The Single Particle Path Integral and Its Calculations

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- Introduction and Motivation
- Some Examples in Calculating Path Integrals
  - The Free Particle
  - The Harmonic Oscillator
- Perturbation Expansions

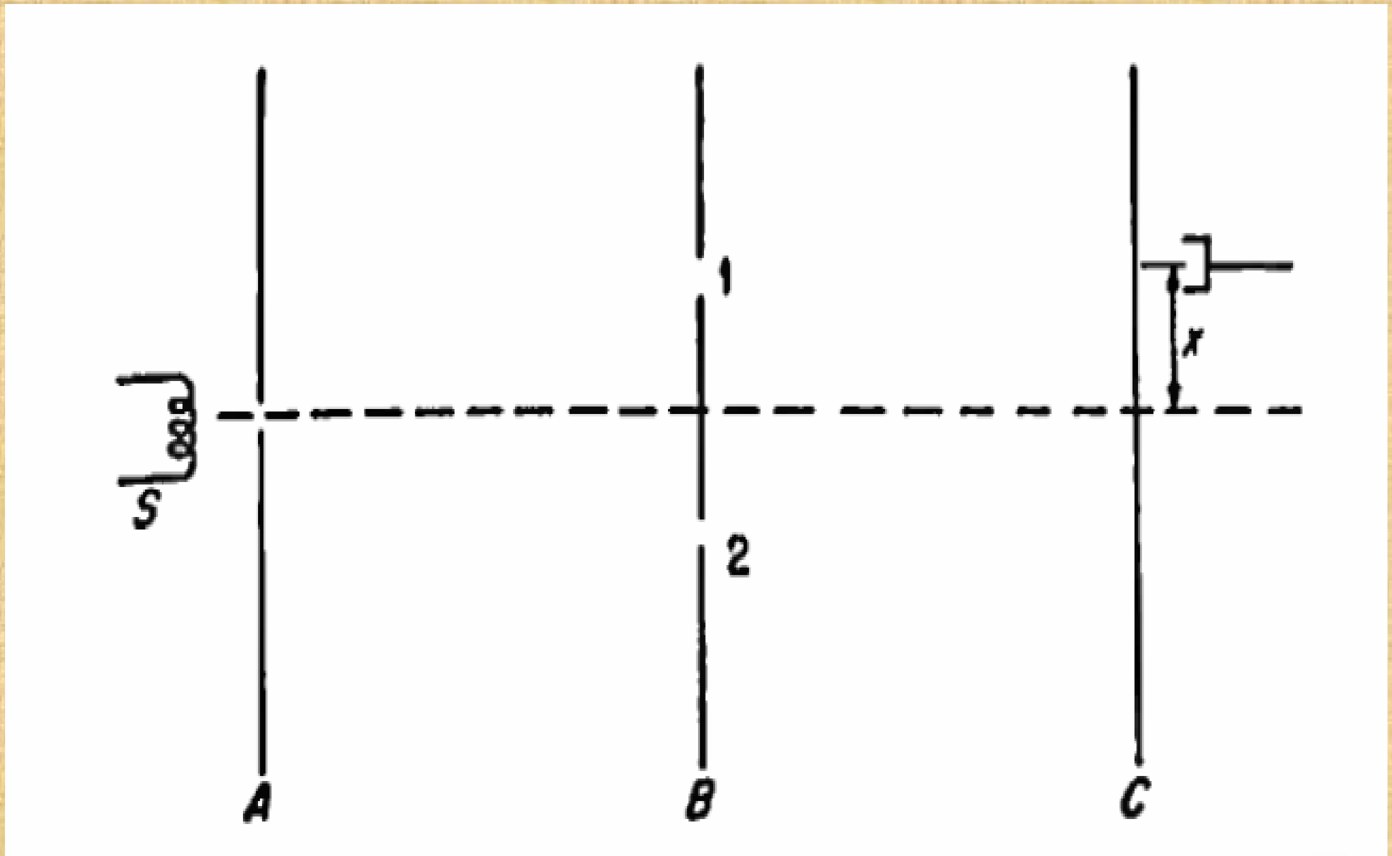
Introduction and Motivation

- In Q.M. – a probability amplitude associated with every method whereby an event in Nature can take place.

- Also associate an amplitude with the overall event by adding together the amplitudes of each alternative method.

- Can be seen via the famous double-slit experiment

The Double Slit Experiment



- ϕ_1 Amplitude for reaching the detector while passing through hole 1

  ϕ_2 Amplitude for reaching the detector while passing through hole 2

  Total amplitude of reaching detector $\phi = \phi_1 + \phi_2$

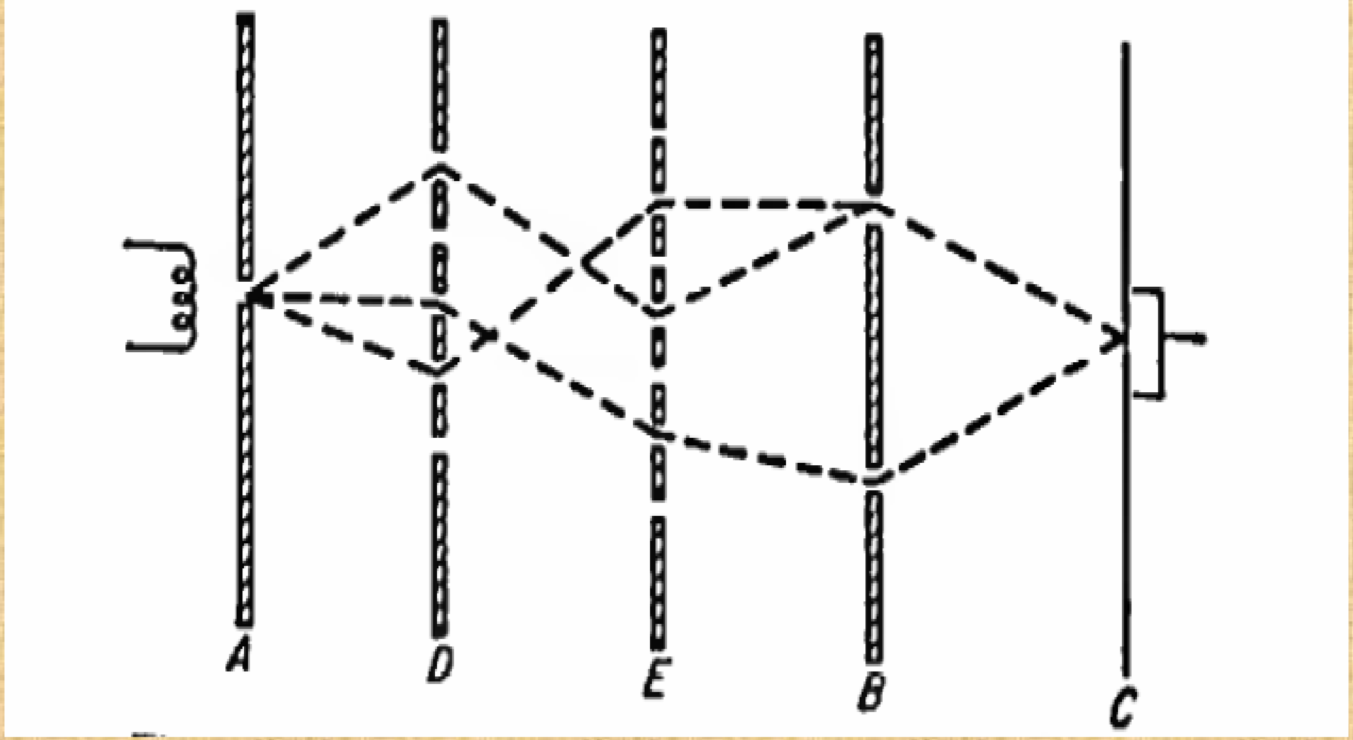
since $\text{Probability} = \left|\text{Probability Amplitude}\right|^2$

