Density matrix and entropy

Probability for state with energy E_n $\qquad P_n = \frac{1}{Z}\exp\left(-E_n/k_BT\right)$

Partition function defined $\qquad Z = \sum_n \exp\left(-E_n/k_BT\right)$

Free energy minimized for system interacting with environment at temperature T is directly related to the partition function,

$$F = U - TS = -k_BT\ln Z$$

So entropy , $\qquad S = k_B \ln Z + U/T \qquad$ With $\ln(P_nZ) = -\frac{E_n}{k_BT}$

$$\frac{U}{T} = \frac{1}{T}\sum E_nP_n = -k_B\sum P_n \ln\left(P_nZ\right) = -k_B\sum P_n\left[\ln z + \ln P_n\right] = -k_B\ln Z - k_B\sum P_n \ln P_n$$

Now we can relate the entropy S to the density matrix (see Commins):

Giving $S = -k_B \sum P_n \ln P_n$

In terms of density matrix $\rho = \sum P_n \left| E_n \right\rangle \left\langle E_n \right|$ with $tr(\rho) = \sum P_n = 1$

$$\ln \rho = \text{diag}\left(\ln P_1 \ldots \ln P_n\right)$$

$$\rho \ln \rho = \text{diag}\left(P_1 \ln P_1 \ldots P_n \ln P_n\right)$$

$$tr\left(\rho ln \rho\right) = \sum P_n \ln P_n$$

Giving the relation $S = -tr\left(\rho ln \rho\right)$

Generalize to entropy for any system in terms of density matrix, known as the **Von Neumann entropy**. The connection between entropy and information was made by Shannon.

Lecture 10:
Feynman Path Integral

See Quantum Mechanics and Path Integrals, Feynman and Hibbs

And Techniques and Applications of Path Integration, L.S. Schulman

$$\langle x_b | \Psi(t_b) \rangle = \int_{-\infty}^{\infty} dx_a \, \underline{\langle x_b | U(t_b, t_a) | x_a \rangle} \, \langle x_a | \Psi(t_a) \rangle$$

the propagator

Note that using completeness for energy eigenstates $\psi_n(x) = \langle x | E_n \rangle$ with energy E_n, the propagator can be expanded as

$$\langle x_b | U(t_b, t_a) | x_a \rangle = \sum_n \langle x_b | E_n \rangle \langle x_a | E_n \rangle^{\star} e^{-i(t_b - t_a)E_n/\hbar}$$

Feynman propagator notation:

$$\langle x_1, t_1 | x_0, t_0 \rangle \equiv \langle x_1 | U(t_1, t_0) | x_0 \rangle$$

(or see Heisenberg picture in Sakurai, $\left|\Psi(t)\right\rangle_S = U(t,0)\left|\Psi(0)\right\rangle_H$) where operators are time dependent)

Composition rule

$$U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)$$

$$\left\langle x_2; t_2 \,|\, x_0; t_0 \right\rangle = \int dx_1 \left\langle x_2; t_2 \,|\, x_1; t_1 \right\rangle \left\langle x_1; t_1 \,|\, x_0; t_0 \right\rangle$$

Space integrals from $-\infty$ to $-\infty$, and so forth, dividing time into smaller intervals

Feynman's Conjecture

$$\langle x_1|U(t_1,t_0)|x_0\rangle = \sum_{\text{all paths}} \exp\left(iS[x]/\hbar\right)$$

Where the sum is over **all** paths from (t_0,x_0) to (t_1,x_1) and S[x] is the classical action along the path. We will derive a more general path integral and prove the conjecture for special cases.

$$B_z = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho A_\phi) = \begin{cases} 0 & \rho > a \\ B_0 & \rho < a \end{cases}$$

$$\psi_{det} = \psi_0\left(1 + e^{i\Delta S/\hbar}\right)$$

$$\Delta S = \frac{e}{c}\oint \vec{A}\cdot\vec{v}\,dt = \frac{e}{c}\oint \vec{A}\cdot d\vec{s} = \frac{e}{c}\Phi_B$$

1 minus 2 gives closed path

magnetic flux $\Phi_B = B_0 \pi a^2$

$$P_{det} = \frac{1}{2}\left[1 + \cos\left(\frac{e\Phi_B}{\hbar c}\right)\right]$$

There is no magnetic field (classical force) where electron propagates, but there produces physical effect.

note that Φ_B is gauge invariant.

Screenshot

Classical Vs Quantum

Recall that for classical particles, $S[x]/\hbar$ is extremely large (>10^30 in our ball drop example).

This means the phase varies so rapidly away from the classical path that the they sum to zero (destructive interference) except exactly on the classical path.

