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Condition for the existence of local magnetisation in a d-dimensional planar model with arbitrary exchange interactions

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Abstract. Making use of the Bogoliubov inequality, a necessary condition for spontaneous local magnetisation is derived for a d-dimensional classical planar model with exchange interactions of arbitrary distribution and range except for systems with infinite energies of elementary excitations. For ferromagnetic systems with long-range interaction $Y^{-d-\sigma}$, it gives the new result that the ferromagnetic phase is ruled out for $d \leqslant \sigma$ with $2 > \sigma > 0$. For spin glass systems of the planar model the condition is $y > 1$ for the density of spin wave states with $N(E) \sim E^y$ for small E.

1. Introduction

Recently random spin systems have attracted much interest. Especially in spin glass systems that have strong competing interactions, there has been much discussion whether they undergo a phase transition with spins frozen at low temperatures in two and three dimensions (for example, see Morgenstern and Binder (1980) and references therein). The Bogoliubov inequality is quite useful to decide whether or not in some kinds of spin systems the phase transition occurs, and has been used by Mermin and Wagner (1966), and Mermin (1967). However, they confined themselves to the ferromagnetic and antiferromagnetic phase with short-range interactions. By making use of a generalised Bogoliubov inequality, recently Vuillermot (1977) made a rigorous treatment to get the absence of ordering in a class of one- and two-dimensional quenched random systems including spin glasses. His result is applicable to classical and quantum spin systems with three spin components, though interactions are limited to being of finite range. Schuster (1980) extended the Bogoliubov inequality to the replica spin glass Hamiltonian and showed vanishing of the Edwards–Anderson order parameter below four dimensions in XY and Heisenberg spin glasses with nearest-neighbour interactions. His treatment seems still to involve the problem of the instability of solutions that appears below the freezing temperature (de Almeida and Thouless 1978, Pytte and Rudnick 1979).

In this paper we investigate, making use of the Bogoliubov inequality, a condition necessary for the existence of a generalised ordered state at non-zero temperatures in classical planar models in which pair spin interactions can have any distribution and any distance dependences as long as the elementary excitations have finite energies.

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The generalised ordered state is defined here to be that in which local magnetisations exist spontaneously. The condition applies to spin glasses as well as ferromagnetic systems with long-range interactions. It is stated as a condition restricted to the elementary excitation (i.e. spin wave) density of states, which enables us to use this quantity (which may be obtained experimentally or theoretically) to determine whether a generalised ordered state exists or not. Therefore, this condition is regarded as one against the instability of a frozen state due to spin waves. In spin glasses where there are a large number of degenerate ground states and metastable states, there may exist other mechanisms to make a frozen state collapse. Therefore, there may be a stronger condition than that to be obtained here. In pure systems, one can theoretically obtain the property of spin waves at low temperatures so that the problem can be solved directly, as will be seen later in ferromagnetic systems with a general type of interaction.

2. Theory

Let us express the Hamiltonian of a classical planar model in an arbitrary dimension. In the ground state or one of the degenerate ground states, each spin is assumed to be oriented with angle θ_i at the ith site in a certain fixed plane common to all the spins. Denoting the deviation from θ_i by ϕ_i we then have

$$\mathscr{H} = -\tfrac{1}{2}\sum_{i,j} J_{ij}\cos(\phi_i - \phi_j + \theta_i - \theta_j) - h\sum_i \cos\phi_i \qquad (1)$$

where h is the strength of an external field in the same direction as the spins. The angles $\{\theta_i\}$ are determined by $\Sigma\, J_{ij}\sin(\theta_i - \theta_j) = 0$.

Let us consider the elementary excitation which can be obtained by the harmonic approximations, that is, the spin waves, since the present method treats the stability of the system against the spin waves. Employing the harmonic approximation and neglecting the constant term, we obtain

$$\mathscr{H}_0 = \tfrac{1}{2}\sum_{i,j} J'_{ij}(\phi_i^2 - \phi_i\phi_j) + \tfrac{1}{2}h\sum_i \phi_i^2 \qquad (2)$$

where $J'_{ij} = J_{ij}\cos(\theta_i - \theta_j)$. This problem is solved formally by diagonalising the matrix $A_{ij} = \delta_{ij}\,\Sigma_k J'_{ik} - J'_{ij}$:

$$\sum_j A_{ij}a_j(\lambda) = \varepsilon_\lambda a_i(\lambda). \qquad (3)$$

Here ε_λ is the eigenvalue of mode λ and $a_i(\lambda)$ is the normalised eigenfunction at site i. Introducing the spin variable $\phi_\lambda = \Sigma_i\, a_i(\lambda)\phi_i$ we then have, for (2), $\mathscr{H}_0 = \frac{1}{2}\Sigma_\lambda\,(\varepsilon_\lambda + h)\phi_\lambda^2$. By adding the kinetic term $\frac{1}{2}I\dot{\phi}_\lambda^2$ to it as in Edwards and Anderson (1976) we get the spin wave energy:

$$\omega_\lambda = [(\varepsilon_\lambda + h)/I]^{1/2}. \qquad (4)$$

As seen from (2) or (3) the lowest energy mode is a rotation of all the spins towards the same direction with $\omega_\lambda = 0$.

