c_1 and c_2 in Fig. 6.7. It was the good fortune of Kac and Ward that they all add up to zero.

On larger than 4×2 lattices, there are more elaborate loops. They can, for example, have crossings (see, for example, the loop in Fig. 6.8). There, the cycle configurations c_1 and c_2 correspond to loops in the generalization of Fig. 6.6 to larger lattices, whereas the cycles c_3 and c_4 are superfluous. However, c_3 makes six left turns and two right turns, so that the overall weight is $\alpha^4 = -1$, whereas the cycle c_4 makes three left turns and three right turns, so that the weight is $+1$, the opposite of that of c_3. The weights of c_3 and c_4 thus cancel.

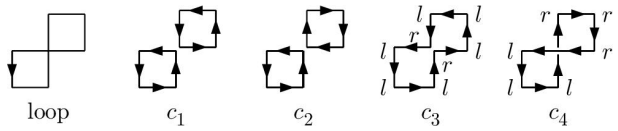

Figure 6.8: Loop and cycle configurations. The weights of c_3 and c_4 cancel.

For larger lattices, it becomes difficult to establish that the sum of cycle configurations in the determinant indeed agrees with the sum of loop configurations of the high-temperature expansion, although rigorous proofs exist to that effect. However, at our introductory level, it is more rewarding to proceed heuristically. We can, for example, write down the 144×144 matrix $U_{6\times6}$ of the 6×6 lattice for various temperatures (using Alg. combinatorial-ising.py), and evaluate the determinant $\det U_{6\times6}$ with a standard linear-algebra routine. Partition functions thus obtained are equivalent to those resulting from Gray-code enumeration, even though the determinant is evaluated in on the order of $144^3 \simeq 3\times10^6$ operations, while the Gray code goes over $2^{35} \simeq 3\times10^{10}$ configurations. The point is that the determinant can be evaluated for lattices that are much too large to go through the list of all configurations.

The matrix $U_{L\times L}$ for the $L \times L$ lattice contains the key to the analytic solution of the two-dimensional Ising model first obtained, in the thermodynamic limit, by Onsager (1944). To recover Onsager's solution, we would have to compute the determinant of U, not numerically as we did, but analytically, as a product over all the eigenvalues. Analytic expressions for the partition functions for Ising models can also be obtained for finite lattices with periodic boundary conditions. To adapt for the changed boundary conditions, one needs four matrices, generalizing the matrix U (compare with the analogous situation for dimers in chapter xx. Remarkably, evaluating $Z(\beta)$ on a finite lattice reduces to evaluating an explicit function (see the classical papers by Kaufman (1949) [13] and Ferdinand and Fisher (1969) [16].

The analytic solutions of the Ising model have not been generalized to higher dimensions, where only Monte Carlo simulations, high-temperature expansions, and renormalization-group calculations allow to compute to high precision the properties of the phase transition. These properties, as mentioned, are universal, that is, they are the same for a wide class of systems, called the Ising universality

class.

6.3 Density of states from thermodynamics

FIXME {TO FINISH In this chapter, we have computed the thermodynnamics of the two-dimensional Ising model by two different approaches that differ in the role played by the density of states. In Alg. enumerateising_dos, it was appropriate to first compute $\mathcal{N}(E)$, and later determine partition functions, internal energies, and specific heat capacities at any temperature. In contrast, in the counting procedure of Kac and Ward, as in the Onsager solution of the Ising model, we determined the partition function $Z(\beta)$, not the density of states. Computing $Z(\beta)$ from $\mathcal{N}(E)$ is straightforward, but how to recover $\mathcal{N}(E)$ from $Z(\beta)$ requires some thought:

$$\mathcal{N}(E) \underset{??}{\overset{\text{easy}}{\rightleftarrows}} Z(\beta).$$

The mathematical problem of computing the density of states from the partition function is one of the basic problems in statistical and solid state physics, and it appears also in the interpretation of experimental or Monte Carlo data. In the presence of statistical uncertainties, it is very difficult to solve, and may often be ill-defined. This means, in our case, that algorithms exist for computing $\mathcal{N}E$ if the partition functions were computed exactly. If, however, $Z(\beta)$ is known only to limited precision, the output generated by the slightly perturbed input can be drastically different from the exact output.

