Homework 9

due April 19, 2017 (at 18:00) [in PDF with LaTeX to Tong Wang twang92@illinois.edu]

As I announced, HWs are regarded as substitutes for Discussion, so you may submit your ‘draft’
electronically for my comments/suggestions/hints (by the time reasonably before the deadline).
Also you can freely discuss with your friends as long as it facilitates your understanding. I hope all
of you will get 100%.

1. [Tonks gas with ‘the standard statistical mechanics’]
We have derived the equation of state for the Tonks gas in two ways (‘intuitive graphics’ and ‘com-
binatorial entropy estimate’). Let us use the ‘standard canonical formalism’ to study the ‘hard rod
gas.’ Let \(L\) be the ‘container tube’ length and there are \(N\) rods of length \(\sigma\) in it. The tempera-
ture is maintained at \(T\). The canonical partition function \(Q\) (or rather, the configuration partition
function) reads
\[
Q = \int \cdots \int _{\sigma < x_1 < x_2 - \sigma < x_3 - 2\sigma < \cdots < x_n -(n-1)\sigma < \cdots < x_N -(N-1)\sigma < L -(N-1)\sigma} dx_1 dx_2 \cdots dx_n, \tag{HW9.1}
\]
where \(x_n\) is the position coordinate of the ‘right end’ of the \(n\)th rod.

(1) Confirm that the above integral is the right configurational partition function. We assume that all the particles are indistinguishable. Do not worry about the distinction between < and \(\leq\).

(2) Calculate the integral with the aid of the variables \(y_n = x_n - (n - 1)\sigma\) \((n = 1, \cdots , N)\).

(3) Can you get Tonk’s equation of state from your result for (2)?

2. [Ising model-lattice gas correspondence on the honeycomb lattice]
Consider the 2D Ising model on the honeycomb lattice (thus each lattice point is connected to three
nearest neighbor lattice points) with \(V \gg 1\) lattice points. We wish to convert this model into
the lattice gas model on the honeycomb lattice, regarding the down spins as the particles (up spins
correspond to empty sites). Let \([D]\) be the total number of down spins, and \([DD]\) the number of
down spin pairs.

(1) Express the following quantities in terms of \([D]\), \([DD]\) and \(V\):
   (i) \(M = \sum _{i=1}^{V} s_i\).
   (ii) \(-J \sum _{(i,j)} s_i s_j\).

(2) What is the chemical potential for the gas particles in this correspondence?

3. [Junior high algebra exercise]
Let us taste a bit (only a small bit) of the proof of the Lee-Yang circle theorem due to Asano. The
circle theorem reads:
Let the real numbers \(a\{\{i,j\}\} \in [-1,1]\) for all \(\{i,j\}\) \(\{i,j \in I = \{1,\cdots , V\}\}\). Then, all the zeros of
the following polynomial are on the unit circle:
\[
P(z) = \sum _{X \in I} z^{|X|} \prod _{i \in X} \prod _{j \notin X} a\{\{i,j\}\}. \tag{HW9.2}
\]
Here, the terms of order 0 and the highest order are, respectively, 1 and \( z^V \), and \( |X| \) is the number of elements in \( X \) (the cardinality of \( X \)). The summation is over all the subsets of \( I \). That is, we take the sum over all the particle placement patterns on the lattice. \( X \) is the set of lattice points occupied by the particles.

1. Let
   \[ p(i, j) = z_iz_j + a(z_i + z_j) + 1. \]  
   (HW9.3)

Notice that this is the partition function for the system consisting of two lattice points \( i \) and \( j \) only, if we set \( z_i = z_j = z \) to be the particle fugacity \( (z = e^{\beta \mu}) \) and \( a = e^{-\beta \varepsilon} \), where \( \varepsilon (> 0) \) is the pair interaction energy.

Show that the quadratic equation \( p(i, j) = 0 \) with \( z_i = z_j = z \) has zeros on the unit circle, if \( a \in [-1, 1] \).

2. Asano discovered that the polynomial \( P \) can be constructed recursively as follows: Suppose we have the polynomial (HW9.2) for a finite lattice \( Y \) containing lattice point \( j \). We wish to introduce a new pair interaction between \( j \) and \( i \) to this system, adding a new lattice point \( i \). Make
   \[ P_Y p(i, j) = Az_j^2 + Bz_j + C, \]  
   (HW9.4)

where \( A, B, C \) contain all the \( z \)’s other than \( z_j \). That is, we regard \( P_Y p \) as a polynomial of \( z_j \). Then, (HW9.2) corresponding to this new system \( Y \cup \{j\} \) is given by (the procedure is called Asano contraction)

\[ \rightarrow A_{z_j} + C. \]  
   (HW9.5)

That is: replace \( z_j^2 \) with \( z_j \) and the original \( z_j \) coefficient is set to be zero \( (B = 0) \).

Thus, starting a pair \((i, j)\) in (1), we can add bonds and vertices (= lattice points) one by one to make \( P \). Then, the circle theorem is restated as:

The polynomial constructed recursively according to the method explained above has all the zeros on the unit circle.

At each step zeros are always on the unit circle.\(^1\)

A proof is in the already posted circle.pdf, but let us taste one step: We start from \( p(1, 2) \):

\[ p(1, 2) = z_1z_2 + a(z_1 + z_2) + 1. \]  
   (HW9.6)

Then, to this ‘lattice’ we add one more point 3 and the 2-3 bond. This is described by \( p(2, 3) \)

\[ p(2, 3) = z_2z_3 + b(z_2 + z_3) + 1. \]  
   (HW9.7)

Here, \( a, b \in [-1, 1] \). Asano contract \( p(1, 2)p(2, 3) \) and actually demonstrate that the resultant polynomial with all \( z_i \)’s identified as \( z \) has all three zeros on the unit circle.

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\(^1\)This is a remarkable theorem, and is likely deep, but so far no connection to other deep mathematical results is known.