6 May

Recap: Mean-field self-consistency condition

\( \text{Im} \) = \text{tanh} \left( \text{ZBd(hn)} + \text{BH} \right) \quad \text{B} = '/T

\( \text{Im} \right) = 0 \rightarrow \text{Im} \text{to} \quad \text{qs} \quad \text{Tectages} \\

\( \text{Second-order phase transition at } \text{T}\_c = 2d

\( \text{with critical exponent '/z} \)

\( \text{Im} \rightarrow \text{(Te-T)'/z} \)

\( \text{Im} \rightarrow \text{Te} \)

\( \text{from below} \)

The situation improves for the two-dimensional Ising model. Onsager's exact H=0 solution features a second-order phase transition, at an inverse critical temperature  $\beta_c=\frac{1}{2}\log\left(1+\sqrt{2}\right)\approx0.44$  that had been exactly determined a few years before his work. For  $T\lesssim T_c$ , the magnetization vanishes as  $\langle m\rangle\propto (T_c-T)^{1/8}$ , corresponding to a critical exponent 1/8. While the mean-field prediction of a second-order phase transition is now qualitatively correct, at a quantitative level its predicted  $\beta_c=\frac{1}{2d}=0.25$  is off by almost a factor of 2, while the mean-field critical exponent b=1/2 is four times larger than the true b=1/8.

3 May 6 Max

For higher dimensions d > 3 there is no known exact solution for the Ising model, but the existence of a second-order phase transition can be established and the corresponding critical temperature and critical exponents can be computed numerically, as we will discuss in Unit 10. In three dimensions the meanfield  $T_c=2d=6$  and b=1/2 are still significantly different from the true  $T_c\approx 4.5$ and  $b \approx 0.32$ . The mean-field prediction for the critical exponent b = 1/2 turns out to be correct for  $d \geq 4$ , while the critical temperature  $T_c = 2d$  gradually approaches the true value as the number of dimensions increases. Numerical computations find  $T_c \approx 6.7, 8.8, 10.8$  and 12.9 for d = 4, 5, 6 and 7, respectively, so that the mean-field result improves from being  $\sim 19\%$  too high for d=4 to only  $\sim 9\%$  too high for d=7. Formally, the mean-field approximation exactly reproduces the Ising model in the abstract limit of infinite dimensions,  $d \to \infty$ . Roughly speaking, the greater reliability of the mean-field approach in higher dimensions is due to the larger number of nearest neighbours for each site, 2d. The larger number of nearest-neighbour spins produces a more reliable approximation of the mean spin in the effective field seen by each site in the mean-field approach.

## 9.4 Supplement: Ising model exact results

If time permits, it is not too hard to prove some of the exact results mentioned above, for Ising models in one and two dimensions where the mean-field approximation is least reliable.

## 9.4.1 One-dimensional partition function and magnetization

The <u>special property</u> of the one-dimensional Ising model that helps us derive a closed-form expression for its partition function is the fact that it has exactly as many links as it has sites. Looking back to the illustration on page 134, we can rewrite the nearest-neighbour interaction term as

$$\sum_{(jk)} s_j s_k = \sum_{n=1}^N \underline{s_n} s_{n+1},$$

where the periodic boundary conditions identify  $s_{N+1} = s_1$ . If we also rewrite  $H \sum_{n=1}^{N} s_n = \frac{H}{2} \sum_{n=1}^{N} (s_n + s_{n+1})$ , then the full internal energy is

$$E_i = -\sum_{n=1}^{N} \left[ s_n s_{n+1} + \frac{H}{2} \left( \underline{s_n} + \underline{s_{n+1}} \right) \right]. \qquad \qquad \mathbf{Z} = \mathbf{S} \mathbf{S} \mathbf{S}$$

Inserting this into the partition function  $Z(\beta, N, H) = \sum_{\{s_n\}} \exp[-\beta E(s_n)]$ , we can convert the exponential of the sum into a product of exponentials,

$$Z = \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} \prod_{n=1}^{N} \exp \left[ \underline{\beta s_n s_{n+1}} + \frac{\beta H}{2} (s_n + s_{n+1}) \right].$$

