G25.2651: Statistical Mechanics

Notes for Lecture 26

I. MEAN FIELD THEORY CALCULATION OF MAGNETIC EXPONENTS

The calculation of critical exponents is nontrivial, even for simple models such as the Ising model. Here, we will introduce an approximate technique known as *mean field theory.* The approximation that is made in the mean field theory (MFT) is that fluctuations can be neglected. Clearly, this is a severe approximation, the consequences of which we will see in the final results.

Consider the Hamiltonian for the Ising model:

$$H = \frac{1}{2}\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j + h\sum_i \sigma_i$$

The partition function is given by

$$\Delta(N,h,T) = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} e^{\beta\left[\frac{1}{2}\sum_{\langle i,j\rangle}\sigma_i\sigma_j + h\sum_i\sigma_i\right]}$$

Notice that we have written the partition function as an isothermal-isomagnetic partition function in analogy with the isothermal-isobaric ensemble. (Most books use the notation Q for the partition function and A for the free energy, which is misleading). This sum is nontrivial to carry out.

In the MFT approximation, one introduces the magnetization

$$m = \frac{1}{N}\langle\sum_{i=1}^N \sigma_i\rangle$$

explicitly into the partition function by using the identity

$$\begin{aligned}\sigma_i\sigma_j &= (\sigma_i - m + m)(\sigma_j - m + m)\\ &= m^2 + m(\sigma_i - m) + m(\sigma_j - m) + (\sigma_i - m)(\sigma_j - m)\end{aligned}$$

The last term is quadratic in the spins and is of the form $(\sigma_i - \langle\sigma\rangle)(\sigma_j - \langle\sigma\rangle)$, the average of which measures the spin fluctuations. Thus, this term is neglected in the MFT. If this term is dropped, then the spin-spin interaction term in the Hamiltonian becomes:

$$\begin{aligned}\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j &\approx \frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}\left[m^2 + m(\sigma_i+\sigma_j) - 2m^2\right]\\ &= \frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}\left[-m^2 + m(\sigma_i+\sigma_j)\right]\end{aligned}$$

We will restrict ourselves to isotropic magnetic systems, for which $\sum_j J_{ij}$ is independent of i (all sites are equivalent). Define $\sum_j J_{ij} \equiv \tilde{J}z$, where z is the number of nearest neighbors of each spin. This number will depend on the number of spatial dimensions. Since this dependence on spatial dimension is a trivial one, we can absorb the z factor into the coupling constant and redefine $J \equiv= \tilde{J}z$. Then,

$$\frac{1}{2}\sum_i J = \frac{1}{2}NJ$$

where N is the total number of spins. Finally,

$$\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij} m(\sigma_i + \sigma_j) = Jm\sum_i \sigma_i$$

and the Hamiltonian now takes the form

$$\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j + h\sum_i \sigma_i \longrightarrow -\frac{1}{2}NJm^2 + (Jm+h)\sum_i \sigma_i$$

and the partition function becomes

$$\begin{aligned}
\Delta(N,h,T) &= e^{-\beta NJm^2/2}\sum_{\sigma_1}\cdots\sum_{\sigma_N} e^{\beta(Jm+h)\sum_i \sigma_i} \\
&= e^{-\beta NJm^2}\left(\sum_{\sigma=\pm 1} e^{\beta(Jm+h)\sigma}\right)^N \\
&= e^{-\beta NJm^2/2}\left[2\cosh\beta(Jm+h)\right]^N
\end{aligned}$$

The free energy per spin $g(h,T) = G(N,h,T)/N$ is then given by

$$\begin{aligned}
g(h,T) &= -\frac{1}{N\beta}\ln\Delta(N,h,T) \\
&= \frac{1}{2}Jm^2 - \frac{1}{\beta}\ln\left[2\cosh\beta(Jm+h)\right]
\end{aligned}$$

The magnetization per spin can be computed from

$$\begin{aligned}
m &= -\left(\frac{\partial g}{\partial h}\right)_h \\
&= \tanh\beta(Jm+h)
\end{aligned}$$

