n chain Ising model

February 20, 2019

1 PROBLEM 4

We have n chains with N spins in each, obeying periodic boundary conditions. Hamiltonian:

$$H = -J_{\parallel} \sum_{m=1}^{n} \sum_{i=1}^{N} \sigma_{m,i}\sigma_{m,i+1} - J_{\perp} \sum_{m=1}^{n} \sum_{i=1}^{N} \sigma_{m,i}\sigma_{m+1,i} - B \sum_{m=1}^{n} \sum_{i=1}^{N} \sigma_{m,i} \tag{1}$$

Here $\sigma_{m,N+1} = \sigma_{m,1}$ and $\sigma_{n+1,i} = \sigma_{1,i}$. This corresponds to wrapping the two dimensional surface of the chains around a torus.

1.0.1 a) Every possible spin-configuration for one chain

For a given i in $\{1, 2, ..., N\}$, we want to generate every possible spin state for the i-th component of the n chains. One systematic way to do this, is to consider all binary numbers up to 2^n (these can be expressed with n digits), and make spin up/down correspond to 1 or 0.

```
In [1]: import numpy as np

        def genAllStates(n):
            #int n = number of chains
            #returns: 2^n x n array (int)

            #Initially, place all spins up
            states = np.ones((2**n, n), dtype=int)
            intToBin = lambda n: bin(n)[2:]
            for i in range(2**n):
                #Convert i into a binary string with appropriate amount of zeros in front
                b = intToBin(i)
                b = b.zfill(n)
                for j in range(n):
                    #Subtract the j-th digit of the binary representation of i for all j spins
                    states[i][j] -= 2*int(b[j])
            return states
```

In particular, the case n=5 yields:

```
In [2]: print(genAllStates(5))
```

```
[[ 1  1  1  1  1]
 [ 1  1  1  1 -1]
 [ 1  1  1 -1  1]
 [ 1  1  1 -1 -1]
 [ 1  1 -1  1  1]
 [ 1  1 -1  1 -1]
 [ 1  1 -1 -1  1]
 [ 1  1 -1 -1 -1]
 [ 1 -1  1  1  1]
 [ 1 -1  1  1 -1]
 [ 1 -1  1 -1  1]
 [ 1 -1  1 -1 -1]
 [ 1 -1 -1  1  1]
 [ 1 -1 -1  1 -1]
 [ 1 -1 -1 -1  1]
 [ 1 -1 -1 -1 -1]
 [-1  1  1  1  1]
 [-1  1  1  1 -1]
 [-1  1  1 -1  1]
 [-1  1  1 -1 -1]
 [-1  1 -1  1  1]
 [-1  1 -1  1 -1]
 [-1  1 -1 -1  1]
 [-1  1 -1 -1 -1]
 [-1 -1  1  1  1]
 [-1 -1  1  1 -1]
 [-1 -1  1 -1  1]
 [-1 -1  1 -1 -1]
 [-1 -1 -1  1  1]
 [-1 -1 -1  1 -1]
 [-1 -1 -1 -1  1]
 [-1 -1 -1 -1 -1]]
```

1.0.2 b) Transfer matrix P

For a single lattice site τ_i:

$$P_{\tau_i\tau_{i+1}} = exp\left[\beta J_{\parallel}\sum_{k=1}^{n}\sigma_i^{(k)}\sigma_{i+1}^{(k)} + \beta J_{\perp}\sum_{k=1}^{n}\sigma_i^{(k)}\sigma_i^{(k+1)} + \frac{\beta B}{2}\sum_{k=1}^{n}(\sigma_i^{(k)} + \sigma_{i+1}^{(k)})\right] \tag{2}$$

can be expressed as a $2^n \times 2^n$ -matrix with all the possible (binary) combinations of $\sigma_i^{(k)}$ and $\sigma_{i+1}^{(k)}$ for $k = \{1, 2, ..., n\}$. I.e. $P_{\tau_i\tau_{i+1}} \to P_{l,m}$ for $l, m \in \mathbb{N}$.

