29 April

Ising model

$$E = -\sum_{(jk)} s_j s_k - H \sum_n s_n \qquad s_n = \pm 1$$

(jk) ← nearest neighbours from lattice w/ periodic boundary conditions

$H=0$ limits

$T \to \infty \to$ all $p_i = \frac{1}{2^N}$

→ degeneracies win → $n_+ \approx n_-$ → disordered

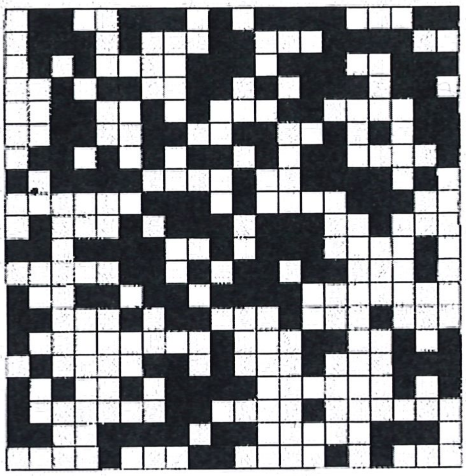
→ Magnetization $|m| = \frac{|M|}{N} = \frac{|n_+ - n_-|}{n_+ + n_-} \to 0$ as $N \to \infty$

$T \to 0 \to$ exponentially suppressed p_i

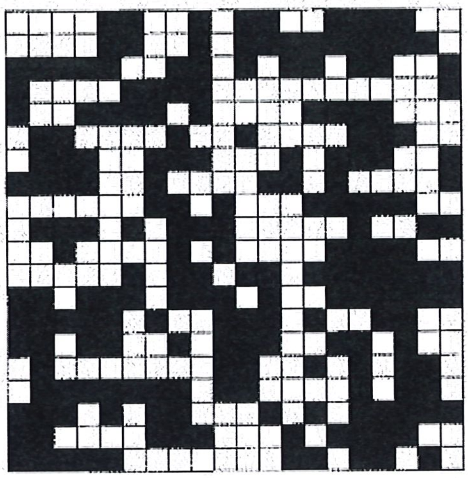
→ ground state wins

→ Ordered phase $|m| \to 1$ as $T \to 0$

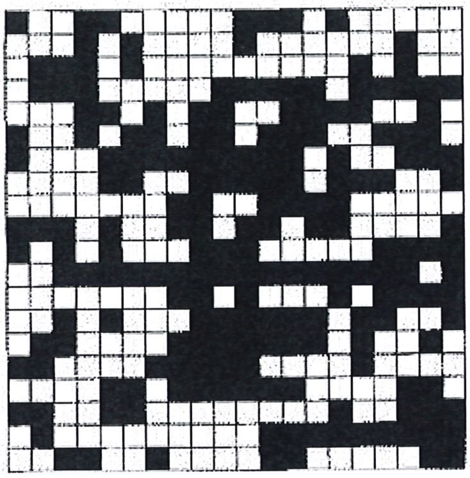
20×20



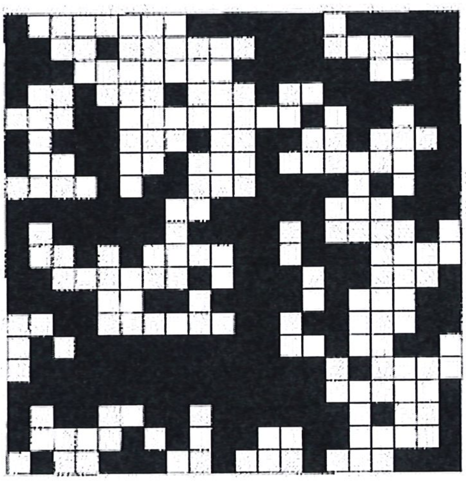
Random initial state



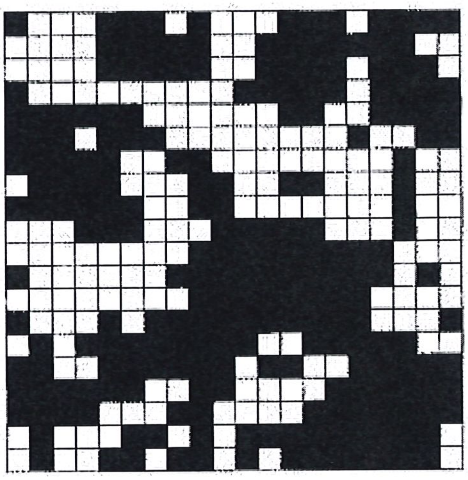
T = 10



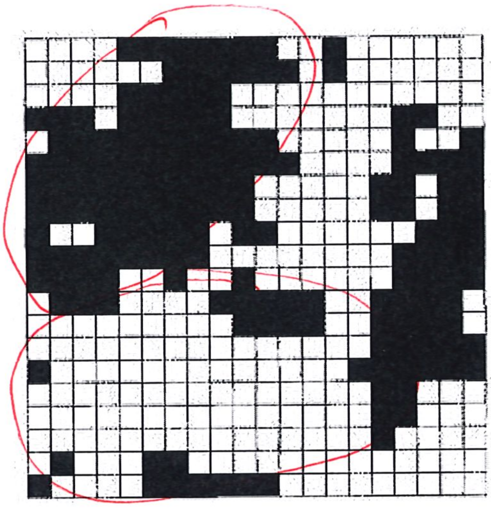
T = 5



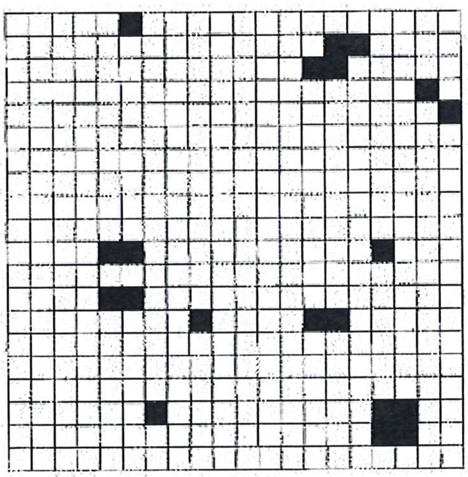
