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Ground state phase diagram of a diluted fcc magnet with modified RKKY interaction in an external magnetic field

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A model of a diluted fcc magnet with modified RKKY interaction in an external magnetic field has been considered. The stability regions of paramagnetic, ferromagnetic and some typical antiferromagnetic phases in the ground state have been studied. In particular, the influence of the dilution and the external field on the phase diagrams has been discussed.

Key words: *diluted magnetic semiconductor; phase diagram; RKKY interaction*

1. Introduction

In diluted magnetic semiconductors (DMS) such as (Ga,Mn)As which acquire ferromagnetic properties owing to impurity ions [1, 2], the indirect coupling of magnetic moments via the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction is believed to contribute mainly to ferromagnetic ordering [3–5]. An immense importance of these materials serves as motivation to study the models of site-diluted fcc magnets driven by the RKKY interaction. A recent example is a Monte Carlo-based work [6] focused mainly on the ferromagnetic phase stability region. However, for the oscillatory, carrier concentration-dependent nature of the interaction, the phase diagrams should indicate a variety of possible magnetic orderings, including antiferromagnetic phases such as presented in [7]. On the other hand, the ground-state phase diagrams for the RKKY interaction in the presence of an external magnetic field have not been studied so far. Therefore, the aim of the present paper is to fill the gap and to study these diagrams for the site-diluted model in the field.

The RKKY interaction is modified here by the damping factor responsible for the free-carriers localization, and by the short-range superexchange antiferromagnetic

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interaction. Such a model is a prototype which can be used to describe roughly the situation occurring in (Ga,Mn)As [6].

2. Theory

We consider a diluted magnet with fcc lattice where the localized spins occupy the lattice sites at random with an equal probability n_i. The system is embedded in an external magnetic field B oriented in the z direction. We assume the Ising-like Hamiltonian in the form:

$$\mathcal{H} = -\sum_{<i,j>} J^{\mathrm{RKKY}}\left(r_{ij}\right)\ \xi_i \xi_j S_i^z S_j^z - \sum_{<i,j>'} J^{\mathrm{AF}} \xi_i \xi_j S_i^z S_j^z + g_{\mathrm{eff}} \mu_{\mathrm{B}} B \sum_i \xi_i S_i^z \tag{1}$$

In Equation (1), the first summation is over all the site pairs (for the long-range RKKY indirect interaction), whereas the second summation is only for the nearest-neighbour (NN) superexchange antiferromagnetic interaction J^{AF}. The third term incorporates the external field B. The occupation operators ($\xi_I = 0, 1$) describe the site dilution, so that the configurational averages $\langle \ldots \rangle_r$ yield $\langle \xi_i \rangle_r = n_i$ and $\left\langle \xi_i \xi_j \right\rangle_r \approx n_i^2$. The RKKY exchange interaction in the spherical approximation is given in the form [8–11]:

$$J^{\mathrm{RKKY}}\left(r\right) = C\ \left(k_{\mathrm{F}} a\right)^4 \frac{\sin\left(2k_{\mathrm{F}} r\right) - 2k_{\mathrm{F}} r \cos\ \left(2k_{\mathrm{F}} r\right)}{\left(2k_{\mathrm{F}} r\right)^4}\ \mathrm{e}^{-r/\lambda} \tag{2}$$

The Fermi wave vector k_F for the fcc lattice is $k_F = (12\pi^2 n_c)^{1/3}/a$, where a is the lattice constant, and n_c stands for the free-carriers concentration. The energetic constant C in Eq. (2) is given by $C = 2A^2 m^*/(\pi h^2 a^4)$, for the contact potential A and the effective mass of the carriers m^*. The exponential damping factor, with the characteristic length λ, takes into account a possible localization of the carriers [11] in the inhomogeneous system.

In Equation (1), the effective gyromagnetic factor g_{eff} contains both the localized spin component, g_S, and the factor of the free carriers, g_c. As shown in the paper [12], the total effective gyromagnetic factor should be of the form:

$$g_{\mathrm{eff}} = g_S + \frac{g_c m^* A k_F}{h^2}$$

The stable ground state magnetic phases under consideration include the disordered paramagnetic phase (P) as well as the ordered ferromagnetic (F) and three antiferromagnetic phases, which are characteristic of the fcc structure [13–15]. According to [13–15], the antiferromagnetic phases are the following: 1st kind (AF1), 1st kind improved (AF1), and 2nd kind (AF2) orderings. The stability regions of each phase in the ground state are determined by the enthalpy minimization, where the enthalpy H

per one lattice site is defined by $H = \left\langle \left\langle \mathcal{H} \right\rangle \right\rangle_r / N$, and $\langle ... \rangle$ is the thermal average in the limit $T \to 0$. For the Hamiltonian (1), the exact expression for the enthalpy is given in the form:

$$H = \begin{cases} -\frac{1}{2} n_i^2 S^2 \left[\sum_k \left(z_k^{\uparrow\uparrow} - z_k^{\uparrow\downarrow} \right) J^{\mathrm{RKKY}} \left(r_k \right) + \left(z_1^{\uparrow\uparrow} - z_1^{\uparrow\downarrow} \right) J^{\mathrm{AF}} \right] & \text{for AF phases} \\ -\frac{1}{2} n_i^2 S^2 \left[\sum_k z_k \, J^{\mathrm{RKKY}} \left(r_k \right) + z_1 \, J^{\mathrm{AF}} \right] - g_{\mathrm{eff}} n_i \mu_{\mathrm{B}} B S & \text{for F phase} \\ 0 & \text{for P phase} \end{cases} \quad (3)$$