Allowing $h \longrightarrow 0$, one finds a transcendental equation for m

$$m = \tanh(\beta mJ)$$

which can be solved graphically as shown below:

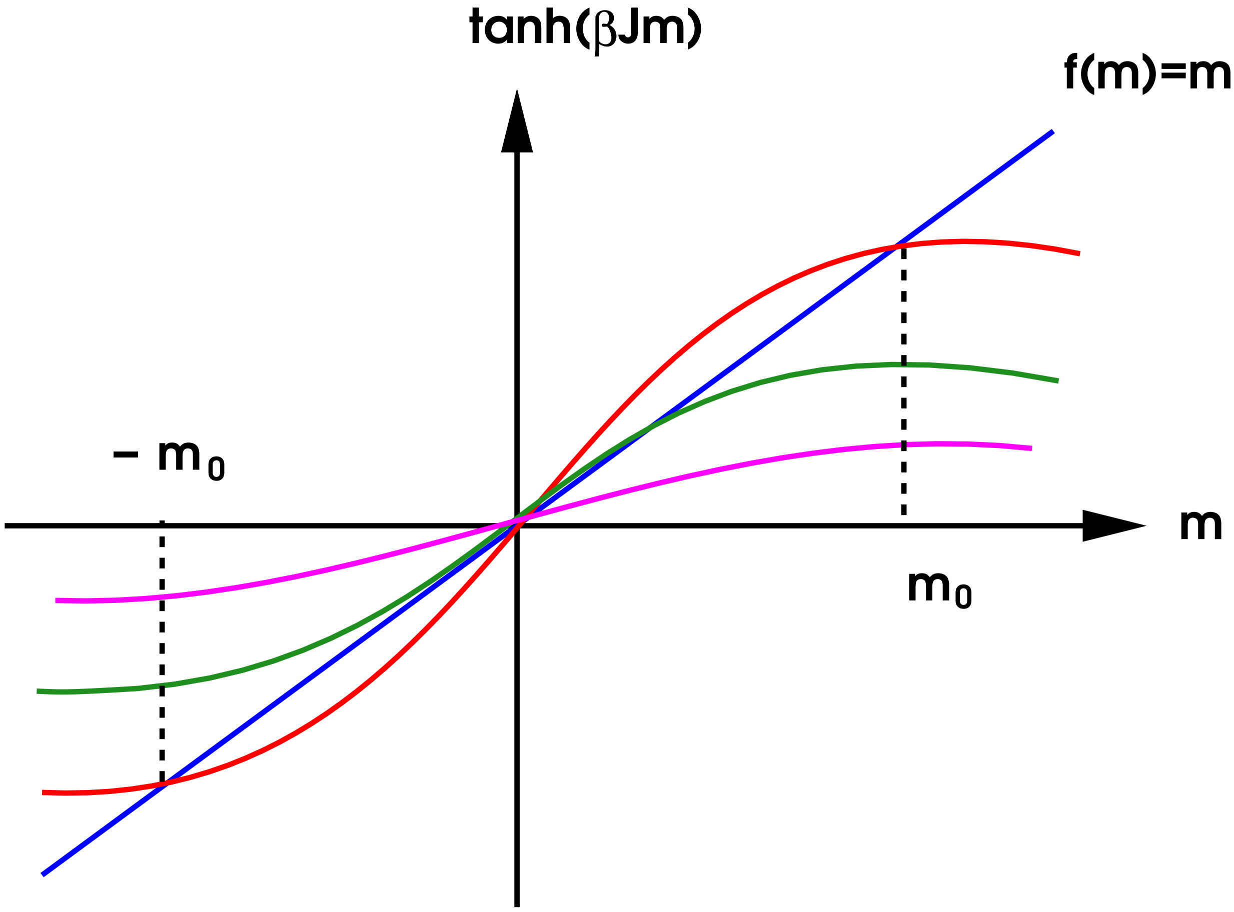

FIG. 1.

