Computer modeling of physical phenomena: path integrals

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Plan

1. Density matrix – central object of quantum statistics
2. Path integrals (by Feynman)
3. Path integral Monte Carlo simulation

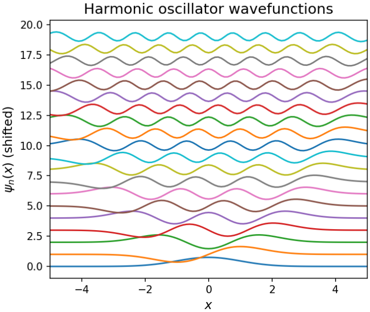
Plan

Quantum harmonic oscillator

- quantum particle in a potential

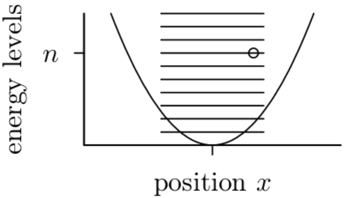
$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2, \quad p = -i\hbar\partial_x$$

- $\hbar = m = \omega = 1$ in our numerics
- wave functions $\psi_n(x)$ and eigenvalues $E_n = n + \frac{1}{2}$



procedure harmonic-wavefunction
input x
$\psi_{-1}^{\text{h.o.}}(x) \leftarrow 0$ (unphysical, starts recursion)
$\psi_0^{\text{h.o.}}(x) \leftarrow \pi^{-1/4} \exp\left(-x^2/2\right)$ (ground state)
for $n = 1, 2, \ldots$ **do**
$\left\{ \psi_n^{\text{h.o.}}(x) \leftarrow \sqrt{\frac{2}{n}} x \psi_{n-1}^{\text{h.o.}}(x) - \sqrt{\frac{n-1}{n}} \psi_{n-2}^{\text{h.o.}}(x) \right.$
output $\{\psi_0^{\text{h.o.}}(x), \psi_1^{\text{h.o.}}(x), \ldots\}$

Thermal occupation



- thermodynamics – partition function:

$$\mathcal{Z}(\beta) = \sum_n e^{-\beta E_n} = \ldots = \frac{1}{2\sinh(\beta/2)}$$

- particle at level "n" at position x, probability:

$$|\psi_n(x)|^2 \times e^{-\beta E_n}/\mathcal{Z}$$

Density matrix

- thermal occupation (prob. of being at x):

$$\pi(x) = \frac{1}{\mathcal{Z}} \sum_n e^{-\beta E_n} |\psi_n(x)|^2$$

- general object, encapsulates knowledge of ψ_n, E_n

$$\rho(x, x', \beta) = \sum_n \psi_n^*(x) \psi_n(x') e^{-\beta E_n}$$

- diagonal part of density matrix

$$\mathcal{Z}(\beta) = \int dx\, \rho(x, x, \beta), \quad \pi(x) = \rho(x, x, \beta)/\mathcal{Z}$$

Free density matrix

- kinetic Hamiltonian $H_0 = \frac{1}{2m}p^2$; plane waves

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx} \quad (p = \hbar k)$$

- introducing resolution of unity

$$\rho_0(x, x', \beta) = \langle x|e^{-\beta H_0}|x'\rangle = \int \frac{dk}{2\pi}\, e^{ik(x-x')} e^{-\beta \frac{\hbar^2 k^2}{2m}}$$

- performing the Gaussian integral we finaly get

$$\rho_0(x, x', \beta) = \sqrt{\frac{m}{2\pi\hbar^2\beta}}\, e^{-\frac{m}{2\hbar^2\beta}(x-x')^2}$$

Plan

Imaginary time

- note: there is a close analogy (formal mapping) between the density matrix and the unitary evolution (propagator):

$$\langle x|e^{-\beta H}|x'\rangle \;\longleftrightarrow\; \langle x|e^{-itH}|x'\rangle$$

- imaginary time $\beta \longleftrightarrow it$ real time
- convolution property (combined evolution in real time):

$$\int dx'\,\rho(x,x',\beta_1)\rho(x',x'',\beta_2) = \ldots = \rho(x,x'',\beta_1+\beta_2)$$

