PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #2 SOLUTIONS

(1) Consider a model in which there are three possible states per site, which we can denote by A, B, and V. The states A and B are for our purposes identical. The energies of A-A, A-B, and B-B links are all identical and equal to W. The state V represents a vacancy, and any link containing a vacancy, meaning A-V, B-V, or V-V, has energy 0.

(a) Suppose we write $\sigma = +1$ for A, $\sigma = -1$ for B, and $\sigma = 0$ for V. How would you write a Hamiltonian for this system? Your result should be of the form

$$\hat{H} = \sum_{\langle ij \rangle} E(\sigma_i \, , \, \sigma_j) \quad .$$

Find a simple and explicit function $E(\sigma, \sigma')$ which yields the correct energy for each possible bond configuration.

(b) Consider a triangle of three sites. Find the average total energy at temperature T. *There are* $3^3 = 27$ *states for the triangle. You can just enumerate them all and find the energies.*

(c) For a one-dimensional ring of N sites, find the 3×3 transfer matrix R. Find the free energy per site $F(T, N)/N$ and the ground state entropy per site $S(T, N)/N$ in the $N \to \infty$ limit for the cases $W < 0$ and $W > 0$. Interpret your results. *The eigenvalue equation for* R *factorizes, so you only have to solve a quadratic equation.*

Solution:

(a) The quantity σ_i^2 is 1 if site i is in state A or B and is 0 in state V. Therefore we have

$$\hat{H} = W \sum_{\langle ij \rangle} \sigma_i^2 \sigma_j^2 \quad .$$

(b) Of the 27 states, eight have zero vacancies – each site has two possible states A and B – with energy $E = 3W$. There are 12 states with one vacancy, since there are three possible locations for the vacancy and then four possibilities for the remaining two sites (each can be either A or B). Each of these 12 single vacancy states has energy $E = W$. There are 6 states with two vacancies and 1 state with three vacancies, all of which have energy $E = 0$. The partition function is therefore

$$Z = 8 \, e^{-3\beta W} + 12 \, e^{-\beta W} + 7 \quad .$$

Note that $Z(\beta = 0) = \text{Tr} \, 1 = 27$ is the total number of 'microstates'. The average energy is then

$$E = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = \left(\frac{24 \, e^{-3\beta W} + 12 \, e^{-\beta W}}{8 \, e^{-3\beta W} + 12 \, e^{-\beta W} + 7} \right) W$$

(c) The transfer matrix is

$$R_{\sigma\sigma'} = e^{-\beta W \sigma^2 \sigma'^2} = \begin{pmatrix} e^{-\beta W} & e^{-\beta W} & 1 \\ e^{-\beta W} & e^{-\beta W} & 1 \\ 1 & 1 & 1 \end{pmatrix} \quad ,$$

where the row and column indices are A (1), B (2), and V (3), respectively. The partition function on a ring of N sites is

$$Z = \lambda_1^N + \lambda_2^N + \lambda_3^N \quad ,$$

where $\lambda_{1,2,3}$ are the three eigenvalues of R. Generally the eigenvalue equation for a 3×3 matrix is cubic, but we can see immediately that $\det R = 0$ because the first two rows are identical. Thus, $\lambda = 0$ is a solution to the characteristic equation $P(\lambda) = \det\big(\lambda\mathbb{I} - R\big) = 0$, and the cubic polynomial $P(\lambda)$ factors into the product of λ and a quadratic. The latter is easily solved. One finds

$$P(\lambda) = \lambda^3 - (2x+1)\,\lambda^2 + (2x-2)\,\lambda \quad ,$$

where $x = e^{-\beta W}$. The roots are $\lambda = 0$ and

$$\lambda_\pm = x + \tfrac{1}{2} \pm \sqrt{x^2 - x + \tfrac{9}{4}} \quad .$$

The largest of the three eigenvalues is λ_+, hence, in the thermodynamic limit,

$$F = -k_B T \ln Z = -N k_B T \ln\!\left(e^{-W/k_B T} + \tfrac{1}{2} + \sqrt{e^{-2W/k_B T} - e^{-W/k_B T} + \tfrac{9}{4}} \right) \quad .$$

The entropy is $S = -\frac{\partial F}{\partial T}$. In the limit $T \to 0$ with $W < 0$, we have

$$\lambda_+(T \to 0\,,\, W < 0) = 2\, e^{|W|/k_B T} + e^{-|W|/k_B T} + \mathcal{O}\big(e^{-2|W|/k_B T}\big) \quad .$$

Thus

$$\begin{aligned} F(T \to 0\,,\, W < 0) &= -N\,|W| - N k_B T \ln 2 + \ldots \\ S(T \to 0\,,\, W < 0) &= N \ln 2 \quad . \end{aligned}$$

When $W > 0$, we have

$$\lambda_+(T \to 0\,,\, W > 0) = 2 + \tfrac{2}{3}\, e^{-W/k_B T} + \mathcal{O}\big(e^{-2W/k_B T}\big) \quad .$$

Then

$$\begin{aligned} F(T \to 0\,,\, W > 0) &= -N k_B T \ln 2 - \tfrac{1}{3} N k_B T\, e^{-W/k_B T} + \ldots \\ S(T \to 0\,,\, W > 0) &= N \ln 2 \quad . \end{aligned}$$

Thus, the ground state entropies are the same, even though the allowed microstates are very different. For $W < 0$, there are no vacancies. For $W > 0$, every link must contain at least one vacancy.

