Lecture 16

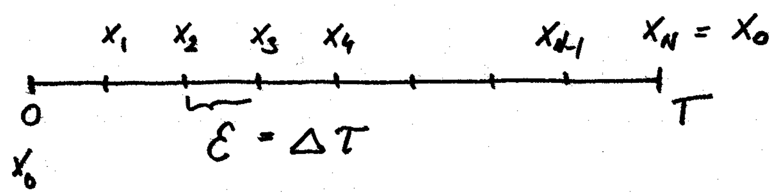
Quantum Monte Carlo and Harmonic Oscillator

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

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

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

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:

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

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

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

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

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

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

Metropolis procedure:

$\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet$

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

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 discretization 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:

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

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

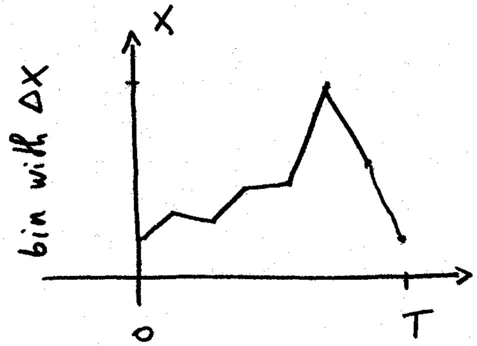
$N = 1000 \qquad \tilde{\omega} = 1.002\,\omega$

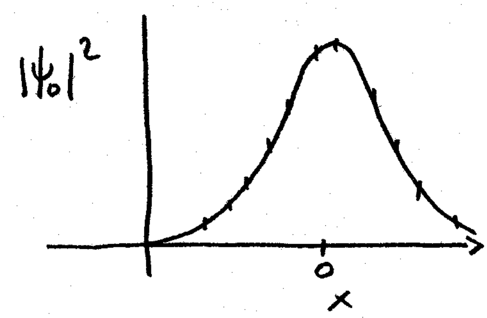
(1) Write update code

$\Delta \sim 2\sqrt{a}$ should keep acceptance around 50%

(2) Calculate E_0 from virial theorem

(3) Calculate ground state wavefunction by histogram method





Monte Carlo implementation

1. Consider the harmonic oscillator with

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2$$

(a) Evaluate the ground state energy and plot the histogram of the ground state |wavefunction|^2 with the following parameters:

$m a = 1$

$\omega \cdot a = 0.15$

$N =$

Recommended run parameters:

$\Delta = 3$ ($\sim 60\%$ acceptance)

10^5 warmup sweeps

10^6 measurement sweeps with 100 sweep separation between measurements

$\sim$ 8 min run

Include an error calculation in the analysis

(b) Calculate first and second excited energies from the $x(0)\,x(\tau)$ and $x^2(0)\,x^2(\tau)$ correlators, respectively.

$$E_1 - E_0 = -\frac{1}{\Delta\tau} \ln\left[\frac{\langle x(0)\, x(\tau+\Delta\tau)\rangle}{\langle x(0)\, x(\tau)\rangle}\right] \qquad \tau \to \infty$$

$$E_2 - E_0 = -\frac{1}{\Delta\tau} \ln\left[\frac{\langle x^2(0)\, x^2(\tau+\Delta\tau)\rangle}{\langle x^2(0)\, x^2(\tau)\rangle}\right] \qquad \tau \to \infty$$

$E_1 - E_0$ in 5–12 τ range

$E_2 - E_0$ in 2–12 τ range

Include an error calculation in the analysis

2. Anharmonic Double Well Potential

$$L = \frac{1}{2} m \dot{x}^2 - \lambda (x^2 - v^2)^2$$

(a) Evaluate the ground state energy and plot the histogram of $|\Psi_0|^2$ with the following parameters:

$a \cdot m = \frac{1}{4}$

$v^2 = 2$

$\lambda = 1$

$\Delta = 2$

10^5 warmup sweeps

10^6 sweeps with 100 sweep separation between measurements

~ 10 min run

Include an error calculation in the analysis

(b) How would you determine the tunneling rate between the two minima?

