Transfer Matrices & Duality

This problem set is partly intended to introduce the *transfer matrix method*, which is used to solve a variety of one-dimensional models with near-neighbor interactions. As an example, consider a linear chain of N Ising spins ($\sigma_i = \pm 1$), with a nearest–neighbor coupling K, and a magnetic field h. To simplify calculations, we assume that the chain is closed upon itself such that the first and last spins are also coupled (periodic boundary conditions), resulting in the Hamiltonian

$$-\beta\mathcal{H} = K\left(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \cdots + \sigma_{N-1}\sigma_N + \sigma_N\sigma_1\right) + h\sum_{i=1}^{N}\sigma_i \ . \tag{1}$$

The corresponding partition function, obtained by summing over all states, can be expressed as the product of matrices, since

$$\begin{aligned} Z &= \sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1}\prod_{i=1}^{N}\exp\left[K\sigma_i\sigma_{i+1} + \frac{h}{2}\left(\sigma_i+\sigma_{i+1}\right)\right] \\ &\equiv \mathrm{tr}\left[\langle\sigma_1|T|\sigma_2\rangle\langle\sigma_2|T|\sigma_3\rangle\cdots\langle\sigma_N|T|\sigma_1\rangle\right] = \mathrm{tr}\left[T^N\right]; \end{aligned} \tag{2}$$

where we have introduced the 2×2 *transfer matrix* T, with elements

$$\langle\sigma_i|T|\sigma_j\rangle = \exp\left[K\sigma_i\sigma_j + \frac{h}{2}(\sigma_i+\sigma_j)\right], \quad \text{i.e.} \quad T = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}. \tag{3}$$

The expression for trace of the matrix can be evaluated in the basis that diagonalizes T, in which case it can be written in terms of the two eigenvalues $\lambda_\pm$ as

$$Z = \lambda_+^N + \lambda_-^N = \lambda_+^N\left[1 + \left(\lambda_-/\lambda_+\right)^N\right] \approx \lambda_+^N. \tag{4}$$

We have assumed that $\lambda_+ > \lambda_-$, and since in the limit of $N\to\infty$ the larger eigenvalue dominates the sum, the free energy is

$$\beta f = -\ln Z/N = -\ln\lambda_+. \tag{5}$$

Solving the characteristic equation, we find the eigenvalues

$$\lambda_\pm = e^K\cosh h \pm \sqrt{e^{2K}\sinh^2 h + e^{-2K}}. \tag{6}$$

We shall leave a discussion of the singularities of the resulting free energy (at zero temperature) to the next section, and instead look at the averages and correlations in the limit of $h = 0$.

To calculate the average of the spin at site i, we need to evaluate

$$\begin{aligned}\langle\sigma_i\rangle &= \frac{1}{Z}\sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1}\sigma_i\prod_{j=1}^{N}\exp\left(K\sigma_j\sigma_{j+1}\right)\\ &\equiv \frac{1}{Z}\mathrm{tr}\left[\langle\sigma_1|T|\sigma_2\rangle\cdots\langle\sigma_{i-1}|T|\sigma_i\rangle\sigma_i\langle\sigma_i|T|\sigma_{i+1}\rangle\cdots\langle\sigma_N|T|\sigma_1\rangle\right]\\ &= \frac{1}{Z}\,\mathrm{tr}\left[T^{i-1}\hat{\sigma}_z T^{N-i+1}\right] = \frac{1}{Z}\,\mathrm{tr}\left[T^N\hat{\sigma}_z\right],\end{aligned} \tag{7}$$

where have permuted the matrices inside the trace, and $\hat{\sigma}_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$, is the usual 2×2 Pauli matrix. One way to evaluate the final expression in Eq.(7) is to rotate to a basis where the matrix T is diagonal. For $h = 0$, this is accomplished by the unitary matrix $U = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$, resulting in

$$\langle\sigma_i\rangle = \frac{1}{Z}\,\mathrm{tr}\left[\begin{pmatrix}\lambda_+^N & 0\\ 0 & \lambda_-^N\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right] = \frac{1}{Z}\begin{pmatrix}0 & \lambda_+^N\\ \lambda_-^N & 0\end{pmatrix} = 0. \tag{8}$$

Note that under this transformation the Pauli matrix $\hat{\sigma}_z$ is rotated into $\hat{\sigma}_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$.

