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RKKY interaction between quantum dot spins tuned by the quantum dot level

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We have investigated the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between two quantum dot (QD) spins mediated by a two-dimensional electron gas in the simplest case. The oscillation of the RKKY interaction versus the distance between the two QDs consists of two ingredients with different periods. The RKKY interaction undulates with the variation of the singly occupied QD level, which provides us a way to tune the magnitude and the sign of the RKKY interaction by pushing the QD level up and down. These conclusions are quite different from the usual result obtained by replacing the *s-d* exchange interaction with its value at the Fermi level. The influence on the RKKY interaction brought about under more realistic conditions is also discussed.

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The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction[1–3] is a fundamental ingredient in magnetic physics. It results in long range magnetic orders and brings about various magnetic ground states.[4] It is believed that the RKKY interaction leads to the ferromagnetism of dilute magnetic semiconductors.[5–7] Because of the resemblance between impurity atoms buried in a host material and quantum dots (QDs) embedded in a two-dimensional electron gas (2DEG), the RKKY theory can also be applied to the study of the interaction between QD spins mediated by free carriers outside the QDs. Since the quantum computation scheme based on the QD system was proposed,[8–10] direct or indirect interaction between the spins of QDs has been a hot topic. Because the RKKY interaction can result in magnetic order between two QD spins, the control of one QD spin could be achieved by modulating another QD spin that is *separated in space* from the former. Recently, Craig *et al.* demonstrated the nonlocal control of QD spins by a RKKY interaction.[11] Thus the RKKY interaction between QD spins, which is deemed a possible way to couple qubits consisting of QDs to construct universal quantum logic gates,[12] has drawn much attention from many theorists.[13–16] Further studies of the RKKY interaction based on the work of Craig *et al.* have been carried out,[13,14] new model devices with tunable RKKY interaction have been proposed,[15,16] and the magnitude of the RKKY interaction between two QDs in semiconductors was estimated.[17]

However, there is a difference between magnetic impurities in a host metal and QD spins in a 2DEG, which has a strong effect on the RKKY interaction. The singly occupied local level (double occupation is prohibited by the strong Coulomb repulsion) at the impurity often lies below the conduction band of the host material and far from the Fermi level. Thus the *s-d* exchange interaction $J_{kk'}$ is a slowly varying function of k and k' (k and k' are the wave vectors of Bloch waves). In this case, $J_{kk'}$ can be replaced by its value at the Fermi level, say, $J_{k_Fk_F}$ (k_F is the Fermi wave vector). Previously the calculation of the RKKY interaction was based on this approximation.[1] But the approximation is not longer valid for a system of vertical QDs grown over a 2DEG or lateral QDs buried in a 2DEG (see Fig. 1), because the singly occupied QD level often lies between the bottom of the conduction band and the Fermi level. The *s-d* exchange interaction is pinned at the energy of the singly occupied level and cannot be substituted by the value at the Fermi level. The position of the singly occupied level in a QD, unlike that of an impurity, can be tuned by changing the voltages applied to the gates. The study of the relation between this parameter and the RKKY interaction could be important for the modulation of QD spin coupling, but it has not been paid sufficient attention before now.

Motivated by the reason mentioned above, we investigate the RKKY interaction between two QD spins (either two vertical QD spins or two lateral QD spins; see Fig. 1) mediated by a 2DEG. For simplicity, we consider only the most basic case, in which the temperature is zero; the Coulomb on-site repulsion is infinite; only one orbital level with energy ϵ_0 in each QD lies below the Fermi level; and the linewidth of the level ϵ_0 is energy independent. The RKKY interaction decays and oscillates with increase of the distance between the two QDs. The oscillation includes two ingredients of two different periods, one larger than λ_F (λ_F is the Fermi wavelength) and the other shorter. The dependence of the RKKY interaction on ϵ_0 is of an oscillating manner also, which allows one to tune the RKKY interaction by pushing ϵ_0 up and down. This result is much different from the usual one obtained by regarding the *s-d* interaction as a constant, which argues that the period of oscillation is $\lambda_F/2$ and the

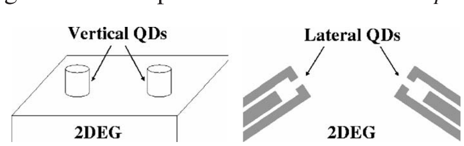

FIG. 1. Schematic diagram of two vertical QDs above a 2DEG and two lateral QDs buried in a 2DEG.

