Exact calculation of finite Ising chain

1. The Hamiltonian for the Ising chain in 1D with open boundary conditions is

$$H = -J\sum_{j=1}^{N-1}\sigma_j\sigma_{j+1} - h\sum_{j=1}^{N}\sigma_j, \quad \sigma_j = \pm 1$$

   Write down formal expressions (*e.g.* expressed as summation but not evaluated) for the partition function Z, the free energy F, the internal energy U, the heat capacity C, the magnetization $M = \sum_j \sigma_j$, and the magnetic susceptibility $\chi = \partial M/\partial h$.

2. For a given chain length N, how many terms are in these sums? 2^N

3. Devise a scheme for sequentially listing all possible states of the chain $\vec{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ that can be programmed in Python. Binary 0,1 → Ising ±1

4. Write a program to calculate U, C and χ as functions of temperature for an arbitrary value of N. Run the program for N=5 and 10. How does the run time vary with N? For each N, plot your results for $k_B T/J$ ranging from 0.1 to 2. Compare the behavior for h/J=0, 0.1, 0.2. For h=0 compare U and C with the exact analytic result.

1.

$$Z = \sum_{\vec{\sigma}} e^{-\beta H(\vec{\sigma})} \qquad F = -kT \ln Z$$

$$U = -\frac{\partial \ln Z}{\partial \beta} = \langle H \rangle = \frac{1}{Z}\sum_{\sigma} H(\sigma) e^{-\beta H(\sigma)}$$

$$C = \frac{\partial U}{\partial T} = \frac{1}{kT^2}\left(\langle H^2\rangle - \langle H\rangle^2\right)$$

$$\langle M \rangle = -kT\frac{\partial \ln Z}{\partial h} = \frac{1}{Z}\sum_{\vec{\sigma}}\left\{\left(\sum_j \sigma_j\right) e^{-\beta H}\right\}$$

$$\chi = \frac{\partial \langle M\rangle}{\partial h} = -kT\frac{\partial^2 \ln Z}{\partial h^2} = \frac{1}{kT}\left(\langle M^2\rangle - \langle M\rangle^2\right)$$