Lecture 16

Path Integral, Simulations and Quantum Algorithms

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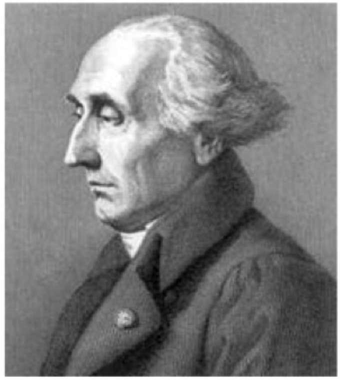
Introduction to Algorithms for Data Science and Physics IMP@Fudan, 2026

Topics of this lecture:

- least action principle $\delta S = 0$
- sum over paths->path integral $e^{\sum \text{paths}}$
- transition amplitude, quantum fluctuation $\langle x_{\rm f}|e^{-iH(t_{\rm f}-t_{\rm i})/\hbar}|x_{\rm i}\rangle = \mathcal{F}(t_{\rm f}, t_{\rm i})e^{iS_{\rm cl}/\hbar}$
- quantum harmonic oscillator
- imaginary time simulations $\beta\hbar = it$
- Grover's square root speedup for searching $t \approx \pi\sqrt{N}/4 \leftrightarrow P(i) \gtrsim 1 - \mathcal{O}(N^{-1})$

