Advanced Quantum Mechanics

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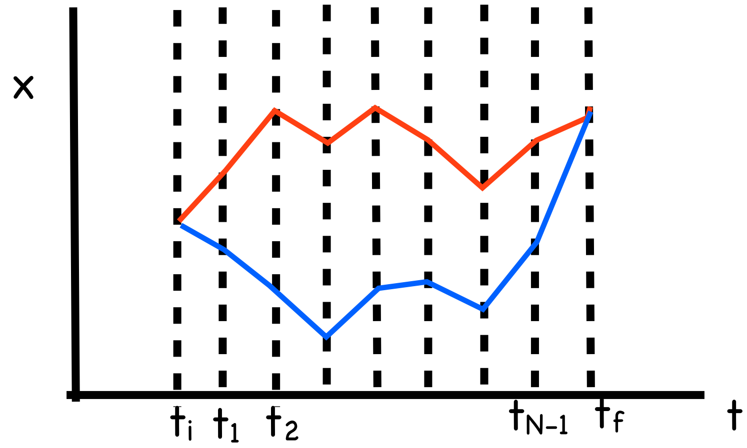
Lecture #20

Path Integrals and QM

Recap of Last Class

Path Integral Formulation of QM

For a particle moving in a potential:



The prob. amplitude of a particle traveling from x_i to x_f through any path is equal in magnitude and has a phase proportional to the classical action along the path.

$$U(x_f, t_f; x_i, t_i) = \left(\frac{mN}{2\pi i(t_f - t_i)}\right)^{1/2} \int \mathcal{D}[x(t)] e^{iS[x(t)]}$$

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2} m\dot{x}^2(t) - V(x(t))\right] = \int_{t_i}^{t_f} dt \mathcal{L}[x(t), \dot{x}(t)]$$

To calculate the amplitude of the particle traveling from x_i to x_f, we must sum over the amplitude contribution from all paths.

- If additional information about intermediate states of the system is available (say through measurements at intermediate times), the routes have to be restricted accordingly. E.g. if it is known through measurement that the particle is at x_k at intermediate time t_k, one should sum up prob. ampl. contributions from only those paths which pass through (x_k, t_k)

Quadratic Lagrangians and classical paths

In general, the matrix element of the time evolution operator is given by

$$U(x_f, t_f; x_i, t_i) = A(t_f, t_i) \int \mathcal{D}[x(t)] e^{iS[x(t)]}$$

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2} m \dot{x}^2(t) - V(x(t)) \right] = \int_{t_i}^{t_f} dt \mathcal{L}[x(t), \dot{x}(t)]$$

Let us simplify to the case where V is at most a quadratic function of x.

$$V(x) = V_1 x + V_2 x^2$$

The Lagrangian then is a quadratic function of positions as well as velocities

Let us relabel all trajectories by $x(t) = x_{cl}(t) + y(t) \qquad \dot{x}(t) = \dot{x}_{cl}(t) + \dot{y}(t)$

where the classical trajectory follows the Euler Lagrange equations $\left[\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} \right] \Bigg|_{x_{cl}(t)} = 0$

Since the endpoints of the trajectory are fixed, i.e. $x(t_i)=x_{cl}(t_i)$ and $x(t_f)=x_{cl}(t_f)$ the boundaries for y are given by $y(t_i)=y(t_f)=0$. i.e the boundary cond. for y is independent of the classical trajectory.

The action is given by:

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2} m (\dot{x}_{cl} + \dot{y})^2 - V_1 (x_{cl} + y) - V_2 (x_{cl} + y)^2 \right]$$

Quadratic Lagrangians and classical paths

$$V(x) = V_1 x + V_2 x^2$$

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2}m(\dot{x}_{cl}+\dot{y})^2 - V_1(x_{cl}+y) - V_2(x_{cl}+y)^2\right]$$

$$= \int_{t_i}^{t_f} dt \left[\frac{1}{2}m(\dot{x}_{cl}^2+\dot{y}^2+2\dot{x}_{cl}\dot{y}) - V_1(x_{cl}+y) - V_2(x_{cl}^2+2x_{cl}y++y^2)\right]$$

$$= S[x_{cl}(t)] + \underbrace{\int_{t_i}^{t_f} dt\,[m\dot{x}_{cl}\dot{y} - 2V_2 x_{cl} y]}_{\text{indep of } x_{cl} \text{ by Euler Lagrange}} + \int_{t_i}^{t_f} dt\left[\frac{1}{2}m\dot{y}^2 - V_1 y - V_2 y^2\right]$$

$$= \underbrace{m\dot{x}_{cl}y\big|_{t_i}^{t_f}}_{=0,\text{ as } y=0 \text{ at endpoints}} - \int_{t_i}^{t_f} dt\,[m\ddot{x}_{cl} + 2V_2 x_{cl}]\,y$$

Euler Lagrange Equation:

$$m\ddot{x}_{cl} + 2V_2 x_{cl} + V_1 = 0$$

$$= \int_{t_i}^{t_f} dt V_1 y$$

$$= \underbrace{S[x_{cl}(t)]}_{\text{where}} + \int_{t_i}^{t_f} dt\left[\frac{1}{2}m\dot{y}^2 - V_2 y^2\right]$$

$$\boxed{S[x_{cl}(t)] = \int_{t_i}^{t_f} dt\left[\frac{1}{2}m\dot{x}_{cl}^2 - V_1 x_{cl} - V_2 x_{cl}^2\right]}$$

