Homework 7, Statistical Mechanics: Concepts and applications
2019/20 ICFP Master (first year)

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In lecture 07 (Ising model: from van der Waerden to Kac and Ward's combinatorial solution) we treated high-temperature expansions of the two-dimensional Ising model, leading up to its exact solution through a method that identifies the high-temperature undirected loops with the directed permutation cycles of a corresponding matrix. This also provides the theme for the present homework session.

I. PERMUTATION CYCLES AND DETERMINANTS

A. Preparation (general matrix)

Consider a general 4×4 matrix A with real elements:

$$A = \begin{pmatrix} 1 & a_{12} & a_{13} & a_{14} \\ a_{21} & 1 & a_{23} & a_{24} \\ a_{31} & a_{32} & 1 & a_{34} \\ a_{41} & a_{42} & a_{43} & 1 \end{pmatrix} \tag{1}$$

and its determinant

$$\det A = \sum_P \operatorname{sign}(P) a_{1P(1)} a_{2P(2)} a_{3P(3)} a_{4P(4)}. \tag{2}$$

where P are the 24 permutations of the elements $(1, 2, 3, 4)$. Write down the terms in the determinant corresponding to some of the permutations, and explain that the formula

$$\det A = \sum_{\substack{\text{cycle}\\ \text{configs}}} (-1)^{\#\text{ of cycles}} \underbrace{a_{P_1P_2} a_{P_2P_3} \dots a_{P_MP_1}}_{\text{weight of first cycle}} \underbrace{a_{P'_1P'_2} \dots}_{\text{other cycles}}$$

$$= \sum_{\substack{\text{cycle}\\ \text{configs}}} \begin{Bmatrix} (-1)\cdot \text{ weight of} \\ \text{first cycle} \end{Bmatrix} \times \dots \times \begin{Bmatrix} (-1)\cdot \text{ weight of} \\ \text{last cycle} \end{Bmatrix}. \tag{3}$$

is OK for even N (no proof needed, just provide the "feel" that eq. (2) is correct). Illustrate the presence of “hairpin” terms in the determinant. if a_{ij} is available alongside a_{ji}.

All the permutations could be decomposed into a series of operations of exchanging two elements. Forming a k-cycle (from the identity permutation) requires $k-1$ operations. Thus, the total number of operations of a permutation is

$$N_{ex} = \sum_{i=1}^{n} (k_i - 1)$$

where N_{ex} is the total number of exchanges, i denotes cycles and n is the total number of cycles. Since $\sum_{i=1}^{n} k_i = N$ and N is even, what matters for the sign of this permutation is then $\sum_{i=1}^{n} 1 = n$.

If a_{ij} appears along with a_{ji}, They form a cycle on their own.

B. Naive matrix $\tilde{U}_{2\times2}$

In lecture 07, we considered the naive matrix:

$$\hat{U}_{2\times2} = \begin{bmatrix} 1 & \gamma\tanh(\beta) & \cdot & \cdot \\ \cdot & 1 & \cdot & \gamma\tanh\beta \\ \gamma\tanh(\beta) & \cdot & 1 & \cdot \\ \cdot & \cdot & \gamma\tanh(\beta) & 1 \end{bmatrix}.$$

where any "$\cdot$" stand for "0" and $\gamma = \mathrm{e}^{i\pi/4} = \sqrt[4]{-1}$. Write down the determinant of this matrix in terms of permutation cycles. Show that

$$Z_{2\times2} = (2^4 \cosh^4\beta) \det\left(\hat{U}_{2\times2}\right) \tag{4}$$

corresponds to the partition function of the 2×2 partition function of the Ising model without periodic boundary conditions. Familiarize yourself with how to visualize cycles in the matrix (from one element of the matrix, you move vertically to the diagonal, then horizontally to the next element, etc).

There are two permutations which gives none 0 terms, one of them is identity, i.e. $\left(\begin{smallmatrix}1&2&3&4\\1&2&3&4\end{smallmatrix}\right)$. This permutation gives 1. The other permutation contains one cycle. The cycle is identified as in Fig. 1 and its contribution (including the sign introduced by the cycle) is $-\gamma^4\tanh^4(\beta)$. Thus, the determinant is $1+\tanh(\beta)$ and $Z_{2\times2} = 2^4\cosh^4\beta\det\left(\hat{U}_{2\times2}\right)$

$$\begin{bmatrix} 1 & \gamma\tanh(\beta) & \cdot & \cdot \\ & 1 & & \gamma\tanh\beta \\ \gamma\tanh(\beta) & & 1 & \\ \cdot & \cdot & \gamma\tanh(\beta) & 1 \end{bmatrix}$$

FIG. 1: Identifying the cycle in the matrix

II. THE $4N \times 4N$ KAC-WARD MATRIX FOR THE ISING MODEL ON N SITES

We now treat the Kac-Ward matrix U, whose determinant is connected to the square of the partition function Z:

$$Z = 2^N \cosh(\beta)^{N_e} \sqrt{\det(U)} \tag{5}$$

where N is the number of sites and $N_e = 2L(L-1)$ the number of edges. The key idea has to do with car traffic (see Fig. 2).

