Phase Transitions in an Ising Lattice with Superexchange

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An Ising lattice with superexchange is investigated. The intermediate atom responsible for the exchange interaction may be in either of two states that differ by an energy ϵ and have different exchange integrals between the neighboring nodes J_1 and J_2. For certain relations between the parameters ϵ, J_1, and J_2, the system under consideration may possess three phase-transition temperatures.

IN certain magnetic materials with a complicated crystal lattice, the exchange interaction between the spins of magnetically active nodes proceeds via magnetically neutral intermediate ions or atoms. Such a transfer of exchange interaction is called superexchange. We consider the simplest model of a lattice with superexchange, assuming that it is described by the Ising model, in which the interaction of each pair of sites (circles with arrows on Fig. 1) is "transferred" by means of a single intermediate atom (circles without arrows in Fig. 1). We shall assume that the intermediate atom, which ensures the exchange interaction, can be in one of two states, which differ in energy by ϵ, and which have different exchange integrals with the neighboring sites J_1 and J_2. If σ_n and σ_{n+1} are the spin variables of the two neighboring sites in the Ising lattice ($\sigma = \pm 1$), then the energy for each single bond (i.e., the line connecting σ_n and σ_{n+1}) can be written as $\mathscr{E}_1 = -J_1\sigma_n\sigma_{n+1}$ or $\mathscr{E}_2 = -J_2\sigma_n\sigma_{n+1} - \epsilon$, depending on the state of the intermediate atom.

The partition function of the entire system can be written in the form

$$Z = \sum_{\{\sigma\}} \prod_{n,j} Z^*(\sigma_n\sigma_{n+j}), \tag{1}$$

where $\mathbf{n}$ is the vector of the corresponding lattice site and $\mathbf{j}$ is a vector connecting the given site with one of its nearest neighbors. In writing (1), use has been made of the notation

$$Z^*(\sigma_1\sigma_2) = \exp\{\beta J_1\sigma_1\sigma_2\} + \exp\{\beta J_2\sigma_1\sigma_2 + \beta\varepsilon\} \equiv Q\exp\{\beta J^*\sigma_1\sigma_2\};$$

the quantities J^* and Q in this formula are easily found by using the theorem of the "transformation" of the Ising lattice.[1] It is seen that

$$\eta \equiv e^{-2\beta J^*} = \frac{e^{-2x} + e^{x(\gamma-\alpha)}}{1 + e^{x(\gamma+\alpha)}}, \tag{2}$$

$$Q = \{1 + e^{x(\gamma+\alpha)}\}^{1/2}\{1 + e^{x(\gamma-\alpha+2)}\}^{1/2};$$
$$\alpha = J_2/J_1, \quad \gamma = \varepsilon/J_1 - 1, \quad x = \beta J_1;$$

($\beta = 1/kT$). The partition function of the Ising lattice with superexchange Z is easily expressed in terms of the partition function of the ordinary Ising lattice $Z_0(e^{-2\beta J})$ by means of the formula

$$Z = Q^N Z_0(\eta),$$

where N is the number of intermediate atoms in the lattice. The function Q has no singularities; therefore all the singularities of Z as a function of $e^{-2\beta J^*}$ are identical with the singularities of the function $Z_0(\eta)$. We recall some properties of $Z_0(\eta)$. If $0 < \eta < 1$, then a phase

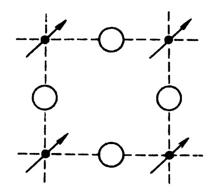

FIG. 1

transition of the ferromagnetic-paramagnetic type takes place for $\eta = \eta_0 < 1$. If $1 < \eta < \infty$, then, for $\eta = 1/\eta_0 > 1$, the transition is of the antiferromagnetic-paramagnetic type. It is important to note that the quantity η_0 is a number characteristic of the lattice type under consideration: for example, for primitive, body-centered, and face-centered cubic lattices, the corresponding values of η_0 are 0.641, 0.727 and 0.815, respectively.[2]

For the ordinary Ising lattice, the quantity η changes monotonically with increasing T. Here only a single Curie point or Neel point is possible. In the model formulated by us, as follows from (2), the quantity η can in principle change nonmonotonically with changing T. It can therefore be shown that several points of phase transition from the ordered to the disordered states and vice versa can be realized in a similar system. The number of possible types of phase transitions in the studied system depends on how many times the curve $\eta = \eta(x)$ crosses the lines $\eta = \eta_0$ and $\eta = 1/\eta_0$ when x varies in the interval $(0, \infty)$. Analyzing the function $\eta = \eta(x)$, we shall show that there are actually sets of values of the parameters α and γ for which the system possesses three phase-transition points.