Total Probability of Electron Reaching Detector

$$P = \left|\phi_1 + \phi_2\right|^2$$

- But – many ways to analyze concept of amplitude.
- In this example – associate amplitude with each possible motion of electron from A to B .
- Hence – total amplitude = sum of a contribution from each of the paths

A Thought Experiment

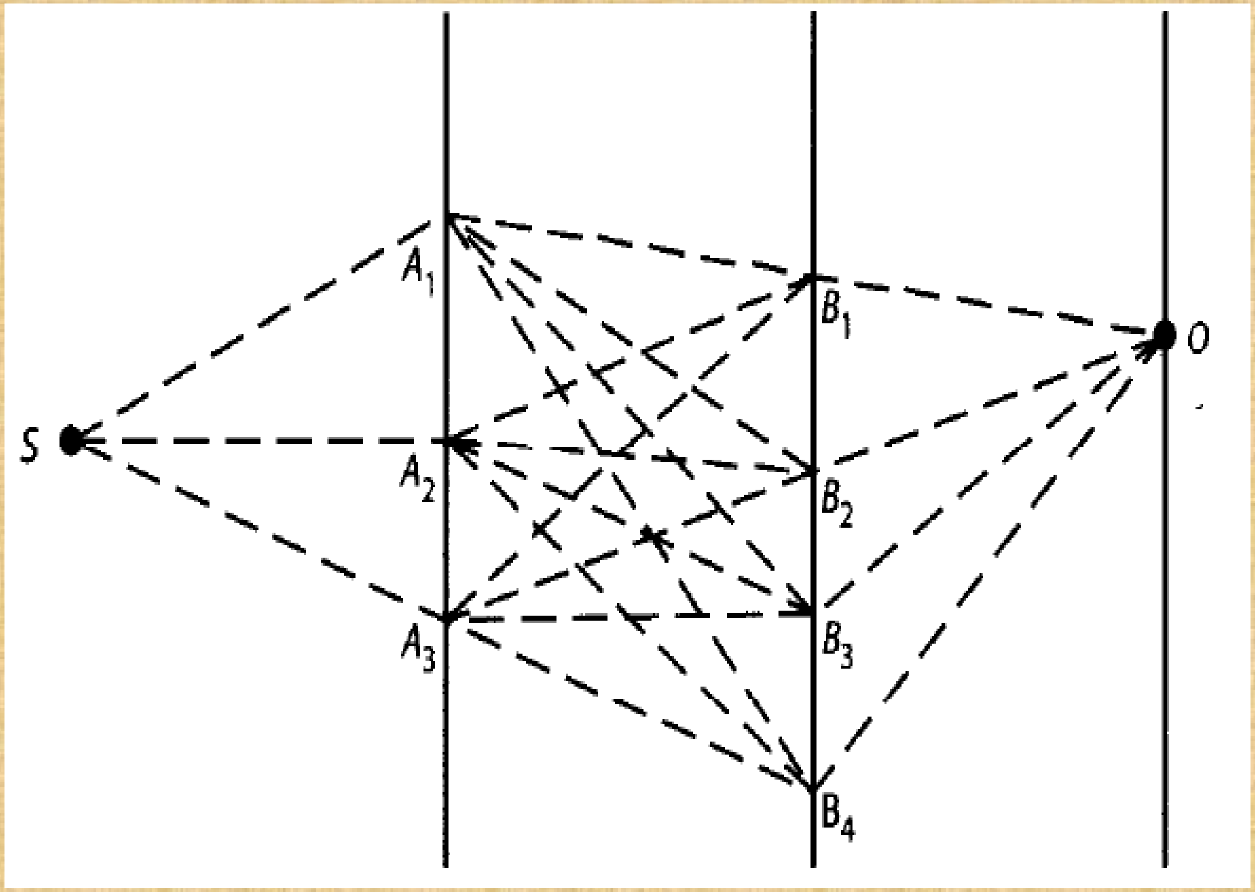


- Each alternative path has own amplitude – Complete amplitude is sum of all possible paths.

