Homework 6, Statistical Mechanics: Concepts and applications
2016/17 ICFP Master (first year)

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This homework will count for your grade. Please hand in on Wednesday,

26 October 2016, at the start of the lecture (extended deadline).

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In lecture 06 (Ising model: from Kramers-Wannier duality 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

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

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

$$
\det U = \sum_{\substack{\text{cycle} \\ \text{configs}}} (-1)^{\text{\# of cycles}} \underbrace{u_{P_1 P_2} u_{P_2 P_3} \cdots u_{P_M P_1}}_{\text{weight of first cycle}} \underbrace{u_{P'_1 P'_2} \cdots}_{\text{other cycles}}
$$

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

is OK (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}.

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

In lecture 06, 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 "·" stand for "0" and $\gamma = e^{i\pi/4} = \sqrt[4]{-1}$. Write down the determinant of this matrix in terms of permutation cycles. Show that

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

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).

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:

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

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. 1).
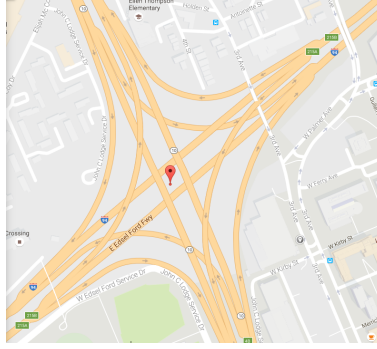
FIG. 1: Highway crossing. To solve the two-dimensional Ising model, Kac and Ward used a high-way crossing strategy to allow traversing each site of the Ising model in all different directions, yet to avoid hair-pins. One crossing corresponds to one site of the lattice, and it is broken up into four different 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 $U_{2\times2}$

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

$$
U_{2\times2} =
\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 \\
\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 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \nu & \alpha & \cdot & \overline{\alpha} \\
\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 \\
\alpha & \cdot & \overline{\alpha} & \nu & \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 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & \alpha & \cdot & \overline{\alpha} & \nu & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1
\end{bmatrix}.
\tag{6}
$$

As discussed in lecture 06, 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.

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

- Compute the determinant of $U_{2\times2}$ from the cycle-sum representation of eq. (3), and show that it agrees with the determinant of $\hat{U}_{2\times2}$.

TABLE I: The matrix elements of the first row of the Kac–Ward matrix $U_{2\times2}$ (see eq. (6)).

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

B. Compact notation for $U_{2\times2}$

Show that the matrix $U_{2\times2}$ can be compactly written as a matrix of 4×4 matrices:

$$U_{2\times2} = \begin{bmatrix} 1 & u_\rightarrow & u_\uparrow & \cdot \\ u_\leftarrow & 1 & \cdot & u_\uparrow \\ u_\downarrow & \cdot & 1 & u_\rightarrow \\ \cdot & u_\downarrow & u_\leftarrow & 1 \end{bmatrix} \tag{7}$$

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

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

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

Using the compact notation of Section II B, write down the matrix $U_{4\times4}$, in complete analogy with what you did for $U_{2\times2}$. Compute its determinant, using a computer algorithm at a few different temperatures. For your convenience, a mathematica notebook file setting up the matrix $U_{2\times2}$ 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.

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

- 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.

- 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. 2, and in particular, its figure caption).

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.
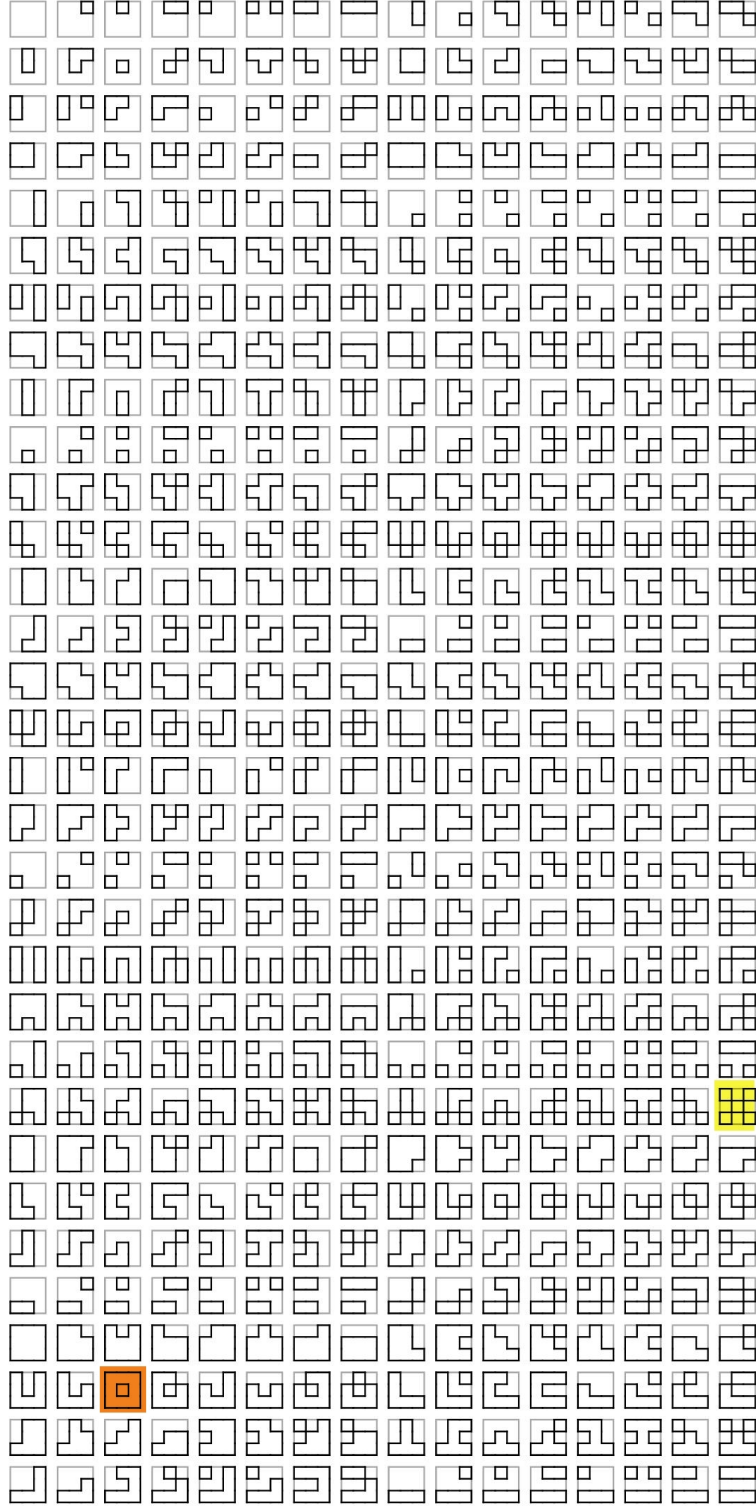
FIG. 2: All the 512 loops that make up the high-temperature expansion of the 4×4 Ising model without periodic boundary conditions. Note that there is one loop with zero edges. There are, in addition, 9 loops with four edges, 12 loops with 6 edges, 50 loops with 8 edges, 92 loops with 10 edges, 158 loops 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.