

Transfer Matrices & Position space renormalization

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

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

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

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

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

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

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 λ_{\pm} as

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

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

$$\beta f = -\ln Z/N = -\ln \lambda_+. \quad (5)$$

Solving the characteristic equation, we find the eigenvalues

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

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

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

where we 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

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

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

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

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

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

Note that because of the periodic boundary conditions, the above answer is invariant under $r \rightarrow (N - r)$. 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

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

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

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

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

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

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

$$Z = \text{tr} [T^N] \approx \lambda_{\max}^N. \quad (15)$$

Note that for $N \rightarrow \infty$, the trace is dominated by the largest eigenvalue λ_{\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 λ_{\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

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

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

$$Z = \text{tr}_{\vec{s}_i} e^{K \sum_{i=1}^N \vec{s}_i \cdot \vec{s}_{i+1}} = \text{tr}_{\vec{s}_i} e^{K \vec{s}_1 \cdot \vec{s}_2} e^{K \vec{s}_2 \cdot \vec{s}_3} \dots e^{K \vec{s}_N \cdot \vec{s}_1} = \text{tr} T^N, \quad (17)$$

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

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

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,

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

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

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

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 $\lambda_1 = 4\pi j_1(-ik) = 4\pi [\cosh K/K - \sinh K/K^2]$.

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 $\langle s | T | s' \rangle = e^{K s s'}$ 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 $K \rightarrow \infty$.
- (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.

2. Clock model: Each site of the lattice is occupied by a q -valued spin $s_i \equiv 1, 2, \dots, q$, with an underlying translational symmetry modulus q , i.e. the system is invariant under

$s_i \rightarrow (s_i + n)_{\text{mod } q}$. The most general Hamiltonian subject to this symmetry with nearest-neighbor interactions is

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

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 $Z = \text{tr}[\exp(-\beta\mathcal{H})]$ can be written as

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

where $T \equiv \langle s_i|T|s_j \rangle = \exp[J(s_i - s_j)]$ 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 $N \rightarrow \infty$. 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

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

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

3. Potts chain (RG): Consider a one-dimensional array of N Potts spins $s_i = 1, 2, \dots, q$, 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 the system critical at zero temperature 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.

4. (Optional) *One dimensional ‘Tonks’ gas:* The transfer matrix method also works for a one dimensional gas of particles with short-range interactions, as described below.

(a) Show that for a potential with a hard core that screens the interactions from further neighbors, the Hamiltonian for N particles can be written as

$$\mathcal{H} = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i=2}^N \mathcal{V}(x_i - x_{i-1}).$$

The (indistinguishable) particles are labeled with coordinates $\{x_i\}$ such that

$$0 \leq x_1 \leq x_2 \leq \dots \leq x_N \leq L,$$

where L is the length of the box confining the particles.

(b) Write the expression for the partition function $Z(T, N, L)$. Change variables to $\delta_1 = x_1$, $\delta_2 = x_2 - x_1$, \dots , $\delta_N = x_N - x_{N-1}$, and carefully indicate the allowed ranges of integration and the constraints.

(c) Consider the Gibbs partition function obtained from the Laplace transformation

$$\mathcal{Z}(T, N, P) = \int_0^\infty dL \exp(-\beta PL) Z(T, N, L),$$

and by extremizing the integrand find the standard formula for P in the canonical ensemble.

(d) Change variables from L to $\delta_{N+1} = L - \sum_{i=1}^N \delta_i$, and find the expression for $\mathcal{Z}(T, N, P)$ as a product over one-dimensional integrals over each δ_i .

(e) At a fixed pressure P , find expressions for the mean length $L(T, N, P)$, and the density $n = N/L(T, N, P)$ (involving ratios of integrals which should be easy to interpret).

Since the expression for $n(T, P)$ in part (e) is continuous and non-singular for any choice of potential, there is in fact no condensation transition for the one-dimensional gas. By contrast, the approximate van der Waals equation (or the mean-field treatment) incorrectly predicts such a transition.

(f) For a hard sphere gas, with minimum separation a between particles, calculate the equation of state $P(T, n)$. Compare the excluded volume factor with the approximate result obtained in earlier problems, and also obtain the general virial coefficient $B_\ell(T)$.

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

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

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

(a) Construct the transfer matrix of this 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 coupling⁷ 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?

6. (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 $T \propto K^{-1} \rightarrow 0$.

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

7. (Optional) Heisenberg chain: Consider a period chain of N three component unit spins \vec{s}_i , subject to nearest neighbor interactions described by $-\beta\mathcal{H} = K \sum_{i=1}^N \vec{s}_i \cdot \vec{s}_{i+1}$, with $s_{N+1} = \vec{s}_1$.

(a) A standard decomposition of plane waves into spherical harmonics Y_{lm} takes the form

$$\exp(i\vec{k} \cdot \vec{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \lambda_{\ell}(K) Y_{\ell m}^*(\hat{k}) Y_{\ell m}(\hat{r}),$$

where \hat{k} and \hat{r} are unit vectors, and in terms of the modified Bessel functions I_{ℓ} ,

$$\lambda_{\ell}(K) = 4\pi i^{\ell} j_{\ell}(-iK) = 4\pi \sqrt{\frac{\pi}{2K}} I_{\ell+1/2}(K).$$

Show that the partition function can be written as $Z = \sum_{\ell} (2\ell + 1) \lambda_{\ell}^N(K)$.

(b) Noting that $\lambda_0(K) = 4\pi \sinh(K)/K$ is the largest eigenvalue, compute the energy per site as $N \rightarrow \infty$, and comment on the behavior of the heat capacity as $T \propto K^{-1} \rightarrow 0$.
