Ising model

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Part 1

Given the Hamiltonian, which is the total energy of the system in a given configuration

$$E = \mathcal{H}(\{\sigma\}) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{1}$$

the goal is to compute $\Delta E = E(Y) - E(X)$ where the difference between the configurations X and Y is that one spin changed sign. J is the coupling constant and each spin is coupled to four of its neighbors (up, down, left, right).

The total Energy for the configuration X can be written as

$$E(X) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{2}$$

If we assume that spin σ_i is flipped to $(-\sigma_i)$ in configuration Y, the total energy is then given by

$$E(Y) = -J \sum_{\langle i,j \rangle} (-\sigma_i)\sigma_j = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{3}$$

The difference between the system can therefore be written as

$$\Delta E = E(Y) - E(X) = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - (-J \sum_{\langle i,j \rangle} \sigma_i \sigma_j) = 2J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{4}$$

we can now define the neighbor field as $h_i = \sum_{\langle i,j \rangle} \sigma_j$ by factoring out σ_i since it's constant with respect to the summation resulting in the following equation

$$\Delta E = 2J\sigma_i h_i. \tag{5}$$

Now in our Ising model we flip the spin if $\Delta E \leq 0$, otherwise accept the configuration with probability $\exp\left[-\frac{\Delta E}{k_B T}\right]$.

Part 3