

Ising Model Partition Functions

$$\mathcal{H} = -\frac{J}{2} \sum_n \sum_{n'}' \sigma_n \sigma_{n'}$$

↖ nearest neighbors

In 1-D: (no field, no periodic boundaries)

$$\mathcal{H} = -\frac{J}{2} (\underbrace{\sigma_1 \sigma_2 + \sigma_2 \sigma_1}_{\text{}} + \underbrace{\sigma_2 \sigma_3 + \sigma_3 \sigma_2}_{\text{}}) + \dots$$

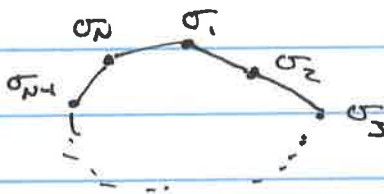
We can recombine these terms together

$$\mathcal{H} = -J \sum_{n=1}^{N-1} \sigma_n \sigma_{n+1}$$

↖ written so each spin only couples to the next one in line

With Periodic Boundaries:

(edge effects are gone because $\sigma_{N+1} = \sigma_1$)



$$\mathcal{H} = -J \sum_{n=1}^N \sigma_n \sigma_{n+1}$$

↖ one more term

We can define a bond variable $b_i = \sigma_i \sigma_{i+1}$

σ_i	σ_{i+1}	b_i
+1	+1	+1
+1	-1	-1
-1	+1	-1
-1	-1	+1

we'll need an additional factor of 2 for each lattice to account for degenerate states!

For N spins, we need N-1 bond variables (and a factor of 2) to visit all states

$$Q_N = \sum_{\{\sigma_i = \pm 1\}} e^{\beta J \sum_i \sigma_i \sigma_{i+1}} = 2 \sum_{\{b_i = \pm 1\}} e^{\beta J \sum_i b_i}$$

$$Q_N = 2 \sum_{\{b_i = \pm 1\}} e^{\beta J b_1} e^{\beta J b_2} e^{\beta J b_3} \dots e^{\beta J b_{N-1}}$$

$$= 2 \left(\sum_{b_1 = \pm 1} e^{\beta J b_1} \right) \left(\sum_{b_2 = \pm 1} e^{\beta J b_2} \right) \dots \left(\sum_{b_{N-1}} e^{\beta J b_{N-1}} \right)$$

$$= 2 (e^{\beta J} + e^{-\beta J}) (e^{\beta J} + e^{-\beta J}) \dots (e^{\beta J} + e^{-\beta J})$$

$$Q_N = 2 (2 \cosh \beta J)^{N-1}$$

Next, without periodic boundaries on dual-lattice bond variables:

$$H = -J \sum_{n=1}^{N-1} \sigma_n \sigma_{n+1}$$

$$Q_N = \sum_{\{\sigma_i = \pm 1\}} e^{\beta J \sum_{n=1}^{N-1} \sigma_n \sigma_{n+1}}$$

$$= \sum_{\{\sigma_i = \pm 1\}} e^{\beta J \sigma_1 \sigma_2} e^{\beta J \sigma_2 \sigma_3} \dots e^{\beta J \sigma_{N-2} \sigma_{N-1}} e^{\beta J \sigma_{N-1} \sigma_N}$$

Let's do the last spin first ($\sigma_N = \pm 1$):

$$Q_N = \sum_{\{\sigma_i = \pm 1\}} e^{\beta J \sigma_1 \sigma_2} \dots e^{\beta J \sigma_{N-2} \sigma_{N-1}} \underbrace{(e^{\beta J \sigma_{N-1}} + e^{-\beta J \sigma_{N-1}})}_{\parallel}$$

If $\sigma_{N-1} = +1$: $(e^{\beta J} + e^{-\beta J})$
 If $\sigma_{N-1} = -1$: $(e^{-\beta J} + e^{\beta J})$
 \parallel
 $2 \cosh \beta J$

$$Q_N = 2 \cosh \beta J \sum_{\{\sigma_i = \pm 1\}} e^{\beta J \sum_{n=1}^{N-2} \sigma_n \sigma_{n+1}} = (2 \cosh \beta J) Q_{N-1}$$