Note that for $\beta J > 1$, there are three solutions. One is at $m = 0$ and the other two are at finite values of m, which we will call $\pm m_0$. For $\beta J < 1$, there is only one solution at $m = 0$. Thus, for $\beta J > 1$, MFT predicts a nonzero magnetization at $h = 0$. The three solutions coalesce onto a single solution at $\beta J = 1$. The condition $\beta J = 1$ thus defines a critical temperature below which ($\beta J > 1$) there is a finite magnetization at $h = 0$. The condition $\beta J = 1$ defines the critical temperature, which leads to

$$kT_c = J$$

To see the physical meaning of the various cases, consider expanding the free energy about $m = 0$ at zero-field. The expansion gives

$$g(0, m) = \text{const} + J(1 - \beta J)m^2 + cm^4$$

where c is a (possibly temperature dependent) constant with $c > 0$. For $\beta J > 1$, the sign of the quadratic term is negative and the free energy as a function of m looks like:

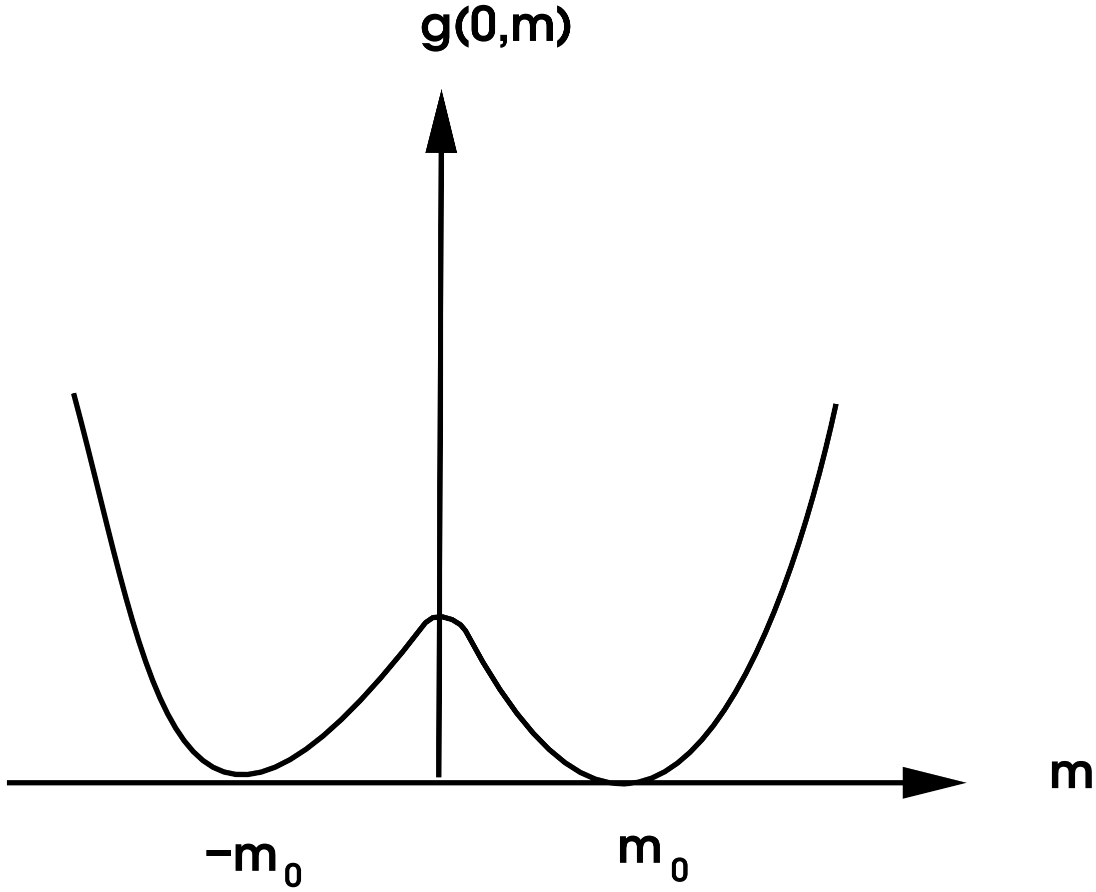

FIG. 2.

