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Spin-glass transition in a system with competing ferromagnetic and antiferromagnetic interaction

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Using the recently developed method of Edwards and Anderson we obtain the free energy for a system of spins interacting with an exchange potential having a distribution in the form of the sum of two Gaussians centered about $\pm J_0$ with widths J. When $J \neq 0$, the system undergoes a spin-glass transition only, with the ferromagnetic or antiferromagnetic phases absent. When $J = 0$ the system shows no transition in the molecular-field approximation used even though J_0 is finite. For very low temperatures and for $J/J_0 \lesssim \frac{1}{2}$ the method gives a negative specific heat and magnetic susceptibility. These unphysical results also arose in connection with the negative entropy obtained previously for spin glasses.

In a recent paper Edwards and Anderson[1] have developed a new method to evaluate the free energy for a set of spins which interact with a Gaussian random exchange potential. Sherrington and Kirkpatrick[2] (SK) used the method of Edwards and Anderson to obtain the free energy for a system of spins interacting via a random Gaussian exchange potential J_{ij} centered about J_0, where J_0 is ferromagnetic. They showed that depending on the parameters entering the Gaussian the systems may undergo a ferromagnetic or spin-glass transition. In the spin-glass phase the magnetization for the system is zero, however, the mean-square local magnetic moment averaged over the spatial coordinates of the system is nonzero.

The purpose of this paper is to examine the behavior of a system having a distribution of exchange potentials in which J_0 is ferromagnetic and antiferromagnetic with equal probability. For this purpose we choose a distribution function $P(J_{ij})$ of the exchange interaction J_{ij} as the sum of two Gaussians, one centered about $+J_0$, tending to give a ferromagnetic ordering like the model discussed by SK, the other centered about $-J_0$, tending to give antiferromagnetic ordering. For simplicity we use here a distribution in which each Gaussian has the same strength and the same width J. Our work not only demonstrates the influence of the choice of the distribution on the nature of the transition, but also represents an interesting analogy to the Ruderman-Kittel-Kasuya-Yosida potential.[3] It can be shown that the latter can be approximated by a completely symmetric distribution about $J_0 = 0$. That the details of the distribution strongly influence the thermodynamic properties of the system was recently demonstrated by Riess and Klein[4] using the self-consistent molecular-field theory of Klein.[5]

We find that for $J \neq 0$ the system undergoes a spin-glass transition only. The magnetic susceptibility and the specific heat are both continuous at $T = T_c$, where T_c is the spin-glass transition temperature. However, both of these quantities have discontinuous derivatives at T_c, thus we have a "third-order phase transition." Furthermore, the maximum in the specific heat and magnetic susceptibility both occur below the transition temperature. For $J = 0$, we have the sum of two δ functions and for this case there is no phase transition.

It is interesting to compare this result with the case considered by Mattis[6] in which the "sites" (and not the potentials, or "bonds") are random variables. For his case Mattis obtains a phase transition.

A serious difficulty arises in our theory when $T \ll T_c$ and the ratio of $J_0/J \gtrsim 2$. For these low temperatures the specific heat and magnetic susceptibility both become negative, giving rise to unphysical results. Such unphysical results were also noted by SK who found that the entropy is negative for $T \to 0$. SK suggested that a possible reason for this behavior is that the interchange of the $\lim N \to \infty$ and $n \to 0$ may not be valid in the n expansion. Another possible reason for our difficulty is given later in the paper. In any case, these anomalous results indicate that caution has to be exercised in applying the n expansion to real physical systems for low temperatures.

Consider an Ising Hamiltonian of the form

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} S_i S_j , \tag{1}$$

where J_{ij} is a random exchange potential, each J_{ij} is assumed to have a symmetric probability distribution of the form

$$P(J_{ij}) = \frac{1}{2J\sqrt{2\pi}} \left\{ \exp\left[-\frac{1}{2} \left(\frac{J_{ij} - J_0}{J} \right)^2 \right] + \exp\left[-\frac{1}{2} \left(\frac{J_{ij} + J_0}{J} \right)^2 \right] \right\}. \tag{2}$$