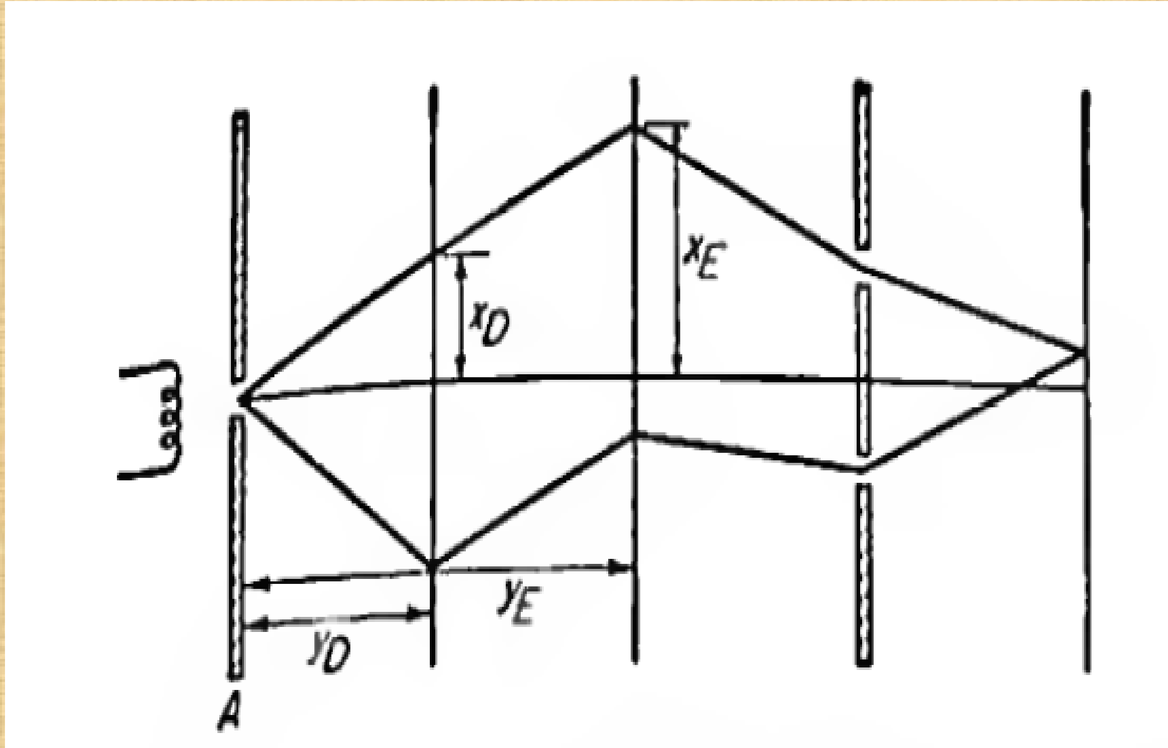
- Now suppose: More and more holes are drilled – till nothing more is left of the screens…

- At each screen, path of electron specified by heights x_D, x_E at which the electron passes positions y_D, y_E

A Thought Experiment II



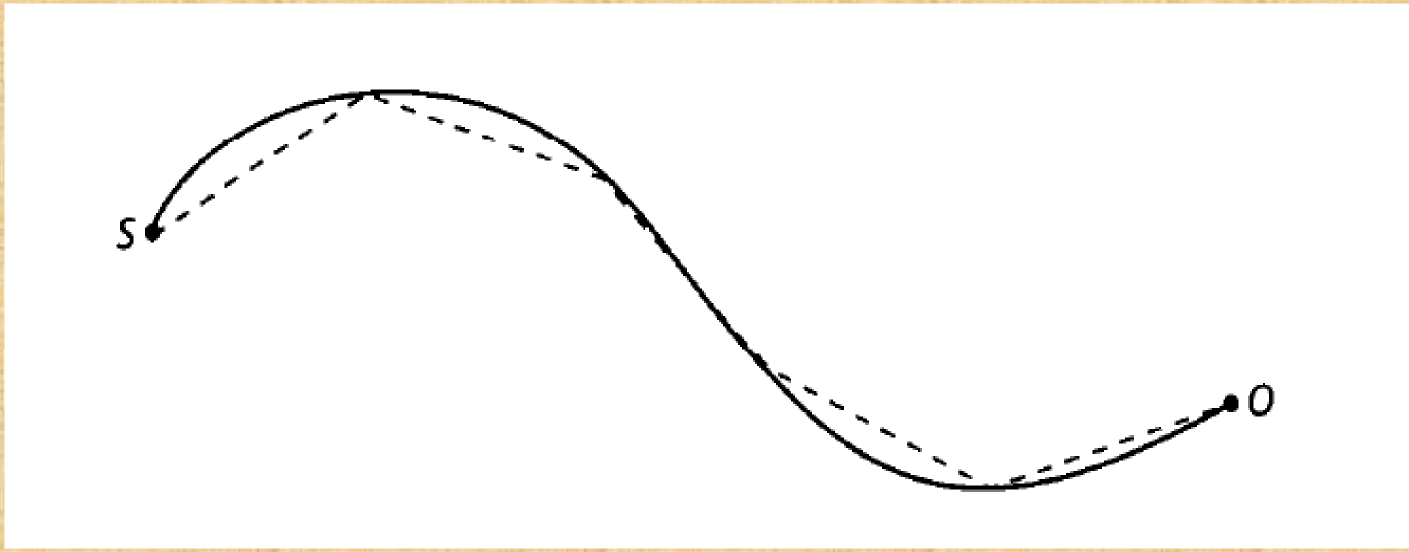
A Thought Experiment III



- To each pair of heights corresponds an amplitude.
- Need to take integral of the amplitudes over all possible values of x_D, x_E .
- Also, the time at which the electron passes each point in space – $y(t)$.
- Thus – a path is defined through $x(t), y(t)$
- Total amplitude = sum over the amplitude for source – detector travel following all possible paths.

- But how does one define a sum over a path?

- One way is to approximate it by line segments + let segments → 0



- Unitarity of Q.M.: Amplitude of the whole path is product of the amplitudes of each infinitesimal path

- Amplitude to propagate from q_i to q_f in time T is given in terms of the unitary operator such that

$$\mathrm{Amplitude} = \left\langle q_f \left| e^{-iHT} \right| q_i \right\rangle$$

- Dividing time T into N infinitesimal segments each of length $\delta t = T / N$, one has

$$\langle q_f | e^{-iHT} | q_i \rangle = \langle q_f | e^{-iH\delta t} \cdots e^{-iH\delta t} | q_i \rangle$$

Completeness of $|q\rangle$ means that

$$\int dq |q\rangle\langle q| = 1$$

- And thus

$$\left\langle q_f \left| e^{-iHT} \right| q_i \right\rangle$$
$$= \left(\prod_{j=1}^{N-1} \int dq_j \right) \left\langle q_f \left| e^{-iH\delta t} \right| q_{N-1} \right\rangle \left\langle q_{N-1} \left| e^{-iH\delta t} \right| q_{N-2} \right\rangle \cdots$$
$$\cdots \left\langle q_2 \left| e^{-iH\delta t} \right| q_1 \right\rangle \left\langle q_1 \left| e^{-iH\delta t} \right| q_i \right\rangle$$