Least action principle

$$S = \int_{t_1}^{t_2} [\mathrm{KE}(t) - \mathrm{PE}(t)]\, dt$$

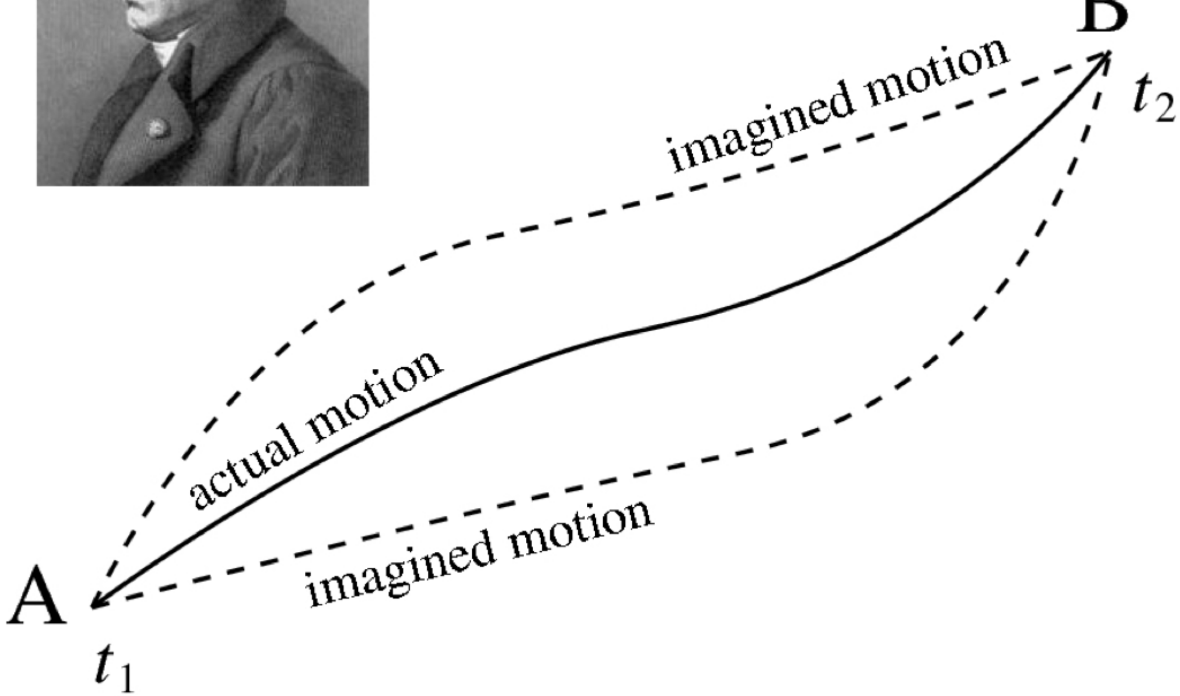


$\min S$

KE: kinetic energy
PE: potential energy

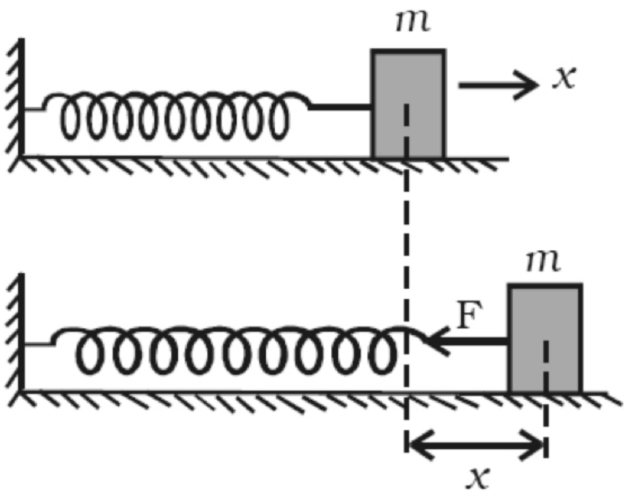
$$\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = 0$$

L=KE-PE



Ex.: Check Lagrange's equation for free particle and harmonic oscillator.

Action for harmonic oscillator



Linear harmonic oscillator

$$KE = \frac{1}{2} m\dot{x}^2, \; PE = \frac{1}{2} kx^2 = \frac{1}{2} m\omega x^2$$

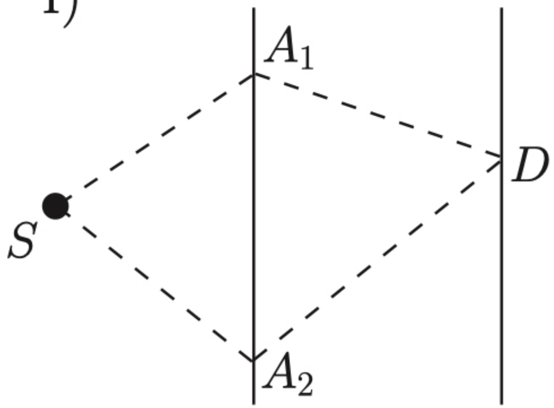
$$S = \frac{m\omega}{2 \sin \omega (t_f - t_i)} \left[\left(x_f^2 + x_i^2 \right) \cos \omega (t_f - t_i) - 2 x_f x_i \right]$$

Ex.: What is limit of $\omega \to 0$?

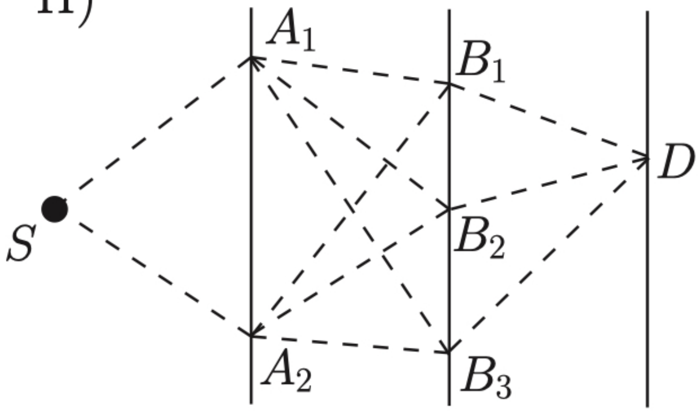
Double-slit experiment

$$\text{Amp.}(D) = \sum_{j=1,2} \text{Amp.}(S \to A_j \to D)$$

I)