Thus, there are two stable minima at $\pm m_0$, corresponding to the two possible states of magnetization. Since a large portion of the spins will be aligned below the critical temperature, the magnetic phase is called an *ordered phase*. For $\beta J > 1$, the sign of the quadratic term is positive and the free energy plot looks like:

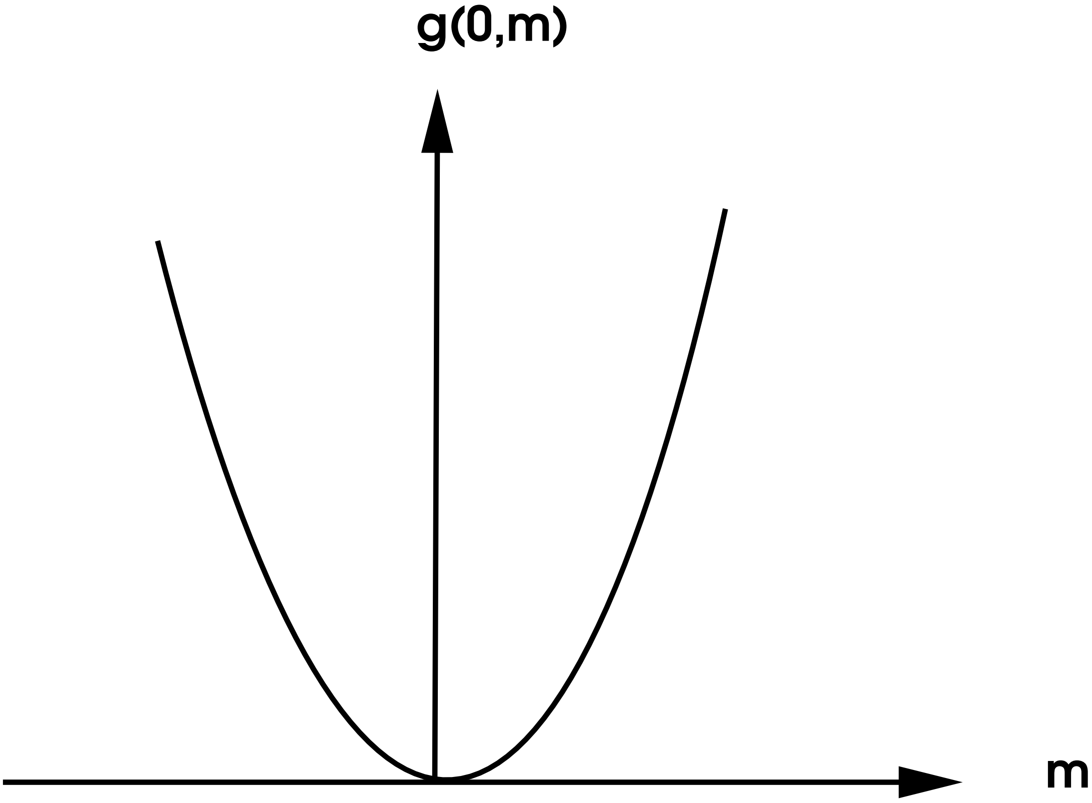

FIG. 3.

i.e., a single minimum function at $m = 0$, indicating no net magnetization above the critical temperature at $h = 0$.

The exponent β can be obtained directly from this expression for the free energy. For $T < T_c$, the value of the magnetization is given by

$$\left.\frac{\partial g}{\partial m}\right|_{m=m_0} = 0$$

which gives

$$\frac{2J}{T}(T - T_c)m_0 + 4cm_0^3 = 0$$
$$m_0 \sim (T_c - T)^{1/2}$$

Thus, $\beta = 1/2$.