The action separates into a classical part and a quantum fluctuation part, which is independent of the classical trajectory

Quadratic Lagrangians and classical paths

$$U(x_f,t_f;x_i,t_i) = e^{iS_{cl}(x_i,t_i;x_f,t_f)} A(t_f,t_i) \underbrace{\int_{y(t_i)=y(t_f)=0} \mathcal{D}[y(t)] e^{i\int_{t_i}^{t_f} \frac{1}{2}m\dot{y}^2 - V_2 y^2}}$$

Normalization,
indep. of x_i and x_f

Sum over trajectories starting and ending at origin, indep. of x_i and x_f

$$= e^{iS_{cl}(x_i,t_i;x_f,t_f)} A^{'}(t_f,t_i)$$

The propagator for a system with a quadratic Lagrangian is (upto an x-indep normalization factor) is a pure phase, with the phase given by the classical action of the system.

Example: Free Particle $V_1=0$, $V_2=0$

$$x_{cl}(t) = x_i + \frac{(x_f - x_i)}{(t_f - t_i)}(t - t_i) \qquad \dot{x}_{cl}(t) = \frac{(x_f - x_i)}{(t_f - t_i)}$$

$$S[x_{cl}(t)] = \frac{1}{2}m\frac{(x_f - x_i)^2}{t_f - t_i}$$

$$U(x_f,t_f;x_i,t_i) = A^{'}(t_f,t_i) e^{\frac{im}{2}\frac{(x_f - x_i)^2}{t_f - t_i}}$$

Quadratic Lagrangians and classical paths

Example: Harmonic Oscillator $V_1=0$

$$\mathcal{L} = \frac{m}{2}\dot{x}^2 - \frac{m}{2}\omega_0^2 x^2$$

Classical EOM: $\ddot{x} + \omega_0^2 x = 0$ $\qquad \omega_0 = \sqrt{\frac{2V_2}{m}}$

$x_{cl}(t) = A\cos\omega_0 t + B\sin\omega_0 t$ with boundary condition

$$x_i = A\cos\omega_0 t_i + B\sin\omega_0 t_i$$
$$x_f = A\cos\omega_0 t_f + B\sin\omega_0 t_f$$

$$x_{cl}(t) = \frac{x_i\sin[\omega_0(t_f-t)] + x_f\sin[\omega_0(t-t_i)]}{\sin[\omega_0(t_f-t_i)]} \qquad \dot{x}_{cl}(t) = \omega_0\frac{x_f\cos[\omega_0(t-t_i)] - x_i\cos[\omega_0(t_f-t)]}{\sin[\omega_0(t_f-t_i)]}$$

for $t_f - t_i \neq \pi/\omega_0$

$$S[x_{cl}(t)] = \frac{m}{2}\int_{t_i}^{t_f} dt[\dot{x}_{cl}^2 - \omega_0^2 x_{cl}^2] = \frac{m}{2}x_{cl}(t)\dot{x}_{cl}(t)\Big|_{t_i}^{t_f} - \frac{m}{2}\int_{t_i}^{t_f} dt x_{cl}\underbrace{[\ddot{x}_{cl} + \omega_0^2 x_{cl}]}_{\text{0 by classical EOM}}$$

$$= \frac{m}{2}[x_{cl}(t_f)\dot{x}_{cl}(t_f) - x_{cl}(t_i)\dot{x}_{cl}(t_i)]$$

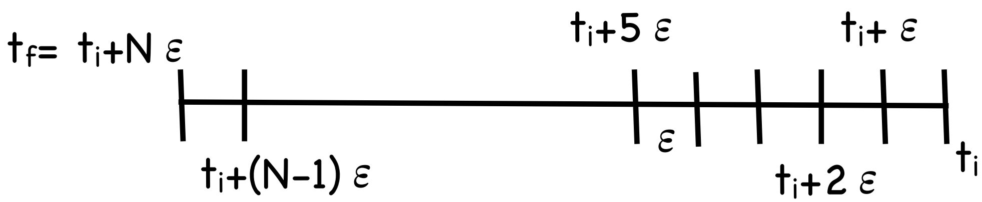
$$= \frac{m\omega_0}{2\sin[\omega_0(t_f-t_i)]}[(x_f^2 + x_i^2)\cos[\omega_0(t_f-t_1)] - 2x_i x_f]$$

Quadratic Lagrangians and Quantum Fluctuations

We have shown that for quadratic Lagrangians $\quad U(x_f,t_f;x_i,t_i) = e^{iS_{cl}(x_f,t_f;x_i,t_i)}A^{'}(t_f,t_i)$

General form for the factor A′ $\quad A^{'}(t_f,t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\int_{y(t_i)=y(t_f)=0}\mathcal{D}[y(t)]e^{i\int_{t_i}^{t_f} dt\,\frac{m}{2}[\dot{y}^2-\omega_0^2y^2]}$

