

Cyman Path Integral

• Review of Classical Mechanics (work in 1D)

- Hamiltonian Formulation (familiar from Quantum)

- Start with a Hamiltonian function of x and p

+ Represents total energy $H(x, p) = K + V$

+ p is the "canonically conjugate momentum" to x

- Evolution determined by Hamilton's eqns

$$\dot{x} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial x}$$

+ In our example with $K = p^2/2m$

$$\dot{x} = p/m, \quad \dot{p} = -\partial V/\partial x \equiv \text{Newton's Laws}$$

+ Related to Ehrenfest's theorem in QM

- There is a known "quantization" procedure, though really one should derive classical from quantum.

- Lagrangian Formulation

- We have a Lagrangian $L(x, \dot{x}) = K - V$, $\dot{x} = dx/dt$

+ The integral of L over time is the action functional

$$S[x(t)] = \int_{t_i}^{t_f} dt L(x(t), \dot{x}(t))$$

+ The action is a function of the full path $x(t)$. So you tell me how the particle moves as a function of time, I give you a single number = the action S .

- Evolution determined by the "principle of least action"

$$\frac{\delta S}{\delta x(t)} = 0$$

+ Formally, say $\frac{\delta x(t')}{\delta x(t)} = \delta(t' - t)$, $\frac{\delta \dot{x}(t')}{\delta x(t)} = \frac{d}{dt} \delta(t' - t)$

Then do integrals

Example $L = \frac{1}{2}m\dot{x}^2 - V(x)$, $S = \int dt' L(x, \dot{x})$

$$\frac{\delta S}{\delta x(t)} = \int dt' \left(m\dot{x}(t') \frac{d}{dt'} \delta(t' - t) - \frac{dV}{dx}(x(t')) \delta(t' - t) \right)$$

$$= -m\ddot{x}(t) - \frac{dV}{dx}(x(t)) = 0 \quad \text{Makes sense!}$$

+ More informally, we can use $x + \delta x$ and write

$$S + \delta S = \int dt L(x + \delta x, \dot{x} + \delta \dot{x}) = \int dt L + \int dt \left(\frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right)$$

$$\Rightarrow \delta S = \int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x \Rightarrow \frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0$$

This is the same as above! Called Euler-Lagrange equations.

- + Note: We've swept some stuff about boundary conditions under the rug.
- We can also define a canonical momentum & relate L to H :

+ $P = \frac{\partial L}{\partial \dot{x}}$ much like $\dot{x} = \frac{\partial H}{\partial P}$

+ Then $H = p\dot{x} - L$ with \dot{x} written in terms of p

and $L = p\dot{x} - H$ with p written in terms of \dot{x}

+ These two approaches are equivalent & equivalent to Newton's laws.

A big advantage of Lagrangians is being able to change variables easily.
Also manifests symmetries (like Lorentz invariance) clearly.

QM in Lagrangian Form

- Look at time evolution

- $\langle \psi_f | e^{-iH(t_f - t_i)} | \psi_i \rangle$ = amplitude to start in state ψ_i at time t_i and evolve to $|\psi_f\rangle$ at time t_f .

+ We can insert dyads

$$\int dx_f \langle \psi_f | x_f \rangle \langle x_f | e^{-iH(t_f-t_i)/\hbar} | x_i \rangle \langle x_i | \psi_i \rangle$$

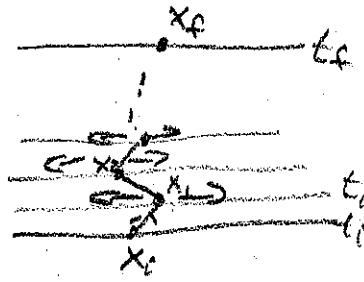
where $|x_{if}\rangle$ are position eigenstates