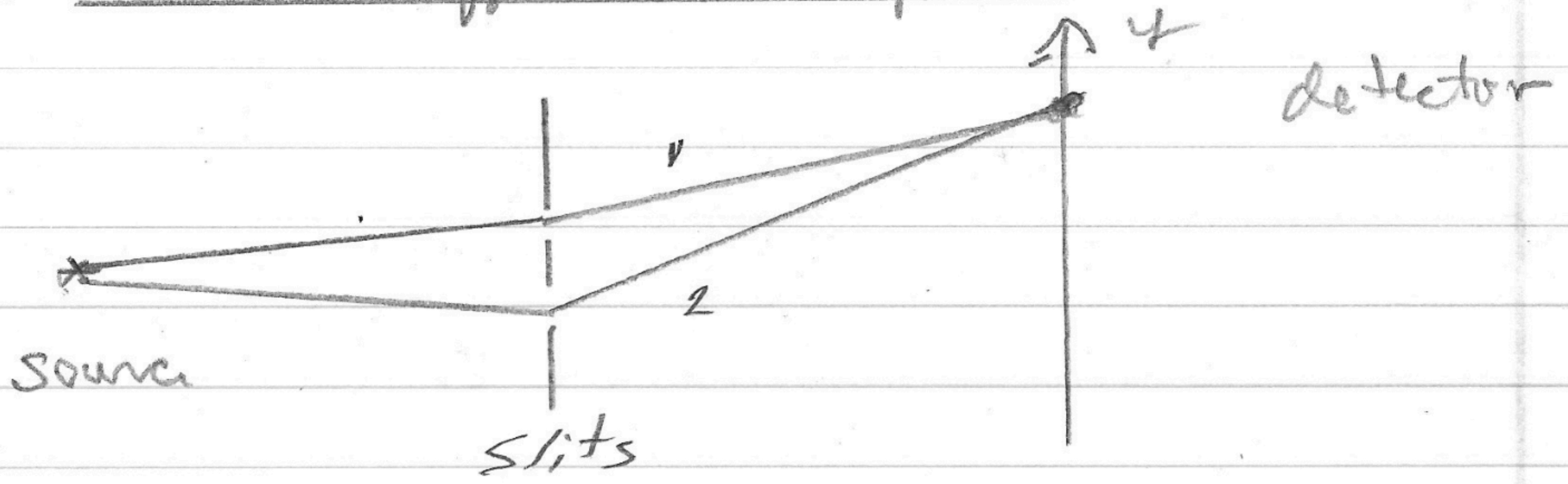
However, a QM particle can have $S[x]/\hbar \sim 1$ so that all paths contribute to the propagator.

The action:

$$S\,[x(t)] = \int_{t_0}^{t_1} L(x, \dot{x}, t)\,dt$$

Examples with interfering paths

Electron diffraction experiment



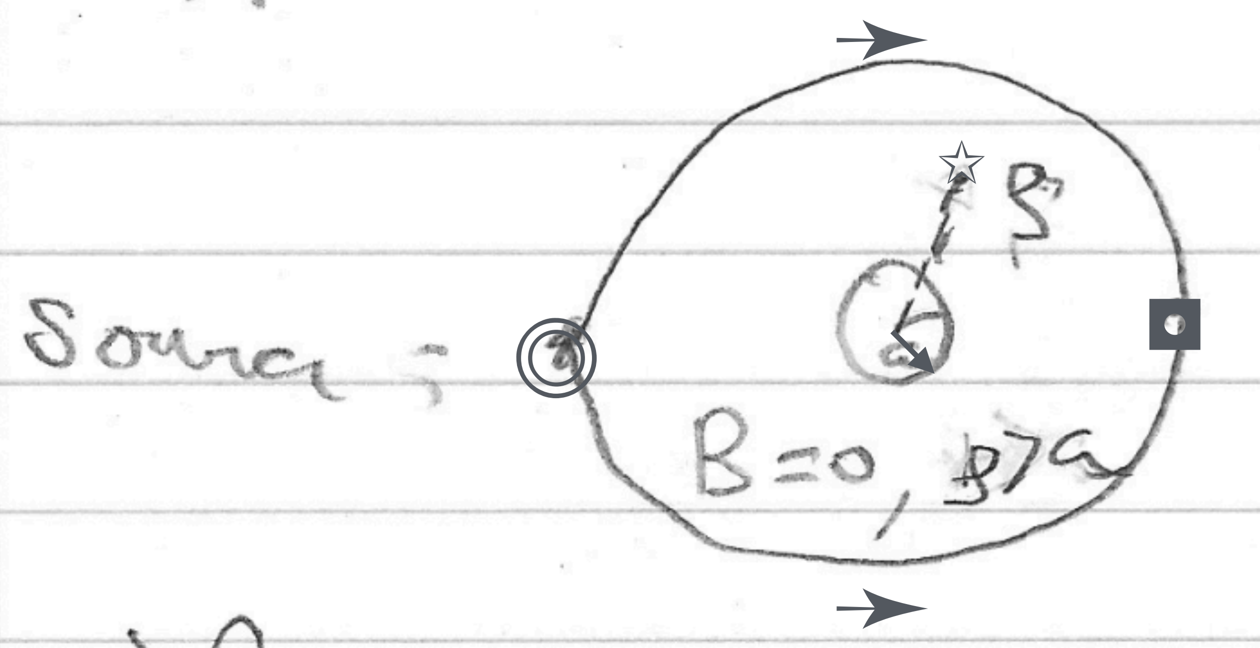
amplitude $\Psi(y) = \psi_0 \left(e^{iS_1/\hbar} + e^{iS_2/\hbar} \right)$

