METROPOLIS SIMULATIONS IN THE ISOBARIC-ISOTHERMAL ENSEMBLE

partition function

$$\Delta(N,p,T) = \int_0^\infty dV\, e^{-\beta p V} \frac{1}{\lambda^{3N} N!} \int d^{3N}q\, e^{-\beta U(\bar{q}_1, \dots \bar{q}_N)}$$

In this ensemble we must update both the coordinates of the particles and the volume V.

Note that V appears indirectly [$\vec{q}$ should be integrated in the volume V].

We assume a cubic box $V = L^3$ and set $\vec{r} = \bar{s} L$

$$\Delta(N,p,T) = \frac{3}{\lambda^{3N} N!} \int_0^\infty dL\, L^{2+3N} e^{-\beta p L^3} \int d^{3N}\bar{s}\, e^{-\beta U(\bar{s}_1 L, \dots, \bar{s}_N L)}$$

We should perform an update of the variables $\{\bar{s}_i\}$ and an update of L.

(a) update of the variables $\vec{s}_i$.
It can be performed as in the canonical case (it is enough to replace $\vec{r}$ with $\vec{s}$).

(b) update of the variables L.

UPDATE OF THE SIZE L : METROPOLIS

Proposal :

$$\begin{cases} x = L \\ y = L + \Delta_L (RAN - 0.5) = L_n \end{cases}$$

Δ_L: a parameter to be tuned with acceptance 30-50%

To proposal is symmetric

Acceptance

$$A = \min\left(1, \frac{\pi_y}{\pi_x}\right) = \min\left[1, \left(\frac{L_n}{L}\right)^{2+3N} e^{-\beta p (L_n^3 - L^3)} \times e^{-\beta\left[U(\bar{s}_1 L_n, \dots \bar{s}_N L_n) - U(\bar{s}_1 L, \dots, \bar{s}_N L)\right]}\right]$$

Note that the acceptance does not only depend on the energy difference.