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Twisted exchange interaction between localized spins embedded in a one- or two-dimensional electron gas with Rashba spin-orbit coupling

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We study theoretically the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in one- and two-dimensions in presence of a Rashba spin-orbit (SO) coupling. We show that rotation of the spin of conduction electrons due to SO coupling causes a twisted RKKY interaction between localized spins which consists of three different terms: Heisenberg, Dzyaloshinsky-Moriya, and Ising interactions. We also show that the effective spin Hamiltonian reduces to the usual RKKY interaction Hamiltonian in the twisted spin space where the spin quantization axis of one localized spin is rotated.

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There has been a great deal of interest in the field of spintronics where spin degrees of freedom of electrons are manipulated to produce a desirable outcome.[1,2] Eminent examples are given by the giant magnetoresistance (GMR) effect[3–5] and the interlayer exchange coupling in magnetic multilayers.[6–8] The interlayer exchange coupling is explained in the context of Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction,[9,10] equivalently, or in terms of spin-dependent electron confinement.[11,12] The RKKY interaction is an indirect exchange interaction between two localized spins via the spin polarization of conduction electrons.[13–16]

Recently, much attention has been focused on the effect of the Rashba spin-orbit (SO) coupling in two-dimensional electron gases (2DEG).[17] Investigation of the Rashba effect of 2DEG in semiconductor heterostructures has been stimulated by the proposition of a spin field effect transistor.[18] It has been established the Rashba SO coupling can be controlled by means of a gate voltage.[19–22] The Rashba effect has also been observed in 2DEG formed from surface states electrons at metal surfaces such as Au(111),[23–27] Li/W(110) or Li/Mo(110).[28] It has also been found that confinement of the surface state due to atomic steps on vicinal surfaces leads to quasi-one-dimensional (1D) surface states, which also exhibit the Rashba effect.[29–31]

Usually the RKKY interaction yields a parallel or antiparallel coupling of localized spins (Heisenberg coupling). However, if spin of conduction electrons precesses due to the spin–orbit coupling, it can be possible to produce a noncollinear Dzyaloshinsky-Moriya (DM) coupling of localized spins.[32–34] In this paper, we investigate the RKKY coupling between localized spins embedded in a 1D- or 2DEG with Rashba SO coupling. We show that rotation of the spin of conduction electrons due to the Rashba SO coupling causes a *twisted* RKKY interaction between localized spins which consists of three different terms: Heisenberg, Dzyaloshinsky-Moriya, and Ising interactions. We point out that a perturbative treatment of the SO coupling as is usually done[32–34] is valid only for small distances between the localized spins; in this case the DM and Ising terms are, respectively, linear and quadratic with respect to the SO coupling strength. In the limit of large distances, a nonperturbative treatment of the SO coupling is necessary, and one obtains DM and Ising terms that have the same oscillation amplitude as the Heisenberg term, independently of the SO coupling strength. This peculiar behavior of the twisted RKKY interaction for a pair of localized spins can be explained by introducing a twisted spin space where the spin quantization axis of one of the localized spins is rotated.

We consider a system consisting of two localized spins embedded in a 1D- or 2DEG with a Rashba-type spin–orbit coupling.[17] The Hamiltonian for the conduction electrons is given by

$$H_0 = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \alpha(-i\hbar\boldsymbol{\nabla}\times\hat{\boldsymbol{z}})\cdot\boldsymbol{\sigma}, \tag{1}$$

where α represents the strength of the spin–orbit coupling, $\hat{\boldsymbol{z}}$ is a unit vector along the z-axis, and $\boldsymbol{\sigma}$ is the vector of Pauli spin matrices. We assume that the conduction electrons are confined in a wire along the x-axis (one-dimensional system) or in the $x-y$ plane (two-dimensional system). The direction of the effective electric field of spin–orbit coupling is taken to be along the z-axis for both one- and two-dimensional systems.

Since the Hamiltonian H_0 commutes with the momentum operator $-i\hbar\boldsymbol{\nabla}$, the wave vector $\boldsymbol{k}$ is a good quantum number. The Green function of the conduction electrons in the real space can be expressed as

$$G(\boldsymbol{R};z) \equiv \frac{1}{(2\pi)^D}\int d^D\boldsymbol{k}e^{i\boldsymbol{k}\cdot\boldsymbol{R}}G(\boldsymbol{k};z), \tag{2}$$

where $D=1$ or 2 is the dimension of the system and the Green function in the momentum space is given by

$$G(\boldsymbol{k};z) = \left[z - \left\{\frac{\hbar^2k^2}{2m}\sigma_0 + \alpha(\boldsymbol{k}\times\hat{\boldsymbol{z}})\cdot\boldsymbol{\sigma}\right\}\right]^{-1}. \tag{3}$$

Here σ_0 is the (2×2) unit matrix in the spin space of conduction electrons.

