PHYSICS 210A : STATISTICAL PHYSICS
HW ASSIGNMENT #6 SOLUTIONS

(1) The Blume-Capel model is a spin-1 version of the Ising model, with Hamiltonian

$$H = -J \sum_{\langle ij \rangle} S_i \, S_j - \Delta \sum_i S_i^2 \ ,$$

where $S_i \in \{-1 \, , \, 0 \, , \, +1\}$ and where the first sum is over all links of a lattice and the second sum is over all sites. It has been used to describe magnetic solids containing vacancies ($S = 0$ for a vacancy) as well as phase separation in ${}^4\text{He} - {}^3\text{He}$ mixtures ($S = 0$ for a ${}^4\text{He}$ atom). This problem will give you an opportunity to study and learn the material in §§5.2,3 of the notes. For parts (b), (c), and (d) you should work in the thermodynamic limit. The eigenvalues and eigenvectors are such that it would shorten your effort considerably to use a program like `Mathematica` to obtain them.

(a) Find the transfer matrix for the $d = 1$ Blume-Capel model.

(b) Find the free energy $F(T, \Delta, N)$.

(c) Find the density of $S = 0$ sites as a function of T and Δ.

(d) *Exciting!* Find the correlation function $\langle \, S_j \, S_{j+n} \, \rangle$.

Solution :

(a) The transfer matrix R can be written in a number of ways, but it is aesthetically pleasing to choose it to be symmetric. In this case we have

$$R_{SS'} = e^{\beta J S S'} e^{\beta \Delta (S^2 + S'^2)/2} = \begin{pmatrix} e^{\beta(\Delta+J)} & e^{\beta\Delta/2} & e^{\beta(\Delta-J)} \\ e^{\beta\Delta/2} & 1 & e^{\beta\Delta/2} \\ e^{\beta(\Delta-J)} & e^{\beta\Delta/2} & e^{\beta(\Delta+J)} \end{pmatrix} \ .$$

(b) For an N-site ring, we have

$$Z = \mathsf{Tr} \, e^{-\beta H} = \mathsf{Tr} \left(R^N \right) = \lambda_+^N + \lambda_0^N + \lambda_-^N \ ,$$

where λ_+, λ_0, and λ_- are the eigenvalues of the transfer matrix R. To find the eigenvalues, note that

$$\vec{\psi}_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

is an eigenvector with eigenvalue $\lambda_0 = 2 \, e^{\beta\Delta} \sinh(\beta J)$. The remaining eigenvectors must be orthogonal to ψ_0, and hence are of the form

$$\vec{\psi}_\pm = \frac{1}{\sqrt{2 + x_\pm^2}} \begin{pmatrix} 1 \\ x_\pm \\ 1 \end{pmatrix} \ .$$

We now demand

$$R\begin{pmatrix}1\\x\\1\end{pmatrix}=\begin{pmatrix}2\,e^{\beta\Delta}\cosh(\beta J)+x\,e^{\beta\Delta/2}\\ 2\,e^{\beta\Delta/2}+x\\ 2\,e^{\beta\Delta}\cosh(\beta J)+x\,e^{\beta\Delta/2}\end{pmatrix}=\begin{pmatrix}\lambda\\ \lambda x\\ \lambda\end{pmatrix}\ ,$$

resulting in the coupled equations

$$\begin{aligned}\lambda&=2\,e^{\beta\Delta}\cosh(\beta J)+x\,e^{\beta\Delta/2}\\ \lambda x&=2e^{\beta\Delta/2}+x\ .\end{aligned}$$

Eliminating x, one obtains a quadratic equation for λ. The solutions are

$$\begin{aligned}\lambda_\pm&=\Big(e^{\beta\Delta}\cosh(\beta J)+\tfrac{1}{2}\Big)\pm\sqrt{\Big(e^{\beta\Delta}\cosh(\beta J)+\tfrac{1}{2}\Big)^2+2\,e^{\beta\Delta}}\\ x_\pm&=e^{-\beta\Delta/2}\bigg\{\Big(\tfrac{1}{2}-e^{\beta\Delta}\cosh(\beta J)\Big)\pm\sqrt{\Big(\tfrac{1}{2}-e^{\beta\Delta}\cosh(\beta J)\Big)^2+2\,e^{\beta\Delta}}\bigg\}\ .\end{aligned}$$