Using periodic boundary conditions, we sidestep possible issues with the above sums running out of of indices. Also, there is no inert connection between lattice sites i and $i+1$ before we determine it with the Hamiltonian, so we may assume the energy contribution between such sites is the same for all pairs. As such, $P = P_{\tau_i\tau_j}$ for some lattice sites τ_i and τ_j, and is non-zero for all $j = i+1$. Otherwise, P is independent of i.

```
In [17]: #Parameters
         Jpar = 1
         Jperp = 1
         B = 1e-2
         beta = 0.5 #Dummy value

         #Matrix element (l,m)
         def P_lm(l, m, n, beta):
             #int l, m = row & column position in P
             #int n = number of chains
             #returns: float

             #Select a possible spin state given by l and k (NB! 0-indexed)
             states = genAllStates(n)
             sig = lambda l, k: states[l][k]
             #Sums in Hamiltonian
             Spar, Sperp, Smag = 0, 0, 0
             for k in range(n):
                 Spar += sig(l, k)*sig(m, k)
                 Sperp += sig(l, k)*sig(m, (k+1)%n)
                 Smag += sig(l, k) + sig(m, k)
             return np.exp( beta*Jpar*Spar + beta*Jperp*Sperp + 1/2*beta*B*Smag )

         #Generate matrix
         def P(n, beta):
             #int n = number of chains
             #returns: 2^n x 2^n array (float)

             mat = np.zeros((2**n, 2**n))
             for l in range(2**n):
                 for m in range(2**n):
                     mat[l][m] = P_lm(l, m, n, beta)
             return mat
```

NB: The matrices P are symmetric, so one could save time by only computing the upper/lower triangular part of P.

