
Algorithm 1 MC Path Integral

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1: procedure SAMPLEQUANTUMDIST
2:    $\hbar, m, k_b, \omega \leftarrow 1$ 
3:    $\theta \leftarrow$  temperature of heat bath
4:    $\beta \leftarrow \hbar/k_b\theta$ 
5:    $N_s \leftarrow$  # of steps
6:    $N_d \leftarrow$  # of lattice points
7:    $\epsilon \leftarrow T/N_d$ 
8:
9:   // Initialize lattice
10:   $x \leftarrow \{x_0, \dots, x_{N_d-1}\}$  //  $x_k \sim \mathcal{N}(0, 1)$ 
11:   $x' \leftarrow x$ 
12:
13:  for  $i = 0, \dots, N_s$  do
14:    for  $k = 0, \dots, N_d$  do
15:       $x'[k] \leftarrow x[k] + \mathcal{N}(0, 1)$  // Proposition
16:       $E \leftarrow \text{energy}(x, \epsilon)$ 
17:       $E' \leftarrow \text{energy}(x', \epsilon)$ 
18:       $\pi \leftarrow e^{\beta(E' - E)}$ 
19:      if  $(E' \leq E)$  then
20:         $x[k] \leftarrow x'[k]$ 
21:      else
22:        if  $(\text{randUniform}(0,1) \leq \pi)$  then
23:           $x[k] \leftarrow x'[k]$ 
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$$E_{\text{path}} = \frac{m}{2\epsilon} \sum_{i=1}^N (x_i - x_{i-1})^2 + \frac{\epsilon}{8} m \omega \sum_{i=1}^N (x_{i-1} + x_i)^2$$

$$\langle E(T) \rangle = \frac{\sum_{n=0}^{\infty} E_n e^{E_n/kT}}{\sum_{n=0}^{\infty} e^{E_n/kT}} = \frac{\sum (n + \frac{1}{2}) \hbar \omega e^{(n+\frac{1}{2})\hbar\omega/kT}}{\sum e^{(n+\frac{1}{2})\hbar\omega/kT}} = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2kT}\right)$$

$$E = \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \omega^2 x^2$$

$$E_n = \left(n + \frac{1}{2} \right) \hbar \omega$$

$$\langle E \rangle = \frac{\int \mathcal{D}[x(\tau)] \left(\frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \omega^2 x^2 \right) e^{-\frac{1}{\hbar} S[x]}}{\int \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar} S[x]}}$$

$$S[x] = \int_0^T \left[\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 + \frac{1}{2} m \omega^2 x^2 \right] d\tau$$

$$E_o = \lim_{T \rightarrow \infty} \frac{\int \mathcal{D}[x(\tau)] \left(\frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \omega^2 x^2 \right) e^{-\frac{1}{\hbar} S[x]}}{\int \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar} S[x]}}$$

$$\psi_o(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2}$$