Note $\lambda_+>\lambda_0>0>\lambda_-$ and that λ_+ is the eigenvalue of the largest magnitude. This is in fact guaranteed by the *Perron-Frobenius theorem*, which states that for any positive matrix R (*i.e.* a matrix whose elements are all positive) there exists a positive real number p such that p is an eigenvalue of R and any other (possibly complex) eigenvalue of R is smaller than p in absolute value. Furthermore the associated eigenvector $\vec{\psi}$ is such that all its components are of the same sign. In the thermodynamic limit $N\to\infty$ we then have

$$F(T,\Delta,N)=-Nk_{\rm B}T\ln\lambda_+\ .$$

(c) Note that, at any site,

$$\langle S^2\rangle=-\frac{1}{N}\frac{\partial F}{\partial\Delta}=\frac{1}{\beta}\frac{\partial\ln\lambda_+}{\partial\Delta}\ ,$$

and furthermore that

$$\delta_{S,0}=1-S^2\ .$$

Thus,

$$\nu_0\equiv\frac{N_0}{N}=1-\frac{1}{\beta}\frac{\partial\ln\lambda_+}{\partial\Delta}\ .$$

After some algebra, find

$$\nu_0=1-\frac{r-\frac{1}{2}}{\sqrt{r^2+2\,e^{\beta\Delta}}}\ ,$$

where

$$r=e^{\beta\Delta}\cosh(\beta J)+\tfrac{1}{2}\ .$$

It is now easy to explore the limiting cases $\Delta\to-\infty$, where we find $\nu_0=1$, and $\Delta\to+\infty$, where we find $\nu_0=0$. Both these limits make physical sense.

(d) We have

$$C(n)=\langle\,S_j\,S_{j+n}\,\rangle=\frac{\mathsf{Tr}\left(\Sigma\,R^n\,\Sigma\,R^{N-n}\right)}{\mathsf{Tr}\left(R^N\right)}\ ,$$

where $\Sigma_{SS'} = S\,\delta_{SS'}$. We work in the thermodynamic limit. Note that $\langle + | \Sigma | + \rangle = 0$, therefore we must write

$$R = \lambda_+ \, | + \rangle\langle + | + \lambda_0 \, | 0 \rangle\langle 0 | + \lambda_- \, | - \rangle\langle - | \ ,$$

and we are forced to choose the middle term for the n instances of R between the two Σ matrices. Thus,

$$C(n) = \left(\frac{\lambda_0}{\lambda_+}\right)^n \big|\langle + | \Sigma | 0 \rangle\big|^2 \ .$$

We define the correlation length ξ by

$$\xi = \frac{1}{\ln\big(\lambda_+/\lambda_0\big)} \ ,$$

in which case

$$C(n) = A\, e^{-|n|/\xi} \ ,$$

where now we generalize to positive and negative values of n, and where

$$A = \big|\langle + | \Sigma | 0 \rangle\big|^2 = \frac{1}{1 + \frac{1}{2}x_+^2} \ .$$

(2) DC Comics superhero Clusterman and his naughty dog Henry are shown in fig. 1. Clusterman, as his name connotes, is a connected diagram, but the diagram for Henry contains some disconnected pieces.

(a) Interpreting the diagrams as arising from the Mayer cluster expansion, compute the symmetry factor s_γ for Clusterman.

(b) What is the *total* symmetry factor for Henry and his disconnected pieces? What would the answer be if, unfortunately, another disconnected piece of the same composition were to be found?

(c) What is the lowest order virial coefficient to which Clusterman contributes?

Solution :

First of all, this is really disgusting and you should all be ashamed that you had anything to do with this problem.

