Statistical Mechanics—a lightning course

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Outline

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Two-dimensional Ising model

- First, we wrap the square lattice onto an $n \times m$ cylinder, labelling the spins at site i, j as $s_{i,j}$.
- We have $s_{i,n+1} = s_{i,1}$, and denote a column configuration as $\sigma_j = (s_{1,j}, s_{2,j}, \dots s_{m,j}.)$. (There are 2^m possible configurations for a column).
- We have

$$\begin{aligned} \mathcal{H}\{s\} &= -J \sum_{i=1}^{m-1} \sum_{j=1}^{n} s_{i,j} s_{1+1,j} - J \sum_{i=1}^{m} \sum_{j=1}^{n} s_{i,j} s_{1,j+1} \qquad (1) \\ & \quad -H \sum_{i=1}^{m} \sum_{j=1}^{n} s_{i,j}. \end{aligned}$$

Setting up the transfer matrix

- We now rewrite (1) as the sum of the interaction energies within a column, $V_1(\sigma_j)$, and the interaction energies between columns, $V_2(\sigma_j, \sigma_{j+1})$.
- $$V_1(\sigma_j) = -J \sum_{i=1}^{m-1} s_{i,j} s_{1+1,j} - H \sum_{i=1}^{m} s_{i,j},$$
- $$V_2(\sigma_j, \sigma_{j+1}) = -J \sum_{i=1}^{m} s_{i,j} s_{1,j+1}.$$

Transfer matrix–cont.

- Then, noting that $\sigma_{n+1} = \sigma_1$,

$$\mathcal{H}\{s\} = \mathcal{H}\{\sigma_1, \sigma_2, \ldots, \sigma_n\} = \sum_{j=1}^{n} [V_1(\sigma_j) + V_2(\sigma_j, \sigma_{j+1})].$$

- The partition function is then

$$\begin{aligned} Z_{n,m} &= \sum_{\{s\}} exp(-\beta \mathcal{H}\{s\}) \\ &= \sum_{\{\sigma_1,\sigma_2,\ldots,\sigma_n\}} exp\left[-\beta\left(\sum_{j=1}^{n}\{V_1(\sigma_j) + V_2(\sigma_j, \sigma_{j+1})\}\right)\right] \\ &= \sum_{\{\sigma_1,\sigma_2,\ldots,\sigma_n\}} L(\sigma_1, \sigma_2) L(\sigma_1, \sigma_2) \cdots L(\sigma_{n-1}, \sigma_n) L(\sigma_n, \sigma_1) \\ &= \sum_{\sigma_1} L^n(\sigma_1, \sigma_1) \end{aligned}$$

Transfer matrix—continued

- Here

$$\begin{aligned} L_{\sigma,\sigma'} &= exp[-\beta V_1(\sigma)]exp[-\beta V_2(\sigma,\sigma')] \quad (2) \\ &= exp\left(K\sum_{i=1}^{m-1} s_i s_{i+1} + B\sum_{i=1}^{m} s_i\right) exp\left(K\sum_{i=1}^{m} s_i s_i'\right) \end{aligned}$$

  with $K = \beta J$ and $B = \beta H$.
- We can also symmetrise this matrix, as we did in the 1d case. In the above equation, $L^n(\sigma_1, \sigma_1)$ denotes the (σ_1, σ_1) component of the $2^m \times 2^m$ matrix **L**, with elements (2) (symmetrised), raised to the *n*th power.
- So

$$Z_{n,m} = Tr(\mathbf{L^n}) = \sum_{\mathbf{j=1}}^{\mathbf{2^m}} \lambda_{\mathbf{j}}^{\mathbf{n}},$$

  where $\lambda_1 > \lambda_2 \geq \ldots \geq \lambda_{2^m}$ are the eigenvalues of the matrix.

Transfer matrix—continued

- The thermodynamic properties are then found from the free energy,

$$-\beta\psi = \lim_{m\to\infty}\lim_{n\to\infty}\frac{1}{mn}\log Z_{n,m} = \lim_{m\to\infty}\frac{1}{m}\log\lambda_1.$$

- By a masterly application of Lie algebras and group representations, Onsager found the largest eigenvalue (with H=0) to be

$$\lambda_1 = (2\sinh 2K)^{m/2} exp[\frac{1}{2}(\gamma_1+\gamma_3+\cdots+\gamma_{2m-1})],$$

where

$$\cosh\gamma_k = \cosh 2K \coth 2K - \cos\left(\frac{\pi k}{m}\right).$$

The free energy

- So

$$-\beta\psi = \frac{1}{2}\log(2\sinh 2K) + \lim_{m\to\infty}\frac{1}{2m}\sum_{k=0}^{m-1}\gamma_{2k+1}.$$

