VI.G Exact free energy of the Square Lattice Ising model

As indicated in eq.(VI.35), the Ising partition function is related to a sum S, over collections of paths on the lattice. The allowed graphs for a square lattice have 2 or 4 bonds per site. Each bond can appear only once in each graph, contributing a factor of $t \equiv \tanh K$. While it is tempting to replace S with the exactly calculable sum S', of all phantom loops of random walks on the lattice, this leads to an overestimation of S. The differences between the two sums arise from intersections of random walks, and can be divided into two categories:

(a) There is an over-counting of graphs which intersect at a *site*, i.e. with 4 bonds through a point. Consider a graph composed of two loops meeting at a site. Since a walker entering the intersection has three choices, this graph can be represented by *three distinct random walks.* One choice leads to two disconnected loops; the other two are single loops with or without a self–crossing in the walker's path.

(b) The independent random walkers in S' may go through a particular lattice *bond* more than once.

Including these constraints amounts to introducing interactions between paths. The resulting interacting random walkers are non–Markovian, as each step is no longer independent of previous ones and of other walkers. While such interacting walks are not in general amenable to exact treatment, in two dimensions an interesting topological property allows us to make the following assertion:

$$S = \sum \text{collections of loops of random walks } \textit{with no } \text{U } \textit{turns} \\ \times t^{\text{number of bonds}} \times (-1)^{\text{number of crossings}}. \tag{VI.55}$$

The negative signs for same terms reduce the overestimate and render the exact sum.

Proof: We shall deal in turn with the two problems mentioned above.

(a) Consider a graph with many intersections and focus on a particular one. A walker must enter and leave such an intersection twice. This can be done in three ways only one of which involves the path of the walker crossing itself (when the walker proceeds straight through the intersection). This configuration carries an additional factor of (-1) according to eq.(VI.55). Thus, independent of other crossings, these three configurations sum up to contribute a factor of 1. By repeating this reasoning at each intersection, we see that the over-counting problem is removed and the sum over all possible ways of tracing the graph leads to the correct factor of one.

(b) Consider a bond that is crossed by two walkers (or twice by the same walker). We can imagine the bond as an avenue with two sides. For each configuration in which the two paths enter and leave on the same side of the avenue, there is another one in which the paths go to the opposite side. The latter involves a crossing of paths and hence carries a minus sign with respect to the former. The two possibilities thus cancel out! The reasoning can be generalized to multiple passes through any bond. The only exception is when the doubled bond is created as a result of a U–turn. This is why such backward steps are explicitly excluded from eq.(VI.55).

Let us label random walkers with no U–turns, and weighted by $(-1)^{\text{number of crossings}}$, as RW*s. Then as in eq.(VI.37) the terms in S can be organized as

$$\begin{aligned} S =& \sum(\text{RW}^*\text{s with 1 loop}) + \sum(\text{RW}^*\text{s with 2 loops}) + \sum(\text{RW}^*\text{s with 3 loops}) + \cdots \\ =& \exp\left[\sum(\text{RW}^*\text{s with 1 loop})\right]. \end{aligned} \tag{VI.56}$$

The exponentiation of the sum is justified, since the only interaction between RW*s is the sign related to their crossings. As two RW* loops always cross an even number of times, this is equivalent to no interaction at all. Using eq.(VI.35), the full Ising free energy is calculated as

$$\ln Z = N\ln 2 + 2N\ln\cosh K + \sum\left(\text{RW}^*\text{s with 1 loop} \times t^{\#\text{ of bonds}}\right). \tag{VI.57}$$

