Feynman's Quantum Paths

(Advanced $\Rightarrow$ Relativity, Quantum Chromodynamics)

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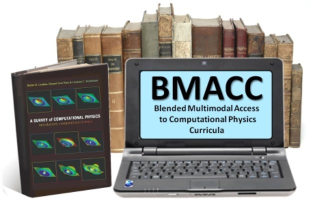
Based on *A Survey of Computational Physics* by Landau, Páez, & Bordeianu

with Support from the National Science Foundation

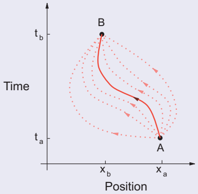
Course: **Computational Physics II**



Feynman: Quantum Mech $\leftrightarrow$ Classical Mech?

Generalize Classical Trajectory to QM Probability

- Classical Mech: single $x(t)$ path $=\bar{x}$
- QM: waves = statistical, no path
- Dirac: Hamilton's least-action prin

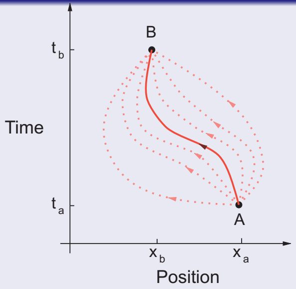


  - F: Look for quantum least-action principle
  - Hamilton: space-time path variation δ calculus
  - F: quantum particle @ $B = (x_b,\ t_b)$
  - From all A via *Green's function* (*propagator*) G

$$\psi(x_b, t_b) = \int dx_a\, G(x_b, t_b; x_a, t_a)\psi(x_a, t_a)$$

Huygen-Feynman Quantum Wavelets

Classical Becomes Quantum



$$\psi(x_b, t_b) = \int dx_a \, G(b,a) \, \psi(x_a, t_a)$$

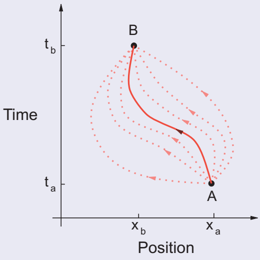
$$G(b,a) = \frac{\exp\left[i \frac{m(x_b - x_a)^2}{2(t_b - t_a)} \right]}{\sqrt{2\pi i (t_b - t_a)}}$$

- $\sim$ Huygens's principle
- $G(b;a)$ = spherical wavelet
- $\psi(x_b, t_b) = \sum$ wavelets
- F's vision: $\psi \leftrightarrow$ path
- $\psi_B = \sum_{\rm all}$ paths, A
- Δ paths Δ probabilities
- All paths possible!
- Also relativity, fields

Hamilton's Principle of Least Action (Classical)

Newton's Law $\equiv \delta S[\bar{x}(t)] = 0$

"The most general motion of a physical particle moving along the classical trajectory $\bar{x}(t)$ from time t_a to t_b is along a path such that the action $S[\bar{x}(t)]$ is an extremum."



$$\delta S = S[\bar{x}(t) + \delta x(t)] - S[\bar{x}(t)] = 0 \quad (1)$$

$$\text{(Constraint)} \quad \delta(x_a) = \delta(x_b) = 0 \quad (2)$$

$$[x(t)] = \text{functional}$$

$$S[\bar{x}(t)] = \int_{t_a}^{t_b} dt\, L[x(t), \dot{x}(t)] \quad (3)$$

$$L = \text{Lagrangian} = T[x, \dot{x}] - V[x] \quad (4)$$

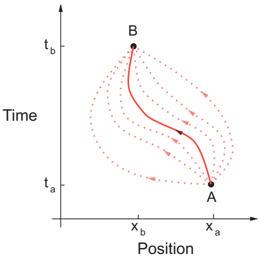
Connecting CM Hamilton's Prin to QM Paths

Consider Free Particle ($V = 0$)

$$S[b,a] = \int_{t_a}^{t_b} dt\,(T - V)$$

$$= \frac{m}{2}\dot{x}^2(t_b - t_a) = \frac{m}{2}\frac{(x_b - x_a)^2}{t_b - t_a} \qquad (1)$$

$$\Rightarrow \quad G(b,a) = \frac{e^{iS[b,a]/\hbar}}{\sqrt{2\pi i(t_b - t_a)}} \qquad (2)$$



$$\Rightarrow \quad G(b,a) = \sum_{\text{paths}} e^{iS[b,a]/\hbar} \qquad (3)$$

- F: QM = path integrals
- All paths $\exists$, Δ prob
- Mainly classical

- $\hbar \simeq 10^{-34}$ Js $\Rightarrow \sim \bar{x}$
- $S_{\bar{x}}$ = extremum

