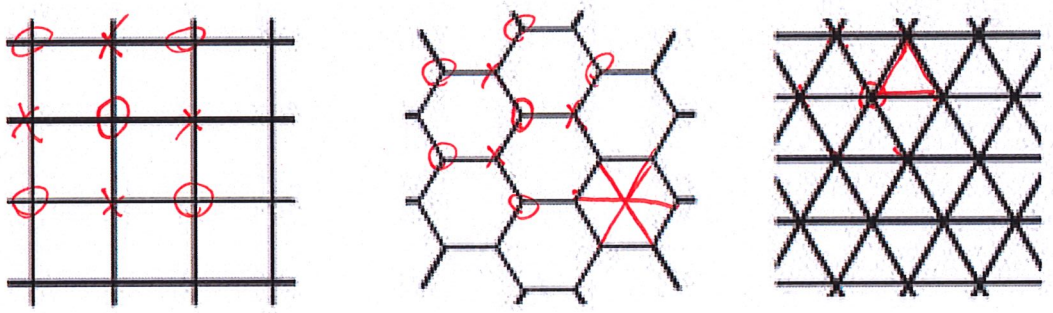
MATH327: Statistical Physics, Spring 2022

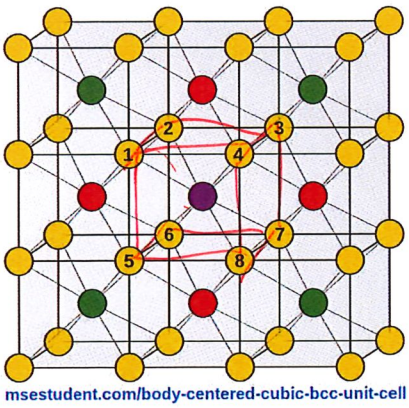
Tutorial problem — Lattices

In the module we are focusing on simple cubic lattices with periodic boundary conditions, but other lattice structures play important roles in both nature and mathematics. Some of the remarkable electronic properties of graphene, for example, are due to its two-dimensional honeycomb lattice structure, while more elaborate three-dimensional lattices play central roles in the search for materials exhibiting high-temperature superconductivity.

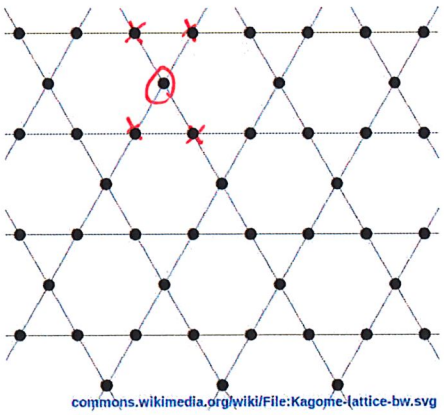
The figure below shows three simple two-dimensional lattices, each of which has a different **coordination number** — the number of nearest neighbours for each site (with periodic boundary conditions). We have already seen that the square lattice has coordination number $C = 2d = 4$, and generalizes to simple cubic and hyper-cubic lattices in higher dimensions.



The honeycomb lattice of graphene has a smaller coordination number $C = d + 1 = 3$, and generalizes to 'hyper-diamond' lattices in higher dimensions. Finally, the triangular lattice essentially fills in the middle of each honeycomb cell, leading to coordination number $C = 2(d + 1) = 6$. Its higher-dimensional generalizations are known as A_d^* lattices, of which the simplest example is the three-dimensional body-centered cubic lattice shown below. Also shown below is the 'kagome' lattice, which has the same $C = 4$ as the square lattice, illustrating that the coordination number is insufficient to completely characterize a lattice.



msestudent.com/body-centered-cubic-bcc-unit-cell



commons.wikimedia.org/wiki/File:Kagome-lattice-bw.svg

Things become more interesting when we consider generalizing the Ising model to have energy

$$E = -J\sum_{(jk)} s_j s_k - H\sum_{n=1}^{N} s_n,$$

with nearest neighbours (jk) defined by any of the three simple two-dimensional lattices above. While any positive interaction strength $J > 0$ can be rescaled to $J = 1$ without loss of generality, the case of a constant negative $J < 0$ is qualitatively different. Specializing to $d = 2$ and $H = 0$, let's consider a couple of **conceptual questions**: What are the minimum-energy ground states for each case $J > 0$ and $J < 0$, for each of the square, honeycomb and triangular lattices? Can you think of an order parameter distinguishing these ground states from the disordered micro-states that dominate at high temperatures?