RKKY interaction is a monotonic function of ϵ_0.

The QD spins we consider in this paper are separated in space and cannot couple to each other directly. But the free carriers outside the QDs can mediate an indirect RKKY interaction when the double occupation of the QDs is prohibited by the on-site Coulomb repulsion. The RKKY interaction Hamiltonian of the two QD spins is

$$H = F{\sum_{i,j}}' \mathbf{S}_i \cdot \mathbf{S}_j, \quad i,j = 1,2, \tag{1}$$

where Σ'_{ij} means the summation over i and j avoiding $i=j$. F is the intensity of the RKKY interaction, which depends on the distance between the two QDs and the position of the singly occupied level in the QDs. Its sign determines whether the coupling between the two spins is ferromagnetic or antiferromagnetic. $\mathbf{S}_i$ is the spin operator of the ith QD. In the following calculations we will set $\hbar=2m=1$ for simplicity, where m is the effective mass of the conduction electron. From second-order perturbation theory, the RKKY interaction can be calculated. It reads

$$F = {\sum_{\mathbf{k},\mathbf{k}'}}' f_{\mathbf{k}}(1-f_{\mathbf{k}'})|J_{\mathbf{kk}'}|^2 \frac{e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}} \tag{2}$$

where $\mathbf{k}=(k\cos\phi, k\sin\phi)$ is the in-plane wave vector of electrons outside the QDs with ϕ the polar angle, $\mathbf{R}$ is the vector originating from one QD and ending at the other one, parallel to which the polar axis is established, $f_{\mathbf{k}}$ is the Fermi-Dirac distribution function, and J is the s-d exchange interaction. According to Schrieffer and Wolff's transform,[18] the s-d exchange interaction in the infinite Coulomb repulsion limit reads[18]

$$J_{\mathbf{kk}'} = \frac{-V_{\mathbf{k}}^* V_{\mathbf{k}'}}{\epsilon_{\mathbf{k}} - \epsilon_0 + i\gamma/2} + (\mathbf{k} \leftrightarrow \mathbf{k}'), \tag{3}$$

where $V_{\mathbf{k}}$ is the coupling strength between the QD state ϵ_0 and the free carrier state $\mathbf{k}$ and γ is the linewidth of the state ϵ_0. The condition for Schrieffer and Wolff's transform, $\epsilon_F - \epsilon_0 \gg \gamma$ (ϵ_F is the Fermi level), is assumed to be satisfied.

We first consider the RKKY interaction between two vertical QD spins. In this case the electronic states in the QDs couple to the two-dimensional free electron states via a tunneling barrier, and the ϕ dependence of $V_{\mathbf{k}}$ can be neglected. Generally, $V_{\mathbf{k}}$ is energy dependent and its energy dependence is difficult to model. To simplify the calculation, we neglect its energy dependence (i.e., $V_{\mathbf{k}}=V$), as most publications do, which leads to a constant linewidth $\gamma=2\pi\rho|V|^2$, where $\rho=1/4\pi$ is the density of states of the 2DEG. The effect induced by the breakdown of this presumption will be stated after our calculation. Replacing the summation in Eq. (2) with integrals, we obtain

$$F = \frac{1}{(2\pi)^2}\int_0^{k_F}\int_{k_F}^{\infty} |J_{kk'}|^2 \frac{kk'}{k^2 - k'^2} J_0(kR) J_0(k'R) dk' dk, \tag{4}$$

where J_μ is the Bessel function of order μ. In deriving the above equation, the identity $\int_0^{2\pi} e^{in\phi} e^{ikR\cos\phi} d\phi = 2\pi i^n J_n(kR)$ is used. The inner integration in Eq. (4) can be worked out analytically by means of the residue theorem. We will show the calculation details in the Appendix. In the case of $0 < \epsilon_0 < \epsilon_F$ we have

$$F = -\frac{\gamma}{\pi} J_0(k_0 R) \int_{k_F}^{\infty} \frac{k J_0(kR)}{k^2 - k_0^2} dk, \tag{5}$$

where $k_0 = \sqrt{\epsilon_0}$ is the wave vector corresponding to the energy ϵ_0. Though the integration in Eq. (5) cannot be calculated analytically, the approximate result can be found when $R \gg \lambda_F$ and ϵ_0 is neither too close to the bottom of the conduction band nor too near the Fermi level. Finally, we have

$$F = A \frac{\cos[(k_F + k_0)R] - \sin[(k_F - k_0)R]}{R^2}, \tag{6}$$

where $A = -\pi^{-2}[\gamma/(\epsilon_F - \epsilon_0)]\sqrt{k_F/k_0}$. In the approximate calculation, we have replaced $J_0(kR)$ with its asymptotic form $\sqrt{2/\pi kR}\cos(kR - \pi/4)$, which is a good approximation if $kR > 1$.

