Chapter 2
Quantum Dynamics

We discuss the dynamic development of state kets and/or observables (change with time).

2.1 Time Evolution and the Schrödinger Equ.;

t : is a parameter in Q.M. not op. (not observable).

The relativistic Q. Theory of fields does treat the time and space coords on the same footing, but it does so only at the expense of demoting position from the status of being an observable to that of being just a parameter

Time Evolution Op.:

$|\alpha, t_0\rangle$ the system at t_0

$|\alpha, t_0; t\rangle$ " " " t

Since t is a continuous parameter;

$$\lim_{t \to t_0} |\alpha, t_0; t\rangle = |\alpha, t_0\rangle \equiv |\alpha\rangle$$

or $\quad |\alpha, t_0; t_0\rangle = |\alpha, t_0\rangle$

We want to study $\quad |\alpha, t_0\rangle \equiv |\alpha\rangle \xrightarrow[?]{\text{time evolution}} |\alpha, t_0, t\rangle$

Put in another way; $\quad |\quad " \quad\rangle \xrightarrow[\substack{\text{under } t_0 \to t \\ \text{displacement}}]{\text{change?}} |\quad " \quad\rangle$

We make this relation by;

$$|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0)\,|\alpha, t_0\rangle$$

time-evolution op

What are the properties of $\mathcal{U}(t, t_0)$?

i) From the probability conservation;

$\langle \alpha, t_0 | \alpha, t_0\rangle = \langle \alpha, t_0; t | \alpha, t_0, t\rangle = 1$

$\rightarrow \quad \mathcal{U}(t_0, t)$ must be unitary $\qquad \mathcal{U}^{\dagger}(t, t_0)\,\mathcal{U}(t, t_0) = I$

Explanation;

Suppose at $t = t_0 \quad |\alpha, t_0\rangle = \sum_{a'} c_{a'}(t_0)\,|a'\rangle$

At a later time $\quad |\alpha, t_0; t\rangle = \sum_{a'} c_{a'}(t)\,|a'\rangle$

In general;

$$|c_{a'}(t_0)| \neq |c_{a'}(t)|$$

But if $[A, H] = 0 \longrightarrow |c_{a'}(t_0)| = |c_{a'}(t)|$

For exaple; spin $\frac{1}{2}$ case

Consider a spin $\frac{1}{2}$ system with its spin magnetic moment subjected to a uniform magnetic field in the z-dir.

To be specific; suppose;

at $t = t_0$ state $= |S_x, +\rangle$

as time goes $\longrightarrow$ the spin precesses in the xy-plane

i.e. at $t = t_0$ $|C_{S_x^+}(t_0)|^2 = 1$

but $t > t_0$ $|C_{S_x^+}(t)|^2 \neq 1$

Yet, $|C_{S_x^+}(t_0)|^2 + |C_{S_x^-}(t_0)|^2 = |C_{S_x^+}(t)|^2 + |C_{S_x^-}(t)|^2$

Generally; $\sum_{a'} |C_{a'}(t_0)|^2 = \sum_{a'} |C_{a'}(t)|^2$

ii) Composition property (a reasonable requirement)

$$\mathcal{U}(t_2, t_0) = \mathcal{U}(t_2, t_1)\, \mathcal{U}(t_1, t_0) \qquad t_2 > t_1 > t_0$$

iii) Let's consider an infinitesimal change in time;

$$|\alpha, t_0; t_0+dt\rangle = \mathcal{U}(t_0+dt, t_0)|\alpha, t_0\rangle$$

Because of continuity;

$$\lim_{dt \to 0} \mathcal{U}(t_0+dt, t_0) = I$$

Note that; $\mathcal{U}(t_2,t_0) = \mathcal{U}(t_2,t_1)\,\mathcal{U}(t_1,t_0)$

$\xrightarrow{\text{as } t_1 \to t_0}$ $\mathcal{U}(t_2,t_0) = \mathcal{U}(t_2,t_0)\,\mathcal{U}(t_0,t_0) \rightarrow \mathcal{U}(t_0,t_0) = I$

We assert that all these requirements are satisfied by;

$$\mathcal{U}(t_0+dt, t_0) - I = -i\Omega\, dt$$ first order in dt (we expect)

$\rightarrow \mathcal{U}(t_0+dt, t_0) = I - i\Omega\, dt$

where $\Omega = \Omega^{\dagger}$ (op.) dim. $= \frac{1}{t}$ (frequency)

Remark: If Ω op. depends on t explicitly, it must be evaluated at t_0.

The unitary property;

$$\mathcal{U}^{\dagger}(t_0+dt, t_0)\,\mathcal{U}(t_0+dt, t_0) = (1 + i\Omega^{\dagger} dt)(1 - i\Omega dt)$$

If $\Omega^{\dagger} = \Omega \rightarrow \mathcal{U}^{\dagger}(t_0+dt, t_0)\,\mathcal{U}(t_0+dt, t_0) \simeq I$ ignoring the $(dt)^2$ and higher terms

From the classical mechanics,

H : the generator of time evolution

$\xrightarrow{\text{in Q.M.}}$ $\Omega = \frac{H}{\hbar}$

$\rightarrow \mathcal{U}(t_0+dt, t_0) = I - \frac{iHdt}{\hbar}$

Is this $\hbar$, the famous $\hbar$?

We will see later if it is not, we are unable to obtain the relation $\frac{dx}{dt} = \frac{p}{m}$

as the classical limit of the corresponding Q. mechanical relation.

The Schrödinger Equ.:

Using the composition property:

$$\mathcal{U}(t+dt, t_0) = \mathcal{U}(t+dt, t)\,\mathcal{U}(t, t_0) = \left(I - \frac{iHdt}{\hbar}\right)\mathcal{U}(t, t_0)$$

where $t - t_0$: need not to be infinitesimal

$$\rightarrow \mathcal{U}(t+dt, t_0) - \mathcal{U}(t, t_0) = -i\left(\frac{H}{\hbar}\right)dt\,\mathcal{U}(t, t_0)$$

$$\rightarrow i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t_0) = H\,\mathcal{U}(t, t_0) \qquad (1)$$

This differential equ. is the Schrödinger equ for the Time-evolution op.

$$(1) \longrightarrow \quad i\hbar \frac{\partial}{\partial t} \mathcal{U}(t,t_0)\,|\alpha,t_0\rangle = H\,\mathcal{U}(t,t_0)\,|\alpha,t_0\rangle \qquad (1')$$

Also $\frac{\partial}{\partial t} |\alpha, t_0\rangle = 0$

$$(1') \longrightarrow \quad i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t\rangle = H\,|\alpha, t_0; t\rangle \qquad (2)$$

Alternative derivation;

$$|\alpha, t; t+\epsilon\rangle = \mathcal{U}(t, t+\epsilon)\,|\alpha, t\rangle$$

$$|\alpha,t\rangle + \epsilon \frac{d}{dt}|\alpha,t\rangle = \left(I - \frac{i\epsilon}{\hbar} H(t)\right)|\alpha,t\rangle$$

$$\rightarrow \quad i\hbar \frac{d}{dt}|\alpha,t\rangle = H(t)\,|\alpha,t\rangle$$

where $\frac{d}{dt}|\alpha,t\rangle = \lim_{\epsilon\to 0} \frac{|\alpha,t,t+\epsilon\rangle - |\alpha,t\rangle}{\epsilon}$

If $\mathcal{U}(t_0,t)$ is given, and we know how $\mathcal{U}(t_0,t)$ acts on $|\alpha,t_0\rangle$, then is no need to be involved with the Schrödinger equ.

Formal sol. to Schrödinger equ. for $\mathcal{U}(t_0,t)$:

$$i\hbar \frac{\partial}{\partial t} \mathcal{U}(t,t_0) = H\,\mathcal{U}(t,t_0)$$

Case 1 — H is indep. of t.

Ex. — H for a spin-magnetic moment interacting with a time-indep. mag. field.