The localized spins are denoted by $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ and located at positions $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, respectively. The coupling between conduction electrons and localized spins is expressed as the s–d interaction Hamiltonian

$$H_1 = J \sum_{i=1,2} \delta(\boldsymbol{r} - \boldsymbol{R}_i) \boldsymbol{S}_i \cdot \boldsymbol{\sigma}, \tag{4}$$

where J represents the strength of the s–d interaction. Note that J has the following dimensionality: (energy) $\times$(length)^D.

The total Hamiltonian is given by the sum of H_0 and H_1. We assume that the coupling constant J is so small that we can treat H_1 as a perturbation on H_0. The RKKY interaction between $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ is calculated from the second order perturbation theory as

$$H_{1,2}^{\mathrm{RKKY}} = -\frac{1}{\pi} \mathrm{Im}\, J^2 \int_{-\infty}^{\varepsilon_F} d\varepsilon\, \mathrm{Tr}[(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma}) G(\boldsymbol{R}_{12}; \varepsilon + i0^+) \times (\boldsymbol{S}_2 \cdot \boldsymbol{\sigma}) G(-\boldsymbol{R}_{12}; \varepsilon + i0^+)], \tag{5}$$

where ε_F is the Fermi energy, $\boldsymbol{R}_{12} \equiv \boldsymbol{R}_1 - \boldsymbol{R}_2$, $i0^+$ represents an infinitesimal imaginary energy, and Tr means a trace over the spin degrees of freedom of conduction electrons.[12,35]

Let us first consider the one-dimensional case. The Green function of conduction electrons in the momentum space is expressed as

$$G(k; \varepsilon + i0^+) = \left[\varepsilon + i0^+ - \left\{ \frac{\hbar^2 k^2}{2m} \sigma_0 - \alpha k \sigma_y \right\} \right]^{-1}. \tag{6}$$

After some algebras, Eq. (6) can be written as

$$G(k; \varepsilon + i0^+) = G_0(k; \varepsilon) \sigma_0 + G_1(k; \varepsilon) \sigma_y, \tag{7}$$

where the diagonal and off-diagonal Green functions are defined as

$$G_0(k; \varepsilon) \equiv \frac{m}{\hbar^2} \left[\frac{1}{k_\varepsilon^2 - k^2 - 2kk_R + i0^+} + \frac{1}{k_\varepsilon^2 - k^2 + 2kk_R + i0^+} \right], \tag{8}$$

$$G_1(k; \varepsilon) \equiv \frac{m}{\hbar^2} \left[\frac{1}{k_\varepsilon^2 - k^2 - 2kk_R + i0^+} - \frac{1}{k_\varepsilon^2 - k^2 + 2kk_R + i0^+} \right] \tag{9}$$

with $k_\varepsilon^2 \equiv 2m\varepsilon/\hbar^2$ and $k_R \equiv m\alpha/\hbar^2$.

A straightforward contour calculation gives

$$G(R; \varepsilon + i0^+) = G_0(R; \varepsilon) \sigma_0 + G_1(R; \varepsilon) \sigma_y, \tag{10}$$

where

$$G_0(R; \varepsilon) = -i \frac{m}{\hbar^2 (q + i0^+)} e^{iq|R|} \cos(k_R R), \tag{11}$$

$$G_1(R; \varepsilon) = \frac{m}{\hbar^2 (q + i0^+)} e^{iq|R|} \sin(k_R R), \tag{12}$$

with

$$q \equiv \sqrt{k_\varepsilon^2 + k_R^2} = \sqrt{\frac{2m}{\hbar^2} \varepsilon + k_R^2}. \tag{13}$$