The vanishing of the magnetization at zero field is of course expected by symmetry. A more interesting quantity is the two-spin correlation function

$$\begin{aligned}\langle\sigma_i\sigma_{i+r}\rangle &= \frac{1}{Z}\sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1}\sigma_i\sigma_{i+r}\prod_{j=1}^{N}\exp\left(K\sigma_j\sigma_{j+1}\right)\\ &= \frac{1}{Z}\,\mathrm{tr}\left[T^{i-1}\hat{\sigma}_z T^r\hat{\sigma}_z T^{N-i-r+1}\right] = \frac{1}{Z}\,\mathrm{tr}\left[\hat{\sigma}_z T^r\hat{\sigma}_z T^{N-r}\right].\end{aligned} \tag{9}$$

Once again rotating to the basis where T is diagonal simplifies the trace to

$$\begin{aligned}\langle\sigma_i\sigma_{i+r}\rangle &= \frac{1}{Z}\,\mathrm{tr}\left[\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\lambda_+^r & 0\\ 0 & \lambda_-^r\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\lambda_+^{N-r} & 0\\ 0 & \lambda_-^{N-r}\end{pmatrix}\right]\\ &= \frac{1}{Z}\,\mathrm{tr}\begin{pmatrix}\lambda_+^{N-r}\lambda_-^r & 0\\ 0 & \lambda_-^{N-r}\lambda_+^r\end{pmatrix} = \frac{\lambda_+^{N-r}\lambda_-^r + \lambda_-^{N-r}\lambda_+^r}{\lambda_+^N + \lambda_-^N}.\end{aligned} \tag{10}$$

Note that because of the periodic boundary conditions, the above answer is invariant under $r \to (N-r)$. We are interested in the limit of $N \gg r$, for which

$$\langle\sigma_i\sigma_{i+r}\rangle \approx \left(\frac{\lambda_-}{\lambda_+}\right)^r \equiv e^{-r/\xi}, \tag{11}$$

with the correlation length

$$\xi = \left[\ln\left(\frac{\lambda_+}{\lambda_-}\right)\right]^{-1} = -\frac{1}{\ln\tanh K}. \tag{12}$$

The above transfer matrix approach can be generalized to any one dimensional chain with variables $\{s_i\}$ and nearest neighbor interactions. The partition function can be written as

$$Z = \sum_{\{s_i\}} \exp\left[\sum_{i=1}^{N} B(s_i, s_{i+1})\right] = \sum_{\{s_i\}} \prod_{i=1}^{N} e^{B(s_i, s_{i+1})}, \tag{13}$$

where we have defined a *transfer matrix* T with elements,

$$\langle s_i|T|s_j\rangle = e^{B(s_i, s_j)}. \tag{14}$$

In the case of *periodic boundary conditions*, we then obtain

$$Z = \mathrm{tr}\left[T^N\right] \approx \lambda_{\max}^N. \tag{15}$$

Note that for $N \to \infty$, the trace is dominated by the largest eigenvalue $\lambda_{\max}$. Quite generally the largest eigenvalue of the transfer matrix is related to the free energy, while the correlation lengths are obtained from ratios of eigenvalues. *Frobenius' theorem* states that for any finite matrix with finite positive elements, the largest eigenvalue is always non-degenerate. This implies that $\lambda_{\max}$ and Z are analytic functions of the parameters appearing in B, and that one dimensional models can exhibit singularities (and hence a phase transition) only at zero temperature (when some matrix elements become infinite).

