PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #3 SOLUTIONS

(1) For the Mayer cluster expansion, write down all possible unlabeled connected subgraphs γ which contain four vertices. For your favorite of these animals, identify its symmetry factor s_γ, and write down the corresponding expression for the cluster integral b_γ. For example, for the $\square$ diagram with four vertices the symmetry factor is $s_\square = 8$ and the cluster integral is

$$
\begin{aligned}
b_\square &= \frac{1}{8V} \int d^d r_1 \int d^d r_2 \int d^d r_3 \int d^d r_4 \, f(r_{12}) \, f(r_{23}) \, f(r_{34}) \, f(r_{14}) \\
&= \frac{1}{8} \int d^d r_1 \int d^d r_2 \int d^d r_3 \, f(r_{12}) \, f(r_{23}) \, f(r_1) \, f(r_3) \quad .
\end{aligned}
$$

(You'll have to choose a favorite other than $\square$.) If you're really energetic, compute s_γ and b_γ for all of the animals with four vertices.

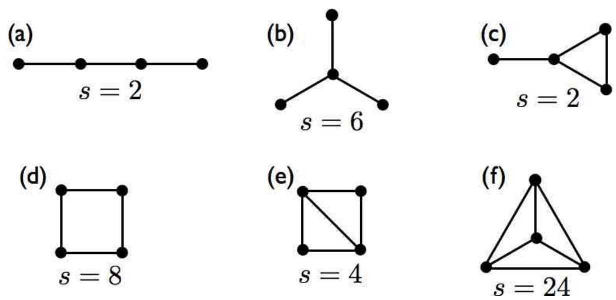

Figure 1: Connected clusters with $n_\gamma = 4$ sites.

Solution :

The animals and their symmetry factors are shown in fig. 1.

$$
\begin{aligned}
b_{\rm a} &= \frac{1}{2} \int d^d r_1 \int d^d r_2 \int d^d r_3 \, f(r_1) \, f(r_{12}) \, f(r_{23}) \\
b_{\rm b} &= \frac{1}{6} \int d^d r_1 \int d^d r_2 \int d^d r_3 \, f(r_1) \, f(r_2) \, f(r_3) \\
b_{\rm c} &= \frac{1}{2} \int d^d r_1 \int d^d r_2 \int d^d r_3 \, f(r_1) \, f(r_{12}) \, f(r_{13}) \, f(r_{23}) \\
b_{\rm d} &= \frac{1}{8} \int d^d r_1 \int d^d r_2 \int d^d r_3 \, f(r_1) \, f(r_2) \, f(r_{13}) \, f(r_{23}) \\
b_{\rm e} &= \frac{1}{4} \int d^d r_1 \int d^d r_2 \int d^d r_3 \, f(r_1) \, f(r_2) \, f(r_{12}) \, f(r_{13}) \, f(r_{23}) \\
b_{\rm f} &= \frac{1}{24} \int d^d r_1 \int d^d r_2 \int d^d r_3 \, f(r_1) \, f(r_2) \, f(r_3) \, f(r_{12}) \, f(r_{13}) \, f(r_{23}) \quad .
\end{aligned}
$$

(2) For each of the cluster diagrams in Fig. 2, find the symmetry factor s_γ and write an expression for the cluster integral b_γ.

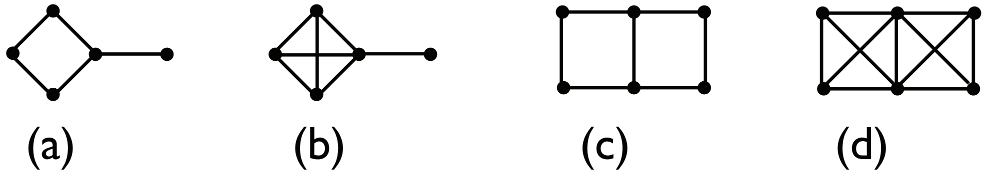

Figure 2: Cluster diagrams for problem 2.

Solution : Choose labels as in Fig. 3, and set $\boldsymbol{x}_{n_\gamma} \equiv 0$ to cancel out the volume factor in the definition of b_γ.

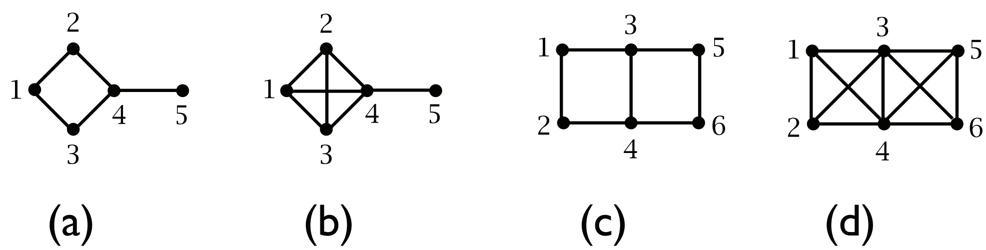

Figure 3: Labeled cluster diagrams.

