Tutorial 4, Statistical Mechanics: Concepts and applications
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Tutorial exercises

I. WORKSHEET: CAN 1D CLASSICAL SYSTEMS HAVE PHASE TRANSITIONS?

1. **The tennis ball problem (variant of the Kittel's model.)**

   Reminder: A phase transition occurs when the free energy is not an analytic function of some thermodynamic quantity, e.g. the temperature. The corresponding values of the parameters are called *critical*.

   The model: we have a very long tube full of tennis balls, that can only be extracted from one end of the tube, one by one at the energy cost of ϵ each. The extracted balls are placed in one of G containers with equal probability.

   (a) Let the number of balls be $N-1$. Compute the free energy.

   (b) Simplify the expression in the thermodynamic limit $N \to \infty$. Is the free energy an analytic function of β? What is the difference between $G = 1$ and $G > 1$ cases?

   (c) Compute the average number of balls in the tube at temperature T.

   (d) Let us now assume that a ball can go into a container only if there is no other container with fewer balls. Is there a phase transition? If yes, what is the critical temperature?

   Hint: You do not need to work out the entire expression for the free energy to answer this question.

2. **Ising model in a staggered field.**

Reminder: In physics, transfer matrices appear in diverse contexts. In classical statistical physics they are employed to compute partition functions. The basic idea is to construct a matrix $T(\beta)$ such that the partition function can be written in the form

$$Z = \mathrm{Tr}[T^N(\beta)W]\,, \tag{1}$$

where W is a matrix that depends on the boundary conditions and N is an integer that in one dimensional chains is proportional to the number of sites. For the sake of simplicity, let us assume that $T(\beta)$ is symmetric. We have

$$Z = \sum_{i=1}^{n} \lambda_i^N(\beta)\mathrm{Tr}[\Pi_i W]\,, \tag{2}$$

where n is the dimensionality of the transfer matrix (essentially the number of states each constituent can assume), $\lambda_i(\beta)$ are the eigenvalues of $T(\beta)$ and Π_i the corresponding projectors on the eigenspace (*i.e.*, if $\vec{v}_i$ is an eigenvector, $[\Pi_i]_{\ell n} = [\vec{v}_i]_\ell[\vec{v}_i]_n$).

Reminder: A matrix M is reducible if and only if it can be placed into block upper-triangular form by simultaneous row/column permutations, i.e.

$$P^t M P = \begin{pmatrix} X & Y \\ 0 & Z \end{pmatrix}\,. \tag{3}$$

where P is a permutation matrix and X and Z are square matrices.

Reminder: Phase transitions are generally forbidden in one dimensional systems by virtue of the following theorems:

- *[Perron-Frobenious] Let A be an irreducible matrix with non-negative elements; the maximum eigenvalue is positive and non-degenerate.*
- *If $T(\beta)$ is a complex matrix with elements analytic functions of β, the eigenvalues are (branches) of analytic functions of β with only algebraic singularities localized at the points at which eigenvalues split or coalesce.*

Specifically, if the transfer matrix $T(\beta)$ is finite-dimensional and does not have zeros, the free energy is an analytic function of β. Since the elements of the transfer matrix are generally the exponentials of real numbers (*i.e.* strictly positive number), there can not be phase transitions at finite temperature. Can you think of any exceptions? In what circumstances would there be zeros present in the transfer matrix?

The model: We consider a classical Ising model in a staggered field:

$$E(\{s\}) = -J\sum_{\ell=1}^{L} s_\ell s_{\ell+1} + (-1)^\ell h s_\ell\,. \tag{4}$$

Here s_ℓ are classical spin variables $s_\ell \in \{-1, 1\}$, J has the dimensions of an energy, and h is the absolute value of the staggered field.

(a) Write down a transfer matrix for this model.

(b) Show the formal structure of the partition function both for periodic ($s_{L+1} \equiv s_1$) and open ($s_{L+1} \equiv 0$) boundary conditions.

(c) Are there phase transitions at finite temperature?

3. **Generalized Kittel's model**

The model: our model can be described by the following Hamiltonian

$$H = \varepsilon(1 - \delta_{s_1 0}) + \sum_{i=1}^{N-2} (\varepsilon + \Lambda \delta_{s_i 0})(1 - \delta_{s_{i+1} 0}) \tag{5}$$

where label $s_i = 0, 1, ..., G$ signifies the state of the ith constituent. Roughly, you can think of it as a generalized version of problem 1, where it is now possible to extract balls from any position in the tube (not just the open end) at the cost of energy Λ. Λ is an auxiliary variable that is used to parametrize the forbidden configurations of the original problem.

(a) In what limit do you get the original problem 1 back?

(b) Write down a transfer matrix for the model.

(c) Compute the free energy.

(d) Take the thermodynamics limit. Is the free energy an analytic function of β if $G = 1$ (only one container in the tennis ball problem)? And if $G > 1$?

(e) Compute the average energy of the system at temperature T.

(f) Explain in what this model differs from the one of Exercise 1.