- Taking a look at one individual factor

$$\left\langle q_{j+1} \left| e^{-iH\delta t} \right| q_j \right\rangle$$

- for free particle case, $V(q)=0$, along with the completeness of $|p\rangle$ gives

$$\left\langle q_{j+1}\left|e^{-i\delta t(\hat{p}^2/2m)}\right|q_j\right\rangle = \int\frac{dp}{2\pi}\left\langle q_{j+1}\left|e^{-i\delta t(\hat{p}^2/2m)}\right|p\right\rangle\left\langle p\middle|q_j\right\rangle$$

$$=\int\frac{dp}{2\pi}e^{-i\delta t(p^2/2m)}\left\langle q_{j+1}\middle|p\right\rangle\left\langle p\middle|q_j\right\rangle$$

$$=\int\frac{dp}{2\pi}e^{-i\delta t(p^2/2m)}e^{ip(q_{j+1}-q_j)}$$

- The integral over p yields, noting that it is Gaussian and employing the relation

$$\int_{-\infty}^{+\infty} dx e^{-\frac{1}{2}ax^2} = \sqrt{\frac{2\pi}{a}}$$

$$\left\langle q_{j+1} \left| e^{-iH\delta t(p^2/2m)} \right| q_j \right\rangle = \left(\frac{-i2\pi m}{\delta t} \right)^{\frac{1}{2}} e^{[im(q_{j+1}-q_j)^2]/2\delta t}$$

$$= \left(\frac{-i2\pi m}{\delta t} \right)^{\frac{1}{2}} e^{i\delta t(m/2)[(q_{j+1}-q_j)/\delta t]^2}$$

- Substituting the integrated expression into the expression for the product of $\langle q_{j+1} | e^{-iH\delta t} | q_j \rangle$ yields

$$\langle q_f | e^{-iHT} | q_i \rangle = \left(\frac{-i2\pi m}{\delta t} \right)^{\frac{N}{2}} \prod_{j=0}^{N-1} \int dq_j e^{i\delta t (m/2) \sum_{j=0}^{N-1} [(q_{j+1} - q_j)/\delta t]^2}$$

- Taking the continuum limit $\delta t \to 0$ one replaces $[(q_{j+1} - q_j)/\delta t]^2 \to \dot{q}^2$ and $\sum_{j=0}^{N-1} \delta t \to \int_0^T dt$

$$\int Dq(t) = \lim_{N \to \infty} \left(\frac{-i2\pi m}{\delta t} \right)^{\frac{N}{2}} \prod_{j=0}^{N-1} \int dq_j$$

- One has then the path integral representation:

$$\langle q_f | e^{-iHT} | q_i \rangle = \int Dq(t) e^{i\int_0^T dt \frac{1}{2} m\dot{q}^2}$$

- To obtain $\langle q_f | e^{-iHT} | q_i \rangle$, one simply integrates over all possible paths $q(t)$ such that $q(0) = q_i$ and $q(T) = q_f$
- Hamiltonian for a particle in a potential $V(\hat{q})$

$$\langle q_f | e^{-iHT} | q_i \rangle = \int Dq(t) e^{i\int_0^T dt [\frac{1}{2} m\dot{q}^2 - V(\hat{q})]}$$

- But $\frac{1}{2}m\dot{q}^2 - V(q) = L(\dot{q}, q)$, and in general

$$\langle q_f | e^{-iHT} | q_i \rangle = \int Dq(t) e^{i\int_0^T dtL(\dot{q},q)}$$

- As $\int_0^T dtL(\dot{q}, q) = S(q)$, and restoring the Planck's constant, the final expression is then

$$\langle q_f | e^{-\frac{i}{\hbar}HT} | q_i \rangle = \int Dq(t) e^{\frac{i}{\hbar}S(q)}$$

Some Examples in Calculating Path Integrals

I. The Free Particle

- The Lagrangian $L(\dot{q}, q)$ for a free particle is noted to be

$$L(\dot{q}, q) = \frac{m\dot{q}^2}{2}$$

- The full amplitude (or kernel) is then

$$K(q_f, q_i) = \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \delta t} \right)^{\frac{N}{2}}$$

$$\times \prod_{j=0}^{N-1} \int dq_j \exp\left(\frac{im}{2\hbar \delta t} \sum_{j=0}^{N} (x_j - x_{j-1})^2 \right)$$

- The full expression can be obtained by substituting the Lagrangian into the action $\int_0^T dt L(\dot{q}, q) = S(q)$ and performing the time integration.

- Alternatively, one can also apply the action principle along with the Hamilton equations for the free particle.

- Taking note of the identity

$$\int_{-\infty}^{\infty} du \sqrt{\frac{a}{u}} e^{-a(x-u)^2} \sqrt{\frac{b}{\pi}} e^{-b(u-y)^2}$$

$$= \sqrt{\frac{ab}{\pi(a+b)}} \exp\left[-\frac{a}{a+b}(x-y)^2 \right]$$

one first considers the first integral over q_1 in the sum of terms in the exponent.

- Including two of the $\left(\frac{m}{2\pi i\hbar\delta t}\right)^{1/2}$ terms one has

$$\left(\frac{m}{2\pi i\hbar\delta t}\right)\int dq_1 \exp\left[\frac{im}{2\hbar\delta t}(q_1-q_0)^2+\frac{im}{2\hbar\delta t}(q_2-q_1)^2\right]$$

$$=\sqrt{\frac{m}{2\pi i\hbar(2\delta t)}}\exp\left[\frac{im}{2\hbar(2\delta t)}(q_2-q_0)^2\right]$$

according to the integral identity displayed in the previous slide

- It can be seen that the effect of integration on the q_i is the replacements

$$q_2 \text{ integration} : 2\delta t \to 3\delta t$$

(both in the square root and in the exponential)

$$\left(q_3 - q_2\right)^2 + \left(q_2 - q_0\right)^2 \to \left(q_3 - q_0\right)^2$$

$$q_3 \text{ integration} : 3\delta t \to 4\delta t$$

(both in the square root and in the exponential)

$$\left(q_4 - q_3\right)^2 + \left(q_3 - q_0\right)^2 \to \left(q_4 - q_0\right)^2$$