$$= \psi_0 e^{iS_1/\hbar} \left(1 + e^{i\Delta S/\hbar} \right)$$

$$P(y) = |\psi|^2 = \frac{1}{2}\left[1 + \cos\left(\frac{\Delta S}{\hbar}\right) \right]$$

Aharnov-Bohm effect

Consider electrons moving in plane $\perp$ long solinoid of radius a along $\hat{z}$ direction.



$$\vec{B} = \begin{cases} B_0\,\hat{z} & \rho < a \\ 0 & \rho > a \end{cases}$$

$$\mathcal{L}_{EM} = -e\phi + \frac{e}{c}\vec{A}\cdot\vec{v} \qquad q = -e$$

vector potential:

$$\rho > a \qquad \vec{A}_{\rho>a} = \frac{B_0 a^2}{2\rho}\hat{\phi}$$

$$\rho < a \qquad \vec{A}_{\rho<a} = \frac{B_0\rho}{2}\hat{\phi}$$

Summing over paths

Discretize path to implement arbitrary path— example for 2 paths

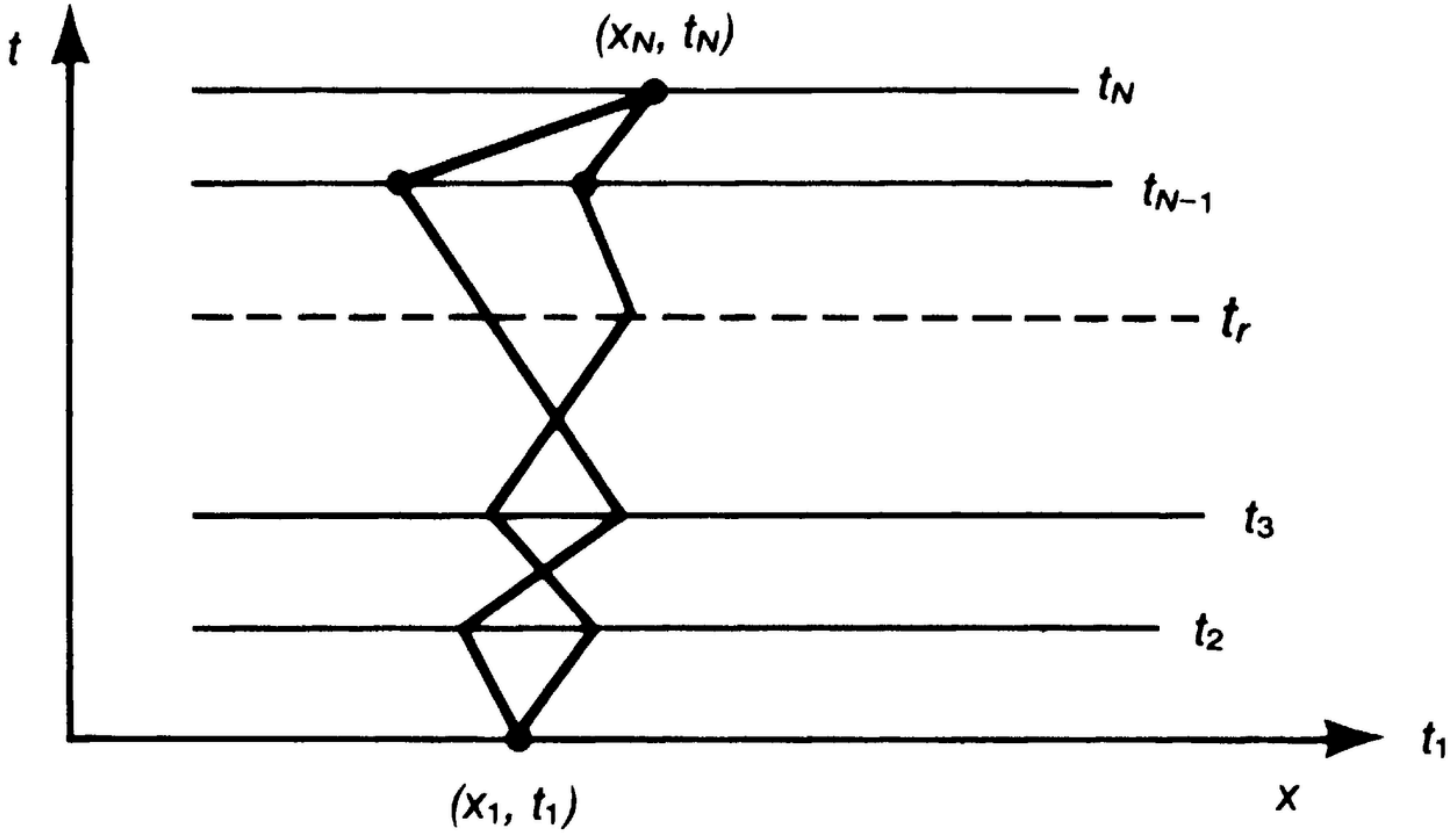
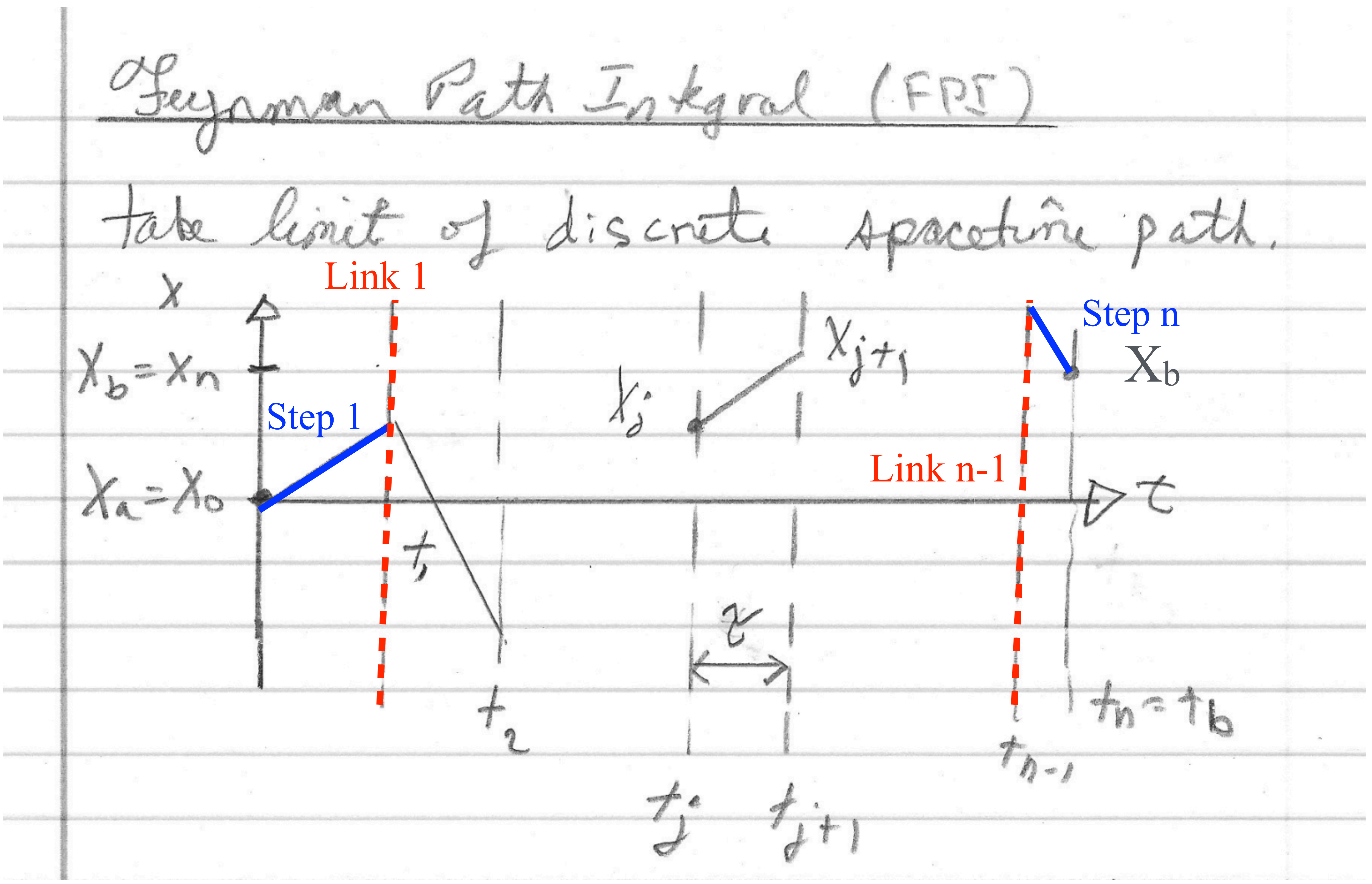


FIGURE 2.2. Paths in *xt*-plane.