T = 4



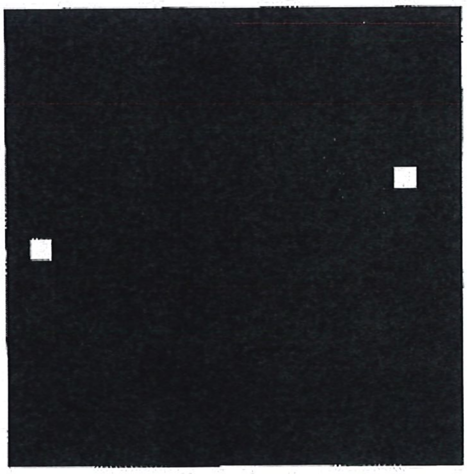
T = 3



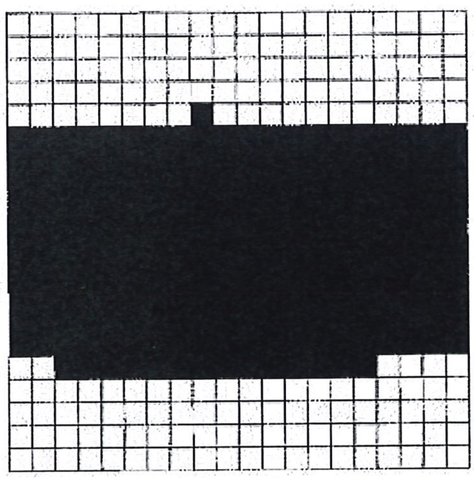
T = 2.5



T = 2



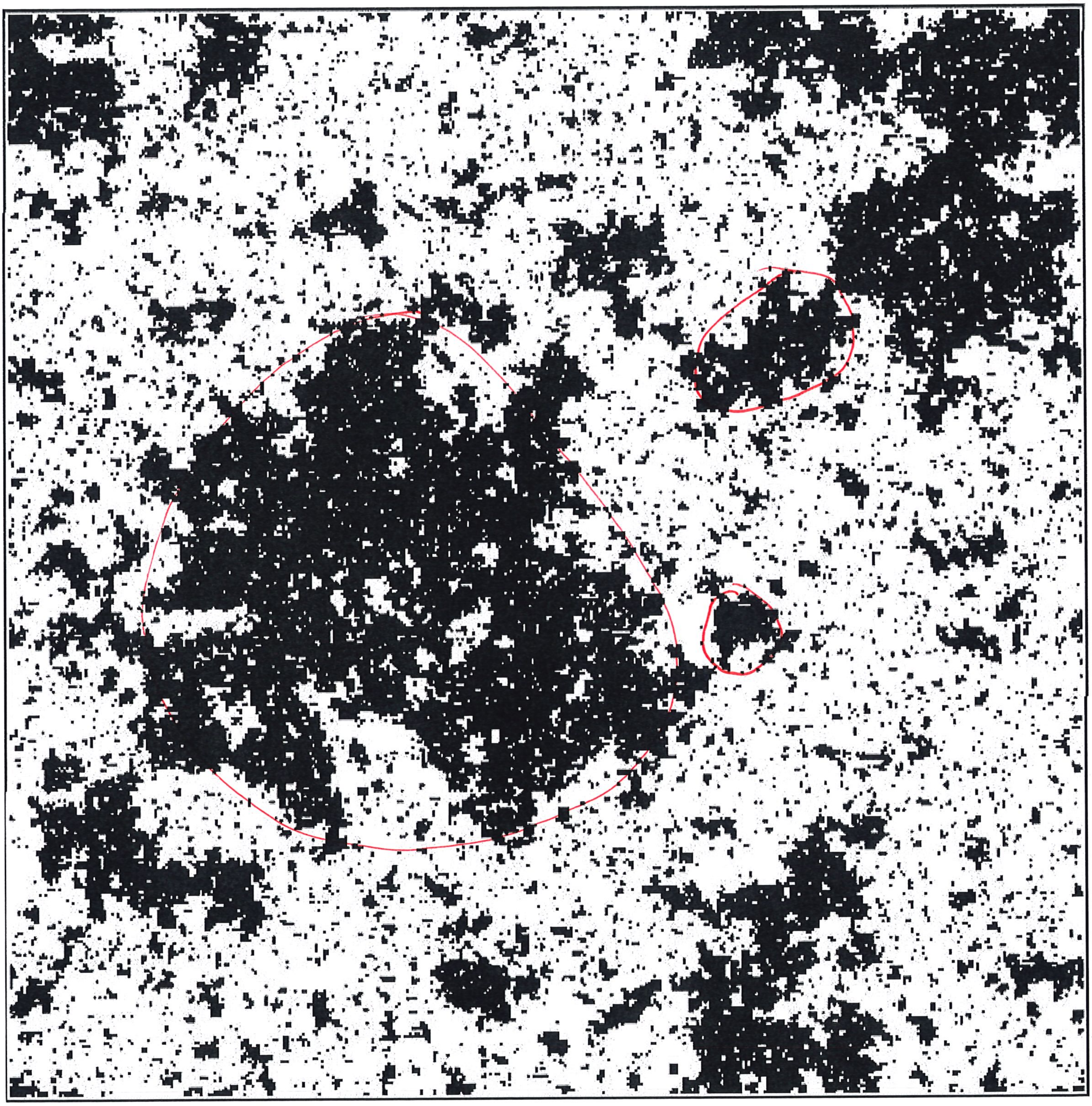
T = 1.5



T = 1

$2^{400} \sim 10^{120}$

$400 \times 400 \quad T = 2.27$



$2^{160,000} \sim 10^{48,164}$

The key factor is the probability for the system to be in one of these micro-states, which depends on the value of the energy E_1 for the first excited energy level. What is this E_1 for the N-site Ising model in d dimensions?

$E_1 = 2d - (d \cdot N - 2d) = -(d \cdot N - 4d)$

+1 from $2d$ links connected to flipped spin

−1 from all other $d \cdot N - 2d$ links

Let's bring everything together by computing the relative probability for the d-dimensional Ising model to be in its ground state with $|m| = 1$ compared to its first excited state with $|m| = 1 - \frac{2}{N}$. This probability is the product of the degeneracy of each energy level times the Boltzmann factor that governs the probability of the system adopting any of these degenerate micro-states:

$$\frac{P(E_0)}{P(E_1)} = \frac{2 \cdot \exp\left[\beta d \cdot N\right]}{2N \cdot \exp\left[\beta\left(d \cdot N - 4d\right)\right]} = \frac{\exp\left[4\beta d\right]}{N}.$$

For any fixed N, a sufficiently low temperature will cause the ground state to dominate, with exponentially suppressed contributions from higher energy levels, just as we previously found for simpler non-interacting systems. This characterizes an **ordered phase** with essentially all spins aligned in the same direction, producing a large expectation value for the magnetization, $\langle |m| \rangle \to 1$.