In this case the sol. of (1) is,

$$\mathcal{U}(t_0,t) = e^{-\frac{iH(t-t_0)}{\hbar}} \qquad (3)$$

To prove this:

$$e^{-\frac{iH(t-t_0)}{\hbar}} = I - \frac{iH(t-t_0)}{\hbar} + \frac{(-i)^2}{2!}\left[\frac{H(t-t_0)}{\hbar}\right]^2 + \cdots \qquad (4)$$

$$\frac{\partial}{\partial t} e^{-\frac{iH(t-t_0)}{\hbar}} = -\frac{iH}{\hbar} + \frac{(-i)^2}{2!}\, 2\left(\frac{H}{\hbar}\right)^2 (t-t_0) + \cdots \qquad (5)$$

→ (3) obviously satisfies (1).

The <u>boundary</u> cond. is also satisfied.

$$\lim_{t\to t_0} \mathcal{U}(t_0,t) = \lim_{t\to t_0} e^{-\frac{iH(t-t_0)}{\hbar}} = I$$

Alternative way:

$$\mathcal{U}(t,t_0) = \lim \left[I - \frac{\left(\frac{iH}{\hbar}\right)(t-t_0)}{N} \right]^N = e^{-\frac{iH(t-t_0)}{\hbar}}$$

Case 2 — $\quad H = H(t) \quad$, but $\quad [H(t_1), H(t_2)] = 0$

Ex. — spin mag. moment subjected to mag. field whose strength varies with Time but whose dir. is always unchanged.

Formal sol.: $\quad \mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')}$

This can be proved in a similar way, by replacing $H(t-t_0)$ in (4) and (5) by $\int_{t_0}^{t} dt' \, H(t')$

Case 3 — $\quad [H(t_1), H(t_2)] \neq 0$

Ex. — H for spin-mag. moment interacting with Time dependent mag. field which changes in direction.

say, at $t = t_1$ the mag. field is in x-dir.
at $t = t_2$ " " " " " y-dir.
and so forth —

$H = \gamma S \cdot B$

$H(t_1) = \gamma S_x B_x \qquad H(t_2) = \gamma S_y B_y \cdots$

Since $[S_x, S_y] \neq 0 \rightarrow [H(t_1), H(t_2)] \neq 0$

Formal sol.;

$$\mathcal{U}(t,t_0) = I + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, H(t_1) \cdots H(t_n)$$

Dyson series

F. J. Dyson developed a perturbation expansion of this form in quanta field theory.

Proof.– When $[H(t_1), H(t_2)] \neq 0$

We cannot write $i\hbar \dfrac{d\mathcal{U}(t,t_0)}{\mathcal{U}(t,t_0)} = H(t)\, dt$

Now, $i\hbar \dfrac{\partial \mathcal{U}(t,t_0)}{\partial t} = H(t)\, \mathcal{U}(t,t_0)$

$$\partial\, \mathcal{U}(t,t_0) = -\frac{i}{\hbar} H(t)\, \mathcal{U}(t,t_0)\, dt$$

$$\rightarrow \mathcal{U}(t,t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} H(t')\, \mathcal{U}(t',t_0)\, dt'$$

satisfying the initial cond. (at $t=t_0$ $\mathcal{U}(t_0,t_0) = I$)

Dyson's series can be obtained by iteration.

Remark:

$$\mathcal{U}(t_2,t_0) = \mathcal{U}(t_2,t_1)\,\mathcal{U}(t_1,t_0)$$

$$\rightarrow \mathcal{U}(t,t) = \mathcal{U}(t,t_0)\,\mathcal{U}(t_0,t) = I$$

For unitary op. ; $\mathcal{U}^{\dagger}(t,t_0) = \mathcal{U}^{-1}(t,t_0)$

$$\begin{cases} \mathcal{U}(t,t_0)\,\mathcal{U}^{\dagger}(t,t_0) = I \\ \mathcal{U}(t,t_0)\,\mathcal{U}(t_0,t) = I \end{cases} \rightarrow \quad \mathcal{U}(t_0,t) = \mathcal{U}^{\dagger}(t,t_0) = \mathcal{U}^{-1}(t,t_0)$$

In the remaining part of this chap. we assume H : time-indep.

Energy Eigenkets:

How does $\mathcal{U}(t,t_0) = e^{-\frac{iH(t-t_0)}{\hbar}}$ act on $|\alpha\rangle$?

This is straightforward if the base kets used are eigenkets of A (i.e. $\{|a'\rangle\}$), such that:

$$[A, H] = 0$$

The eigenkets of A are *also* eigenkets of H, are called *energy* eigenkets;

$$H|a'\rangle = E_{a'}|a'\rangle$$

also $\quad A|a'\rangle = a'|a'\rangle$

$$e^{-\frac{iHt}{\hbar}} = \sum_{a'}\sum_{a''}|a''\rangle\langle a''|\, e^{-\frac{iHt}{\hbar}}\,|a'\rangle\langle a'| = \sum_{a'}|a'\rangle e^{-\frac{iE_{a'}t}{\hbar}}\langle a'|$$

$$|\alpha, t_0=0\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle = \sum_{a'} C_{a'}|a'\rangle$$

$$|\alpha, t_0=0; t\rangle = e^{-\frac{iHt}{\hbar}}|\alpha, t_0=0\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle\, e^{-\frac{iE_{a'}t}{\hbar}}$$

In other words;

$$C_{a'}(t=0) \longrightarrow C_{a'}(t) = C_{a'}(t=0)\, e^{-\frac{iE_{a'}t}{\hbar}}$$

with its *modulus* unchanged.

Notice that the relative *phases* (i.e. $e^{-\frac{i}{\hbar}(E_{a'}-E_{a''})t}$) do vary with time because the oscillation *frequencies* (i.e $\frac{E_{a'}}{\hbar}$) are *different*.

If $|\alpha, t_0 = 0\rangle = |a'\rangle$ eigenstate

$\rightarrow |\alpha, t_0 = 0; t\rangle = |a'\rangle e^{-\frac{iE_{a'}t}{\hbar}}$

Then if the system is initially a simultaneous eigenstate of A and H $\longrightarrow$ it remains so at all times.

Just we have phase modulation $e^{-\frac{iE_{a'}t}{\hbar}}$.

In this sense; if $[A, H] = 0 \longrightarrow A$: const. of motion

Generalization:

$$[A, B] = [B, C] = [A, C] = \cdots = 0$$
$$[A, H] = [B, H] = [C, H] = \cdots = 0$$

$$\rightarrow \quad e^{-\frac{iHt}{\hbar}} = \sum_{K'} |K'\rangle e^{-\frac{iE_{K'}t}{\hbar}} \langle K'|$$

where $K' \equiv (a', b', c', \ldots)$

$\rightarrow$ It is important to find a complete set of mutually compatible observables that also to commute with H.

Time Dependence of Expectation Values

Suppose at $t=0$ state $= |a'\rangle$ and $[A,H]=0$

Now we look at $\langle B\rangle$ where $[A,B]\neq 0$, $[B,H]\neq 0$ in general

Because, $|a', t_0=0, t\rangle = \mathcal{U}(t,0)|a'\rangle$

$$\rightarrow \langle a', t_0=0; t|B|a', t_0=0; t\rangle = \left(\langle a'|\mathcal{U}^\dagger(t,0)\right)\cdot B\cdot\left(\mathcal{U}(t,0)|a'\rangle\right)$$

$$= \langle a'|e^{+\frac{iE_{a'}t}{\hbar}} B e^{-\frac{iE_{a'}t}{\hbar}}|a'\rangle = \langle a'|B|a'\rangle$$

<u>indep. of t</u>

→ Expectation value of an observable taken with respect to an energy eigenstate <u>does not</u> change with <u>t</u>.

<u>For this reason</u> → An energy eigenstate is often referred to as a <u>stationary</u> state.