For the two-dimensional Ising model, a procedure put together by Beale has allowed to compute the density of states for system sizes up to 200×200. **}**

6.4 Explicit calculations of Partition function (Python + Diagonalization)

On the website, one may find the 20-line program `combinatorial_ising.py`, which actually computes the partitition function via the matrix diagonalization shown in the previous section. The complex-valued matrix in question, as mentioned, is of size $4N \times 4N$, it gives directly the partition function of the Ising model without periodic boundary conditions. From this function, through an a bit pedestrian procedure, we can obtain the internal energy, the heat capacity, and all the thermodynamic properties. Of course, our program only works for small lattices, it would have to be written more carefully in order to avoid numerical overflow. The matrices that we have written down can be diagonalized explicitly, and all the eigenvalues computed (TODO). The result agrees very well with the exact result.

A magnificent result is due to Kaufman in 1949[13]. She has computed the exact partition function of the $N \times N$ lattice with periodic boundary conditions,

and obtained an explicit formula for it. This explicit formula is programmed in `kaufman_formula.py`.

6.5 General results for the NxN Ising model, Kaufman, Ferdinand & Fisher

Let us consider, for a moment, the formulas for the free energy

$$Z(\beta) = \overbrace{\sum_{\sigma_1=\pm1,\ldots,\sigma_N=\pm1} \exp -\beta E(\sigma_1,\ldots,\sigma_N)}^{\propto 2^N \text{ terms}} = \overbrace{\sum_E dosE \exp -\beta E}^{\propto N \text{ terms}}.$$

Similarly, the mean energy $\langle E \rangle$ can be computed from $Z(\beta)$ by numerical differentiation, that is,

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log Z, \tag{6.12}$$ {OD_mean_energy_derivative}

but we are again better off using an average over the density of states:

$$\langle E \rangle = \frac{\sum_\sigma E_\sigma \exp -\beta E_\sigma}{\sum_\sigma \exp -\beta E_\sigma} = \frac{1}{Z} \sum_E E dosE \exp -\beta E, \tag{6.13}$$ {OD_mean_energy}

$$\langle E \rangle = \frac{\sum_\sigma E_\sigma \exp -\beta E_\sigma}{\sum_\sigma \exp -\beta E_\sigma} = \frac{1}{Z} \sum_E E dosE \exp -\beta E, \tag{6.14}$$ {OD_mean_energy}

where we have used σ as a shorthand for $\{\sigma_1,\ldots,\sigma_N\}$. Higher moments of the energy can also be expressed via $dosE$:

$$\langle E^2 \rangle = \frac{\sum_\sigma E_\sigma^2 \exp -\beta E_\sigma}{\sum_\sigma \exp -\beta E_\sigma} = \frac{1}{Z} \sum_E E^2 dosE \exp -\beta E. \tag{6.15}$$ {OD_mean_square_energy}

The specific heat capacity C_V, the increase in internal energy caused by an infinitesimal increase in temperature,

$$C_V = \frac{\partial \langle E \rangle}{\partial T} = \frac{\partial \beta}{\partial T} \frac{\partial \langle E \rangle}{\partial \beta} = -\beta^2 \frac{\partial \langle E \rangle}{\partial \beta}, \tag{6.16}$$ {OD_specific_head_derivati

can be expressed via Eq. 6.12 as a second-order derivative of the partition function:

$$C_V = \beta^2 \frac{\partial^2}{\partial \beta^2} \log Z.$$

Again, there is a more convenient expression, which we write for the specific heat capacity per particle c_V,

