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Asymmetrical Ising model*

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A model is introduced, which shows a discontinuous or first-order phase transition in temperature coordinate. As temperature increases, its long-range order undergoes a discontinuity at the condensation point, but contrary to the conventional assumption it does not vanish after the phase change. The long-range order remains nonzero at all finite temperatures and vanishes only at infinite temperature.

A great deal of studies have been made to understand continuous or second-order phase transitions. However, most phase changes occurring in nature are discontinuous or first-order transitions and much less is known about them. Believing that it is always desirable to have a simple model which shows any resemblance to those occurring in nature, we introduce in this short paper an asymmetrical Ising model which exhibits discontinuous phase transitions. In two dimensions exact properties of this model in the transition region can be deduced from that of the ordinary Ising model. The new model is, in some respects, similar to the Maier-Saupe quadrupole-interaction model[1] for nematic liquid crystals. We compare the rigorous results with the mean-field approximations on which most current theories of liquid crystals are based. It is found that the well-known mean-field result that the long-range order vanishes identically above the transition point is inaccurate.

Consider a usual Ising lattice and let S_i' denote the value of the dynamic variable associated with the ith lattice site. Each S_i' $(i=1,2,\ldots,N)$ can take on two eigenvalues: $-1/\lambda$, which is λ-fold degenerate $(\lambda>1)$; and $+1$, which is nondegenerate. The total energy of the system is given in the usual Ising form

$$U'=-G'\sum_{\langle ij\rangle}S_i'S_j'-H'\sum_i S_i' , \tag{1}$$

where G' and H' are, respectively, the coupling constant and the external "magnetic" field, and the symbol $\langle ij\rangle$ denotes a nearest-neighboring pair of lattice sites. This asymmetrical Ising model reduces to the usual nearest-neighbor interaction Ising model if λ equals one. In the following λ will be allowed to take any real value greater than one.

The statistical mechanical properties of the asymmetrical Ising model can be conveniently calculated by first transforming it into an equivalent Ising model. To do so we use the notation $\uparrow$ to denote an S_i' taking on the positive value $(+1)$, $\downarrow$ is an S_i' taking on the negative value $(-1/\lambda)$, $N_\uparrow$ is the number of $\uparrow$ lattice sites, and $N_{\uparrow\uparrow}$ is the number of nearest-neighboring pairs of lattice sites with both variables $\uparrow$, etc. Then the U' [Eq. (1)] can be expressed as

$$U'=-N(\tfrac{1}{2}G'\gamma\lambda^{-2}-H'\lambda^{-1})-N_\uparrow[H'(1+\lambda^{-1}) - G'\gamma\lambda^{-1}(1+\lambda^{-1})]-N_{\uparrow\uparrow}G'(1+\lambda^{-1})^2. \tag{2}$$

where γ is the coordination number of the lattice. The partition function is therefore

$$e^{-N\beta F'(H',T)}=e^{N\beta(G'\gamma\lambda^{-2}/2-H'\lambda^{-1})}\times\sum_{N_\uparrow}e^{N_\uparrow\beta[H'(1+\lambda^{-1})-G'\gamma\lambda^{-1}(1+\lambda^{-1})]}\times\sum_{N_{\uparrow\uparrow}}{}' C(N_\uparrow,N_{\uparrow\uparrow})\lambda^{N_\downarrow}e^{N_{\uparrow\uparrow}\beta G'(1+\lambda^{-1})^2} , \tag{3}$$

where $\beta=(kT)^{-1}$, the summation $\sum'$ extends over all possible $N_{\uparrow\uparrow}$ with $N_\uparrow$ positive sites, and the configuration factor $C(N_\uparrow,N_{\uparrow\uparrow})$ is the number of different configurations for a given $N_\uparrow$ and $N_{\uparrow\uparrow}$. The factor $\lambda^{N_\downarrow}$ is due to the degeneracy of the negative state. In comparison with an Ising model which has an interaction energy