+ We might as well just look at matrix elements

$$M = \langle x_f | e^{-iH(t_f-t_i)/\hbar} | x_i \rangle$$

* Break up the interval t_i to t_f into N steps of δt each

+ Set $|x_f\rangle \equiv |x_{N+1}\rangle$, $|x_i\rangle \equiv |x_0\rangle$



+ Insert dyads $\int dx_n |x_n\rangle \langle x_n|$ at each timestep

$$M = \int_{t_i}^{t_f} dt \prod_{n=1}^N \int_{x_{n-1}}^{x_n} dx_n \langle x_{n+1} | e^{-iH\delta t/\hbar} | x_n \rangle$$

+ We start to see an "integral over all possible paths" emerging

* Now consider that $H = P^2/2m + V(x)$

+ We can write

$$e^{-iH\delta t/\hbar} = e^{-i(P^2/2m)\delta t/\hbar} e^{-iV(x)\delta t/\hbar} e^{O(\delta t^2)} \text{ [commutator stuff]}$$

+ As $\delta t \rightarrow 0$, we drop the $O(\delta t^2)$ terms

+ Now insert a momentum dyad at each timestep

$$\begin{aligned} \langle x_{n+1} | e^{-iH\delta t/\hbar} | x_n \rangle &= \int dp_n \langle x_{n+1} | p_n \rangle \langle p_n | e^{-i(P^2/2m)\delta t/\hbar} e^{-iV(x)\delta t/\hbar} | x_n \rangle \\ &= \int dp_n \left(\frac{1}{\sqrt{2\pi}} e^{ip_n x_{n+1}} \right) e^{-i(P^2/2m + V(x_n))\delta t/\hbar} \left(\frac{1}{\sqrt{2\pi}} e^{-ip_n x_n} \right) \end{aligned}$$

That replaces operators with eigenvalues and uses the momentum state wavefunction $\langle x | p \rangle$.

+ Putting it all together,

$$\mathcal{M} = \int \prod_{n=1}^N dx_n \left(\prod_{n=0}^N \frac{dp_n}{2\pi} \right) \exp \left[+i \frac{8t}{\hbar} \sum_{n=0}^{\infty} \left(p_n \dot{x}_n - \frac{p_n^2}{2m} - V(x_n) \right) \right]$$

where we used $p_n \dot{x}_{n+1} - p_{n+1} \dot{x}_n \approx -p_n \dot{x}_n \delta t$.

+ We can call this a phase-space path integral

$$\mathcal{M} = \int Dx Dp e^{iS[t](p \dot{x} - H)/\hbar}$$

• We would really like just to integrate over Dx .

+ Notice that the Dp integrals are all Gaussian of the form

$$\int_{-\infty}^{\infty} dy e^{-by^2 + ay} = \sqrt{\frac{\pi}{b}} e^{a^2/4b} \quad (\text{by completing squares})$$

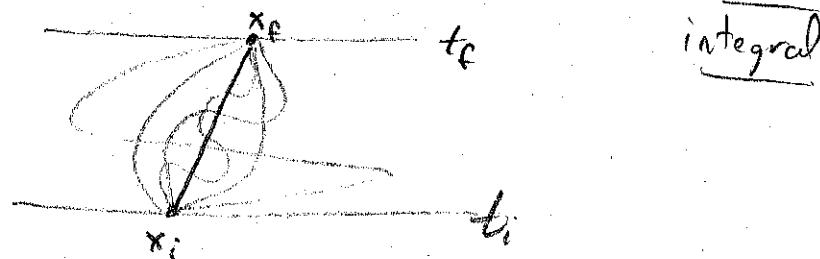
+ Therefore,

$$\begin{aligned} \langle x_{n+1} | e^{-iH\delta t/\hbar} | x_n \rangle &= \frac{1}{2\pi} e^{-iV(x_n)\delta t/\hbar} \int Dp e^{-i(P_n^2/2m - p_n \dot{x}_n)\delta t/\hbar} \\ &= \sqrt{\frac{m\hbar}{2\pi i \delta t}} e^{-i(\frac{m}{2}\dot{x}_n^2 - V(x_n))\delta t/\hbar} \end{aligned}$$