While the above formulation is framed in the language of discrete variables $\{s_i\}$, the method can also be applied to continuous variables as illustrated in the following problems. As an example of the latter, let us consider three component *unit* spins $\vec{s}_i = (s_i^x, s_i^y, s_i^z)$, with the *Heisenberg model* Hamiltonian

$$-\beta\mathcal{H} = K \sum_{i=1}^{N} \vec{s}_i \cdot \vec{s}_{i+1}. \tag{16}$$

Summing over all spin configurations, the partition function can be written as

$$Z = \mathop{\mathrm{tr}}_{\vec{s}_i} e^{K\sum_{i=1}^{N} \vec{s}_i\cdot\vec{s}_{i+1}} = \mathop{\mathrm{tr}}_{\vec{s}_i} e^{K\vec{s}_1\cdot\vec{s}_2} e^{K\vec{s}_2\cdot\vec{s}_3} \cdots e^{K\vec{s}_N\cdot\vec{s}_1} = \mathrm{tr}\, T^N, \tag{17}$$

where $\langle \vec{s}_1 | T | \vec{s}_2 \rangle = e^{K \vec{s}_1 \cdot \vec{s}_2}$ is a transfer function. Quite generally we would like to bring T into the diagonal form $\sum_\alpha \lambda_\alpha |\alpha\rangle\langle\alpha|$ (in Dirac notation), such that

$$\langle \vec{s}_1 | T | \vec{s}_2 \rangle = \sum_\alpha \lambda_\alpha \langle \vec{s}_1 | \alpha \rangle \langle \alpha | \vec{s}_2 \rangle = \sum_\alpha \lambda_\alpha f_\alpha(\vec{s}_1) f_\alpha^*(\vec{s}_2). \tag{18}$$

From studies of plane waves in quantum mechanics you may recall that the exponential of a dot product can be decomposed in terms of the spherical harmonics $Y_{\ell m}$. In particular,

$$e^{K \vec{s}_1 \cdot \vec{s}_2} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} 4\pi i^\ell j_\ell(-ik) Y_{\ell m}^*(\vec{s}_1) Y_{\ell m}(\vec{s}_2), \tag{19}$$

is precisely in the form of Eq.(18), from which we can read off the eigenvalues $\lambda_{\ell m}(k) = 4\pi i^\ell j_\ell(-ik)$, which do not depend on m. The partition function is now given by

$$Z = \operatorname{tr} T^N = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \lambda_{\ell m}^N = \sum_{\ell=0}^{\infty} (2\ell+1) \lambda_\ell^N \approx \lambda_0^N, \tag{20}$$

with $\lambda_0 = 4\pi j_0(-ik) = 4\pi \sinh K / K$ as the largest eigenvalue. The second largest eigenvalue is three fold degenerate, and given by $\lambda_1 = 4\pi j_1(-ik) = 4\pi \left[\cosh K/K - \sinh K/K^2\right]$.

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1. *The spin–1 model:* Consider a linear chain where the spin s_i at each site takes on three values $s_i = -1,\ 0,\ +1$. The spins interact via a Hamiltonian

$$-\beta\mathcal{H} = \sum_i K s_i s_{i+1}.$$

(a) Write down the transfer matrix $\langle s | T | s' \rangle = e^{Kss'}$ explicitly.

(b) Use symmetry properties to find the largest eigenvalue of T and hence obtain the expression for the free energy per site ($\ln Z/N$).

(c) Obtain the expression for the correlation length ξ, and note its behavior as $K \to \infty$.

(d) If we try to perform a renormalization group by decimation on the above chain we find that additional interactions are generated. Write down the simplest generalization of $\beta\mathcal{H}$ whose parameter space is closed under such RG.

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2. *Potts chain (RG):* Consider a one-dimensional array of N Potts spins $s_i = 1, 2, \cdots, q$, subject to the Hamiltonian $-\beta\mathcal{H} = J \sum_i \delta_{s_i, s_{i+1}}$.

(a) Using the transfer matrix method (or otherwise) calculate the partition function Z, and the correlation length ξ.

(b) Is zero temperature a critical point (infinite correlation length) for antiferromagnetic couplings $J < 0$?