(2) Consider a longer-ranged Ising model on a ring with Hamiltonian

$$\hat{H} = \sum_{n=1}^{L} E(\sigma_n, \sigma_{n+1}, \sigma_{n+2}) \quad ,$$

where the length $L > 2$ is even and the energy function $E(\sigma.\sigma', \sigma'')$ is arbitrary. Note that this chain involves second-neighbor interactions.

(a) Show that the partition function can be written as

$$Z(T, L) = \operatorname*{Tr}_{\boldsymbol{\sigma}} \prod_{k=1}^{K} T(\sigma_{2k-1}, \sigma_{2k} \,|\, \sigma_{2k+1}, \sigma_{2k+2})$$

where $K = \frac{1}{2}L$. and find $T(\sigma_{2k-1}, \sigma_{2k} \,|\, \sigma_{2k+1}, \sigma_{2k+2})$ in terms of $E(\sigma_n, \sigma_{n+1}, \sigma_{n+2})$.

(b) Show that $T(\sigma, \sigma' \,|\, \sigma'', \sigma''')$ can be considered a 4×4 matrix, whence $Z = \text{Tr}\, T^K$.

(c) Suppose

$$E(\sigma_n, \sigma_{n+1}, \sigma_{n+2}) = \begin{cases} -J & \text{if } \sigma_n = \sigma_{n+1} = \sigma_{n+2} \\ 0 & \text{otherwise} \quad . \end{cases}$$

Find the 4×4 transfer matrix.

`Solution:`

(a) Define

$$T(\sigma_{2k-1}, \sigma_{2k} \,|\, \sigma_{2k+1}, \sigma_{2k+2}) \equiv e^{-\beta E(\sigma_{2k-1}, \sigma_{2k}, \sigma_{2k+1})} \, e^{-\beta E(\sigma_{2k}, \sigma_{2k+1}, \sigma_{2k+2})} \quad .$$

Then

$$Z(T, L) = \operatorname*{Tr}_{\boldsymbol{\sigma}} e^{-\beta E(\sigma_1, \sigma_2, \sigma_3)} \, e^{-\beta E(\sigma_2, \sigma_3, \sigma_4)} \cdots e^{-\beta E(\sigma_{L-2}, \sigma_{L-1}, \sigma_L)} \, e^{-\beta E(\sigma_{L-1}, \sigma_L, \sigma_1)} \, e^{-\beta E(\sigma_L, \sigma_1, \sigma_2)} \quad ,$$

which is the partition function for the L-site chain.

(b) Since the pair (σ, σ') can take four possible values, *i.e.* $(+,+)$, $(+,-)$, $(-,+)$, and $(-,-)$, which we respectively define as states $a = 1$, 2, 3, and 4, we have

$$T_{a,a'} = e^{-\beta \mathcal{E}(a,a')}$$

and clearly $Z = \text{Tr}\, T^K$.

(c) For the given energy function $E(\sigma_n, \sigma_{n+1}, \sigma_{n+2})$, we have

$$\mathcal{E}(a, a') = \begin{cases} -2J & \text{if } a = (+,+) \text{ and } a' = (+,+) \text{ or } a = (-,-) \text{ and } a' = (-,-) \\ -J & \text{if } a = (+,+) \text{ and } a' = (+,-) \text{ or } a = (-,-) \text{ and } a' = (-,+) \\ -J & \text{if } a = (-,+) \text{ and } a' = (+,+) \text{ or } a = (+,-) \text{ and } a' = (-,-) \\ 0 & \text{otherwise} \quad . \end{cases}$$

In matrix form,

$$\mathcal{E}(a,a') = \begin{pmatrix} -2J & -J & 0 & 0 \\ 0 & 0 & 0 & -J \\ -J & 0 & 0 & 0 \\ 0 & 0 & -J & -2J \end{pmatrix}$$

and

$$T_{a,a'} = e^{-\beta \mathcal{E}(a,a')} = \begin{pmatrix} x^2 & x & 1 & 1 \\ 1 & 1 & 1 & x \\ x & 1 & 1 & 1 \\ 1 & 1 & x & x^2 \end{pmatrix} \quad ,$$

where $x = \exp(\beta J)$. The characteristic polynomial $P(\lambda) = \det(\lambda \mathbb{I} - T)$ factors into a product of binomials, with roots

$$\lambda_1 = \tfrac{1}{2}x^2 + \tfrac{1}{2}\sqrt{x^4 + 2x^2 + 8x + 5} + \tfrac{3}{2} \quad , \quad \lambda_3 = \tfrac{1}{2}x^2 + (x-1)^{3/2}(x+3)^{1/2} - \tfrac{1}{2}$$
$$\lambda_2 = \tfrac{1}{2}x^2 - \tfrac{1}{2}\sqrt{x^4 + 2x^2 + 8x + 5} + \tfrac{3}{2} \quad , \quad \lambda_4 = \tfrac{1}{2}x^2 - (x-1)^{3/2}(x+3)^{1/2} - \tfrac{1}{2} \quad .$$

The largest eigenvalue is λ_1 and thus in the thermodynamic limit we have $Z = \lambda_1^K$.

(3) 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 ${}^4\mathrm{He} - {}^3\mathrm{He}$ mixtures ($S = 0$ for a ${}^4\mathrm{He}$ 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

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

(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

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

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

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

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

$$F(T, \Delta, N) = -N k_B T \ln \lambda_+ \ .$$

(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

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

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

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

(4) 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 $Z(K,N) = \mathsf{Tr} \; e^{-\mathcal{H}(K,N)}$. 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,

$$\begin{aligned} 2\cosh 2K &= e^{-c}\, e^{K'} \\ 2 &= e^{-c}\, e^{-K'} \ . \end{aligned}$$

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.