$$U=-G\sum_{\langle ij\rangle}S_iS_j-H\sum_i S_i , \tag{4}$$

where S_i takes on the eigenvalues $+1$ and -1, both nondegenerate, and has a partition function

$$e^{-N\beta F(H,T)}=e^{N\beta(G\gamma/2-H)}\sum_{N_\uparrow}e^{\beta N_\uparrow(2H-2G\gamma)}\times\sum_{N_{\uparrow\uparrow}}{}' C(N_\uparrow,N_{\uparrow\uparrow})e^{4\beta GN_{\uparrow\uparrow}} , \tag{5}$$

we conclude that

$$\mathrm{Tr}\exp\Big(\beta G'\sum_{\langle ij\rangle}S_i'S_j'+\beta H'\sum S_i'\Big)=e^{\beta KN}\,\mathrm{Tr}\exp\Big(\beta G\sum_{\langle ij\rangle}S_iS_j+\beta H\sum S_i\Big) \tag{6}$$

or

$$F'(H',T)=F(H,T)-K , \tag{7}$$

provided

$$G = \tfrac{1}{4}G'(1+\lambda^{-1})^2 , \tag{8.1}$$

$$H = \tfrac{1}{2}H'(1+\lambda^{-1}) + \tfrac{1}{4}G'\gamma(1-\lambda^{-2}) - \tfrac{1}{2}kT\ln\lambda , \tag{8.2}$$

$$K = \tfrac{1}{8}G'\gamma(1-\lambda^{-1})^2 + \tfrac{1}{2}H'(1-\lambda^{-1}) + \tfrac{1}{2}kT\ln\lambda . \tag{8.3}$$

In other words, the asymmetrical Ising model is equivalent to an Ising model if the H and G of the latter are given by (8.1) and (8.2).

We can now apply the Lee-Yang circle theorem[2] to the asymmetrical model. If one varies one of H' and T while keeping the other constant, the system cannot undergo more than one phase transition, which must occur, if at all, at the point where $H=0$. Together with Yang's rigorous result for the spontaneous magnetization of the two-dimensional Ising model,[3] one concludes that first-order phase transitions do occur in two-dimensional asymmetrical models at temperatures below the critical point[4] $T_c = (2G/k)/\ln(1+\sqrt{2})$ [henceforth a square lattice ($\gamma=4$) is assumed]. At $H'=0$, the condensation temperature is given by ($H=0$)

$$T_D = 4\left(\frac{\lambda-1}{\lambda+1}\right)\frac{\ln(1+\sqrt{2})}{\ln\lambda}T_c , \tag{9}$$

provided $T_D < T_c$, that implies λ has to be greater than a value $\lambda_c = 26.217\,722\,5\ldots$. (The model also condenses at $H'=0$ for $\lambda < 1/\lambda_c$.) Figure 1 shows the phase diagrams of the asymmetrical Ising model compared with the Ising model. Although the new model is nonsymmetric by Fisher's definition,[5] i.e., $H' \to -H'$ does not imply $(\partial F'/\partial H')_T = -M' \to +M'$, the coexistence curve diameter is constant.[2,5]