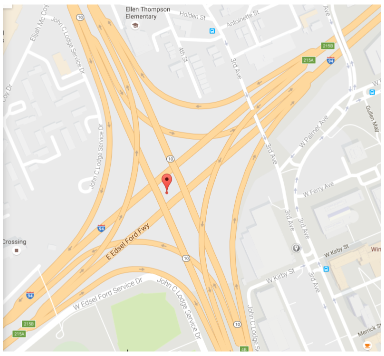

FIG. 2: Highway crossing. To solve the two-dimensional Ising model, Kac and Ward used a high-way crossing strategy to allow traversing each site of the Ising model in all different directions, yet to avoid hair-pins. One crossing corresponds to one site of the lattice, and it is broken up into four different directions ("right" = 1, "up" = 2, "left" = 3, "down" = 4). Straight traversals count as ν, left turns = α, hairpin turns = 0, right turns = $\overline{\alpha}$ (see Table I).

A. The not-so-naive matrix $U_{2\times 2}$

A not-so-naive Kac-Ward matrix for the 2×2 problem is given by the following:

$$U_{2\times 2} = \begin{bmatrix}
1 & \cdot & \cdot & \cdot & \nu & \alpha & \cdot & \overline{\alpha} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \overline{\alpha} & \nu & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \nu & \alpha & \cdot & \overline{\alpha} \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\alpha & \cdot & \overline{\alpha} & \nu & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \overline{\alpha} & \nu & \alpha & \cdot & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & \cdot & \alpha & \cdot & \overline{\alpha} & \nu & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1
\end{bmatrix}. \tag{6}$$

As discussed in lecture 07, rows and columns 1-4 of this matrix correspond to site 1 of the Ising model, column 5-8 to site 2, columns 9-12 to site 3, and columns 13-16 to site 4.

- Explain the values of $u_{6,13}$, $u_{6,14}$, $u_{6,15}$ in this matrix.

  The sites in the system are labeled as $\begin{pmatrix} 3 & 4 \\ 1 & 2 \end{pmatrix}$.

  - $u_{6,13}$ *means turning right at site 4*
  - $u_{6,14}$ *means going upward through site 4*
  - $u_{6,15}$ *means turning left at site 4*

- Expose, by direct inspection, the four non-trivial permutations in this matrix.

  There are 2 cycles in the matrix, which correspond to the clockwise loop of traffic $(1 \to 4 \to 3 \to 2)$ *and anti-clockwise loop of traffic* $(1 \to 2 \to 3 \to 4)$ *in the configuration. The cycles in the matrix are shown in Fig. 3. Each cycle provides a permutation. Since all of the terms which contribute to the cycles never appears in the same row or column, the multiplication of the cycles also yields a permutation. And the last non-trivial permutation is identity.*

- Compute the determinant of $U_{2\times 2}$ from the cycle-sum representation of eq. (3), and show that it agrees with the determinant of $\hat{U}_{2\times 2}$.

  The two cycles give α^4 *and* $\overline{\alpha}^4$ *respectively, thus*

$$\det\left(U_{2\times 2}\right) = 1 - \alpha^4 - \overline{\alpha}^4 + (\alpha\overline{\alpha})^4 = (1 + \tanh^4(\beta))^2 = \left[\det\left(\hat{U}_{2\times 2}\right)\right]^2$$

$$\begin{bmatrix}
1 & \cdot & \cdot & \cdot & \nu & \alpha & \cdot & \overline{\alpha} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \overline{\alpha} & \nu & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \overline{\alpha} & \nu & \alpha & \cdot \\
\cdot & \overline{\alpha} & \nu & \alpha & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\alpha & \cdot & \overline{\alpha} & \nu & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \overline{\alpha} & \nu & \alpha & \cdot & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & \cdot & \alpha & \cdot & \overline{\alpha} & \nu & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1
\end{bmatrix}$$

FIG. 3: Cycles in the matrix. The orange cycle is for anti-clockwise loop, while the blue cycle is for clockwise loop. The loops do not overlap, which means none of the elements, which contribute to the cycles, are in the same row or column.