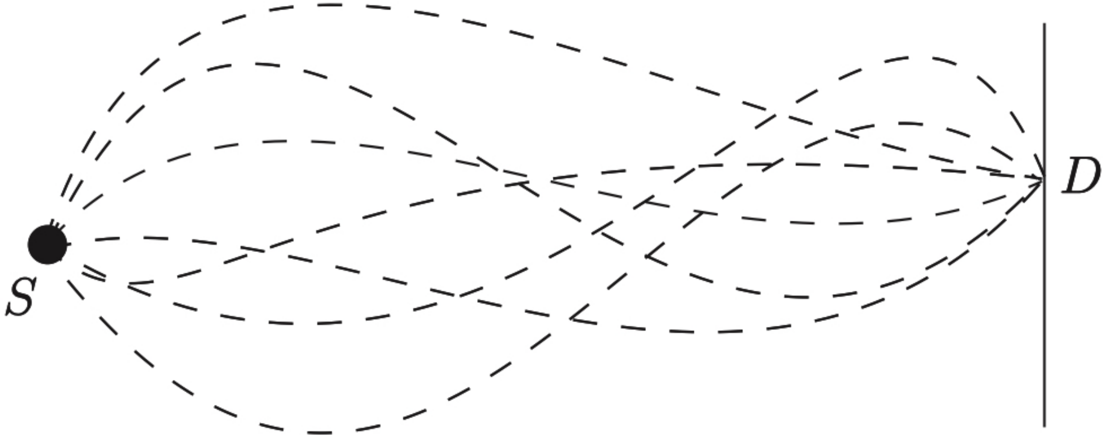


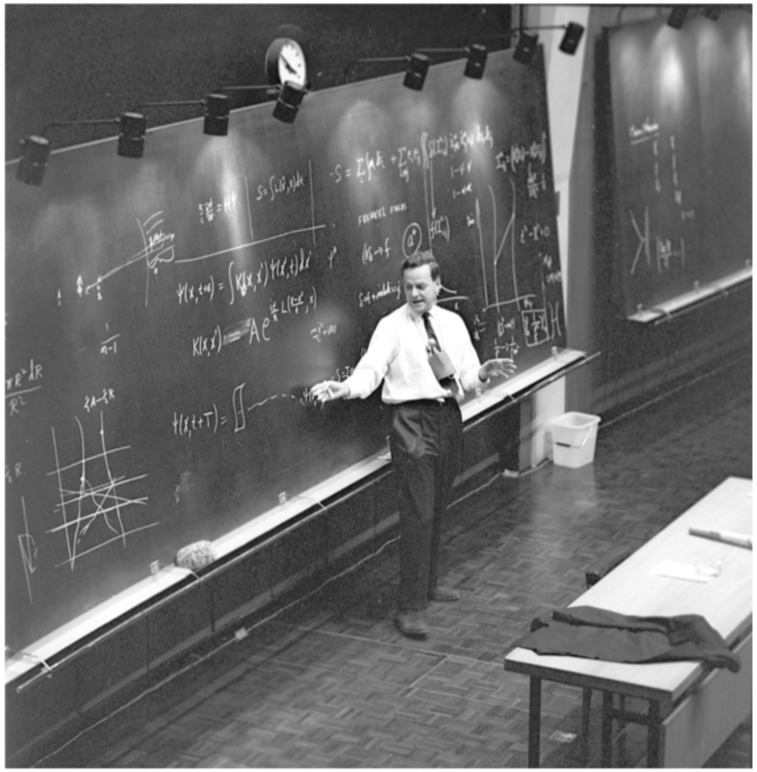
II)



$$\text{Amp.}(D) = \sum_{j,k} \text{Amp.}(S \to A_j \to B_k \to D)$$

What happens if there is no slit/wall?





$$\text{Amp.}(D) = \sum_{\text{all path } (S \to D)} \text{Amp.}(S \to \cdots \to D)$$

Amplitude for free particle

$$\mathcal{O} = \sum_n |n\rangle\langle n|, \quad \langle i|j\rangle = \delta_{ij}$$

$$\Psi(x,t) = e^{-iHt/\hbar}\Psi(x,0)$$

Ex.: What is $\mathcal{O}|m\rangle$?

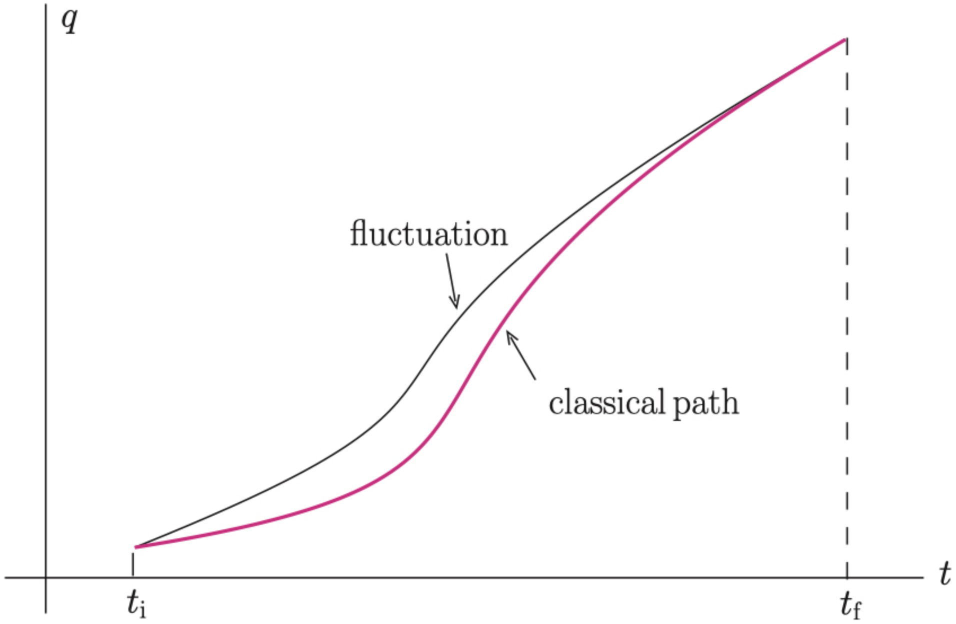
transition amplitude: $\langle x_\mathrm{f}|e^{-iHt/\hbar}|x_\mathrm{i}\rangle$