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We have now seen how the behaviour of the magnetization $\langle |m| \rangle$ distinguishes the high- and low-temperature phases of the zero-field Ising model in d dimensions. In the high-temperature disordered phase, the magnetization is small and $\langle |m| \rangle \to 0$ in the thermodynamic limit $N \to \infty$. In the low-temperature ordered phase, the magnetization is large and $\langle |m| \rangle \to 1$ as $T \to 0$.

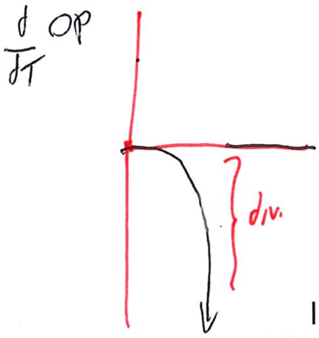
This contrast between ordered and disordered phases is typical behaviour for interacting statistical systems. These two phases are distinguished by an **order parameter** — an observable (related to a derivative of the free energy) that is zero in the disordered phase but non-zero in the ordered phase.[14] The magnetization is the order parameter for the Ising model, which we will connect to the free energy in the next section. Note that the order parameter need not reach its maximum value in the ordered phase — in the case of the Ising model, we don't need complete domination by the fully ordered ground state. So long as there is a tendency towards order, mathematically defined by a non-zero order

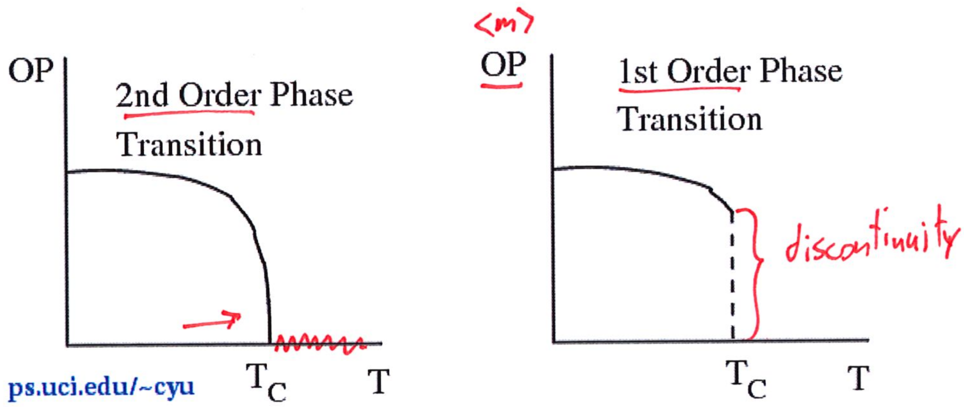
[14] There are atypical (but interesting and important) *topological phase transitions* that are not characterized by such an order parameter. The most famous example is the BKT phase transition named after Vadim Berezinskii, J. Michael Kosterlitz and David Thouless, which was awarded the 2016 Nobel Prize in Physics. It is also possible for a single system to have multiple distinct phase transitions, each characterized by a different order parameter.

parameter, the system is in the ordered phase. The details of how the order parameter changes between zero and non-zero values are what distinguish gradual crossovers from rapid phase transitions.

A **phase transition** is defined by a discontinuity or divergence in the order parameter or its derivative(s), in the $N \to \infty$ thermodynamic limit. The value(s) of the control parameter(s) at which the discontinuity occurs define the *critical point(s)* corresponding to the transition.

For the zero-field Ising model, since we have set $H = 0$, the only remaining control parameter is the temperature T. Any phase transition would therefore occur at a **critical temperature** T_C. The sketches below illustrate the most common types of phase transitions. When the order parameter (OP) itself is discontinuous (shown by a dashed line), the transition is said to be a *first-order* phase transition. When the order parameter is continuous at T_C but its first derivative with respect to the control parameter is discontinuous (typically divergent), the transition is said to be a *second-order* phase transition. This naming scheme can be generalized to higher-order phase transitions, for which discontinuities don't occur until higher derivatives of the order parameter are considered, but in general any phase transition with a continuous order parameter is called a second-order transition.





