$$\boxed{\langle f \rangle = \frac{\int f(x)\, p(x)\, dx}{\int p(x)\, dx}} = \int f(x)\, p(x)\, dx$$

(if $p(x)$ is normalised)

Analogy to 1D SHO: $E(x) = x^2$ for $k_B T = 1$

$$\langle E \rangle = \frac{\int x^2 e^{-x^2} dx}{\int e^{-x^2} dx}$$

Here, we perform MC simulation on the energy surface: $E(x) = x^2$

Now, consider: $E(x) = x^4$.

So, $$\langle E \rangle = \frac{\int x^4 e^{-x^4} dx}{\int e^{-x^4} dx}$$

$\longrightarrow$ Just perform MC simulation over energy surface $E(x) = x^4$ & compute $\langle E \rangle$!

---

* Other importance sampling:

$$I = \int f(x)\, dx = \frac{1}{N} \sum_{i=1}^{N} f(x_i) = \langle f \rangle,$$

where, x_i is drawn from uniform distribution

$$I = \int f(x)\, dx = \int \frac{f(x)}{W(x)} W(x)\, dx = \left\langle \frac{f}{W} \right\rangle,$$

where, x_i is drawn with a distribution function $W(x)$.

Monte Carlo of 3D LJ particles:

① We'll use truncated LJ function

$$U_{fullLJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$U_{trunc}(r) = \begin{cases} U_{fullLJ}(r) - U_{fullLJ}(r_c) & : \text{for } r \leq r_c \\ 0 & : \text{for } r > r_c \end{cases}$$

* No interaction beyond cut-off distance r_c.

* Shifted so that $U_{trunc}(r)$ is continuous at $r = r_c$.

② Periodic Boundary Condition (PBC):

Wrap particles inside box of length L:

Box : $[0, L]$

If $x > L$:

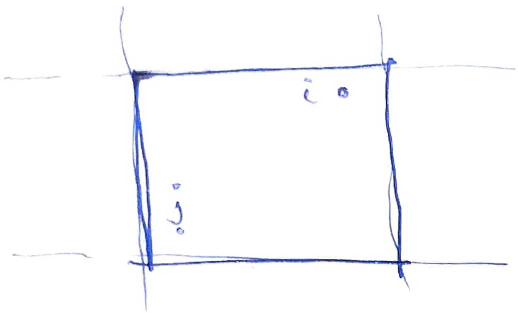
$x = x - L$

If $x < 0$:

$x = x + L$

(3) Minimum Image Convention:

Energy of i-th particle: E_i




```
For j = 1 to N:
    if i ≠ j:
        E_i += E_ij(r)
```

Note: For calculating $E_{ij}(r)$, we must use the nearest image of j (to i).

Following transformation is required:

$$r^2 = \Delta x^2 + \Delta y^2 + \Delta z^2$$

If $\Delta x > L/2$:

$$\Delta x' = \Delta x - L$$

If $\Delta x < -L/2$:

$$\Delta x' = \Delta x + L$$

Same for $\Delta x, \Delta y, \Delta z$ $\longrightarrow$ then calculate r.

$$r'^2 = \Delta x'^2 + \Delta y'^2 + \Delta z'^2$$

(4) Run MC & compute following:

$\langle E \rangle$, C_v, P (pressure)

* How to compute P as ensemble average? Find out! Hint: "virial" (Google is your friend! :))

* Plot P vs. $1/\rho$ at different T