(a) Clusterman's head gives a factor of 6 because the upper three vertices can be permuted among themselves in any of $3! = 6$ ways. Each of his hands gives a factor of 2 because each hand can be rotated by π about its corresponding arm. The arms themselves can be interchanged, by rotating his shoulders by π about his body axis (Clusterman finds this invigorating). Finally, the analysis for the hands and arms applies just as well to the feet and legs, so we conclude

$$s_\gamma = 6 \cdot \big(2^2 \cdot 2\big)^2 = 3 \cdot 2^7 = 384 \ .$$

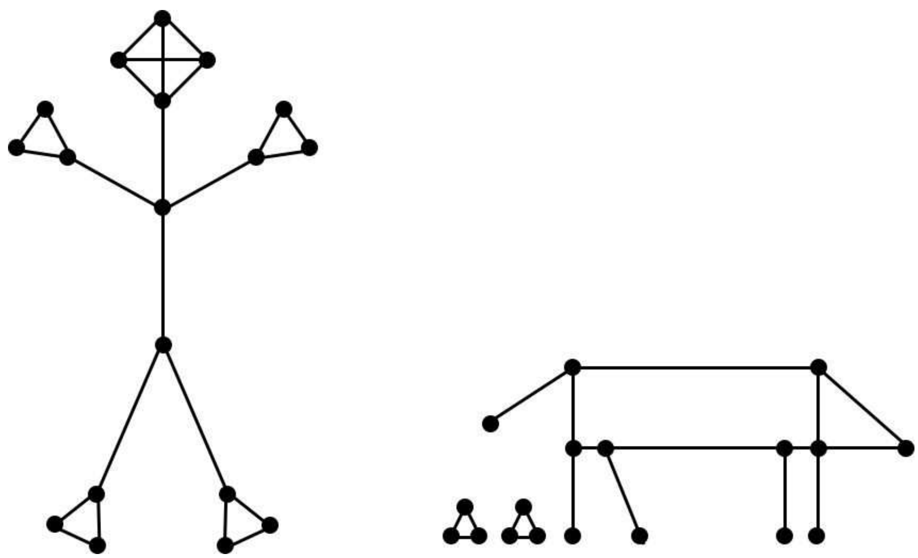

Figure 1: Mayer expansion diagrams for Clusterman and his dog.

Note that an arm cannot be exchanged with a leg, because the two lower vertices on Clusterman's torso are not equivalent. Plus, that would be a really mean thing to do to Clusterman.

(b) Henry himself has no symmetries. The little pieces each have $s_{\triangle} = 3!$, and moreover they can be exchanged, yielding another factor of 2. So the total symmetry factor for Henry plus disconnected pieces is $s_{\triangle\triangle} = 2! \cdot (3!)^2 = 72$. Were another little piece of the same…er…consistency to be found, the symmetry factor would be $s_{\triangle\triangle\triangle} = 3! \cdot (3!)^3 = 2^4 \cdot 3^4 = 1296$, since we get a factor of 3! from each of the $\triangle$ pieces, and a fourth factor of 3! from the permutations among the $\triangle$s.

(c) There are 18 vertices in Clusterman, hence he will first appear in B_{18}.

(3) The Tonks gas is a one-dimensional generalization of the hard sphere gas. Consider a one-dimensional gas of indistinguishable particles of mass m interacting via the potential

$$u(x - x') = \begin{cases} \infty & \text{if } |x - x'| < a \\ 0 & \text{if } |x - x'| \geq a \ . \end{cases}$$

Let the gas be placed in a finite volume L. The hard sphere nature of the particles means that no particle can get within a distance $\frac{1}{2}a$ of the ends at $x = 0$ and $x = L$. That is, there is a one-body potential $v(x)$ acting as well, where

$$v(x) = \begin{cases} \infty & \text{if } x < \frac{1}{2}a \\ 0 & \text{if } \frac{1}{2}a \leq x \leq L - \frac{1}{2}a \\ \infty & \text{if } x > L - \frac{1}{2}a \ . \end{cases}$$

(a) Compute the N particle partition function $Z(T, L, N)$ for the Tonks gas. Present a clear derivation of your result. Please try your best to solve this, either by yourself or in collaboration with classmates. If you get stuck there is an $\mathrm{S}k\log Wiki$ page on the web on "1-dimensional hard rods" where you can look up the derivation.

(b) Find the equation of state $p = p(T, L, N)$.