Now suppose we have a <u>nonstationary</u> state;

that is, $|\alpha, t_0=0\rangle = \sum_{a'} c_{a'}|a'\rangle$

$$\langle B\rangle = \left[\sum_{a'} C^*_{a'}\langle a'| e^{+\frac{iE_{a'}t}{\hbar}}\right]\cdot B\cdot\left[\sum_{a''} C_{a''} e^{-\frac{iE_{a''}t}{\hbar}}|a''\rangle\right]$$

$$= \sum_{a'}\sum_{a''} C^*_{a'} C_{a''}\langle a'|B|a''\rangle e^{-\frac{i(E_{a''}-E_{a'})t}{\hbar}} \qquad (1)$$

So, $\langle B\rangle$ consists of oscillating term with angular frequency; $\omega_{a''a'} = \frac{E_{a''}-E_{a'}}{\hbar}$

Spin Precession

The int. of spin mag. moment with an external mag. field B: $\quad H = -\mu\cdot B = -\frac{e}{m_e c} S\cdot B \quad (e<0)$

If $\bar{B} = B\hat{z}$ static, uniform

$\rightarrow \quad H = -\left(\frac{eB}{m_e c}\right) S_z$

Then $[H, S_z] = 0$

$\rightarrow$ Eigenstates of S_z are also energy eigenstates

$\rightarrow E_\pm = \mp\frac{e\hbar B}{2m_e c}$ for $|S_z,\pm\rangle$ (corresponding energy eigenvalues)

we define $\omega \equiv \frac{|e|B}{m_e c}$

$\rightarrow E_- - E_+ = \hbar\omega$

and $H = \omega S_z$

$$\mathcal{U}(t,0) = e^{-\frac{iH(t-t_0)}{\hbar}} = e^{-\frac{i\omega S_z t}{\hbar}}$$

Now $|\alpha, t_0=0\rangle = C_+|+\rangle + C_-|-\rangle$

$$\mathcal{U}(t,0)|\alpha, t_0=0\rangle = |\alpha, t_0=0; t\rangle = C_+ e^{-\frac{i\omega t}{2}}|+\rangle + C_- e^{+\frac{i\omega t}{2}}|-\rangle \quad (1)$$

where we have used $H|\pm\rangle = \frac{\pm\hbar\omega}{2}|\pm\rangle$

i) Now let us suppose that $C_+ = 1$, $C_- = 0$

i.e. $|\alpha, t_0=0\rangle = |+\rangle$

Equ. (1) tells us at a later time the state is still in spin-up state (which is no surprise, because it is a stationary state)

ii) Now let us suppose

$$|\alpha, t_0=0\rangle = |S_x, +\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle$$

i.e. $C_1 = C_2 = \frac{1}{\sqrt{2}}$

The probabilities for the system to be found in the $|S_x;\pm\rangle$ state at some later time t;

$$|\langle S_x,\pm|\alpha, t_0=0; t\rangle|^2 =$$

$$= \left|\left[\tfrac{1}{\sqrt{2}}\langle +| \pm \tfrac{1}{\sqrt{2}}\langle -|\right]\cdot\left[\tfrac{1}{\sqrt{2}} e^{\frac{-i\omega t}{2}}|+\rangle + \tfrac{1}{\sqrt{2}} e^{\frac{+i\omega t}{2}}|-\rangle\right]\right|^2$$

$$= \left|\tfrac{1}{2} e^{\frac{-i\omega t}{2}} \pm \tfrac{1}{2} e^{\frac{+i\omega t}{2}}\right|^2 = \begin{cases} \cos^2\frac{\omega t}{2} & \text{for } |S_x;+\rangle \\ \sin^2\frac{\omega t}{2} & ,\ |S_x;-\rangle \end{cases}$$

Eventhough the spin is initially in the positive x-dir., (i.e. $|S_x,+\rangle$), the $\bar{B}$ along $\hat{z}$-dir $\xrightarrow{\text{Causes}}$ it to rotate.

$|C_+(t)|^2 + |C_-(t)|^2 = 1$ in agreement with the unitary property of $\mathcal{U}$.

Using. $\langle A\rangle = \sum_{a'} a' |\langle a'|\alpha\rangle|^2$

$$\rightarrow \langle S_x\rangle = \frac{\hbar}{2}\cos^2\frac{\omega t}{2} + \left(-\frac{\hbar}{2}\right)\sin^2\frac{\omega t}{2} = \frac{\hbar}{2}\cos\omega t$$

This is in agreement with Equ. (1) P93.

We may check also,

$\langle S_y\rangle = \frac{\hbar}{2}\sin\omega t \qquad \langle S_z\rangle = 0$

$\xrightarrow{\text{result}}$ The spin precesses in the xy-plane.

Correlation Amplitude and Energy-Time Uncertainty Relation:

$|\alpha, t_0=0, t_1\rangle \xleftrightarrow[\text{times are correlated with each other ?}]{\text{How state kets at different}} |\alpha, t_0=0, t_2\rangle \qquad t_1 \neq t_2$

Now;

$$C(t) = \langle \alpha, t_0=0 | \alpha, t_0=0; t\rangle = \langle \alpha, t_0=0 | \mathcal{U}(t,0) | \alpha, t_0=0\rangle$$

The extent of similarity of the states ket at $t=0$ and $t=t$.

(or Correlation Amplitude)

The modulus $C(t)$ $\xrightarrow{\text{Provides}}$ a quantitative measure of resemblance between the state kets at different times.

Ex. — initial state $= |a'\rangle$ one of the eigenstates of H

$$\longrightarrow \quad C(t) = \langle a' | a', t_0=0, t\rangle = e^{\frac{-iE_{a'}t}{\hbar}}$$

$\rightarrow |C(t)| = 1 \quad \forall t$ (which is not surprizing for stationary state)

Ex- More general situation;

$$\text{initial state} = \sum_{a'} C_{a'} |a'\rangle \qquad \{|a'\rangle\}\text{; eigenkets of } H$$

$$C(t) = \left(\sum_{a'} C_{a'}^* \langle a'|\right)\left[\sum_{a''} C_{a''} e^{\frac{-iE_{a''}t}{\hbar}} |a''\rangle\right]$$

$$= \sum_{a'} |C_{a'}|^2 e^{\frac{-iE_{a'}t}{\hbar}} \qquad (1)$$

As $t \longrightarrow$ large $\longrightarrow$ A strong cancellation is possible.

We expect;

$C(0) = 1 \longrightarrow C(t) \rightarrow$ decrease (with Time)

To estimate (1) in a more concrete manner; suppose that;

$|\ \rangle$ = Superposition of so many energy eigenkets with similar energies (quasi-continuous spectrum)

$$\sum_{a'} \rightarrow \int dE\, \rho(E) \qquad C_{a'} \rightarrow g(E)\Big|_{E=E_{a'}}$$

$$(1) \longrightarrow C(t) = \int dE\, |g(E)|^2 \rho(E)\, e^{-\frac{iEt}{\hbar}}$$

Subject to the normalization cond.;

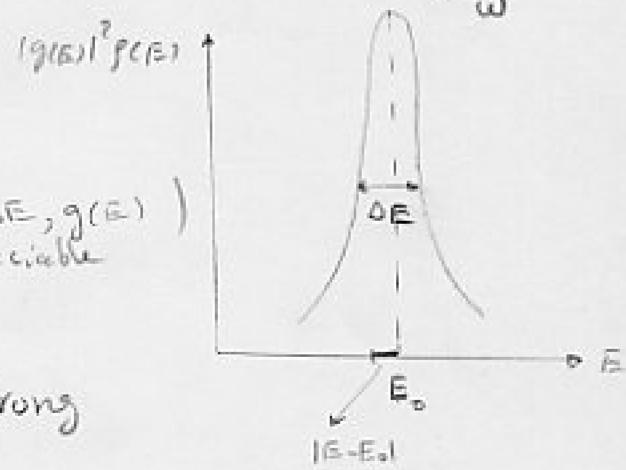
$$\int dE\ |g(E)|^2\ \rho(E) = 1$$

In realistic physical situation;