Generalizing the Ising model in this way opens up a vast landscape of possible applications both practical and abstract. As one example (with both practical and abstract relevance), a **spin glass** can be modeled by allowing the interaction strength to vary from site to site,

$$E_{\text{SG}} = -\sum_{(jk)} J_{jk} s_j s_k.$$

Giorgio Parisi was awarded part of the 2021 Nobel Prize in Physics for his work studying the mathematics of such spin glass systems. In particular, he was able to solve the so-called Sherrington–Kirkpatrick model

$$E_{\text{SG}} = -\sum_{j<k} J_{jk} s_j s_k,$$

where the values J_{jk} are randomly drawn from a gaussian distribution around some mean J_0 and the system is defined on a fully connected lattice (or **complete graph**) where every site j is a nearest neighbour of every other site $k \neq j$. (Summing only over $j < k$ and not $j > k$ avoids double-counting the link jk.) As shown on the next page, a fully connected lattice with N sites has $\frac{1}{2}N(N-1) = \binom{N}{2}$ links.

While we may look a bit more closely at spin glasses if time permits during the next couple of weeks, for now let's consider a simpler Ising system with constant interaction strength on the fully connected lattice:

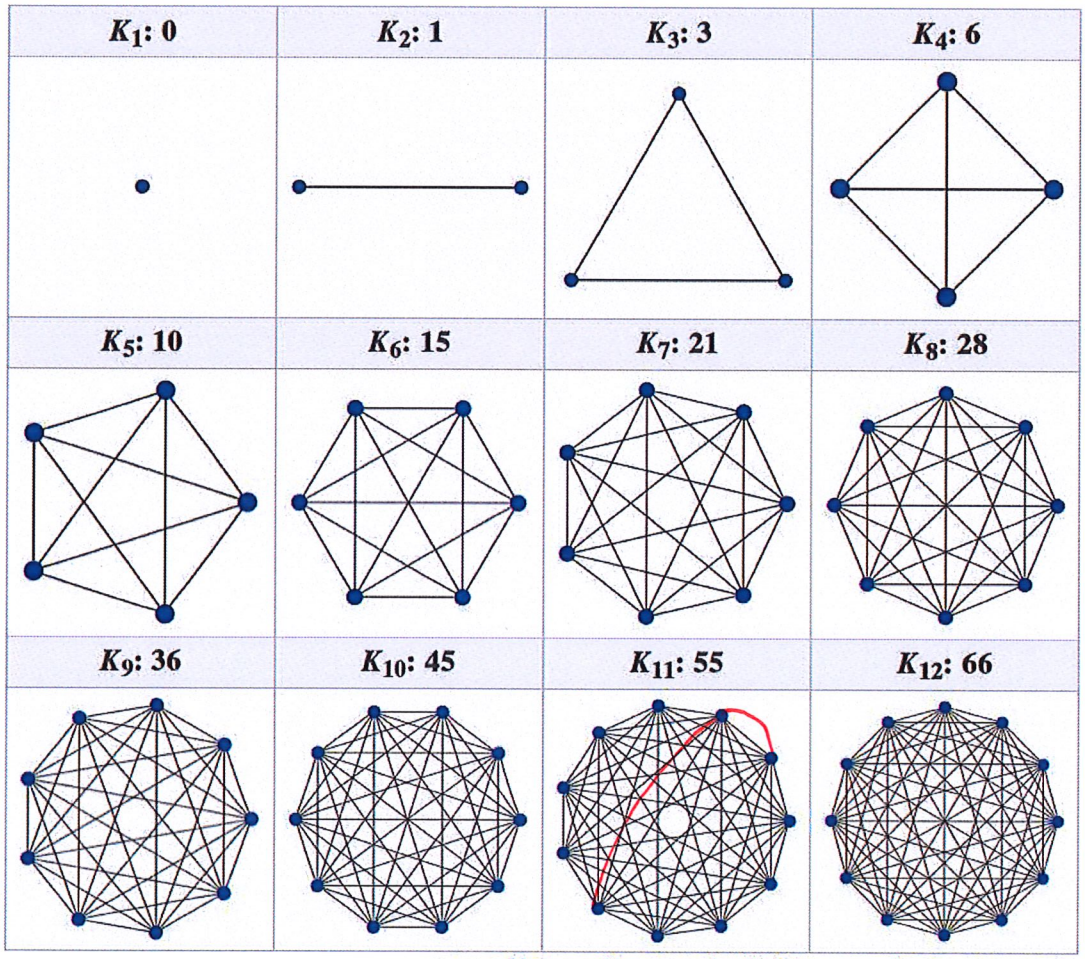
$$E = -\frac{J}{N}\sum_{j<k} s_j s_k - H\sum_{n=1}^{N} s_n.$$