(c) Construct a renormalization group (RG) treatment by eliminating every other spin. Write down the recursion relations for the coupling J, and the additive constant g.

(d) Discuss the fixed points, and their stability.

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3. (Optional) *Helical Potts model:* Consider a variant of the chain of 3-state Potts spins $s_i = 1, 2, 3$, subject to the Hamiltonian

$$-\beta\mathcal{H} = \sum_{i=1}^{N} \left[K\delta_{s_i,s_{i+1}} + L\delta_{s_i,s_{i+1}+1}\right] .$$

For $L > K$, the ground state switches to alternating spins $\{1, 2, 3, 1, 2, 3, \cdots\}$, encoding a helical (chiral) preference to the sequence $\{1, 3, 2, 1, 3, 2, \cdots\}$.

(a) Construct the transfer matrix of this Hamiltonian, and find its eigenvalues.

(b) Construct a renormalization group (RG) treatment by eliminating every other spin. Write down the recursion relations for the coupling' K, L, and the additive constant g.

(c) Construct the recursion relation $K'(K, L)$ and $L'(K, L)$ in d–dimensions for $b = 2$, using the Migdal–Kadanoff bond moving scheme.

(d) For $d = 2$, obtain the fixed point K^* for $L^* = 0$.

(e) From the above RG equations, is a finite helicity, $L \neq 0$, expected change the nature of the phase transition of the 3 state Potts model?

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4. *Clock model:* Each site of the lattice is occupied by a q-valued spin $s_i \equiv 1, 2, \cdots, q$, with an underlying translational symmetry modulus q, i.e. the system is invariant under $s_i \to (s_i + n)_{\text{mod}q}$. The most general Hamiltonian subject to this symmetry with nearest–neighbor interactions is

$$\beta\mathcal{H}_C = -\sum_{<i,j>} J\left(|(s_i - s_j)_{\text{mod } q}|\right) ,$$

where $J(n)$ is any function, e.g. $J(n) = J\cos(2\pi n/q)$. *Potts models* are a special case of Clock models with full *permutation symmetry*; the Ising model is obtained for $q = 2$.

(a) For a closed linear chain of N clock spins subject to the above Hamiltonian show that the partition function $Z = \mathrm{tr}\left[\exp(-\beta\mathcal{H})\right]$ can be written as

$$Z = \mathrm{tr}\left[\langle s_1|T|s_2\rangle\langle s_2|T|s_3\rangle\cdots\langle s_N|T|s_1\rangle\right] \ ;$$

where $T \equiv \langle s_i|T|s_j\rangle = \exp\left[J(s_i - s_j)\right]$ is a $q \times q$ transfer matrix.

(b) Write down the transfer matrix explicitly and diagonalize it. Note that you do not have to solve a q^{th} order secular equation; because of the translational symmetry, the eigenvalues are easily obtained by discrete Fourier transformation as

$$\lambda(k) = \sum_{n=1}^{q} \exp\left[J(n) + \frac{2\pi i n k}{q}\right] .$$

(c) Show that $Z = \sum_{k=1}^{q} \lambda(k)^N \approx \lambda(0)^N$ for $N \to \infty$. Write down the expression for the free energy per site $\beta f = -\ln Z/N$.

(d) Show that the correlation function can be calculated from

$$\left\langle \delta_{s_i, s_{i+\ell}} \right\rangle = \frac{1}{Z}\sum_{\alpha=1}^{q} \mathrm{tr}\left[\Pi_\alpha T^\ell \Pi_\alpha T^{N-\ell}\right] ,$$

where Π_α is a projection matrix. Hence show that $\left\langle \delta_{s_i, s_{i+\ell}} \right\rangle_c \sim \left[\lambda(1)/\lambda(0)\right]^\ell$. (You do not have to explicitly calculate the constant of proportionality.)