From the equation for the magnetization at nonzero field, the exponent δ is obtained as follows:

$$\begin{aligned} m &= \tanh\beta(Jm + h) \\ \beta(Jm + h) &= \tanh^{-1}m \\ h &\approx kT\left[m + \frac{m^3}{3} + \cdots\right] - Jm \\ &= mk(T - T_c) + \frac{kT}{3}m^3 \end{aligned}$$

where the second line is obtained by expanding the inverse hyperbolic tangent about $m = 0$. At the critical temperature, this becomes

$$h \sim m^3$$

so that $\delta = 3$.

For the exponent α, we need to compute the heat capacity at zero-field, which is either C_h or C_m. In either case, we have, for $T > T_c$, where $m = 0$,

$$G = -NkT \ln 2$$

so

$$C_h = -T \left(\frac{\partial^2 G}{\partial T^2} \right) = 0$$

from which is it clear that $\alpha = 0$. For $T < T_c$, C_h approaches a different value as $T \to T_c$, however, the dependence on $|T - T_c|$ is the same, so that $\alpha = 0$ is still obtained.

Finally, the susceptibility, which is given by

$$\chi = \frac{\partial m}{\partial h} = \frac{1}{\partial h / \partial m}$$

but, near $m = 0$,

$$h = mk(T - T_c) + \frac{kT}{3} m^3$$
$$\frac{\partial h}{\partial m} = k(T - T_c) + kTm^2$$

As the critical temperature is approached, $m \to 0$ and

$$\chi \sim |T - T_c|^{-1}$$

which implies $\gamma = 1$.

The MFT exponents for the Ising model are, therefore

$$\alpha = 0 \qquad \beta = 1/2 \qquad \gamma = 1 \qquad \delta = 3$$

which are exactly the same exponents that the Van der Waals theory predict for the fluid system. The fact that two (or more) dissimilar systems have the same set of critical exponents (at least at the MFT level) is a consequence of a more general phenomenon known as *universality*, which was alluded to in the previous lecture.

Systems belonging to the same *universality class* will exhibit the same behavior about their critical points, as manifested by their having the same set of critical exponents.

A universality class is characterized by two parameters:

1. The spatial dimension d.
2. The dimension, n, of the *order parameter*.

An *order parameter* is defined as follows:

> Suppose the Hamiltonian H_0 of a system is invariant under all the transformations of a group $\mathcal{G}$. If two phases can be distinguished by the appearance of a thermodynamic average $\langle \phi \rangle$, which is not invariant under $\mathcal{G}$, then $\langle \phi \rangle$ is an *order parameter* for the system.

The Ising system, for which H_0 is given by

$$H_0 = -\frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j$$

is invariant under the group Z_2, which is the group that contains only two elements, an identity element and a spin reflection transformation: $Z_2 = 1, -1$. Thus, under Z_2, the spins transform as

$$\sigma_i \to \sigma_i \qquad\qquad \sigma_i \to -\sigma_i$$

From the form of H_0 is can be seen that $H_0 \to H_0$ under both transformations of Z_2, so that it is invariant under Z_2. However, the magnetization

$$m = \frac{1}{N} \langle \sum_i = 1^N \sigma_i \rangle$$

is not invariant under a spin reflection for $T < T_c$, when the system is magnetized. In a completely ordered state, with all spins aligned, under a spin reflection $m \rightarrow -m$. Thus, m is an order parameter for the Ising model, and, since it is a scalar quantity, its dimension is 1.