TABLE I: The matrix elements of the first row of the Kac–Ward matrix $U_{2\times 2}$ (see eq. (6)).

Matrix element (example)	value	type
$u_{1,5}$	$\nu = \tanh\beta$	(straight traversal of site 2)
$u_{1,6}$	$\alpha = \mathrm{e}^{i\pi/4}\tanh\beta$	(left turn at site 2)
$u_{1,7}$	0	(hairpin turn at site 2)
$u_{1,8}$	$\overline{\alpha} = \mathrm{e}^{-i\pi/4}\tanh\beta$	(right turn at site 2)

B. Compact notation for $U_{2\times 2}$

Show that the matrix $U_{2\times 2}$ can be compactly written as a matrix of 4×4 matrices:

$$U_{2\times 2} = \begin{bmatrix} 1 & u_{\rightarrow} & u_{\uparrow} & \cdot \\ u_{\leftarrow} & 1 & \cdot & u_{\uparrow} \\ u_{\downarrow} & \cdot & 1 & u_{\rightarrow} \\ \cdot & u_{\downarrow} & u_{\leftarrow} & 1 \end{bmatrix} \tag{7}$$

where 1 is the 4×4 unit matrix, and furthermore, the 4×4 matrices $u_{\rightarrow}$, $u_{\uparrow}$, $u_{\leftarrow}$, and $u_{\downarrow}$ are given by

$$
\begin{aligned}
u_{\rightarrow} &= \begin{bmatrix} \nu & \alpha & \cdot & \overline{\alpha} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}, \quad u_{\uparrow} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \overline{\alpha} & \nu & \alpha & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}, \\
u_{\leftarrow} &= \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \overline{\alpha} & \nu & \alpha \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}, \quad u_{\downarrow} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \alpha & \cdot & \overline{\alpha} & \nu \end{bmatrix}.
\end{aligned}
\tag{8}
$$

One can check explicitly that this matrix is identical to the 16×16 matrix. This matrix can also be interpreted in the following way: Each column and each row in (compact) $U_{2\times 2}$ stands for a site. If one can reach site j by moving upward from site i, there are non-trivial elements in block $U_{2\times 2,ij}$. (For other directions, this interpretation also works.) This block is denoted by $u_{\uparrow}$. In u, rows means the directions of going from site i to site j, and columns means the directions of going out of site j. Thus, only the second row of $u_{\uparrow}$ contains non-trivial elements. And the value of these elements could be found by using similar argument as constructing Table I. As long as the two directions are fixed, the elements in matrices u are irrelevant to the positions of the sites. So the matrices u works for arbitrary sites and arbitrarily large systems. By using the compact notion, the Kac-Ward matrix could by written down by examining how the sites are connected, instead of analyzing explicitly what are the elements.

III. KAC-WARD MATRIX FOR THE 4×4 ISING MODEL

Using the compact notation of Section II B, write down the matrix $U_{4\times 4}$, in complete analogy with what you did for $U_{2\times 2}$. Compute its determinant, using a computer algorithm at a few different temperatures. For your convenience, a mathematica notebook file setting up the matrix $U_{2\times 2}$ is made available on the website. Note that the conversion factor of eq. (5) must be introduced in order to yield the partition function Z.

- Explain what this program does.

This program build the $U_{2\times 2}$ using the compact notion, and calculate the determinant of this matrix.

- Explain in particular why you have to take the square root of the determinant.

The non-trivial contribution to the determinant comes from the loops of traffic in the configuration. The loops appear here are identical to the loops which appear in the high temperature expansion, and their contribution are also identical. However, loops in the Kac-Ward matrix formalism are directed, which means the contribution of each loop is counted twice, not to mention the combination of the clockwise and anti-clockwise loop also contributes to the determinant. Taking square root is thus needed to get rid of these contributions.

- Modify this program to make it work for $U_{4\times 4}$ (or write your own) and compute the partition function of the 4×4 Ising model (without periodic boundary conditions), version Kac and Ward. Notice that we have not proven that this matrix actually gives the exact result.

Please check the mathematica file for solution. Though not proven, the Kac-Ward method does give correct result.

- To check this latter point, compare the partition function with the partition function of the 4×4 Ising model obtained from the high-temperature expansion (see Fig. 4, and in particular, its figure caption).

Please check the mathematica file for solution.

