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Chapter 6

Lattice models and phase transitions

Lattice models are quite ubiquitous in physics. We have already encountered such lattice models when we had a look at a coupled harmonic system. It should be clear that there are many instances of such models. Here, one thinks of having a graph $G = (V, E)$ given, with a quantum or a classical degree of freedom per lattice site. This graph could reflect a cubic lattice, or a simple line – such as in the case of the simple harmonic chain above. Or a more sophisticated lattice, such as a Kagome lattice, or a triagonal lattice. It should be clear that in particular in the condensed-matter context, such lattice models are everywhere. Also, for systems of cold atoms in optical lattices one encounters such lattice models: The lattice is then the one given by the laser light itself. Interactions are usually local. This means that systems directly interact only with finitely many neighbours, such as nearest neighbours.

Local Hamiltonians: A local Hamiltonian is a Hamiltonian on a lattice defined by a graph $G = (V, E)$. Interactions are finite-ranged in the sense that there exists an r such that whenever $j, k \in V$ with

$$\mathrm{dist}(j, k) > r \tag{6.1}$$

then the two constituents do not interact.

This is a somewhat sophisticated way of putting it. For practical purposes, one is usually interested in cubic lattices of some dimension D, and nearest-neighbor interactions, for which $r = 1$. One then often writes $\langle j, k\rangle$ for nearest neighbors in the lattice, that is, for sites $j, k \in V$ for which

$$\mathrm{dist}(j, k) = 1. \tag{6.2}$$

One distinguishes then periodic boundary conditions from open boundary condi-

tions. For periodic boundary conditions, one has $V = \mathbb{Z}_L^D$, that is, one considers the sites in each dimension modulo N. For open boundary conditions, the sites at the boundary are only coupled to neighbours in the interior. For such local interactions, a common translationally invariant quantum Hamiltonian with open boundary conditions then looks as follows.

Hamiltonian with nearest-neighbor interaction in a cubic lattice: With V being the cubic lattice, the Hamiltonian is of the form

$$H = \sum_{j \in V} h_j + \sum_{\langle j,k \rangle} v_{j,k}. \tag{6.3}$$

Each of the terms h_j are the same then, respectively, only translates of each other, and supported on sites j only. In case of $v_{j,k}$, again all terms are either translates of each other, or appropriately rotated instances. Again, it is always the same Hamiltonian term, only the support is different. Of course, it is a small step to accommodate also more complicated periodicities: We can think of elementary cells in a crystal structure and have not a fully translationally invariant Hamiltonian. In condensed matter physics, one often encounters such Hamiltonians.

Now there is an intricate feature about such lattice models: They are easy to describe. We have just done so: For a translationally invariant model, it is sufficient to give the on-site term h_j for some j and the coupling term $v_{j,k}$ for some j, k. That is it! These are only very, very few numbers. Yet, it is usually very difficult to grasp properties of such models. They can exhibit a very sophisticated behaviour, and can show phase transitions, topological order, string order, and so on. And of course, this is all a property of the Hamiltonian. Still, these intricate properties are in a way an emergent property. Still today, a lot of research is dedicated to finding out properties from such lattice models.

6.1 Classical lattice models

6.1.1 Ising model

We start by discussing classical lattice models. Here, each degree of freedom per site in V is a classical degree of freedom. The most famous model of that kind is the Ising model, where each site is associated with a classical spin degree of freedom. In fact, it is the simplest mathematical model of ferromagnetism in statistical mechanics that already shows very important features of the phenomenon. It has also been used to describe the behaviour of lattice gases, binary alloys melting of DNA, and other situations. The Ising model was invented by Wilhelm Lenz, who gave this model as a problem to be solved to Ising, who indeed presented the solution for the one-dimensional situation given below. To be fair, this is a very simple problem. The big breakthrough was the exact

solution for the two-dimensional case given by Onsager. We will only have the time to hint at that. In the Ising model, the underlying lattice is

$$V = L^{\times D}, \tag{6.4}$$

so L in one dimension, $L \times L$ in two dimensions, and so on. At each site, there is a spin that can take the values $s_j \in \{+1, -1\}$. A configuration is hence a collection of all values

$$s = (s_1, \ldots, s_{L^D}). \tag{6.5}$$

$s = (-1, -1, \ldots, -1)$ is a configuration in which all spins are pointing downwards, for $s = (1, 1, \ldots, 1)$ all are going up.