$$\langle x_\mathrm{f}|e^{-iHT/\hbar}|x_\mathrm{i}\rangle = \sqrt{\frac{m}{2\pi\hbar i T}} \times \exp\left[\frac{i}{\hbar}\frac{m(x_\mathrm{f}-x_\mathrm{i})^2}{2T}\right]$$

General result for amplitude

$$\mathcal{F}(t_f, t_i) = \int \mathcal{D}[\delta x(t)] \times \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f} dt \times \left[\alpha(t)\delta\dot{x}^2 + \beta(t)\delta x\delta\dot{x} + \gamma(t)\delta x^2\right]\right]$$

$$L(x,\dot{x},t) = \alpha(t)\dot{x}^2(t) + \beta(t)x(t)\dot{x}(t) + \gamma(t)x^2(t) + \delta(t)\dot{x}(t) + \chi(t)x(t) + \varphi(t)$$



$$\langle x_f | e^{-iH(t_f - t_i)/\hbar} | x_i \rangle = \mathcal{F}(t_f, t_i) e^{iS_{cl}/\hbar}$$

Quantum harmonic oscillator

$$\langle x_{\mathrm{f}}|e^{-iH(t_{\mathrm{f}}-t_{\mathrm{i}})/\hbar}|x_{\mathrm{i}}\rangle = \left(\frac{m\omega}{2\pi i\hbar \sin\omega(t_{\mathrm{f}}-t_{\mathrm{i}})}\right)^{1/2} \times \exp\left[\frac{i}{\hbar}\frac{m\omega}{2\sin\omega(t_{\mathrm{f}}-t_{\mathrm{i}})}\left[(x_{\mathrm{f}}^2+x_{\mathrm{i}}^2)\cos\omega(t_{\mathrm{f}}-t_{\mathrm{i}})-2x_{\mathrm{f}}x_{\mathrm{i}}\right]\right]$$

Ex.: Take the limit of $\omega \to 0$.

Ex.: Obtain the zero-point energy using Heisenberg's uncertainty principle.

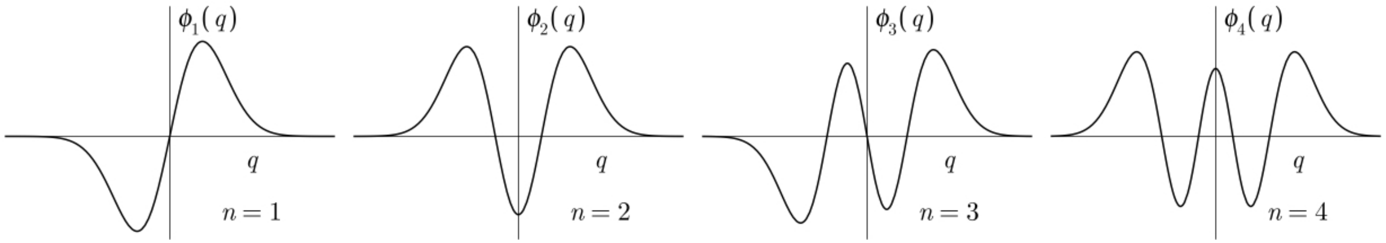
energy: $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$

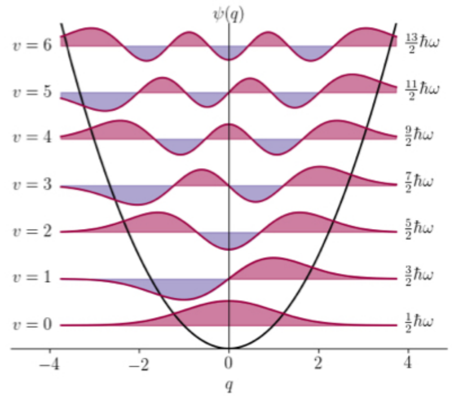
wave function: $\phi_n(x) = 2^{-n/2}(n!)^{-1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$