Substituting Eqs. (10)–(12) into Eq. (5), and using the relations $G_0(-R; \varepsilon) = G_0(R; \varepsilon)$ and $G_1(-R; \varepsilon) = -G_1(R; \varepsilon)$, we have

$$\begin{aligned} H_{1,2}^{\mathrm{RKKY}} = -\frac{1}{\pi} J^2\, \mathrm{Im} \Bigg[& \mathrm{Tr}\{(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma})(\boldsymbol{S}_2 \cdot \boldsymbol{\sigma})\} \int_{-\infty}^{\varepsilon_F} d\varepsilon\, G_0(R_{12}; \varepsilon)^2 \\ & + \mathrm{Tr}\{(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma}) \sigma_y (\boldsymbol{S}_2 \cdot \boldsymbol{\sigma})\} \int_{-\infty}^{\varepsilon_F} d\varepsilon\, G_1(R_{12}; \varepsilon) \\ & \times G_0(R_{12}; \varepsilon) - \mathrm{Tr}\{(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma}) \\ & \times (\boldsymbol{S}_2 \cdot \boldsymbol{\sigma}) \sigma_y\} \int_{-\infty}^{\varepsilon_F} d\varepsilon\, G_0(R_{12}; \varepsilon) G_1(R_{12}; \varepsilon) \\ & - \mathrm{Tr}\{(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma}) \sigma_y (\boldsymbol{S}_2 \cdot \boldsymbol{\sigma}) \sigma_y\} \int_{-\infty}^{\varepsilon_F} d\varepsilon\, G_1(R_{12}; \varepsilon)^2 \Bigg]. \end{aligned} \tag{14}$$

The traces over the spin operators can be calculated by using the relation $(\boldsymbol{A} \cdot \boldsymbol{\sigma})(\boldsymbol{B} \cdot \boldsymbol{\sigma}) = (\boldsymbol{A} \cdot \boldsymbol{B}) \sigma_0 + i(\boldsymbol{A} \times \boldsymbol{B}) \cdot \boldsymbol{\sigma}$, repeatedly[36]:

$$\mathrm{Tr}\{(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma})(\boldsymbol{S}_2 \cdot \boldsymbol{\sigma})\} = 2 \boldsymbol{S}_1 \cdot \boldsymbol{S}_2, \tag{15}$$

$$\mathrm{Tr}\{(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma}) \sigma_y (\boldsymbol{S}_2 \cdot \boldsymbol{\sigma})\} = -2i(\boldsymbol{S}_1 \times \boldsymbol{S}_2)_y, \tag{16}$$

$$\mathrm{Tr}\{(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma})(\boldsymbol{S}_2 \cdot \boldsymbol{\sigma}) \sigma_y\} = 2i(\boldsymbol{S}_1 \times \boldsymbol{S}_2)_y, \tag{17}$$

$$\mathrm{Tr}\{(\boldsymbol{S}_1 \cdot \boldsymbol{\sigma}) \sigma_y (\boldsymbol{S}_2 \cdot \boldsymbol{\sigma}) \sigma_y\} = 2(2 S_1^y S_2^y - \boldsymbol{S}_1 \cdot \boldsymbol{S}_2). \tag{18}$$

Thus, using Eqs. (11)–(18) we find

$$\begin{aligned} H_{1,2}^{\mathrm{RKKY}} = F_1(|R_{12}|)[& \cos(2k_R R_{12}) \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 + \sin(2k_R R_{12}) \\ & \times (\boldsymbol{S}_1 \times \boldsymbol{S}_2)_y + \{1 - \cos(2k_R R_{12})\} S_1^y S_2^y], \end{aligned} \tag{19}$$

where the range function $F_1(|R|)$ is defined as

$$F_1(|R|) \equiv \frac{2J^2}{\pi} \left(\frac{m}{\hbar^2} \right)^2 \mathrm{Im} \int_{-\infty}^{\varepsilon_F} \frac{e^{2iq|R|}}{(q + i0^+)^2} d\varepsilon. \tag{20}$$

Performing the change of variable $\varepsilon \to q$ and using standard complex-plane integration techniques, one eventually obtains:

$$F_1(|R|) = \frac{2J^2}{\pi} \frac{m}{\hbar^2} \left[\mathrm{Si}(2q_F|R|) - \frac{\pi}{2} \right], \tag{21}$$

where $q_F \equiv \sqrt{2m\varepsilon_F/\hbar^2 + k_R^2}$ and Si() is the sine integral function.[37] The range function of Eq. (21) is the same form as that of the usual one-dimensional RKKY interaction[38,39] except that the Fermi wave vector $k_F(\equiv\sqrt{2m\varepsilon_F/\hbar^2})$ is replaced by q_F.