Organizing the sum in terms of the number of bonds, and taking advantage of the translational symmetry of the lattice (up to corrections due to boundaries),

$$\frac{\ln Z}{N} = \ln\left(2\cosh^2 K\right) + \sum_{\ell}^{\infty}\frac{t^\ell}{\ell}\left\langle \mathbf{0}|W^*(\ell)|\mathbf{0}\right\rangle, \tag{VI.58}$$

where

$$\begin{aligned} \langle \mathbf{0}|W^*(\ell)|\mathbf{0}\rangle =& \text{number of closed loops of } \ell \text{ steps, with no U turns, from } \mathbf{0} \text{ to } \mathbf{0} \\ & \times (-1)^{\#\text{ of crossings}}. \end{aligned} \tag{VI.59}$$

The absence of U–turns, a local constraint, does not complicate the counting of loops. On the other hand, the number of crossings is a function of the complete configuration of the loop and is a non–Markovian property. Fortunately, in two dimensions it is possible to obtain the *parity* of the number of crossings from local considerations. The first step is to construct the loops from *directed* random walks, indicated by placing an arrow along the direction that the path is traversed. Since any loop can be traversed in two directions,

$$\langle \mathbf{0}|W^*(\ell)|\mathbf{0}\rangle = \frac{1}{2}\sum \textit{directed}\ \mathrm{RW}^*\ \text{loops of } \ell \text{ steps, no U turns, from } \mathbf{0} \text{ to } \mathbf{0} \times (-1)^{n_c}, \tag{VI.60}$$

where n_c is the number of self–crossings of the loop. We can now take advantage of the following topological result:

Whitney's Theorem: The number of self–crossings of a planar loop is related to the total angle Θ, through which the tangent vector turns in going around the loop by

$$(n_c)_{\mathrm{mod}\ 2} = \left(1 + \frac{\Theta}{2\pi}\right)_{\mathrm{mod}\ 2}. \tag{VI.61}$$

This theorem can be checked by a few examples. A single loop corresponds to $\Theta = \pm 2\pi$, while a single intersection results in $\Theta = 0$.

Since the total angle Θ, is the sum of the angles through which the walker turns at each step, the parity of crossings can be obtained using *local* information alone as

$$(-1)^{n_c} = e^{i\pi n_c} = \exp\left[i\pi\left(1 + \frac{\Theta}{2\pi}\right)\right] = -e^{\frac{i}{2}\sum_{j=1}^{\ell}\theta_j}, \tag{VI.62}$$

where θ_j is the angle through which the walker turns on the j^{th} step, leading to

$$\begin{aligned}\langle \mathbf{0}|W^*(\ell)|\mathbf{0}\rangle = -\frac{1}{2}\sum \textit{directed}\ \mathrm{RW}^*\ &\text{loops of } \ell \text{ steps, with no U turns, from } \mathbf{0} \text{ to } \mathbf{0}\\ &\times \exp\left(\frac{1}{2}\sum \text{ local change of angle by the tangent vector}\right).\end{aligned} \tag{VI.63}$$

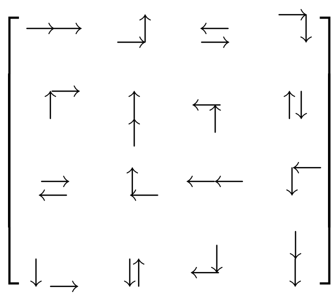
The angle turned can be calculated at each site, if we keep track of the directions of arrival and departure of the path. To this end, we introduce a label μ for the 4 directions *going out* of each site, e.g. $\mu = 1$ for right, $\mu = 2$ for up, $\mu = 3$ for left, and $\mu = 4$ for down. We next introduce a set of $4N \times 4N$ matrices generalizing eq.(VI.39) as

$$\begin{aligned}\langle x_2y_2, \mu_2|W^*(\ell)|x_1y_1, \mu_1\rangle = \sum &\text{directed random walks of } \ell \text{ steps, with no U turns,}\\ &\text{departing } (x_1, y_1) \text{ along } \mu_1, \text{ proceeding along } \mu_2 \text{ after reaching } (x_2, y_2) \times e^{\frac{i}{2}\sum_{j=1}^{\ell}\theta_j}.\end{aligned} \tag{VI.64}$$