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We can continue this sequence all the way down to Q_1 :

$$Q_N = (2 \cosh \beta J)^{N-1} Q_1$$

$$= (2 \cosh \beta J)^{N-1} \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} e^{\beta J \sigma_1 \sigma_2}$$

These last terms we can do explicitly:

$$Q_N = (2 \cosh \beta J)^{N-1} \left(\underbrace{e^{\beta J}}_{\substack{\sigma_1=1 \\ \sigma_2=1}} + \underbrace{e^{-\beta J}}_{\substack{\sigma_1=1 \\ \sigma_2=-1}} + \underbrace{e^{-\beta J}}_{\substack{\sigma_1=-1 \\ \sigma_2=1}} + \underbrace{e^{\beta J}}_{\substack{\sigma_1=-1 \\ \sigma_2=-1}} \right)$$

$$Q_N = (2 \cosh \beta J)^{N-1} 2(e^{\beta J} + e^{-\beta J})$$

$$Q_N = 2 \cdot (2 \cosh \beta J)^N$$

← without periodic boundaries

$$Q_N = 2 \cdot (2 \cosh \beta J)^{N-1}$$

← with periodic boundaries

Free Energies, Heat Capacities

$$A(N, V, T) = -k_B T \ln Q_N = -k_B T [\ln 2 + N \ln (2 \cosh \beta J)]$$

$$= -k T \ln 2 - N k T \ln [2 \cosh \beta J]$$

$$\langle E \rangle = +k T^2 \left(\frac{\partial \ln Q}{\partial T} \right) = - \left(\frac{\partial \ln Q}{\partial \beta} \right) = -N \frac{1}{2 \cosh \beta J} \cdot 2 \sinh \beta J \cdot J$$

$$= -N J \tanh \beta J$$

$$C_V = \frac{\partial \langle E \rangle}{\partial T} = \frac{+J^2 N}{k T^2} \left(\operatorname{sech} \frac{J}{k_B T} \right)^2 \leftarrow \text{why might this be a problem?}$$

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With a field

$$\mathcal{H} = -H \sum_{i=1}^N \sigma_i - J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} \stackrel{\text{PBC}}{=} -\frac{H}{2} \sum_{i=1}^N (\sigma_i + \sigma_{i+1}) - J \sum_{i=1}^N \sigma_i \sigma_{i+1}$$

$$Q = \sum_{\{\sigma_i = \pm 1\}} e^{\beta J \sum \sigma_i \sigma_{i+1} + \beta \frac{H}{2} \sum (\sigma_i + \sigma_{i+1})}$$

Let's define a transfer matrix \underline{P} :
it connects adjacent spins σ & σ'

$$\langle \sigma | P | \sigma' \rangle = e^{\beta J \sigma \sigma' + \beta H (\sigma + \sigma')/2}$$

$$\langle +1 | P | +1 \rangle = e^{\beta(J+H)}$$

$$\langle +1 | P | -1 \rangle = e^{-\beta J}$$

$$\langle -1 | P | +1 \rangle = e^{-\beta J}$$

$$\langle -1 | P | -1 \rangle = e^{\beta(J-H)}$$

$$\underline{P} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} \leftarrow \text{connects states of two adjacent spins}$$

$$Q = \sum_{\{\sigma_i = \pm 1\}} \langle \sigma_1 | P | \sigma_2 \rangle \langle \sigma_2 | P | \sigma_3 \rangle \dots \langle \sigma_N | P | \sigma_1 \rangle$$

$\hat{=}$ this includes all possible states:

$$\sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \dots \sum_{\sigma_N = \pm 1}$$

If we use the closure relation: $\sum_{\sigma_i = \pm 1} |\sigma_i\rangle \langle \sigma_i| = 1$

$$Q = \sum_{\sigma_1 = \pm 1} \langle \sigma_1 | \underline{P}^N | \sigma_1 \rangle = \text{Tr} [\underline{P}^N]$$

