Computer modeling of physical phenomena: path integrals and quantum Monte Carlo

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Plan

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

References

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2. W. Krauth “Statistical Mechanics: Algorithms and Computations” Oxford (2006).
2. G. G. Batrouni “Quantum phase transitions” in Les Houches Lecture Notes (2009).
3. M.J.E. Westbroek, P.R. King, D.D. Vvedensky, S. Durr “Users guide to Monte Carlo methods for evaluating path integrals” American Journal of Physics **86**, 293 (2018).

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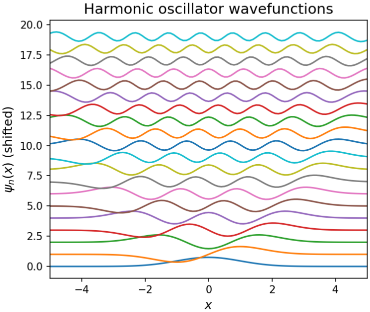
Quantum harmonic oscillator

- quantum particle in a potential

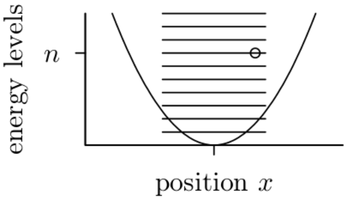
$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2, \quad p = -i\hbar\partial_x$$

- $\hbar = m = \omega = 1$ 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

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

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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:

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

- path is a sequence $\{x_0, \dots, x_N\}$, 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 $\{x_0, \dots, x_N\}$ (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.)

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

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

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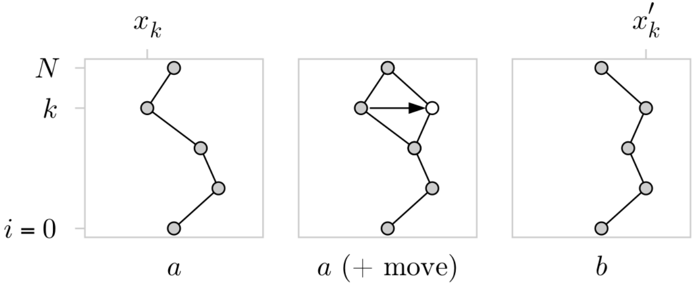
Path sampling algorithm



- 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 $\{x_0, \ldots, x_{N-1}\}$

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