$|g(E)|^2 \rho(E)$ may be peaked around $E=E_0$ with width $=\Delta E$

$$(1)\quad C(t) = e^{-\frac{iE_0t}{\hbar}} \int dE\ |g(E)|^2\ \rho(E)\ e^{-\frac{i(E-E_0)t}{\hbar}}$$

As $t \to$ large $\longrightarrow$ the integrand oscillates very rapidly unless $|E-E_0| < \frac{\hbar}{t}$ (or $\underbrace{\frac{|E-E_0|}{\hbar}}_{\omega} < \frac{1}{t}$)

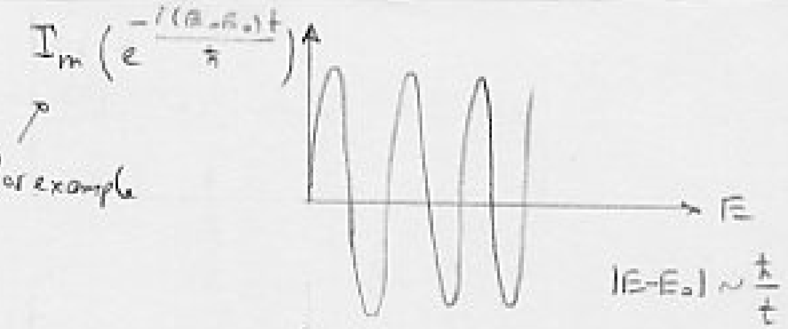


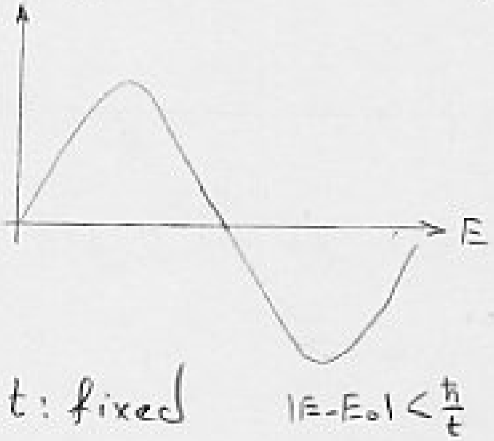
If the interval for which ($|E-E_0| \approx \frac{\hbar}{t}$) $\ll \Delta E$ (within ΔE, $g(E)$ is appreciable)

$\longrightarrow C(t) \to 0$ because of strong oscillations

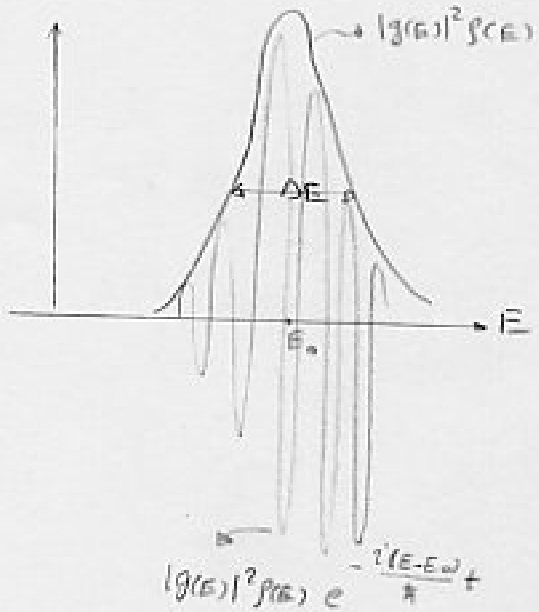
$t \simeq \frac{\hbar}{\Delta E}$ the characteristic time at which $|C(t)|$ starts becomming $|C(t)| \neq 1$ appreciably

Explanation:





Eventhough $t \simeq \frac{\hbar}{\Delta E}$ is obtained for a superposition state with quasi-continuous energy spectrum, it make sense for a two level system.



$|E-E_0| \approx \frac{\hbar}{t} << \Delta E$

In spin precession prob.;

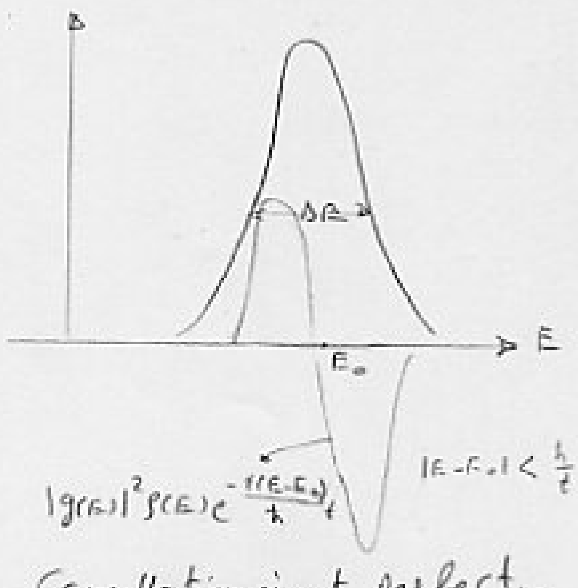
$$|\langle S_{x},+|\alpha, t_0=0; t\rangle|^2 = \cos^2\frac{\omega t}{2}$$

The initially $|S_x,+\rangle$ state starts losing its identity after $t \sim \frac{1}{\omega} = \frac{\hbar}{E_+ - E_-}$

Conclusion:

A physical system ceases to retain its original form after $\Delta t \sim \frac{\hbar}{\Delta E}$

$\rightarrow \Delta t \, \Delta E \simeq \hbar$ Time-energy uncertainty relation



Cancellation is not perfect.

But its nature is different from the uncertainty relation for two incompatible observables.

2.2 The Schrödinger Versus Heisenberg Picture;

Unitary OPs.;

Schrödinger Picture: $|\alpha, t_0; t\rangle = \mathcal{U}(t,t_0)|\alpha, t_0\rangle$ They change with t

A,s : They are fixed in t

Heisenberg Picture: $|\alpha, t_0\rangle$: Fixed in t

A,s : They change with t

These two formulation of Q.M. are equivalent.

General Comments on Unitary OPs.:

We use them for different purposes in Q.M.,

i) Ex.

$$\{|a'\rangle\} \xleftrightarrow{\mathcal{U}} \{|b'\rangle\}$$

In this example the state kets are assumed not to change as we switch from $\{|a'\rangle\}$ to $\{|b'\rangle\}$, even though the numerical values of the expansion coeffs for $|\alpha\rangle$ are of course different in different representations.

ii) Ex. $|\alpha\rangle \xrightarrow{\mathcal{T}(dx)} |\alpha'\rangle$ (translation)

$|\alpha, t_0\rangle \xrightarrow{\mathcal{U}(t,t_0)} |\alpha, t_0, t\rangle$ (time-evolution)

These two <u>actually change</u> the state kets.

Under unitary transformation; $|\alpha\rangle \to \mathcal{U}|\alpha\rangle$

$\langle\beta|\alpha\rangle \to \langle\beta|\mathcal{U}^{\dagger}\mathcal{U}|\alpha\rangle = \langle\beta|\alpha\rangle$ inner product unchanged

Using the <u>fact</u> that <u>these</u> transformations <u>affect the state kets</u> <u>but not</u> <u>OPS.</u>;

$\langle\beta|X|\alpha\rangle \longrightarrow (\langle\beta|\mathcal{U}^{\dagger}) \cdot X \cdot (\mathcal{U}|\alpha\rangle) = \langle\beta|\mathcal{U}^{\dagger}X\mathcal{U}|\alpha\rangle$

From A. A. M $\to$ $(\langle\beta|\mathcal{U}^{\dagger}) \cdot X \cdot (\mathcal{U}|\alpha\rangle) = \langle\beta|\cdot(\mathcal{U}^{\dagger}X\mathcal{U})\cdot|\alpha\rangle$

This identity suggests <u>two</u> approaches to unitary tr.;

Approach 1: $|\alpha\rangle \to \mathcal{U}|\alpha\rangle$ with operators unchanged

" 2: $X \to \mathcal{U}^{\dagger}X\mathcal{U}$ " state kets "

In <u>Classical</u> Phys. ;

We <u>don't</u> introduce state kets, yet we talk about translation, time-evolution and the like.