Notice that there are many non-zero cycles in the matrix $U_{4\times 4}$ that have no relation to loops in the high-temperature expansion of the Ising model. It was the "good fortune" of Kac and Ward that they all sum up to zero. Your program does provide a constructive prove of this property for small loops and cycles.

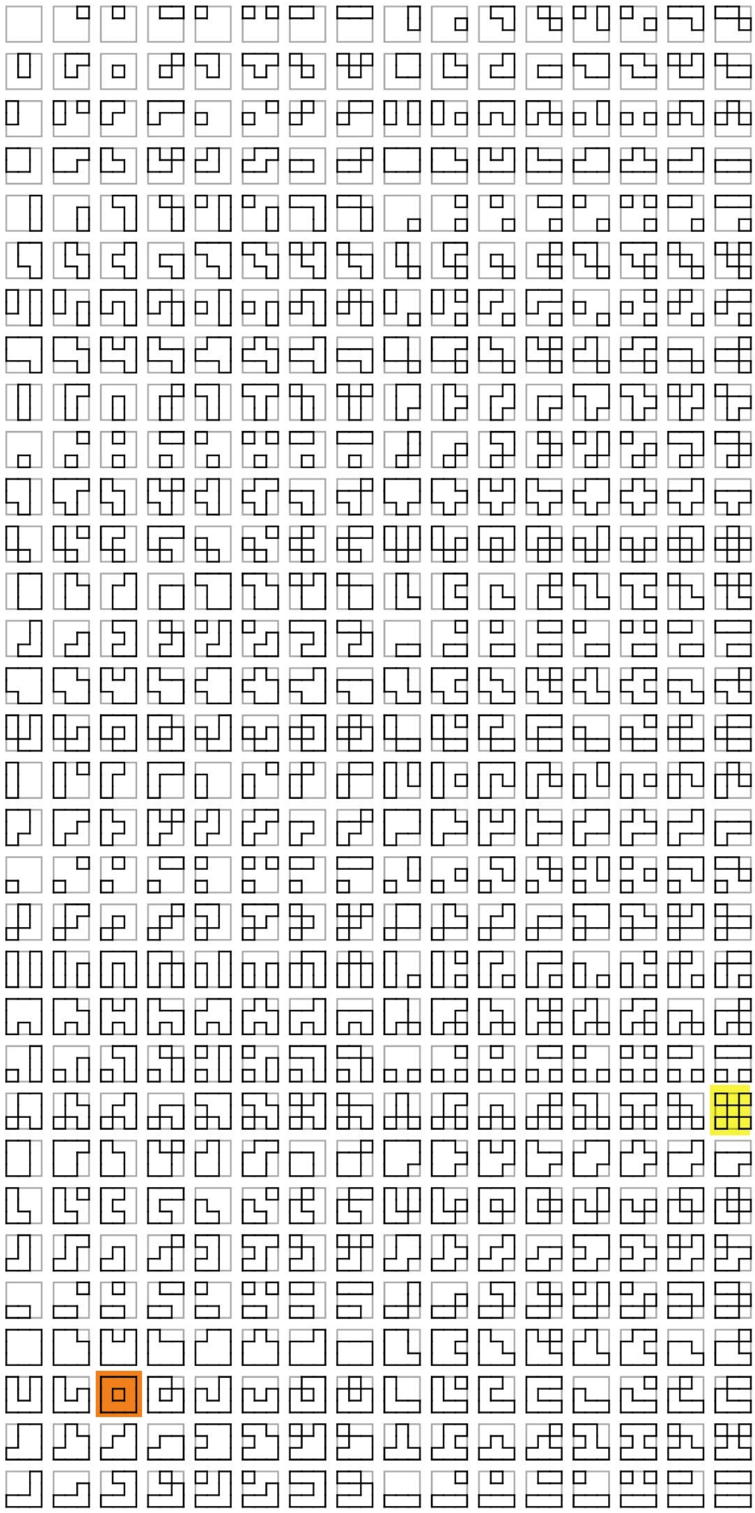

FIG. 4: All the 512 loops that make up the high-temperature expansion of the 4×4 Ising model without periodic boundary conditions. Note that there is one loop with zero edges. There are, in addition, 9 loops with four edges, 12 loops with 6 edges, 50 loops with 8 edges, 92 loops with 10 edges, 158 loops with 12 edges, 116 loops with 14 edges, 69 loops with 16 edges, 4 loops with 18 edges, 1 loop with 20 edges (in yellow). The "golden" configuration presents a loop within a loop.