PHYSICS 210A : EQUILIBRIUM STATISTICAL PHYSICS
HW ASSIGNMENT #5 SOLUTIONS

(1) Consider a spin-1 Ising chain with Hamiltonian

$$\hat{H} = -J \sum_n S_n \, S_{n+1} \ ,$$

where each S_n takes possible values $\{-1, 0, 1\}$.

(a) Find the transfer matrix for the this model.

(b) Find an expression for the free energy $F(T, J, N)$ for an N-site chain and for an N-site ring.

(c) Suppose a magnetic field term $\hat{H}' = -\mu_0 H \sum_n S_n$ is included. Find the transfer matrix.

Solution :

(a) The transfer matrix is

$$R_{SS'} = e^{\beta J S S'} = \begin{pmatrix} e^{\beta J} & 1 & e^{-\beta J} \\ 1 & 1 & 1 \\ e^{-\beta J} & 1 & e^{\beta J} \end{pmatrix} \ .$$

(b) The partition function is

$$Z_{\text{ring}} = \text{Tr}\left(R^N\right) \qquad , \qquad Z_{\text{chain}} = \sum_{S,S'} \left[R^{N-1}\right]_{SS'} \ .$$

We can derive the eigenvalues and eigenvectors of R almost by inspection. Clearly one eigenvector is

$$\psi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \qquad , \qquad \lambda_0 = 2 \sinh \beta J \ .$$

The remaining two eigenvectors are orthogonal to $\psi^{(0)}$ and may be written as

$$\psi_\pm = \frac{1}{\sqrt{2 + \alpha^2}} \begin{pmatrix} 1 \\ \alpha \\ 1 \end{pmatrix} \ ,$$

where there are two possible solutions for α which we call $\alpha_\pm$. Applying R to $\psi_\pm$, we have

$$\begin{aligned} 2 \cosh \beta J + \alpha &= \lambda \\ 2 + \alpha &= \lambda \, \alpha \end{aligned}$$

Using the second equation to solve for λ, we have $\lambda = 1 + 2\alpha^{-1}$. Plugging this into the first equation, we obtain

$$\alpha_\pm = \tfrac{1}{2} - \cosh \beta J \pm \sqrt{\left(\tfrac{1}{2} - \cosh \beta J\right)^2 + 2}$$

and

$$\lambda_{\pm} = \tfrac{1}{2} + \cosh\beta J \pm \sqrt{\tfrac{9}{4} - \cosh\beta J + \cosh^2\!\beta J}$$

The roots $\alpha_{\pm}$ satisfy $\alpha_+\alpha_- = -2$, which guarantees that $\langle\, \psi_+ \,|\, \psi_- \,\rangle = 0$. Note that

$$\langle\, S \,|\, \psi_0 \,\rangle\langle\, \psi_0 \,|\, S' \,\rangle = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

$$\langle\, S \,|\, \psi_{\pm} \,\rangle\langle\, \psi_{\pm} \,|\, S' \,\rangle = \frac{1}{2+\alpha_{\pm}^2}\begin{pmatrix} 1 & \alpha_{\pm} & 1 \\ \alpha_{\pm} & \alpha_{\pm}^2 & \alpha_{\pm} \\ 1 & \alpha_{\pm} & 1 \end{pmatrix}$$

and, for any J,

$$\big[R^J\big]_{SS'} = \lambda_+^J \cdot \langle\, S \,|\, \psi_+ \,\rangle\langle\, \psi_+ \,|\, S' \,\rangle + \lambda_0^J \cdot \langle\, S \,|\, \psi_0 \,\rangle\langle\, \psi_0 \,|\, S' \,\rangle + \lambda_-^J \cdot \langle\, S \,|\, \psi_- \,\rangle\langle\, \psi_- \,|\, S' \,\rangle \,.$$