As shown in Eq. (19), the resulting RKKY interaction consists of three physically quite different interactions: Heisenberg, Dzyaloshinsky-Moriya, and Ising interactions. The Heisenberg and Ising couplings favor a collinear alignment of localized spins. On the contrary, the DM coupling favors a noncollinear alignment of localized spins. For distances (more precisely, for $k_R|R_{12}|\ll 1$), the DM and Ising terms are, respectively, linear and quadratic in the Rashba SO coupling α; this corresponds to the result obtained from a perturbative treatment of the SO coupling. However, for large distances ($k_R|R_{12}|\gg 1$), a perturbative treatment of the SO coupling would completely fail: indeed, in this regime, one finds that the DM and Ising couplings oscillate with the same amplitude as the Heisenberg term.

This peculiar twisted coupling of localized spins can be easily understood by introducing the twisted spin space where the spin quantization axis of the second localized spin $\boldsymbol{S}_2$ is rotated by an angle $\theta_{12}=2k_RR_{12}$ around the y-axis. The spin operators for the second localized spin in the twisted spin space are given by

$$S_2^x(\theta_{12})=\cos\theta_{12}S_2^x+\sin\theta_{12}S_2^z, \tag{22}$$

$$S_2^y(\theta_{12})=S_2^y, \tag{23}$$

$$S_2^z(\theta_{12})=\cos\theta_{12}S_2^z-\sin\theta_{12}S_2^x. \tag{24}$$

From the above equations, one can easily show that the inner product of $\boldsymbol{S}_1$ and $\boldsymbol{S}_2(\theta_{12})$ is

$$\begin{aligned}\boldsymbol{S}_1\cdot\boldsymbol{S}_2(\theta_{12})=&\cos\theta_{12}\boldsymbol{S}_1\cdot\boldsymbol{S}_2+\sin\theta_{12}(\boldsymbol{S}_1\times\boldsymbol{S}_2)_y\\&+\{1-\cos\theta_{12}\}S_1^yS_2^y,\end{aligned} \tag{25}$$

so that the RKKY interaction of Eq. (19) can be expressed as

$$H_{1,2}^{\mathrm{RKKY}}=F_1(|R_{12}|)\boldsymbol{S}_1\cdot\boldsymbol{S}_2(\theta_{12}). \tag{26}$$

Equation (26) shows that in presence of spin–orbit coupling the RKKY interaction results in a collinear coupling of localized spins in the θ_{12}-twisted spin space.

Next we address the two-dimensional case. The Green function of conduction electrons now takes the form

$$G(\boldsymbol{R};\varepsilon+i0^+)=G_0(R;\varepsilon)\sigma_0+G_1(R;\varepsilon)(\hat{\boldsymbol{z}}\times\hat{\boldsymbol{R}})\cdot\boldsymbol{\sigma}, \tag{27}$$

where $R\equiv\|\boldsymbol{R}\|$ and $\hat{\boldsymbol{R}}\equiv\boldsymbol{R}/R$ is the unit vector parallel to $\boldsymbol{R}$. The Green functions $G_0(R;\varepsilon)$ and $G_1(R;\varepsilon)$ can be calculated in the similar way as in Ref. 40. A straightforward calculation yields

$$\begin{aligned}G_0(R;\varepsilon)=-\frac{im}{4\hbar^2}\bigg[&\left(1+\frac{k_R}{q}\right)H_0^{(1)}[(q+k_R+i0^+)R]\\&+\left(1-\frac{k_R}{q}\right)H_0^{(1)}[(q-k_R+i0^+)R]\bigg],\end{aligned} \tag{28}$$

$$\begin{aligned}G_1(R;\varepsilon)=-\frac{m}{4\hbar^2}\bigg[&\left(1+\frac{k_R}{q}\right)H_1^{(1)}[(q+k_R+i0^+)R]\\&-\left(1-\frac{k_R}{q}\right)H_1^{(1)}[(q-k_R+i0^+)R]\bigg],\end{aligned} \tag{29}$$

where $H_0^{(1)}[\ ]$ and $H_1^{(1)}[\ ]$ are Hankel functions.[37] Hereafter, we restrict ourselves to the region $qR\gg 1$ and $k_R\ll q$. In this case we can use the asymptotic form of Hankel's functions,[37]

$$H_n^{(1)}(z)\simeq\sqrt{\frac{2}{\pi z}}e^{i(z-(n\pi/2)-(\pi/4))}\quad(|z|\to\infty). \tag{30}$$