Let us go back to the picture of time slices

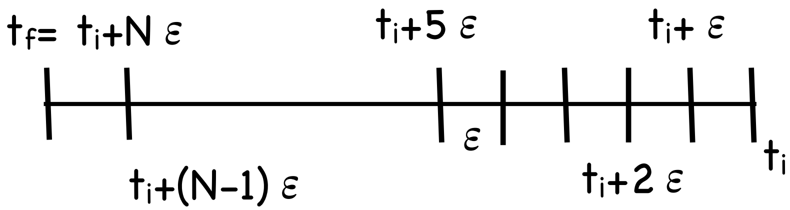


$$A^{'}(t_f,t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2}\int dy_1\int dy_2..\int dy_{N-1}e^{i\epsilon\sum_k \frac{m}{2}\left[\frac{(y_{k+1}-y_k)^2}{\epsilon^2}-\omega_0^2y_k^2\right]}$$

The time slicing is like a lattice in along the time axis with spacing ε. We will work with this lattice version of the problem and take the $\varepsilon \to 0$ limit (continuum limit) at the end

Quadratic Lagrangians and Quantum Fluctuations

$$A'(t_f,t_i)=\left(\frac{m}{2\pi i\epsilon}\right)^{N/2}\int dy_1\int dy_2..\int dy_{N-1}e^{i\epsilon\sum_k \frac{m}{2}\left[\frac{(y_{k+1}-y_k)^2}{\epsilon^2}-\omega_0^2y_k^2\right]}$$



Lattice derivatives: $\nabla y_n=\frac{1}{\epsilon}[y_{n+1}-y_n]$ $\quad\bar\nabla y_n=\frac{1}{\epsilon}[y_n-y_{n-1}]$

$$\sum_{k=0}^{N}(\nabla y_k)^2=\underbrace{y_k\nabla y_k|_{k=0}^{k=N}}_{\text{0 by b.c.}}-\sum_{k=1}^{N}y_k\bar\nabla\nabla y_k=-\sum_{k=1}^{N}y_k\bar\nabla\nabla y_k$$

$$A'(t_f,t_i)=\left(\frac{m}{2\pi i\epsilon}\right)^{N/2}\int dy_1\int dy_2..\int dy_{N-1}e^{-i\epsilon\sum_k \frac{m}{2}y_k\left[(\bar\nabla\nabla)_{kk'}+\omega_0^2\delta_{kk'}\right]y_{k'}}$$

$$A'(t_f,t_i)=\left(\frac{m}{2\pi i\epsilon}\right)^{N/2}\left(\frac{2\pi i}{m\epsilon}\right)^{(N-1)/2}\left(Det\left[(\bar\nabla\nabla)_{kk'}+\omega_0^2\delta_{kk'}\right]\right)^{-1/2}$$

Quadratic Lagrangians and Quantum Fluctuations

$$A'(t_f, t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2} \left(\frac{2\pi i}{m\epsilon}\right)^{(N-1)/2} \left(Det\left[(\bar{\nabla}\nabla)_{kk'} + \omega_0^2 \delta_{kk'}\right]\right)^{-1/2}$$

Free Particle:

$$\bar{\nabla}\nabla y_n = \frac{1}{\epsilon}\bar{\nabla}[y_{n+1} - y_n] = \frac{1}{\epsilon^2}[y_{n+1} - y_n - y_n + y_{n-1}]$$

$$\bar{\nabla}\nabla = \frac{1}{\epsilon^2}\begin{pmatrix} -2 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ . & & & & & & . \\ . & & & & & & . \\ . & & & & & & . \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & -2 \end{pmatrix}$$

To Find the Determinant:

$$Det_{N=1}[-\epsilon^2\bar{\nabla}\nabla] = 2$$

$$Det_{N=2}[-\epsilon^2\bar{\nabla}\nabla] = \begin{vmatrix} 2 & -1 \\ -1 & 2 \end{vmatrix} = 3$$

Recursion Relation:

$$Det_n[-\epsilon^2\bar{\nabla}\nabla] = 2Det_{n-1}[-\epsilon^2\bar{\nabla}\nabla] - Det_{n-2}[-\epsilon^2\bar{\nabla}\nabla]$$

$$Det_n[-\epsilon^2\bar{\nabla}\nabla] = n + 1 \qquad Det_{N-1}[\bar{\nabla}\nabla] = \left(\frac{-1}{\epsilon^2}\right)^{N-1} N$$

$$A'(t_f, t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2} \left(\frac{2\pi i}{m\epsilon}\right)^{(N-1)/2} (\epsilon^2)^{(N-1)/2} \frac{1}{N^{1/2}} = \left(\frac{m}{2\pi i\epsilon N}\right)^{1/2} = \left(\frac{m}{2\pi i(t_f - t_i)}\right)^{1/2}$$

$$\boxed{U(x_f, t_f; x_i, t_i) = \left(\frac{m}{2\pi i(t_f - t_i)}\right)^{1/2} e^{i\frac{m}{2}\frac{(x_f - x_i)^2}{(t_f - t_i)}}}$$

Quadratic Lagrangians and Quantum Fluctuations

Alternative: work in Fourier space $A'(t_f, t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2} \int dy_1 \int dy_2 .. \int dy_{N-1} e^{i\epsilon \sum_k \frac{m}{2}\left[\frac{(y_{k+1}-y_k)^2}{\epsilon^2} - \omega_0^2 y_k^2\right]}$