- Grouping and integrating N times, one finally has

$$\delta t \rightarrow (N+1)\delta t = T$$

$$\text{Distance squared} \rightarrow (q_{N+1} - q_0)^2 = (q_f - q_i)^2$$

- The final expression of the integral is

$$K(q_f, q_j) = \sqrt{\frac{m}{2\pi i\hbar T}}\exp\left[\frac{im}{2\hbar T}(q_f - q_i)^2\right]$$

II. The Harmonic Oscillator

- The harmonic oscillator Lagrangian → special case of the quadratic Lagrangian

$$L = \frac{1}{2} m\dot{x}^2 + b(t)x\dot{x} - \frac{1}{2} c(t)x^2 - e(t)x$$

- For the harmonic oscillator (replacing : $q_{f/i} \to x(t_{b/a})$)

$$L = \frac{1}{2} m\dot{x}^2 - \frac{1}{2} m\omega^2 x^2$$

- The action of the Lagrangian is of course

$$S(x(\tau)) = \int L dt$$

- In general, quadratic Lagrangians (such as har. osc.) can be solved by introducing

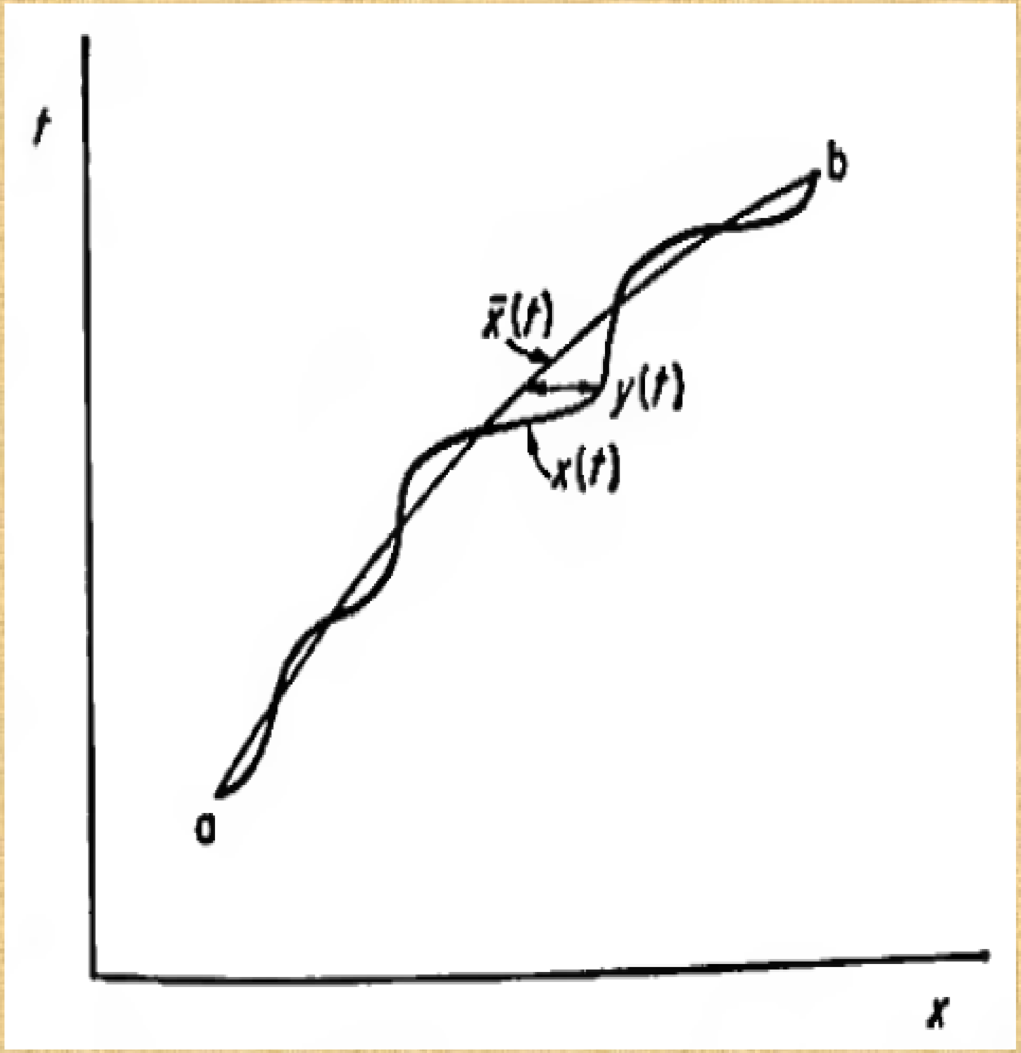
$$x(\tau) = \bar{x}(\tau) + y(\tau)$$

where $\bar{x}(\tau) = \text{classical trajectory}$, i.e., where the action is an extremum (S unchanged in the 1st order if $\bar{x}(\tau)$ is modified slightly.)

- Difference between classical path $\bar{x}(t)$ and a possible alternative path $x(t)$ is $y(t)$.
- Evidently

$$y(t_a) = y(t_b) = 0$$

- Classical path is constant



- Setting a new "integration variable"

$$y(t) = x(t) - \bar{x}(t)$$

$$\dot{y}(t) = \dot{x}(t) - \dot{\bar{x}}(t)$$

- the Lagrangian can be Taylor-expanded around $\bar{x}(t), \dot{\bar{x}}(t)$ as

$$L(x,\dot{x};t) = L(\bar{x},\dot{\bar{x}};t) + \left.\frac{\partial L}{\partial x}\right|_{\bar{x}} y + \left.\frac{\partial L}{\partial \dot{x}}\right|_{\dot{\bar{x}}} \dot{y}$$

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

- The Taylor expansion terminates after the second term since $L(x,\dot{x};\tau)$ is a quadratic functional.