- In the limit, the sum becomes an integral, and we have

$$\begin{aligned} -\beta\psi &= \frac{1}{2}\log(2\sinh 2K) \\ &+ \frac{1}{2\pi}\int_0^{\pi}\cosh^{-1}(\cosh 2K \coth 2K - \cos\theta)d\theta. \end{aligned}$$

The free energy—continued

- The using the identity

$$\cosh^{-1}|z| = \frac{1}{\pi}\int_0^\pi \log[2(z-\cos\phi)]d\phi$$

allows us to rewrite this, (after symmetrisation), as

$$-\beta\psi = \log 2 + \frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \log[\cosh^2 2K - \sinh 2K(\cos\theta_1+\cos\theta_2)]d\theta_1 d\theta_2.$$

- Exercise: Calculate the internal energy

$$U = -kT^2\frac{\partial}{\partial T}\frac{\psi}{kT}$$

and hence show that it diverges logarithmically at the origin $\theta_1 = \theta_2 = 0$. Hence show that the specific heat $C_V = \frac{\partial U}{\partial T}$ has a logarithmic divergence.

The significance

- This remarkable result was the first demonstration that statistical mechanics, alone, could produce a phase transition. It is also arguably the first mathematical treatment of the collective behaviour that is studied widely under the heading of complex systems.

Ising model–a mathematician's description

- Onsager used the algebra

$$[A_m, A_n] = 4G_{m-n}$$

$$[G_m, A_n] = 2A_{n+m} - 2A_{n-m}$$

$$[G_m, G_n] = 0$$

This algebra is isomorphic to an SL_2 loop algebra with a Z_2 automorphism modded out.

Generalisations of the Ising model–Potts model

- Rewrite the Hamiltonian as

$$\mathcal{H} = -J \sum_{\{i,j\}} \delta(\sigma_i, \sigma_j) - H \sum_i \delta(\sigma_i, 1)$$

  where $\sigma_i = 1, 2, \ldots, q$. This is the q-state Potts model that Alan has been discussing.
- When $q = 2$ it reduces to the Ising model (with a trivial rescaling of the coupling J by a factor of 2, and an energy shift, which makes no contribution to thermodynamic quantities).
- In two-dimensions, the Potts model has a second order phase transition for $q = 2, 3$ and 4 on a regular planar lattice.

Potts model–continued

- A *first-order* phase transition is characterised by a discontinuity in a first-derivative of the free-energy, while a second-order phase transiiton ....
- For $q > 4$ the Potts model has a first order phase transition.
- In three-dimensions the result is not rigorously known, but it is believed to be first order for $q \geq 2.8$ or so.
- The $q = 3$ state Potts model in three-dimensions is believed to be in the same universality class as the quantum chromodynamics phase transition when quark-hadrons emerged from the quark-gluon plasma at the time of formation of the universe.

The O(n) model–another generalisation of the Ising model

- Another generalization arises if we allow the spin variables to be unit vectors of dimension n.
- This gives rise to the O(n) model. Let $\mathbf{s_i} = (\mathbf{s_i^{(1)}}, \mathbf{s_i^{(2)}}, \ldots, \mathbf{s_i^{(n)}})$ be an n-component vector such that $|\mathbf{s_i}| = \mathbf{1}$.

$$\mathcal{H} = -J \sum_{\{i,j\}} \mathbf{s_i} \cdot \mathbf{s_j} - \mathbf{H} \sum_{\mathbf{i}} \mathbf{s_i^{(1)}}$$

- Clearly, when $n = 1$ we recover the Ising model.
- For $n = 2$ the model is called the planar classical Heisenberg model (or planar model). It exhibits no phase transition for $d = 2$, but does for $d = 3$.

The O(n) model–continued

- For $n = 3$ the model is called the classical Heisenberg model (there is a quantum version). It also exhibits no phase transition for $d = 2$, but does for $d = 3$.
- As $n \to \infty$ we recover the spherical model of Kac-Berlin, in which a spherical constraint can be imposed on the spins $\sum \mathbf{s_i^2} = \mathbf{N}$.
- Of the greatest interest is the $n \to 0$ limit, when we recover (de Gennes) the SAW model. This is a rather non-rigorous result. There is a half-believable derivation in the book by Madras and Slade called *The self-avoiding walk*.
- Other interesting limits are $n = -1$ (spanning forests, Caracciolo, Jacobsen, Saleur, Sokal, Sportiello), $n = -2$ (Gaussian model), $n = -3, \ -5, \ -7 \ \cdots$ which are all conjectured to have a combinatorial interpretation (Sokal).