Phase Diagram of a Spin-One Ising System

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Phase diagram is determined for the spin-1 Ising system described by the Hamiltonian

\[ H = H \sum_i s_i + J \sum_{\langle i,j \rangle} s_i s_j \]

where \( s_i = \pm 1 \) 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 \( \langle i, j \rangle \). This Hamiltonian differs from that considered in Refs. 2 and 3 in the absence of the bilinear interactions \( -J s_i s_j \). The Hamiltonian (1) is therefore a special case of the most general spin-1 system.

Griffiths\(^\text{a}\) has pointed out that when \( H = 0 \) and \( J > 0 \) the spin-1 model (1) is equivalent to a spin-1/2 Ising model and, consequently, exhibits a first-order transition. We shall here consider more generally \( H \neq 0 \) and determine the phase diagram in the \((H, J, T)\) space for both \( J > 0 \) and \( J < 0 \).

The partition function to consider is

\[ Z = \sum_{\{s_i = \pm 1\}} e^{-\beta H} \]

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where $\beta=1/kT$. Following Griffiths\(^\text{(6)}\), we write
\[ \sigma_i=2z_j-1, \quad (3) \]
and further use the identity
\[ \sum_{\sigma_i=\pm 1} e^{J\sigma_iH} = \sum_{\sigma_i=\pm 1} (2 \cosh \beta H)^{z_j(z_j+1)} f\left(\frac{\sigma_z+1}{2}\right) \quad (4) \]
which is readily established by identifying the terms $\sigma_\pm=1(0)$ 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 lattice be of $N$ sites and coordination number $z$. We find
\[ Z=e^{-\Delta H_0} Z_{1/2}(L, K) \quad (5) \]
where
\[ Z_{1/2}(L, K) = \sum_{\{\sigma_i=\pm 1\}} \exp(L \sum_i \sigma_i + K \sum_{<ij>} \sigma_i \sigma_j) \quad (6) \]
is the partition function of a spin-1/2 Ising model defined by (6). In (5) and (6) we have
\[ F_L = \frac{1}{2} \left[ -\frac{1}{\beta} \ln(2 \cosh \beta H) - \Delta + \frac{1}{4} zJ \right] \]
\[ L = \frac{1}{2} \left[ \ln(2 \cosh \beta H) - \Delta + \frac{1}{2} z^2 \right] \]
\[ K = \frac{1}{4} \beta J. \quad (7) \]

The free energy per spin, $F_{1/2} = -kT \ln N^{-1} \ln Z$, of the spin-1 model is now related to that of the spin-1/2 model, $F_{1/2}$, through
\[ F(T, H, \Delta, J) = F_{1/2}(L, K) \quad (8) \]

A phase transition occurs in the spin-1 system when $F$ becomes nonanalytic in $T$. The locus of the nonanalytic points is then the phase boundaries in the $(H, A, T)$ space, which separate regions characterized by different kinds of long-range orderings. This yields the phase diagram for the spin-1 system.

Since the functions $F_L$, $L$ 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-1/2 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-1/2 model; $F_{1/2}$ is nonanalytic at the phase boundary
\[ L=0, \quad K^2+K^4>0 \quad (9) \]
where $K_0$ is a positive constant depending only the geometry of the lattice. Specifically we have for the following regular lattices\(^\text{(6)}\)
\[ K_0 = \frac{1}{2} \ln(\sqrt{2}+1) \quad \text{square} (z=4) \]
\[ = \frac{1}{2} \ln(\sqrt{3}+3) \quad \text{honeycomb} (z=3) \]
\[ = \frac{1}{4} \ln 3 \quad \text{triangular} (z=6) \]
\[ = 0.2217 \quad \text{simple cubic} (z=6) \]
\[ = 0.1575 \quad \text{bcc} (z=8) \]
\[ = 0.1021 \quad \text{fcc} (z=12) \]
The derivative $\partial F_{ia}/\partial L$ is discontinuous across the boundary (9)).

For $K<0$ which corresponds to an antiferromagnetic spin-$1/2$ model, the exact situation is not so clear. However, in the case of bipartite lattices at least, it is known that $F_{ia}(0,K)$ 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. The current belief is that a second-order transition occurs along this phase boundary. The phase boundary is expected to reach $K=0$ (zero temperature in the spin-$1/2$ model) at some point $L/K=\epsilon=\text{constant}$ 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, $\epsilon=z$, the coordination number.

The transformation (7) now maps the phase boundaries of Fig. 1 into the phase boundaries for the spin-$1$ 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

$$2 \cosh \beta H = e^{H(\Delta-1/2J)}; \quad 0<T<T_i$$

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

$$T=0:\quad |H|=\Delta - \frac{1}{2} zJ,$$

$$H=0:\quad \Delta = \frac{1}{2} zJ+kT \ln 2; \quad T_i > T > 0$$

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 $\partial F_{ia}/\partial L$. The critical surface terminates at a line of critical end points, the heavy line in Fig. 2(a), at $T=T_{i}(\Delta = J/K_0)$ beyond which there is no distinction of the different phases.

For large $A$ the system exhibits a long-range order with a thermal average $\langle \phi \rangle$ induced by the crystal field $A$. This ordering disappears in the region below the critical surface. The projection of the critical surface on the $(A, H)$ 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 reasonable

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behavior of the critical line in Fig. 1(b), we may obtain the critical surface for the spin-1 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

\[
|H| = \Delta, \quad T = O \\
|H| = \Delta + z |J|, \quad T = O
\]

Furthermore, the exact critical point \( L=0, K=-K_c \) maps into the exact critical line

\[
2 \cosh \beta sH = \beta (\Delta^{1/2} z |J|)
\]

where \( \beta_s = 1/kT_s \). 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 \( T=T_s \) 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 fashion. 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.