(c) Find the grand potential $\Omega(T, L, \mu)$. *Hint : There is a small subtlety you must appreciate in order to obtain the correct answer.*

Solution :

(a) The partition function is

$$Z(T, L, N) = \frac{\lambda_T^N}{N!} \int_0^L \! dx_1 \cdots \int_0^L \! dx_N \; \chi(x_1, \ldots, x_N) \ ,$$

where $\chi = e^{-U/k_\mathrm{B}T}$ is zero if any two 'rods' (of length a) overlap, or if any rod overlaps with either boundary at $x = 0$ and $x = L$, and $\chi = 1$ otherwise. Note that χ does not depend on temperature. Without loss of generality, we can integrate over the subspace where $x_1 < x_2 < \cdots < x_N$ and then multiply the result by $N!$. Clearly x_j must lie to the right of $x_{j-1} + a$ and to the left of $Y_j \equiv L - (N-j)a - \frac{1}{2}a$. Thus,

$$\begin{aligned} Z(T, L, N) &= \lambda_T^N \int_{a/2}^{Y_1} \! dx_1 \int_{x_1+a}^{Y_2} \! dx_2 \cdots \int_{x_{N-1}+a}^{Y_N} \! dx_N \\ &= \lambda_T^N \int_{a/2}^{Y_1} \! dx_1 \int_{x_1+a}^{Y_2} \! dx_2 \cdots \int_{x_{N-2}+a}^{Y_{N-1}} \! dx_{N-1} \left(Y_{N-1} - x_{N-1} \right) \\ &= \lambda_T^N \int_{a/2}^{Y_1} \! dx_1 \int_{x_1+a}^{Y_2} \! dx_2 \cdots \int_{x_{N-3}+a}^{Y_{N-2}} \! dx_{N-2} \, \tfrac{1}{2} \left(Y_{N-2} - x_{N-2} \right)^2 \\ &= \cdots = \frac{\lambda_T^N}{N!} \left(X_1 - \tfrac{1}{2}a \right)^N = \frac{\lambda_T^N}{N!} \left(L - Na \right)^N \ . \end{aligned}$$

The λ_T^N factor comes from integrating over the momenta; recall $\lambda_T = \sqrt{2\pi\hbar^2/mk_\mathrm{B}T}$.

(b) The free energy is

$$F = -k_\mathrm{B}T \ln Z = -Nk_\mathrm{B}T \left\{ \ln \lambda_T + 1 + \ln \left(\frac{L}{N} - a \right) \right\} \ ,$$

where we have used Stirling's rule to write $\ln N! \approx N \ln N - N$. The pressure is

$$p = -\frac{\partial F}{\partial L} = \frac{k_\mathrm{B}T}{\frac{L}{N} - a} = \frac{nk_\mathrm{B}T}{1 - na} \ ,$$

where $n = N/L$ is the one-dimensional density. Note that the pressure diverges as n approaches a^{-1} from below, and $n > a^{-1}$ is not allowed.

(c) We have

$$\Xi(T,L,\mu) = \sum_{N=0}^{N_{\rm max}} e^{N\mu/k_{\rm B}T}\, Z(T,L,N) \ ,$$

where $N_{\rm max} = [L/a]$, where $[x]$ is the greatest integer less than or equal to x. Then $\Omega = -k_{\rm B}T \ln \Xi$. Not much more we can do with this.

(4) In §5.5.3 of the notes, the virial equation of state is derived for a single species of particle.

(a) Generalize eqn. 5.160 to the case of two species interacting by $u_{\sigma\sigma'}(r)$, where σ and σ' are the species labels.

(b) For a plasma, show from Debye-Hückel theory that the pair correlation function is $g_{\sigma\sigma'} \propto \exp\big(-\sigma\sigma' q^2 \phi(r)/k_{\rm B}T\big)$, where σ and σ' are the signs of the charges (magnitude q), and $\phi(r)$ is the screened potential due to a unit positive test charge.

(c) Find the equation of state for a three-dimensional two-component plasma, in the limit where T is large.

