4 C_3]$ , which places the reference function values in the range  $[-1, 1]$ . Again, for large  $r$ , the only influence of  $\sigma$  on the  $J_{3D}$  exchange integral is a strong damping of the amplitude of oscillations. The presentation of Figs. 1–3 with the use of the dimensionless abscissa axis ( $2k_F r$ ) makes it universal for all charge carriers concen-

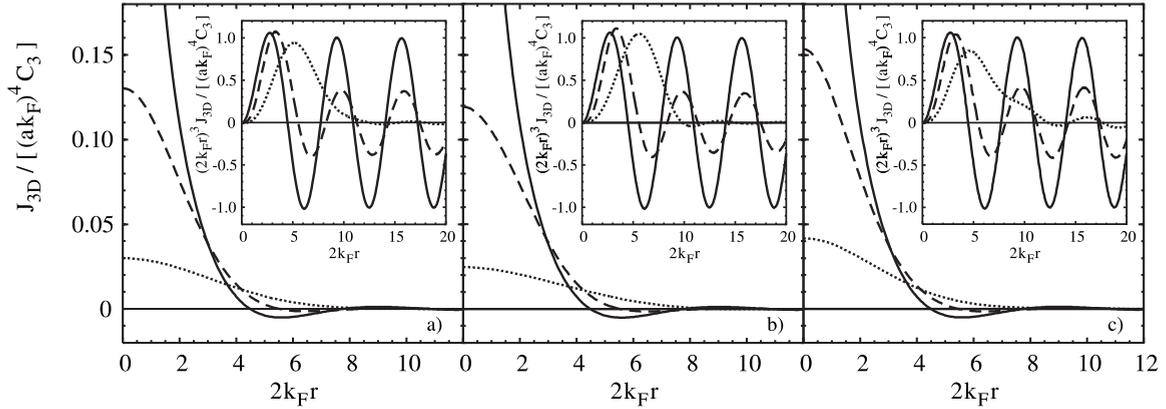


FIG. 3. The dependence of RKKY exchange integral on dimensionless distance  $2k_F r$  in three dimensions for Gaussian (a), uniform (b), and exponential (c) probability distributions. Solid line is for standard deviation  $2k_F \sigma = 0$ , dashed for  $2k_F \sigma = 1$ , and dotted for  $2k_F \sigma = 2$ .

trations since no particular expression of  $k_F$  is then necessary.

One of the most spectacular result presented in Figs. 1–3 is a finite value of the RKKY exchange integral when  $r \rightarrow 0$  and  $\sigma > 0$ . Let us inspect this finding more thoroughly. For  $r \rightarrow 0$  and  $\sigma = 0$ , the well-known divergencies obtained for 2D and 3D cases are of the asymptotic form:  $J_{2D} \sim \ln(1/\sqrt{r})$  and  $J_{3D} \sim 1/r$ , respectively.<sup>13</sup> These divergencies are unphysical, being in contradiction with an assumption that the perturbation calculus can be adopted in derivation of the RKKY interaction. Our results show that a diffusion of the contact potential, which better describes the physical situation, removes this contradiction. In order to discuss the strength of the effect in Fig. 4, we present the RKKY exchange integral for  $r=0$  vs dimensionless parameter  $2k_F \sigma$  in a double-logarithmic scale. The three parts of Figs. 4(a), 4(b), and 4(c) correspond to 1D, 2D, and 3D cases, respectively. The solid lines denote the results for Gaussian and uniform distributions (which are indistinguishable cases in the figure scale) whereas the dotted line represents the exponential distribution. For the exponential contact potential, the exchange integral takes slightly higher values than for other distributions, which is well seen in the range  $2k_F \sigma > 1$ . However, for  $2k_F \sigma < 1$ , the differences between all the three distributions become negligible for all dimensions. Generally, a strong decrease in the exchange integral for  $r=0$  vs  $\sigma$  is seen although the slope of the curves is different for various dimensions. The highest slope is for 3D system and the lowest

is for the 1D one. Moreover, the changes are slower for  $2k_F \sigma < 1$  while for higher dispersion parameters ( $2k_F \sigma > 1$ ), the changes become more rapid. Figure 4 illustrates the general fact that, for obtaining the finite value of  $J_{nD}$  (for  $r=0$ ), the  $\sigma$  parameter is absolutely crucial whereas a shape of the particular distribution becomes less important.