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5. *Clock model duality:* Consider spins $s_i = (1, 2, \cdots, q)$ placed on the sites of a square lattice, interacting via the clock model Hamiltonian

$$\beta\mathcal{H}_C = -\sum_{<i,j>} J\left((s_i - s_j)_{\mathrm{mod}q}\right) ,$$

(a) Change from the N site variables to the $2N$ bond variables $b_{ij} = s_i - s_j$. Show that the difference in the number of variables can be accounted for by the constraint that around each plaquette (elementary square) the sum of the four bond variables must be zero modulus q.

(b) The constraints can be implemented by adding "delta–functions"

$$\delta\left[S_p\right]_{\mathrm{mod}q}=\frac{1}{q}\sum_{n_p=1}^{q}\exp\left[\frac{2\pi i n_p S_p}{q}\right],$$

for each plaquette. Show that after summing over the bond variables, the partition function can be written in terms of the dual variables, as

$$Z=q^{-N}\sum_{\{n_p\}}\prod_{\langle p,p'\rangle}\lambda\left(n_p-n_{p'}\right)\equiv\sum_{\{n_p\}}\exp\left[\sum_{\langle p,p'\rangle}\tilde{J}\left(n_p-n_{p'}\right)\right],$$

where $\lambda(k)$ is the discrete Fourier transform of $e^{J(n)}$.

(c) Calculate the dual interaction parameter of a Potts model, and hence locate the critical point $J_c(q)$.

(d) Construct the dual of the anisotropic Potts model, with

$$-\beta\mathcal{H}=\sum_{x,y}\left(J_x\delta_{s_{x,y},s_{x+1,y}}+J_y\delta_{s_{x,y},s_{x,y+1}}\right);$$

i.e. with bonds of different strengths along the x and y directions. Find the line of self–dual interactions in the plane (J_x,J_y).

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6. (Optional) *Cubic lattice:* The geometric concept of duality can be extended to general dimensions d. However, the dual of a geometric element of dimension D is an entity of dimension $d-D$. For example, the dual of a bond ($D=1$) in $d=3$ is a plaquette ($D=2$), as demonstrated in this problem.

(a) Consider a clock model on a cubic lattice of N points. Change to the $3N$ bond variables $b_{ij}=s_i-s_j$. (Note that one must make a convention about the positive directions on the three axes.) Show that there are now $2N$ constraints associated with the plaquettes of this lattice.

(b) Implement the constraints through discrete delta-functions by associating an auxiliary variable n_p with each plaquette. It is useful to imagine n_p as defined on a bond of the dual lattice, perpendicular to the plaquette p.

(c) By summing over the bond variables in Z, obtain the dual Hamiltonian

$$\beta\tilde{\mathcal{H}}=\sum_p\tilde{J}\left(n_{12}^p-n_{23}^p+n_{34}^p-n_{41}^p\right),$$

where the sum is over all plaquettes p of the dual lattice, with $\{n_{ij}^p\}$ indicating the four bonds around plaquette p.

(d) Note that $\beta\tilde{\mathcal{H}}$ is left invariant if all the six bonds going out of any site are simultaneously increased by the same integer. Thus unlike the original model which only had a *global translation symmetry*, the dual model has a *local*, i.e. *gauge symmetry*.

(e) Consider a Potts gauge theory defined on the plaquettes of a four dimensional hyper-cubic lattice. Find its critical coupling $J_c(q)$.

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7. (Optional) *XY model:* Consider two component unit spins $\vec{s_i} = (\cos\theta_i, \sin\theta_i)$ in one dimension, with the nearest neighbor interactions described by $-\beta\mathcal{H} = K\sum_{i=1}^N \vec{s_i}\cdot\vec{s_{i+1}}$.

(a) Write down the transfer matrix $\langle\theta|T|\theta'\rangle$, and show that it can be diagonalized with eigenvectors $f_m(\theta) \propto e^{im\theta}$ for integer m.

(b) Calculate the free energy per site, and comment on the behavior of the heat capacity as $T \propto K^{-1} \to 0$.

(c) Find the correlation length ξ, and note its behavior as $K \to \infty$.

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