This is possible because these operations actually change quantities such as $\bar{x}$ and $\bar{L}$ (which are observables of Classical M.).

<u>Conjecture</u> $\longrightarrow$ A <u>closer</u> connection may be established if we follow <u>approach 2</u>.

<u>Ex.</u> - Translation $\tau(dx')$

Approach 1 — $$|\alpha\rangle \longrightarrow \left(I - \frac{iP \cdot dx'}{\hbar}\right)|\alpha\rangle$$

$$x \longrightarrow x$$

Approach 2 — $$|\alpha\rangle \longrightarrow |\alpha\rangle$$

$$x \rightarrow \left(I + \frac{iP\cdot dx'}{\hbar}\right) x \left(I - \frac{iP\cdot dx'}{\hbar}\right)$$

$$= x + \frac{i}{\hbar}[P\cdot dx', x]$$

$$= x + dx' I$$

It can be shown;

$\langle x \rangle_{\tau(dx')|\alpha\rangle}$ and $\langle x \rangle_{|\alpha\rangle} + \langle dx' I \rangle_{|\alpha\rangle}$ lead to the same result.

State Kets and Observables in the Schrödinger and the Heisenberg Pictures:

We set $t_0 = 0 \quad \rightarrow \mathcal{U}(t, t_0 = 0) \equiv \mathcal{U}(t) = e^{-\frac{iHt}{\hbar}}$

Def.- $\quad A^{(H)}(t) \equiv \mathcal{U}^{\dagger}(t)\, A^{(S)}\, \mathcal{U}(t)$ $\qquad$ Heisenberg picture Observable

$\rightarrow \quad A^{(H)}(0) = A^{(S)}$

$|\alpha, t_0 = 0; t\rangle_H = |\alpha, t_0 = 0\rangle$ $\qquad$ Heisenberg picture state ket is frozen to what it was at $t=0$ (indep. of t)

while; $|\alpha, t_0 = 0; t\rangle_S = \mathcal{U}(t)\, |\alpha, t_0 = 0\rangle$

Obviously: $\langle A\rangle_S = \langle A\rangle_H$

$${}_S\langle\alpha, t_0=0; t|\, A^{(S)}\, |\alpha, t_0 = 0, t\rangle = \langle\alpha, t_0 = 0|\, \mathcal{U}^{\dagger}(t)\, A^{(S)}\, \mathcal{U}(t)\, |\alpha, t_0 = 0\rangle$$

$$= {}_H\langle\alpha, t_0 = 0; t|\, A^{(H)}(t)\, |\alpha, t_0 = 0; t\rangle_H$$

The Heisenberg Equ. of Motion:

Assuming $A^{(S)} \neq A^{(S)}(t)$ explicitly — which is the case in most physical situations

$$A^{(H)}(t) \equiv \mathcal{U}^{+}(t)\, A^{(S)}\, \mathcal{U}(t) \quad , \quad \mathcal{U}(t) = e^{\frac{-iHt}{\hbar}}$$

$$\longrightarrow \frac{dA^{(H)}}{dt} = \frac{\partial U^{+}}{\partial t} A^{(S)} U + U^{+} A^{(S)} \frac{\partial U}{\partial t} + 0$$

$$= -\frac{1}{i\hbar} U^{+} H U \underbrace{U^{+} A^{(S)} U}_{A^{(H)}} + \frac{1}{i\hbar} \underbrace{U^{+} A^{(S)} U}\, U^{+} H U = \frac{1}{i\hbar}\left[A^{(H)}, U^{+} H U\right]$$

where we have used; $\frac{\partial U}{\partial t} = \frac{1}{i\hbar} H U$, $\frac{\partial U^{+}}{\partial t} = -\frac{1}{i\hbar} U^{+} H$

But since $H^{(H)} = U^{+} H U = H \qquad ([H, U] = 0)$

$$\longrightarrow \frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}\left[A^{(H)}, H\right]$$

Equ. of motion in the Heisenberg picture

Comparison with the classical equ. of motion in Poisson bracket form:

$$\frac{dA}{dt} = [A, H]_{cl.} \qquad \text{where } A = A(q, p)$$

Dirac quantization rule $[\,,\,]_{cl} \longrightarrow \frac{[\,,\,]}{i\hbar}$ leads to the correct equ. in Q.M.

This makes sense if $A^{(H)}$ has a classical analogue.

For example the spin op. in Heisenberg picture satisfies

$$\frac{dS_i^{(H)}}{dt} = \frac{1}{i\hbar}\left[S_i^{(H)}, H\right]$$

but this equ. has <u>no</u> classical counterpart, because S_z <u>cannot</u> be written as a func. of q_i's and p_i's.

<u>Rather</u> we may argue that for quantities possessing classical counterparts, the correct classical equ. can be obtained in the following way:

$$\frac{[\ ,\ ]}{i\hbar} \longrightarrow [\ ,\ ]_{cl.}$$

$$Q.M \longrightarrow Cl.M.$$

Free Particles; <u>Ehrenfest's</u> Theorem;

For physical systems with classical <u>analogues</u>,

$H_{cl} \xrightarrow{\text{Assume}} H_{cl}$ but x_i's, p_i's $\xrightarrow[\text{by the}]{\text{replaced}}$ corresponding ops.

Cl.M. $\qquad\qquad$ Q.M

Whenever an ambiguity arises because of noncommuting observables, we attempt to resolve it by requiring H to be Hermitian

Ex.

$$XP \longrightarrow \frac{1}{2}(XP+PX)$$

in cl.M.

When the physical system in question has no classical analogues, we can only guess the structure of H op.

The empirical observations must confirm it.

For free-particle of mass m;

$$H = \frac{P^{(H)2}}{2m} = \frac{(P_x^{(H)2} + P_y^{(H)2} + P_z^{(H)2})}{2m}$$

$$\frac{dP_i^{(H)}}{dt} = \frac{1}{i\hbar}\left[P_i^{(H)}, H\right] = \frac{1}{i\hbar}\left[P_i^{(H)}, H^{(H)}\right] = 0$$

Remark; $\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}[A^{(H)}, H] = \frac{1}{i\hbar}[A^{(H)}, H^{(H)}] = \frac{1}{i\hbar}\mathcal{U}^{+}(t)[A, H]\mathcal{U}(t) = \frac{1}{i\hbar}[A, H]^{(H)}$

For free particle $P_i^{(H)}(t) = P_i^{(H)}(0)$ const. of motion

Quite generally; if $[A^{(H)}, H] = 0 \rightarrow$

$\frac{dA^{(H)}}{dt} = 0$ const. of motion

Next;

$$\frac{dx_i^{(H)}}{dt} = \frac{1}{i\hbar}\left[x_i^{(H)}, H\right] = \frac{1}{i\hbar}\left\{\frac{1}{2m} i\hbar \frac{\partial}{\partial p_i}\left(\sum_{j=1}^{3} p_j^2\right)\right\}^{(H)}$$

$$= \frac{p_i^{(H)}}{m} = \frac{p_i^{(H)}(0)}{m} \rightsquigarrow \text{for free particle}$$

where we have used $\quad [x_i, F(\bar{p})] = i\hbar \frac{\partial F}{\partial p_i}$

$$\longrightarrow x_i(t) = x_i(0) + \frac{p_i(0)}{m} t$$

which is a reminiscent of classical trajectory equ. for a uniform rectilinear motion.