As to the large distance range, it has been found from Figs. 1–3 that the nonzero standard deviation  $\sigma$  changes only the amplitude of interaction. Neither the period of oscillations changes nor the phase shift occurs. It has been found numerically that, due to diffusion of the contact potential, the damping of oscillations for large  $2k_F r$  fulfills the relationship

$$\frac{J(r, \sigma)}{J(r, \sigma = 0)} = \varphi^2(2k_F \sigma, \sigma), \quad (30)$$

and does not depend on  $r$ .

The numerical formula (30) is presumably fulfilled for arbitrary dimension only with the characteristic function  $\varphi(q, \sigma)$  appropriately chosen. In order to illustrate the relationship [Eq. (30)] in Fig. 5 in the parts (a), (b) and (c), we present the results for 1D, 2D, and 3D systems, respectively. The solid lines in Fig. 5 correspond to the Gaussian contact potential, the dashed lines denote the uniform distribution, and the dotted lines the exponential one. It has been found that for small dispersion (when  $2k_F \sigma < 1$ ), the damping is practically the same for all distributions. For the value  $2k_F \sigma = 1$  and  $r \rightarrow \infty$ , the decrease in the RKKY exchange in-

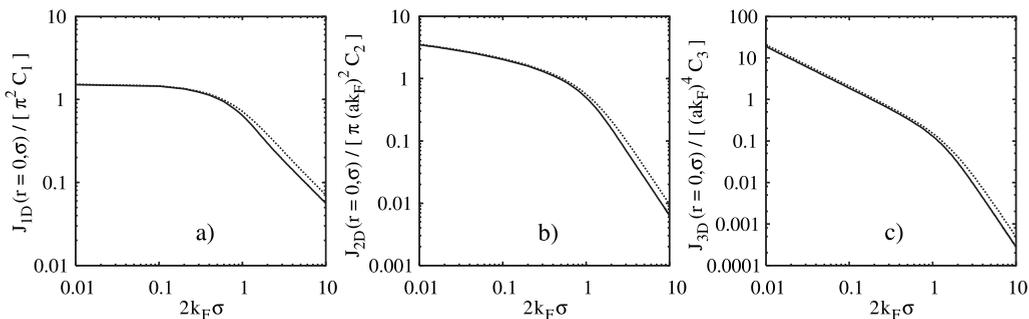


FIG. 4. The value of RKKY exchange integral at the point  $r=0$  as a function of standard deviation  $2k_F \sigma$  for one (a), two (b), and three dimensions (c). The solid line is plotted for the Gaussian and uniform probability distribution; the dotted one for exponential distribution.

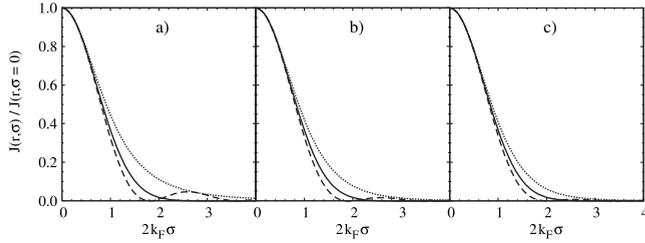


FIG. 5. The damping factor for RKKY exchange integral at large distances as a function of standard deviation  $2k_F\sigma$  in one (a), two (b), and three dimensions (c). The solid line is plotted for the Gaussian probability distribution, the dashed line for uniform one, and the dotted line for exponential one.

tegral owing to the damping  $\varphi^2$  approximates the factor  $1/2$ . For higher dispersions, when  $2k_F\sigma > 1$ , some differences between various distributions occur in the damping curves. It is seen in Fig. 5 that the slowest damping can be attributed to the exponential distribution. Some oscillations connected with the characteristic function of the uniform distribution (dashed curve) appear to be the strongest for 1D case and they weaken as the dimensionality increases.

For the small and intermediate distances  $r$ , one of the important consequences resulting from the diffused contact potential is a phase shift of the exchange integral, as illustrated in Figs. 1–3. In particular, this effect leads to the shift of the first-zero point of the range function toward higher distances. It means that due to the nonzero standard deviation  $\sigma$ , the ferromagnetic range of the exchange integral becomes wider. The effect of the first-zero-point shift has been illustrated in Fig. 6. The (a), (b) and (c) parts of this figure correspond to the 1D, 2D, and 3D cases, respectively. The first-zero position of the range function is denoted by  $r_1$ . Again, the solid, dashed, and dotted lines correspond to the Gaussian, uniform, and exponential distributions, respectively. It can be seen in Fig. 6 that for small dispersions (when  $2k_F\sigma < 1$ ), the shift of the first-zero point expressed by the  $2k_F r_1$  position does not depend on the particular distribution. The differences are seen only when  $2k_F\sigma > 1$  and they increase with  $\sigma$ . The interesting observation is that for the Gaussian and exponential distributions, the increase in  $r_1$  is not continuous with the first jump around  $2k_F\sigma \approx 1.5$ . As a result, the ferromagnetic range increases rapidly at the jump points whereas, for the uniform distribution, the increase in