In spin glasses one might think that in the ground state with $h = 0$ there are clusters of spins that can rotate freely as a whole independent of the surroundings and therefore the harmonic approximation breaks down even at $T = 0$. However, we can prove that there are no such clusters. Let us assume that there is such a cluster and consider a spin (at the ith site) on the border of the cluster. One has $\Sigma_{j:\text{in}} J_{ij}\sin(\theta_i-\theta_j)+\Sigma_{k:\text{out}} J_{ik}\sin(\theta_i-\theta_k)=0$ for one state of the cluster and $\Sigma_{j:\text{in}}\sin(\psi_i-\psi_j)+\Sigma_{k:\text{out}} J_{ik}\sin(\psi_i-\theta_k)=0$ for another state. As $\theta_i-\theta_j=\psi_i-\psi_j$ for the spins in the cluster one gets $\Sigma_{k:\text{out}} J_{ij}[-\sin(\theta_i-\theta_k)+\sin(\psi_i-\theta_k)]=0$. Since ψ_i can take arbitrary values one only has the solution that $J_{ik}=0$, hence the first assumption is wrong. This proof does not deny the existence of the ground state degeneracy. There may be a lot of degenerate ground states with finite energy barriers among them. We have no idea how far the properties of elementary excitations reflect the properties of degenerate ground states, but it is possible and meaningful to investigate the stability of a ground state at $T\neq 0$ against elementary excitations as a necessary condition for it, besides the effects due to other causes.

Now we shall apply the classical Bogoliubov inequality (Mermin 1967) to the problem,

$$\langle |A|^2\rangle \geqslant k_BT|\langle [C,A^*]\rangle|^2/\langle [C,[C^*,\mathscr{H}]]\rangle \tag{5}$$

where $[A, B]$ is the Poisson bracket and $\langle\ldots\rangle$ the thermal average. Inequality (5) is valid provided that each constituent part in (5) is finite and the validity is not directly related to whether the system is uniform or not. It is convenient to define A and C as

$$A_\lambda=\sum_i a_i(\lambda)\sin\phi_i, \qquad C_\lambda=\sum_i a_i(\lambda)p_i. \tag{6}$$

p_i is the angular momentum perpendicular to the plane of rotation, which is the canonical variable conjugate to ϕ_i. Using (1) and (6) we get $[C_\lambda,\mathscr{H}]=-\Sigma_i a_i(\lambda)\partial\mathscr{H}/\partial\phi_i$. Similarly we obtain

$$\begin{aligned}\langle [C_\lambda,[C_\lambda^*,\mathscr{H}]]\rangle \\ &=\sum_{i,j} a_i(\lambda)a_j^*(\lambda)\langle \partial^2\mathscr{H}/\partial\phi_i\partial\phi_j\rangle \\ &=\sum_{i,j} J_{ij}(|a_i(\lambda)|^2-a_i(\lambda)a_j^*(\lambda))\langle\cos(\phi_i-\phi_j+\theta_i-\theta_j)\rangle+h\sum_i |a_i(\lambda)|^2\langle\cos\phi_i\rangle \\ &\equiv E_\lambda(T,h)+hM_\lambda\end{aligned} \tag{7}$$

where

$$M_\lambda=\sum_i |a_i(\lambda)|^2 m_i, \qquad m_i=\langle\cos\phi_i\rangle. \tag{8}$$

In (8) m_i is the local magnetisation. On the right-hand side of (7) one always has $E_\lambda(T,h)+hM_\lambda\geqslant 0$ since

$$k_BT\langle [C^*,[C,\mathscr{H}]]\rangle=\langle |B|^2\rangle\geqslant 0 \tag{9}$$

holds, where $B=[C,\mathscr{H}]$.

Performing a similar calculation as above, we obtain

$$\langle [A_\lambda, C_\lambda]\rangle=\sum_i |a_i(\lambda)|^2\langle\cos\phi_i\rangle=M_\lambda \tag{10}$$

and

$$\sum_\lambda \langle |A_\lambda|^2\rangle=\sum_i\langle\sin^2\phi_i\rangle\leqslant N, \tag{11}$$

where N is the total number of spins. Substituting (7) and (10) into (5) and summing over λ and then using (11), we get

$$1 \geqslant k_B T N^{-1} \sum_\lambda |M_\lambda|^2/(E_\lambda + hM_\lambda) \tag{12}$$

for finite N. When obtaining (12) we have kept h some positive value to prevent any of the denominators from falling into zero and to use it as a trigger to break the symmetry of the system.