Relate Paths to Ground State Wave Function

Hermitian $\tilde{H}$ $\Rightarrow$ Complete Orthonormal Set $\Rightarrow$ Propagator

$$\tilde{H}\psi_n = E_n\psi_n \tag{1}$$

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n\, e^{-iE_nt}\, \psi_n(x) \tag{2}$$

$$c_n = \int_{-\infty}^{+\infty} dx\, \psi_n^*(x,0)\psi(x,0) \tag{3}$$

$$\rightarrow \quad \underline{\psi(x,t)} = \int_{-\infty}^{+\infty} dx_0 \sum_n \psi_n^*(x_0)\psi_n(x)e^{-iE_nt}\, \underline{\psi(x_0, t=0)} \tag{4}$$

$$\text{Recall:} \quad \psi(x_b,t_b) = \int dx_a\, G(x_b,t_b;x_a,t_a)\psi(x_a,t_a) \tag{5}$$

$$\Rightarrow \quad G(x,t;x_0,0) = \sum_n \psi_n^*(x_0)\psi_n(x)e^{-iE_nt} \tag{6}$$

Relate Space-Time Paths to Ψ_0 (cont)

Hermitian $\tilde{H} \Rightarrow$ Complete Orthonormal Set

$$G(x, t; x_0, t=0) = \sum_n \psi_n^*(x_0)\psi_n(x)e^{-iE_n t} \tag{1}$$

- Evaluate @ imaginary t (Wick rotation):

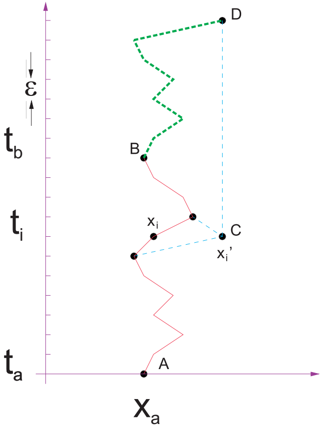
$$G(x, -i\tau; x_0, t=0) = \sum_n \psi_n^*(x_0)\psi_n(x)e^{-E_n \tau} \tag{2}$$

- Im time $\tau \to \infty$ only $n = 0$
- For $|\psi_0|^2$: paths start & end at $x_0 = x$

$$G(x, -i\tau; x, 0) = \sum_n |\psi_n(x)|^2 e^{-E_n\tau} = |\psi_0|^2 e^{-E_0\tau} + |\psi_1|^2 e^{-E_1\tau} + \cdots \tag{3}$$

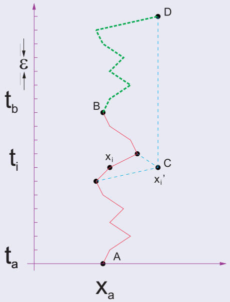
$$\Rightarrow \quad |\psi_0(x)|^2 = \lim_{\tau\to\infty} e^{E_0\tau} G(x, -i\tau; x, 0) \tag{4}$$

Break Now, Compute Later



Lattice Quantum Mechanics (Algorithm)

Easy: Discrete Times & Positions Only!



$$\frac{dx_j}{dt} \simeq \frac{x_j - x_{j-1}}{\varepsilon} \quad (1)$$

$$S_j \simeq L_j \, \Delta t \quad (2)$$

$$\simeq \frac{m\Delta x^2}{2\varepsilon} - V(x_j)\varepsilon \quad (3)$$

- Add actions for N-links
- $G(b, a) \leftrightarrow \sum_{\mathrm{a-b\ paths}}$
- Ea path $= \sum_{\mathrm{links}}$
- Path: $\sum$ links
- Euler + Time step ε:

$$G(b, a) = \int dx_1 \cdots dx_{N-1} \, e^{iS[b,a]} \quad (4)$$

Rotate t: Lagrangian $(-i\tau)$ $=$ -Hamiltonian (τ)

Wick Rotation into Imaginary Time

$$G(x, t; x_0, t_0) = \sum\!\!\!\!\!\!\int dx_1\, dx_2 \cdots dx_{N-1}\, e^{iS[x,x_0]} \tag{1}$$

$$S[x, x_0] \simeq \sum_{j=1}^{N-1} L\,(x_j, \dot{x}_j)\,\varepsilon \tag{2}$$

$$L\,(x, \dot{x}) = T - V(x) = +\frac{1}{2} m \left(\frac{dx}{dt}\right)^2 - V(x) \tag{3}$$

$$\Rightarrow L\left(x, \frac{dx}{-id\tau}\right) = -\frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2 - V(x) = -H \tag{4}$$

Put Pieces Together Sum Over Paths

Related to Wave Function

$$G(x, -i\tau; x_0, 0) = \int dx_1 \ldots dx_{N-1}\, e^{-\int_0^\tau H(\tau')d\tau'} \tag{5}$$

Individual path integral:

$$\int H(\tau)\, d\tau \simeq \sum_j \varepsilon E_j = \varepsilon \mathcal{E} \tag{6}$$