Breakup propagator into n time **steps**, n-1 intermediate times ("links")

$$t_a = t_0 \; ; t_b = t_n \; ; \tau = (t_b - t_a)/n \; ; t_b = t_a + n\tau$$

Then break up time evolution into n steps,

$$U(t_b, t_a) = \exp\left\{-\frac{i}{\hbar}H(t_b - t_a)\right\} = \left(U(\tau)\right)^n$$

Insert identity $I = \int_{-\infty}^{\infty} dx_j \left|x_j\right\rangle\left\langle x_j\right|$ n-1 intermediate time links

Take $H = \dfrac{\hat{p}^2}{2m} + V(\hat{x})$

$$\left\langle x_b; t_b \,|\, x_a; t_a \right\rangle = \int_{-\infty}^{\infty} dx_1 \cdots dx_{n-1} \Pi_{j=0}^{n-1} \left\langle x_{j+1} \,|\, U(\tau) \,|\, x_j \right\rangle$$

All integrals from $-\infty$ to $+\infty$ including paths with $\dot{x} > c$!

Can prove propagator with **relativistic Hamiltonian** is Lorentz invariant.

For Infinitesimal τ, $\quad U(\tau) \approx 1 - \frac{i\tau}{\hbar} H(\hat{x}, \hat{p}) \quad$ With $H = \frac{\hat{p}^2}{2m} + V(\hat{x})$

The operator $\hat{x}$ gives the eigenvalue

$$V(\hat{x}) \left| x_j \right\rangle = V(x_j) \left| x_j \right\rangle$$

However, for $\hat{p}$ we need to use the momentum basis. Insert **n** identity operators one for each step

$$I = \int_{-\infty}^{\infty} dp_j \left| p_j \right\rangle \left\langle p_j \right|$$

Into each step n,

$$I_j = \int_{-\infty}^{\infty} dp_j \left\langle x_{j+1} \left| \left(1 - \frac{i\tau}{\hbar} \left[\frac{\hat{p}^2}{2m} + V(x_j) \right] \right) \right| p_j \right\rangle \left\langle p_j | x_j \right\rangle$$

$$= \int dp_j \left(1 - \frac{i\tau}{\hbar} E_j \right) \left\langle x_{j+1} | p_j \right\rangle \left\langle p_j | x_j \right\rangle$$

where the energy is $E_j = \dfrac{p_j^2}{2m} + V(x_j)$

Then approximate

$$1 - \frac{i\tau E_j}{\hbar} \approx \exp\left[\frac{-i\tau E_j}{\hbar}\right]$$

Use explicit plane waves as

$$\left\langle x_{j+1} \,|\, p_j \right\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{i}{\hbar} p_j x_{j+1}\right)$$

To get for each link

$$\left\langle x_{j+1} \,|\, U(\tau) \,|\, x_j \right\rangle = \frac{1}{2\pi\hbar} \exp\left(-iE_j\tau/\hbar\right) \exp\left(+iP_j x_{j+1}/\hbar\right) \exp\left(-iP_j x_j/\hbar\right)$$

Using the exponents sum to

$$\exp \frac{i\tau}{\hbar}\left[p_j\left(\frac{x_{j+1}-x_j}{\tau}\right)-E_j\right]$$

And, voila! we see a Legendre Transformation where the velocity is

$$\dot{x}_j = \frac{x_{j+1}-x_j}{\tau},$$

$$\mathscr{L}\left(x_j, \dot{x}_j\right) = p_j\dot{x}_j - E_j = p_j\dot{x}_j - H(x_j, p_j)$$

Before returning to this, lets put everything together:

$$\left\langle x_b; t_b \,|\, x_a; t_a \right\rangle = \left\langle x_b \,|\, U(t_b, t_a) \,|\, x_a \right\rangle = \Pi_{j=1}^{n-1} \int dx_j \cdot \Pi_{j=1}^{n} \int \frac{dp_j}{2\pi\hbar} \exp \frac{i\tau}{\hbar} \left(p_j \left(\frac{x_{j+1} - x_j}{\tau} \right) - E_j \right)$$

In the limit $\tau \to 0,\ n \to \infty$

$$\lim \begin{pmatrix} \tau \to 0 \\ n \to \infty \end{pmatrix} \Pi_{j=1}^{n} \exp \frac{i\tau}{\hbar} \left[p_j \left(\frac{x_{j+1} - x_j}{\tau} \right) - E_j \right] = \exp \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[p\dot{x} - E(p, x) \right] = \exp \left[\frac{i}{\hbar} S(t_a, t_b) \right]$$

Where we have written the result in terms of the action S as a functional of x(t) and p(t).