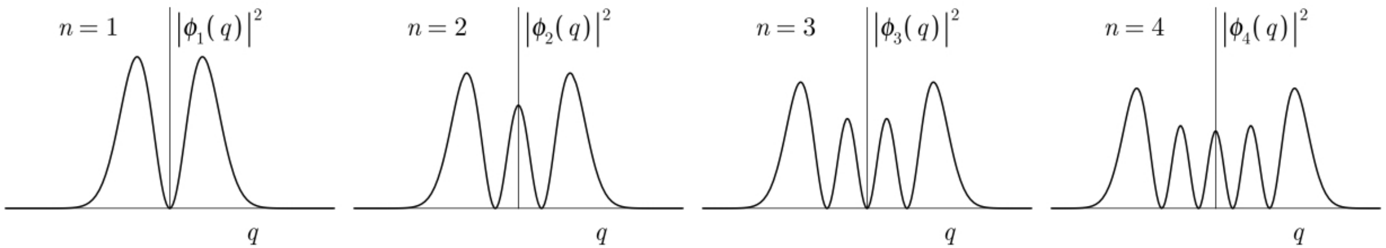
Ex.: Features of GS wave function.

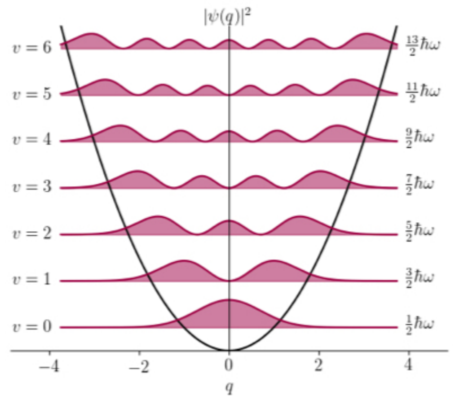
$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}$$

Wave functions for quantum HO









Probability at the origin

$$\mathrm{prob}_0^{\mathsf{quan}}(x)/\mathrm{prob}_0^{\mathsf{quan}}(0) = e^{-\beta x^2}$$

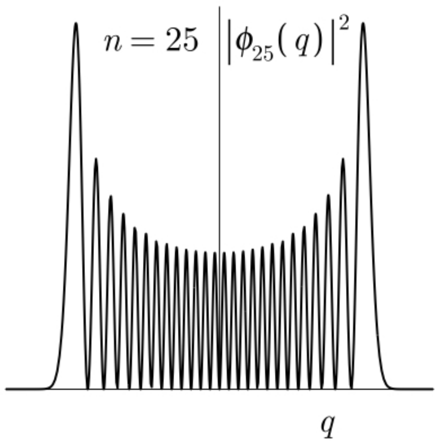
$$x(t) = X \sin \omega t$$

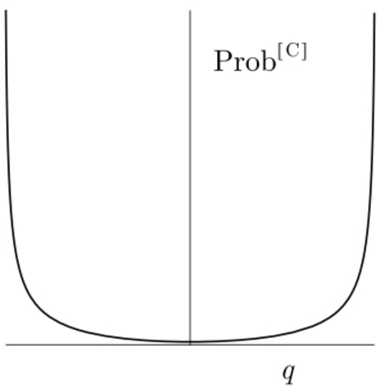
$$v(t) = X\omega \cos \omega t = \omega\sqrt{X^2 - x^2}$$

