CHINESE JOURNAL OF PHYSICS VOL. 16, NO 2, 3 SUMMER AUTUMN 1978

A Paper Contributed to the Special Issue of the Chinese Journal of Physics Celebrating Seventieth Birthday of Prof. Ta-You Wu

Phase Diagram of a Spin-One Ising System

F. Y. Wu (吳法岳)*

Department of Physics Northeastern University
Boston, Massachusetts 02115 , U. S. A.

(Received July 10, 1978)

Phase diagram is determined for the spin-l Ising system described by the Hamiltonian $\mathcal{H}=H\sum_i s_i+\Delta\sum_i s_i^2-J\sum_{<ij>}s_i^2 s_j^2$. The determination is exact for ferromagnetic interactions ($J>0$) and schematic for antiferromagnetic interactions ($J<0$).

THE spin-one Ising model has been of interest in recent years. The model is useful in explaining the occurrence of certain magnetic transitions such as that existing in UO_2[1]; it has also been adopted as a model in a qualitative description of the λ transition and phase separation in He^3-He^4 mixture[2]. These discussions, while leading to a qualitative understanding of the critical behavior of the spin-l systems, are based on the molecular field approximations. More recently, the renormalization group has been used to investigate the spin-l system in two dimensions[3]. As in all studies associated with the renormalization group, the result is also not exact, and the degree of accuracy is not known in the critical region of interest. Therefore, it is of interest to report the exact determination of the phase diagram for a special spin-l system, which appears to have hitherto escaped attention.

We consider a spin-l system described by the Hamiltonian

$$\mathcal{H}=H\sum_i s_i+\Delta\sum_i s_i^2-J\sum_{<ij>}s_i^2 s_j^2 \tag{1}$$

where $s_i=0,\pm 1$ denotes the spin variable at the site i, H the external magnetic field, and -J the strength of a biquadratic interaction between all nearest neighbors $\langle ij\rangle$. This Hamiltonian differs from that considered in Refs. 2 and 3 in the absence of the bilinear interactions $-J'\sum_{<ij>}s_i s_j$. The Hamiltonian (1) is therefore a special case of the most general spin-l system.

Griffiths[4] has pointed out that when $H=O$ and $J>O$ the spin-l model (1) is equivalent to a spin-l/2 Ising model and, consequently, exhibits a first-order transition. We shall here consider more generally $H\#O$ and determine the phase diagram in the (H, Δ, T) space for both $J>0$ and $J<O$.

The partition function to consider is

$$Z=\sum_{\{s_i=0,\pm 1\}} e^{-\beta\mathcal{H}} \tag{2}$$

---

* Work supported in part by the National Science Foundation Grant No. DMR76-20643.

(1) M. Blume, Phys. Rev. **141, 517** (1966). See also earlier works by H. W. Capel, Physica 32, 966 (1966); 33, 295 (1967); 37, 423 (1967); M. Blume and R.E. Watson, J. App. Phys. 38, 991 (1967).
(2) M. Blume, V. J. Emery and R.B. Griffiths, Phys. Rev. ***A4, 1071*** (1971).
(3) A. N. Berker and M. Wortis, Phys. Rev. B14, 4946 (1976).
(4) R. B. Griffiths, Physica 33, 690 (1967).

where $\beta=1/kT$. Following Griffiths[4], we write

$$\sigma_i=2s_i^2-1\,, \tag{3}$$

and further use the identity

$$\sum_{s=0,\pm1} e^{-\beta Hs} f(s^2)=\sum_{\sigma=\pm1}(2\cosh\beta H)^{1/2(\sigma+1)} f\left(\frac{\sigma+1}{2}\right) \tag{4}$$

which is readily established by identifying the terms $s=\pm1(0)$ on the LHS as $\sigma=1(-1)$ on the RHS. The partition function (2) is then transformed into that of a spin-1/2 Ising model with a nonzero magnetic field. More precisely, let the lettice be of N sites and coordination number z. We find

$$Z=e^{-N\beta F_0}Z_{1/2}(L,K) \tag{5}$$

where

$$Z_{1/2}(L,K)=\sum_{\{\sigma_i=\pm1\}}\exp(L\sum_i\sigma_i+K\sum_{<ij>}\sigma_i\sigma_j) \tag{6}$$

is the partition function of a spin-l/2 Ising model defined by (6). In (5) and (6) we have

$$\begin{aligned} F_0&=-\frac{1}{2}\left[\frac{1}{\beta}\ln(2\cosh\beta H)-\Delta+\frac{1}{4}zJ\right]\\ L&=\frac{1}{2}\left[\ln(2\cosh\beta H)-\beta\Delta+\frac{1}{2}z\beta J\right]\\ K&=\frac{1}{4}\beta J\,. \end{aligned} \tag{7}$$

The free energy per spin, $F\equiv-kT\lim_{N\to\infty}N^{-1}\ln Z$, of the spin-1 model is now related to that of the spin-l/2 model, $F_{1/2}$, through

$$F(T,H,\Delta,J)F_0+F_{1/2}(L,K) \tag{8}$$

A phase transition occurs in the spin-l system when F becomes nonanalytic in T. The locus of the nonanalytic points is then the phase boundaries in the (H,Δ,T) space, which separate regions characterized by different kinds of long-range orderings. This yields the phase diagram for the spin-l system.