We normalize the interaction strength by N so that the system retains a finite energy per spin in the $N \to \infty$ thermodynamic limit.

Can you compute a closed-form expression for the partition function of this Ising model on the fully connected lattice? As a hint, it may be profitable to reorganize the calculation into a sum over the $N + 1$ possible values of the magnetization $-1 \leq m \leq 1$, and counting how many micro-states there are with a given magnetization. (This is analogous to the fugacity expansion that reorganizes the

grand-canonical partition function into a sum over possible particle numbers.) The energy above would need to be rewritten in terms of the magnetization, which is easier when summing over all $j < k$ compared to considering only nearest neighbours. Finally, for large N we can approximate the $N + 1$ possible values of m as continuously varying, and integrate

$$Z = \int_{-1}^{1} (\cdots)\, dm.$$



en.wikipedia.org/wiki/Complete_graph

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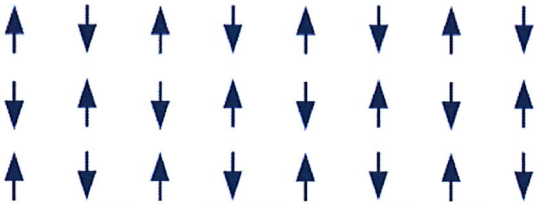
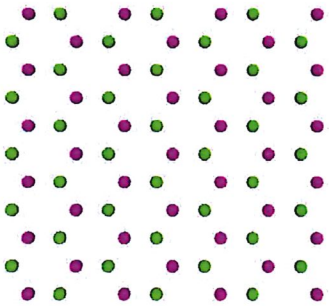
Tutorial comments — Lattices

Beginning with the qualitative questions, it's straightforward to appreciate that the $J > 0$ case leads to the same doubly degenerate ground state that we previously considered, independent of the lattice structure: All of the spins align with each other, either all $s_n = 1$ or all $s_n = -1$, and the magnetization $\langle m \rangle \propto \frac{\partial}{\partial H} F$ is the corresponding order parameter. Interpreting the spins as molecular magnetic dipoles, their alignment corresponds to a *ferromagnetic* phase of the sort Lenz and Ising initially aimed to investigate in the 1920s.

When we consider instead $J < 0$, we can note that each pair of aligned nearest-neighbour spins would now make a positive contribution to the energy. To lower the energy and reach the ground state, we want all of these pairs to be anti-aligned instead, which is possible for the square and honeycomb lattices as illustrated below. (In the honeycomb case, think of the green and purple sites as respectively representing $s_n = 1$ and $s_n = -1$.) These patterns correspond to an *anti-ferromagnetic* phase.