We can define the product of integrals as ``functional measures" and write in a final pretty form hiding our ignorance of ``measure"

$$\left\langle x_b; t_b \,|\, x_a; t_a \right\rangle = \int \mathscr{D}x[t] \int \mathscr{D}p[t] \exp\left(\frac{i}{\hbar} S(t_a, t_b)\right)$$

This very *formal* expression is the **phase space path integral**.

Deriving Feynman's Conjecture

$\Rightarrow$ do Gaussian integrals over momenta

With $E_j = \dfrac{p_j}{2m} + V(x_j)$ we can do the phase space integrals by completing the square

$$I_j = \int \frac{dp_j}{2\pi\hbar} \exp \frac{i\tau}{\hbar}\left(p_j\left(\frac{x_{j+1}-x_j}{\tau}\right) - E_j\right)$$

$$= \int \frac{dp_j}{2\pi\hbar} \exp \frac{i\tau}{\hbar}\left(p_j\left(\frac{x_{j+1}-x_j}{\tau}\right) - \frac{p_j^2}{2m} - V(x_j)\right)$$

Factor out V which does not depend on p_j

$$I_j = \exp\left(-\frac{i\tau}{\hbar}V(x_j)\right)\int \frac{dp_j}{2\pi\hbar}\exp\frac{i\tau}{\hbar}\left(p_j\left(\frac{x_{j+1}-x_j}{\tau}\right)-\frac{p_j^2}{2m}\right)$$

Complete the square in p_j

$$() = \frac{-i\tau}{2m\hbar}\left[p_j^2 - \frac{m}{\tau}p_j\left(x_{j+1}-x_j\right)\right]$$

$$() = \frac{-i\tau}{2m\hbar}\left[p_j - \frac{m}{\tau}\left(x_{j+1}-x_j\right)\right]^2 + \frac{i\tau}{2m\hbar}\left(\frac{m}{\tau}\right)^2\left(x_{j+1}-x_j\right)^2$$

Change variables $$p_j' = p_j - \frac{m}{\tau}\left(x_{j+1}-x_j\right)$$

$$I_j = \exp\left(-\frac{i\tau}{2\hbar}V(x_j)\right)\exp\left(\frac{im\tau}{\hbar}\left(\frac{x_{j+1}-x_j}{\tau}\right)^2\right)\int_{-\infty}^{\infty}\frac{dp'_j}{2\pi\hbar}\exp\left\{\frac{-i\tau}{2m\hbar}p'^2_j\right\}$$

With $a = \dfrac{i\tau}{2m\hbar}$ we find the Gaussian integral,

$$\int_{-\infty}^{\infty}\frac{dp'_j}{2\pi\hbar}\exp\left(-ap'^2_j\right) = \frac{1}{2\pi\hbar}\sqrt{\frac{\pi}{a}} = \sqrt{\frac{m}{2\pi i\hbar\tau}}$$

$$\left\langle x_b \,|\, U(t_b, t_a) \,|\, x_a \right\rangle = \Pi_{j=1}^{n-1} \int dx_j \sqrt{\frac{m}{2\pi i\hbar\tau}} \exp\left\{ \frac{i\tau}{\hbar} \Sigma_{j=1}^{n} \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{\tau} \right)^2 - V(x_j) \right] \right\}$$

In limit $\tau \to 0,\ n \to \infty$

$$\left\langle x_b \,|\, U(t_b, t_a) \,|\, x_a \right\rangle = \int \mathscr{D}'[x] \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left(\frac{m\dot{x}^2}{2} - V(x) \right) \right\}$$

Where we define the measure

$$\mathscr{D}'[x] = \lim \begin{pmatrix} \tau \to 0 \\ n \to \infty \end{pmatrix} \Pi_{j=1}^{n-1} dx_j \sqrt{\frac{m}{2\pi i\hbar\tau}}$$

note that $\sqrt{\ }$ makes measure dimensionless

We now have the Feynman path integral,

$$\left\langle x_b \,|\, U(t_b, t_a) \,|\, x_a \right\rangle = \int_{x_a}^{x_b} \mathscr{D}'[x] \exp\left\{ \frac{i}{\hbar} S(t_a, t_b) \right\}$$