Note that even though;

$$[x_i(0), x_j(0)] = 0 \qquad \text{at equal times}$$

but $\quad [x_i(t_1), x_j(t_2)] \neq 0 \qquad t_1 \neq t_2$

Specifically; $[x_i(t), x_i(0)] = \left[\frac{p_i(0)}{m}, x_i(0)\right] = \frac{-i\hbar t}{m}$

Applying $\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$ to this commutator

$$\langle(\Delta x_i)^2_t\rangle\langle(\Delta x_i)^2_{t=0}\rangle \geq \frac{\hbar^2 t^2}{4m^2}$$

$\longrightarrow$ Even if the particle is well localized at $t=0$, its position becomes more and more uncertain with t. (which can be concluded also by studying the time-evolution behavior of free-particle wave packets.) (But it still remains at its initial energy eigenstate)

We now add a pot. $V(\bar{x})$ to free-particle H;

$$H = \frac{P^2}{2m} + V(\bar{x}) \qquad V(\bar{x}) \equiv V(x,y,z)$$

Using $[P_i, G(\bar{x})] = -i\hbar \frac{\partial G}{\partial x_i}$

$$\frac{dP_i^{(H)}}{dt} = \frac{1}{i\hbar}[P_i^{(H)}, H] = \frac{1}{i\hbar}[P_i, V(\bar{x})]^{(H)} = -\frac{\partial}{\partial x_i} V(\bar{x}) \qquad (1)$$

On the other hand $\frac{dx_i^{(H)}}{dt} = \frac{P_i^{(H)}}{m}$ still holds;

because $[x_j, V(\bar{x})] = 0$

We use once again the Heisenberg equ. of motion;

$$\frac{d^2 x_i}{dt^2} = \frac{1}{i\hbar}\left[\frac{dx_i^{(H)}}{dt}, H\right] = \frac{1}{i\hbar}\left[\frac{P_i^{(H)}}{m}, H\right] = \frac{1}{i\hbar}\left[\frac{P_i}{m}, H\right]^{(H)}$$

$$= \frac{1}{m}\frac{dP_i^{(H)}}{dt} \quad \text{from Heisenberg equ.} \qquad (2)$$

$$(1)(2) \longrightarrow \quad m\frac{d^2\bar{x}^{(H)}}{dt^2} = -\nabla V(x)^{(H)} \quad (3)$$

Q. mechanical analogue of Newton's Second law

$$m\frac{d^2}{dt^2}\langle \bar{x}^{(H)}\rangle_H = \frac{d\langle \bar{p}^{(H)}\rangle_H}{dt} = -\langle \nabla V(x)^H \rangle_H \quad (4)$$

Ehrenfest Theorem

Equ (4) is valid also in the Schrödinger picture.

(expectation values are the same in two picture)

while equ. (3) has meaning only when x and p are written in Heisenberg picture.

We note that $\hbar$'s have completely disappeared in (4).

$\longrightarrow$ The center of a wave packet moves like a classical particle subjected to $V(\bar{x})$.

Base Kets and Transition Amplitudes;

How the base Kets evolve in time?

A common misconception:

It is not true to say;

As Time goes on, all Kets move in the Schrödinger picture and are stationary in the Heisenberg picture!!!

The important point is to distinguish the behavior of state kets from that of base kets.

What happens to $A|a'\rangle = a'|a'\rangle$ with Time?

In the Schrödinger picture;

$A^{(s)}$: does not change with t

$\longrightarrow$ So the base kets obtained as the sols. to $A|a'\rangle = a'|a'\rangle$ at $t=0$ (for instance) must remain unchanged.

$\longrightarrow$ The base kets do not change in the Schrödinger picture (unlike the state kets)

In the Heisenberg picture:

$$A^{(H)}(t) = \mathcal{U}^{+} A^{S}\, \mathcal{U} = \mathcal{U}^{+} A(0)\, \mathcal{U}$$

From $A|a'\rangle = a'|a'\rangle$ (evaluated at $t=0$) when the two pictures coincide,

$$\longrightarrow \quad \mathcal{U}^{+} A(0)|a'\rangle = a'\, \mathcal{U}^{+}|a'\rangle$$

$$\longrightarrow \quad \mathcal{U}^{+} A(0)\, \mathcal{U}\mathcal{U}^{+}|a'\rangle = a'\, \mathcal{U}^{+}|a'\rangle$$

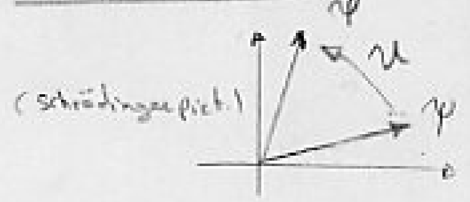
$$\longrightarrow \quad A^{(H)}(t)\left(\mathcal{U}^{+}|a'\rangle\right) = a'\left(\mathcal{U}^{+}|a'\rangle\right) \qquad (1)$$

Now, if we continue to <u>maintain</u> the view that the eigenkets of observables form the base kets $\longrightarrow \{\mathcal{U}^{+}|a'\rangle\}$ <u>must</u> be used as the base kets in the <u>Heisenberg</u> picture.

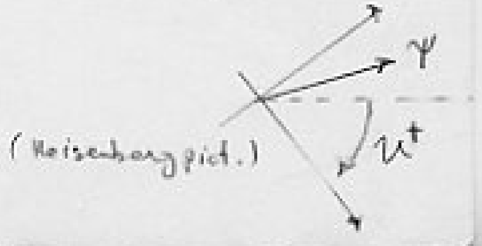
$$|a',t\rangle_H = \mathcal{U}^{+}|a'\rangle$$ base kets in Heisenberg picture

Because of $\mathcal{U}^{+}$ they are seen to rotate oppositely when compared with the Schrödinger picture <u>state kets</u>.

Specifically: $|a',t\rangle_H$ satisfies <u>wrong-sign</u> Schrödinger equ.



$$i\hbar \frac{\partial}{\partial t}|a',t\rangle_H = -H|a',t\rangle$$



As for the eigenvalues themselves,

(1) $\xrightarrow{\text{Shows}}$ They are <u>unchanged</u> with <u>t</u>.

This is consistent with the theorem on <u>unitary equivalent</u> <u>observables</u> (P 56).

$\left\{ \begin{array}{l} \text{Remark: in this case } \mathcal{U} \to \mathcal{U}^{+} = \mathcal{U}^{-1} \\ \text{and } \mathcal{U}^{-1} \to \mathcal{U} \end{array} \right.$

Notice also, the following expansion;

$$A^{(H)}(t) = \sum_{a'} |a',t\rangle_H \, a' \, {}_H\langle a',t| = \sum_{a'} \mathcal{U}^{+}|a'\rangle a' \langle a'|\mathcal{U}$$

$$= \mathcal{U}^{+} A^{(S)} \mathcal{U}$$

which shows everything is quite consistent provided;

$$|a',t\rangle_H = \mathcal{U}^{+}|a'\rangle$$

Also,

$$C_{a'}(t) = \langle a'|\alpha, t_0=0, t\rangle = \underbrace{\langle a'|}_{\text{base bra}} \cdot \underbrace{(\mathcal{U}|\alpha, t_0=0\rangle)}_{\text{state ket}}$$

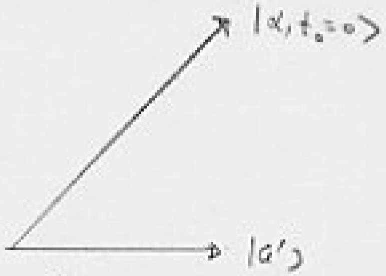
in the schrödinger picture

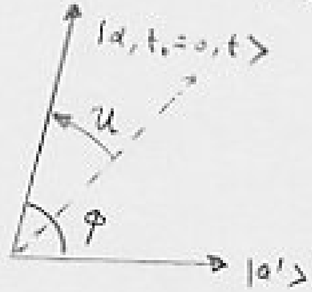
$$C_{a'}(t) = \underbrace{(\langle a'|\mathcal{U})}_{\text{base bra}} \cdot \underbrace{|\alpha, t_0=0\rangle}_{\text{state ket}}$$

" " Heisenberg "

$C_{a'}(t)$ (expansion coeffs. of a state ket) are <u>same</u> in both picture.