Thus,

$$\begin{aligned} Z_{\text{ring}} &= \lambda_+^N + \lambda_0^N + \lambda_-^N \\ Z_{\text{chain}} &= \lambda_+^{N-1} \cdot \frac{(\alpha_+ + 2)^2}{\alpha_+^2 + 2} + \lambda_-^{N-1} \cdot \frac{(\alpha_- + 2)^2}{\alpha_-^2 + 2} \\ &= \frac{\big(2\lambda_+ - 3\big)^2 \cdot \lambda_+^{N-1}}{2\big(\lambda_+ - 2\big)^2 + 1} + \frac{\big(2\lambda_- - 3\big)^2 \cdot \lambda_-^{N-1}}{2\big(\lambda_- - 2\big)^2 + 1} \,. \end{aligned}$$

(c) With a magnetic field, we have

$$R_{SS'} = e^{\beta J S S'}\, e^{\beta\mu_0 H(S+S')/2} = \begin{pmatrix} e^{\beta(J+\mu_0 H)} & e^{\beta\mu_0 H/2} & e^{-\beta J} \\ e^{\beta\mu_0 H/2} & 1 & e^{-\beta\mu_0 H/2} \\ e^{-\beta J} & e^{-\beta\mu_0 H/2} & e^{\beta(J-\mu_0 H)} \end{pmatrix} \,.$$

(2) Consider an N-site Ising ring, with N even. Let $K = J/k_{\rm B}T$ be the dimensionless ferromagnetic coupling ($K > 0$), and $\mathcal{H}(K,N) = H/k_{\rm B}T = -K\sum_{n=1}^N \sigma_n\,\sigma_{n+1}$ the dimensionless Hamiltonian. The partition function is $Z(K,N) = \text{Tr}\; e^{-\mathcal{H}(K,N)}$. By 'tracing out' over the even sites, show that

$$Z(K,N) = e^{-N'c}\, Z(K',N') \,,$$

where $N' = N/2$, $c = c(K)$ and $K' = K'(K)$. Thus, the partition function of an N site ring with dimensionless coupling K is related to the partition function *for the same model* on an $N' = N/2$ site ring, at some *renormalized* coupling K', up to a constant factor.

Solution :

We have

$$\sum_{\sigma_{2k}=\pm} e^{K\sigma_{2k}(\sigma_{2k-1}+\sigma_{2k+1})} = 2\cosh\big(K\sigma_{2k-1} + K\sigma_{2k+1}\big) \equiv e^{-c}\, e^{K'\sigma_{2k-1}\,\sigma_{2k+1}}$$

Consider the cases $(\sigma_{2k-1}, \sigma_{2k+1}) = (1, 1)$ and $(1, -1)$, respectively. These yield two equations,

$$2\cosh 2K = e^{-c}\, e^{K'}$$
$$2 = e^{-c}\, e^{-K'} \ .$$

From these we derive

$$c(K) = -\ln 2 - \tfrac{1}{2} \ln \cosh K$$

and

$$K'(K) = \tfrac{1}{2} \ln \cosh 2K \ .$$

This last equation is a realization of the *renormalization group*. By thinning the degrees of freedom, we derive an effective coupling K' valid at a new length scale. In our case, it is easy to see that $K' < K$ so the coupling gets weaker and weaker at longer length scales. This is consistent with the fact that the one-dimensional Ising model is disordered at all finite temperatures.

(3) For each of the cluster diagrams in Fig. 1, find the symmetry factor s_γ and write an expression for the cluster integral b_γ.

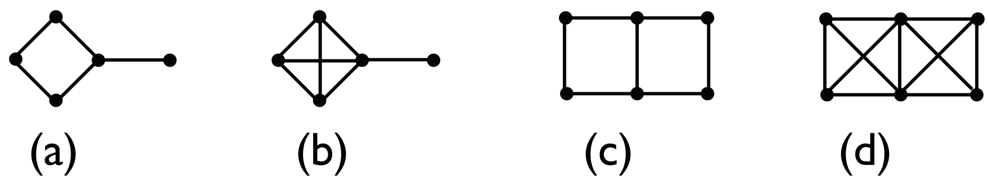

Figure 1: Cluster diagrams for problem 1.