- Substituting the Lagrangian for the harmonic oscillator yields for the action:

$$S = \int dt L(x,\dot{x};t) = \int_{t_i}^{t_f} L(\bar{x},\dot{\bar{x}};t) + \int_{t_i}^{t_f} dt \left(\frac{\partial L}{\partial x} y + \frac{\partial L}{\partial \dot{x}} \dot{y} \right)\Bigg|_{\bar{x},\dot{\bar{x}}}$$

$$+ \int_{t_i}^{t_f} dt \frac{1}{2} m \left(\dot{y}^2 - \omega^2 y^2 \right)$$

- Performing integration by parts and using $\left.\frac{\delta S}{\delta x}\right|_{\bar{x}} = 0$ from the definition of the classical path yields the expression

$$S = S_{cl} + \int_{t_i}^{t_f} dt \frac{1}{2} m\left(\dot{y}^2 - \omega^2 y^2\right)$$

Which gives for the amplitude

$$K(x_f, t_f; x_i, t_i) = \exp\left[\frac{iS(x_f, t_f; x_i, t_i)}{\hbar}\right]\tilde{K}(0, t_f; 0, t_i)$$

as the path integral only depends on time

- Employing the usual definitions of the path integral one writes

$$\tilde{K}(0,t_b;0,t_a) = \lim_{N\to\infty}\int dy_1 \ldots dy_N \left(\frac{m}{2\pi i\hbar\delta t}\right)^{\frac{N}{2}}$$

$$\times\exp\left\{\frac{i}{\hbar}\sum_{j=0}^{N}\left[\frac{m}{2\delta t}\left(y_j - y_{j-1}\right)^2 - \frac{1}{2}\delta t\omega^2 y_j{}^2\right]\right\}$$

- To deal with the multitude of integrals, one resorts to a method introduced by Gelfand and Yaglom

Gelfand-Yaglom Method

- The expression

$$\exp\left\{\frac{i}{\hbar}\sum_{j=0}^{N}\left[\frac{m}{2\delta t}\left(y_j - y_{j-1}\right)^2 - \frac{1}{2}\delta t\,\omega^2 y_j{}^2\right]\right\}$$

can be written in terms of matrix elements such that

$$\eta = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix}$$

and thus

$$\frac{i}{\hbar}\sum_{j=0}^{N}\left[\frac{m}{2\delta t}\left(y_j - y_{j-1}\right)^2 - \frac{1}{2}\delta t\,\omega^2 y_j{}^2\right] = -\eta^T \sigma \eta$$

- Here σ is the matrix defined by

$$\sigma = \frac{m}{2\delta t\hbar i}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{pmatrix} + \frac{i\delta t}{2\hbar}\begin{pmatrix} c_1 & & & & \\ & c_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & c_N \end{pmatrix}$$

and thus the amplitude can be written

$$\tilde{K} = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\delta t}\right)^{\frac{N}{2}}\int d^N\eta \exp\left(-\eta^T\sigma\eta\right)$$

- σ is of the form $i\tilde{\sigma}$ with $\tilde{\sigma}$ real and Hermitian → diagonalizable by a unitary matrix

$$\sigma = U^{+}\sigma_D U$$

where σ_D is the diagonal matrix of eigenvalues of σ . For real eigenvectors U is also real; one can set $\xi = U\eta$. Since $\left|\det U\right| = 1$ it is true that

$$\int d^N\eta e^{-\eta^T\sigma\eta} = \int d^N\xi e^{-\xi\sigma_D\xi} = \prod_{\alpha=1}^{N}\sqrt{\frac{\pi}{\sigma_\alpha}} = \frac{\pi^{N/2}}{\sqrt{\det\sigma}}$$

- The amplitude is then written as

$$\tilde{K}(0,t_f;0,t_i) = \lim_{N\to\infty}\left[\left(\frac{m}{2\pi i\hbar\delta t}\right)^{N+1}\frac{\pi^N}{\det\sigma}\right]^{1/2}$$

$$= \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar}\cdot\frac{1}{\delta t}\cdot\frac{1}{\left(\frac{2i\hbar\delta t}{m}\right)^N\det\sigma}\right]$$

- The factor

$$\left(\frac{2i\hbar\delta t}{m}\right)^N \det\sigma = \det\left\{\begin{bmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix} - \frac{(\delta t)^2}{m}\begin{bmatrix} c_1 & & & \\ & \ddots & & \\ & & \ddots & \\ & & & c_N \end{bmatrix}\right\}$$

$$\equiv \det\sigma'_N \equiv p_N$$

- The determinant can be calculated by considering truncated $j\times j$ matrices from σ'_N

- By expanding σ'_{j+1} in minors, it can be seen that they obey the recursion formula

$$p_{j+1} = \left(2 - \frac{(\delta t)^2}{m}\omega \right) p_j - p_{j-1}$$, where $j = 1, \ldots, N$

and $p_1 = 2 - (\delta t)^2 \omega / m$,

- Rewriting yields $p_0 = 1$

$$\frac{p_{j+1} - 2p_j + p_{j-1}}{(\delta t)^2} = -\frac{\omega p_j}{m}$$

- If one writes $\varphi(t) = \delta t p_j$ for $t = t_a + j\delta t$, then in the limit of $\delta t \to 0$, $\varphi(t)$ satisfies

$$\frac{d^2\varphi}{dt^2} = -\frac{\omega}{m}\varphi$$

with initial values

$$\varphi(0) = \delta t p_0 \to 0$$

$$\frac{d\varphi(0)}{dt} = \delta t\left(\frac{p_1 - p_0}{\delta t}\right) = 2 - \frac{(\delta t)^2}{m}\omega - 1 \to 1 \quad \text{as } N \to \infty$$

- Thus

$$f(t_f, t_i) = \lim_{N\to\infty}\left[\varepsilon\left(\frac{2i\hbar\delta t}{m}\right)^N \det\sigma\right] = \varphi(t_f)$$

is obtained by solving the differential equation

$$m\frac{\partial^2 f(t_f, t_i)}{\partial t^2} + \omega f(t_f, t_i) = 0$$

with initial conditions

$$f(t_i, t_i) = 0, \qquad \left.\frac{\partial f}{\partial t}(t, t_i)\right|_{t=t_a} = 1$$

- And thus, one arrives at the amplitude for the harmonic oscillator

$$K(x_f, t_f; x_i, t_i) =$$

$$\sqrt{\frac{m}{2\pi i\hbar f(t_f, t_i)}} \exp\left[\frac{i}{\hbar} S_c(x_f, t_f; x_i, t_i)\right]$$

Perturbation Expansions

- On general quadratic actions are relatively easy to solve using the path integral method.
- For general class of potentials → perturbation expansion of path integral.
- Start with a general expression for the potential → specialize to scattering problem.

- a particle moving in a potential $V(x,t)$ has the kernel

$$K_V(f,i) = \int_i^f \left(\exp\left\{ \frac{i}{\hbar} \int_{t_i}^{t_f} \left[\frac{m}{2}\dot{x}^2 - V(x,t) \right] dt \right\} \right) Dx(t)$$

where $Dx(t)$ is as previously defined.