In other words ; $\cos\varphi = \cos\varphi'$





Remark:

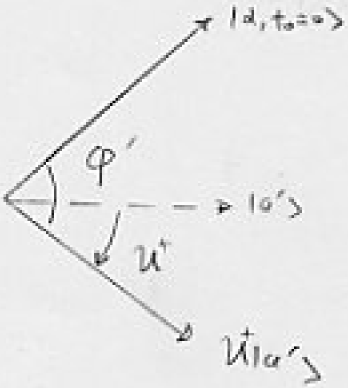
$U|\alpha,t=0\rangle = |\alpha,t=0,t\rangle = \sum_{a'} \langle a'|U|\alpha,t=0\rangle\, |a'\rangle$

$|\alpha,t=0\rangle = \sum_{a'} (\langle a'|U)\,|\alpha,t=0\rangle\, (U^\dagger|a'\rangle)$

$= \sum_{a'} \langle a'|U|\alpha,t=0\rangle\, U^\dagger|a'\rangle$

$\varphi = \varphi'$ ←

$\cos\varphi = \cos\varphi'$



These considerations apply equally well to base kets that exhibit a continuous spectrum.

Further equivalence between the two picture,

Suppose; a physical system $= |a'\rangle$ at $t=0$ (eigenstate of A)

What is the probability amplitude to be found in $|b'\rangle$ (or transition ")

(eigenstate of B) at some later time t ?

Transition amplitude $= \underbrace{\langle b'|}_{\substack{\text{base bra} \\ \text{(fixed)}}} \cdot \underbrace{(U|a'\rangle)}_{\text{state ket}}$ Schrödinger picture

$= \underbrace{(\langle b'|U)}_{\text{base bra}} \cdot \underbrace{|a'\rangle}_{\substack{\text{state ket} \\ \text{(fixed)}}}$ Heisenberg "

Obviously they are the <u>same</u>. $= \langle b'|\mathcal{U}(t,0)|a'\rangle$

	Schrödinger picture	Heisenberg picture
State ket	Moving	Stationary
Observable	Stationary	Moving
Base ket	"	" oppositely

Ex.-- A state : $|a', t_0=0\rangle$ at t_0

" : $|a', t_0=0, t\rangle = U|a', t_0=0\rangle$ at t

The base : $\{|a', t_0=0\rangle\}$

Schrödinger picture

The same state : $|a', t_0=0, t\rangle_H = |a', t_0=0\rangle$ at all t

The base : $\{U^{+}|a', t_0=0\rangle\}$

Heisenberg Picture

See Fig (P113)

2.3 Simple Harmonic Osc.:

Energy Eigenkets and Energy Eigenvalues:

The basic Hamiltonian: $H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$ $\qquad \omega = \sqrt{\frac{k}{m}}$

x, p: Hermitian ops.,

Dirac's operator method:

We define two non-Hermitian ops.:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), \qquad a^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

(annihilation op) $\qquad\qquad$ (creation op.)

$$[a, a^{+}] = \left(\frac{1}{2\hbar}\right)\left(-i[x,p] + i[p,x]\right) = I$$

We also define the number op.:

$$N = a^{+}a \qquad \text{(obviously } N = N^{+}\text{)}$$

$$a^{+}a = \left(\frac{m\omega}{2\hbar}\right)\left(x^2 + \frac{p^2}{m^2\omega^2}\right) + \left(\frac{i}{2\hbar}\right)[x,p] = \frac{H}{\hbar\omega} - \frac{1}{2}$$

$$\longrightarrow H = \hbar\omega\left(N + \tfrac{1}{2}\right) \qquad \longrightarrow [H, N] = 0$$

$$\longrightarrow \begin{cases} N|n\rangle = n|n\rangle \\ H|n\rangle = \hbar\omega\left(n + \tfrac{1}{2}\right)|n\rangle \end{cases}$$

where $|n\rangle$ is simultaneous eigenket of N and H

i.e. $\rightarrow$ $E_n = (n+\frac{1}{2})\hbar\omega$

Note also that $[N,a] = [a^+a, a] = a^+[a,a] + \underbrace{[a^+,a]}_{-1}a = -a$

Likewise; $[N, a^+] = a^+$

As a result; $Na^+|n\rangle = ([N,a^+] + a^+N)|n\rangle = (n+1)a^+|n\rangle$ (1)

and $Na|n\rangle = ([N,a] + aN)|n\rangle = (n-1)a|n\rangle$ (2)

$\rightarrow$ $\begin{cases} a^+|n\rangle : \text{ eigenket of } N \text{ with eigenvalue of } (n+1) \\ a|n\rangle : \quad " \quad " \quad " \quad " \quad " \quad (n-1) \end{cases}$

(2) $a|n\rangle \sim |n-1\rangle \longrightarrow a|n\rangle = c|n-1\rangle$

but since $\langle n|n\rangle = 1$, $\langle n-1|n-1\rangle = 1$

$\langle n|\underbrace{a^+a}_{N}|n\rangle = |c|^2 \rightarrow n = |c|^2$

c: Real, positive by convention

$a|n\rangle = \sqrt{n}\,|n-1\rangle$

Similarly $a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$

Applying annihilation op. repeatdly:

$$a^2|n\rangle = \sqrt{n(n-1)}\ |n-2\rangle$$
$$a^3|n\rangle = \sqrt{n(n-1)(n-2)}\ |n-3\rangle$$
$$\vdots$$

This sequence will terminate if n is $\begin{cases}\text{Positive} \\ \text{integer}\end{cases}$

If n is not integer $\longrightarrow$ the sequence will not terminate

(coeff $\xrightarrow[\text{go to}]{\text{will not}}$ 0)

leading to eigenkets with a negative value of n.

But we also have the possibility requirement for the norm of $a|n\rangle$

$$n = \langle n|N|n\rangle = (\langle n|a^{+})\cdot(a|n\rangle) \geqslant 0$$

$\longrightarrow$ The sequence must terminate with $n=0$ and

allowed values of n are $\begin{cases}\text{non-negative} \\ \text{integer}\end{cases}$.

For $n=0$ $\quad E_0 = \frac{1}{2}\hbar\omega$ $\qquad$ for the ground state

$|0\rangle$: ground state

Now; using $a^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$$|1\rangle = a^{+}|0\rangle$$

$$|2\rangle = \left(\frac{a^{+}}{\sqrt{2}}\right)|1\rangle = \left[\frac{(a^{+})^{2}}{\sqrt{2}}\right]|0\rangle$$

$$|3\rangle = \left(\frac{a^{+}}{\sqrt{3}}\right)|2\rangle = \left[\frac{(a^{+})^{3}}{\sqrt{3!}}\right]|0\rangle$$

$$\vdots$$

$$|n\rangle = \left[\frac{(a^{+})^{n}}{\sqrt{n!}}\right]|0\rangle$$

Simultaneous eigenkets of N and H

$$E_n = (n+\tfrac{1}{2})\hbar\omega \qquad n = 0, 1, 2 \ldots$$

Also

$$\begin{cases} \langle n'|a|n\rangle = \sqrt{n}\,\langle n'|n-1\rangle = \sqrt{n}\,\delta_{n',n-1} \\ \langle n'|a^{+}|n\rangle = \sqrt{n+1}\,\langle n'|n+1\rangle = \sqrt{n+1}\,\delta_{n',n+1} \\ X = \sqrt{\frac{\hbar}{2m\omega}}\,(a+a^{+}) \qquad P = i\sqrt{\frac{m\hbar\omega}{2}}\,(-a+a^{+}) \end{cases}$$

$$\longrightarrow \langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{n',n-1} + \sqrt{n+1}\,\delta_{n',n+1}\right)$$

$$\langle n'|P|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left(-\sqrt{n}\,\delta_{n',n-1} + \sqrt{n+1}\,\delta_{n',n+1}\right)$$

