Notes on Metropolis algorithm

The Boltzmann distribution is a function that gives the probability distribution of a thermodynamics system at temperature T:

$$P_i = \frac{\exp(-\frac{E_i}{k_B T})}{\sum_{i=1}^{N} \exp(-\frac{E_i}{k_B T})} = \frac{\exp(-\frac{E_i}{k_B T})}{Z}$$

The denominator Z is sum over all the energy states, it is known as *partition function* and it is constant quantity.

If the system is isolated, a transition from a state energy to another can happen only if the new state has a lower energy, i.e. if it has a higher probability (looking at the Boltzmann distribution). Other transitions would be forbidden.
If the system is not isolated, it can take energy from the environment and make also transitions from a lower state energy to a higher state energy, overcoming the energy gap. The probability to make a forbidden transition depends on the temperature of the environment. The following algorithm, known as *Metropolis algorithm* is a technique to formalize this process and to decide if a transition from a state energy E_0 to a state energy E_1 can happen.

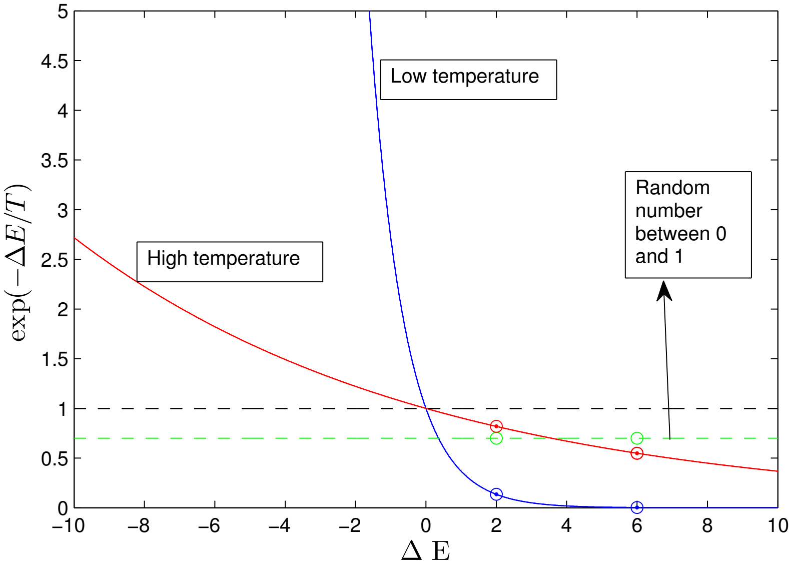
1. Compute the initial state energy E_0.
2. Make a transition and compute the new state energy E_1.
3. Compute $\Delta E = E_1 - E_0$
4. if $\Delta E <= 0$, then the transition is accepted.
5. if $\Delta E > 0$:
   (a) Extract a random number $r \in [0, 1)$ from a uniform distribution.
   (b) If $\exp\left(-\frac{\Delta E}{k_b \cdot T}\right) > r$, then the transition is accepted. Otherwise transition is rejected and the system does not change configuration.

The term $\exp\left(-\frac{\Delta E}{k_b \cdot T}\right)$ is the ratio between the Boltzmann distribution of the new state and the old state:

$$\frac{P(E_1)}{P(E_0)} = \frac{\exp(-\frac{E_0}{k_B T})}{Z} \cdot \frac{Z}{\exp(-\frac{E_1}{k_B T})} = \exp\left(-\frac{\Delta E}{k_b \cdot T}\right)$$

This means that if $\exp\left(-\frac{\Delta E}{k_b \cdot T}\right) > 1$, the probability of the new state is higher.

To better understand the Metropolis algorithm, can be useful to give a look to the graph of the function $\exp\left(-\frac{\Delta E}{k_b \cdot T}\right)$ (fig.1).
When $\Delta E <= 0$, the graph is always greater then 1 (the transition is always allowed). When $\Delta E > 0$, the probability to make a transition depends on the random number generated and on the temperature of the system.
Let's consider two different transitions, one when $\Delta E = 2$ and the second when $\Delta E = 6$. The random number used in the example is 0.7 (green line).
When the temperature is low (blue line), both the transitions cannot happen, because the blue line is under the green line ($\Delta E = 2$ and $\Delta E = 6$).
If the temperature is higher (red line), the transition $\Delta E = 2$ can happen, but the other transition is not allowed yet.
On the other hand a transition is never forbidden: higher is the temperature (i.e. higher is the energy of the environment), higher is the probability to find a number between 0 and 1 such that $\exp\left(-\frac{\Delta E}{k_b \cdot T}\right) > r$.



For the Ising model, a transition happens when a single atom changes sign. Then you should apply the Metropolis algorithm for each atom of the grid. One time-step of the simulation is concluded, after you have tried to flip all the atoms (i.e. when you have concluded the double for loop through the grid).