Feynman’s Quantum Paths
(Advanced ⇒ Relativity, Quantum Chromodynamics)

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Course: Computational Physics II
Feynman: Quantum Mech ↔ 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 $\delta$ 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

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

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

- F’s vision: \( \psi \leftrightarrow \text{path} \)
- \( \psi_B = \sum \text{all paths, A} \)
- \( \Delta \) paths \( \Delta \) probabilities
- All paths possible!
- Also relativity, fields

\( \sim \) Huygens’s principle

\( G(b; a) = \) spherical wavelet

\[ \psi(x_b, t_b) = \sum \text{wavelets} \]
Hamilton’s Principle of Least Action (Classical)

Newton’s Law ≡ \( \delta S[\bar{x}(t)] = 0 \)

"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."

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

(Constraint) \( \delta(x_a) = \delta(x_b) = 0 \) \( (2) \)

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

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

\[
L = \text{Lagrangian} = T [x, \dot{x}] - V[x] \quad (4)
\]
Connecting CM Hamilton’s Prin to QM Paths

Consider Free Particle \((V = 0)\)

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

\[
= \frac{m}{2} \dot{x}^2 (t_b - t_a) = \frac{m}{2} \frac{(x_b - x_a)^2}{t_b - t_a}
\]

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

- \(F: QM = \text{path integrals}\)
- All paths \(\exists, \Delta \text{ prob}\)
- Mainly classical

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

\[
\hbar \approx 10^{-34} \text{ Js} \quad \Rightarrow \sim \bar{x}
\]

\[
S_{\bar{x}} = \text{extremum}
\]
Relate Paths to Ground State Wave Function

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

\[ \tilde{H}\psi_n = E_n\psi_n \quad (1) \]

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

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

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

Recall: \[ \psi(x_b, t_b) = \int dx_a G(x_b, t_b; x_a, t_a)\psi(x_a, t_a) \quad (5) \]

\[ \Rightarrow G(x, t; x_0, 0) = \sum_n \psi_n^*(x_0)\psi_n(x)e^{-iE_nt} \quad (6) \]
Relate Space-Time Paths to $\Psi_0$ (cont)

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

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

- Evaluate @ imaginary t (Wick rotation):
  $$G(x, -i\tau; x_0, t = 0) = \sum_n \psi_n^*(x_0) \psi_n(x) e^{-E_n \tau} \quad (2)$$

- Im time $\tau \to \infty$ only $n = 0$

- For $|\psi_0|^2$: paths start & end at $x_0 = x$
  $$G(x, -i\tau; x, 0) = \sum_n |\psi_n(x)|^2 e^{-E_n \tau} = |\psi_0|^2 e^{-E_0 \tau} + |\psi_1|^2 e^{-E_1 \tau} + \cdots \quad (3)$$

  $\Rightarrow$  $$|\psi_0(x)|^2 = \lim_{\tau \to \infty} e^{E_0 \tau} G(x, -i\tau; x, 0) \quad (4)$$
Break Now, Compute Later
Lattice Quantum Mechanics (Algorithm)

Easy: Discrete Times & Positions Only!

Path: \[ \sum \text{links} \]

Euler + Time step \( \varepsilon \):

\[
\frac{dx_j}{dt} \approx \frac{x_j - x_{j-1}}{\varepsilon} \quad (1)
\]

\[
S_j \approx L_j \Delta t \quad (2)
\]

\[
\approx \frac{m\Delta x^2}{2\varepsilon} - V(x_j)\varepsilon \quad (3)
\]

- Add actions for \( N \)-links
- \( G(b, a) \leftrightarrow \sum_{a-b \text{ paths}} \)
- Ea path = \( \sum_{\text{links}} \)

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

\( \psi_0 \) Lattice \( t \to -i\tau \) Trick Implementation Assessment

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

**Wick Rotation into Imaginary Time**

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

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

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

\[
\Rightarrow L (x, \frac{dx}{-id\tau}) = - \frac{1}{2} m \left( \frac{dx}{d\tau} \right)^2 - V(x) = -H \tag{4}
\]
Put Pieces Together Sum Over Paths

Related to Wave Function

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

Individual path integral:

\[ \int H(\tau) d\tau \simeq \sum_j \epsilon E_j = \epsilon \mathcal{E} \]  

Ground State Wave Function via Feynman:

\[ |\psi_0(x)|^2 = \frac{1}{Z} \lim_{\tau \to \infty} \int_{\text{paths}} dx_1 \ldots dx_{N-1} e^{-\epsilon \mathcal{E}} \]
Imaginary Time Relates QM to Thermodynamics

Schrödinger Equation $\rightarrow$ Heat Diffusion Equation

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

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

- Boltzmann $\mathcal{P} = e^{-\varepsilon\mathcal{E}}$ weights ea Feynman path

- Temperature $\Leftrightarrow$ time step:

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

- $\Rightarrow \lim_{\varepsilon \to 0} = \lim_{T \to \infty}$

- $\psi_0$: long imaginary $\tau$ vs $\hbar/\Delta E$

- Like equilibration in Ising model
Feynman’s Path Integral Formulation of QM

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

Quantum Monte Carlo (QMC) Applet
A Time-Saving Trick

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

$$|\psi_0(x)|^2 = \int dx_1 \cdots dx_N e^{-\varepsilon E(x, x_1, \ldots)} = \int dx_0 \cdots dx_N \delta(x - x_0) e^{-\varepsilon E(\ldots)}$$

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

- Integrate all $x$ sites
- Don’t compute $\delta(x)$!
- Accumulate $\psi(x')$
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 \( \rho @ \) turning pts

5. Each \( x_j \), running sum \( |\psi_0(x_j)|^2 \)

6. \( \Delta \) seed; many runs > 1 long run
Assessment and Exploration

1. Plot classical trajectory, some actual space-time paths
2. Explore effect of smaller $\Delta x$, smaller $\Delta t$
3. Assume $\psi(x) = \sqrt{\psi^2(x)}$, calculate:
   \[
   E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\omega}{2 \langle \psi | \psi \rangle} \int_{-\infty}^{+\infty} \psi^*(x) \left( \frac{-d^2}{dx^2} + x^2 \right) \psi(x) \, dx
   \] (1)
4. Explore effect of larger, smaller $\hbar$
5. Test $\psi$ with quantum bouncer:
   \[
   V(x) = mg|x|
   \] (2)
   \[
   x(t) = x_0 + v_0 t + \frac{1}{2} gt^2.
   \] (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