1 Spin-1 Partition functions

We're told for this problem that we have a 1-D array of N spins $s_1, \ldots, s_N$, where $s_i \in \{-1, 0, 1\}$. We're also, importantly, given periodic boundary conditions $s_{N+1} = s_1$. Our Hamiltonian has no external field:

$$\mathcal{H} = -J \sum_{i=1}^{N} s_i s_{i+1} \tag{1}$$

We're asked to effectively find the transfer matrix, and show that the Helmholtz free energy A satisfies

$$A = -N k_{\mathrm{B}} T \log \lambda_+, \tag{2}$$

where λ_+ is the largest eigenvalue of the transfer matrix $\mathcal{T}$.

(a) Helmholtz free energy

We want to start by finding the partition function Q, as we know that $A = -k_{\mathrm{B}} T \log Q$. For Q, summing over all values of each spin:

$$\begin{aligned} Q &= \sum_{s_1} \cdots \sum_{s_N} e^{-\beta \mathcal{H}} && (3) \\ &= \sum_{s_1} \cdots \sum_{s_N} e^{-\beta\left(-J \sum_{i=1}^{N} s_i s_{i+1}\right)} && (4) \\ &= \sum_{s_1} \cdots \sum_{s_N} e^{\sum_{i=1}^{N} \beta J s_i s_{i+1}} && (5) \\ &= \sum_{s_1} \cdots \sum_{s_N} \prod_{i=1}^{N} e^{\beta J s_i s_{i+1}} && (6) \end{aligned}$$

This is the point where we can define a matrix $\mathcal{T}$ such that

$$\mathcal{T}_{ab} = e^{\beta J a b}, \tag{7}$$

where the indices run over possible spin values. Substituting this in for Q leads to:

$$\begin{aligned} Q &= \sum_{s_1} \cdots \sum_{s_N} \prod_{i=1}^{N} \mathcal{T}_{s_i s_{i+1}} && (8) \\ &= \sum_{s_1} \cdots \sum_{s_N} \mathcal{T}_{s_1 s_2} \mathcal{T}_{s_2 s_3} \cdots \mathcal{T}_{s_{N-1} s_N} \mathcal{T}_{s_N s_1} && (9) \end{aligned}$$

We recognise this sum over repeated indices as basic matrix multiplication:

$$Q = \sum_{s_1} \mathcal{T}^N_{s_1 s_1} \tag{10}$$

It's important here that we had a periodic boundary condition, or we'd have some extra work to do for the first and last spin and the next step wouldn't be possible. We have only the s_1 index left to sum over, and we recognise here the trace of $\mathcal{T}^N$:

$$Q = \operatorname{Tr} \mathcal{T}^N \tag{11}$$

Why's this good? We know that $\operatorname{Tr} \mathcal{T} = \sum \lambda_i$, where the λ are the eigenvalues of $\mathcal{T}$, and we also know that $\operatorname{Tr} \mathcal{T}^N = \sum \lambda_i^N$. As with the examples of the transfer matrix method, we can make the assumption that the three eigenvalues for this Hamiltonian's transfer matrix have a T- and J- independent order, and name them λ_+, λ_0 and λ_- (where $\lambda_+ > \lambda_0 > \lambda_-$). Thus we write

$$\begin{aligned} Q &= \operatorname{Tr} \mathcal{T}^N && (12)\\ &= \lambda_+^N + \lambda_0^N + \lambda_-^N && (13)\\ &= \lambda_+^N \left(1 + \left(\frac{\lambda_0}{\lambda_+}\right)^N + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right) && (14) \end{aligned}$$

For sufficiently large N, the quantity in parentheses goes to 1 (because each parenthesised quantity therein contained goes to 0), so

$$Q = \lambda_+^N \tag{15}$$

The Helmholtz free energy is trivial:

$$\begin{aligned} A &= -k_\mathrm{B} T \log Q && (16)\\ A &= -k_\mathrm{B} T \log \left(\lambda_+^N\right) && (17)\\ A &= -N k_\mathrm{B} T \log \lambda_+ && (18) \end{aligned}$$

This is what we wanted to show for this part.

(b) The components of the transfer matrix

We can go back to (7):, $\mathcal{T}_{ab} = e^{\beta J ab}$, and recall that a and b ran over the values for the spins, $\{-1, 0, 1\}$. If either a or b is 0, $\mathcal{T}_{ab} = 1$, and the other components are only slightly more complicated:

$$\begin{array}{cc} & \begin{array}{ccc} s=1 & s=0 & s=-1 \end{array} \\ \mathcal{T} = & \begin{pmatrix} e^{\beta J} & 1 & e^{-\beta J} \\ 1 & 1 & 1 \\ e^{-\beta J} & 1 & e^{\beta J} \end{pmatrix} \begin{array}{c} s=1 \\ s=0 \\ s=-1 \end{array} \end{array} \tag{19}$$

(c) Equation for $\boldsymbol{\lambda}_+$

We want to find the eigenvalues of $\mathcal{T}$. Let's solve our standard eigenvalue equation:

$$\begin{align} 0 &= \det(\mathcal{T} - \lambda I) \tag{20} \\ &= \det \begin{pmatrix} e^{\beta J} - \lambda & 1 & e^{-\beta J} \\ 1 & 1-\lambda & 1 \\ e^{-\beta J} & 1 & e^{\beta J} - \lambda \end{pmatrix} \tag{21} \end{align}$$

To spare my fingers the extra typing, we'll define $a = e^{\beta J}$ and $b = e^{-\beta J}$.

$$\begin{align} 0 &= \det \begin{pmatrix} a-\lambda & 1 & b \\ 1 & 1-\lambda & 1 \\ b & 1 & a-\lambda \end{pmatrix} \tag{22} \\ &= (a-\lambda)\left((1-\lambda)(a-\lambda)-1\right) - \left((a-\lambda)-b\right) + b\left(1-(1-\lambda)\,b\right) \tag{23} \\ &= (a-\lambda)\left(a+\lambda^2-\lambda(1+a)-1\right) - a + \lambda + b + b\left(1-b+b\lambda\right) \tag{24} \\ &= (a-\lambda)\left(\lambda^2-\lambda(1+a)+a-1\right) - a + \lambda + b + b - b^2 + b^2\lambda \tag{25} \\ &= (a-\lambda)\left(\lambda^2-\lambda(1+a)+a-1\right) + \lambda(1+b^2) - a + 2b - b^2 \tag{26} \\ &= a\lambda^2 - \lambda(a+a^2) + a^2 - a - \lambda^3 + \lambda^2(1+a) - \lambda a + \lambda \nonumber \\ &\quad + \lambda(1+b^2) - a + 2b - b^2 \tag{27} \\ &= -\lambda^3 + \lambda^2\,(2a+1) + \lambda\left(-a-a^2-a+1+1+b^2\right) \nonumber \\ &\quad + a^2 - a - a + 2b - b^2 \tag{28} \\ &= -\lambda^3 + \lambda^2\,(2a+1) + \lambda\left(b^2-a^2-2a+2\right) + a^2 - b^2 - 2a + 2b \tag{29} \end{align}$$

This cubic equation seems rather ugly, but not unexpectedly so. I'm sure this can be simplified further by plugging in for a and b and writing some hyperbolic trig functions, but I don't think that helps, particularly given that we're not going to be solving this. It's exactly solvable though, and that's quite cool.