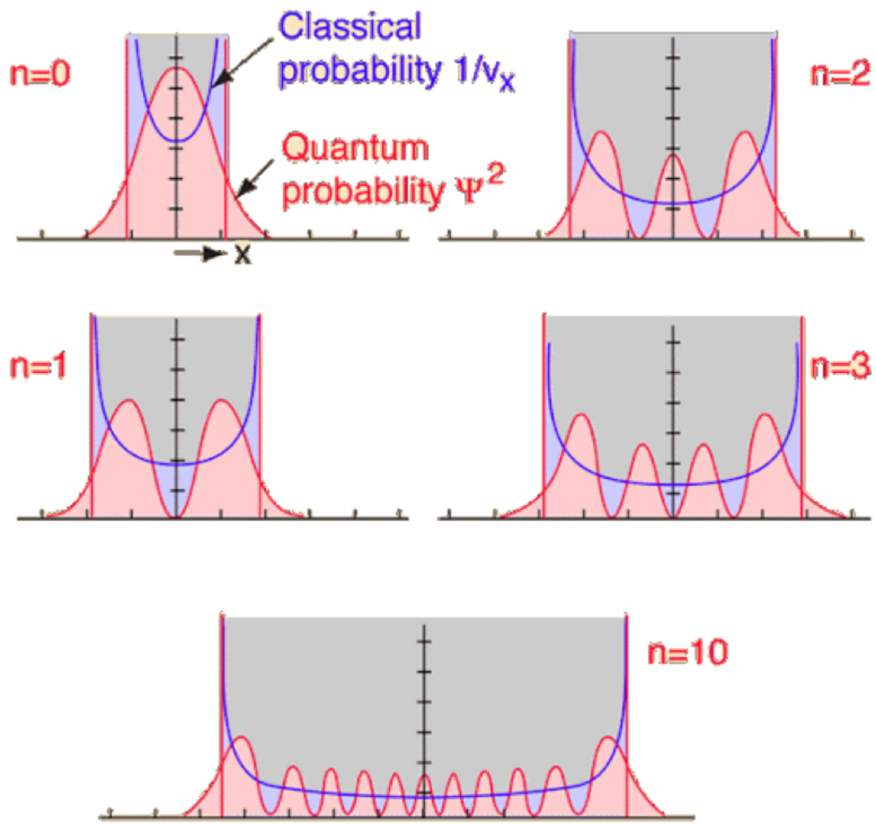
$$\mathrm{prob}^{\mathsf{class}}(x)dx = \frac{1}{T}\frac{2dx}{v(x)} = \frac{\omega}{2\pi}\frac{2dx}{\omega\sqrt{X^2 - x^2}} = \frac{1}{\pi}\frac{dx}{\sqrt{X^2 - x^2}}$$

$$\mathrm{prob}^{\mathsf{class}}(x) = \frac{1}{\pi X}\left[1 - \left(\frac{x}{X}\right)^2\right]^{-1/2}$$

Large *n*: correspondence principle







*Density matrix and partition function (statistical mechanics)

density matrix: $\langle x_\mathrm{f}|e^{-\beta H}|x_\mathrm{i}\rangle = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2} \exp\left[-\frac{m(x_\mathrm{f}-x_\mathrm{i})^2}{2\beta\hbar^2}\right]$

propagator: $\langle x_\mathrm{f}|e^{-iHt/\hbar}|x_\mathrm{i}\rangle = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \exp\left[\frac{i}{\hbar}\frac{m(x_\mathrm{f}-x_\mathrm{i})^2}{2t}\right]$

imaginary time: $\beta\hbar = it$

Wick rotation <-> Euclidean action

$$\rightarrow iS|_{t=-i\tau} = \int_{\tau_\mathrm{i}}^{\tau_\mathrm{f}} d\tau \left[-\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 - U(x)\right] = -S_\mathrm{E}$$

$$\rightarrow Z(\beta) = \mathrm{tr}(e^{-\beta H}) = \int dx\langle x|e^{-\beta H}|x\rangle = \int_{x(0)=x(\beta)} \mathcal{D}[x(\tau)] \exp\left[-\frac{1}{\hbar}\int_0^\beta d\tau \left[\frac{1}{2}m\dot{x}(\tau) + U(x(\tau))\right]\right]$$

