Estimation of the magnitude of the Ruderman-Kittel interaction in 3d and 2d GaAs crystals

Journal of Physics: Conference Series **1482** (2020) 012001 doi:10.1088/1742-6596/1482/1/012001

Estimation of the magnitude of the Ruderman-Kittel interaction in 3d and 2d GaAs crystals

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Abstract. In this paper, estimates are made of the Ruderman-Kittel interaction in a gallium arsenide crystal and in GaAs quantum wells of varying widths. The calculation results indicate that this interaction may be weaker than the magnetic dipole-dipole interaction by an order of magnitude. Also discovered was a relatively strong dependence of this interaction on the level of doping.

1. Introduction

The study of spontaneous order in the nuclear spin systems of various materials is largely of academic interest. It may, however, have certain applications in spintronics. That is because the spontaneous ordering of nuclear spins would decrease the scattering of electron spin by the nuclear spin system, thereby increasing it's lifetime.

The goal of studies on spontaneous ordering is to achieve the ordering in experiments, and to be able to predict the ordering temperature as well as the resulting spin configuration. For an accurate prediction, the interactions between nuclear spins must be known as precisely as possible.

The most well-known nuclear spin-spin interaction is the magnetic dipole interaction, which has a classical counterpart. Another important spin-spin interaction is the indirect exchange interaction. The magnitude of the fluctuation of the dipole-dipole interaction in GaAs is known (e.g [1], [2]). However, no information about the relative importance of various indirect exchange interactions in GaAs has been previously published. The aim of this work is to make the first step in this direction and give a basic estimate of the magnitude of indirect exchange interactions in bulk GaAs as well as in quantum wells based on GaAs.

2. Indirect exchange interaction

When a free electron (or a hole) is scattered by the hyperfine interaction with a nucleus, their states change. If this electron is then scattered by another nuclear spin and returns to it's original state, then the electron is the same as before the double scattering, while the states of both nuclear spins are altered. The effective coupling between nuclear spins which results from this virtual process is called the indirect exchange interaction.

2.1. Importance of the RK-interaction in GaAs

The different indirect exchange interactions are born from different interactions between electrons and nuclear spins. For example, the Ruderman-Kittel interaction is caused by the

contact term, and is isotropic. On the other hand, the dipole-dipole and orbital interactions are anisotropic, giving rise to anisotropic exchange interactions.

The contact interaction is usually much greater in magnitude than the others in the case of spherical wave functions. This means that e.g. in GaAs the primary indirect exchange mechanism for electrons is the RK interaction. Holes in GaAs, however, have p-type wave functions, thus the contact interaction between hole and nuclear spins is negligible. For this reason it was assumed that the electron-mediated RK interaction between nuclear spins was the greatest contributor to energy out of all the different indirect exchange mechanisms.

2.2. Theory of the RK-interaction

Originally, the subject of indirect exchange interactions mediated by the contact interaction between electrons and nuclei was explored in a 1954 paper by Ruderman and Kittel [3]. The article showed that the interaction energy H_{n-n}^{RK} is of the exchange form:

$$H_{n-n}^{RK} = -\sum_{i,j} J_{ij}\ \mathbf{I}_i \cdot \mathbf{I}_j. \tag{1}$$

A mathematical expression was also given for the exchange constant J_{ij} in a three-dimensional material. Later, the formula was somewhat rearranged and generalized to simultaneously describe three-, two- and one-dimensional materials [4]:

$$J_{ij} = \frac{\rho_d(\varepsilon_F) k_F^d A_i A_j V^2}{2\pi} \mathrm{F}_d(2k_F r_{ij}) |\varphi_0(\boldsymbol{\zeta}_i)|^2 |\varphi_0(\boldsymbol{\zeta}_j)|^2, \tag{2}$$

where $\rho_d(\varepsilon_F)$ is the density of states of a d-dimensional electron gas at the Fermi level, k_F is the d-dimensional Fermi vector, $A_{i,j}$ is the hyperfine constant of the respective nucleus, V is the unit cell volume, $\varphi_0(\boldsymbol{\zeta})$ is the wave function of electrons in the confining potential (this term is absent in the case of $d = 3$), and F_d is the range function. This function is not the same for different d, but is always decreasing and oscillating. In the cases $d = 2, 3$, the functions are

$$\mathrm{F}_2(x) = \int_1^\infty \frac{\mathrm{J}_1(xt)}{xt(t^2-1)^{1/2}}\,\mathrm{d}t, \tag{3}$$

$$\mathrm{F}_3(x) = \frac{1}{x^4}(\sin x - x\cos x), \tag{4}$$

where J_1 is the first Bessel function.