Thus μ_2 specifies a direction taken *after* the walker reaches its destination. It serves to exclude some paths (arriving along -μ_2), and leads to an additional phase. As in eq.(VI.43), due to their Markovian property, these matrices can be calculated recursively as

$$\begin{aligned}&\langle x_2 y_2, \mu_2 | W^*(\ell) | x_1 y_1, \mu_1 \rangle \\ &\qquad = \sum_{x'y',\mu'} \langle x_2 y_2, \mu_2 | T^* | x'y', \mu' \rangle \langle x'y', \mu' | W^*(\ell-1) | x_1 y_1, \mu_1 \rangle \\ &\qquad = \langle x_2 y_2, \mu_2 | T^* W^*(\ell-1) | x_1 y_1, \mu_1 \rangle = \left\langle x_2 y_2, \mu_2 | T^{*\ell} | x_1 y_1, \mu_1 \right\rangle ,\end{aligned} \tag{VI.65}$$

where $T^* \equiv W^*(1)$ describes one step of the walk. The direction of arrival uniquely determines the nearest neighbor from which the walker departed, and the angle between the two directions fixes the phase of the matrix element. We can thus generalize eq.(VI.46) to a 4×4 matrix that keeps track of both connectivity and phase between pairs of sites. The steps taken can be represented diagrammatically as

$T =$  , (VI.66)

and correspond to the matrix

$$\langle x'y' | T^* | xy \rangle =$$

$$\begin{bmatrix} \langle x', y' | x+1, y \rangle & \langle x', y' | x+1, y \rangle \, e^{\frac{i\pi}{4}} & 0 & \langle x', y' | x+1, y \rangle \, e^{-\frac{i\pi}{4}} \\ \langle x', y' | x, y+1 \rangle \, e^{-\frac{i\pi}{4}} & \langle x', y' | x, y+1 \rangle & \langle x', y' | x, y+1 \rangle \, e^{\frac{i\pi}{4}} & 0 \\ 0 & \langle x', y' | x-1, y \rangle \, e^{-\frac{i\pi}{4}} & \langle x', y' | x-1, y \rangle & \langle x', y' | x-1, y \rangle \, e^{\frac{i\pi}{4}} \\ \langle x', y' | x, y-1 \rangle \, e^{\frac{i\pi}{4}} & 0 & \langle x', y' | x, y-1 \rangle \, e^{-\frac{i\pi}{4}} & \langle x', y' | x, y-1 \rangle \end{bmatrix} , \tag{VI.67}$$

where $< x, y | x', y' > \equiv \delta_{x,x'} \delta_{y,y'}$.

Because of its translational symmetry, the $4N \times 4N$ matrix takes a *block diagonal* form in the Fourier basis, $\langle xy | q_x q_y \rangle = e^{i(q_x x + q_y y)} / \sqrt{N}$, i.e.

$$\sum_{xy} \langle x'y', \mu' | T^* | xy, \mu \rangle \langle xy | q_x q_y \rangle = \langle \mu' | T^*(\mathbf{q}) | \mu \rangle \langle x'y' | q_x q_y \rangle . \tag{VI.68}$$

Each 4×4 block is labelled by a wavevector $\mathbf{q} = (q_x, q_y)$, and takes the form

$$T^*(\mathbf{q}) = \begin{bmatrix} e^{-iq_x} & e^{-i(q_x - \frac{\pi}{4})} & 0 & e^{-i(q_x + \frac{\pi}{4})} \\ e^{-i(q_y + \frac{\pi}{4})} & e^{-iq_y} & e^{-i(q_y - \frac{\pi}{4})} & 0 \\ 0 & e^{i(q_x - \frac{\pi}{4})} & e^{iq_x} & e^{i(q_x + \frac{\pi}{4})} \\ e^{i(q_y + \frac{\pi}{4})} & 0 & e^{i(q_y - \frac{\pi}{4})} & e^{iq_y} \end{bmatrix} . \tag{VI.69}$$