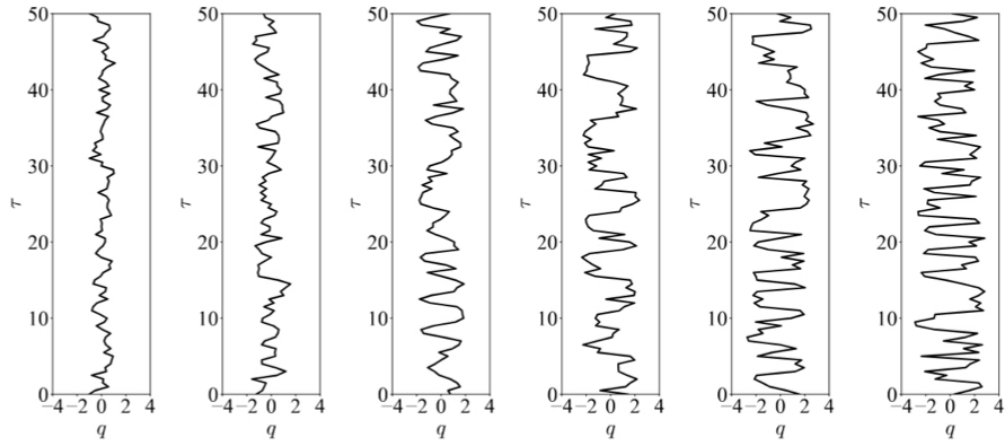
partition function; periodic orbits

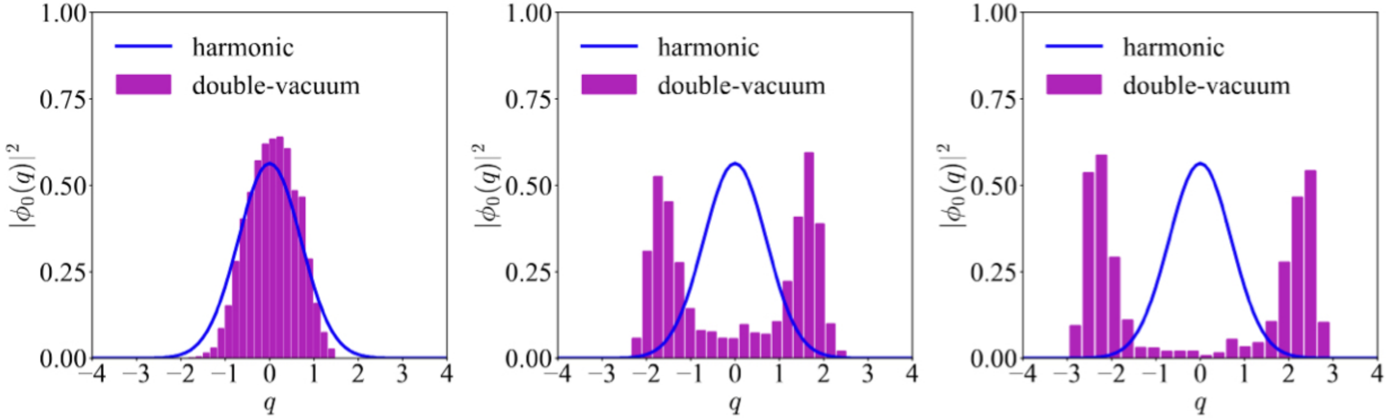
Ground state probabilities

$$iG(x,\tau;x,0) = \sum_n \phi_n(x)\phi_0(x_0)e^{-\tau E_n/\hbar}$$

$$\rightarrow \phi_0^2(x) = \lim_{\tau\to\infty} e^{-\tau E_0/\hbar} iG(x,\tau;x,0)$$

