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STATIC FLUCTUATION OF SPINS IN SYSTEMS WITH COMPETING ANISOTROPIES

H. Mano

Department of Physics, Gakushuin University, 1-5-1 Mejiros, Toshima-ku, Tokyo, Japan

Abstract. — Spin structure and phase transition of mixtures with competing anisotropies are investigated by a theory which takes static fluctuation of thermal averages of spins into consideration. It is found that random off-diagonal interaction between neighboring spins induces orientational distribution of spins and affect the second order phase transition.

Random mixtures of two kinds of spins with orthogonal anisotropies have three distinct ordered phases. For a mixture composed of A- and B-spins which prefer to align to the x- and y-axes, respectively, the x-component of the spin has the long range order (LRO) in the high concentration range of A-spin and the y-component has LRO in the low concentration range. In the intermediate concentration range both components achieve LRO and a phase called the oblique phase appears. (We denote these phases as [z], [x] and [xz] phases in this report.) One of characteristic features of the mixture is that the thermal average of each spin points to various directions depending on its local environment in [xz] phase [1, 2]. On the other hand the spin structure of [z] or [x] phases is rather simple. All spins point to z- or x-axes. This situation changes drastically if there exists random off-diagonal interaction which couples the x- and y-components of neighboring spins. Such interaction is expected to appear generally, even if its magnitude is small, in random mixtures since the bulk crystal symmetry is destroyed locally [3].

In this work I investigate how the off-diagonal interaction affects the spin structure of the ordered phases and the phase transition paying main attention to the orientational distribution of spins.

For this purpose I consider a ferromagnetic mixture of A- and B-spins whose magnitudes are one. Its Hamiltonian, $H = H_0 + H'$, is given as

$$H_0 = -2 \sum_{i,j} (J_{ij}^x S_i^x S_j^x + J_{ij}^y S_i^y S_j^y + J_{ij}^z S_i^z S_j^z),$$

$$H' = -2 \sum_{i,j} J_{ij}^z (S_i^x S_j^x + S_i^y S_j^y),$$

where the summations are taken over the nearest neighbor pairs in the simple cubic lattice. The exchange integrals are taken as $J_{AA} = J_{BB} = J_{AB} = J$, $J_{zz}^x = J_{BB} = 0$ or $1 - p_B$, and $J_{AB} = J_{AB} = r J / 2$. The random off-diagonal interaction is assumed to act between A- and B-spin pair and take values $+J^{zz}$ and $-J^{zz}$ with equal probabilities.

If there exists the orientational distribution of spins, the effective field acting on a spin from the neighboring spins fluctuates in its direction. I have developed a theory where the fluctuation of the directions of the thermal averages of spins are taken into consideration. The effective field acting on a spin is obtained by replacing each neighboring spin operator by $S_{p, 1}$ or $S_{p, 2}$ ($P = A$ or $B$) with probability $p_P$ or $1 - p_P$, while in the ordinary mean field theory it is replaced by the thermal average of P-spin, $(S_P)$. Two vectors $S_{p, 1}$ and $S_{p, 2}$ are determined by introducing two parameters $S_{p, 1}$ and $S_{p, 2}$.

$$S_{p, 1} = S_{p, n} + S_{p, 1}, t, S_{p, 2} = S_{p, n} + S_{p, 2}, t, \quad (3)$$

where $n$ and $t$ are unit vectors parallel and perpendicular to $(S_P)$ and $S_{p, n}$ is the magnitude of $(S_P)$. The parameters $S_{p, 1}$ and $S_{p, 2}$ represent the degree of the static fluctuation of P-spins and obtained as the averages of the component of $(S_P(E))$, the thermal average of P-spin placed in a local environment designated by $E$, perpendicular to $n$ under the condition that $(S_P(E))$ is positive and negative, respectively. They satisfy a equation that $p_P S_{p, 1} + (1 - p_P) S_{p, 2} = 0$. In this theory local environment of a spin is classified into 462 types for the simple cubic lattice. The parameters $(S_P)$, $S_{p, 1}$, $S_{p, 2}$ are determined self-consistently in the framework of a single site approximation.

The phase diagrams for $r = 0.1$ and $J^{zz} / J = 0, 0.1, 0.2$ are shown in figure 1. The transition temperature Fig. 1. — Phase diagrams in the temperature vs. concentration $c_A$ of A-spin plane for $r = 0.1$. Three lines between [x] or [z] phase and [xz] phase correspond to $J^{zz} / J = 0, 0.1, 0.2$ from outer to inner.
$T_L$ between $[x]$ or $[z]$ phases and $[x]z$ phase decreases as $J^{xx}$ increases while the Curie temperature $T_C$ between the para phase and $[x]$ or $[z]$ phases is unchanged. An important point is that existence of the random off-diagonal interaction causes the directions of thermal averages of spins to distribute even in $[x]$ and $[z]$ phases. As an example the temperature dependence of $\langle S_A^x \rangle$, $\langle S_A^y \rangle$, and $\langle S_A^z \rangle$ are shown in figure 2 for $r = 0.1$, $J^{xx} = 0.1$ J and $c_A = 0.3$. The probability distribution of the angle of $\langle S_A(\theta) \rangle$ is shown in figure 3. In $[x]$ phase the $x$ component of spins achieves LRO. On the other hand, as can be seen from figure 3a, the $z$ component of each spin takes positive or negative values with equal probability. As the temperature decreases $\langle S_A^z \rangle$ starts to take a finite value at $T = T_L$ but for $T \approx T_L$ the $z$ component of almost half of spins has opposite sign to the LRO parameter as can be seen from figure 3b. These spins do not contribute to LRO of the $z$ component. Their number decreases continuously with decreasing temperature (see Fig. 3c). From the point of view of the ordering of the $z$ component of spins the transition at $T_L$ is considered to be that from a glass phase to an ordered phase. Thus the second order phase transition at $T = T_L$ is not considered to be the ordinary one. For cases where anisotropy of spin is described by a single-ion one the transition between $[x]$ phase and $[x]z$ phase becomes the first order one. When $J^{xx} = 0$, $T_L$ is the ordinary second order transition point since no static fluctuation occurs in $[x]$ and $[z]$ phases. The smearing or disappearance of the phase transition at $T_L$ has been found experimentally in some antiferromagnetic mixtures and it is interpreted as random field effect [3]. The present work will provide another point of view for it.