In practice, any system with a finite number of degrees of freedom will not exhibit a true discontinuity or divergence in any observable. As a result, it is sometimes said that true phase transitions only occur in the $N \to \infty$ thermodynamic limit, but I consider this excessively pedantic, especially given the finite number of atoms in the universe. We are still able to distinguish crossovers from true phase transitions when considering a finite number of degrees of freedom, by analyzing the way in which the system approaches the thermodynomic limit. If there is time and inclination, we may explore such *finite-size scaling*, but first we will develop a useful approximation technique, and apply it to the Ising model to investigate its (dimensionality-dependent) phase transition in more detail.

9.3 The mean-field approximation

Having identified the ordered and disordered phases of the zero-field Ising model, respectively at low and high temperatures, let's now restore a non-zero external magnetic field, $H > 0$. This will allow us to gain a deeper appreciation of the magnetization — now with no absolute value — by noting that Eq. 113 means the magnetization is just the average spin:

$$m = \frac{M}{N} = \frac{1}{N}(n_+ - n_-) = \frac{1}{N}\sum_{n=1}^{N} s_n.$$

We can benefit from this observation in two ways. First, we can recognize the magnetization in the internal energy of the full Ising model with $H > 0$:

$$E_i = -\sum_{(jk)} s_j s_k - H\sum_{n=1}^{N} s_n = -\sum_{(jk)} s_j s_k - HNm = -\sum_{(jk)} s_j s_k - HM.$$

$Z = \sum e^{-\beta E_i}$

The corresponding canonical partition function is

$$Z = \sum_{\{s_i\}} \exp\left[\beta \sum_{(jk)} s_j s_k + \beta H M\right].$$

Based on this expression, and our earlier experience with the entropy and internal energy, we can anticipate that $\langle m\rangle = \langle M\rangle / N$ is related to the derivative of the Helmholtz free energy $F = -T\log Z$ with respect to the field strength H:

$$\frac{\partial}{\partial H}F = -T\frac{\partial}{\partial H}\log Z = -T\frac{1}{Z}\frac{\partial Z}{\partial H}$$

$$= -T\frac{1}{Z}\sum_{\{s_i\}} \beta M \exp\left[\beta \sum_{(jk)} s_j s_k + \beta H M\right]$$

$$= -\langle M\rangle = -N\langle m\rangle$$

$$\langle m\rangle = \frac{1}{N\beta}\frac{\partial}{\partial H}\log Z$$

As promised in the previous section, this relation ensures that the magnetization is an appropriate order parameter for the Ising model phase transition.

The second way we can benefit from relating the magnetization to the average spin is to express the Ising model in terms of the expectation value

$$\langle m\rangle = \frac{1}{Z}\sum_{\{s_n\}} m\, e^{-\beta E(s_n)} = \frac{1}{N}\sum_{n=1}^{N}\langle s_n\rangle.$$

The expectation value of the average spin, $\frac{1}{N}\sum_{n=1}^{N}\langle s_n\rangle$, is independent of the spin configuration $\{s_n\}$ and is simply a function of the inverse temperature β and

$\langle s_n \rangle (\beta, H)$

magnetic field strength H. By adding and subtracting factors of $\langle m\rangle$, we can exactly rewrite each nearest-neighbour term in the Ising model energy, Eq. 111, as

$$\begin{aligned} s_j s_k &= [(s_j - \langle m\rangle) + \langle m\rangle] \times [(s_k - \langle m\rangle) + \langle m\rangle] \\ &= \underbrace{(s_j - \langle m\rangle)(s_k - \langle m\rangle)}_{\text{negligible}} + (s_j + s_k)\langle m\rangle - \langle m\rangle^2 . \end{aligned} \tag{114}$$

This is beneficial because we can note that the factors of $(s_j - \langle m\rangle)$ correspond to the spins' fluctuations around their mean value $\langle m\rangle$. By conjecturing that these fluctuations are small *on average*, we can approximate the Ising model energy by neglecting the first term in Eq. 114 when summing over all links:

$$E_i = -\sum_{(jk)} s_j s_k - H\sum_{n=1}^{N} s_n \quad \longrightarrow \quad E_{\text{MF}} = -\sum_{(jk)} \left[(s_j + s_k)\langle m\rangle - \langle m\rangle^2\right] - H\sum_{n=1}^{N} s_n .$$