Similarly to Eq. 41 for the non-interacting case, we are going to distribute the summations. Now, however, we have to keep track of the fact that a given spin  $s_i$ will appear both when n=j and when n+1=j, and for each spin configuration it must have the same value both times it appears. An elegant way to account for all allowed possibilities is through matrix multiplication. Use the  $2 \times 2$  matrix

$$\underline{T_n} = \begin{pmatrix} e^{\beta + \beta H} & e^{-\beta} \\ e^{-\beta} & e^{\beta - \beta H} \end{pmatrix} \tag{119}$$

to collect the exponential factors for the four possibilities

$$\{s_n, s_{n+1}\} = \begin{pmatrix} \{1, 1\} & \{1, -1\} \\ \{-1, 1\} & \{-1, -1\} \end{pmatrix}.$$

The matrix product  $T_n \cdot T_{n+1}$  then provides the sum over all contributions with consistent values for  $s_{n+1}$ . Repeating this for all terms in  $\prod_{n=1}^{N}$ , the periodic boundary conditions produce the (cyclic) trace, making the exact partition function simply

$$Z = \operatorname{Tr}\left[\prod_{n=1}^{N} T_{n}\right]. = \underbrace{Z}_{i,k} \operatorname{Til}_{i,k} \operatorname{Til}_{k} \operatorname{Til}_{k} \operatorname{Til}_{k}$$

What's more, since  $\underline{T}_n \equiv T$  is actually independent of n, this simplifies further to

$$Z = \operatorname{Tr}\left[T^{N}\right]. \tag{120}$$

T is known as the **transfer matrix** — roughly speaking, it 'transfers' information about the values of the spins from one link to the next. At this point we can appreciate that our earlier rewriting of the magnetic-field term in the energy just helped to make T more symmetric. If we now diagonalize

$$T = \begin{pmatrix} e^{\beta}e^{\beta H} & e^{-\beta} \\ e^{-\beta} & e^{\beta}e^{-\beta H} \end{pmatrix} \longrightarrow \begin{pmatrix} \lambda_{+} & 0 \\ 0 & \lambda_{-} \end{pmatrix},$$

the partition function will become simply

$$Z = \operatorname{Tr} \left[ \begin{pmatrix} \lambda_{+} & 0 \\ 0 & \lambda_{-} \end{pmatrix}^{N} \right] = \operatorname{Tr} \left( \begin{matrix} \lambda_{+}^{N} & 0 \\ 0 & \lambda_{-}^{N} \end{matrix} \right) = \underbrace{\lambda_{+}^{N} + \lambda_{-}^{N}}.$$

$$H=0: \lambda_{\pm} = e^{\beta} \pm \sqrt{e^{2\beta} - (e^{\beta} - e^{-2\beta})}$$
  
=  $e^{\beta} \pm e^{-\beta}$ 

What are the two eigenvalues  $\lambda_{\pm}$  of T?

$$|T - \lambda I | = \left| \frac{e^{\beta}e^{\beta H} - \lambda}{e^{-\beta}} \right| = \frac{e^{-\beta}}{e^{\beta}e^{-\beta H} - \lambda} = \frac{e^{-\beta}}{e^{-\beta}e^{-\beta H}} + \frac{e^{-\beta}e^{-\beta H}}{e^{\beta}e^{-\beta H}} + \frac{e^{-\beta}e^{$$

With  $\beta \geq 0$  and  $H \geq 0$ , we can check that both eigenvalues are real and  $\lambda_+ > \lambda_-$ . For asymptotically high temperatures,  $\beta \to 0$ , the eigenvalues reduce to  $\lambda_+ = 2$  and  $\lambda_- = 0$  independent of H. In the special case H = 0, the eigenvalues are  $\lambda_+ = 2\cosh\beta$  and  $\lambda_- = 2\sinh\beta$ , while H > 0 typically produces  $\lambda_+ \gg \lambda_-$ . Because  $\lambda_-/\lambda_+ < 1$ , for sufficiently large  $N \gg 1$  we can further simplify

$$Z = \lambda_{+}^{N} \left[ 1 + \left( \frac{\lambda_{+}}{\lambda_{+}} \right)^{N} \right] \approx \lambda_{+}^{N} = e^{N\beta} \cosh^{N}(\beta H) \left[ 1 + \sqrt{1 - \frac{2 \sinh(2\beta)}{e^{2\beta} \cosh^{2}(\beta H)}} \right]^{N}.$$