When we turn to the RKKY interaction between two lateral QD spins, there is additional complexity that should be considered carefully. Because the lateral QDs couple to the 2DEG via quantum point contacts and the profile of the 2DEG is irregular due to the metallic gates above the 2DEG, the hybrid term $V_{\mathbf{k}}$ depends on ϕ, i.e., $V_{\mathbf{k}} = V_k(\phi)$. We can expand the term $|V_{\mathbf{k}}|^2$, which is hidden in $|J_{\mathbf{kk}'}|^2$ in Eq. (2), into the Fourier series $|V_{\mathbf{k}}|^2 = |\bar{V}_k|^2 \Sigma_n c_n e^{in\phi}$ with $c_n = |\bar{V}_k|^{-2} \int_0^{2\pi} |V_k(\phi)|^2 e^{-in\phi} d\phi / 2\pi$ and $|\bar{V}_k|^2 = \int_0^{2\pi} |V_k(\phi)|^2 d\phi / 2\pi$. Correspondingly, the term $J_0(kR)J_0(k'R)$ in Eq. (4) is replaced by $\Sigma_{nn'} i^{n+n'} c_n c_{n'} J_n(kR) J_{n'}(k'R)$. Because $c_0 = 1$ and $c_0 > c_n$ for $n \neq 0$, the term $J_n(kR)J_{n'}(k'R)$ with $n = n' = 0$ in this summation remains the predominant one and apparently results in the same conclusion as Eq. (6). Other terms in the summation only lead to some unimportant rectifications, such as different weights for the two trigonometric functions in Eq. (6) and other phase differences between them. Therefore, Eq. (6), while derived for two vertical QDs, also contains the main physics for two lateral QDs coupled by a 2DEG.

Equation (6) is the essential result of this paper, and reveals the relation of the RKKY interaction to R and ϵ_0. It implies that the RKKY interaction decays as R^{-2} and oscillates when R increases, which is the same as the usual argument that we will discuss later. However, there are two conclusions much different from the usual result: (1) the oscillation consists of two ingredients with two different periods $2\pi/(k_F + k_0)$ and $2\pi/(k_F - k_0)$, one of which is larger than λ_F and the other of which is shorter; (2) the RKKY interaction oscillates when k_0 changes, and therefore undulates as ϵ_0 changes, which can be seen more clearly by combining the two trigonometric functions in Eq. (6) into one term $2\cos(k_F R + \pi/4)\cos(k_0 R - \pi/4)$. Figure 2 shows F as a function of R and of ϵ_0. The solid and dashed lines are calculated numerically from Eq. (4) and calculated according to Eq. (6), respectively. One can see that the solid and the dashed lines in Fig. 2(a) fit each other better when R increases, and those in Fig. 2(b) agree well with each other in

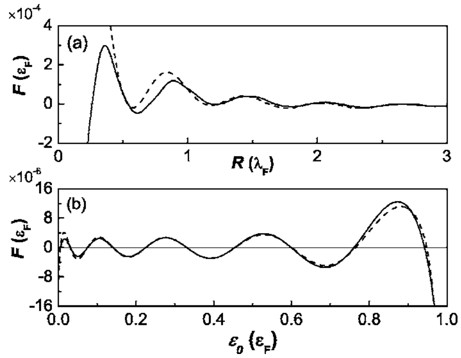

FIG. 2. The RKKY interaction calculated numerically from Eq. (4) (solid lines) and calculated according to Eq. (6) (dashed lines). (a) F versus R with the parameters $\gamma=0.01\epsilon_F$, and $\epsilon_0=0.5\epsilon_F$. (b) F versus ϵ_0 with the parameters $\gamma=0.01\epsilon_F$ and $R=5\lambda_F$.

the region where ϵ_0 is far from the bottom of the band and the Fermi level. For a 2DEG of a GaAs/GaAlAs heterostructure with the electron density $10^{15}\ \mathrm{m}^{-2}$, the Fermi wavelength is about 80 nm and the Fermi energy is about 3.4 meV. According to the parameters in Fig. 2, the linewidth of the QD level is about 3.4×10^{-2} meV. These sample parameters are experimentally reachable.

