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Twisted exchange interaction between localized spins in presence of Rashba spin-orbit coupling

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Abstract. We theoretically study the RKKY interaction between localized spins embedded in a 1D- or 2DEG with Rashba spin-orbit coupling. We show that rotation of spin of conduction electrons due to the Rashba spin-orbit coupling causes a twisted RKKY interaction between localized spins which consists of three different terms: Heisenberg, Dzyaloshinsky-Moriya, and Ising interactions. We also study the spin-configuration of linear- and ring-shaped artificial molecules consisting localized spins coupled via the twisted RKKY interaction. We find that the square-norm of the total spin of an artificial molecule oscillates with the twist angle θ and has maxima at $\theta =$ an odd integer times π. The square-norm of the total spin of the ring-shaped artificial molecules change drastically at certain values of θ where the lowest two energy levels cross each other.

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. Eminent examples are given by the giant magnetoresistance (GMR) effect and the interlayer exchange coupling in magnetic multilayers. The interlayer exchange coupling is explained in the context of Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction[1]. Recently, much attention has been focused on the effect of the Rashba spin-orbit (RSO) coupling in two-dimensional electron gases (2DEG)[2, 3, 4] . It has been established the RSO coupling can be controlled by means of a gate voltage. The RSO coupling has also been observed in 2DEG formed from surface states at metal surfaces such as Au(111)[5]. It has also been found that confinement of the surface state due to atomic steps on vicinal surfaces leads to quasi one-dimensional surface states, which also exhibit the RSO coupling[6].

We consider the system consisting of localized spins embedded in a 1D or 2DEG with RSO coupling. The Hamiltonian of two localized spins, $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$, located at positions $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ is given by

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \alpha\left(-i\hbar\nabla\times\hat{\boldsymbol{z}}\right)\cdot\boldsymbol{\sigma} + J\sum_{i=1,2}\delta(\boldsymbol{r}-\boldsymbol{R}_i)\boldsymbol{S}_i\cdot\boldsymbol{\sigma}, \tag{1}$$

where α represents the strength of the spin-orbit coupling, $\hat{\boldsymbol{z}}$ is a unit vector along the z-axis, $\boldsymbol{\sigma}$ is the vector of Pauli spin matrices, and J represents the strength of the s-d interaction. 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.

The RKKY interaction between $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ is calculated from the second order perturbation theory as

$$H_{1,2}^{\mathrm{RKKY}} = F_d(R)\Big[\cos(2k_R R)\boldsymbol{S}_1\cdot\boldsymbol{S}_2 + \sin(2k_R R)(\boldsymbol{S}_1\times\boldsymbol{S}_2)_y + \{1-\cos(2k_R R)\}\, S_1^y S_2^y\Big], \tag{2}$$

where $k_R \equiv m\alpha/\hbar^2$, $R \equiv |\boldsymbol{R}_1 - \boldsymbol{R}_2|$, and $F_d(R)$ is the range function for d-dimensional system[7]. We take the coordinate system so that the vector $\boldsymbol{R}$ is aligned with the x-axis, i. e., $\boldsymbol{R}_1 - \boldsymbol{R}_2 = R\,\hat{\boldsymbol{x}}$. The resulting RKKY interaction of Eq.(2) consists of three physically quite different interactions: Heisenberg, Dzyaloshinsky-Moriya (DM) and, Ising interactions. The Heisenberg and Ising interactions favor a collinear alignment of localized spins. On the contrary, the DM interaction favors a non-collinear alignment of localized spins.

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 $\theta \equiv 2k_R R$ around the y-axis. One can easily show that the RKKY interaction of Eq. (2) can be expressed as

$$H_{1,2}^{\mathrm{RKKY}} = F_d(R)\boldsymbol{S}_1\cdot\boldsymbol{S}_2(\theta). \tag{3}$$

Eq.(3) implies that the twisted RKKY interaction results in a collinear coupling of localized spins in the θ-twisted