Solution : Choose labels as in Fig. 2, and set $\boldsymbol{x}_{n_\gamma} \equiv 0$ to cancel out the volume factor in the definition of b_γ.

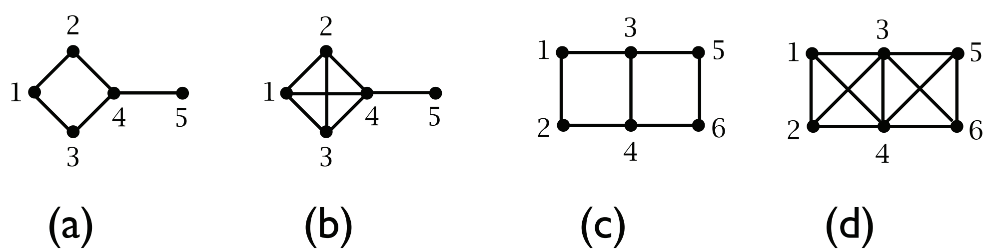

Figure 2: Labeled cluster diagrams.

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

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

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

$$b_\gamma = \tfrac{1}{6}\int\! d^dx_1\!\int\! d^dx_2\!\int\! d^dx_3\!\int\! d^dx_4\; f(r_{12})\, f(r_{13})\, f(r_{24})\, f(r_{34})\, f(r_{14})\, f(r_{23})\, f(r_4)\, .$$

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

$$b_\gamma = \tfrac{1}{4}\int\! d^dx_1\!\int\! d^dx_2\!\int\! d^dx_3\!\int\! d^dx_4\!\int\! d^dx_5\; f(r_{12})\, f(r_{13})\, f(r_{24})\, f(r_{34})\, f(r_{35})\, f(r_4)\, f(r_5)\, .$$

(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

$$b_\gamma = \tfrac{1}{16}\int\! d^dx_1\!\int\! d^dx_2\!\int\! d^dx_3\!\int\! d^dx_4\!\int\! d^dx_5\; f(r_{12})\, f(r_{13})\, f(r_{14})\, f(r_{23})\, f(r_{24})\, f(r_{34})\, f(r_{35})\, f(r_{45})\, f(r_3)\, f(r_4)\, f(r_5)\, .$$

(4) The grand potential for an interacting system in a finite volume V is given by

$$\Xi(z) = (1+z)^M \prod_{j=1}^{j} \frac{1-(z/\sigma_j)^{L_j+1}}{1-(z/\sigma_j)} \quad .$$

(a) Find all the zeros of $\Xi(z)$ in the complex plane, along with their orders.

(b) Define the normalized density of states like function,

$$g(\sigma) = \frac{1}{L}\sum_{j=1}^{J} L_j\, \delta(\sigma - \sigma_j) \quad ,$$

with $L = \sum_{j=1}^{j} L_j$. In the thermodynamic limit, take $V \to \infty$, $M \to \infty$, $L_j \to \infty$ with $v_0 \equiv V/M$ and $\alpha \equiv L/M$ constant. Then define the dimensionless density $\nu = Nv_0/V$ and dimensionless pressure $\pi \equiv pv_0/k_B T$. Derive expressions for $\nu(z)$ and $\pi(z)$ in terms of z, α, and the function $g(\sigma)$. *Hint: you may find it helpful to consult Example Problem 6.12.*

(c) Suppose $g(\sigma) = A\,(b-\sigma)^t\,\Theta(b-\sigma)$ with $A = (t+1)/b^{t+1}$ and $t > -1$. Show that there is a phase transition at all values of $b > 0$, and find expressions for $\nu_c(b)$ and $\pi_c(b)$.

(d) Find the leading singularity in $\pi(\nu)$ as a function of $(\nu - \nu_c)$ on either side of the critical point (*i.e.* for $\nu < \nu_c$ and $\nu > \nu_c$).