Equation (6) can be easily understood from a physical view. Because the QD level ϵ_0 lies in the conduction band, the *s-d* exchange interaction between the states k_0 and ϵ_0 is predominant. Therefore the RKKY interaction is mainly mediated by two types of processes as follows, which interfere with each other. The electron in the state $\mathbf{k}_0$ interacts with the state ϵ_0 of the first QD and thus has a probability of being scattered into an empty state above the Fermi level, say $\mathbf{k}_F$. It then travels in this state until it is scattered by the second QD into the state $\mathbf{k}_0$, which has just been emptied due to the scattering of the electron from it. In this process the wave function of the electron acquires the phase factor $e^{i\mathbf{k}_F\cdot\mathbf{R}}$. Meanwhile the electron in the state $\mathbf{k}_0$ has a probability of propagating to the second dot without experiencing scattering, and thus its wave function acquires another phase factor $e^{i\mathbf{k}_0\cdot\mathbf{R}}$. The phase difference between the two branches is $(\mathbf{k}_F-\mathbf{k}_0)\cdot\mathbf{R}$, and the interference between them results in the oscillation of the RKKY interaction in the manner of $\cos[(\mathbf{k}_F-\mathbf{k}_0)\cdot\mathbf{R}]$. Furthermore, all possible orientations of the initial and the mediated wave vectors and all possible moduli of the mediated wave vectors larger than k_F should be taken into account. The effect is renormalized into two special cases: case 1 is that $\mathbf{k}_F$ and $\mathbf{k}_0$ are both parallel or antiparallel to $\mathbf{R}$, which means that the RKKY interaction oscillates as $\cos[(k_F-k_0)R+\alpha]$; case 2 is that one of them is parallel but the other is antiparallel to $\mathbf{R}$, which leads the RKKY interaction to oscillate as $\cos[(k_F+k_0)R+\beta]$. Here α and β are two parameters that depend on the physical model adopted. They are 0 and $\pi/2$ in this paper, respectively.

Though the case in which ϵ_0 is much below the bottom of the conduction band is not of interest to us, we have to review this case and compare it with our result. In this case Eq. (5) is no longer valid, and we must recalculate from Eq. (4). Because the poles in $J_{kk'}$ are outside the conduction band, the RKKY interaction can be calculated by regarding $J_{kk'}$ as a constant $J_{k_Fk_F}$. Thus, only the pole $\sqrt{k^2+i0^+}$ in the inner integral needs to be considered. After applying the residue theorem, we have $F\sim|J_{k_Fk_F}|^2k_F^2[J_0(k_FR)N_0(k_FR)+J_1(k_FR)N_1(k_FR)]$, which is the same as in a few earlier papers that used other methods,[19–21] where N_μ is the Neuman function of order μ. When $R\gg\lambda_F$, we have $F\sim|J_{k_Fk_F}|^2R^{-2}\sin 2k_FR$. This implies that the RKKY interaction oscillates with the period $\lambda_F/2$ when R increases, and varies monotonically when ϵ_0 approaches the bottom of the band from negative infinity because $J_{k_Fk_F}$ is still a function of ϵ_0 [see Eq. (3)]. Clearly, the conclusion is much different from the result implied by Eq. (6).

Though only the most basic case is studied in this paper, the main features of the RKKY interaction in more complicated and more realistic cases can be predicted to some extent from our conclusion. A nonzero temperature has little effect on the RKKY interaction except that the temperature broadening is comparable to the separation between the QD level and the Fermi level. The finiteness of the Coulomb repulsion leads the oscillation of the RKKY interaction versus R and versus k_0 to contain new ingredients with other periods. The energy dependence of $V_{\mathbf{k}}$ or γ results in the RKKY interaction being modulated by the linewidth in Eq. (6) [see the definition of A after Eq. (6)].

In summary, we have investigated the RKKY interaction between two QD spins mediated by a 2DEG in the most basic case. The RKKY interaction decays and oscillates as the distance between the two QDs increases. The oscillation has two ingredients with different periods. The RKKY interaction undulates with the position of the singly occupied level in the QDs. We have discussed the possible features of the RKKY interaction under more realistic conditions. The result could be useful for QD spin control via the RKKY interaction.