- If the potential is small, then the potential part is:

$$\exp\left[-\frac{i}{\hbar} \int_{t_i}^{t_f} V(x,t)dt \right] = 1 - \frac{i}{\hbar} \int_{t_i}^{t_f} V(x,t)dt + \frac{1}{2!}\left(\frac{i}{\hbar}\right)^2 \left[\int_{t_i}^{t_f} V(x,t) \right]^2 \ldots$$

- Substituting into the original expression:

$$K_V(f,i) = K_0(f,i) + K^{(1)}(f,i) + K^{(2)}(f,i) + \ldots$$

where:

$$K_0(f,i) = \int_i^f \left[\exp\left(\frac{i}{\hbar} \int_{t_i}^{t_f} \frac{m\dot{x}^2}{2} dt \right) \right] Dx(t)$$

$$K^{(1)}(f,i) = -\frac{i}{\hbar} \int_i^f \left[\exp\left(\frac{i}{\hbar} \int_{t_a}^{t_b} \frac{m\dot{x}^2}{2} dt \right) \right] \int_{t_a}^{t_b} V[x(s),s] ds Dx(t)$$

$$K^{(2)}(f,i) = -\frac{1}{2\hbar^2} \int_i^f \left[\exp\left(\frac{i}{\hbar} \int_{t_a}^{t_b} \frac{m\dot{x}^2}{2} dt \right) \right] \int_{t_i}^{t_f} V[x(s)] ds$$

$$\times \int_{t_i}^{t_f} V[x(s'),s'] ds' Dx(t)$$

- Interchanging integration order and writing

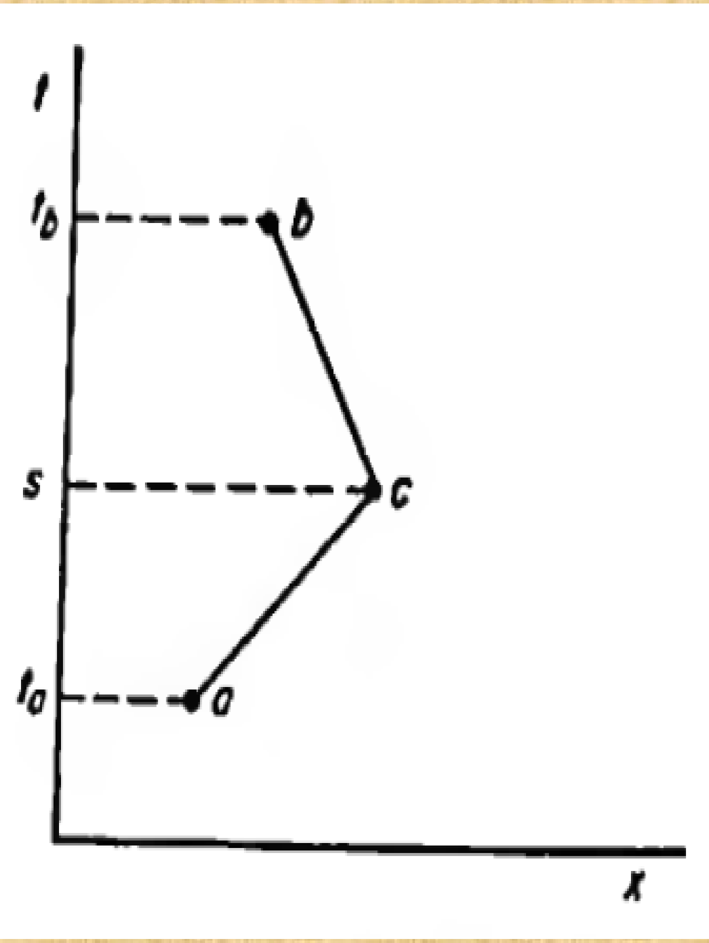
$$K^{(1)}(f,i) = -\frac{i}{\hbar}\int_{t_i}^{t_f} F(s)ds$$

where

$$F(s) = \int_i^f \left[\exp\left(\frac{i}{\hbar}\int_{t_i}^{t_f}\frac{m\dot{x}^2}{2}dt\right)\right] V\left[x(s), s\right] Dx(t)$$

- $F(s)$ is the sum over all paths of the free-particle amplitude; potential term can be additionally interpreted.

- However – weighted at time ***s*** by $V[x(s),s]$



- Before and after ***s*** – free particle.

- Unitarity of propagators → sum over all paths between ***i*** to ***c*** & ***c*** to ***f*** can be written $K_0(f,c)K_0(c,i)$