Let us briefly mention some properties of M_λ and m_i in disordered systems. Since those systems have no translational symmetry the $a_i(\lambda)$ are real and thus $a_i(\lambda)$ (and probably m_i) varies depending on site i. This means from (8) that M_λ is not generally non-vanishing if $m_i \neq 0$. However M_λ should not be confused with $\tilde{m}_\lambda = \Sigma_i a_i(\lambda) m_i$ which represents the component of mode λ in condensation, although there may be a possibility that even $\tilde{m}_\lambda$ for general λ does not vanish as well as for the lowest energy mode. Therefore the M_λ are not the order parameter itself, but they can be considered to indicate roughly the degree of magnitude of the local magnetisations.

In those systems which have strong and many frustrations, if the system is in an ordered state for $h = 0$, all the m_i may not necessarily be positive depending on temperature. This property of the m_i does not prevent us from proceeding further as seen in (12), although one may be able to keep every M_λ positive if the temperature is much lower than the critical point.

In order to ask for a condition necessary for non-vanishing m_i at non-zero temperatures from (12), let us introduce the density of states for $E_\lambda(T, h = 0)$

$$\rho(E) = N^{-1} \sum_\lambda \delta(E - E_\lambda(T, 0)) \sim E^Y \qquad (N \to \infty) \tag{13}$$

where we have defined the exponent Y of the leading term (the one with the lowest exponent) as $E \to 0$. Here we have assumed that $\rho(E)$ is continuous in E from $E = 0$, which is plausible because there is always a lowest energy mode of $E_\lambda(T, 0) = 0$ corresponding to a rotation of all the spins; if $\rho(E)$ has a gap, it follows immediately that the system can have a stable ordered state. Using $E(T, h) = E(T, 0) + O(h^2)$ in (12), taking the limit $N \to \infty$ and replacing $M(E)$ by a constant M in the resulting integral, we find that the right-hand side has the asymptotic form $-k_B T M^{2+Y} h^Y/Y$ as $h \to 0$. Thus if $M > 0$ we must have

$$Y > 0 \tag{14}$$

since otherwise the bound (12) could be violated by letting $h \to 0$.

It is not clear whether Y depends on temperature or not. First we suppose Y is constant. If $E_\lambda(T, 0)$ is a continuous function of T, one can then put $E_\lambda(0, 0)$ $(= {\omega_\lambda}^2)$ in place of $E_\lambda(T, 0)$ in (12) to give Y an expression in terms of spin waves, introducing the density of states for spin waves:

$$N(E) = N^{-1} \sum_\lambda \delta(E - \omega_\lambda) \sim E^y \qquad (N \to \infty). \tag{15}$$

We thus obtain the condition

$$y > 1. \tag{16}$$

Let us think about the case when $E_\lambda(T, 0)$ is discontinuous in T. This discontinuity means that correlation functions $\langle \cos(\phi_i - \phi_j + \theta_i - \theta_j) \rangle$ are discontinuous at some temperature T_d, so that there occurs a first-order phase transition. Even the occurrence of a first-order phase transition does not, however, prevent us from considering our present subject and obtaining (16) unless $T_d = 0$.

Next we show that there is no change in (16) even if Y is supposed to depend on temperature. Because Y depends on T, it follows from (14) and (12) that $Y > 0$ must be fulfilled at least below T_c or T_d for systems which undergo a second- or first-order phase transition. Therefore (14) at $T = 0$, namely (16), gives a necessary condition on which a system can have an ordered state with non-vanishing m_i at low but non-zero temperatures. This statement is not applicable only for the two unusual cases; one is $T_d = 0$ and the other is that $Y(T)$ increases with rising temperature, which means, for instance, that there is a disordered state at low temperatures but there appears an ordered state at larger temperatures as found in bond annealed Ising spin systems (Kasai and Syoji 1973, Ueno and Oguchi 1975).

In order that the inequality (5) be valid, each part in it should be finite. $\langle |A_\lambda|^2 \rangle$ is always finite and $k_B T |\langle [C_\lambda, A_\lambda] \rangle|^2$ is finite for $T < \infty$. As for the denominator, it is required from (7) at $T = 0$ that the energies of the spin waves should be bounded, i.e. $\omega_\lambda < \infty$.

It should be noted that the condition (16) is invalid for the Heisenberg model since in ferromagnetic Heisenberg systems (14) holds but $\sqrt{E_k}$ is not a spin wave energy.