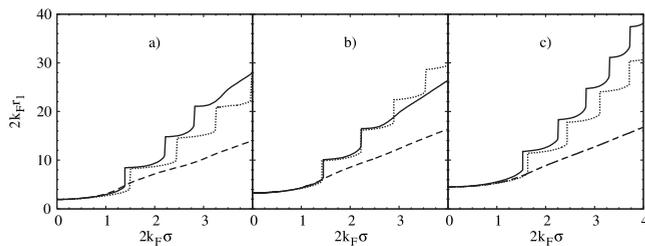


FIG. 6. The position of the first zero of the RKKY exchange integral as a function of standard deviation  $2k_F\sigma$  in one (a), two (b), and three dimensions (c). The solid line corresponds to the Gaussian probability distribution, the dashed line to the uniform one, and the dotted line to the exponential one.

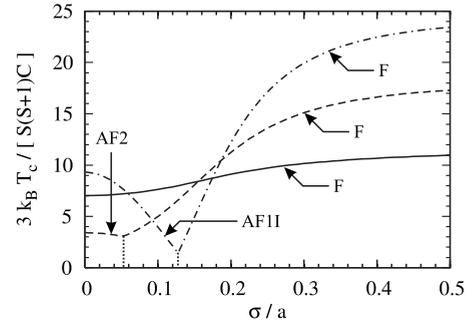


FIG. 7. The MFA critical temperature for model Ising spin- $S$  system on fcc lattice with RKKY interactions vs “diffusion” of the contact potential. The solid curve corresponds to the charge carrier concentration  $N_e/N=0.05$ , the dashed one to  $N_e/N=0.2$ , and the dashed-dotted one to  $N_e/N=0.5$ .

this range is monotonous and takes place more slowly.

In summary, one can conclude that the diffusion of the contact potential has a great influence on the RKKY exchange integral. The effect has been examined in all dimensions ( $n=1,2,3$ ) with different probability distributions (instead of the conventional Dirac’s  $\delta$  function) taken into account. One of the main conclusions of the paper is that an unphysical divergency of the RKKY exchange integral (which appears for 2D and 3D cases at  $r=0$ ) is removed as an outcome of the nonzero dispersion  $\sigma^2$ . The asymptotic behavior of the range functions for  $r \rightarrow \infty$  remains unchanged with accuracy to the damping factor  $\varphi^2(2k_F, \sigma)$ . Some enhancement of the exchange integral for intermediate distances results in the first-zero-point shift and, at the same time, an increase in the ferromagnetic range occurs. It can be predicted that all the changes resulting from diffusion of the contact potential should have a remarkable influence on the magnetic properties of the systems in which the RKKY interaction takes place.

For instance, in order to illustrate the influence of the finite spatial extension of the exchange coupling potential on the thermodynamic properties, we present an example of the critical temperature. In Fig. 7 we plot the magnetic phase diagram for Ising spin system on the fcc lattice with 3D RKKY interaction [given by the formula (20)]. The Curie temperatures for ferromagnetic phase (F), as well as the Néel temperatures for first kind improved antiferromagnetic phase (AF11) and second kind antiferromagnetic phase (AF2), are plotted. These critical temperatures are obtained in the molecular-field approximation for the Gaussian exchange coupling potential as a function of its standard deviation  $\sigma/a$ , normalized to the lattice constant. The three curves: solid, dashed, and dashed dotted correspond to the free-charge carrier densities of  $N_e/N=0.05$ , 0.2, and 0.5, respectively.

It is visible that by increasing the diffusion of the coupling potential, we observe a rather fast decrease in the Néel temperature if the antiferromagnetic magnetic ordering is present for  $\sigma=0$ . For these cases, at some value of standard deviation  $\sigma$ , the thermodynamically stable phase changes from the antiferromagnetic to the ferromagnetic one. For the

ferromagnetic phase itself, the increase in the spatial extension of the exchange coupling potential results in noticeably higher Curie temperature. Its value is quite sensitive to the choice of  $\sigma$  for the range of small dispersions before some kind of saturation is reached for larger  $\sigma$ .

It is worth noticing that the predicted changes in the phase

diagram occur for rather realistic values of the exchange potential spatial extension, being a fraction of the lattice constant. The presented results support the finding that increasing  $\sigma$  favors ferromagnetism and emphasize the importance of the diffusion of the contact potential for the description of thermodynamic properties.

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