Since $y(t_i)=y(t_f)=0$, it can be expanded in a discrete sine series

$$y_n = y(t_n) = \sum_{l=1}^{N-1} \sqrt{\frac{2}{N}} y(\omega_l) \sin[\omega_l(t_n - t_i)] \qquad \omega_l = \frac{2\pi l}{N(t_f - t_i)} \qquad l = 1, 2, ...N-1$$

Complete orthonormal basis sets for expansion

$$\frac{2}{N}\sum_{n=1}^{N-1} \sin[\omega_l(t_n - t_i)] \sin[\omega_{l'}(t_n - t_i)] = \delta_{ll'} \qquad \frac{2}{N}\sum_{l=1}^{N-1} \sin[\omega_l(t_n - t_i)] \sin[\omega_l(t_{n'} - t_i)] = \delta_{nn'}$$

Jacobian for the transformation is 1

$$-\frac{m}{2}\epsilon \sum_n y_n \bar{\nabla}\nabla y_n = -\frac{m}{2\epsilon}\sum_n y_n[y_{n+1} - 2y_n + y_{n-1}]$$

$$-\frac{m}{2\epsilon}\frac{2}{N}\sum_{ll'} y(\omega_l) y(\omega_{l'}) \sum_n \sin[\omega_{l'}(t_n - t_i)](\sin[\omega_l(t_n - t_i + \epsilon)] - 2\sin[\omega_l(t_n - t_i)] + \sin[\omega_l(t_n - t_i - \epsilon)])$$

$$= \frac{m}{2\epsilon}\frac{2}{N}\sum_{ll'} y(\omega_l) y(\omega_{l'}) \sum_n \sin[\omega_{l'}(t_n - t_i)](2\sin[\omega_l(t_n - t_i)] - \sin[\omega_l(t_n - t_i + \epsilon)] - \sin[\omega_l(t_n - t_i - \epsilon)])$$

$$= \frac{m}{\epsilon}\frac{2}{N}\sum_{ll'} y(\omega_l) y(\omega_{l'}) \sum_n \sin[\omega_{l'}(t_n - t_i)] \sin[\omega_l(t_n - t_i)](1 - \cos[\omega_l \epsilon]) = \frac{m}{\epsilon}\sum_l y(\omega_l) y(\omega_l)(1 - \cos[\omega_l \epsilon])$$

Quadratic Lagrangians and Quantum Fluctuations

$$A^{'}(t_f,t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2} \int dy(\omega_1) \int dy(\omega_2) .. \int dy(\omega_{N-1}) e^{i\frac{m}{2\epsilon}\sum_l y(\omega_l)y(\omega_l)(2-2\cos[\omega_l\epsilon])}$$

$$= \left(\frac{m}{2\pi i\epsilon}\right)^{N/2} \left(\frac{2\pi i\epsilon}{m}\right)^{(N-1)/2} \left(\prod_{l=1}^{(N-1)} (2-2\cos[\omega_l\epsilon])\right)^{-1/2}$$

$$= \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \left(\prod_{l=1}^{(N-1)} (2-2\cos[\omega_l\epsilon])\right)^{-1/2} = \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \left(\prod_{l=1}^{(N-1)} (2-2\cos\left[\frac{\pi l}{N}\right])\right)^{-1/2}$$

Use $\prod_{l=1}^{(N-1)} (1+x^2-2x\cos\left[\frac{\pi l}{N}\right]) = \frac{x^{2N}-1}{x^2-1}$ with x ⟶ 1 to get $\left(\prod_{l=1}^{(N-1)} (2-2\cos\left[\frac{\pi l}{N}\right])\right)^{-1/2} = \frac{1}{\sqrt{N}}$

Recover for the free particle:

$$\boxed{U(x_f,t_f;x_i,t_i) = \left(\frac{m}{2\pi i(t_f-t_i)}\right)^{1/2} e^{i\frac{m}{2}\frac{(x_f-x_i)^2}{(t_f-t_i)}}}$$

Quadratic Lagrangians and Quantum Fluctuations

Harmonic Oscillator:

Work in Fourier space: $$A^{'}(t_f,t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2}\int dy_1\int dy_2..\int dy_{N-1}e^{i\epsilon\sum_k \frac{m}{2}\left[\frac{(y_{k+1}-y_k)^2}{\epsilon^2}-\omega_0^2 y_k^2\right]}$$

For free particle: $$A^{'}(t_f,t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2}\int dy(\omega_1)\int dy(\omega_2)..\int dy(\omega_{N-1})e^{i\frac{m}{2\epsilon}\sum_l y(\omega_l)y(\omega_l)(2-2\cos[\omega_l\epsilon])}$$

For SHO:

$$A^{'}(t_f,t_i) = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2}\int dy(\omega_1)\int dy(\omega_2)..\int dy(\omega_{N-1})e^{i\frac{m}{2\epsilon}\sum_l y(\omega_l)y(\omega_l)(2-2\cos[\omega_l\epsilon]-\epsilon^2\omega_0^2)}$$

$$= \left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\left(\prod_{l=1}^{(N-1)}(2-2\cos\left[\frac{\pi l}{N}\right]-\epsilon^2\omega_0^2)\right)^{-1/2}$$

$$= A^{\prime}_{fp}(t_f,t_i)\left(\frac{\left(\prod_{l=1}^{(N-1)}(2-2\cos\left[\frac{\pi l}{N}\right]-\epsilon^2\omega_0^2)\right)}{\left(\prod_{l=1}^{(N-1)}(2-2\cos\left[\frac{\pi l}{N}\right])\right)}\right)^{-1/2}$$