To carry out the trace, we must first diagonalize \underline{P}

A brief interlude on 2x2 matrices

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$$\underline{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

$$\underline{B} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

$$[A \cdot B]_{ij} = \sum_{k=1}^2 A_{ik} B_{kj}$$

$$\text{Tr}[\underline{A}] = A_{11} + A_{22} = \sum_{k=1}^2 A_{kk}$$

The trace is conserved for cyclic permutations

$$\text{tr}[A \cdot B \cdot C] = \text{tr}[C \cdot A \cdot B] = \text{tr}[B \cdot C \cdot A]$$

but not for acyclic permutations:

$$\text{tr}[A \cdot B \cdot C] \neq \text{tr}[B \cdot A \cdot C]$$

Diagonalization

$$\underline{M} = \underline{U}^T \cdot \underline{A} \cdot \underline{U}$$

For an arbitrary square matrix \underline{A} , there is a unitary transformation which results in a diagonal matrix \underline{M}

$$\underline{M} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \leftarrow \lambda_1 \text{ \& } \lambda_2 \text{ are the } \underline{\text{eigenvalues}} \text{ of } \underline{A}$$

\underline{U} = matrix of unit eigenvectors of \underline{A}
columns of \underline{U} are eigenvectors of \underline{A}

$$\left. \begin{aligned} \underline{A} \cdot \underline{u}_1 &= \lambda_1 \underline{u}_1 = \lambda_1 \begin{pmatrix} u_{11} \\ u_{12} \end{pmatrix} \\ \underline{A} \cdot \underline{u}_2 &= \lambda_2 \underline{u}_2 = \lambda_2 \begin{pmatrix} u_{21} \\ u_{22} \end{pmatrix} \end{aligned} \right\} \rightarrow \underline{U} = \begin{pmatrix} u_{11} & u_{21} \\ u_{12} & u_{22} \end{pmatrix}$$

⑥

The diagonalization transform is a unitary similarity transform:

$$\underline{U}^T = \underline{U}^{-1}$$

$$\underline{U}^T \cdot \underline{U} = \underline{U}^{-1} \cdot \underline{U} = \underline{I} \quad \leftarrow \text{The Identity Matrix}$$

Now, consider: $\text{Tr}[\underline{P}^N] = \sum_k [\underline{P}^N]_{kk}$
 $\hat{=}$ hard to determine

Suppose we diagonalize \underline{P} first:

$$\underline{M} = \underline{U}^T \cdot \underline{P} \cdot \underline{U}$$

$$\underline{M}^N = (\underline{U}^T \cdot \underline{P} \cdot \underline{U})(\underline{U}^T \cdot \underline{P} \cdot \underline{U})(\underline{U}^T \cdot \underline{P} \cdot \underline{U}) \dots$$

$$= \underline{U}^T \cdot \underline{P} \cdot (\underline{U} \cdot \underline{U}^T) \cdot \underline{P} \cdot (\underline{U} \cdot \underline{U}^T) \cdot \underline{P} \dots$$

$\hat{=} \underline{U}^{-1} = \underline{U}^T$

$$= \underline{U}^T \cdot \underline{P} \cdot \underline{I} \cdot \underline{P} \cdot \underline{I} \cdot \underline{P} \dots$$

$$\underline{M}^N = \underline{U}^T \cdot \underline{P}^N \cdot \underline{U}$$

So:

$$\begin{aligned} \text{Tr}[\underline{M}^N] &= \text{Tr}[\underline{U}^T \cdot \underline{P}^N \cdot \underline{U}] \\ &= \text{Tr}[\underline{U} \cdot \underline{U}^T \cdot \underline{P}^N] \end{aligned}$$

\leftarrow cyclic permutation

$$\text{Tr}[\underline{M}^N] = \text{Tr}[\underline{P}^N]$$

$$\therefore Q_N = \text{tr} \left[\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}^N \right] = \text{tr} \left[\begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} \right] = \lambda_1^N + \lambda_2^N$$

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Now, back to the Ising problem:

$$\mathcal{H} = \sum_n \left[-J \sigma_n \sigma_{n+1} - \frac{H}{2} (\sigma_n + \sigma_{n+1}) \right]$$

$$Q_N = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \langle \sigma_1 | \underbrace{e^{\beta J \sigma_1 \sigma_2 + \frac{\beta H}{2} (\sigma_1 + \sigma_2)}}_{P} | \sigma_2 \rangle \langle \sigma_2 | \cdots \rangle$$