It is important to note that the Fermi vector and density of states at the Fermi level depend on the electron concentration, therefore the relative importance of the RK interaction may be quite different in semiconductors with different doping levels.

Despite the RK interaction being generally antiferromagnetic in metals [5], the interaction in semiconductors turns out to be ferromagnetic due to the relatively small Fermi wave vector, i.e., the coupling constant J is positive for nearest neighbors. Consequently, the dipole-dipole interaction will compete with it, and the ordering temperature may be significantly lowered if the RK interaction is of a similar magnitude.

3. Estimating the magnitude of the RK interaction in 3d and 2d GaAs crystals

Two different but easy to calculate values were chosen to make the estimates, designated as $E^{(1)}$ and $E^{(2)}$. $E^{(1)}$, or the complete order energy, is the energy of a specific nuclear spin i in the effective RK field of all other spins $j \neq i$ in the case of full ferromagnetic order. On the other hand, $E^{(2)}$, or the complete disorder energy, is the fluctuation of said energy in a situation where

the orientations of spins are completely independent and chaotic. The expression used for the calculations of $E^{(1)}$ is especially simple:

$$E^{(1)} = \sum_j J_{ij}\mathbf{I}_i \cdot \mathbf{I}_j = \mathrm{I}_i \sum_j J_{ij}\mathrm{I}_j = \mathrm{I}^2 \sum_j J_{ij}. \tag{5}$$

In order to obtain an analogous expression for $E^{(2)}$, we must first calculate the fluctuation $B_i^{(fl)}$ of the effective field $\mathbf{B}_i = \sum_j J_{ij}\mathbf{I}_j$, which is exerted on the spin i by the surrounding non-interacting spins.

$$(B_i^{(fl)})^2 = \langle (\sum_j J_{ij}\mathbf{I}_j)^2 \rangle = \sum_j \sum_{j'} J_{ij}J_{ij'}\langle \mathbf{I}_j \cdot \mathbf{I}_{j'} \rangle = \\ = \sum_j J_{ij}^2 \langle \mathbf{I}_j^2 \rangle = \mathrm{I}^2 \sum_j J_{ij}^2.$$

Thus, the expression for the complete disorder energy may be written as

$$E^{(2)} = \mathrm{I}^2 \sqrt{\sum_j J_{ij}^2}. \tag{6}$$

The task is therefore reduced to evaluating J_{ij} along the GaAs lattice for various concentrations of carriers.

4. Results and discussion

The results of calculations are presented in the form of charts (see figures 1, 2, 3). All of the necessary calculations were carried out using MATLAB. Overall, these results suggest a fairly steep dependence of the RK interaction strength on the carrier concentration, both in bulk GaAs and in quantum wells. In units of temperature, the energy of the RK interaction seems to be of the order of tenths or hundredths of μK, depending on the energy and structure in question.

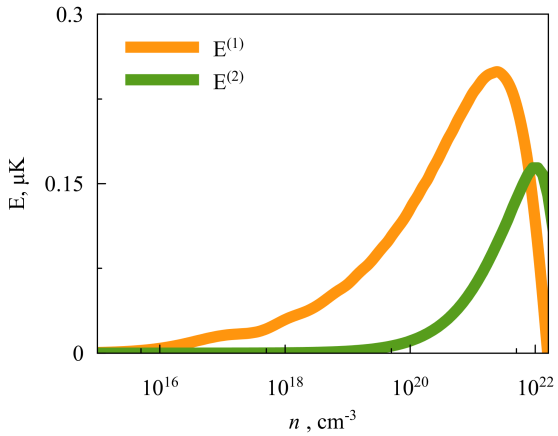

Figure 1: The dependencies of $E^{(1)}$ and $E^{(2)}$ on the carrier concentration n in bulk n-GaAs. The complete order energy reaches it's maximum at $n \sim 10^{21}$ cm^{-3}.