Solution :

(a) $\Xi(z)$ has one zero of order M at $z = -1$, and $L = \sum_{j=1}^{J} L_j$ simple zeros at $z = \sigma_j\, e^{2\pi i \ell_j/(L_j+1)}$ for $j \in \{1,\ldots,J\}$ and $\ell_j \in \{1,\ldots,L_j\}$.

(b) We have

$$\pi = \frac{pv_0}{k_{\rm B}T} = \frac{1}{M}\ln \Xi(z) = \ln(1+z) + \frac{1}{M}\sum_{j=1}^{J} L_j \, \ln\!\Big(\frac{z}{\sigma_j}\Big)\,\Theta\big(|z|-\sigma_j\big)$$

$$= \ln(1+z) + \alpha\int\limits_0^z\! d\sigma\, g(\sigma)\ln\!\Big(\frac{z}{\sigma}\Big)$$

and consequently[1]

$$\nu = \frac{Nv_0}{V} = z\,\frac{\partial\pi}{\partial z} = \frac{z}{1+z} + \frac{1}{M}\sum_{j=1}^{J} L_j\,\Theta\big(|z|-\sigma_j\big)$$

$$= \frac{z}{1+z} + \alpha\int\limits_0^z\! d\sigma\, g(\sigma) \quad .$$

In our final expressions for $\pi(z)$ and $\nu(z)$, we have taken $z \in \mathbb{R}_+$. If you are wondering where the temperature T is implicit in all this, it is in the quantities $\sigma_j = \sigma_j(T)$, and thus in the distribution $g(\sigma) = g(\sigma, T)$. Note that

$$g(\sigma) = \frac{1}{L}\sum_{j=1}^{J} L_j\,\delta(\sigma-\sigma_j)$$

is normalized, *i.e.* $\int\limits_0^\infty d\sigma\, g(\sigma) = 1$.

(c) There is a phase transition at $z = z_{\rm c} = b$, where the function $g(\sigma)$ is singular, and hence where integrals of the form $\int\limits_0^z d\sigma\, g(\sigma)\, F(\sigma)$ are singular, where $F(\sigma)$ is any smooth function. Therefore,

$$\nu_{\rm c} = \frac{b}{1+b} + \alpha$$

$$\pi_{\rm c} = \ln(1+b) + \alpha\, f(t) \quad ,$$

where

$$f(t) = -(t+1)\int\limits_0^1\! du\,(1-u)^t\,\ln u = \sum_{k=1}^\infty \frac{1}{k}\cdot\frac{t+1}{t+1+k} \quad .$$

[1]Note that when differentiating $\Theta(z-\sigma_j)$ with respect to z, one obtains $\delta(z-\sigma_j)$. However, this vanishes when multiplied by $\ln(z/\sigma_j)$, which vanishes linearly as a function of $z-\sigma_j$. This is because the distribution $x\,\delta(x)$ may be set to zero provided it is not weighted by a divergent function of x which would effectively cancel the x prefactor.

(d) With $g(\sigma) = (t+1)\,(b-\sigma)^t\,\Theta(b-\sigma)/b^{t+1}$, defining $\sigma \equiv bu$, we have

$$\nu(z) = \frac{z}{1+z} + (t+1)\,\alpha \int\limits_0^{z/b} du\,(1-u)^t\,\Theta(1-u)$$

$$\pi(z) = \ln(1+z) + (t+1)\,\alpha \int\limits_0^{z/b} du\,(1-u)^t \left\{ \ln\!\left(\frac{z}{b}\right) - \ln u \right\} \Theta(1-u)$$

Let us write $z = b \pm \varepsilon$ with $\varepsilon > 0$ and expand in powers of ε. We must separately consider the cases $z > b$ and $z < b$.