Hamiltonian of the Ising model: For $J, B \in \mathbb{R}$, the Hamiltonian is

$$H(s) = -J \sum_{\langle j,k \rangle} s_j s_k - B \sum_j s_j. \tag{6.6}$$

This is a model for spins in a solid-state system: J is the magnetic interaction energy between nearest-neighbour spins in the lattice. B reflects an external magnetic field. This is usually written as μB with a chemical potential μ, but this we have absorbed in our definition of B to keep the discussion simpler. In this model, both positive and negative values for J make sense. If

- $J > 0$, the interaction is called ferromagnetic,
- $J < 0$, the interaction is called antiferromagnetic,
- $J = 0$, the spins are noninteracting.

We will also subsequently freely move between different boundary conditions; but it should be clear that for each dimension, one can consider all boundary conditions separately. At this point, we are in the position to formulate the partition function of the classical canonical ensemble for inverse temperature $\beta > 0$,

$$Z = \sum_s \exp\left(\beta J \sum_{\langle j,k \rangle} s_j s_k + \beta B \sum_j s_j\right). \tag{6.7}$$

Here, the sum s is the sum over all 2^{L^D} many configurations of the spins in the lattice. Clearly, this is a daunting sum, and it is not easy to perform naively. In 1D and in 2D, one can still solve the model exactly. In 1D, this is a very easy task, in 2D not so much. But already at this level, we can roughly grasp what is going on here. At low temperatures, we expect the lattice to be ordered. As we increase the temperature, at some point the order should disappear and the spins should become randomly oriented.

6.1.2 Absence of a phase transition in the 1D Ising model

For our discussion in 1D, let us pick periodic boundary conditions. This does not alter the problem compared to open boundary conditions here, but the notation becomes a bit simpler. We hence consider spins on a ring, with sites $(1, \dots, L)$. We identify $s_{j+N} = s_j$. The Hamiltonian is hence

$$H(s) = -J \sum_{j=1}^{L} s_j s_{j+1} - B \sum_{j=1}^{L} s_j. \tag{6.8}$$

Again, the partition function in the canonical ensemble becomes

$$Z = \sum_{s_1=\pm 1} \cdots \sum_{s_L=\pm 1} \exp\left(\beta \sum_{j=1}^{L} \left(J s_j s_{j+1} + \frac{1}{2} B (s_j + s_{j+1}) \right) \right), \tag{6.9}$$

where we have used that

$$\sum_{j=1}^{L} s_j = \frac{1}{2} \sum_{j=1}^{L} (s_j + s_{j+1}) \tag{6.10}$$

for a periodic lattice. At this point, it seems infeasible to perform the sum over all configurations. We can, however, introduce a trick of a transfer operator. In fact, this trick is quite magic: Be astonished by the simplicity of it. This amounts to reordering the sum in a way such that the entire expression can be written as a matrix power of a transfer operator. In modern terms, one could also say that the tensor network describing this can be efficiently contracted. The trick is as follows. Let us introduce a 2×2-matrix, called the transfer matrix,

$$P = \begin{pmatrix} e^{\beta(J+B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} \end{pmatrix}. \tag{6.11}$$

We identify the matrix elements with a kernel of a quadratic form over $(+1, -1)$, so the elements of this matrix are

$$\langle +1|P|+1\rangle = e^{\beta(J+B)}, \tag{6.12}$$
$$\langle +1|P|-1\rangle = \langle -1|P|+1\rangle = e^{-\beta J}, \tag{6.13}$$
$$\langle -1|P|-1\rangle = e^{\beta(J-B)}. \tag{6.14}$$

That is to say, we have

$$\langle s_j|P|s_k\rangle = e^{\beta(J s_j s_{j+1} + \frac{1}{2} B(s_j + s_{j+1})}. \tag{6.15}$$

