The energy of the lattice is calculated using the formula. The circshift calculates the energy difference between the neighbouring atoms in the lattice

Numerically it is impractical to solve for all possible evolutions in the Ising model as there are simply too many possible evolutions. The partition function for the Ising model which can be used to calculate the macroscopic properties is given by the formula

$$Z = \sum\_{s\_i} e^{-\beta U}$$

As an example, for a tiny matrix of 10 by 10 molecules the partition function contains 2^100 terms, a number impossibly big for a computer to calculate in any reasonable timeframe [3].

While it is impossible to compute the probabilities of all the possible states, using the Metropolis algorithm we can evolve the system using the Boltzmann factors as probability of a particular evolution of the system. This algorithm, as described in the 341 Thermal textbook by Schroeder [3], chooses a random molecule

If the molecule has a high energy

A picture containing crossword puzzle

Description automatically generated

such as its spin is opposite to its neighbors, flipping the molecule would reduce the energy of the system. If this is the case the molecule is flipped.

On the other hand, if the molecule has low energy

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Such as its spin is aligned with its neighbors, flipping the molecule would reduce the energy of the system. In this case it would make sense to not flip the molecule as energy is required to do so. However, In the Ising model the molecule is flipped with probability given by the formula $P = e^{-\beta \Delta E}$. Meaning When Temperature increases probability of flipping increases even if energy increases.

Representing this in code we can make a function that can return the probability of flipping a particular node at each step.

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This process is then repeated to simulate the evolution of the system.

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To find the critical temperature at which phase transition occurs, computationally, we would run the Metropolis algorithm for sufficient number of evolutions at different temperatures and compare the energy in the final state using the formula