So there we have it — the solution of the Ising model in one dimension. As usual, the partition function Z is not so revelatory in and of itself. Its principal value lies in enabling us to predict observables like the <u>magnetization</u> — so let's do that, returning to the zero-field case for which we computed the mean-field critical temperature and critical exponent in the previous section:

$$\langle m \rangle = \frac{1}{N\beta} \frac{\partial}{\partial H} \log Z \Big|_{H=0} = \frac{1}{N\beta} \frac{\partial}{\partial H} \log_{\lambda} \lambda_{+}^{N} \Big|_{H=0} = \frac{1}{1+\beta} \frac{\partial \lambda_{+}}{\partial H} \Big|_{H=0}$$

$$\frac{\partial \lambda_{+}}{\partial H} = \frac{\partial}{\partial H} \left[ e^{\beta} \cosh(\beta H) + N e^{\beta} \cosh(\beta H) - 2 \sinh(\beta H) \right]$$

$$\ll \sinh(\beta H) \rightarrow 0$$

Note that we set H=0 only <u>after</u> computing the derivative of the free energy, which avoids the need to consider the absolute value. Upon setting  $\underline{H}=0$ , something remarkable happens:  $\langle \underline{m} \rangle = 0$  for all temperatures!

As claimed at the end of the previous section, the one-dimensional Ising model has no phase transition at all. It is always in the disordered phase, even in the limit of absolute zero  $T \to 0$ . In addition to revealing that the mean-field approximation fails in one dimension, this result also contradicts our general consideration of the phases of the  $\underline{d}$ -dimensional Ising model in Section 9.2. What went wrong there?

The problematic argument in Section 9.2 was our claim that all the degenerate micro-states of the first excited energy level correspond to flipping a single spin to oppose the full alignment of the ground state. This is true for any d>1 simple cubic lattice, and even in one dimension this does account for 2N of the micro-states with next-to-minimal energy  $E_1$ . However, uniquely in one dimension there are additional micro-states with  $E_1$ .

Fixing d=1, suppose we start from the ground state and flip spin  $s_j$  to reach the first excited energy level. Relative to the ground-state energy  $E_0=-N$ , the energy of this micro-state is increased to  $E_1=-N+4$  due to the positive contributions from the  $s_{j-1}s_j$  and  $s_js_{j+1}$  links. But if we now consider also flipping spin  $s_{j+1}$ , the  $s_js_{j+1}$  link goes back to providing a negative contribution while the positive contribution shifts to the  $s_{j+1}s_{j+2}$  link. This gives us an additional 2N micro-states featuring a flipped nearest-neighbour pair of spins, with the same energy  $E_1$  but a smaller magnetization  $|m|=1-\frac{4}{N}$ . And we can continue this process, finding more degenerate micro-states with a flipped block of any number of neighbouring spins up to N-1, and hence any magnetization, including m=0.

Therefore, for d=1 only, our argument that the first excited energy level of the Ising model corresponds to the unique magnetization  $|m|=1-\frac{2}{N}\to 1$  was incorrect. As we have now seen from our exact solution, there is actually no ordered phase in one dimension. A useful way to visualize this sort of behaviour is to think of all these micro-states in the first excited energy level as consisting of two *domains* — one in which the spins point up and the other in which they point down. The two **domain walls** separating these domains are able to move freely through the lattice without changing the energy, but as the domain walls move the magnetization samples the full range of values  $-\left(1-\frac{2}{N}\right) \leq m \leq 1-\frac{2}{N}$ .

## 6 May

## 9.4.2 Two-dimensional critical temperature

While the zero-field Ising model on the d=2 square lattice has also been exactly solved, both Onsager's original calculation and subsequent re-derivations using simpler techniques go substantially beyond this module. However, a few years before Onsager published his famous result, Hans Kramers and G. H. Wannier were able to determine the exact d=2 critical temperature in 1941. They did this by identifying a relation between two Ising model partition functions, without actually evaluating either sum over micro-states:

$$\frac{Z(\beta)}{2^N\cosh^{2N}\beta} = \frac{Z(\widetilde{\beta})}{2e^{2N\widetilde{\beta}}},$$

where the two inverse temperatures  $\beta$  and  $\widetilde{\beta}$  are related by

$$\sinh(2\beta) = \frac{1}{\sinh(2\widetilde{\beta})}.$$

This relation is now known as Kramers–Wannier duality, and the general concept of duality has become a powerful tool in modern theoretical physics. Note that small  $\beta$  implies large  $\widetilde{\beta}$  and vice versa — the duality relates one d=2 Ising model at a high temperature to another one at a low temperature.

150