8.334 Statistical Mechanics II: Statistical Physics of Fields
Spring 2008

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

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

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

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

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

$$Z = \mathrm{tr}\, T^N = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} \lambda^N_{\ell m} = \sum_{\ell=0}^{\infty}(2\ell+1)\lambda^N_\ell \approx \lambda^N_0, \tag{20}$$

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. *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

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

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

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*, and Ising model is obtained in the limit of $q = 2$.

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

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

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 $N \to \infty$. 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 $\left\langle \delta_{s_i, s_{i+\ell}} \right\rangle_c \sim [\lambda(1)/\lambda(0)]^\ell$. (You do not have to explicitly calculate the constant of proportionality.)

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3. *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) Calulate 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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4. (Optional) *One dimensional gas:* The transfer matrix method can also be applied to a one dimensional gas of particles with short-range interactions, as described in this problem.

(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

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

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 $\delta_1 = x_1$, $\delta_2 = x_2 - x_1$, $\cdots$, $\delta_N = x_N - x_{N-1}$, and carefully indicate the allowed ranges of integration and the constraints.

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

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

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 $B_\ell(T)$.

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5. *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 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.

(e) Write the expression for $\ln Z$ in terms of the additive constants of successive rescalings.

(f) Show that the recursion relations are simplified when written in terms of $t(J) \equiv e^{-1/\xi(J)}$.

(g) Use the result in (f) to express the series in (e) in terms of t. Show that the answer can be reduced to that obtained in part (a), upon using the result

$$\sum_{n=0}^{\infty} \frac{1}{2^{n+1}} \ln\left(\frac{1+t^{2^n}}{1-t^{2^n}}\right) = -\ln(1-t).$$

(h) Repeat the RG calculation of part (c), when a small symmetry breaking term $h\sum_i \delta_{s_i,1}$ is added to $-\beta\mathcal{H}$. You will find that an additional coupling term $K\sum_i \delta_{s_i,1}\delta_{s_{i+1},1}$ is generated under RG. Calculate the recursion relations in the three parameter space (J, K, h).

(i) Find the magnetic eigenvalues at the zero temperature fixed point where $J \to \infty$, and obtain the form of the correlation length close to zero temperature.

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6. *Cluster RG:* Consider Ising spins on a *hexagonal lattice* with nearest neighbor interactions J.

(a) Group the sites into clusters of four in preparation for a position space renormalization group with $b = 2$.

(b) How can the majority rule be modified to define the renormalized spin of each cluster.

(c) For a scheme in which the central site is chosen as the tie–breaker, make a table of all possible configurations of site–spins for a given value of the cluster–spin.

(d) Focus on a pair of neighboring clusters. Indicate the contributions of intra–cluster and inter–cluster bonds to the total energy.

(e) Show that in zero magnetic field, the Boltzmann weights of parallel and anti-parallel clusters are given by

$$R(+,+) = x^8 + 2x^6 + 7x^4 + 14x^2 + 17 + 14x^{-2} + 7x^{-4} + 2x^{-6},$$

and

$$R(+,-) = 9x^4 + 16x^2 + 13 + 16x^{-2} + 9x^{-4} + x^{-8},$$

where $x = e^J$.

(f) Find the expression for the resulting recursion relation $J'(J)$.

(g) Estimate the critical *ferromagnetic* coupling J_c, and the exponent ν obtained from this RG scheme, and compare with the exact values.

(h) What are the values of the magnetic and thermal exponents (y_h, y_t) at the zero temperature ferromagnetic fixed point?

(i) Is the above scheme also applicable for anti-ferromagnetic interactions? What symmetry of the original problem is not respected by this transformation?

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7. (Optional) *Transition probability matrix:* Consider a system of two Ising spins with a coupling K, which can thus be in one of four states.

(a) Explicitly write the 4×4 transition matrix corresponding to single spin flips for a Metropolis algorithm. Verify that the equilibrium weights are indeed a left eigenvector of this matrix.

(b) Repeat the above exercise if both single spin and double spin flips are allowed. The two types of moves are chosen randomly with probabilities p and $q = 1 - p$.

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