With Lagrangian

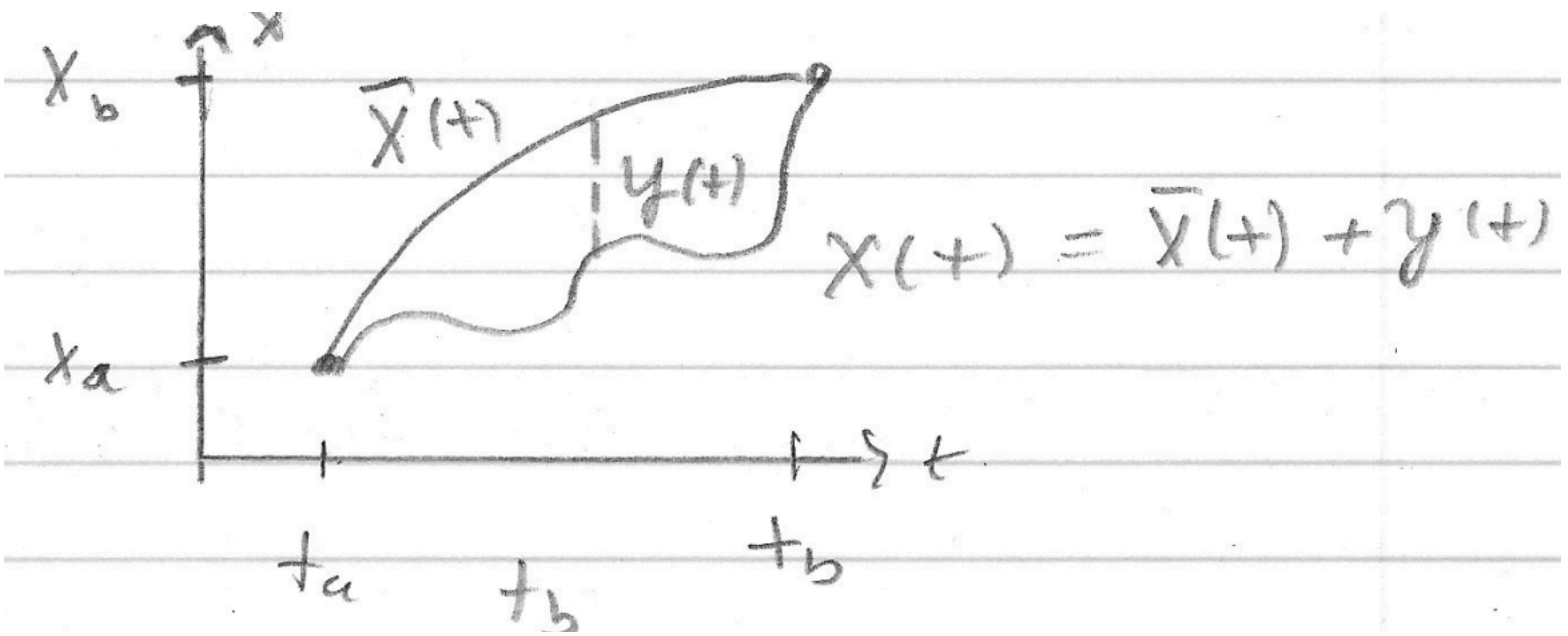
$$\mathscr{L} = \frac{m\dot{x}^2}{2} - V(x)$$

But wait, there is more…

Feynman went further for a certain class of potentials:

$$V(x) = a + bx + cx^2 + d\dot{x} + ex\dot{x}$$

Expand about classical path $x(t) = \bar{x}(t) + y(t)$



$$S[x] = S[\bar{x} + y] = \int \mathscr{L}\left(\bar{x} + y, \dot{\bar{x}} + \dot{y}\right) dt$$

$$\mathscr{L}(x, \dot{x}) \approx \mathscr{L}(\bar{x}, \dot{\bar{x}}) + y\frac{\partial \mathscr{L}}{\partial x}|_{\bar{x}\dot{\bar{x}}} + \dot{y}\frac{\partial \mathscr{L}}{\partial \dot{x}}|_{\bar{x}\dot{\bar{x}}} + \frac{1}{2}y^2\frac{\partial^2 \mathscr{L}}{\partial^2 x^2}|_{\bar{x}\dot{\bar{x}}} + y\dot{y}\frac{\partial^2 \mathscr{L}}{\partial x \partial \dot{x}}|_{\bar{x}\dot{\bar{x}}} + \frac{1}{2}\dot{y}^2\frac{\partial^2 \mathscr{L}}{\partial^2 \dot{x}}|_{\bar{x}\dot{\bar{x}}}$$

Terms linear in y and $\dot{y}$ cancel due to the extremal condition (Euler-Lagrange equations) (you show). So,

Kinetic energy

$$S[x] = S[\bar{x}] + \int_{t_a}^{t_b} dt \left[\frac{1}{2}m\dot{y}^2 - ey\dot{y} + cy^2\right]$$

Define A which depends only on the time difference,

$$A(t_b, t_a) = \int \mathscr{D}'[y] \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left(\frac{m\dot{y}^2}{2} - cy^2 - ey\dot{y} \right) \right\}$$

And we get the result for the propagator

$$\left\langle x_b \,|\, U(t_b, t_a) \,|\, x_a \right\rangle = A(t_b, t_a) \times \exp\left(\frac{i}{\hbar} S[\bar{x}] \right)$$

An amazing result that depends only on the action evaluated along the classical path.