From Eq. (7) one has

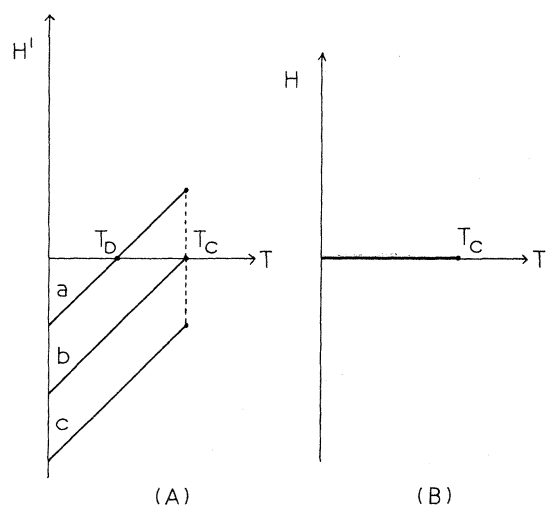

FIG. 1. Phase diagrams for (A) the asymmetrical Ising model and (B) for the Ising model. In (A) the phase boundaries a, b, and c correspond to $\lambda > \lambda_c$, $\lambda = \lambda_c$, and $\lambda < \lambda_c$ respectively. If temperature varies along an H' = const. line which intersects a phase boundary, a first-order phase transition occurs at the intersection.

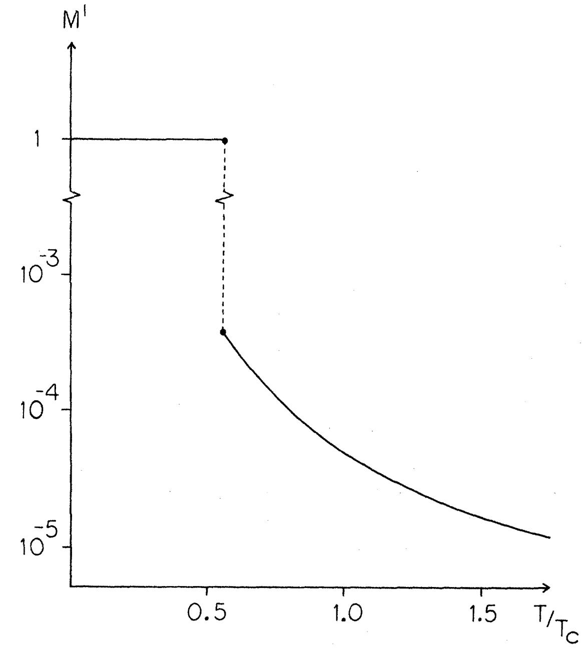

FIG. 2. M'-T diagram for an asymmetrical Ising model with $\lambda = 500$. The dots are exact values of M' at the condensation temperature T_D. The curves are obtained from cluster expansions.

$$M'(H', T) = [(1+\lambda)/2\lambda]M(H, T) + (\lambda-1)/2\lambda , \tag{10}$$

where $M(H, T) = -[\partial F(H, T)/\partial H]_T$. Since M is a continuous function of T but as a function of H is discontinuous at $H=0$ if $T < T_c$, from Eq. (8.2) one has

$$M'(0, T_D\pm) = \tfrac{1}{2}(1+\lambda^{-1})M(0\mp, T_D) + \tfrac{1}{2}(1-\lambda^{-1}) , \tag{11}$$

where $M(0\pm, T)$ have been calculated by Yang.[3] The latent heat associated with the condensation can also be calculated from the relation [Eq. (6)]

$$T_D[S'(0, T_D+) - S'(0, T_D-)] = \tfrac{1}{2}kT_D(\ln\lambda)[M(0+, T_D) - M(0-, T_D)] , \tag{12}$$

where $S'(H', T) = -[\partial F'(H', T)/\partial T]_{H'}$. For temperatures not equal to T_D, exact solutions are not available. However, the Mayer cluster expansion[6] for M' or M is convergent for $H<0$,

$$M(H, T) = -1 + 2y + y^2(8x^{-1} - 10) + y^3(36x^{-2} - 96x^{-1} + 62) + y^4(8x^{-4} + \ldots) + \cdots , \tag{13}$$

where $y = x^2 e^{2H/kT}$, $x = -4G/kT$. Therefore [from Eq. (8.2)], one sees that the series expansion is applicable for $T > T_D$. The temperatures lower than T_D correspond to $H>0$. If H and T are independent as in the usual Ising model, then $F(H, T) = F(-H, T)$. One can expand the magnetization in powers of y^{-1} for $H>0$,[2]

TABLE I. Discontinuities of the long-range order M' at the condensation points T_D for various values of λ when the external field is absent.