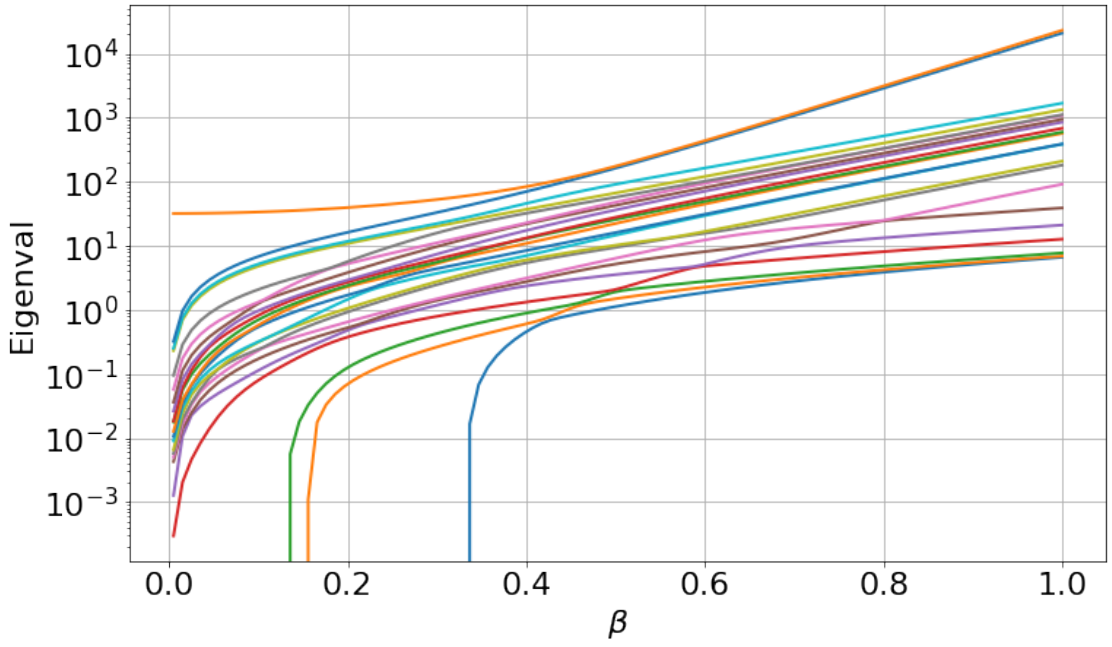
1.0.3 c) Eigenvalues

Now, I plot (the real part of) all the eigenvalues of a single P for n chains (there are n of them) as a function of β. The parameters are all set to unity.

```
In [23]: import matplotlib
         matplotlib.rcParams['figure.figsize'] = [12, 7]
         matplotlib.rcParams.update({'font.size': 22})
         import matplotlib.pyplot as plt

         #Plot in beta
```

```
def plotOverBeta(n):
    #int n = number of chains
    #returns: Nan

    num = 100
    betaRange = np.linspace(0.005, 1.0, num)
    plotVals = np.zeros((num,2**n))
    #Solve eigenvalues for every value of beta in the given range
    for i in range(num):
        s, S = np.linalg.eigh(P(n, betaRange[i]))
        plotVals[i] = np.real(s)
    # We end up with 2**n different eigenvalue-plots
    for i in range(2**n):
        plt.semilogy(betaRange, plotVals[:,i], lw=2)
    plt.grid()
    plt.xlabel(r'$\beta$')
    plt.ylabel(r'Eigenval')
    plt.show()
    return None

plotOverBeta(5)
```

```
/home/svein/anaconda3/lib/python3.6/site-packages/matplotlib/ticker.py:2198: UserWarning: Data
  "Data has no positive values, and therefore cannot be "
```



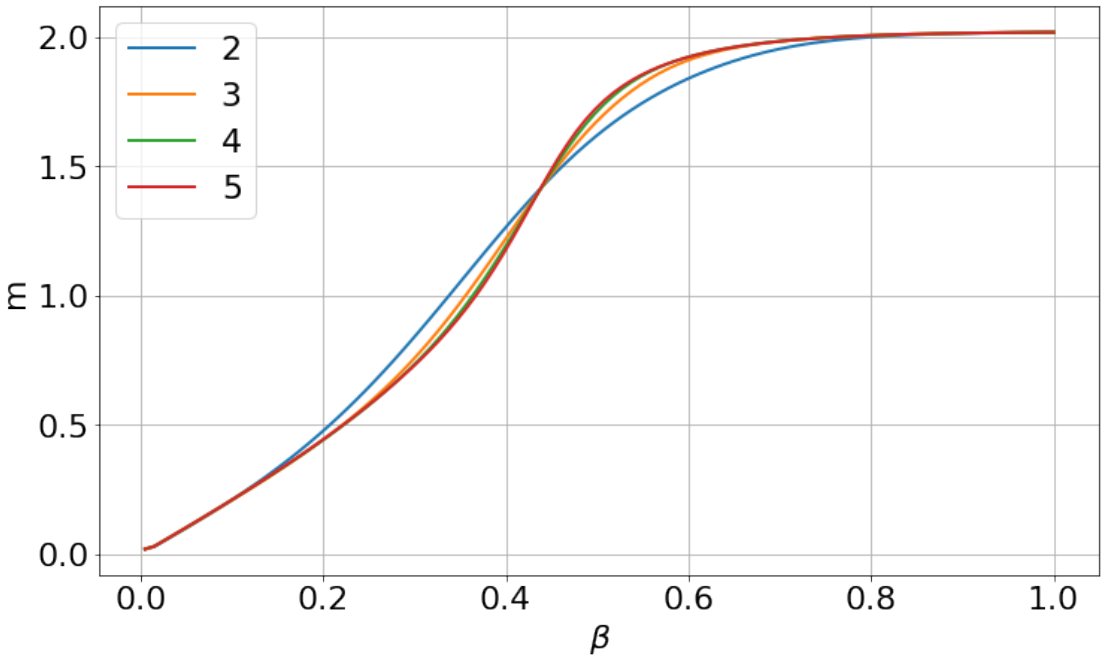
We notice that the largest eigenvalue is the largest for all values of β. This motivates our choice to approximate Z as being only the largest eigenvalue.