λ more negative $\rightarrow$

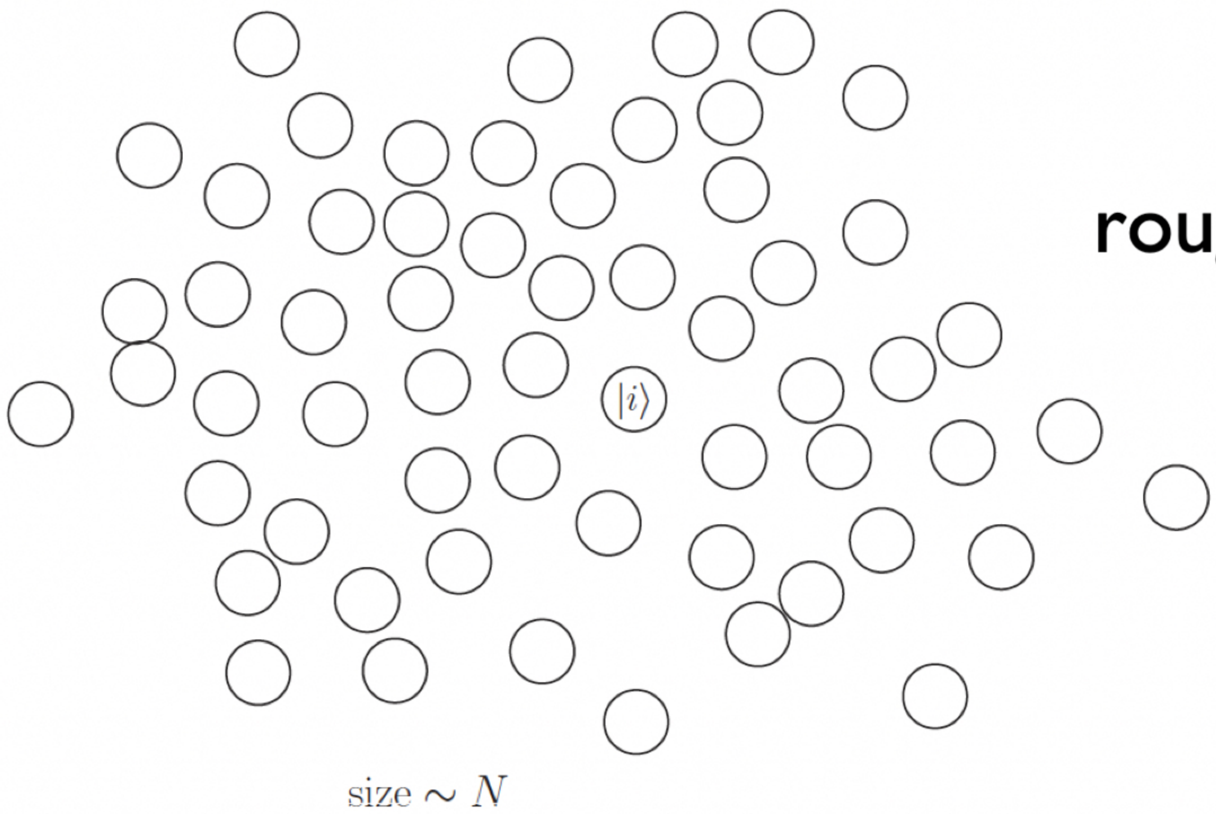




$$U(x) = x^4 + \lambda x^2$$
$$\lambda = 0,\ -6,\ -12$$

$$E_1 - E_0 = -\frac{1}{\epsilon}\ln\left(\frac{\langle x(0)x(\tau+\epsilon)\rangle}{\langle x(0)x(\tau)\rangle}\right)$$

How many times do we need to find the needle?



roughly $\sim \mathcal{O}(N)$

Grover's square root speedup

1. reflection: $\mathrm{R}_u = 2|u\rangle\langle u| - \vec{1}$
2. oracle and diffusion: $\mathrm{U} = \vec{1} - 2|i\rangle\langle i|$, $\mathrm{D} = 2|u\rangle\langle u| - \vec{1}$
3. 2D subspace: $V = \mathrm{span}\{|i\rangle, |v\rangle\}$
4. Grover iteration: $\mathrm{G} = \mathrm{DU}$ = two reflections=rotation by 2ϑ
5. after repeated rotations: $|u\rangle \to |i\rangle$

remaining state

$$|v\rangle = \frac{1}{\sqrt{N-1}} \sum_{j \neq i} |j\rangle = \frac{\sqrt{N}|u\rangle - |i\rangle}{\sqrt{N-1}}$$

$$|\Phi\rangle = \underbrace{\mathbf{DUDU}\cdots\mathbf{DU}}_{t\,\text{times}}|u\rangle = (\mathbf{DU})^t|u\rangle$$

Ex.: What is role of U acting on $|i\rangle$ or $|j\rangle$?

Ex.: Write down the form of D and show $\mathrm{D}^\dagger\mathrm{D} = \vec{1}$.

number of steps to rotate $|\Phi\rangle$ from the initial state toward $|i\rangle$: $\sim t \approx \frac{\pi/2}{2\vartheta} = \frac{\pi}{4\vartheta}$

angle between $|u\rangle$ and $|v\rangle$: $\langle u|v\rangle = \frac{\sqrt{N}\langle u|u\rangle}{\sqrt{N-1}} = \cos\vartheta = \sqrt{1 - \frac{1}{N}} \approx 1 - \frac{1}{2N} + \mathcal{O}\left(\frac{1}{N^2}\right)$

$$\cos\vartheta \approx 1 - \vartheta^2/2 + \mathcal{O}(\vartheta^4) \to t \approx \frac{\pi}{4}\sqrt{N}$$

probability of finding $|i\rangle$ after t steps: $P(i) = |\langle\Phi|i\rangle|^2 \geq \cos^2\vartheta = 1 - \mathcal{O}(\vartheta^2) = 1 - \mathcal{O}\left(\frac{1}{N}\right)$