Since the functions F_0, L and K are analytic in T, the nonanalyticity of F, if any, coincides with that of $F_{1/2}$ in L and K. While the spin-l/2 Ising model in a nonzero magnetic field has not been solved exactly, the analytic properties of $F_{1/2}$ are well-known, and this is sufficient for our purposes. We first summarize the known properties of $F_{1/2}$.

The phase diagram of the spin-1/2 Ising model is shown in Fig. 1. For $K>0$ which corresponds to a ferromagnetic spin-l/2 model; $F_{1/2}$ is nonanalytic at the phase boundary

$$L=0,\qquad K_0^{-1}>K^{-1}>0 \tag{9}$$

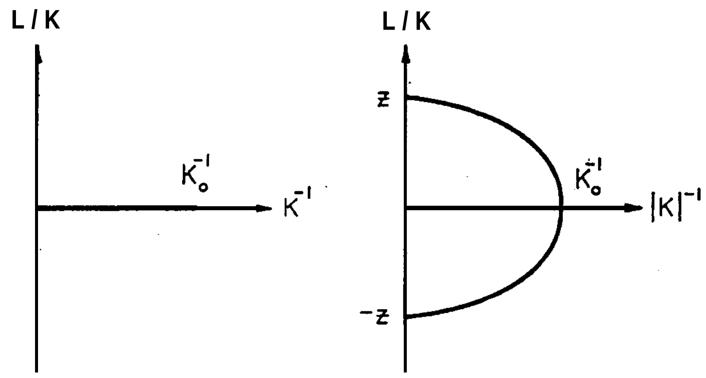
where K_0 is a positive constant depending only the geometry of the lattice. Specifically we have for the following regular lattices[5]

$K_0=\frac{1}{2}\ln(\sqrt{2}+1)$	square	$(z=4)$
$=\frac{1}{2}\ln(\sqrt{2}+3)$	honeycomb	$(z=3)$
$=\frac{1}{4}\ln 3$	triangular	$(z=6)$
$=0.2217$	simple cubic	$(z=6)$
$=0.1575$	bcc	$(z=8)$
$=0.1021$	fcc	$(z=12)$

(5) See, e.g., M. E. Fisher, Rep. Progr. Phys. 30, 615 (1967).

The derivative $\partial F_{1/2}/\partial L$ is discontinuous across the boundary (9)[6].

For $K<O$ which corresponds to an antiferromagnetic spin-l/2 model, the exact situation is not so clear. However, in the case of bipartite lattices at least, it is known that $F_{1/2}(0,K)$ is nonanalytic in K at $K=-K_0$. Furthermore, the phase boundary is expected to extend to the region $L\neq 0$ as shown schematically in Fig. 1[7]. The current belief is that a second-order transition occurs along this phase boundary. The phase boundary is expected to reach $K^{-1}=0$ (zero temperature in the spin-1/2 model) at some point $|L/K|=c=\text{constant}$ when the magnetic field is just enough to overcome the antiferromagnetic ordering. It can be argued from a simple energetic consideration that for bipartite lattices, $c=z$, the coordination number.



(a) K > 0 (b) K < 0

Fig. 1. Phase diagram for the spin-% Ising model.
(a) Ferromagnetic.
(b) Antiferromagnetic (schematic, bipartite lattices).

The transformation (7) now maps the phase boundaries of Fig. 1 into the phase boundaries for the spin-l model. These are the critical surfaces in the (T, H, A) space. We consider the cases $J>0$ and $J<0$ separately.

For $J>0$ the critical line (9) yields the *exact* critical surface

$$2\cosh\beta H=e^{\beta(\Delta-1/2zJ)},\quad 0<T<T_0 \tag{10}$$

which is shown in Fig. 2(a). We note the following intercepts:

$$T=O:\quad |H|=\Delta-\frac{1}{2}zJ, \tag{11}$$

$$H-O:\quad \Delta=\frac{1}{2}zJ+kT\ \mathrm{In}\ 2,\qquad T_0>T>0 \tag{12}$$

Eq. (10) now gives rise to a critical surface of first-order transition across which the transition is accompanied with a nonzero latent heat. This corresponds to the discontinuity in $\partial F_{1/2}/\partial L$. The critical surface terminates at a line of critical end points, the heavy line in Fig. 2(a), at $T=T_0(\equiv J/kK_0)$ beyond which there is no distinction of the different phases.