Quadratic Lagrangians and Quantum Fluctuations

Harmonic Oscillator:

$$A'(t_f,t_i) = A'_{fp}(t_f,t_i)\left(\frac{\left(\prod_{l=1}^{(N-1)}(2-2\cos\left[\frac{\pi l}{N}\right]-\epsilon^2\omega_0^2)\right)}{\left(\prod_{l=1}^{(N-1)}(2-2\cos\left[\frac{\pi l}{N}\right])\right)}\right)^{-1/2} \qquad \sin[x/2]=\epsilon\omega_0/2$$

$$\frac{\left(\prod_{l=1}^{(N-1)}(2-2\cos\left[\frac{\pi l}{N}\right]-\epsilon^2\omega_0^2)\right)}{\left(\prod_{l=1}^{(N-1)}(2-2\cos\left[\frac{\pi l}{N}\right])\right)} = \prod_{l=1}^{(N-1)}\left(1-\frac{\sin^2\left[\frac{x}{2}\right]}{\sin^2\left[\frac{\pi l}{2N}\right]}\right)$$

$$\prod_{l=1}^{(N-1)}\left(1-\frac{\sin^2\left[\frac{x}{2}\right]}{\sin^2\left[\frac{\pi l}{2N}\right]}\right) = \frac{\sin[2Nx]}{N\sin[2x]}$$

Define: $x=\epsilon\bar{\omega}/2$

$\bar{\omega}\to\omega_0 \quad as \quad \epsilon\to 0$

Then as $\epsilon\to 0 \quad \prod_{l=1}^{(N-1)}\left(1-\frac{\sin^2\left[\frac{x}{2}\right]}{\sin^2\left[\frac{\pi l}{2N}\right]}\right) = \frac{\sin[\omega_0(t_f-t_i)]}{\omega_0(t_f-t_i)}$

$$A'(t_f,t_i) = A'_{fp}(t_f,t_i)\left(\frac{\omega_0(t_f-t_i)}{\sin[\omega_0(t_f-t_i)]}\right)^{1/2} = \left(\frac{m\omega_0}{2\pi i\sin[\omega_0(t_f-t_i)]}\right)^{1/2}$$

Finally, collecting everything together:

$$\boxed{U(x_f,t_f;x_i,t_i) = \left(\frac{m\omega_0}{2\pi i\sin[\omega_0(t_f-t_i)]}\right)^{1/2} e^{i\frac{m\omega_0}{2\sin[\omega_0(t_f-t_i)]}[(x_f^2+x_i^2)\cos\omega_0(t_f-t_i)-2x_ix_f]}}$$

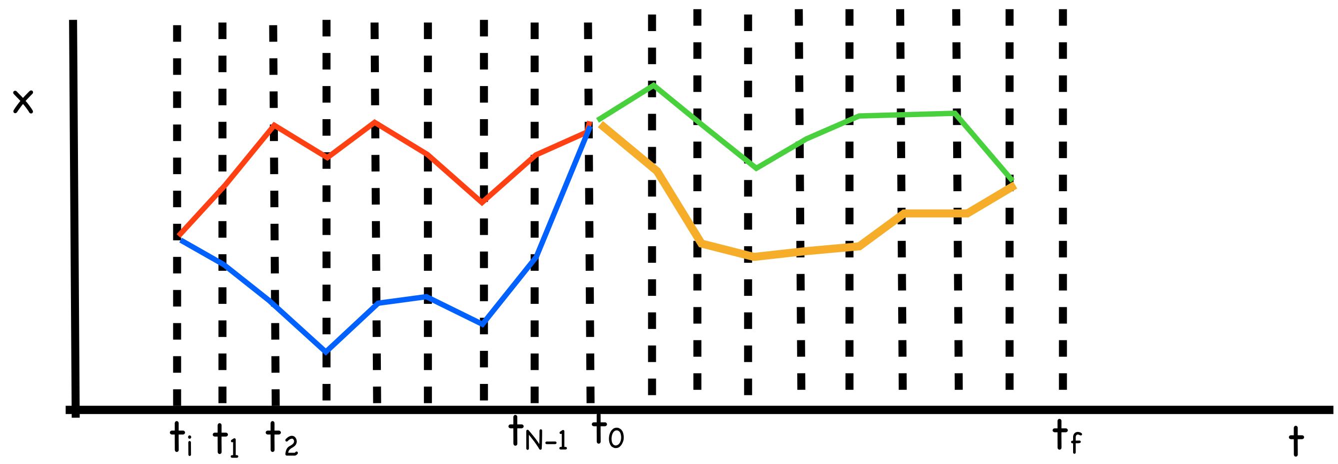
Matrix Elements of Operators

In QM, we are interested in evaluating matrix elements of various operators between different states. How does that work out in path integral language?