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APPENDIX: CALCULATION DETAILS

In the appendix, we will show how to obtain Eq. (5) from Eq. (4) using the residue theorem. The twofold integration $\int_0^{k_F}\int_{k_F}^{\infty}dk\,dk'$ in Eq. (4) can be replaced with $(\int_0^{k_F}\int_0^{\infty}-\int_0^{k_F}\int_0^{k_F})dk\,dk'$, and the latter integration in the parentheses vanishes because the integrand changes its sign when we exchange k and k'. After changing the lower integration limit of k' from k_F to 0, we rewrite Eq. (4) as

$$F=\frac{1}{(2\pi)^2}\int_0^{k_F}g(k)J_0(kR)k\,dk, \tag{A1}$$

where

$$g(k)=\int_0^{\infty}|J_{kk'}|^2\frac{k'}{k^2-k'^2}J_0(k'R)dk' \tag{A2}$$

contains the integration over k', which we will calculate first. There are six poles in the integrand of Eq. (A2), $\pm\sqrt{k^2+i0^+}$,

$\pm\sqrt{k_0^2+i\gamma/2}$, and $\pm\sqrt{k_0^2-i\gamma/2}$ [the first two poles can be found immediately, while the remaining four poles are hidden in $J_{kk'}$; see Eq. (3)], lying on the complex plane of k', three on the upper half plane and three on the lower half plane. Because the integrand is an odd function of k' [note $J_0(k'R)$ is even about k'] and the range of integration runs from 0 to ∞, the residue theorem cannot be applied directly. So we first replace the even function $J_0(k'R)$ with an odd one:

$$\tilde{J}_0(k'R) = \begin{cases} J_0(k'R) & \text{for } k' > 0, \\ 0 & \text{for } k' = 0, \\ -J_0(k'R) & \text{for } k' < 0. \end{cases} \quad \text{(A3)}$$

Obviously, the value of the integral remains unchanged if we replace $J_0(k'R)$ with $\tilde{J}_0(k'R)$, but the parity of the integrand changes. For the odd function we can find the odd Fourier integration representation, i.e., the sinusoidal representation

$$\tilde{J}_0(k'R) = \frac{2}{\pi}\int_1^\infty \frac{\sin(k'Rx)}{\sqrt{x^2-1}}dx. \quad \text{(A4)}$$

Substitute it into Eq. (2), we have

$$g(k) = \frac{1}{i\pi}\int_1^\infty \frac{dx}{\sqrt{x^2-1}}\int_{-\infty}^\infty |J_{kk'}|^2 \frac{e^{ik'Rx}}{k^2-k'^2}k'\,dk'. \quad \text{(A5)}$$

One can see immediately that the residue theorem can be applied directly on the above equation. Performing the contour integration around every pole on the upper half complex plane of k' and working out the integral over x, we obtain

$$g(k) = 2^2\pi^2\gamma N_0(k_0R)\,\delta(k^2-k_0^2) + 2^2\pi\gamma\frac{k^2-k_0^2}{(k^2-k_0^2)^2+(\gamma/2)^2}J_0(k_0R), \quad \text{(A6)}$$

where the identity $N_0(kR)=-\frac{1}{\pi}\int_1^\infty e^{ikRx}(x^2-1)^{-1/2}dx+\text{c.c.}$ and the approximation $\{\gamma/[(k^2-k_0^2)^2+\gamma^2/4]\}_{\gamma\to 0}=2\pi\delta(k^2-k_0^2)$ are used. Because of the relation $\frac{1}{(2\pi)^2}\int_0^\infty g(k)J_0(kR)k\,dk=0$, we can change the range of the integration over k to simplify the RKKY interaction as

$$\begin{aligned} F &= -\frac{1}{(2\pi)^2}\int_{k_F}^\infty g(k)J_0(kR)k\,dk \\ &= -\frac{\gamma}{\pi}J_0(k_0R)\int_{k_F}^\infty kJ_0(kR)\frac{(k^2-k_0^2)}{(k^2-k_0^2)^2+(\gamma/2)^2}dk \\ &\simeq -\frac{\gamma}{\pi}J_0(k_0R)\int_{k_F}^\infty \frac{kJ_0(kR)}{k^2-k_0^2}dk. \end{aligned} \quad \text{(A7)}$$

So we obtain Eq. (5).

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