(a) The symmetry factor is $s_\gamma = 2$, so

$$b_\gamma = \tfrac{1}{2} \int d^d\!x_1 \int d^d\!x_2 \int d^d\!x_3 \int d^d\!x_4 \; f(r_{12})\, f(r_{13})\, f(r_{24})\, f(r_{34})\, f(r_4) \quad .$$

(b) Sites 1, 2, and 3 may be permuted in any way, so the symmetry factor is $s_\gamma = 6$. We then have

$$b_\gamma = \tfrac{1}{6} \int d^d\!x_1 \int d^d\!x_2 \int d^d\!x_3 \int d^d\!x_4 \; f(r_{12})\, f(r_{13})\, f(r_{24})\, f(r_{34})\, f(r_{14})\, f(r_{23})\, f(r_4) \quad .$$

(c) The diagram is symmetric under reflections in two axes, hence $s_\gamma = 4$. We then have

$$b_\gamma = \tfrac{1}{4} \int d^d\!x_1 \int d^d\!x_2 \int d^d\!x_3 \int d^d\!x_4 \int d^d\!x_5 \; f(r_{12})\, f(r_{13})\, f(r_{24})\, f(r_{34})\, f(r_{35})\, f(r_4)\, f(r_5) \quad .$$

(d) The diagram is symmetric with respect to the permutations (12), (34), (56), and $(15)(26)$. Thus, $s_\gamma = 2^4 = 16$. We then have

$$b_\gamma = \tfrac{1}{16} \int d^d\!x_1 \int d^d\!x_2 \int d^d\!x_3 \int d^d\!x_4 \int d^d\!x_5 \; f(r_{12})\, f(r_{13})\, f(r_{14})\, f(r_{23})\, f(r_{24})\, f(r_{34})\, f(r_{35})\, f(r_{45})\, f(r_3)\, f(r_4)\, f(r_5) \quad .$$

(3) Compute the partition function for the one-dimensional Tonks gas of hard rods of length a on a ring of circumference L. This is slightly tricky, so here are some hints. Once again, assume a particular ordering so that $x_1 < x_2 < \cdots < x_N$. Due to translational invariance, we can define the positions of particles $\{2, \ldots, N\}$ relative to that of particle 1, which we initially place at $x_1 = 0$. Then periodicity means that $x_N \leq L - a$, and in general one then has

$$x_{j-1} + a \leq x_j \leq Y_j \equiv L - Na + (j-1)a \quad .$$

Now integrate over $\{x_2, \ldots, x_N\}$ subject to these constraints. Finally, one does the x_1 integral, which is over the entire ring, but which must be corrected to eliminate overcounting from cyclic permutations. How many cyclic permutations are there?

Solution :

There are N cyclic permutations, hence

$$Z(T, L, N) = \lambda_T^{-N} \, \frac{L}{N} \int\limits_a^{Y_2} \! dx_2 \int\limits_{x_2+a}^{Y_3} \! dx_3 \, \cdots \int\limits_{x_{N-1}+a}^{Y_N} \! dx_N = \frac{L(L - Na)^{N-1} \lambda_T^{-N}}{N!} \quad .$$

(4) Consider a three-dimensional gas of point particles interacting according to the potential

$$u(r) = \begin{cases} +\Delta_0 & \text{if } r \leq a \\ -\Delta_1 & \text{if } a < r \leq b \\ 0 & \text{if } b < r \quad , \end{cases}$$

where $\Delta_{0,1}$ are both positive. Compute the second virial coefficient $B_2(T)$ and find a relation which determines the inversion temperature in a throttling process.

Solution :

The Mayer function is

$$f(r) = \begin{cases} e^{-\Delta_0/k_\mathrm{B}T} - 1 & \text{if } r \leq 0 \\ e^{\Delta_1/k_\mathrm{B}T} - 1 & \text{if } a < r \leq b \\ 0 & \text{if } b < r \quad . \end{cases}$$

The second virial coefficient is

$$\begin{aligned} B_2(T) &= -\tfrac{1}{2} \int \! d^3\!r \, f(r) \\ &= \frac{2\pi a^3}{3} \cdot \Big[\big(1 - e^{-\Delta_0/k_\mathrm{B}T}\big) + (s^3 - 1)\big(1 - e^{\Delta_1/k_\mathrm{B}T}\big) \Big] \quad , \end{aligned}$$

where $s = b/a$. The inversion temperature is a solution of the equation $B_2(T) = TB_2'(T)$, which gives

$$s^3 - 1 = \frac{1 + \left(\frac{\Delta_0}{k_\mathrm{B}T} - 1\right) e^{-\Delta_0/k_\mathrm{B}T}}{1 + \left(\frac{\Delta_1}{k_\mathrm{B}T} + 1\right) e^{\Delta_1/k_\mathrm{B}T}} \quad .$$