path integrals

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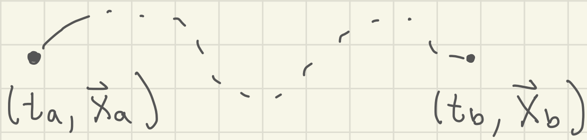
goal: find the most probable path $x(t)$ from position a to position b for a quantum particle in a given potential $V(x)$ between time t_a and time t_b



from classical mechanics:

the path $x(t)$ which minimizes the action $S[x(t)]$ is the physical path taken by the object

$$S[x(t)] = \int_{t_a}^{t_b} \mathcal{L}[\dot{x}, x, t]\, dt$$

where $\mathcal{L}$ is the Lagrangian of the system which is defined as kinetic minus potential energy

$$\mathcal{L} \equiv T - V$$

note that typically $T = T(\dot{x})$ and $V = V(x)$

in quantum mechanics

there is no definite, "physical path"
in QM, there is only the "most probable path"

this is the $x(t)$ that will minimize the action in QM, the $x(t)$ we want to find.

each quantum path has a probability, (and thus a "probability amplitude") which determines the chance of the particle taking that path.

$$\phi[x(t)] = C e^{iS[x(t)]/\hbar}$$

$$= C e^{i\mathcal{L}\delta t/\hbar}$$

we will use this probability amplitude for our second MH condition!

. . . but we need to make a change of variables to get rid of the "i" . . .

let $it = \tau$, so $t = -i\tau$

the kinetic term changes sign with this change of variables

$$T_t = \frac{1}{2} m \left(\frac{dx}{dt}\right)^2 = \frac{1}{2} \frac{m}{i^2} \left(\frac{dx}{d\tau}\right)^2 = -T_\tau$$

$V(x)$ doesn't change

$$\quad\quad\quad\quad T \quad - \quad V$$

$$S[x(\tau)] = \int_{\tau_a}^{\tau_b} \left(-T_\tau - V(x)\right)(-i\, d\tau)$$

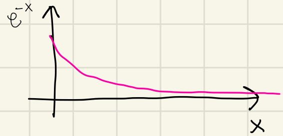
$$= i \int_{\tau_a}^{\tau_b} \left(T_\tau + V(x)\right) d\tau$$

$$= i \int H \, d\tau$$

$$\longrightarrow \quad \phi[x(t)] = C e^{-H\delta\tau/\hbar}$$

yay! no imaginary exponent!

also note, large action paths are decayed



to determine if a path is more probable than another, check if it's action is smaller!

$\delta\tau$ will be the same for all, we can just check if the hamiltonian is smaller!

(aka the energy)

MH algorithm

we will store T full paths

$$\underline{X}[N+2, T] = \begin{array}{c} t_0 \\ t_1 \\ \vdots \\ \vdots \\ \vdots \\ t_{N+1} \end{array} \begin{bmatrix} x_a & x_a & & \\ x_1 & x_1 & & \\ x_2 & x_2 + \delta(2u-1) & & \\ x_3 & x_3 & & \\ \vdots & \vdots & & \\ x_b & x_b & & \end{bmatrix}$$

path 0, path 1, ... path T-1

capital X

same format for $\underline{E}$ except [N+1, T]

set up an initial path X[1:N+1, 0] of random #'s ∈ [-1, 1]
set boundaries x_a & x_b for initial path

copy previous path into new column

choose a random x_i to perturb

$$x_i' = x_i + \delta(2u-1)$$

does this decrease the action (hamiltonian)?

$$H = \frac{1}{2} m \dot{x}^2 + V(x)$$

approx

$$\text{hamiltonian}(x_i, x_{i+1}) = \frac{1}{2} m \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 + V(x_i)$$

we only perturb one x_i at a time, so only two terms in the total energy change.

"hamiltonian" function in code

$$\Delta E = \underbrace{H(x_{i-1}, x'_i) - H(x_{i-1}, x_i)}_{\Delta E \text{ between } x_{i-1} \text{ \& } x_i} + \underbrace{H(x'_i, x_{i+1}) - H(x_i, x_{i+1})}_{\Delta E \text{ between } x_i \text{ \& } x_{i+1}}$$

if $\Delta E < 0$,

keep x'_i in place of x_i

else

we still want a chance to keep x'_i
according to the probability amplitude

- get a random $u \in [0, 1]$ ← a new u!
- if $u \leq \exp(-\epsilon \Delta E / \hbar)$

  keep x'_i in place of x_i

cut off the first "ncut" paths from the beginning & return

$$X[N+2,T] = \begin{array}{cc} 0 & t_0 \\ 1 & t_1 \\ \vdots & \vdots \\ & \\ & \\ N & t_N \\ N+1 & t_{N+1} \end{array} \begin{bmatrix} x_a & x_a & & \\ x_1 & x_1 & & \\ x_2 & x_2 + \delta(2u-1) & & \\ x_3 & x_3 & & \\ \vdots & \vdots & & \\ & & & \\ x_b & x_b & & \end{bmatrix}$$

$$\begin{array}{cccc} \text{path } 0 & \text{path } 1 & \cdots\cdots & \text{path } T-1 \end{array}$$

$$E[N+1,T] = \begin{array}{cc} 0 & t_{1/2} \\ 1 & t_{1+1/2} \\ 2 & t_{2+1/2} \\ \vdots & \vdots \\ N & t_{N+\frac{1}{2}} \end{array} \begin{bmatrix} E_{1/2} & & \\ E_{1\,1/2} & & \\ \vdots & & \\ \vdots & & \\ E_{N+\frac{1}{2}} & & \end{bmatrix}$$

$$\begin{array}{cccc} \text{path } 0 & \text{path } 1 & \cdots\cdots & \text{path } T-1 \end{array}$$

E[i, j] = hamiltonian (x[i, j], x[i+1, j], eps, fPOT)

$$\text{hamiltonian} = \frac{1}{2} m \dot{x}^2 + V(x_i)$$

$$= \frac{1}{2} m \left(\frac{\Delta x}{\Delta t}\right)^2 + V(x_i)$$

$$= \frac{1}{2} m \left(\frac{x_{i+1} - x_i}{\Delta t}\right)^2 + V(x_i)$$

needs position at 2 times