$$\underline{c_V} = -\frac{\beta^2}{N}\frac{\partial \langle E\rangle}{\partial \beta} = -\frac{\beta^2}{N}\frac{\partial}{\partial \beta}\left(\frac{\sum_{\boldsymbol{\sigma}} E_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta E_\sigma}}\right)$$
$$= \frac{\beta^2}{N}\frac{\sum_{\boldsymbol{\sigma}} E^2 \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}} \sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}} - (\sum_{\boldsymbol{\sigma}} E_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}})^2}{(\sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}})^2} = \underline{\frac{\beta^2}{N}(\langle E^2\rangle - \langle E\rangle^2)},$$

which can be evaluated with the second formulas in Eq. 6.14 and Eq. 6.15 and is implemented in Alg. thermo-ising. We can recognize that the specific heat capacity, an experimentally measurable quantity, is proportional to the variance of the energy, a statistical measure of the distribution of energies. Specific-heat-capacity data for small two-dimensional lattices with periodic boundary conditions are shown in Fig. 6.9.

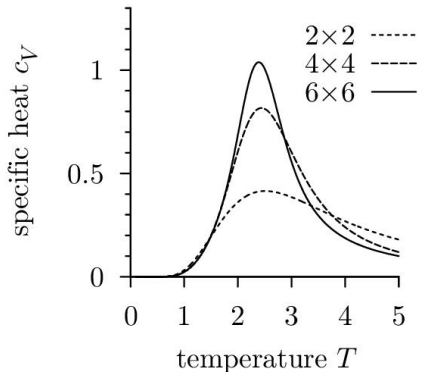

Figure 6.9: Specific heat per spin for small Ising systems with periodic boundary conditions. Data obtained by exact enumeration, using Alg. enumerate_ising.py. The naive python version only works for 2×2 and 4×4 systems.

6.6 Kramers and Wannier duality

We now analyze the $512 = 3^3$ loop configurations in Fig. 6.3 and see where the non-analycity of the partition function (the divergence of its second derivative with respect to temperature, at the critical temperature T_c) can come up.

As discussed before, the loop configurations came from a high-temperature expansion as it is in powers of $\tanh\beta$, that goes as β for small arguments. Kramers and Wannier, in 1941[17], first noted that this same expansion also applies to a low-temperature expansion on the dual lattice (the lattice of edges of the original one). This is sketched in Fig. 6.11: Any loop configuration of

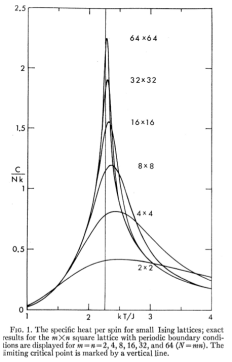

Figure 6.10: Specific heat per spin for the Ising model on a square lattice, with periodic boundary conditions. From Ferdinand and Fisher (1969)[16]. The free energy is everywhere continuous, and so is the energy per particle (a first derivative of the free energy. The second derivative of the free energy, the specific heat, diverges logarithmically at the critical point.

the van der Waerden high-temperature expansion on the $N \times N$ lattice without periodic boundary conditions, where each edge carries a $\tanh \beta$ (shown on the left figure), could correspond to a domain of equally oriented spins within a sea of opposite spins. As shown in the rightmost panel of the figure, the [**?**] loop configurations on the $N \times N$ lattice are isomorohic to domain loops of the $(N+1) \times (N+1)$ lattice where the outer ring of spins are all negative.

By exploiting this property, Kramers and Wannier first obtained the value of the critical temperature, and this of course before Onsager's analytical solution of the model. It should be noted that at the time at which duality was first discussed, Peierls had already proven (see the orgument sketched in Section 6.8) that the two-dimensional Ising model must have a phase transition.

We continue with finite square lattices with periodic boundary conditions: These lattices are self-dual: The $L \times L$ lattice has a dual lattice of same size, with lattice sites at the center of the original cells. **FIXME {**add figure in 1d, 2d, 3d**}**.