To ensure that a path that starts at the origin completes a loop properly, the final arrival direction at the origin must coincide with the original one. Summing over all 4 such directions, the total number of such loops is obtained from

$$\langle \mathbf{0}|W^*(\ell)|\mathbf{0}\rangle = \sum_{\mu=1}^{4} \langle 00, \mu|T^{*\ell}|00, \mu\rangle = \frac{1}{N}\sum_{xy,\mu} \langle xy, \mu|T^{*\ell}|xy, \mu\rangle = \frac{1}{N}\,\mathrm{tr}\left(T^{*\ell}\right). \qquad \text{(VI.70)}$$

Using eq.(VI.58), the free energy is calculated as

$$\begin{aligned}\frac{\ln Z}{N} &= \ln\left(2\cosh^2 K\right) - \frac{1}{2}\sum_{\ell}\frac{t^\ell}{\ell}\langle \mathbf{0}|W^*(\ell)|\mathbf{0}\rangle = \ln\left(2\cosh^2 K\right) - \frac{1}{2N}\,\mathrm{tr}\left[\sum_{\ell}\frac{T^{*\ell}t^\ell}{\ell}\right] \\ &= \ln\left(2\cosh^2 K\right) + \frac{1}{2N}\,\mathrm{tr}\ln\left(1 - tT^*\right) \\ &= \ln\left(2\cosh^2 K\right) + \frac{1}{2N}\sum_{\mathbf{q}}\mathrm{tr}\ln\left(1 - tT^*(\mathbf{q})\right). \end{aligned} \qquad \text{(VI.71)}$$

But for any matrix M with eigenvalues $\{\lambda_\alpha\}$,

$$\mathrm{tr}\ln M = \sum_{\alpha}\ln\lambda_\alpha = \ln\prod_{\alpha}\lambda_\alpha = \ln\det M.$$

Converting the sum over $\mathbf{q}$ in eq.(VI.71) to an integral leads to

$$\begin{aligned}\frac{\ln Z}{N} &= \ln\left(2\cosh^2 K\right) + \\ &\frac{1}{2}\int\frac{d^2\mathbf{q}}{(2\pi)^2}\ln\left\{\det\begin{vmatrix} 1 - te^{-iq_x} & -te^{-i(q_x-\frac{\pi}{4})} & 0 & -te^{-i(q_x+\frac{\pi}{4})} \\ -te^{-i(q_y+\frac{\pi}{4})} & 1 - te^{-iq_y} & -te^{-i(q_y-\frac{\pi}{4})} & 0 \\ 0 & -te^{i(q_x-\frac{\pi}{4})} & 1 - te^{iq_x} & -te^{i(q_x+\frac{\pi}{4})} \\ -te^{i(q_y+\frac{\pi}{4})} & 0 & -te^{i(q_y-\frac{\pi}{4})} & 1 - te^{iq_y}\end{vmatrix}\right\}.\end{aligned} \qquad \text{(VI.72)}$$

Evaluation of the above determinant is straightforward, and the final result is

$$\frac{\ln Z}{N} = \ln\left(2\cosh^2 K\right) + \frac{1}{2}\int\frac{d^2\mathbf{q}}{(2\pi)^2}\ln\left[\left(1+t^2\right)^2 - 2t\left(1-t^2\right)\left(\cos q_x + \cos q_y\right)\right]. \qquad \text{(VI.73)}$$

Taking advantage of trigonometric identities, the result can be simplified to

$$\frac{\ln Z}{N} = \ln 2 + \frac{1}{2}\int_{-\pi}^{\pi}\frac{dq_x dq_y}{(2\pi)^2}\ln\left[\cosh^2(2K) - \sinh(2K)\left(\cos q_x + \cos q_y\right)\right]. \qquad \text{(VI.74)}$$

While it is possible to obtain a closed form expression by performing the integrals exactly, the final expression involves a hypergeometric function, and is not any more illuminating.