Ground State Wave Function via Feynman:

$$|\psi_0(x)|^2 = \frac{1}{Z} \lim_{\tau\to\infty} \int_{paths} dx_1 \cdots dx_{N-1}\, e^{-\varepsilon\mathcal{E}} \tag{7}$$

Imaginary Time Relates QM to Thermodynamics

Schrödinger Equation $\longrightarrow$ Heat Diffusion Equation

- t in QM $\longrightarrow$ $-i\tau$

$$i\frac{\partial\psi}{\partial(-i\tau)} = \frac{-\nabla^2}{2m}\psi \quad \Rightarrow \quad \frac{\partial\psi}{\partial\tau} = \frac{\nabla^2}{2m}\psi \tag{1}$$

- Boltzmann $\mathcal{P} = e^{-\varepsilon\mathcal{E}}$ weights ea Feynman path
- Temperature $\Leftrightarrow$ time step:

$$\mathcal{P} = e^{-\varepsilon\mathcal{E}} = e^{-\mathcal{E}/k_B T} \quad \Rightarrow \quad k_B T = \frac{1}{\varepsilon} \equiv \frac{\hbar}{\varepsilon} \tag{2}$$

- $\Rightarrow \lim_{\varepsilon\to 0} = \lim_{T\to\infty}$
- ψ_0: long imaginary τ *vs* $\hbar/\,\Delta E$
- *Like equilibration in Ising model*

Summary (This is Heavy Stuff)

Feynman's Path Integral Formulation of QM

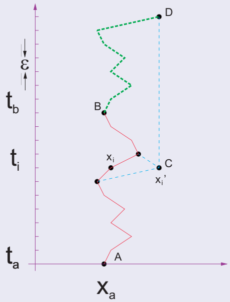
- QM ψ via statistical fluctuations $\sim$ class trajectory
- Propagator($t_a \to t_b$) G = path integral, $\sum_{\text{paths}} \int$
- Hamilton: extremum S $\to$ path integration of H
- Path integral = sum trajectories on x-t lattice
- Paths weighted with probability $e^{-iS/\hbar}$
- Algorithm: Δ path link $\Rightarrow \Delta E$ (like Ising)
- Ψ equilibrates to ground state

Break Before Algorithm

Quantum Monte Carlo (QMC) Applet Applet

A Time-Saving Trick

Compute $\psi(x)$ for All x (x_b) Simultaneously



- Integrate all x sites
- Don't compute $\delta(x)$!
- Accumulate $\psi(x')$

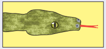
$$|\psi_0(x)|^2 = \int dx_1 \cdots dx_N \, e^{-\varepsilon \mathcal{E}(x, x_1, \ldots)}$$

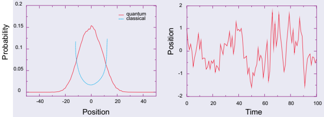
$$= \int dx_0 \cdots dx_N \delta(x - x_0) \, e^{-\varepsilon \mathcal{E}(\ldots)}$$

- Frequent x_j $\Rightarrow$ larger $\psi(x_j)$
- EG: AB, New path + C
- CBD same $\sum E_i$ as ACB
- Equilibrate, flip links, new E

Lattice Implementation

QMC.py





1. Harmonic oscillator

$$V(x) = \frac{1}{2}x^2$$

2. Natural units: $m = 1$,
   L: $\sqrt{\hbar/m\omega}$; t: $1/\omega$; $T = 2\pi$
3. Short $T \sim 2T$, Long $t \sim 20T$
4. Classical: max ρ @ turning pts
5. Each x_j, running sum $|\Psi_0(x_j)|^2$
6. Δ seed; many runs > 1 long run

Assessment and Exploration

1. Plot classical trajectory, some actual space-time paths
2. Explore effect of smaller Δx, smaller Δt
3. Assume $\psi(x) = \sqrt{\psi^2(x)}$, calculate:

$$E = \frac{\langle\psi|\, H \,|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\omega}{2\langle\psi|\psi\rangle} \int_{-\infty}^{+\infty} \psi^*(x) \left(\frac{-d^2}{dx^2} + x^2 \right) \psi(x)\, dx \qquad (1)$$

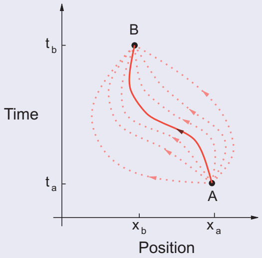
4. Explore effect of larger, smaller $\hbar$
5. Test ψ with quantum bouncer:

$$V(x) = mg|x| \qquad (2)$$

$$x(t) = x_0 + v_0 t + \frac{1}{2} g t^2. \qquad (3)$$

Summary

Feynman Path Integrals



- A different view of quantum mechanics
- It seems to give same answers as traditional QM
- Is at heart of lattice quantum chromodynamics
- Hard to apply beyond ground state
- Satisfying connection to classical mechanics