commons.wikimedia.org/wiki/File:Antiferromagnetic_ordering.svg



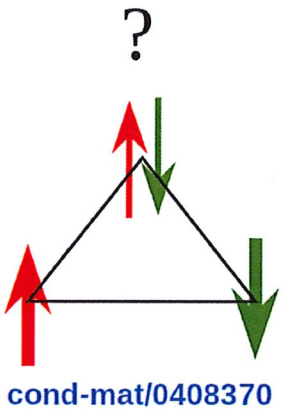
These ground states are also doubly degenerate, with the same energy if all anti-aligned spins are simultaneously flipped. Although the magnetization vanishes for these micro-states, $\langle m \rangle = 0$ as in the disordered phase, the clear order they exhibit suggests that it should be possible to define a corresponding order parameter. This turns out to be the *staggered magnetization* $m_s = \frac{1}{N} \sum_{n=1}^{N} (-1)^n s_n$, where the site indices n are assigned in such a way that even and odd sites alternate in the patterns shown above. For the staggered magnetization to be a true order parameter, it should be related to a derivative of the free energy, which we can ensure by generalizing the internal energy to be

$$E = -J \sum_{(jk)} s_j s_k - H \sum_{n=1}^{N} s_n - H_s \sum_{n=1}^{N} (-1)^n s_n,$$

so that $\langle m_s \rangle \propto \frac{\partial}{\partial H_s} F$ and we typically turn off this 'staggered magnetic field', $H_s = 0$.

Things are more complicated for the triangular lattice, because there is no way to assign indices so that even sites only have odd neighbours and vice-versa.

In technical terminology, the triangular lattice is non-bipartite. As illustrated below, it is not possible to obtain negative contributions to the internal energy from all three links in the elementary unit cell. There are instead six degenerate configurations, with one of the spins aligned against the other two, that all produce the same minimum energy. Generalizing this situation to a lattice with $N \gg 1$ sites, there is no regular order, no order parameter, and a large number of degenerate micro-states — implying to a non-zero entropy even at absolute zero temperature, as first reported by G. H. Wannier in 1950.



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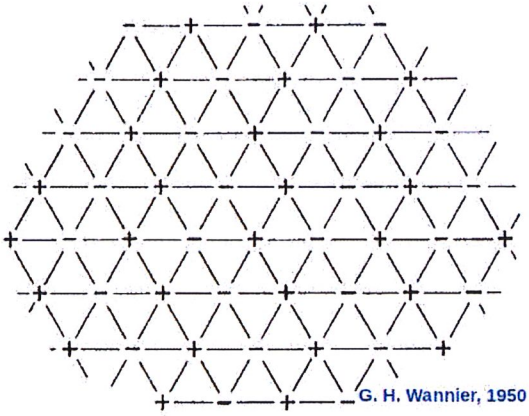

This system is known as a *frustrated anti-ferromagnet*, 'frustrated' in the sense that its lattice structure obstructs the anti-ferromagnetic ordering it 'wants' to achieve in order to minimize its energy at low temperatures. Such systems can be extremely difficult to analyze, as Matthias Troyer and Uwe-Jens Wiese discussed (for an Ising spin glass) in work from 2004 that has motivated quantum computing in recent years. In the language of theoretical computer science, the task of finding the ground states of these frustrated spin glasses falls in the *non-deterministic polynomial* (NP) complexity class. Roughly speaking, given any particular spin configuration it is quick and easy to check whether its energy is smaller than any given E_0, but it requires exponentially large computing resources to search through the 2^N possible spin configurations for minimum-energy micro-states.

Turning now to the Ising model on a fully connected lattice, we begin by following the hint to rewrite the energy in terms of the magnetization $m = \frac{1}{N}\sum_{n=1}^{N} s_n$. This is possible thanks to the presence of links connecting all pairs of distinct sites, which allows us to replace the sum over these links by sums over site:

$$\sum_{j<k} s_j s_k = \frac{1}{2}\sum_{j\neq k} s_j s_k = \frac{1}{2}\left(\sum_{j=1}^{N} s_j\right)\left(\sum_{k=1}^{N} s_k\right) - \frac{1}{2}\sum_{j=1}^{N} s_j^2 = \frac{N^2 m^2}{2} - \frac{N}{2}$$

since $s_j^2 = 1$. Inserting this into the energy, we have

$$E = -\frac{J}{N}\sum_{j<k} s_j s_k - H\sum_{n=1}^{N} s_n = -\frac{JNm^2}{2} + \frac{J}{2} - HNm = -\frac{J}{2}\left(Nm^2 - 1\right) - HNm.$$