In this way, can write the partition function as

$$Z = \sum_{s_1=\pm 1} \cdots \sum_{s_L=\pm 1} \langle s_1|P|s_2\rangle \langle s_2|P|s_3\rangle \dots \langle s_L|P|s_1\rangle. \tag{6.16}$$

At first glance, it seems as if we had not gained much by this reformulation. But we have. We can now perform the sum over each term explicitly, using the completeness relation. We get

$$Z = \sum_{s_1=\pm 1} \langle s_1 | P^L | s_1 \rangle = \mathrm{tr}(P^L). \tag{6.17}$$

So we can reduce the entire sum to a single sum, so to a trace of the transfer matrix. But this is easy. If we denote the largest and the smallest eigenvalues of the symmetric matrix with λ_+ and λ_-, respectively (remember they are real for symmetric matrices), then one finds

$$Z = \lambda_+^L + \lambda_-^L = \lambda_+^L \left(1 + \left(\frac{\lambda_-}{\lambda_+} \right)^L \right). \tag{6.18}$$

We can easily find these eigenvalues explicitly,

$$\lambda_{\pm 1} = e^{\beta J} \left(\cosh(\beta B) \pm \left(\cosh^2(\beta B) - 2^{-2\beta J} \sinh(2\beta J) \right)^{1/2} \right); \tag{6.19}$$

after all, do not forget that P is a simple 2×2 matrix where we can simply solve the equation involving the characteristic polynomial. In the limit $L \to$, only the largest eigenvalue λ_+ contributes to thermodynamic quantities. For example, the free energy per site is in the thermodynamic limit

$$\lim_{L\to\infty} \frac{\beta}{L} \log Z = -\beta \log(\lambda_+). \tag{6.20}$$

Here, we have used that

$$\lim_{L\to\infty} \left(\frac{\lambda_-}{\lambda_+} \right)^L = 0. \tag{6.21}$$

Hence, the free energy per site is

$$f = -L - k \log \left(\cosh(\beta B) + \left(\cosh^2(\beta B) - 2^{-2\beta J} \sinh(2\beta J) \right)^{1/2} \right). \tag{6.22}$$

The order parameter is given by the magnetisation

$$m = \frac{1}{L} \sum_{j=1}^{L} s_j. \tag{6.23}$$

One finds

$$\langle m \rangle = -\left(\frac{\partial f}{\partial B} \right)_T = \frac{\sinh(\beta B)}{(\cosh^2(\beta B) - 2e^{-2\beta J} \sinh(2\beta J))^{1/2}}. \tag{6.24}$$

We see that this model cannot exhibit a phase transition, since when $B \to 0$, the order parameter also goes to zero. That is to say, no spontaneous non-zero value of the order parameter is possible. The reason is that there are for each site not enough neighbours in order to enforce some kind of order. The equivalent 2D model, in fact, does exhibit a phase transition.

6.1.3 Existence of a phase transition in the 2D Ising model

We will now see that the same model in 2D does exhibit a phase transition. This can again be exactly solved with more elaborate methods. We will first have a look at a high-level argument, however. This high level argument will show that there in fact exists a phase transition, but not quite at what point. To keep the discussion simple, let us set $B = 0$: We anyway want to see a spontaneous non-zero value of the order parameter at a vanishing field. We also pick now open boundary conditions, this again to keep the discussion as simple as possible. The Hamiltonian is hence nothing but

$$H(s) = -J \sum_{\langle j,k \rangle} s_j s_k, \tag{6.25}$$

for configurations $s = (s_1, \ldots, s_{L^2}) \in \{-1, 1\}^{\times 2}$. The neighbours of each site are the four sites that are immediately adjacent to each site, so again nearest neighbours only. As we know, the probability that the system takes some configuration s is given by

$$p(s) = \frac{1}{Z} e^{-\beta H(s)}. \tag{6.26}$$

We consider the case of low temperatures, so the limit $\beta \to \infty$, and state that with high probability, the magnetisation

$$m = \frac{1}{L^2} \sum_{j=1}^{L} s_j \tag{6.27}$$

takes values close to $+1$ or -1. This means that all spins then point to the same direction, spontaneously. "Spontaneous" here means, as is common in physics, that the state emerging has less symmetry that the original problem, which is perfectly symmetric under exchange of $+1$ and -1. In many fields of physics, such as in quantum field theory, one encounters such spontaneously broken symmetries all the time, even if in a slightly different sense.