P = transfer matrix connecting σ_1 & σ_2

$$P = \begin{pmatrix} e^{\beta J + \beta H} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta H} \end{pmatrix}$$

$$Q_N = \text{Tr}[P^N] = \text{Tr}[\underline{u}^T \cdot \underline{M}^N \cdot \underline{u}] = \text{Tr}[\underline{M}^N]$$

$$= M_{11}^N + M_{22}^N = \lambda_1^N + \lambda_2^N \leftarrow \lambda_1 \neq \lambda_2 \text{ are eigenvalues of } P$$

$$\det[P - \lambda I] = 0 \Rightarrow \begin{vmatrix} e^{\beta J + \beta H} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta H} - \lambda \end{vmatrix} = 0$$

$$(e^{\beta J + \beta H} - \lambda)(e^{\beta J - \beta H} - \lambda) - e^{-2\beta J} = 0$$

$$e^{2\beta J} - \lambda(e^{\beta J + \beta H} + e^{\beta J - \beta H}) + \lambda^2 - e^{-2\beta J} = 0$$

$$\lambda^2 - \lambda(e^{\beta J}(e^{\beta H} + e^{-\beta H})) + (e^{2\beta J} + e^{-2\beta J}) = 0$$

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$$\lambda^2 - \lambda e^{\beta J} (2 \cosh \beta H) + 2 \sinh(2\beta J)$$

$$\lambda = \frac{e^{\beta J} 2 \cosh \beta H \pm \sqrt{e^{2\beta J} 4 \cosh^2 \beta H - 8 \sinh(2\beta J)}}{2}$$

$$= e^{\beta J} \cosh \beta H \pm \sqrt{e^{2\beta J} \cosh^2 \beta H - 2 \sinh(2\beta J)}$$

$$= e^{\beta J} \cosh \beta H \pm \sqrt{e^{2\beta J} \cosh^2 \beta H - e^{2\beta J} + e^{-2\beta J}}$$

$$= e^{\beta J} \left(\cosh \beta H \pm \sqrt{\cosh^2 \beta H - 1 + e^{-4\beta J}} \right)$$

$$\lambda_{\pm} = e^{\beta J} \left(\cosh \beta H \pm \sqrt{\sinh^2 \beta H + e^{-4\beta J}} \right)$$

$$Q_N = \lambda_+^N + \lambda_-^N$$

← one will always be larger
 $1.1^N + 0.9^N$
 λ_+ will dominate
 as $N \rightarrow \infty$

$$Q_N \approx \left(e^{\beta J} \left(\cosh \beta H + \sqrt{\sinh^2 \beta H + e^{-4\beta J}} \right) \right)^N$$

$$A \approx -N k_B T \ln \left[e^{\beta J} \cosh \beta H + \left(e^{2\beta J} \sinh^2 \beta H + e^{-2\beta J} \right)^{1/2} \right]$$

$$m = \langle \sigma \rangle = -\frac{1}{N} \frac{\partial A}{\partial H} = \frac{1}{\beta \lambda_+} \frac{\partial \lambda_+}{\partial H}$$

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$$m = \frac{\sinh(\beta H)}{\sqrt{\sinh^2 \beta H + e^{-\beta J_4}}}$$

\therefore when $H \rightarrow 0$ there is no spontaneous magnetization at any temperature in 1-D.

In 2D, there is!

An experimental tie:

$$\text{magnetiz susceptibility} : \chi = \frac{\partial \langle m \rangle}{\partial H}$$

A review of what we know:

$$\mathcal{H} = -H \sum_{i=1}^N \sigma_i - \frac{J}{2} \sum_{i=1}^N \sum_{j \in NN_i} \sigma_i \sigma_j$$

↑
nearest neighbor sum

0°K states with H=0;