Path integral

- applying repeatedly the convolution:

$$\rho(x_0, x_N, \beta) = \int \ldots \int dx_1 \ldots dx_{N-1}\, \rho(x_0, x_1, \beta/N) \ldots \rho(x_{N-1}, x_N, \beta/N)$$

- path is a sequence $\{x_0, \ldots, x_N\}$, we imagine x_k at time $k\Delta\tau$ ($\Delta\tau = \beta/N$); path in $d+1$ dimensions
- density functions and partition function are represented as integrals over paths $\{x_0, \ldots, x_N\}$ (formally also $N \to \infty$)

Trotter decomposition

- we use a (sec. order) Suzuki-Trotter decomposition

$$e^{-\Delta\tau(H_0+V)} = e^{-\frac{1}{2}\Delta\tau V} e^{-\Delta\tau H_0} e^{-\frac{1}{2}\Delta\tau V}$$

so

$$\rho(x, x', \Delta\tau) = e^{-\frac{1}{2}\Delta\tau V(x)} \rho_0(x, x', \Delta\tau) e^{-\frac{1}{2}\Delta\tau V(x')}$$

- we know explicit formula for the free density matrix $\rho_0(x, x', \Delta\tau)$

Expansion for $\pi(x)$

- collecting all terms in the path integral (with x_0 fixed and p.b.c.)

$$\pi(x_0) = \frac{1}{\mathcal{Z}} \int \mathcal{D}\{x_i\}\, e^{-\Delta\tau V(x_0)} \rho_0(x_0, x_1, \Delta\tau) \dots \\ e^{-\Delta\tau V(x_{N-1})} \rho_0(x_{N-1}, x_0, \Delta\tau)$$

- form of this path integral with “Euclidean” action S:

$$\pi(x_0) = \frac{1}{\mathcal{Z}} \int \mathcal{D}\{x_i\} e^{-S(\{x_i\})},$$

where $S(\{x_i\}) = \sum_i \frac{1}{2\beta}(x_i - x_{i+1})^2 + \sum_i \Delta\tau V(x_i)$

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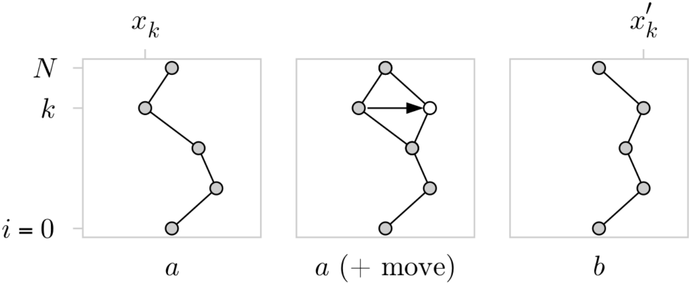
Path sampling algorithm



- choose random element k, accept the move $x_k \to x_k + \delta$ with Metropolis algorithm
- only the segments $\{x_{k-1}, x_k\}$ and $\{x_k, x_{k+1}\}$ are involved

Pseudo-code

procedure `naive-harmonic-path`
input $\{x_0, \ldots, x_{N-1}\}$
$\Delta_\tau \leftarrow \beta/N$
$k \leftarrow \texttt{nran}\,(0, N-1)$
$k_\pm \leftarrow k \pm 1$ modulo N

$x'_k \leftarrow x_k + \texttt{ran}\,(-\delta, \delta)$
$\pi_a \leftarrow \rho^{\text{free}}\left(x_{k_-}, x_k, \Delta_\tau\right) \rho^{\text{free}}\left(x_k, x_{k_+}, \Delta_\tau\right) \exp\left(-\frac{1}{2}\Delta_\tau x_k^2\right)$
$\pi_b \leftarrow \rho^{\text{free}}\left(x_{k_-}, x'_k, \Delta_\tau\right) \rho^{\text{free}}\left(x'_k, x_{k_+}, \Delta_\tau\right) \exp\left(-\frac{1}{2}\Delta_\tau x_k'^2\right)$
$\Upsilon \leftarrow \pi_b/\pi_a$
if $(\texttt{ran}\,(0,1) < \Upsilon) x_k \leftarrow x'_k$
output $\{x_0, \ldots, x_{N-1}\}$