First of all, we note that in the analysis below it suffices to limit ourselves to the $\epsilon > 0$ and $x > 0$ (which corresponds to $J_1 > 0$). Actually, the substitutions $J_1 \to -J_1$ and $J_2 \to -J_2$ transform η into $1/\eta$, the case $x < 0$ reducing thereby to the case $x > 0$. Proceeding to the analysis of the function $\eta(x)$, we consider the expression for the derivative $d\eta/dx = a(x)\lambda(x)$, where $a < 0$ always, and

$$\lambda(x) = 2e^{-(1+\gamma)x} + 2\alpha e^{(1+\gamma)x} + (2+\alpha+\gamma)e^{(\alpha-1)x} + (\alpha-\gamma)e^{(1-\alpha)x}. \tag{3}$$

An elementary investigation of this expression shows that a nonmonotonic behavior of $\lambda(x)$ is possible only for $-1 < \alpha < 1$. It is convenient to carry out further detailed study of (3) in three different cases, which permit in principle the existence of three phase-transition points.

1. Case $\alpha < 0$ and $\gamma < \alpha$. In this case $J_2 < 0$, i.e., the exchange integrals in the different states of the in-

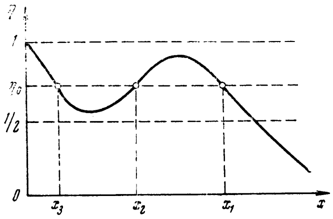

FIG. 2

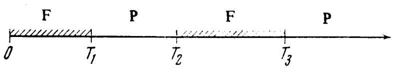

FIG. 3

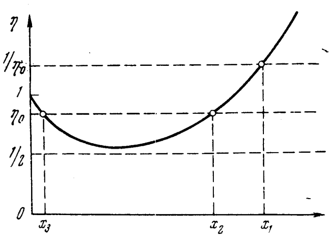

FIG. 4

termediate atom differ in sign (we recall that $J_1 > 0$). The ground state of the system (for T = 0) is ferromagnetic. The greatest nonmonotonicity of $\eta(x)$ occurs at $|\alpha - \gamma| \ll |\alpha + \gamma| \ll 2$. A schematic plot of $\eta = \eta(x)$ will have the form of Fig. 2. It is easy to see that there exist such values of the parameters α and γ for which $\eta_{\min} < \eta_0 < \eta_{\max}$. For example, let $\gamma = -0.11$ and $\alpha = -0.10$. Then, at x = 2 and x = 15, the corresponding values of η are 0.602 and 0.825. Thus, for these values of the parameters α and γ, three phase-transition points are possible in all three cubic lattices. The locations of the corresponding phases on the temperature axis are shown in Fig. 3 (we recall that $x = \beta J_1$). The letters F and P in this figure refers to the ferromagnetic and the paramagnetic phases.

2. The case $\alpha < 0$ and $\alpha < \gamma < |\alpha|$. The ground state of the system is antiferromagnetic in this case. The schematic plot of $\eta(x)$ now has the form of Fig. 4. The most favorable conditions for the appearance of a strong nonmonotonicity (i.e., the sharp drop of the plot of $\eta(x)$ in Fig. 4) are realized as $\alpha \to 0$. For example, for $\alpha = -0.05$, $\gamma = 0$ and x = 2, we obtain $\eta = 0.589$, which satisfies all three cubic lattices with something

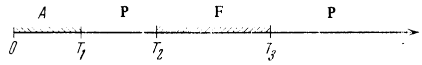

FIG. 5

α	γ	η_{min}	η_{max}	SC	BCC	α	γ	η_{min}	η_{max}	SC	BCC
0.01	0.21	0.585	0.737	+	+						
0.01	0.31	0.617	0.791	+	+	0.03	0.43	0.626	0.679	+	−
0.02	0.32	0.606	0.696	+	−	0.02	0.52	0.656	0.768	−	+
0.02	0.42	0.633	0.737	+	+	0.04	0.54	0.636	0.670	+	−

to spare. The locations of the phases on the temperature axis for the primitive and body-centered cubic lattices in this case are shown in Fig. 5, where A is the symbol for the antiferromagnetic state.

3. The case $\alpha > 0$ and $\gamma > \alpha$. The exchange integrals J_1 and J_2 in this case are of the same sign (positive). The ground state of the system is ferromagnetic. The greatest nonmonotonicity of the plot of $\eta(x)$ occurs upon satisfaction of the inequalities $\alpha \ll \gamma \ll 2$. The schematic dependence of $\eta(x)$ for such conditions is similar to that shown in Fig. 2 with the corresponding phase locations (Fig. 3). Since very small values of α are necessary to achieve strong nonmonotonicity in this case, we have carried out a numerical treatment of $\eta(x)$ for the purpose of finding $\eta_{\min}$ and $\eta_{\max}$ for different values of the parameters α and γ. In the table we show α and γ for which phase transitions take place in primitive and body-centered cubic lattices. (The plus signs in the last two columns indicate the presence of three phase-transition points.)

In conclusion, we note that the problem of the appearance of several phase-transition points in modified Ising lattices has been discussed by many authors.[3] However, the model assumed by us differs from what has been considered previously by the fact that in it the exchange between the sites takes place through "nonmagnetic" ions, with "internal" degrees of freedom.

[1]M. E. Fisher, The Nature of the Critical State, (Russ. transl.), Mir, 1968.

[2]A. M. Kosevich and V. A. Shklovskiĭ, Zh. Eksp. Teor. Fiz. **60**, 1086 (1971) [Sov. Phys.-JETP **33**, 588 (1971)].

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