$$\langle x_f, t_f|\hat{x}(t_0)|x_i, t_i\rangle = \int dx(t_0)\langle x_f, t_f|x(t_0), t_0\rangle x(t_0)\langle x(t_0), t_0|x_i, t_i\rangle$$

$$= \underbrace{\int dx_0}_{\text{Integral over } x_0} \underbrace{\int_{x(t_0)=x_0}^{x(t_f)=x_f} D[x(t)]e^{i\int_{t_0}^{t_f}\mathcal{L}[x(t)]}}_{\text{Integral over paths going through } (x_f,t_f) \text{ and } (x_0,t_0)} x_0 \underbrace{\int_{x(t_i)=x_i}^{x(t_0)=x_0} D[x(t)]e^{i\int_{t_i}^{t_0}\mathcal{L}[x(t)]}}_{\text{Integral over paths going through } (x_0,t_0) \text{ and } (x_i,t_i)}$$

So, we are integrating over all paths starting at (x_i,t_i) and ending at (x_f,t_f)



$$= \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)]x(t_0)e^{i\int_{t_i}^{t_f}\mathcal{L}[x(t)]}$$

Matrix Elements of Operators

Alternative treatment with source terms

Define a new action in presence of source terms

$$S[x(t), J(t)] = \int_{t_i}^{t_f} dt\mathcal{L}[x(t)] - iJ(t)x(t)$$

J(t) is for now an arbitrary function

Write down a new path-integral in terms of this action

$$U_J(x_f, t_f; x_i, t_i) = \int \mathcal{D}[x(t)]e^{iS[x(t),J(t)]}$$

Then $$\langle x_f, t_f|\hat{x}(t_0)|x_i, t_i\rangle = \left.\frac{\partial U_J(x_f, t_f; x_i, t_i)}{\partial J(t_0)}\right|_{J(t)=0}$$

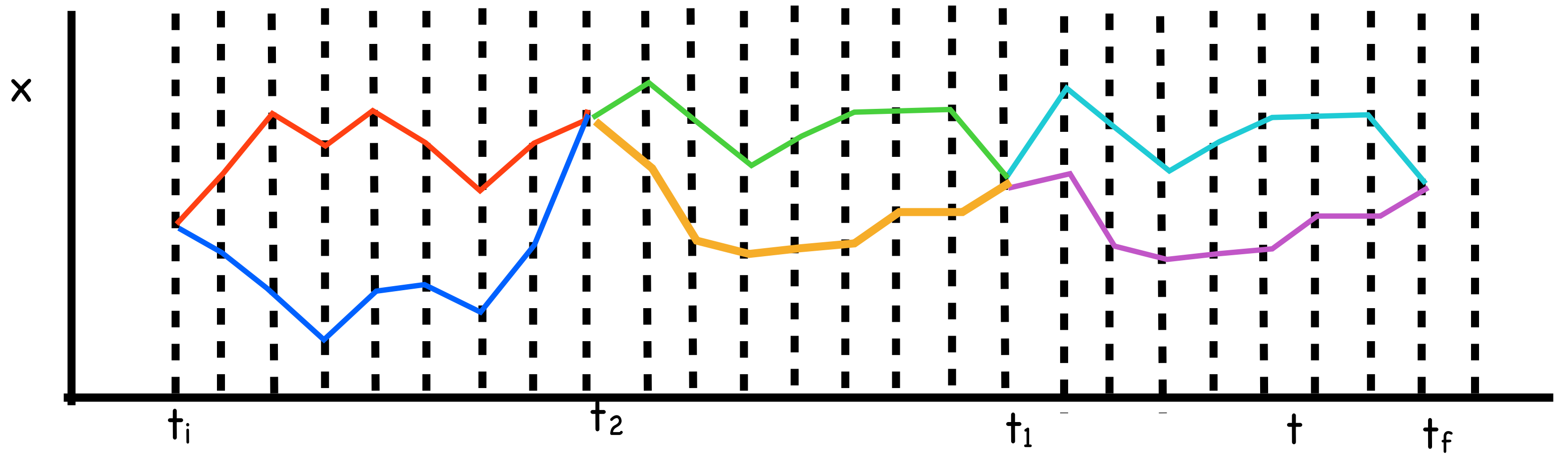
$$= \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)]x(t_0)e^{i\int_{t_i}^{t_f} \mathcal{L}[x(t)]}$$

Matrix Elements of Operators

Let us consider $\langle x_f, t_f | \hat{x}(t_1)\hat{x}(t_2) | x_i, t_i \rangle$

If $t_1 > t_2$, i.e the operator is time ordered

$$\langle x_f, t_f | \hat{x}(t_1)\hat{x}(t_2) | x_i, t_i \rangle = \int dx_1 dx_2 \langle x_f, t_f | x_1, t_1 \rangle x_1 \langle x_1, t_1 | x_2, t_2 \rangle x_2 \langle x_2, t_2 | x_i, t_i \rangle$$



$$\langle x_f, t_f | \hat{x}(t_1)\hat{x}(t_2) | x_i, t_i \rangle = \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x(t)] x(t_1) x(t_2) e^{i \int_{t_i}^{t_f} \mathcal{L}[x(t)]}$$

Alternatively $\langle x_f, t_f | \hat{x}(t_1)\hat{x}(t_2) | x_i, t_i \rangle = \left. \dfrac{\partial^2 U_J(x_f, t_f; x_i, t_i)}{\partial J(t_1) \partial J(t_2)} \right|_{J(t)=0}$

More generally $\langle x_f, t_f | \hat{x}(t_1)\hat{x}(t_2)..\hat{x}(t_n) | x_i, t_i \rangle = \left. \dfrac{\partial^n U_j}{\partial J(t_1) \partial J(t_2) ... \partial J(t_n)} \right|_{J(t)=0}$

Note: Operators should be time ordered

Variation wrt Paths (Endpoints fixed)

In CM, path of extremum action gives Euler Lagrange eqn.s What do we get here?