We can now express the partition function as a sum over the $N+1$ values $-1 \leq m \leq 1$ that correspond to $0 \leq n_+ \leq N$ with multiplicity $\binom{N}{n_+}$:

$$\begin{aligned} Z &= \sum_{n_+=0}^{N} \binom{N}{n_+} \exp\left[\frac{\beta J}{2}\left(Nm^2-1\right)+\beta HNm\right] \\ &\longrightarrow \int_{-1}^{1} \binom{N}{n_+} \exp\left[\frac{\beta J}{2}\left(Nm^2-1\right)+\beta HNm\right]\, dm. \end{aligned}$$

In order to integrate over the magnetization we need to express the binomial coefficient in terms of

$$m = \frac{2n_+}{N} - 1 = 1 - \frac{2n_-}{N} \qquad \Longrightarrow \qquad n_\pm = \frac{N}{2}\left(1 \pm m\right).$$

With a plan to combine this factor with the exponential, let's express it as

$$\binom{N}{n_+} = \frac{N!}{n_+!\, n_-!} = \exp\left[\log\left(\frac{N!}{n_+!\, n_-!}\right)\right] = \exp\left[\log(N!) - \log(n_+!) - \log(n_-!)\right].$$

Applying Stirling's formula as usual, the linear terms cancel and the argument of the exponential becomes

$$N\log N - \frac{N}{2}(1+m)\log\left(\frac{N}{2}(1+m)\right) - \frac{N}{2}(1-m)\log\left(\frac{N}{2}(1-m)\right).$$

The only terms that don't cancel in the expression above are

$$\frac{N}{2}\log\left(\frac{4}{1-m^2}\right) + \frac{Nm}{2}\log\left(\frac{1-m}{1+m}\right).$$

Inserting these back into the exponential in the partition function, and pulling out the m-independent factor, we have

$$\begin{aligned} Z =& e^{-\beta J/2} \int_{-1}^{1} e^{Nf(m)}\, dm = e^{-\beta J/2} \int_{-1}^{1} \left[e^{f(m)}\right]^N\, dm \\ f(m) \equiv& \frac{1}{2}\log\left(\frac{4}{1-m^2}\right) + \frac{m}{2}\log\left(\frac{1-m}{1+m}\right) + \frac{\beta J m^2}{2} + \beta H m. \end{aligned}$$

Along the same lines as the Sommerfeld expansion we considered in Section 8.8, we will expand the integrand around the m for which $f(m)$ is maximized. This maximum value is exponentially preferred in the partition function above, with a further enhancement by $N \gg 1$. Although our approach involves an expansion, it is possible to show that the solution is exact in the thermodynamic limit — see *Statistical Mechanics of Lattice Systems* by Sacha Friedli and Yvan Velenik for more formal proofs. In that book, this Ising model on the fully connected lattice is called the **Curie–Weiss model**.

Anyway, the first step is to find extrema of $f(m)$, by considering its derivative

$$\frac{\partial f}{\partial m} = \frac{\partial}{\partial m}\left[-\frac{1}{2}\log\left(1-m^2\right) + \frac{m}{2}\log\left(\frac{1-m}{1+m}\right) + \frac{\beta J m^2}{2} + \beta H m\right].$$

After some nice cancellations,

$$\frac{\partial f}{\partial m} = \frac{1}{2}\log\left(\frac{1-m}{1+m}\right) + \beta J m + \beta H = 0.$$

Perhaps taking inspiration from our mean-field analysis, we can recognize

$$\operatorname{arctanh}(m) = \frac{1}{2}\log\left(\frac{1+m}{1-m}\right) = -\frac{1}{2}\log\left(\frac{1-m}{1+m}\right)$$

so that

$$\frac{\partial f}{\partial m} = \beta(Jm + H) - \operatorname{arctanh}(m) = 0 \qquad \Longrightarrow \qquad m = \tanh\left[\beta(Jm+H)\right].$$

We have reproduced essentially the same self-consistency condition that we derived for the mean-field approximation! This shouldn't be surprising, because we are considering a system in which every site has $N \gg 1$ nearest neighbours, the regime in which the mean-field approximation should be a reliable guide.