λ	$M'(0, T_D-)$	$M'(0, T_D+)$
26.2178	0.58176	0.38010
27.0	0.820	0.143
30.0	0.889	0.078
40.0	0.942	0.033
100.0	0.985	0.005

$$M(H, T) = 1 - 2y^{-1}x^4 - y^{-2}(8x^7 - 10x^8) - y^{-3}(36x^{10} - 96x^{11} + 62x^{12}) - 8y^{-4}(x^{12} + \cdots) + \cdots . \quad (14)$$

For an asymmetrical model at $H' = 0$, H and T are not independent. However, for $|T - T_D|/T_D \ll 1$, $F(H(T), T_D) \simeq F(-H(T), T_D)$ is a good approximation. Therefore, Eq. (14) provides an approximate expansion for M at $T \lesssim T_D$. Unfortunately, Eqs. (13) and (14) converge very slowly unless the value of λ is very large. Figure 2 shows the M'-T diagram for $\lambda = 500$. Table I shows the discontinuities of M' at the condensation points corresponding to various values of λ.

It is interesting to compare the energy spectrum of S' in the asymmetrical Ising model with that of the Maier-Saupe model for nematic liquid crystals.[1] Figure 3 shows that the energy spectrum of S' may be viewed as a step-function version of the quadrupole potential energy of a rodlike molecule in nematic liquid crystals. The mean-field (MF) approximations of these two models have the same character in every respect. However, in the MF theory, the long-range order (M' in the case of asymmetrical Ising models) equal to zero is always a root of the self-consistency condition, corresponding to a stable state above T_D and an unstable state below T_D. It has always been assumed that the long-range order vanishes identically above T_D when the external field is absent. The rigorous results however indicate that this is not the case, at least in one model. As temperature increases, the long-range order undergoes a discontinuity at the condensation point, but unlike second-order phase transitions it does not vanish after the phase change. It remains nonzero at all finite temperatures and vanishes only at infinite temperature. Note however that above T_D, M' is appreciable only for a very narrow range (out of λ_c to ∞) of λ. It is possible that the vanishing long-range order above T_D is a good approximation for the Maier-Saupe model.

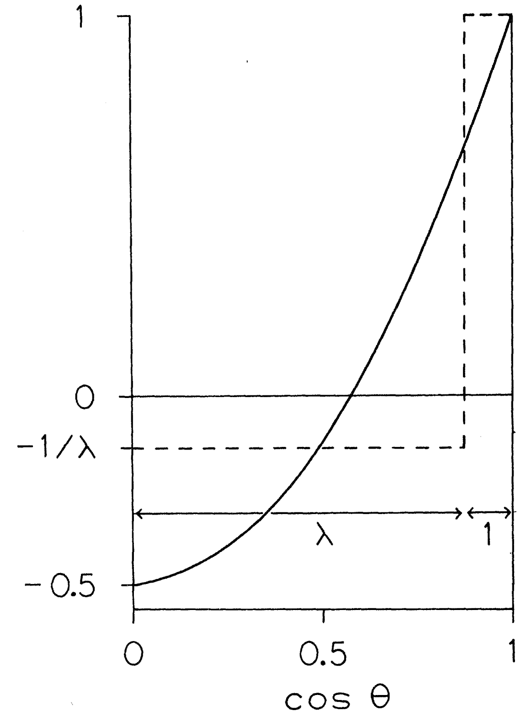

FIG. 3. Comparison of the asymmetrical Ising model with the Maier-Saupe model for nematic liquid crystals. The solid curve $(3\cos^2\theta/2 - 1)$ represents the average potential energy of a rodlike molecule when it makes an angle θ with respect to the nematic direction. The asymmetrical Ising model represented by the dashed line can be viewed as a step-function version of the quadrupole potential in the sense that the rod can only take either parallel or perpendicular orientation with respect to the nematic direction; the latter is λ-fold degenerate compared with the former.

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