On the $L \times L$ lattice with periodic boundary conditions, we can now write down the partition function in two ways: On the one hand we can enumerate domain walls, and compute as follows.

$$Z_{pbc}(\beta) = 2\ \mathrm{e}^{2N\beta} \sum_{l} g(l) \mathrm{e}^{-2l\beta} \tag{6.17}$$ {e:loops_low_T}

where $g(l)$ is the number of loop configurations of length l (the red "2" comes from the fact that we should count each loop configuration twice, once for a "+" domain in a sea of "-" and once for a "-" domain Eq. 6.17, the loop configurations describe domain walls. There can be intersecting loops, or loops within loops, as the "red" configuration in Fig. 6.3.

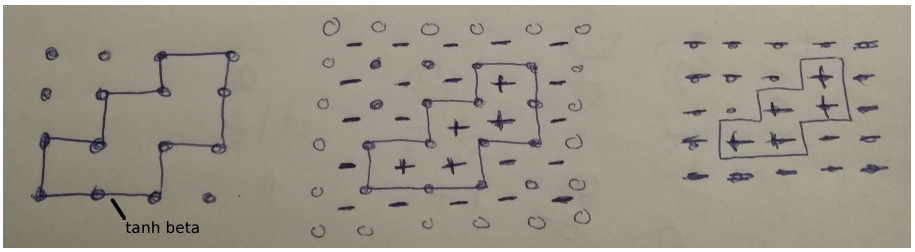

Figure 6.11: Square lattice duality: *Left*: One of the 512 loop configuration on the $4x4$ lattice without periodic boundary condition. Each of the links on the loop carries a $\tanh\beta$ *Center:* Construction of a slightly larger 6×6 lattice, and the *dual* 5×5 lattice made up of its centers. Now, the loop describes a domain wall. Note that on the outer layer of the dual lattice, spins are put to -1. *right*: 5×5 dual lattice, by itself.

An alternative representation of the partition function is given by Eq. 6.5 (the high-temperature expansion of $Z_x x$) adapted to the case of the N-site lattice with periodic boundary conditions. Writing it for a temperature $\tilde{\beta}$, we have

$$Z_{pbc}(\tilde{\beta}) = 2^N \cosh^{2N}\tilde{\beta} \sum_l g(l) \tanh^l \tilde{\beta} \tag{6.18}$$ {e:loops_high_T}

In Eq. 6.17 and Eq. 6.18, the function $g(l)$ describing loop configurations on a finite lattice are exactly the same. In addition, we can choose for any temperature β another temperature $\tilde{\beta}$, by

$$\Upsilon = \mathrm{e}^{-2\beta} = \tanh\tilde{\beta} \tag{6.19}$$

so that everything that the sums in the two equations is the same. We can then write, in Eq. 6.17:

$$\text{in Eq. 6.17: } \mathrm{e}^{2N\beta} = \tanh^{-N}\tilde{\beta} \tag{6.20}$$

So that we arrive at the expression:

$$Z(\tilde{\beta}) = 2^N \cosh^{2N}\tilde{\beta}\ \tanh^N\tilde{\beta}\ Z(\beta) \tag{6.21}$$ {e:Ising_duality}

If there is a single transition, it must take place at the temperature

$$\mathrm{e}^{-2\beta} = \tanh\beta = \frac{\mathrm{e}^{-\beta} - \mathrm{e}^{\beta}}{\mathrm{e}^{-\beta} + \mathrm{e}^{\beta}} \tag{6.22}$$ {e:Ising_duality_critical_T

To find this temperature, we can either, naively, solve Eq. 6.22 by doing

$$\beta \to \beta' = \left[(\beta - \frac{1}{2}\left(\log\tanh\beta\right)\right]/2 \tag{6.23}$$

Then do $\beta' \to \beta''$ etc. In a few steps, we will converge to $\beta = 0.44068679351$. To understand this value, we set $\exp(-\beta) = x$ in Eq. 6.22, and further:

$$x^2 = \frac{1/x - x}{x + 1/x} \tag{6.24}$$

which leads to a quadratic equation for $u = x^2$ with the solution $u = \sqrt{2} - 1$, so that we reach

$$\beta = -\frac{1}{2} \log \frac{1}{\sqrt{2} - 1} = \frac{1}{2} \log \left(1 + \sqrt{2}\right) = 0.44068\ldots \tag{6.25}$$

To better understand the Kramers–Wannier duality, we can further investigate it on a finite lattice. An example for the 4×4 lattice with periodic boundary condition is programmed in Alg. `Ising_dual_4x4.py`. We will notice that the duality works great at small temperature (β large, $\tilde{\beta}$ small), but that there is a finite ratio between the partition functions.