Thus, the Ising model defines a universality class known as the *Ising universality class*, characterized by $d = 3$, $n = 1$ in three dimensions. Note that the fluid system, which has the same MFT critical exponents as the Ising system, belongs to the same universality class. The order parameter for this system, by the analogy table defined in the last lecture, is the volume difference between the gas an liquid phases, $V_{\mathrm{L}} - V_{\mathrm{G}}$, or equivalently, the density difference, $\rho_{\mathrm{L}} - \rho_{\mathrm{G}}$. Although the solid phase is the truly ordered phase, while the gas phase is disordered, the liquid phase is somewhere in between, i.e., it is a *partially* ordered phase. The Hamiltonian of a fluid is invariant under rotations of the coordinate system. Ordered and partially ordered phases break this symmetry. Note also that a true magnetic system, in which the spins can point in any spatial direction, need an order parameter that is the vector generalization of the magnetization:

$$\mathbf{m} = \frac{1}{N}\langle \sum_{i=1}^{N} \sigma_i \rangle$$

Since the dimension of the vector magnetization is 3, the true magnetic system belongs to the $d = 3$, $n = 3$ universality class.

II. EXACT SOLUTIONS OF THE ISING MODEL IN 1 AND 2 DIMENSIONS

Exact solutions of the Ising model are possible in 1 and 2 dimensions and can be used to calculate the exact critical exponents for the two corresponding universality classes.

In one dimension, the Ising Hamiltonian becomes:

$$H = -\sum_{i=1}^{N} J_{i,i+1}\sigma_i\sigma_{i+1} - h\sum_{i=1}^{N}\sigma_i$$

which corresponds to N spins on a line. We will impose periodic boundary conditions on the spins so that $\sigma_{N+1} = \sigma_1$. Thus, the topology of the spin space is that of a circle. Finally, let all sites be equivalent, so that $J_{i,i+1} \equiv J$. Then,

$$H = -J\sum_{i=1}^{N} \sigma_i\sigma_{i+1} - h\sum_{i=1}^{N}\sigma_i$$

The partition function is then

$$\Delta(N, h, T) = \sum_{\sigma_1} \cdots \sum_{\sigma_N} e^{\beta\left[J\sum_i \sigma_i\sigma_{i+1} + \frac{1}{2}h\sum_{i=1}^{N}(\sigma_i + \sigma_{i+1})\right]}$$

In order to carry out the spin sum, let us define a matrix P with matrix elements:

$$\begin{aligned}
\langle\sigma|\mathrm{P}|\sigma'\rangle &= e^{\beta[J\sigma\sigma' + h(\sigma+\sigma')/2]} \\
\langle 1|\mathrm{P}|1\rangle &= e^{\beta(J+h)} \\
\langle -1|\mathrm{P}|-1\rangle &= e^{\beta(J-h)} \\
\langle 1|\mathrm{P}|-1\rangle &= \langle -1|\mathrm{P}|1\rangle = e^{-\beta J}
\end{aligned}$$

Thus, the matrix P becomes is a 2×2 matrix given by

$$\mathrm{P} = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}$$

so that the partition function becomes

$$\begin{aligned}
\Delta(N, h, T) &= \sum_{\sigma_1} \cdots \sum_{\sigma_N} \langle\sigma_1|\mathrm{P}|\sigma_2\rangle\langle\sigma_2|\mathrm{P}|\sigma_3\rangle \cdots \langle\sigma_{N-1}|\mathrm{P}|\sigma_N\rangle\langle\sigma_N|\mathrm{P}|\sigma_1\rangle \\
&= \sum_{\sigma_1} \langle\sigma_1|\mathrm{P}^N|\sigma_1\rangle \\
&= \mathrm{Tr}\left(\mathrm{P}^N\right)
\end{aligned}$$

A simple way to carry out the trace is diagonalize the matrix, P. From

$$\det(\mathrm{P} - \lambda \mathrm{I}) = 0$$

the eigenvalues can be seen to be

$$\lambda = e^{\beta J}\left[\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right] \equiv \lambda_{\pm}$$

where λ_+ corresponds to the choice of + in the eigenvalue expression, etc.
The trace of the P^N is then

$$\mathrm{Tr}\left(\mathrm{P}^N\right) = \lambda_+^N + \lambda_-^N$$

We will be interested in the thermodynamic limit. Note that $\lambda_+ > \lambda_-$ for any h, so that as $N \to \infty$, λ_+^N dominates over λ_-^N. Thus, in this limit, the partition function has the single term:

$$\Delta(N, h, T) \longrightarrow \lambda_+^N$$

Thus, the free energy per spin becomes

$$\begin{aligned} g(h, T) &= -kT \ln \lambda_+ \\ &= -J - kT \ln\left[\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right] \end{aligned}$$

and the magnetization becomes

$$\begin{aligned} m &= \left(\frac{\partial g}{\partial h}\right) \\ &= -\frac{\partial}{\partial(\beta h)} \ln \lambda^+ \\ &= \frac{\sinh(\beta h) + \frac{\sinh(\beta h)\cosh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}}{\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}} \end{aligned}$$

which, as $h \to 0$, since $\cosh(\beta h) \to 1$ and $\sinh(\beta h) \to 0$, itself vanishes. Thus, there is no magnetization at any finite temperature in one dimension, hence no nontrivial critical point.

While the one-dimensional Ising model is a relatively simple problem to solve, the two-dimensional Ising model is *highly* nontrivial. It was only the pure mathematical genius of Lars Onsager that was able to find an analytical solution to the two-dimensional Ising model. This, then, gives an exact set of critical exponents for the $d = 2$, $n = 1$ universality class. To date, the three-dimensional Ising model remains unsolved.

Here, the Onsager solution will be outlined only and the results stated. Consider a two-dimension spin-lattice as shown below:

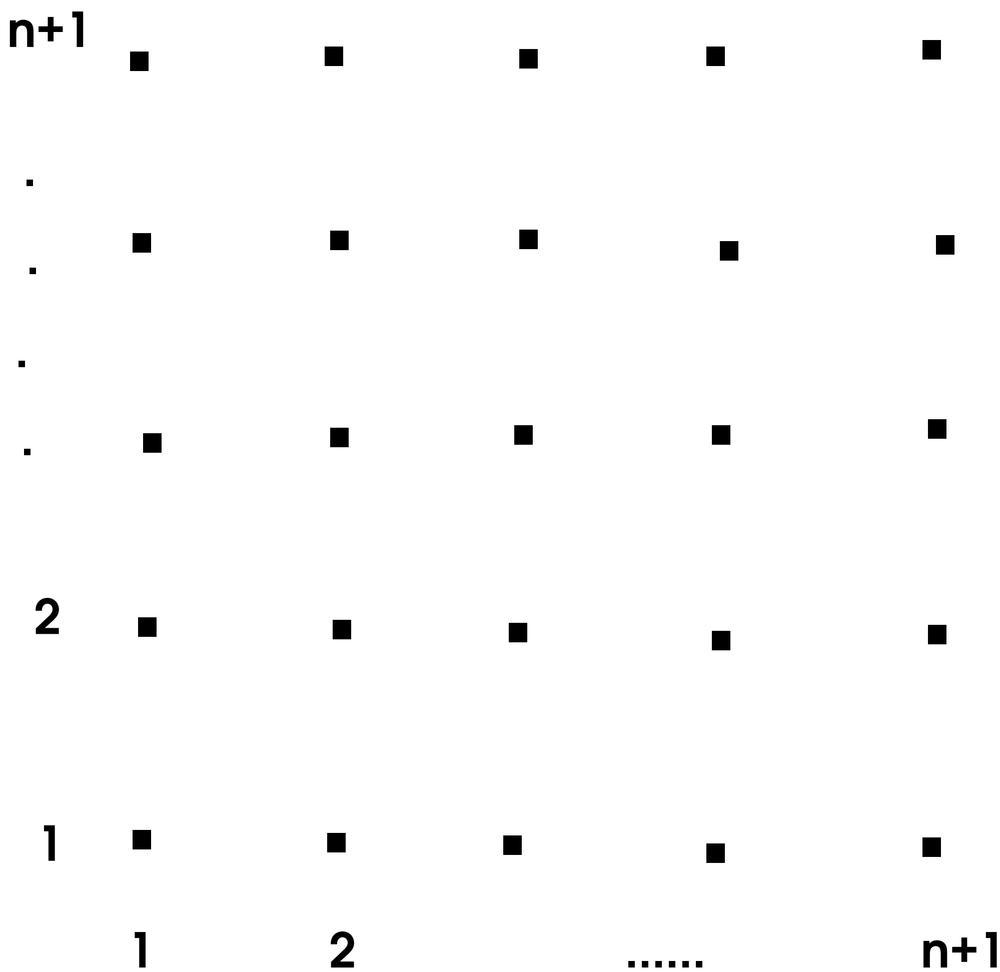

FIG. 4.