J > 0 → degenerate ferromagnetic states
 all up, <m> = +1
 all down, <m> = -1

J < 0 → degenerate anti-ferromagnetic states
 +-+- and -+-+
 both with <m> = 0

At any temperature in 1D, we've shown:

$$Q_N = 2(2 \cosh \beta J)^N \quad \leftarrow \text{no field}$$

$$Q_N = \left(e^{\beta J} (\cosh \beta H + \sqrt{\sinh^2 \beta H - e^{-4\beta J}}) \right)^N \quad \leftarrow \text{field}$$

we got here using a transfer matrix,
diagonalization, and the cyclic invariance of the trace

Here are some derivative tricks:

$$\langle m \rangle = \frac{1}{Q} \sum_{\{\sigma_i = \pm 1\}} \frac{1}{N} \left(\sum_{i=1}^N \sigma_i \right) e^{\beta \left(H \sum_i \sigma_i + \sum_{ij} \sigma_i \sigma_j \cdot \frac{J}{2} \right)}$$

↑
this term in exponent matches

$$\langle m \rangle = \frac{1}{N} \frac{\partial \ln Q}{\partial (\beta H)} = \frac{1}{N} \cdot \frac{1}{Q} \frac{\partial Q}{\partial (\beta H)}$$

$$= \frac{1}{N} \frac{1}{Q} \frac{\partial}{\partial (\beta H)} \sum_{\{\sigma\}} e^{\beta H \sum_i \sigma_i + \frac{\beta J}{2} \sum_{ij} \sigma_i \sigma_j}$$

↑
this derivative pulls down this term

$$= \frac{1}{Q} \sum_{\{\sigma\}} \frac{1}{N} \left(\sum_i \sigma_i \right) e^{\beta H \sum_i \sigma_i + \frac{\beta J}{2} \sum_{i,j} \sigma_i \sigma_j}$$

$$\therefore \langle m \rangle = \frac{1}{N} \frac{\partial \ln Q}{\partial (\beta H)} = \frac{k_B T}{N} \frac{\partial \ln Q}{\partial H}$$

Last time, we also showed:

$$\langle m \rangle = \frac{\sinh(\beta H)}{\sqrt{\sinh^2(\beta H) + e^{-4\beta J}}}$$

The other first derivative property of interest

$$\frac{\langle E \rangle}{N} = \frac{1}{N} - \frac{\partial \ln Q}{\partial \beta} = -J \tanh(\beta J)$$

has no discontinuities

The second derivative properties

Susceptibility

$$\chi = \frac{\partial m}{\partial H} = \frac{\beta \cosh(\beta H)}{(1 + e^{4\beta J} \sinh^2(\beta H))^{3/2}} + \text{other ugly terms}$$

$$\lim_{H \rightarrow 0} \chi = \frac{\beta}{\sqrt{e^{-4\beta J}}} \leftarrow \text{only diverges at } T=0$$

Heat Capacity

$$C_V = \frac{\partial \langle E \rangle}{\partial T} = \frac{J}{kT^2} \text{sech}^2(\beta J)$$

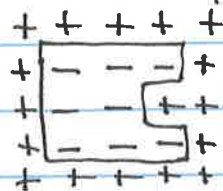
no divergences!

Conclusions: There are no phase transitions in the 1-D ising model!

Peierls Theorem

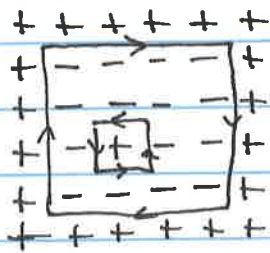
For the 2D Ising model, there exists a temperature T_c at which the probability of "+" spins \neq the probability of "-" spins
 That is, $\langle \sigma_n \rangle \neq 0$ below T_c

Consider an array of spins:



← energy = $J \times$ length of perimeter

N spins on an array, with all edge spins set to "+"



a contour passes through the midpoint of every $+ -$ bond

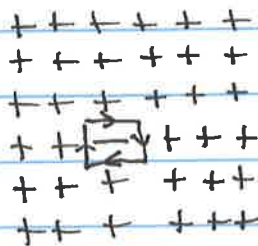
a closed contour meets itself
 ← length

$C(l, i)$
 ← index or label

Energy of a closed contour $E[C] = J l$

Direction: R.H.S. of path has "-" spins

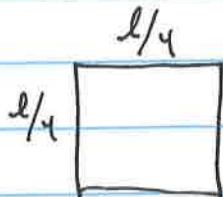
Conjugate: Reverse all spins to R.H.S. of contour