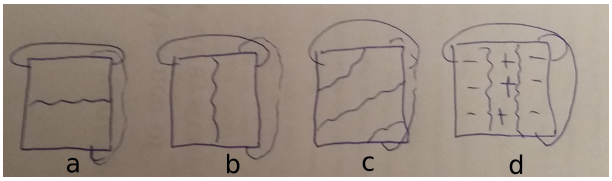

Figure 6.12: a-c: Loop configurations that appear in the high-temperature expansion of the Ising model with periodic boundary conditions, but not in the low-temperature expansion. d: Loop configuration (made up of two loops) that does appear in both expansions.

Unfortunately, for finite lattices, the situation is a bit more complicated: For periodic boundary conditions, a number of graphs in the high-temperature expansion do not appear in the low-temperature expansion. Three example are shown in Fig. **??**, namely paths winding around the lattice in either the x direction or the y direction, or in both x and y. So, although the finite square lattice is self-dual, the partition functions at β and $\tilde{\beta}$ are not exactly related to one another. However, the differences are minor and do not affect the free energy per site in the thermodynamic limit.

6.7 Mean-field solution, mean-field exponents

Mean-field theory is an important model, with which to juxtapose the richer and more physical models. The mean field model consistes in supposing at the same time that every spin has q neighbors but that it is in fact connected to all the $N - 1$ other sites in the lattice. One thus writes

$$E(\sigma) = -\frac{qJ}{N-1} \sum_{i.j} \sigma_i \sigma_j - H \sum_i \sigma_i \tag{6.26}$$

where the sum carries over all the $N(N-1)/2$ distinct pairs (i,j). It is easy to see that the energy of the mean-field model only depends on the total magnetization

$$E(\sigma) = -\frac{1}{2}qJ(M^2 - N)/(N-1) - HM \tag{6.27}$$

where we use that the spins are all of size 1. It is extremely simple to compute the partition function of this model, and one finds:

$$Z = \sum_r c_r \tag{6.28}$$

where

$$c_r = \frac{N!}{r!(N-r)!} \exp\{1/2\beta qJ[(N-2r)^2 - N]/(N-1) + \beta H(N-2r)\} \tag{6.29}$$

This model has a phase transition at $\beta_c = 1/(qJ)$. **FIXME {**Add graphs to discuss mean-field theory**}**

6.8 Spontaneous Magnetization

As mentioned in Section 6.6, duality by itself cannot prove the existence of a phase transition. It rather provides a relation between partition functions on a lattice and its dual lattice at two temperatures, β and $\tilde{\beta}$. It is under the added hypothesis that there is a (unique) phase transition point, this is due to. The question arises how to prove that the Ising model does have a phase transition, without going through the explicit solution that we discussed in Section **??**. It is crucial to realize In this respect, that it is not sufficient to prove that the groundstate (that is realized at strictly zero temperature) is ferromagnetic. The important point here is the existence of a phase transition at finite temperature.

The important step, namely the proof that at small but finite temperature, there is a finite magnetization, was taken by Peierls, in 1936[18]. It is based on an argument about the number of paths in the low-temperature expansion. We will not repeat this argument here.

FIXME { Peierl's argument proves the existence of a spontaneous magnetization, but cannot explain how it decreases to zero at the critical point.

The spontaneous magnetization is predicted by mean-field theory to be, but a famous result of Onsager proves it to go to zero with a power of 1/8.**}**

6.9 Exact solution of the two-dimensional Ising spin glass

In the Ising model, we choose all the interactions to equal $J = +1$. In many cases, however, the interactions can be different, for example all negative, or even, for some pairse $J_{ij} = +1$ and for other pairs $J_{ij} = +1$ (see Fig. **??**), or the