The sum over the links $\ell = (jk)$ in d dimensions simply counts $d \cdot N$ factors of the constant $\langle m\rangle^2$. Similarly, since the first term includes both spins $(s_j + s_k)$ on each end of the link, every individual spin appears $2d$ times in the sum over links. Therefore this term just gives us $2d\langle m\rangle$ times another sum over the spins s_n, which we can combine with the final term above:

$$E_{\text{MF}} = d \cdot N\langle m\rangle^2 - (2d\langle m\rangle + H)\sum_{n=1}^{N} s_n \equiv d \cdot N\langle m\rangle^2 - H_{\text{eff}}\sum_{n=1}^{N} s_n . \tag{115}$$

In this expression we define an effective magnetic field $H_{\text{eff}} = 2d\langle m\rangle + H$ that depends on the mean spin. This is a way to remember that this approach of neglecting the squared fluctuations $(s_j - \langle m\rangle)(s_k - \langle m\rangle)$ is known as the **mean-field approximation**. In essence, this approach supposes that we can average over all $2d$ nearest neighbours of each spin and end up with an approximately constant factor that behaves like a modification of the magnetic field. Given the resulting mean-field energy E_{MF} from Eq. 115, let's check the change in this energy, ΔE_j, upon negating any $s_j \to -s_j$:

$$\left.\begin{aligned} E_{MF} &= d\cdot N\langle m\rangle^2 - H_{eff}\Big(s_j + \sum_{k\neq j} s_k\Big) \\ &\to d\cdot N\langle m\rangle^2 - H_{eff}\Big(-s_j + \sum_{k\neq j} s_k\Big) \end{aligned}\right\} \quad \Delta E_j = 2H_{eff}s_j$$

Independent of s_k for $k\neq j$ $\to$ non-interacting!

In light of this result, it isn't surprising that the mean-field approximation producing Eq. 115 makes it very easy to compute the corresponding canonical partition function

$$\begin{aligned} Z_{\text{MF}} &= \sum_{\{s_n\}} \exp\left[-\beta E(s_n)\right] = \exp\left[-\beta d \cdot N \left\langle m \right\rangle^2\right] \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} \exp\left[-x \sum_{n=1}^{N} s_n\right] \\ &= \exp\left[-\beta d \cdot N \left\langle m \right\rangle^2\right] \left(2 \cosh\left[\beta H_{\text{eff}}\right]\right)^N \\ &= \exp\left[-\beta d \cdot N \left\langle m \right\rangle^2\right] \left(2 \cosh\left[\beta \left(2d \left\langle m \right\rangle + H\right)\right]\right)^N , \end{aligned} \tag{116}$$

where we defined $x \equiv -\beta H_{\text{eff}}$ to put the sums into the same form as in Eq. 41. Although this factorized result is far simpler than the partition function for the full Ising model, it does involve some complicated dependence on $\langle m \rangle$ — especially when we recall that $\langle m \rangle$ itself is related to a derivative of $\log Z_{\text{MF}}$. With

$$\log Z_{\text{MF}} = N \log\cosh\left[\beta \left(2d \left\langle m \right\rangle + H\right)\right] + \{H\text{-independent terms}\} ,$$

the relation we derived above gives us

$$\left\langle m \right\rangle = \frac{1}{N\beta} \frac{\partial}{\partial H} \log Z_{\text{MF}} = \frac{1}{\beta} \frac{1}{\cosh\left[\beta \left(2d \left\langle m \right\rangle + H\right)\right]} \frac{\partial}{\partial H} \cosh\left[\beta \left(2d \left\langle m \right\rangle + H\right)\right] .$$

Simplifying, we obtain a **self-consistency condition** for the Ising model magnetization in the mean-field approximation:

$$\left\langle m \right\rangle = \tanh\left[\beta \left(2d \left\langle m \right\rangle + H\right)\right] . \tag{117}$$

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Solving this equation for $\langle m \rangle$ is equivalent to finding the roots of the equation $\tanh\left[\beta(2d \cdot x + H)\right] - x = 0$.

A straightforward way to inspect such solutions is by plotting both

$$f(\langle m \rangle) = \langle m \rangle \qquad\qquad g(\langle m \rangle) = \tanh\left[\beta(2d \left\langle m \right\rangle + H)\right]$$

and monitoring the intersections of these two functions. Fixing $d = 2$ dimensions, the plot below considers the simplest case $\beta = \frac{1}{4}$ and $H = 0$ for which $g(\langle m \rangle) = \tanh\left[\langle m \rangle\right]$ (the solid line). There is only a single intersection between this function and $f(\langle m \rangle)$ (the dashed line), at $\langle m \rangle = 0$, which we should interpret as a disordered phase.