We have already considered the solutions to this self-consistency condition in some detail. Let's consider expanding $f(m)$ around one of these solutions, which we'll call m_0 (and can be either zero or non-zero). Let m_0 be a solution to the self-consistency To ensure we have a maximum, we need to consider the second derivative, which will also make an appearance in the eventual expansion.

$$\frac{\partial^2 f}{\partial m^2} = \frac{\partial}{\partial m}\left[\frac{1}{2}\log\left(\frac{1-m}{1+m}\right) + \beta J m\right] = \beta J - \frac{1}{1-m^2},$$

so in order to have a maximum, we need $\beta J < \frac{1}{1-m_0^2}$ so that $\frac{\partial^2 f}{\partial m^2} < 0$. For the disordered solution $m_0 = 0$, this requires $\beta < 1/J$ — this is a more analytical way of determining the mean-field critical temperature $T_c = J$ compared to the graphical approach we went through earlier this week. This critical temperature is sometimes called the **Curie temperature** due to the equivalence between the Curie–Weiss model and the mean-field approximation. For lower temperatures, the (unstable) disordered solution is a minimum of $f(m)$, and instead we need to consider non-zero m_0, which allows us to find a maximum at arbitrarily low temperatures (small β) as $|m_0| \to 1$.

Focusing on $m_0 \neq 0$, we can expand around either of the two equivalent minima, and simply double the resulting partition function to account for them both. Starting from

$$\begin{aligned} f(m) &\approx f(m_0) + \frac{1}{2}(m-m_0)^2 \left.\frac{\partial^2 f}{\partial m^2}\right|_{m=m_0} \\ &= \frac{1}{2}\log\left(\frac{4}{1-m_0^2}\right) + m_0\left[\frac{1}{2}\log\left(\frac{1-m_0}{1+m_0}\right) + \frac{\beta J m_0}{2} + \beta H\right] \\ &\qquad + \frac{1}{2}(m-m_0)^2\left(\beta J - \frac{1}{1-m_0^2}\right), \end{aligned}$$

we know that m_0 is a solution to the self-consistency condition

$$\frac{1}{2}\log\left(\frac{1-m_0}{1+m_0}\right) + \beta J m_0 + \beta H = 0,$$

which significantly simplifies the result:

$$f(m) \approx \frac{1}{2}\log\left(\frac{4}{1-m_0^2}\right) - \frac{\beta J m_0^2}{2} + \frac{1}{2}(m-m_0)^2\left(\beta J - \frac{1}{1-m_0^2}\right).$$

In particular, the self-consistency condition removes all dependence on the external magnetic field H, though there is still implicit dependence on H through its effect on the precise value of m_0.

Inserting this back into the partition function, we can pull out all the m-independent factors and repeat our earlier trick of extending the integration domain to include the negligible tails for $|m| > 1$:

$$Z = 2e^{-\beta J(1+Nm_0^2)/2}\left(\frac{4}{1-m_0^2}\right)^{N/2}\int_{-\infty}^{\infty}\exp\left[-\frac{N}{2}(m-m_0)^2\left(\frac{1}{1-m_0^2}-\beta J\right)\right]\,dm.$$

We are now left with a gaussian integral that we know how to do, obtaining

$$Z = 2e^{-\beta J(1+Nm_0^2)/2}\left(\frac{4}{1-m_0^2}\right)^{N/2}\sqrt{\frac{2\pi\left(1-m_0^2\right)}{N\left(1-\beta J+\beta J m_0^2\right)}}.$$

As for the simple one-dimensional Ising model, this closed-form expression for the partition function doesn't itself give us clear intuitive physical insight into the system. However, it can be used to predict observables, including the magnetization — for which we have already found that the result is a transcendental equation that behaves as

$$\langle m\rangle = \begin{cases} \pm\sqrt{3}\,(T_c - T)^{1/2} & \text{for } T \lesssim T_c \\ 0 & \text{for } T \gtrsim T_c \end{cases}$$

around the critical temperature $T_c = J$, with critical exponent $b = 1/2$.