Since the positions of the spins are "frozen-in" we have to average the free energy, i.e., the logarithm of the partition function Z, over all coordinates, rather than Z itself. For this purpose we use the n expansion[1,2] based on the relation

$$\ln Z = \lim_{n\to 0} (1/n)(Z^n - 1). \tag{3}$$

Using Eq. (3) enables us to average Z^n over all coordinates, and then take the limit as $n \to 0$. Thus the free energy is (k_B is taken to be unity)

$$F = -T \lim_{n\to 0} \frac{1}{n}\left[\prod_{i\neq j} \int P(J_{ij}) dJ_{ij} \times \mathrm{Tr}_n \exp\left(\frac{J_{ij}}{2T} \sum_{\alpha=1}^{n} S_i{}^\alpha S_j{}^\alpha\right) - 1\right], \tag{4}$$

where Tr_n is the trace evaluated for a replica of n systems. Substituting Eq. (2) into Eq. (4) and integrating gives

$$F = -T \lim_{n\to 0} \frac{1}{n}\left\{\prod_{i\neq j} \mathrm{Tr}_n \frac{1}{2}\left[\exp\left(\frac{J_0}{T}\sum_{\alpha=1}^{n} S_i{}^\alpha S_j{}^\alpha\right) + \exp\left(-\frac{J_0}{T}\sum_{\alpha=1}^{n} S_i{}^\alpha S_j{}^\alpha\right)\right] \exp\left(\frac{J^2}{4T^2}\sum_{\alpha,\beta} S_i{}^\alpha S_j{}^\alpha S_i{}^\beta S_j{}^\beta\right) - 1\right\}. \tag{5}$$

Similarly to SK we define the order parameters m^α and $q^{\alpha\beta}$ by the relation

$$m^\alpha = \langle S_i^\alpha \rangle_n , \tag{6a}$$

$$q^{\alpha\beta} = \langle S_i^\alpha S_i^\beta \rangle_n, \quad \alpha \neq \beta \tag{6b}$$

and in the mean-field approximation we obtain for z neighbors

$$\sum_{i\neq j} S_i^\alpha S_j^\alpha = z m^\alpha \sum_i (2S_i^\alpha - m^\alpha), \tag{7a}$$

$$\sum_{i\neq j} S_i^\alpha S_j^\alpha S_i^\beta S_j^\beta = z q^{\alpha\beta} \sum_i (2S_i^\alpha S_i^\beta - q^{\alpha\beta}). \tag{7b}$$

We note that instead of the term $\frac{1}{2}[\exp(X) + \exp(-X)]$ arising in our Eq. (5) SK have only e^X, where $X = (J_0/T)\sum_{\alpha=1}^{n} S_i^\alpha S_j^\alpha$. For this reason only terms of the form $(X^2)^k$ appear in our Eq. (5), where

$$(X^2)^k = \left[\left(\frac{J_0}{T}\right)^2 \sum_{\alpha\neq\beta} S_i^\alpha S_j^\alpha S_i^\beta S_j^\beta\right]^k. \tag{8}$$

All the terms containing $\sum_\alpha S_i^\alpha S_j^\alpha$ to odd powers cancel, and the order parameter m given by Eq. (6a) does not even appear in the free energy. This indicates that the system will have neither a ferromagnetic nor anitferromagnetic transition but rather a spin-glass transition (if any) connected with the order parameter q.

Terms with $k \geq 2$ in Eq. (8) give contributions to the free energy involving at least four spins on the same site i. The n average of these kinds of terms requires, in addition to q and m, new order parameters of the form $\langle S_i^{\alpha_1} S_i^{\alpha_2} \cdots S_i^{\alpha_{2k}} \rangle_n$ where $k > 1$. The consideration of such order parameters are beyond the scope of our paper, however, they may have to be considered for $T \ll T_c$.

Expanding the $\cosh[(J_0/T)\sum_{\alpha=1}^{n} S_i^\alpha S_j^\alpha]$ and in accordance with our argument in the previous paragraph keeping only the terms $k=1$ in Eq. (8), gives

$$F = -T \lim_{n\to 0} \frac{1}{n}\left[\prod_{i\neq j} \mathrm{Tr}_n \left(1 + \frac{J_0{}^2}{8T^2}\frac{\partial}{\partial u}\right) \exp\left(u \sum_{\alpha,\beta} S_i^\alpha S_j^\alpha S_i^\beta S_j^\beta\right) - 1\right]. \tag{9}$$

where $u = (J/2T)^2$.

We next substitute Eq. (7b) into Eq. (9), then transform the remaining pairs of spin operators using the relation

$$\sum_i \sum_{\alpha,\beta} z q^{\alpha\beta} (S_i^\alpha S_i^\beta) = z q \sum_i \left[\left(\sum_\alpha S_i^\alpha\right)^2 - n\right],$$

where we assumed that the $q^{\alpha\beta}$ are the same for each α and β.