In the time evolution of the wave function, A(t) is just a constant factor:

$$\left\langle x_b \,|\, \Psi(t_b) \right\rangle = A(t_b, t_a) \int_{-\infty}^{\infty} dx_a \exp\left(\frac{i}{\hbar} S[\bar{x}]\right) \left\langle x_a \,|\, \Psi(t_a) \right\rangle$$

The factor ``A” can be obtained from a simple second order differential equation (see Techniques and Applications of Path Integration, L.S. Schulman) **You will use this method in HW #7.**

Schrödinger equation can be obtained from the path integral (Feynman and Hibbs, Shankar, and lecture 10 notes.)

Path integral equivalence to Schrödinger (Shankar)

Infinitesimal Schrödinger (time τ)

$$\psi(x,\tau) - \psi(x,0) = -\frac{i\tau}{\hbar}\left[-\frac{\partial^2}{2m\partial x^2} + V(x)\right]\psi(x,0) \tag{1}$$

$$\psi(x,\tau) = \int_{-\infty}^{\infty} \langle x|U(\tau)|x'\rangle\, \psi(x',0)\, dx' \tag{2}$$

Propagator for infinitesimal time

$$\langle x|U(\tau)|x'\rangle = C(\tau)\exp\left[\frac{i}{\hbar}\frac{m}{2\tau}(x-x')^2 - \frac{i\tau}{\hbar}V(x)\right] \tag{3}$$

factor out front

$$C(\tau) = \sqrt{\frac{m}{2\pi i\hbar\tau}} \tag{4}$$

Define $y = x' - x$.
For infinitesimal τ:

$$\exp\left(\frac{im}{2\tau}y^2\right) \quad \text{oscillates rapidly with } y \text{ except near} \tag{5}$$

$$\frac{my^2}{2\hbar\tau} < \pi \tag{6}$$

$$|y| < \left(\frac{2\pi\hbar\tau}{m}\right)^{1/2} \tag{7}$$

Coherence region.

Suggests expand propagator to order τ, y^2. With $im/2\hbar\tau = -\pi c^2$,

$$\Psi(x,\tau) = c\int dy\, \exp\left\{-\pi c^2 y^2\right\} \exp\left\{-i\tau\hbar V(x+y)\right\} \Psi(x+y,0) \tag{1}$$

$$\Psi(x+y,0) \approx \Psi(x,0) + y\frac{\partial\Psi}{\partial x} + \frac{1}{2}y^2\frac{\partial^2\Psi}{\partial x^2}$$

$$\exp\left[\frac{i\tau}{\hbar}V(x+y)\right] \approx 1 - \frac{i\tau}{\hbar}V(x)$$

Ignore τy terms:

$$\Psi(x,\tau) = c\int_{-\infty}^{\infty} dy\, \exp\left\{-\pi c^2 y^2\right\}\left[\Psi(x,0) - \frac{i\tau}{\hbar}V(x)\Psi(x,0) + y\frac{\partial\Psi}{\partial x} + \frac{1}{2}y^2\frac{\partial^2\Psi}{\partial x^2}\right] \tag{2}$$

$$\Psi(x,0) - \frac{i\tau}{\hbar}V(x)\Psi(x,0) + y\frac{\partial\Psi}{\partial x} + \frac{1}{2}y^2\frac{\partial^2\Psi}{\partial x^2}$$

Do Gaussian integral:

$$\int dy\ \exp\{-\pi c^2 y^2\} = \frac{1}{c}$$

$$\int dy\, y\ \exp\{-\pi c^2 y^2\} = 0$$

$$\int dy\, y^2\ \exp\{-\pi c^2 y^2\} = \frac{1}{2\pi c^2} \cdot \frac{1}{c} = \frac{1}{2\pi mc}$$

$$\Psi(x,\tau) = \Psi(x,0) + \frac{i\hbar\tau}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i\tau}{\hbar}V(x)\Psi(x,0) \tag{3}$$

$$\frac{\Psi(x,\tau) - \Psi(x,0)}{\tau} = -\frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,0) \tag{4}$$

Which is Schrödinger eq.