For large A the system exhibits a long-range order with a thermal average $\langle s^2\rangle>1/2$ induced by the crystal field A. This ordering disappears in the region below the critical surface. The projection of the critical surface on the $T=O$ plane is shown in Fig. 2(b) where the cross-hatched area denotes the region in the (A, H) plane in which a phase transition is possible.

For $J<0$ the critical surface cannot be located precisely. However, by assuming a reasoable

(6) C. N. Yang, Phys. Rev. 85, 808 (1952).

(7) See, e.g., C. Domb, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London 1974). Vol. 3, p. 372.

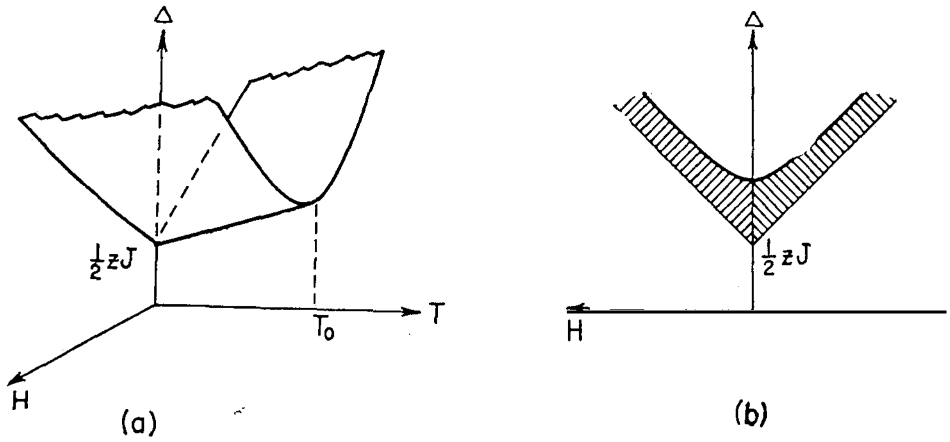


Fig. 2. Phase diagram for the ferromagnetic spin-l Ising model.
(a) Phase diagram.
(b) Region in the (A, H) plane in which a transition is possible.

behavior of the critical line in Fig. l(b), we may obtain the critical surface for the spin-l model on a schematic basis. This is done in Fig. 3(a). First, the exact points $K^{-1}=0$ and $LK=\pm z$ map into the exact intercepts

$$|H|=\Delta, \qquad T=0$$
$$|H|=\Delta+z|J|, \qquad T=0 \tag{13}$$

Furthermore, the exact critical point $L=0, K=-K_0$ maps into the exact critical line

$$2\cosh\beta_0 H=e^{\beta_0(\Delta+1/2\, z|J|)} \tag{14}$$

where $\beta_0=1/kT_0$. These lines are shown in Fig. 3. Assuming a reasonable behavior of the phase boundaries, we then expect the critical surface to be of the general shape as shown. While its equation is not known, the intercepts with $T=0$ and $T=T_0$ are exact. Within the two U-shaped regions enclosed by the ' critical surface, there is a long-range order accompanied with a sublattice ordering. The transition across the phase boundary is expected to be of second order. The cross-hatched area in Fig. 3(b) denotes the projection of the critical surface on the plane $T=0$, and is the region in the (A, H) plane in which a transition is possible.

Finally, we remark that the phase diagram for the antiferromagnetic model on nonbipartite, such as the triangular and Kagomé, lattices can also be constructed in a similar fasion. Since no new feature emerges from these considerations, we shall omit showing these phase diagrams. They are similar to that shown in Fig. 3(a) with more complicated structures.

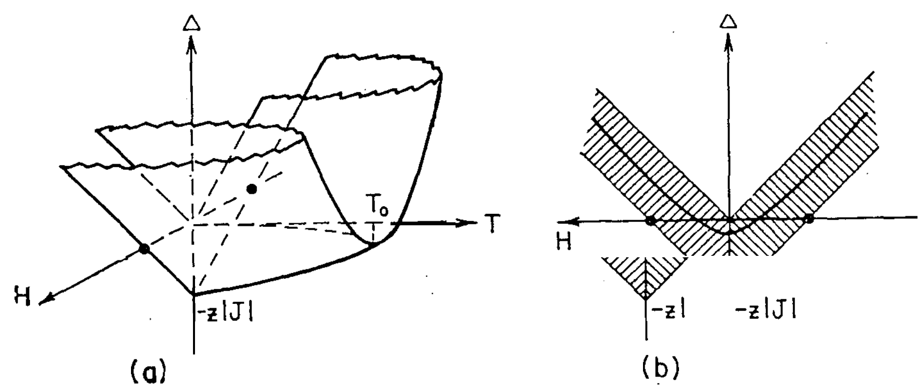


Fig. 3. Phase diagram for the antiferromagnetic spin-l Ising model on bipartite lattices.
(a) Phase diagram (schematic).
(b) Region *in* the (A, H) plane in which a transition is possible.