The basic argument will be that the spins that are in the minority (meaning, the spins not taking the most probable value) are enclosed by a contour which separates $+1$ values from -1 values. Such a contour costs energy and is hence improbable. We will have a closer look at this idea in the following.

Let us first define properly what we think a contour is. A contour C is a line running on the lines of the lattice, which does not cross itself, and which is either closed or which ends on the boundary of the lattice. The length of the contour we denote as $l(C)$. The inner of the contour C is defined as the enclosed surface, if C is closed, or the smaller of the two areas, if C ends at the boundaries and hence cuts the lattice into two parts. We denote this enclosed area with $f(C)$. With this convention, of course we have

$$f(C) = l(C)^2. \tag{6.28}$$

We will also need the number $n(l, L)$ of contours of a given length l. It is not so easy to compute this number, it is a combinatorical problem. Still, this number can somewhat crudely be upper bounded by

$$n(l, L) \leq (L+1)^2 4 3^{l-1}. \tag{6.29}$$

The factor $(L+1)^2$ reflects the choice of the starting point. The factor 4 originates from the freedom of choosing the initial direction. And the factor 3^{l-1} stands for the choice of a direction for the rest of the pieces, respecting the fact that one cannot go back. This is of course not very tight. To start with, not for all lattice sites all 4 initial directions are possible. Also, after a few steps, other directions will be restricted. Still, it is obviously an upper bound, and it will be sufficient for our purposes.

Now we have to bring the concept of a contour together with the spin configurations. For that we define what it means that a contour C fits to a configuration s. We say that C fits to s if C separates $+1$ from -1 everywhere, and if all boundary values in the inner of C have the same value. For a given contour C, the probability $p(C)$ that this contour fits is then

$$p(C) = \frac{\sum_{s,\text{ fits}} e^{\beta J \sum_{\langle j,k\rangle} s_j s_k}}{\sum_s e^{\beta J \sum_{\langle j,k\rangle} s_j s_k}}. \tag{6.30}$$

We now come to an important observation: To each configuration $\tilde{s}$ of the nominator there is a configuration in the nominator s with energy

$$H(\tilde{s}) = 2Jl(C) + H(s), \tag{6.31}$$

which one gets by altering the sign of all spins in the inner of C. In this way, one also alters the interaction terms along the contour line from $-J$ to J, while all other contributions stay the same. This procedure amounts to a change of the interaction energy of $\pm JL(C)$. We can hence single out these terms in the above some, and write

$$p(C) = e^{-2\beta Jl(C)} \frac{\sum_{s,\text{ fits}} e^{\beta J \sum_{\langle j,k\rangle} s_j s_k}}{\sum_{s,\text{ fits}} e^{\beta J \sum_{\langle j,k\rangle} s_j s_k} + \text{further terms}} \leq e^{-2\beta Jl(C)}. \tag{6.32}$$

Here, we have used that the exponential function delivers always positive terms. Up to now, the problem is symmetric under an interchange of $+$ and $-$. For every spin configuration, however, there is at least one spin that is not contained in a fitting contour. Also, according to our convention, no lines of different contours may cross each other and hence there must be at least one site that is not in the inner of a fitting contour. In case there are several spins for a given configuration that are not contained in a fitting contour, then these spins must have the same value: Otherwise, there would be a separating contour between them and one of the spins would be in the inner of this contour. That is to say, we can assign each spin configuration in this way a $+$ or a $-$, called the "outer spin". In this way, we have broken the symmetry between $+$ and $-$ and will

from now on look at only configurations with outer spin +. We will now show that for small temperatures, these configurations will only have a few − spins. We will therefore consider the quantity

$$N_-(s) = \#\{j : s_j = -1\}, \tag{6.33}$$

the number of spins that have in the configuration s the value −. Every − spin has to be contained in a contour, since + spins can only be outside of a contour. We can hence bound the number of − spins by the sum of the areas of all fitting contours. Again the bound is very crude, since contours may be contained within another and hence, for an exact count, some areas have to be counted with a negative sign. But for our purposes, this bound will be tight enough. We get

$$N_-(s) \leq \sum_{C,\text{fits to } s} f(C) \leq \sum_{C,\text{fits to } s} l(C)^2. \tag{6.34}$$