The Hamiltonian can be written as

$$H = -J\sum_{i,j}(\sigma_{i,j}\sigma_{i+1,j} + \sigma_{i,j+1}\sigma_{i,j}) - h\sum_{i,j}\sigma_{i,j}$$

where the spins are now indexed by two indices corresponding to a point on the 2-dimensional lattice. Introduce a shorthand notation for H:

$$H = \sum_{j=1}^{n}[E(\mu_j, \mu_{j+1}) + E(\mu_j)]$$

where

$$E(\mu_j, \mu_k) \equiv -\sum_{i=1}^{n}\sigma_{ij}\sigma_{ik}$$
$$E(\mu_j) \equiv -J\sum_{i=1}^{n}\sigma_{ij}\sigma_{i+1,j} - h\sum_{i,j}\sigma_j$$

and μ_j is defined to be a set of spins in a particular column:

$$\mu_j \equiv \{\sigma_{1j}, ..., \sigma_{nj}\}$$

Then, define a transfer matrix P, with matrix elements:

$$\langle \mu_j | \mathrm{P} | \mu_k \rangle = e^{-\beta[E(\mu_j,\mu_k)+E(\mu_j)]}$$

which is a $2^n \times 2^n$ matrix. The partition function will be given by

$$\Delta = \mathrm{Tr}\left(\mathrm{P}^n\right)$$

and, like, in the one-dimensional case, the largest eigenvalue of P is sought. This is the nontrivial problem that is worked out in 20 pages in Huang's book.

In the thermodynamic limit, the final result at zero field is:

$$g(T) = -kT \ln\left[2\cosh(2\beta J)\right] - \frac{kT}{2\pi}\int_0^\pi d\phi \ln\frac{1}{2}\left(1+\sqrt{1-K^2\sin^2\phi}\right)$$

where

$$K = \frac{2}{\cosh(2\beta J)\coth(2\beta J)}$$

The energy per spin is

$$\varepsilon(T) = -2J\tanh(2\beta J) + \frac{K}{2\pi}\frac{dK}{d\beta}\int_0^\pi d\phi \frac{\sin^2\phi}{\Delta(1+\Delta)}$$

where

$$\Delta = \sqrt{1-K^2\sin^2\phi}$$

The magnetization, then, becomes

$$m = \left\{1-\left[\sinh(2\beta J)\right]^{-4}\right\}^{1/8}$$

for $T < T_c$ and 0 for $T > T_c$, indicating the presence of an order-disorder phase transition at zero field. The condition for determining the critical temperature at which this phase transition occurs turns out to be

$$2\tanh^2(2\beta J) = 1$$
$$kT_c \approx 2.269185J$$

Near $T = T_c$, the heat capacity per spin is given by

$$\frac{C(t)}{k} = \frac{2}{\pi}\left(\frac{2J}{kT_c}\right)^2\left[-\ln\left(1-\frac{T}{T_c}\right)+\ln\left(\frac{kT_c}{2J}\right)-\left(1+\frac{\pi}{4}\right)\right]$$

Thus, the heat capacity can be seen to diverge logarithmically as $T \to T_c$.

The critical exponents computed from the Onsager solution are

$$\alpha = 0 \quad \text{(log divergence)}$$
$$\beta = \frac{1}{8}$$
$$\gamma = \frac{7}{4}$$
$$\delta = 15$$

which are a set of exact exponents for the $d = 2$, $n = 1$ universality class.