Thus we have

$$G_0(R;\varepsilon)\simeq-i\frac{m}{\hbar^2}\frac{1}{\sqrt{2\pi qR}}e^{i(qR-(\pi/4))}\cos(k_RR), \tag{31}$$

$$G_1(R;\varepsilon)\simeq\frac{m}{\hbar^2}\frac{1}{\sqrt{2\pi qR}}e^{i(qR-(\pi/4))}\sin(k_RR). \tag{32}$$

Without restriction, we can take the coordinate system so that the vector $\boldsymbol{R}$ is aligned with the x-axis, i.e., $\boldsymbol{R}=R\hat{\boldsymbol{x}}$. Then the Green function takes the form

$$G(\boldsymbol{R};\varepsilon+i0^+)=G_0(R;\varepsilon)\sigma_0+G_1(R;\varepsilon)\sigma_y. \tag{33}$$

The RKKY interaction can be obtained in the similar way as one-dimensional system, and one gets (for $q_FR\gg 1$)

$$H_{1,2}^{\mathrm{RKKY}}\simeq F_2(R_{12})\boldsymbol{S}_1\cdot\boldsymbol{S}_2(\theta_{12}), \tag{34}$$

where the range function $F_2(R)$ is given by

$$F_2(R)\simeq-\frac{J^2}{2\pi^2}\frac{m}{\hbar^2}\frac{\sin(2q_FR)}{R^2}. \tag{35}$$

Equation (34) is the same as the usual two-dimensional RKKY interaction[39,41] except that k_F and $\boldsymbol{S}_2$ are replaced by q_F and $\boldsymbol{S}_2(\theta_{12})$, respectively. It is reasonable that the twisted coupling of two localized spins takes the same form $\boldsymbol{S}_1\cdot\boldsymbol{S}_2(\theta_{12})$ as for the 1D system, because for $q_FR\gg 1$ a scattering wave of 2D system behaves like a plane wave.

The 2DEG from surface states at metallic surfaces are good candidates for investigating the twisted RKKY interaction. Experiments on Au(111) surfaces have yielded $q_F\simeq 0.17$ Å^{-1} and $k_R\simeq 0.012$ Å^{-1};[26] in complete analogy to the effect of negative gate voltage for 2DEGs at a semiconductor heterojunction,[19,20] the adsorption of a noble gas (e.g., Xe) produces an effective repulsive potential (because of the Pauli exclusion principle) and leads to a decrease of the average Fermi wave vector ($q_F\simeq 0.155$ Å^{-1}) and an increase of the Rashba splitting ($k_R\simeq 0.015$ Å^{-1}).[26] Furthermore, quasi-1D surface states can also be obtained for vicinal surfaces, such as Au(788) and Au(23 23 21), with comparable Rashba splitting.[29–31] The distance between magnetic adatoms deposited on such surfaces can be controlled either directly by atom manipulation using the tip of a scanning tunneling microscope, or by exploiting self-organization processes. Such systems therefore constitute a versatile laboratory to investigate surface states mediated RKKY interactions under the influence of the Rashba effect. With $k_R \simeq 0.015$ Å^{-1} and a distance $R=10$ Å the twist angle $\theta = 2k_R R$ is of the order of 17$^{\mathrm{o}}$, which is quite sizable. In particular, due to the twisted nature of the RKKY interaction, very interesting frustration phenomena may be anticipated.

In semiconductor heterostructures the twisted RKKY interaction may also be of great interest, in particular in view of possibilities for manipulating entanglement between spins of quantum dots connected by a wire with Rashba SO coupling,[42] as needed for a spin-based solid-state quantum computer.[43,44] Considering the value of the Rashba coupling reported for $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ heterostructure[19] one obtains that the twist angle θ can be controlled from $\theta = \pi$ to $\theta = 3\pi/2$ by a gate voltage for $R=400$ nm.

In conclusion, we have studied the twisted RKKY interaction in one- and two-dimensions in presence of Rashba spin–orbit coupling. We have also shown that in the twisted spin space where the spin quantization axis of one localized spin is rotated, the twisted RKKY interaction is expressed in the same form as the usual RKKY interaction. The angle θ between the localized spins can be controlled by the distance between localized spins R and/or the strength of the spin-orbit coupling of conduction electrons.

After finishing this work we became aware of the paper.[45] The twisted spin space we discussed can be justified by the unitary transformation introduced in Ref. 45. We are grateful to Vladimir I. Fal'ko for pointing out this point.

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