$\tilde{C}(l, i)$

$$E[\tilde{C}] = E[C] - lJ$$

The contour with the maximal number of enclosed spins for a given length is a regular polygon:



$$A = N_{\max} = \frac{l^2}{16}$$

$M(l)$ = total number of contours of length l

$M(l) \leq$ total number of contours we can draw

$$\leq N \times 4 \times 3^{l-1} \times \frac{1}{2l} \leftarrow \begin{array}{l} \text{required to} \\ \text{close loop} \end{array}$$

\uparrow places to start \uparrow choices for 1st step \uparrow choices of direction on all following steps

$X(l, i) = \begin{cases} 1 & \text{if configuration contains contour } C(l, i) \\ 0 & \text{otherwise} \end{cases}$

$$N_- \leq \sum_l \left(\frac{l^2}{16} \right) \sum_{i=1}^{M(l)} X(l, i) = \text{overestimate of } N_-$$

\uparrow # of negative spins \uparrow maximal enclosed spins \uparrow does configuration contain this contour

$$\langle X(l, i) \rangle = \frac{\sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}(\{\sigma_n\})} X(l, i)}{\sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}(\{\sigma_n\})}}$$

we can do this as a "constrained" sum over only those configurations containing $C(l, i)$

$$\langle X(l, i) \rangle = \frac{\sum_{\text{Constrained configurations}} e^{-\beta E[C(l, i)]}}{\sum_{\text{all states}} e^{-\beta \mathcal{H}}}$$

we can underestimate the denominator as the same set of constrained set of configurations without the contour

$$\langle X(l, i) \rangle \leq \frac{\sum_{\text{configs}} e^{-\beta E[C(l, i)]}}{\sum_{\text{configs}} e^{-\beta E[\tilde{C}(l, i)]}}$$

$$\langle X(l, i) \rangle \leq e^{-\beta J l} \quad \leftarrow \text{since } E[\tilde{C}] = E[C] - J l$$

So:

$$\begin{aligned} \frac{\langle N \rangle}{N} &\leq \frac{1}{N} \sum_l \left(\frac{l^2}{16}\right) \sum_{i=1}^{m(l)} \langle X(l, i) \rangle \\ &\leq \sum_{l=4}^{\infty} \left(\frac{l^2}{16}\right) 3^{l-1} e^{-J \beta l} \frac{4}{2l} \end{aligned}$$

$$\frac{\langle N \rangle}{N} \leq \frac{5}{24} \frac{e^{-4\alpha}}{1 - e^{-\alpha}} \quad \text{where } \alpha = \frac{J}{T} - \ln 3$$

$$\frac{\langle N \rangle}{N} \ll \frac{1}{2} \quad \text{as } T \rightarrow 0$$

∴ There must be a T_c below which $\frac{\langle N \rangle}{N} < \frac{1}{2}$

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2-D exact solution:

Lars Onsager Phys. Rev. 65, pp. 117-149 (1944).

$$Q(\beta, N) = [2 \cosh(\beta J e^{\pm})]^N$$

$$I = \frac{1}{2\pi} \int_0^\pi d\phi \ln \left\{ \frac{1}{2} [1 + (1 - \kappa^2 \sin^2 \phi)^{1/2}] \right\}$$

$$\kappa = \frac{2 \sinh \beta J}{\cosh^2(2\beta J)}$$

Critical Temperature: $T_c = \frac{2.269 J}{k_B}$

$$\frac{C_v}{N} \sim \frac{8 k_B}{\pi} (\beta J)^2 \ln \left| \frac{1}{T - T_c} \right| \quad \alpha = 0$$

$$m \sim \text{const} (T_c - T)^{1/8} \quad \text{when } T < T_c$$

$$\beta = 1/8$$

3D: No exact solutions yet! Numerically:

$$\frac{C_v}{N} \propto |T - T_c|^{-0.125}$$

$$m \propto (T_c - T)^{0.313} \quad T < T_c$$

$$T_c \sim \frac{4J}{k_B}$$