- Thus, for $s = t_c$, $F(s) = F(t_c)$ can be written as

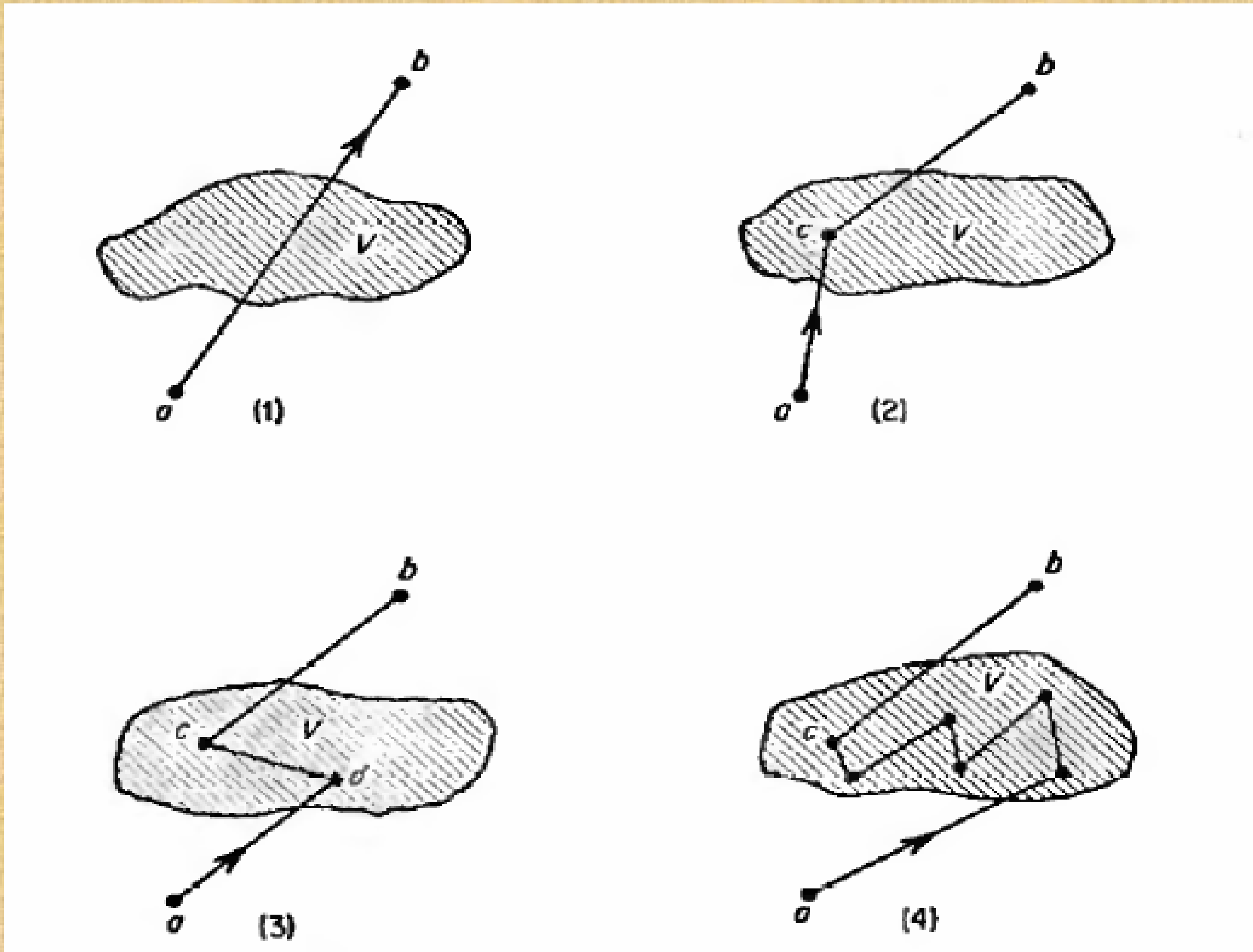
$$F(t_c) = \int_{-\infty}^{\infty} K_0(f, c) V(x_c, t) K_0(c, i) dx_c$$

- Substituting into the expression for $K^{(1)}(f, i)$

$$K^{(1)}(f, i) = -\frac{i}{\hbar} \int_{t_i}^{t_f} K_0(f, c) V(c) K_0(c, i) dx_c dt_c$$

- Can be interpreted as a free particle propagating from ***i*** to ***c***, is scattered, and finally propagates freely to ***f***

$$K_0(f,i), K_1(f,i), K_2(f,i), \ldots$$



- Thus, $K_V(f,i)$ can be written as

$$K_V(f,i) =$$

$$K_0(f,i) - \frac{i}{\hbar}\int K_0(f,c)V(c)K_0(c,i)\,d\tau_c +$$

$$\left(\frac{i}{\hbar}\right)^2 \iint K_0(f,c)V(c)K_0(c,d)V(d)K_0(d,i)\,d\tau_c\,d\tau_a + \ldots$$

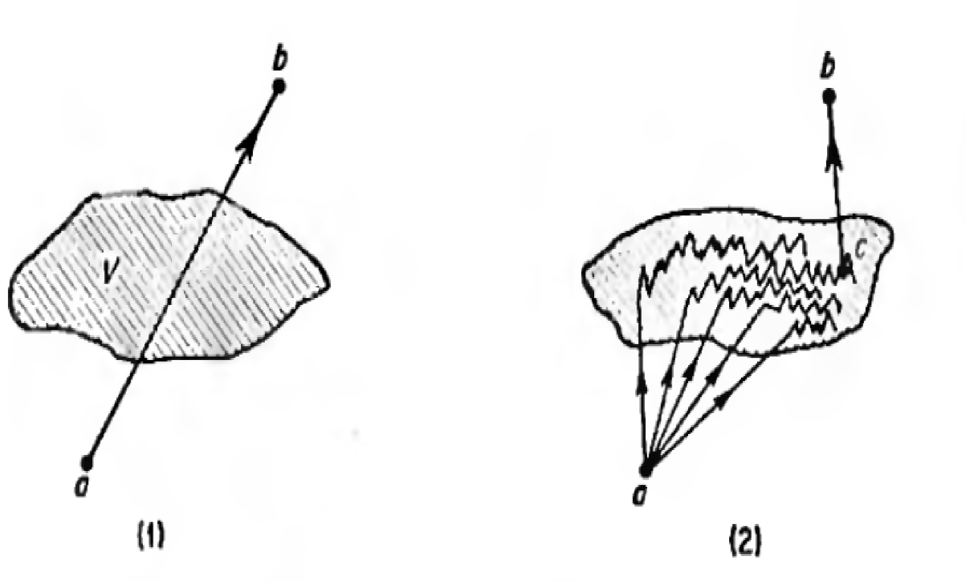
$$= K_0(f,i)$$

$$-\frac{i}{\hbar}\int K_0(f,c)V(c)\left[K_0(c,i) - \frac{i}{\hbar}\int K_0(f,d)V(d)K_0(d,i)\,d\tau_d + \ldots\right]$$

- Thus, one can also write

$$K_V(f,i) = K_0(f,i) - \frac{i}{\hbar}\int K_0(f,c)V(c)K_V(c,i)d\tau_c$$

- An integral equation describing K_V if K_0 is known.



- Operating $K_V(f,i)$ on a wavefunction yields

$$\psi(b) = \int K_V(f,i) f(i) dx_i$$

- Substituting the series expansion of K_V

$$\psi(b) = \int K_0(f,i) f(i) dx_i$$
$$- \frac{i}{\hbar} \int\int K_0(f,c) V(c) K_0(c,i) d\tau_c f(i) dx_i + \ldots$$

- The first term gives the unperturbed wavefunction at time t_f . Calling this term ϕ one has

$$\phi(f) = \int K_0(f,i) f(i) dx_i$$

which yields

$$\psi(b) = \phi(b) - \frac{i}{\hbar}\int K_0(f,c)V(c)\phi(c)d\tau_c$$

$$+\frac{i}{\hbar^2}\int\int K_0(f,c)V(c)K_0(c,d)V(d)\phi(d)d\tau_c d\tau_d + \dots$$

Thank You for Your Patience