$\boxed{\text{Error estimate}}$ (for energy)

$E_i \quad i = 1, 2, \dots N_{samp}$ energy estimators of configurations while sampling

$E_i^2 \quad i = 1, 2, \dots, N_{samp}$ useful to calculate at the same time

$$\overline{E} = \frac{1}{N_{samp}} \sum_{i=1}^{N_{samp}} E_i$$

$$\overline{E^2} = \frac{1}{N_{samp}} \sum_{i=1}^{N_{samp}} E_i^2$$

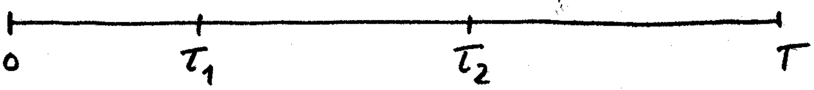
$$E_{error} = \sqrt{\frac{\overline{E^2} - \overline{E}^2}{N_{samp}}}$$

Similar for any other measured quantity

$\overline{E^2} - \overline{E}^2$ determines "intrinsic noise" (variance)

$\frac{1}{\sqrt{N_{samp}}}$ beats the noise in $N_{samp} \to \infty$ limit

$\boxed{\text{Correlation Functions}}$



$$\langle x_0 | \; x(\tau_1)\, x(\tau_2) \; e^{-HT} \; | x_T \rangle =$$

$$= \langle x_0 | \; e^{-H\tau_1} \; x(0) \; e^{H(\tau_1 - \tau_2)} \; x(0) \; e^{H(\tau_2 - T)} \; | x_T \rangle$$

$$|n_1\rangle\langle n_1| \qquad |n_2\rangle\langle n_2| \qquad |n_3\rangle\langle n_3| \qquad |n_4\rangle\langle n_4|$$

$$= \psi_0(x_0)\, e^{-E_0\tau_1} \langle 0 | x(0) | 0 \rangle\, e^{E_0(\tau_1-\tau_2)} \langle 0 | x(0) | 0 \rangle \times$$

$$\times\, \psi^*(x_T)\, e^{E_0(\tau_2 - T)} \quad +$$

$$+ \; \psi_0(x_0)\, e^{-E_0\tau_1} \langle 0 | x(0) | 1 \rangle \langle 1 | x(0) | 0 \rangle\, e^{E_1(\tau_1-\tau_2)} \times$$

$$\times\, e^{E_0(\tau_2 - T)}\, \psi^*(x_T) \qquad + \; \cdots$$

negligible for large T

for large T and large $\tau_2 - \tau_1$

$$\langle x_0 | \, x(\tau_1) \, x(\tau_2) \, e^{-HT} \, | x_T \rangle =$$

$$= \psi_0(x_0) \, \psi^*(x_T) \, e^{-E_0 T} \Big\{ \left| \langle 0 | x(0) | 0 \rangle \right|^2 +$$

$$+ e^{-(E_1 - E_0)(\tau_2 - \tau_1)} \langle 0 | x(0) | 1 \rangle \langle 1 | x(0) | 0 \rangle \Big\}$$

$x_T = x_0$ in our case

zero for first excited state

$$C(\tau_1, \tau_2) = \frac{\mathrm{Tr}\left(x(\tau_1) \, x(\tau_2) \, e^{-HT} \right)}{\mathrm{Tr} \, e^{-HT}} - \Big(\underbrace{\frac{\mathrm{Tr} \, x \, e^{-HT}}{\mathrm{Tr} \, e^{-HT}}}_{} \Big)^2$$

$$= e^{-(E_1 - E_0)(\tau_2 - \tau_1)} \cdot \left| \langle 0 | x | 1 \rangle \right|^2$$

Similar for second excitation

Clarification on Dimensional Analysis:

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

E_n energy eigenvalues

$$\frac{H}{m} = \frac{p^2}{2m^2} + \frac{1}{2} \frac{\omega^2}{m^2} m^2 x^2$$

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

$\frac{H}{m}$, $\frac{p}{m}$, $\frac{\omega}{m}$, mx are dimensionless

$$\frac{p^2}{2m^2} \rightarrow -\frac{d^2}{d\xi^2}$$

$mx = \xi$

$\frac{\omega}{m} = \Omega$

$\hbar = 1$

$$\left(-\frac{d^2}{d\xi^2} + \frac{1}{2} \Omega^2 \cdot \xi^2\right) \psi_n(\xi) = \frac{E_n}{m} \psi_n(\xi)$$

$$\frac{E_n}{m} = \Omega \left(n + \frac{1}{2}\right)$$

If we now discretize ξ, a is dimensionless

$m \cdot T$ is also dimensionless

$$e^{-E_n T} \rightarrow e^{-\frac{E_n}{m} \cdot mT}$$