Lecture 17

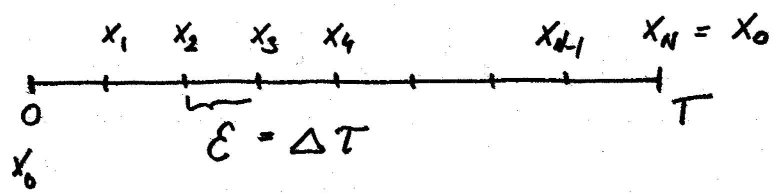
Quantum Monte Carlo and Harmonic Oscillator

$$Z = \int \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_0^T \left[\frac{1}{2}m\left(\frac{dx}{d\tau}\right)^2 + V(x(\tau))\right]d\tau}$$

$$x(0) = x(T)$$

$$Z = \sum_n e^{-\frac{1}{\hbar}E_n T}$$

Discretized form:



$$Z = \int dx_0 \cdots \int dx_{N-1} \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{\frac{N}{2}} \times$$

$$\times \exp\left\{-\frac{m}{2\hbar\varepsilon}\sum_{i=1}^{N}(x_i - x_{i-1})^2 - \frac{\varepsilon}{\hbar}\sum_{i=1}^{N} V\left(\frac{x_{i-1}+x_i}{2}\right)\right\}$$

well-defined N-dimensional integral

V can be taken at endpoint

$$\langle E \rangle = \frac{\sum_n E_n e^{-\frac{1}{\hbar}E_n T}}{\sum_n e^{-\frac{1}{\hbar}E_n T}} = \frac{\sum_n E_n e^{-\frac{1}{\hbar}E_n T}}{Z}$$

$$T = \frac{\hbar}{k\Theta}$$

Θ is the "temperature" of heat bath

Energy (kinetic)

$$\langle v_i^2 \rangle = - \frac{\langle (x_{i+1} - x_i)(x_i - x_{i-1}) \rangle}{\varepsilon^2}$$

$\uparrow$

split point definition of v_i^2

alternative :

$$\frac{1}{2} m \langle v_i^2 \rangle = \frac{1}{2} \langle x V'(x) \rangle$$

Virial theorem classical and quantum mechanical

$$H = \frac{p^2}{2m} + V(x)$$ Hamilton operator

$$[H, xp] = -i\hbar \left(\frac{p^2}{m} - x V'(x) \right)$$

$\langle \psi | [H, xp] | \psi \rangle = 0$ for energy eigenstates

$$\hookrightarrow \langle \psi | \frac{p^2}{m} | \psi \rangle = \langle \psi | x V'(x) | \psi \rangle$$

$$\langle E \rangle = \frac{\sum_n E_n e^{-\frac{1}{\hbar} E_n T}}{Z} =$$

$$= \frac{\int \mathcal{D}[x(\tau)] \left[\frac{1}{2} x V'(x) + V(x) \right] e^{-\frac{1}{\hbar} S[x]}}{\int \mathcal{D}[x(\tau)] \; e^{-\frac{1}{\hbar} S[x]}}$$

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

$$x(T) = x(0)$$

$$E_0 = \lim_{T \to \infty} \frac{\int \mathcal{D}[x(\tau)] \left(\frac{1}{2} x V'(x) + V(x) \right) e^{-\frac{1}{\hbar} S[x]}}{\int \mathcal{D}[x(\tau)] \; e^{-\frac{1}{\hbar} S[x]}}$$

ground state energy

harmonic oscillator

$V = \frac{1}{2} m\omega^2 x^2$ $\qquad \omega = \hbar = m = 1$ units later

$N = 1000$ in discretization

$T = 20 \qquad \varepsilon = \frac{1}{50}$

Discretized form:

$$\langle E\rangle = \frac{1}{Z}\int dx_0\cdots\int dx_{N-1}\left(\frac{m}{2\pi\hbar\varepsilon}\right)^{\frac{N}{2}}\cdot\frac{1}{N}\sum_{i=1}^{N} m\omega^2 x_i^2 \exp\left\{-\frac{m}{2\hbar\varepsilon}\sum_{i=1}^{N}(x_i-x_{i-1})^2 - \frac{\varepsilon}{\hbar}\sum_{i=1}^{N}\frac{1}{2}m\omega^2 x_{i-1}^2\right\} \qquad x_N = x_0$$

$$\frac{1}{2}xV' + V = m\omega^2\left(\frac{1}{2}x\cdot x + \frac{1}{2}x^2\right) = x^2 m\omega^2$$

$\langle E\rangle$ is the ratio of two integrals (N-dimensional)

$$\langle E\rangle = \frac{\int dx_0\cdots\int dx_{N-1}\left(\frac{m}{2\pi\hbar\varepsilon}\right)^{\frac{N}{2}} f\,\frac{1}{N}\sum_{i=1}^{N}x_i^2\, e^{-\frac{1}{\hbar}S(x_0,\dots,x_{N-1})}}{\int dx_0\cdots\int dx_{N-1}\left(\frac{m}{2\pi\hbar\varepsilon}\right)^{\frac{N}{2}} e^{-\frac{1}{\hbar}S(x_0,\dots,x_{N-1})}}$$

$$\langle E\rangle = \frac{\int dx_0\cdots\int dx_{N-1}\, f(x_0,\dots,x_{N-1})\, e^{-\frac{1}{\hbar}S(x_0,\dots,x_{N-1})}}{\int dx_0\cdots\int dx_{N-1}\, e^{-\frac{1}{\hbar}S(x_0,\dots,x_{N-1})}}$$

$$f(x_0,\dots,x_{N-1}) = \frac{1}{N}\sum_{i=0}^{N-1} m\omega^2 x_i^2$$

Metropolis procedure:

$$\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet$$
$$x_0 \quad x_1 \quad x_2 \quad x_3 \quad x_4 \qquad\qquad\qquad x_{N-1}$$

sweep of the lattice: we cycle through the N sites. Only the two neighbors on left and right have to be looked up for the Metropolis move.

Periodic boundary condition on the to ends of the lattice

It is useful to express dimensionful quantities in ε units

$\hbar = 1$

$\varepsilon \equiv a$ in literature (lattice spacing)

$c = 1$

$$V = \frac{1}{2} m\omega^2 x^2$$

$\frac{x}{a}$ dimensionless integration variable:

resolution of the problem is set by the choice of a in ω units

Error of discretitation is not difficult to estimate by Gaussian integration with $m \cdot a = 1$ choice

we find that the energy levels are somewhat shifted at finite $a^2\omega^2$

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

$$\tilde{\omega}^2 = \omega^2 \left(1 + \frac{a^2\omega^2}{4}\right)$$

$$\langle x^2 \rangle = \frac{1}{2\omega\left(1 + \frac{a^2\omega^2}{4}\right)^{\frac{1}{2}}} \left(\frac{1 + R^N}{1 - R^N}\right)$$

$$R = 1 + \frac{a^2\omega^2}{2} - a\omega\left(1 + \frac{a^2\omega^2}{4}\right)^{\frac{1}{2}}$$

$$\psi_0(x) = \left(\frac{\tilde{\omega}}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\tilde{\omega} x^2}$$

lattice wavefunction for ground states

$$Z = (2\pi a R)^{\frac{N}{2}} \frac{1}{1 - R^N}$$

In our laboratory project:

$m = 1 \qquad a = 0.1 \qquad (am) = 0.1$

$\omega^2 = 1 \qquad a^2\omega^2 = \frac{1}{100}$

$N = 1000 \qquad \tilde{\omega} = 1.002\,\omega$

(1) Write update code
$\Delta \sim 2\sqrt{a}$ should keep acceptance around 50%

(2) Calculate E_0 from virial theorem

(3) Calculate ground state wavefunction by histogram method