1.0.4 d)

Using the relations given in the exercise text, one can express m like:

$$m = \frac{1}{n}\frac{\partial}{\partial(\beta B)} ln(\lambda_{n,\max}) = \frac{1}{nB}\frac{\partial}{\partial\beta} ln(\lambda_{n,\max}). \tag{3}$$

```
In [24]: def generateLargestLambda(n):
             num = 100
             betaRange = np.linspace(0.005, 1.0, num)
             Z = np.zeros((num,2**n))
             for i in range(num):
                 s, S = np.linalg.eigh(P(n, betaRange[i]))
                 #Add eigenvalues to Z
                 Z[i] = np.real(s)
             #Return the entire column containing the largest eigenvalue
             return Z[:,np.argmax(Z)%2**n]

         def m(n):
             Z = generateLargestLambda(n)
             return 1/(n*B)*np.gradient(np.log(Z))

         def plotm():
             for n in range(2,6):
                 mag = m(n)
                 betaRange = np.linspace(0.005, 1.0, 100)
                 plt.plot(betaRange, mag, label=n, lw=2)
             plt.xlabel(r'$\beta$')
             plt.ylabel(r'm')
             plt.grid()
             plt.legend()
             plt.show()

         plotm()
```



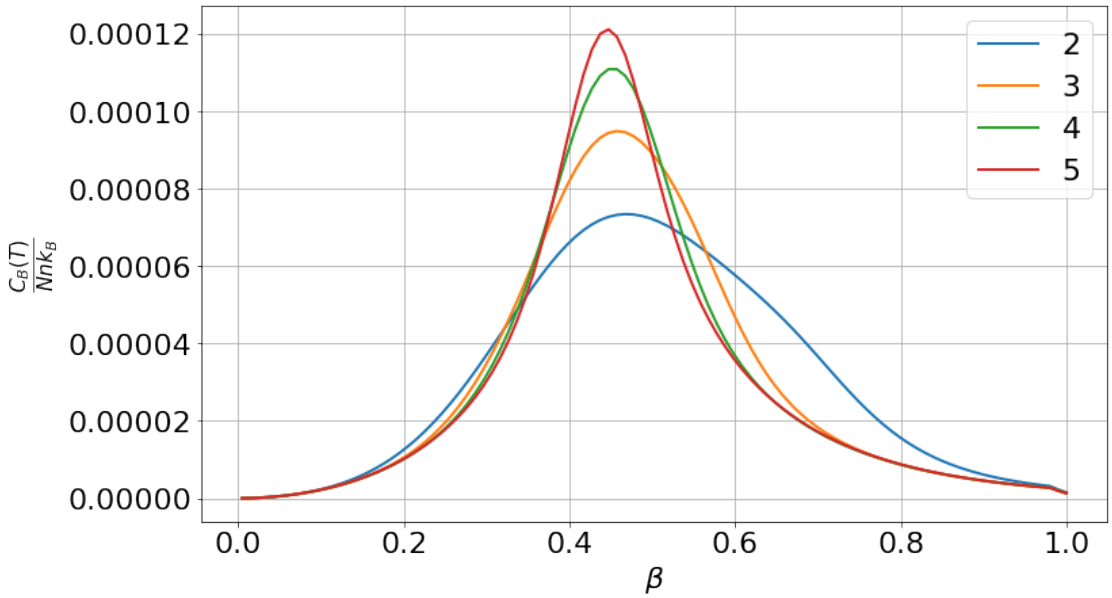
1.0.5 e)

Using the given relations, I calculate and plot

$$\frac{C_B(T)}{Nnk_B} = \frac{\beta^2}{n}\frac{\partial^2 ln(\lambda_{n,\max})}{\partial\beta^2} \tag{4}$$

over β.

```
In [25]: def plotC_B():
             for n in range(2, 6):
                 betaRange = np.linspace(0.005, 1.0, 100)
                 Z = generateLargestLambda(n)
                 plotvals = 1/n * betaRange**2*np.gradient(np.gradient(np.log(Z)))
                 plt.plot(betaRange, plotvals, label=n, lw=2)
             plt.xlabel(r'$\beta$')
             plt.ylabel(r'$\frac{C_{B}(T)}{Nnk_{B}}$')
             plt.grid()
             plt.legend()
             plt.show()

         plotC_B()
```



The dependence of C on B:

Large $|B| \implies C \to 0$ as the enthalpy is completely dominated by the term $B\sum_{m=1}^{n}\sum_{i=1}^{N}\sigma_{m,i}$ in the Hamiltonian. Any increase in T contributes to kinetic energy, but completely dies out in comparison.

Small $|B|$ means all the terms in H are fairly small, so increasing kinetic energy can give a noticable contribution to enthalpy.

All in all; $C(B)$ decreases symmetrically around the origin.