We will now look at the canonical expectation value of N_-, only considering configurations with outer spin +. Again, by this we break the symmetry. We get

$$\begin{aligned} \langle N_- \rangle &\leq \frac{1}{2Z} \sum_{s,+} \left(\sum_{C,\text{fits to } s} l(C)^2 \right) e^{-\beta H(s)} \\ &= \frac{1}{2Z} \sum_C l(C)^2 \sum_{s,\text{fits to } C,+} e^{-\beta H(s)} \\ &= \sum_C l(C)^2 p(C). \end{aligned} \tag{6.35}$$

Remember that $p(C)$ is the probability that the contour C fits to a configuration. The factor $1/2$ is obtained since we only consider configurations with outer spin +. We now put in out bounds derived above and get

$$\begin{aligned} \langle N_- \rangle &\leq \frac{1}{4} \sum_C l(C)^2 e^{-\beta J l(C)} \\ &= \frac{1}{4} \sum_l l^2 e^{-2\beta J l} n(j, L) \\ &\leq \frac{1}{3}(L+1)^2 \sum_{l=2}^{\infty} l^2 e^{-\beta J l} 3^l \\ &\leq \frac{1}{3}(L+1)^2 \sum_{l=0}^{\infty} l^2 (e^{-2\beta J} 3)^l. \end{aligned} \tag{6.36}$$

This sum is convergent if $3e^{-2\beta J} < 1$ or

$$\beta > \log(3)/(2J), \tag{6.37}$$

as one can show by twice differentiating the geometric sum. In particular, the sum goes to 0 if $e^{-2\beta J}$ goes to 0, hence $\beta \to \infty$. For the probability that an arbitrary spin is in the state $-$, we get

$$\left\langle \frac{N_-}{L^2} \right\rangle_+ \to 0 \tag{6.38}$$

for $\beta \to \infty$. Of course we can repeat the calculation with outer spin $-$. One gets in an analogous fashion that the number of $+$ spins is small. In particular, the expectation value for N_- (and of N_+) depends continuously of β, hence also at finite temperatures, with high probability one gets only configurations for which almost all spins take the same value, so either all $+$ or all $-$.

6.1.4 Classical mean field approaches

As we have already mentioned, in 2D the model can be exactly solved, and a closed form of the partition function is known. We will not get into the details of this Onsager solution, however, at this point. Instead, we will pursue a line of thought that gives rise to surprisingly accurate results, in particular for high-dimensional systems (there also is a good reason for that). In this subsection, we will have a look at mean field approaches. The mean field idea is a simple one: One considers each spin to be subject to a "mean field" generated by all of the neighboring ones. Of course, this mean field will again depend on the solution of the problem. The trick is that one takes this mean field as a parameter of the problem, solves the now uncoupled problem, and then asks for self-consistency. We will see how this goes by having another look at the Ising model.

We replace the Hamiltonian of the Ising model in arbitrary dimension (do no longer 1D or 2D) by

$$H(s) = -\frac{1}{2}\sum_j \nu J\langle s\rangle s_j - B\sum_j s_j, \tag{6.39}$$

where ν is the number of nearest-neighbors in the lattice (so the sites with $\mathrm{dist}(j,k) = 1$) and $\langle s\rangle = \langle s_j\rangle$ for each j is the average spin per site. That is, the Hamiltonian can be written as

$$H(s) = -\sum_j E(J,B)s_j, \tag{6.40}$$

where

$$E(J,B) := \frac{1}{2}\nu J\langle s\rangle + \mu B. \tag{6.41}$$

As explained above, we have an uncoupled system, one that we can simply solve – at the expense that the expectation value $\langle s\rangle$ is contained in the expression, which must be determined in a self-consistent manner. The partition function can now be written as

$$Z = \left(\sum_{s_1=\pm 1} e^{\beta E(J,B)s_1}\right)^N = (2\cosh(\beta E))^N. \tag{6.42}$$