For $z = b + \varepsilon$ we have

$$\begin{aligned} \nu(z)\big|_{z=b+\varepsilon} &= \nu_c + \left(\frac{b+\varepsilon}{1+b+\varepsilon} - \frac{b}{1+b} \right) \\ &= \nu_c + \frac{\varepsilon}{(1+b)^2} + \mathcal{O}(\varepsilon^2) \end{aligned}$$

and

$$\begin{aligned} \pi(z)\big|_{z=b+\varepsilon} &= \pi_c + \ln\!\left(\frac{1+b+\varepsilon}{1+b} \right) + \alpha \ln\!\left(1 + \frac{\varepsilon}{b} \right) \\ &= \pi_c + \left(\frac{\alpha}{b} + \frac{1}{1+b} \right) \varepsilon + \mathcal{O}(\varepsilon^2) \quad . \end{aligned}$$

For $z = b - \varepsilon$ we have

$$\begin{aligned} \nu(z)\big|_{z=b-\varepsilon} &= \nu_c + \left(\frac{b-\varepsilon}{1+b-\varepsilon} - \frac{b}{1+b} \right) - \alpha\,\frac{\varepsilon^{t+1}}{b^{t+1}} \\ &= \nu_c - \frac{\varepsilon}{(1+b)^2} - \alpha\,\frac{\varepsilon^{t+1}}{b^{t+1}} + \mathcal{O}(\varepsilon^2) \end{aligned}$$

and

$$\begin{aligned} \pi(z)\big|_{z=b-\varepsilon} &= \pi_c - \frac{\varepsilon}{1+b} - \alpha\,\ln\!\left(1-\frac{\varepsilon}{b}\right) - \alpha\,\ln\!\left(1-\frac{\varepsilon}{b}\right) \frac{\varepsilon^{t+1}}{b^{t+1}} - (t+1)\,\alpha \int\limits_0^{\varepsilon/b} ds\, s^t\,\ln(1-s) \\ &= \pi_c - \left(\frac{\alpha}{b} + \frac{1}{1+b} \right) \varepsilon - \frac{\alpha}{t+2}\,\frac{\varepsilon^{t+2}}{b^{t+2}} + \mathcal{O}(\varepsilon, \varepsilon^{t+3}) \quad . \end{aligned}$$

If $t > 0$, to lowest order in $\Delta\nu = \nu - \nu_c$, we find

$$t > 0 \ : \qquad \pi(\nu) = \pi_c + (1+b)^2 \left(\frac{\alpha}{b} + \frac{1}{1+b} \right) (\nu - \nu_c) + \ \ldots \quad .$$

When $t = 0$, the above result holds for $\nu > \nu_{\mathrm{c}}$, but for $\nu < \nu_{\mathrm{c}}$ the slope is different:

$$t > 0\ ,\ \nu < \nu_{\mathrm{c}}\ : \qquad \pi(\nu) = \pi_{\mathrm{c}} + \left(\frac{\alpha}{b} + \frac{1}{(1+b)^2}\right)^{-1} \left(\frac{\alpha}{b} + \frac{1}{1+b}\right)(\nu - \nu_{\mathrm{c}}) + \ \ldots \quad .$$

When $-1 < t < 0$, provided $\nu > \nu_{\mathrm{c}}$, we still have

$$-1 < t < 0\ ,\ \nu > \nu_{\mathrm{c}}\ : \qquad \pi(\nu) = \pi_{\mathrm{c}} + (1+b)^2 \left(\frac{\alpha}{b} + \frac{1}{1+b}\right)(\nu - \nu_{\mathrm{c}}) + \ \ldots \quad .$$

However when $\nu < \nu_{\mathrm{c}}$, we find a new behavior:

$$-1 < t < 0\ ,\ \nu < \nu_{\mathrm{c}}\ : \qquad \pi(\nu) = \pi_{\mathrm{c}} - \left(\alpha + \frac{b}{1+b}\right)\left(\frac{\nu_{\mathrm{c}} - \nu}{\alpha}\right)^{1/(t+1)} + \ \ldots \quad .$$