Solution :

(a) Let $i = 1, \ldots, N_+ + N_-$ index all the particles, and let $\sigma_i = \pm 1$ denote the sign of the charge of particle i, with $\sigma_i = +1$ for $1 \le i \le N_+$ and $\sigma_i = -1$ for $(N_+ + 1) \le i \le (N_+ + N_-)$. In a globally neutral system, $N_+ = N_- \equiv \frac{1}{2}N$. We define

$$g_{\mu\nu}(\boldsymbol{r}) \equiv \frac{1}{n_\mu n_\nu} \Big\langle \sum_{i\neq j} \delta(\boldsymbol{r} - \boldsymbol{x}_i)\, \delta(\boldsymbol{x}_j)\, \delta_{\sigma_i,\mu}\, \delta_{\sigma_j,\nu} \Big\rangle \ ,$$

where n_μ is the density of particles of species μ, with $\mu = \pm 1$. As defined, $g_{\mu\nu}(\boldsymbol{r}) \to 1$ as $r \to \infty$. If instead we normalize $g_{\mu\nu}$ by dividing by $n_{\rm tot}^2 = (n_+ + n_-)^2$, then we would have $g_{\mu\nu}(r \to \infty) = \frac{1}{4}$. We next work on the virial equation of state,

$$\frac{p}{k_{\rm B}T} = \frac{N_+ + N_-}{V} - \frac{1}{3Vk_{\rm B}T} \sum_{i=1}^{N_+ + N_-} \big\langle \boldsymbol{x}_i \cdot \boldsymbol{\nabla}_i W \big\rangle \ .$$

The potential is

$$W = \sum_{i<j} \frac{\sigma_i\, \sigma_j\, q^2}{|\boldsymbol{x}_i - \boldsymbol{x}_j|} \equiv \sum_{i<j} u_{\sigma_i \sigma_j}\big(|\boldsymbol{x}_i - \boldsymbol{x}_j|\big) \ ,$$

with $u_{\sigma\sigma'}(r) = \sigma\sigma' q^2/r$. Then using translational invariance one has

$$\frac{p}{k_{\rm B}T} = n_+ + n_- - \frac{2\pi}{3k_{\rm B}T} \sum_{\sigma,\sigma'} n_\sigma n_{\sigma'} \int\limits_0^\infty \! dr\, r^3\, u'_{\sigma\sigma'}(r)\, g_{\sigma\sigma'}(r)$$

(b) According to Debye-Hückel theory,

$$g_{\sigma\sigma'}(r) = \exp\bigg(-\frac{\sigma\sigma' q\,\phi(r)}{k_{\rm B}T}\bigg) \ ,$$

where $\phi(r)$ is the screened potential at r due to a point charge q at the origin, which satisfies

$$\nabla^2\phi = 4\pi q\,\sinh\big(q\phi/k_{\rm B}T\big) - 4\pi q\,\delta(\boldsymbol{r}) \ ,$$

where $n_+ = n_- \equiv \frac{1}{2}n$. In the high temperature limit, we can expand the sinh function and we obtain the Yukawa potential

$$\phi(r) = \frac{q}{r}\,e^{-\kappa_{\rm D}r} \ ,$$

where

$$\kappa_{\rm D} = \bigg(\frac{4\pi n q^2}{k_{\rm B}T}\bigg)^{1/2}$$

is the Debye screening wavevector. Thus, we have

$$\begin{aligned}
\frac{p}{k_{\rm B}T} &= n - \frac{\pi n^2}{6k_{\rm B}T}\int\limits_0^\infty\!dr\,r^3\bigg(-\frac{q^2}{r^2}\bigg)\sum_{\sigma,\sigma'}\sigma\sigma'\,g_{\sigma\sigma'}(r) \\
&= n - \frac{2\pi n^2 q^3}{3(k_{\rm B}T)^2}\int\limits_0^\infty\!dr\,r\,\phi(r) = n - \frac{2\pi n^2 q^4}{3(k_{\rm B}T)^2\kappa_{\rm D}} \\
&= n\bigg(1 - \frac{\sqrt{\pi}\,n^{1/2}\,q^3}{3\,(k_{\rm B}T)^{3/2}}\bigg) \ .
\end{aligned}$$