Using the relation

$$\exp\left[-2zuq\left(\sum_\alpha S_i^\alpha\right)^2\right] = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} e^{-x^2/2} \exp\left(2(zqu)^{1/2} x \sum_\alpha S_i^\alpha\right) dx \tag{10}$$

gives for the final expression for the free energy

$$F=-TN\left[\frac{(2\bar{J}^2+\bar{J}_0^{\,2})(1-q)^2}{8T^2}+\frac{1}{(2\pi)^{1/2}}\int_{-\infty}^{\infty}e^{-x^2/2}\ln\left(2\cosh\frac{\bar{J}}{T}q^{1/2}x\right)\left(1-\frac{\bar{J}_0^2}{4\bar{J}^2}+\frac{\bar{J}_0^2}{4\bar{J}^2}x^2\right)dx\right], \tag{11}$$

where $\bar{J}=Jz^{1/2}$, $\bar{J}_0=J_0z^{1/2}$.

The order parameter q is obtained by minimizing the free energy with respect to q. We obtain

$$q=1-\frac{2\bar{J}^2}{2\bar{J}^2+\bar{J}_0^2}\int\frac{dx}{(2\pi)^{1/2}}e^{-x^2/2}\,\frac{\tanh[(\bar{J}/T)q^{1/2}x]}{(\bar{J}/T)q^{1/2}}\left[\left(1-\frac{\bar{J}_0^2}{4\bar{J}^2}\right)x+\frac{\bar{J}_0^2}{4\bar{J}^2}x^3\right]. \tag{12}$$

Equation (12) gives, $q=0$ for $T\geq T_c$, and $q\neq 0$ for $T<T_c$, where the spin glass phase transition T_c is

$$T_c=\bar{J}\left(\frac{2+2(\bar{J}_0/\bar{J})^2}{2+(\bar{J}_0/\bar{J})^2}\right)^{1/2}. \tag{13}$$

Comparing our Eq. (13) with T_c arising from the SK distribution[2] shows that whereas our T_c increases monotonically with J_0 from $T_c=\bar{J}$ when $\bar{J}_0=0$, to $T_c\to\sqrt{2}\,\bar{J}$, when $\bar{J}_0\to\infty$, for the SK distribution $T_c=\bar{J}$ independently of J_0. Equation (13) also shows that T_c increases monotonically with the width of the distribution function J and there is no phase transition when $J=0$.

Expanding Eq. (12) for T slightly below $T_c(T\lesssim T_c^-)$ gives

$$q\approx(T/\bar{J})^2(T_c^2-T^2)/(2\bar{J}^2+3\bar{J}_0^2),$$

thus the "order parameter" $q^{1/2}$ is proportional to $(T_c-T)^{1/2}$ near T_c, in accordance with the standard mean-field theory.

The magnetization and the magentic susceptibility are obtained from the free energy Eq. (11) by adding the term H/T into the argument of the hyperbolic cosine and letting the magnetic field $H\to 0$. We obtain that the magnetic susceptibility χ exhibits a discontinuous derivative at $T=T_c$, with $d\chi/dT=-N/T^2$ for $T\geq T_c^+$ and

$$\frac{d\chi(T_c^-)}{dT}=-N\bar{J}_0^{\,2}/[T_c^{\,2}(2\bar{J}^2+3\bar{J}_0^{\,2})],$$

where $T_c^{\pm}$ is the temperature just above (below) T_c.

The energy U is readily obtained from Eq. (11) and is $U=-(2\bar{J}^2+\bar{J}_0^2)N(1-q^2)/4T$. The specific heat C_v is proportional to T^{-2} for $T>T_c$, is continuous at $T=T_c$ with a discontinuous derivative dC_v/dT at $T=T_c$. It is interesting to note that the sign of dC_v/dT as well as $d\chi/dT$ continue to be negative for $T<T_c$, showing that the maxima in C_v and χ are at some temperature lower than T_c.

We next consider the low-temperature behavior. For low T we obtain that

$$q=1-(2/\pi)^{1/2}(T/\bar{J})(4+y^2)/(4+2y^2)+O(T^2),$$

where $y=J_0/J$. The low-temperature susceptibility and specific heat are

$$\chi=(2/\pi)^{1/2}(N/\bar{J})(1-\tfrac{1}{4}y^2)+O(T),$$

$$C_v=N(T/\bar{J})(\tfrac{1}{2}\pi)^{3/2}[(4-y^2)/12-(2/\pi)^3(2+y^2)^{-2}].$$

In the limit as $J_0\to 0$ all our equations are identical with SK formulas in the same limit. We observe that when $J\lesssim\frac{1}{2}J_0$ the susceptibility and the specific heat become negative provided $T\ll T_c$. The unphysical behavior of χ and C_v has its possible origin in the interchange of the limits $N\to\infty$ and $n\to 0$. This same reason is used by SK as the casue of their negative entropy for low temperatures. Another possible reason for this anomaly may be that the existence of order parameters (other than m and q) defined by Eq. (8) for $k>1$ may effect the low-temperature results, however, these are unimportant near T_c. Clearly these suggestions can only be termed as speculations.

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