+ The whole thing is now

$$\begin{aligned} \mathcal{M} &= \lim_{N \rightarrow \infty} \sqrt{\frac{m\hbar}{2\pi i \delta t}} \int \prod_{n=1}^N \left(\sqrt{\frac{m\hbar}{2\pi i \delta t}} dx_n \right) \exp \left[i \frac{8t}{\hbar} \sum_i \left(\frac{m}{2} \dot{x}_n^2 - V(x_n) \right) \right] \\ &\equiv \int Dx e^{iS[x]/\hbar} \quad \text{We'll ignore normalization concerns.} \end{aligned}$$

• Heuristically, this is integrating over all possible paths between x_i at t_i and x_f at t_f . Feynman Path Integral or functional



Properties

- Really crazy mathematically: normalization is always divergent, but fortunately we can usually divide that out
- The variables in a path integral are variables, not operators
- Classical physics shows up cleanly.
 - + If S varies quickly, oscillating integrand cancels out
 - + Need $\delta S/\delta x(t) = 0$ to avoid that if S/\hbar large
That means classical physics dominates = saddle point approx.

Uses of Path Integrals: You can calculate energy eigenvalues, but better for:

- Correlation Functions

- Haven't really talked about this, but we often want to look at expectation values of operators at different times
 - + Like $\langle x(t_2)x(t_1) \rangle$ \rightsquigarrow Need to keep track of time ordering
 $= \langle x e^{-iH(t_2-t_1)/\hbar} x \rangle$ etc.
 - + These tell you the response of one measurement to any earlier one (done in a different location)
 - + Common in field theories, including material/condensed matter physics
 $\underline{\text{ex}}$ measure current at 2 different places

- These can be messy in Hamiltonian form. + As a path integral

$$\langle x(t_2)x(t_1) \rangle = \int dx x(t_2)x(t_1) e^{iS[x]}$$

- + There are nice tricks to simplify this integral, which really shine for harmonic oscillators + similar

- Semi-classical calculations of tunneling

Since it calculates a probability amplitude of going from x_i to x_f , we can really look at decay rate in potentials like

- Connection to Statistical Mechanics

* In stat mech, we study the partition function $Z = \sum_n e^{-\beta E_n}$

+ In QM, write this as $Z = \sum_i \langle E_n | e^{-\beta H} | E_n \rangle$

+ If we insert position dyads

$$Z = \sum_i \int dx_i \int dx_f \langle E_n | x_0 \rangle \langle x_f | e^{-\beta H} | x_i \rangle \langle x_i | E_n \rangle$$

+ $\int dx$

$$\int dx_i \int dx_f \sum_n \langle x_i | E_n \rangle \langle E_n | x_f \rangle = \int dx_i \int dx_f \delta(x_i - x_f) = \int dx$$

so $Z = \int dx \langle x | e^{-\beta H} | x \rangle$

* That form looks like $\langle x_f | e^{-iHT/\hbar} | x_i \rangle \underset{\text{except}}{\approx} \int_{x(0)=x_i}^{x(T)=x_f} \mathcal{D}x e^{iS[x]/\hbar}$

1) $T = -i\beta\hbar$ 2) Paths are periodic $x(0) = x(\beta\hbar) \forall$ period $\beta\hbar$

+ Define $T = i\beta\hbar$, $t \in [-iT, t]$; t = "Euclidean time" b/c acts like space

$$\begin{aligned} + \text{ Then } S &= \int_0^T \left(\frac{1}{2m}\dot{x}^2 - V(x) \right) = -i \int_0^{\beta\hbar} \left(-\frac{1}{2m} \left(\frac{dx}{dt} \right)^2 - V(x) \right) \\ &= i \int_0^{\beta\hbar} \left(\frac{1}{2m} \left(\frac{dx}{dt} \right)^2 + V(x) \right) \end{aligned}$$

+ The partition function is the Euclidean path integral

$$Z = \int_{\text{periodic}} \mathcal{D}x e^{-S_E/\hbar} \quad \text{over periodic paths}$$

- Technically a little prettier in quantum field theories / particle physics
(though there are aficionados of Hamiltonians, as well)