3. Application

We shall apply the above result to some kinds of systems.

3.1. Ferromagnetic systems

Let us consider interactions with a general form $J(r) = A r^{-d-\sigma}$. Then the eigenvalue ε_λ in (3) is given in terms of momenta as

$$\varepsilon_k = \tilde{J}(0) - \tilde{J}(k) \sim \begin{cases} k^\sigma, & \sigma < 2, \\ k^2, & \sigma \geq 2, \end{cases} \tag{17}$$

where $\tilde{J}(k)$ is a Fourier transformation of $J(r)$. In these systems, one can directly evaluate Y (or y) using the following inequality:

$$\begin{aligned} E_k(T, 0) &= N^{-1} \sum_i \sum_j J_{ij} \{1 - \exp[ik \cdot (r_i - r_j)]\} \langle \cos(\phi_i - \phi_j) \rangle \\ &\leq \tilde{J}(0) - \tilde{J}(k). \end{aligned} \tag{18}$$

Since $\tilde{J}(0)$ is maximum and $\tilde{J}(0) \propto a_0^{-\sigma} - R^{-\sigma}$ where R is the size of the system and a_0 the lattice constant, we require $\sigma > 0$ for $\omega_k < \infty$. Accordingly (16) becomes

$$\begin{aligned} d &> \sigma \qquad \text{for } 2 > \sigma > 0, \\ d &> 2 \qquad \text{for } \sigma \geq 2. \end{aligned} \tag{19}$$

The result for $\sigma \geq 2$ is in agreement with that of Mermin (1967). We have obtained the new result that the ferromagnetic phase is ruled out in $d \leq \sigma$ for $0 < \sigma < 2$.

3.2. *Spin glass systems*

The problem of the spin waves in these systems is still unsettled both theoretically and experimentally (Villain 1980 and references therein). However, the low-temperature specific heat has been confirmed by several experiments (for instance, Wegner and Keesom 1976) to be linear in temperature. The temperature dependence of this quantity can be determined only by the knowledge of the density of states without the details for the spin waves if contributions other than that from the spin waves can be neglected. Assuming $C_m \propto T^{\alpha_l}$ for the low-temperature specific heat and approximating the spin waves as non-interacting bosons, we get instead of (16)

$$\alpha_l > 2. \tag{20}$$

However, no experiments seem to be available which can apply to the planar model.

On the other hand, there are numerical studies for planar models by some authors. Huber *et al* (1979) and Huber and Ching (1980) obtained that the low-frequency excitations are propagating modes with a linear dispersion in $d = 2$ and 3, as already predicted by Edwards and Anderson (1976). This means $y = 1$ for $d = 2$ and $y = 2$ for $d = 3$. Their exact calculation of $N(E)$ is not available because of the finite-size effects. Bray and Moore (1981) obtained $Y = 0.0 \pm 0.1$ for the square lattice and $Y = 0.1 \pm 0.1$ for the simple cubic lattice. If these results are roughly right, the spin glass order is ruled out in two dimensions but is not clear in three dimensions.

4. Conclusion and discussion

We have argued the relation of the low-frequency property of the density of states with a necessary condition for generalised ordered phases in which local magnetisations exist. The condition requires that $y > 1$ for the spin wave density of states (15). The application of this condition is excluded for the unusual cases. First, the elementary excitation energy is infinite; second, as we raise the temperature from $T = 0$, an ordered state appears following a disordered state; and lastly, a first-order phase transition occurs at $T = 0$. The last two cases are, however, unlikely to happen at all in continuous spin systems.

The condition (16) can be reduced to (20) for the low-temperature specific heat in general systems. In ferromagnetic systems with long-range interactions we have a new result, (19).

As seen above, the present method includes the contribution from the spin waves but probably neglects the possibility of the contributions from barrier modes as reversal of spins inside finite domains (Tholence and Tournier 1977) and transitions between quasi-degenerate ground states via thermal activation processes (Fischer 1979) which may be important in spin glass systems. However, as long as there exist spin waves which have no gap in energy spectra and are largely extended, they must give an important contribution at low temperatures.

Recently, Bray and Moore (1981) showed that the dynamics of vector spin glasses at low temperatures is governed by the low-frequency property of the spin wave density of states. Hence this property is quite important and it may be possible to see if the spin glass order occurs or not by observing the dynamics at low temperatures. Stauffer and Binder (1981) observed in Monte Carlo simulations a nearly logarithmic decay of the Edwards–Anderson order parameter with time which, however, did not show any dependence on both $d (2 \leqslant d \leqslant 6)$ and spin dimensionality n $(1 \leqslant n \leqslant 3)$.

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