In Equation (3), by $z_k^{\uparrow\uparrow}$ ($z_k^{\uparrow\downarrow}$) we denote the numbers of spins situated on the *k*th coordination zone of the radius r_k which are parallel (antiparallel) to the central spin, where $z_k = z_k^{\uparrow\uparrow} + z_k^{\uparrow\downarrow}$. These numbers are characteristic of (and different for) each ordered phase in the fcc structure and have to be found numerically.

3. Numerical results and discussion

The ground state phase diagrams have been calculated based on the exact expression (3), where the summation over *k* was performed up to $r_k = 100a$ (which corresponds to 18 335 coordination zones in the fcc structure). For such an interaction range, a good convergence of the enthalpy per site has been achieved. The phase diagrams are presented in n_i and n_c/n_i coordinates, where n_i and n_c are treated as independent variables, being concentrations of the impurity spins and free carriers, respectively. This assumption reflects the fact that in DMS both lattice and interstitial ions make independent contributions to (Ga, Mn)As.

In order to perform the numerical calculations in an external field, some experimental material constants characteristic of (Mn,Ga)As have been assumed such as: $a = 5.65$ Å, $A = -55$ meV·nm^3 and $m^* = 0.5m_e$, whereas the localized spins have the magnitude $S = 5/2$ [2, 16]. For the above values, we obtain the energetic constant $C = 3.1$ meV. Selected phase diagrams are presented in Fig. 1.

The diagram in Fig. 1a corresponds to the initial situation (without the external magnetic field), whereas the RKKY interaction is taken without any damping, i.e., for $\lambda \to \infty$. The antiferromagnetic NN interaction has been neglected, $J^{\mathrm{AF}} = 0$. For these initial parameters, the phase boundaries are of hyperbolic shape. It is noteworthy that in the particular case, for $n_i = 1$, the phases sequence upon n_c (and the boundary positions) are precisely the same as those calculated in [7]. In Figure 1b, an additional NN interaction is taken into account with some moderate magnitude $J^{\mathrm{AF}}/C = -0.5$. The remaining parameters are the same as in Fig. 1a. We see that two new areas of AF1 phase appear for the low carrier concentrations and in the region between AF2 and AF1I phases. Additionally, the paramagnetic state (P) is present in a narrow area. The ferromagnetic region (F) diminished in comparison with Fig. 1b, as should be expected.