In bulk n-GaAs, the dependencies of both $E^{(1)}$ and $E^{(2)}$ on the carrier concentration n are quite simple (figure 1), with the RK interaction magnitude rising with increasing n across

possible doping levels. However, it is important to note that while the complete order energy is of the order of 0.1 μK in highly doped GaAs, the complete disorder energy, or fluctuation, is lower by an order of magnitude in the same regime, and reaches a value of about 0.01 μK at $n \sim 10^{20}$ cm^{-3}.

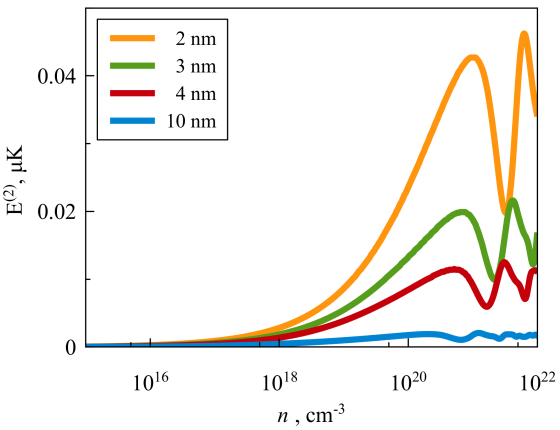

Figure 2: The dependencies of $E^{(2)}$ in various quantum wells. The first maxima correspond to $n \sim 10^{21}$ cm^{-3}.

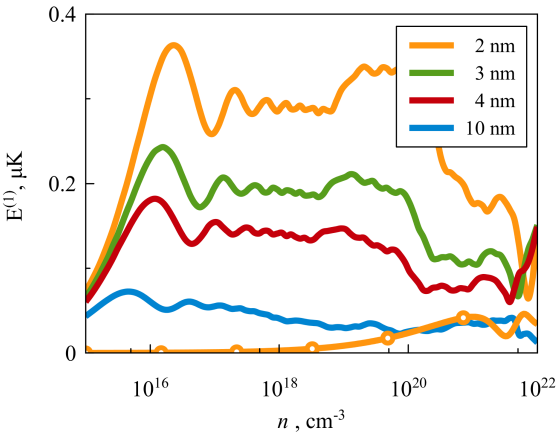

Figure 3: Smooth lines denote the dependence $E^{(1)}(n)$ in various quantum wells. The dotted line represents $E^{(2)}(n)$ in a well of $L = 2$ nm.

The calculations performed for n-GaAs quantum wells give similar results for the fluctuation $E^{(2)}$ (figure 2). In the narrowest well, $L = 2$ nm, the dependency almost mirrors the one seen in figure 1, with both dependencies having similar values and general behaviour across possible carrier concentrations. The complete order energy, on the other hand, is almost constant (figure 3), unlike in bulk GaAs, and has a magnitude of about 0.3 μK in the case of $L = 2$ nm. For both $E^{(1)}$ and $E^{(2)}$, the calculations show a steep decline in interaction strength with increasing well width.

For comparison, the measured value of magnetic dipole-dipole fluctuations in GaAs was shown to be about 0.1 μK [2], which is an order of magnitude higher than our estimates for Ruderman-Kittel fluctuations. Therefore, it is likely that as a rough simplification one may omit the RK interaction when performing estimates of ordering temperatures, especially considering the lack of precision across the different theoretical approaches [5]. The configurations of ordered spins, however, may be significantly different from the simplest antiferromagnetic structure, due to the different symmetries of the interactions.

5. Conclusion

An estimate of the strength of the Ruderman-Kittel interaction in bulk n-GaAs and n-GaAs-based quantum wells has been made. The results suggest that the energy of the RK interaction between a given spin and it's neighbors is in general of the order of 0.1-0.01 μK, with a steep positive dependence on the carrier concentration. In the 2d case, a strong negative relationship between well width and interaction strength has been found. The fluctuation of this interaction across various concentrations and well widths (in the 2d case) is smaller than the measured dipole-dipole fluctuation by an order of magnitude, which suggests that the role of the RK interaction, while not negligible, is significantly smaller than that of the dipole-dipole interaction. Therefore, the ordering temperature is likely determined almost entirely by the

dipole-dipole interaction, while the configurations of ordered spins may differ from the simplest antiferromagnetic structures due to the different symmetries of the interactions.

6. Acknowledgements

The authors acknowledge financial support from the Russian Foundation for Basic Research (RFBR Project No. 19-52-12043) and Deutsche Forschungsgemeinschaft (DFG Project A6) in the framework of International Collaborative Research Center TRR 160.

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