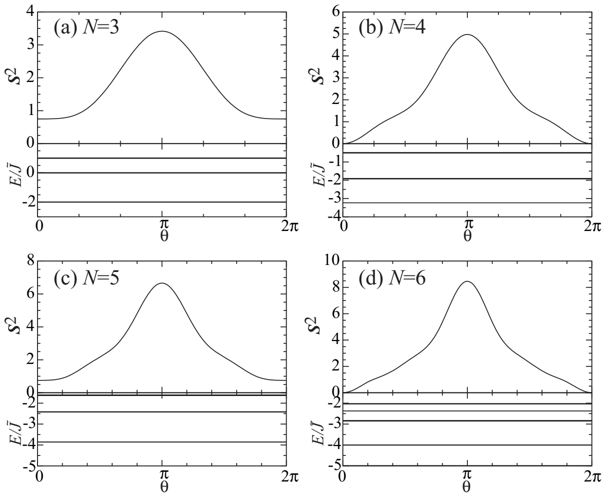

FIGURE 1. The square-norm of the total spin $\boldsymbol{S}^2$ of the ground states and energy levels of linear-shaped AMs with $N = 3, 4, 5$, and 6 are plotted against the twist angle θ in panels (a), (b), (c) and (d), respectively. Energy is normalized by the coupling constant of the RKKY interaction, $\tilde{J}$, and the twist angle takes the same valueθ for all bonds.

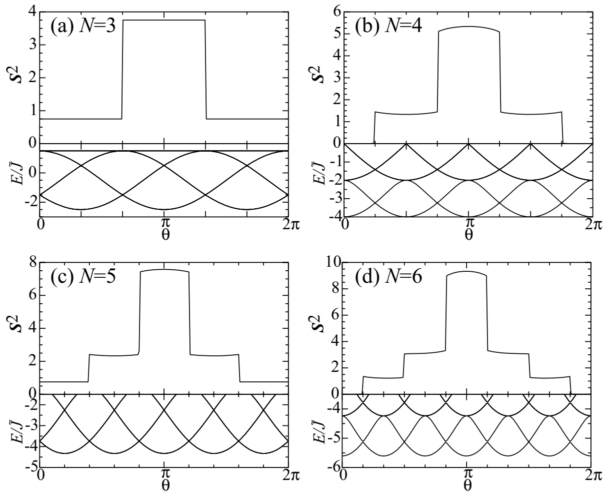

FIGURE 2. The same plot as Fig. 1 but for ring-shaped AMs.

spin space. The energy eigenvalues do not depend on θ and the total spin in the θ-twisted spin space is a conserved quantity.

In order to capture the basic physics of the twisted-RKKY interaction, we set hereafter $F_d(R) = \tilde{J} > 0$. The wavefunction of the ground state of two localized spins is given by $\psi \propto \cos\frac{\theta}{2}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + \sin\frac{\theta}{2}\left(|\uparrow,\uparrow\rangle + |\downarrow,\downarrow\rangle\right)$. Then the square norm of the total spin of the ground state, $\boldsymbol{S}^2 = 2\sin^2\frac{\theta}{2}$, is an oscillating function of θ and takes the maxima at $\theta = \pi$. One should note that the ground state in the θ-twisted spin space is always the singlet. However, the singlet in the π-twisted spin space is in fact the triplet with $\boldsymbol{S}^2 = 2$ ($S = 1$) in the real spin space. The wavefunction in the real spin space changes from singlet $\rightarrow$ triplet $\rightarrow$ singlet as we increase the twist angle θ[8]. For semiconductor artificial molecules (AMs), quantum dots connected via spin field effect transistors, the twist angle θ can be controlled by a gate voltage[3].

The above discussions can be generalized to the linear shaped AMs with $N(\geq 3)$ localized spins, since the Hamiltonian can be mapped to the usual RKKY Hamiltonian by the rotation of the spin quantization axis. In Figs. 1 (a)-(d), we show the square-norm of the ground state and energy levels for the linear-shaped AM consisting of $N = 3, 4, 5$, and 6. The energy levels do not depend on θ. Without RSO coupling, $\theta = 0$, the ground state has the antiferromagnetic spin configuration with $S = 0$ or 1/2. The square-norm $\boldsymbol{S}^2$ is again an oscillating function of θ with a period of 2π.

On the contrary to the linear-shaped AM, the square-norm $\boldsymbol{S}^2$ of the ring-shaped AM is not a smooth function of the twist angle as shown in Figs. 2 (a)-(d). Due to the boundary condition we cannot twist the spin-wavefunction by an arbitrary angle θ. Therefore, the square-norm $\boldsymbol{S}^2$ jumps at a certain value of angle θ where the lowest two energy levels cross each other as shown in Figs. 2 (a)-(b).

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