We have singled out here s_1, but could have taken any other spin as well, as we encounter a completely uncoupled problem. The free energy per site is then

$$f = -kT \lim_{N\to\infty} \left(\frac{1}{N} \log(Z) \right) = -kT \log(2\cosh(\beta E)) \tag{6.43}$$

The expected magnetization is then

$$\langle m \rangle = \frac{\sum_{s_1=\pm 1} s_1 e^{\beta E s_1}}{\sum_{s_1=\pm 1} e^{\beta E s_1}} = \tanh(\beta E) = \tanh\left(\beta(\frac{1}{2}\nu J \langle s \rangle + B) \right). \tag{6.44}$$

The magnetization is the order parameter for the spin lattice. If $B = 0$, then the magnetization will be zero for the high-temperature paramagnetic phase of the lattice. The spins are just randomly ordered. For low temperatures, in contrast, it will be non-zero when the spins have spontaneously aligned. We will now determine the critical temperature at which the lattice starts to become ordered when the temperature is lowered. We start from the expression of $\langle s \rangle$ for the case of $B = 0$. We then get

$$\langle s \rangle = \tanh\left(\frac{1}{2}\beta \nu J \langle s \rangle \right) = \tanh\left(\frac{\nu J \langle s \rangle}{2kT} \right). \tag{6.45}$$

We now must solve this equation for $\langle s \rangle$. There are many ways of doing this. A particularly appealing way is to do it "graphically", and plots $\langle s \rangle \mapsto \langle s \rangle$ versus

$$\langle s \rangle \mapsto \tanh\left(\alpha \langle s \rangle \right), \tag{6.46}$$

calling

$$\alpha := \frac{\nu J}{2kT}. \tag{6.47}$$

The solution will then correspond to the intersections of the two graphs. Now there are two quite different regimes:

- For $\alpha < 1$ there is only one crossing point at $\langle s \rangle = 0$.
- For $\alpha > 1$ there are now three crossing points: One at $\langle s \rangle = 0$ and one each at $\langle s \rangle = \pm s_0$.

The free energy per site in various cases is

$$f = \begin{cases} -kT \log(2), & \text{if } \langle s \rangle = 0, \\ -kT \log(2\cosh(\beta \nu J s_0/2)), & \text{if } \langle s \rangle = s_0. \end{cases} \tag{6.48}$$

Thus the values $\langle s \rangle = \pm s_0$ describe possible states of thermodynamic equilibrium situations since they minimize the free energy. The transition point (the critical point) is at $\alpha = 1$, and hence when

$$\nu J/(2kT) = 1. \tag{6.49}$$

The critical temperature is therefore

$$T_c = \nu J/(2k). \tag{6.50}$$

Mean field theory hence predicts a phase transition for a D-dimensional cubic lattice. This prediction is wrong in 1D, as we already know, and correct in 2D. It is expected to be good in case of a large number of neighbors, so for a large dimension. This indeed turns out to be true.

6.2 Quantum lattice models

We now turn to quantum lattice models. Again, the Hamiltonian is of the form

$$H = \sum_{j \in V} h_j + \sum_{\langle j,k \rangle} v_{j,k}, \tag{6.51}$$

but now both the on-site terms h_j as well as the nearest-neighbor couplings $v_{j,k}$ are operators with a small support. As mentioned before, quantum lattice models are ubiquitous in physics, in particular in the condensed matter context. We will only have time to have a look at some paradigmatic models.

6.2.1 Bose-Hubbard model and other quantum lattice models

6.2.2 Quantum phase transitions at zero temperature

6.2.3 Fermionic chains and phase transitions of second order