$x(t) \longrightarrow x(t) + \delta x(t)$, with $x(t_i)$ and $x(t_f)$ fixed

Reparametrization of paths does not change path integral

$$\int \mathcal{D}[x(t)] e^{iS[x(t)+\delta x(t)]/\hbar} - \int \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar} = \frac{i}{\hbar} \int \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar} \delta S = 0$$

From CM

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

$$= \left(\frac{\partial L}{\partial \dot{x}} \right) \delta x(t) \Big|_{t_i}^{t_f} + \int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t)$$

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

Variation wrt Paths (Endpoints fixed)

So $$\int \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar} \int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t) = 0$$

Since δ x(t) is arbitrary, the integrand (with the path integ.) is zero for each t

$$\int \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar} \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) = 0$$

Euler Lagrange Equation is satisfied as expectation value —— Ehrenfest Theorem

Variation wrt paths (End point variation)

Let us do the same exercise, but allow variation of the final point

$$U(x_f + \delta x_f, t_f; x_i, t_i) - U(x_f, t_f; x_i, t_i) = \frac{\partial U}{\partial x_f} \delta x_f$$

$$= \frac{i}{\hbar} \int \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar} \delta S$$

Now $$\delta S = \left(\frac{\partial L}{\partial \dot{x}} \right) \delta x(t) \Big|_{t_i}^{t_f} + \int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t)$$

Since we allow variation of end location, $\delta x(t_f) \neq 0$, and the boundary term contributes

$$\frac{\partial U}{\partial x_f} \delta x_f = \frac{i}{\hbar} \int \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar} \left[\left(\frac{\partial L}{\partial \dot{x}} \right) \delta x_f + \underline{\int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t)} \right]$$

0 by Ehrenfest Theorem

$$\frac{\partial U}{\partial x_f} = \frac{i}{\hbar} \int \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar} p(t_f) \qquad p \rightarrow \frac{\hbar}{i} \nabla$$

Variation wrt paths (End point variation)

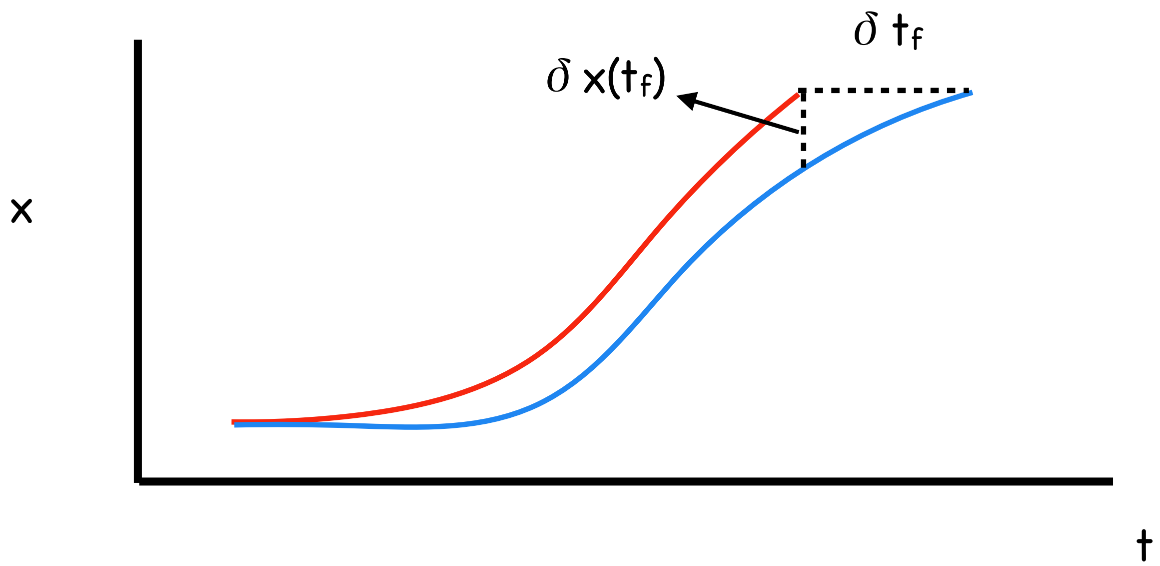
Let us do the same exercise, but allow variation of the final time

$$U(x_f,t_f+\delta t_f;x_i,t_i)-U(x_f,t_f;x_i,t_i)=\frac{\partial U}{\partial t_f}\delta t_f$$
$$=\frac{i}{\hbar}\int\mathcal{D}[x(t)]e^{iS[x(t)]/\hbar}\delta S$$

Now $$\delta S=L[x(t_f),\dot{x}(t_f)]\delta t_f+\left(\frac{\partial L}{\partial\dot{x}}\right)\delta x(t)\Big|_{t_i}^{t_f}+\int_{t_i}^{t_f}dt\left(\frac{\partial L}{\partial x}-\frac{d}{dt}\frac{\partial L}{\partial\dot{x}}\right)\delta x(t)$$

$$\frac{\partial U}{\partial t_f}\delta t_f=\frac{i}{\hbar}\int\mathcal{D}[x(t)]e^{iS[x(t)]/\hbar}\left[L[x(t_f),\dot{x}(t_f)]\delta t_f+\left(\frac{\partial L}{\partial\dot{x}}\right)\delta x(t_f)+\int dt\left(\frac{\partial L}{\partial x}-\frac{d}{dt}\frac{\partial L}{\partial\dot{x}}\right)\delta x(t)\right]$$