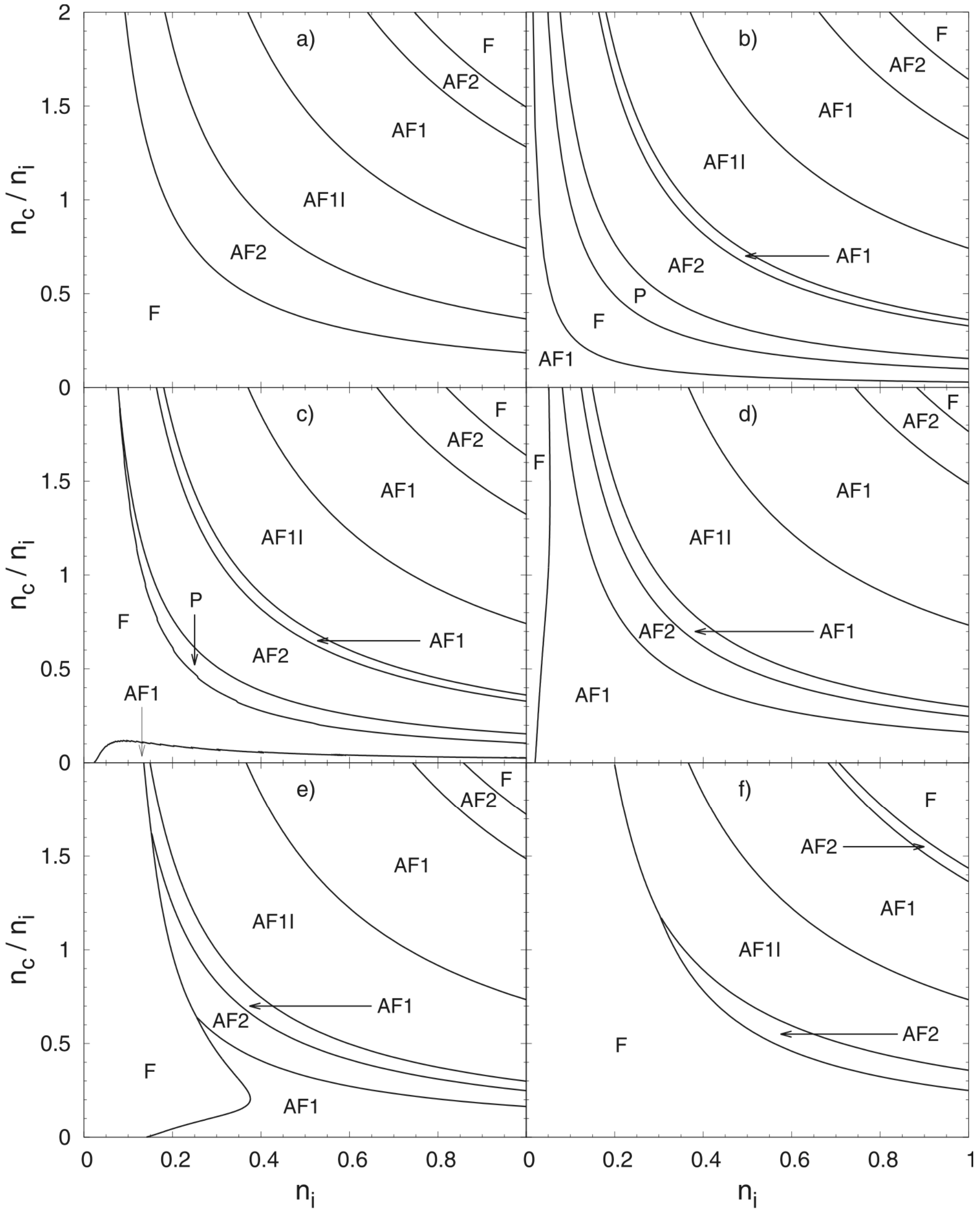

Fig. 1. Ground-state phase diagrams of the diluted fcc magnet in (n_i, n_c/n_i) space, where n_i is the concentration of impurities and n_c/n_i is the number of carriers per an impurity ion: a) $\mu_B B/C = 0$, $J^{AF}/C = 0$, $\lambda/a = \infty$, b) $\mu_B B/C = 0$, $J^{AF}/C = -0.5$, $\lambda/a = \infty$, c) $\mu_B B/C = 0.1$, $J^{AF}/C = -0.5$, $\lambda/a = \infty$, d) $\mu_B B/C = 0.1$, $J^{AF}/C = -0.5$, $\lambda/a = 1$, e) $\mu_B B/C = 0.7$, $J^{AF}/C = -0.5$, $\lambda/a = 1$, f) $\mu_B B/C = 0.7$, $J^{AF}/C = 0$, $\lambda/a = 1$

In Figure 1c, the effect of the external field of a moderate magnitude $\mu_B B/C = 0.1$ is presented. The other parameters are the same as in Fig. 1b. The field restricts the AF1 and P phases and favours the F phase. The effect is most remarkable for the low concentration of carriers. On the other hand, the influence of the strong localization of the carriers is illustrated in Fig. 1d for $\lambda/a = 1$, whereas the other parameters are the same as in Fig.1c. It is worth noting that the effect of damping in the RKKY interaction is opposite to the external field influence, i.e., the AF1 phase grows with the damping at the expense of the F-phase. Additionally, the P phase disappears in Fig. 1d as a result of a strong localization of the carriers. On the other hand, when a relatively strong magnetic field is applied, i.e., $\mu_B B/C = 0.7$ in Fig. 1e, the F phase becomes stronger at the expense of AF1 and AF2 phases. The influence of the external field is most remarkable in Fig. 1e for low concentrations of impurities n_i, contrary to Fig. 1c, where the changes were mainly seen for low concentration of carriers n_c.

Finally, in Fig. 1f the antiferromagnetic NN interaction has been removed, whereas the strong magnetic field and strong damping remained with the values as in Fig. 1e. As a consequence, the areas occupied by the F phase became considerably larger, while all the antiferromagnetic phases have been suppressed. In particular, one of the AF1 areas, indicated by the arrow in Fig. 1e, completely disappears in Fig. 1f. All the phase boundaries presented in the ground state correspond to the 1st order (discontinuous) phase transitions.

4. Conclusions

For the ground-state phase diagrams calculated without the external magnetic field (Figs. 1a and 1b), the phase boundaries are hyperbolic. By including the field (Figs. 1c –1f) some deformation of the boundary lines is observed and the F phase becomes more noticeable. The phase diagrams are most sensitive to the external magnetic field, as well as to other model parameters, for small concentrations of n_i and n_c, i.e., in the area highly relevant to practical applications.

The NN antiferromagnetic superexchange interaction J^{AF} restricts and softens the F phase, in agreement with the simulations for (Ga,Mn)As [6]. However, the free-carriers localization parameter λ has the same effect on the system if embedded in an external field, contrary to the observation made in [6] for zero field situation. The presence of $J^{\mathrm{AF}} < 0$ even enables the paramagnetic phase (P) to occur in the ground state, albeit in a very narrow region. For very low values of n_i (or n_c) only the F and/or AF1 phases have been found. A rich structure of the diagrams for $T = 0$ calls for further temperature studies.

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