

We then calculate the change in energy of the system ΔE , which is caused by the move. If $\Delta E < 0$, i.e., if the move would bring the system to a state of lower energy, we allow the move and put the particle in its new position. If $\Delta E > 0$, we allow the move with probability $\exp(-\Delta E/kT)$; i.e., we take a random number ξ_3 between 0 and 1, and if $\xi_3 < \exp(-\Delta E/kT)$, we move the particle to its new position. If $\xi_3 > \exp(-\Delta E/kT)$, we return it to its old position. Then, whether the move has been allowed or not, i.e., whether we are in a different configuration or in the original configuration, we consider that we are in a new configuration for the purpose of taking our averages. So