0 by Ehrenfest Theorem

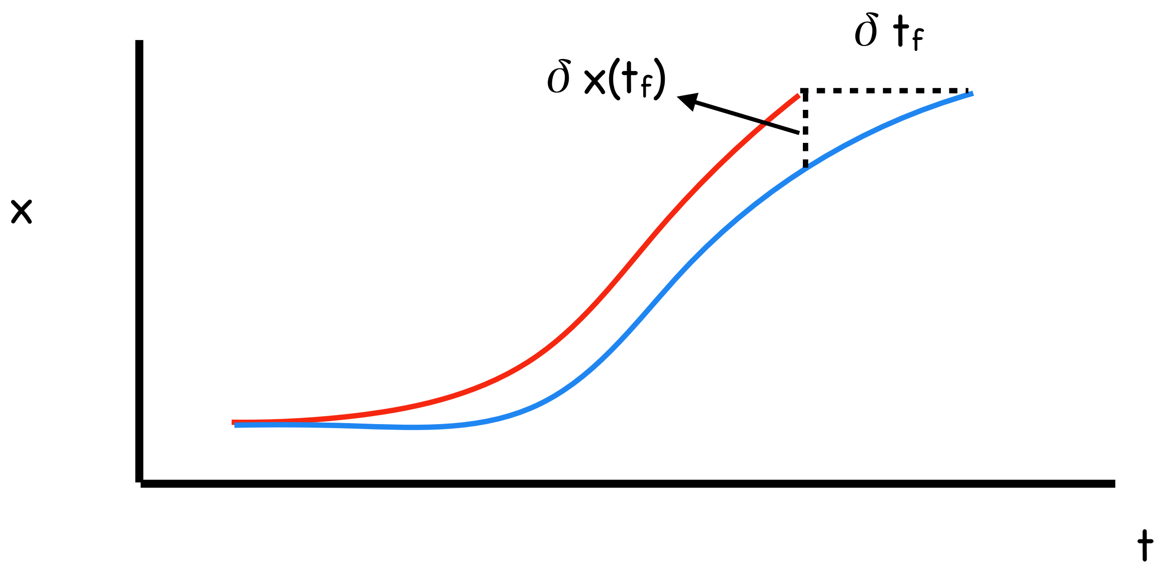


$$\delta x(t_f)=-\dot{x}(t_f)\delta t_f$$

Variation wrt paths (End point variation)

$$\frac{\partial U}{\partial t_f}\delta t_f = \frac{i}{\hbar}\int \mathcal{D}[x(t)]e^{iS[x(t)]/\hbar}\left[L[x(t_f),\dot{x}(t_f)]\delta t_f + \left(\frac{\partial L}{\partial \dot{x}}\right)\delta x(t_f) + \underbrace{\int dt\left(\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}\right)\delta x(t)}_{}\right]$$

0 by Ehrenfest Theorem



$$\delta x(t_f) = -\dot{x}(t_f)\delta t_f$$

$$\frac{\partial U}{\partial t_f}\delta t_f = \frac{i}{\hbar}\int \mathcal{D}[x(t)]e^{iS[x(t)]/\hbar}\underbrace{\left[L[x(t_f),\dot{x}(t_f)] - \dot{x}\left(\frac{\partial L}{\partial \dot{x}}\right)\right]}_{}\delta t_f$$

$$-[p\dot{x} - L] = -H$$

$$i\hbar\frac{\partial U}{\partial t_f} = \int \mathcal{D}[x(t)]e^{iS[x(t)]/\hbar}H(t_f)$$

Schrodinger Equation

Generalizations

We have been essentially looking at 1D QM. This can be generalized to higher dimensions E.g. in 3D you would have (x_1,x_2,x_3) at each time points.

We can extend this formalism to time dependent Hamiltonians: e.g. we can deal with a Harmonic Oscillator whose natural frequency is changing with time.

$$U(t,0) = e^{-i\hat{H}t} \longrightarrow U(t,0) = T[e^{-i\int_0^t H_{1I}(t')dt'}]$$

The main reason that time-dependent Hamiltonians are harder to work with is that the Hamiltonian operator at different times do not commute with each other.

Example: A Harmonic oscillator kicked by a spatially uniform time-dependent external force

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 + f(t)\hat{x} \qquad [\hat{H}(t_1), \hat{H}(t_2)] = \frac{i\hbar(f(t_1)-f(t_2))}{m}\hat{p}$$

Once you break up into infinitesimal time slices, the problem occurs in 2nd order in ε

This is the same order in which Trotter error occurs, $\longrightarrow$ not a problem for path integral

$$U(x_f,t_f;x_i,t_i) = \left(\frac{mN}{2\pi i(t_f-t_i)}\right)^{1/2}\int \mathcal{D}[x(t)]e^{iS[x(t)]} \qquad S[x(t)] = \int_{t_i}^{t_f} dt\frac{m}{2}\dot{x}^2 - V(x,t)$$