Neither x nor p is diagonal in N-representation

because $[x, N] \neq 0 \qquad [P, N] \neq 0$

Let us apply a on $|0\rangle$; $a|0\rangle = 0$

In the x-rep.

$$\langle x'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\,\langle x'|\left(x + \frac{ip}{m\omega}\right)|0\rangle = 0$$

Recalling $\langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle$ (chap. 1)

$$\left(x' + x_0^2\frac{d}{dx'}\right)\langle x'|0\rangle = 0 \qquad \text{where } x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$$

Normalized sol. $\longrightarrow$ $\langle x'|0\rangle = \left(\dfrac{1}{\pi^{1/4}\sqrt{x_0}}\right) e^{-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2}$

Also,

$$\langle x'|1\rangle = \langle x'|a^\dagger|0\rangle = \left(\frac{1}{\sqrt{2}\,x_0}\right)\left(x' - x_0^2\frac{d}{dx'}\right)\langle x'|0\rangle$$

$$\langle x'|2\rangle = \left(\frac{1}{\sqrt{2}}\right)\langle x'|(a^\dagger)^2|0\rangle = \left(\frac{1}{\sqrt{2!}}\right)\left(\frac{1}{\sqrt{2}\,x_0}\right)^2\left(x' - x_0^2\frac{d}{dx'}\right)^2\langle x'|0\rangle$$

In general;

$$\langle x'|n\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{2^n n!}}\right)\left(\frac{1}{x_0^{n+\frac{1}{2}}}\right)\left(x' - x_0^2\frac{d}{dx'}\right)^n e^{-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2}$$

What about $\langle x^2\rangle_0 = ?$ $\langle p^2\rangle_0 = ?$

Note that;

$$x^2 = \left(\frac{\hbar}{2m\omega}\right)\left(a^2 + a^{\dagger 2} + a^\dagger a + a a^\dagger\right)$$

$$p^2 = -\frac{m\hbar\omega}{2}\left(a^2 + a^{\dagger 2} - a^\dagger a - a a^\dagger\right)$$

Only the last term in x^2 has nonvanishing contribution;

$$\langle x^2 \rangle_0 = \frac{\hbar}{2m\omega} = \frac{x_0^2}{2}$$ for the ground state

$$\langle p^2 \rangle_0 = \frac{\hbar m\omega}{2}$$ " " "

$$\rightarrow \left\langle \frac{p^2}{2m} \right\rangle_0 = \frac{\hbar\omega}{4} \quad , \quad \left\langle \frac{m\omega^2 x^2}{2} \right\rangle_0 = \frac{\hbar\omega}{4}$$

$$\langle H \rangle_0 = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

$$\left\langle \frac{p^2}{2m} \right\rangle_0 = \frac{\langle H \rangle_0}{2} \qquad \left\langle \frac{m\omega^2 x^2}{2} \right\rangle_0 = \frac{\langle H \rangle_0}{2}$$

as expected from Virial theorem.

Also $\langle x \rangle_0 = 0 \quad \langle p \rangle_0 = 0$ (also holds for the excited states)

$$\rightarrow \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \frac{\hbar}{2m\omega}$$

$$\langle (\Delta p)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar m\omega}{2}$$

$$\langle (\Delta x)^2 \rangle_0 \langle (\Delta p)^2 \rangle_0 = \frac{\hbar^2}{4}$$ (not surprizing, because the ground state has a gaussian shape)

But

$$\langle (\Delta x)^2 \rangle_n \langle (\Delta p)^2 \rangle_n = (n + \tfrac{1}{2})^2 \hbar^2 \geqslant \frac{\hbar^2}{4}$$

Time Development of the Oscillator;

Using the Heisenberg equ. of motion;

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}\left[A^{(H)}, H\right] \longrightarrow$$

$$\begin{cases} \dfrac{dP_i^{(H)}}{dt} = \dfrac{1}{i\hbar}\left[P_i^{(H)}, H\right] = \dfrac{1}{i\hbar}\left[P_i^{(H)}, V^{(H)}(x)\right] = -\dfrac{\partial}{\partial x_i} V^{(H)}(x) \\ \dfrac{dx_i^{(H)}}{dt} = \dfrac{1}{i\hbar}\left[x_i^{(H)}, H\right] = \dfrac{P_i^{(H)}}{m} \end{cases}$$

$$\rightarrow \begin{cases} \dfrac{dp^{(H)}}{dt} = -m\omega^2 x^{(H)} \\ \dfrac{dx^{(H)}}{dt} = \dfrac{p^{(H)}}{m} \end{cases}$$ coupled diff. equs.

$$\begin{cases} \dfrac{d}{dt}\left(i\sqrt{\dfrac{m\hbar\omega}{2}}\,(-a+a^{+})\right)^{H} = -m\omega^2\left(\sqrt{\dfrac{\hbar}{2m\omega}}\,(a+a^{+})\right)^{H} \\ \dfrac{d}{dt}\left(\sqrt{\dfrac{\hbar}{2m\omega}}\,(a+a^{+})\right)^{H} = \dfrac{i}{m}\sqrt{\dfrac{m\hbar\omega}{2}}\,(-a+a^{+})^{H} \end{cases}$$

$$\longrightarrow \begin{cases} \dfrac{da^{H}}{dt} = \sqrt{\dfrac{m\omega}{2\hbar}}\left(\dfrac{p}{m} - i\omega x\right) = -i\omega a \\ \dfrac{da^{+H}}{dt} = i\omega a^{+} \end{cases}$$ uncoupled

Sols.:

$$\begin{cases} a^H(t) = a(0)\, e^{-i\omega t} \\ a^{+H}(t) = a^+(0)\, e^{+i\omega t} \end{cases} \quad (1)$$

$$\rightarrow \begin{cases} N^H = (a^+a)^H = a^+(0)\,a(0) \\ \text{Also } H^H = H \end{cases}$$

Time-indep. in Heisenberg picture as they must be.

(1) in terms of x, p;

$$\rightarrow \begin{cases} x^H(t) + \dfrac{i\,p^H(t)}{m\omega} = x(0)\, e^{-i\omega t} + i\,\dfrac{p(0)}{m\omega}\, e^{-i\omega t} \\ x^H(t) - \dfrac{i\,p^H(t)}{m\omega} = x(0)\, e^{i\omega t} - i\,\dfrac{p(0)}{m\omega}\, e^{i\omega t} \end{cases}$$

Equating the Hermitian and anti-Hermitian parts of both sides separately;

$$\rightarrow \begin{cases} x^H(t) = x(0)\cos\omega t + \dfrac{p(0)}{m\omega}\sin\omega t \\ p^H(t) = -m\omega\, x(0)\sin\omega t + p(0)\cos\omega t \end{cases}$$

These look the same as the classical equs. of motion.

Remark: $H_{cl} = \dfrac{p^2}{2m} + \dfrac{1}{2}m\omega^2x^2 = \dfrac{p^2}{2m} + \dfrac{1}{2}kx^2 = \text{Const.}$

$F = m\dfrac{d^2x}{dt^2}$ $\quad -kx = m\dfrac{d^2x}{dt^2} \longrightarrow$ similar equs.

or we may use Lagrange formalism.

Alternative derivation:

$$X^H(t) = e^{\frac{iHt}{\hbar}} X(0)\, e^{-\frac{iHt}{\hbar}}$$

Using the Baker-Hausdorff lemma;

$$e^{iB\lambda} A\, e^{-iB\lambda} = A + i\lambda[B,A] + \left(\frac{i^2\lambda^2}{2!}\right)[B[B,A]] + \cdots +$$
$$+\left(\frac{i^n\lambda^n}{n!}\right)[B[B[B\cdots[B,A]]\cdots] + \cdots$$

B: Hermitian op $\quad \lambda$: real number

$$\rightarrow e^{\frac{iHt}{\hbar}} X(0)\, e^{-\frac{iHt}{\hbar}} = X(0) + \left(\frac{it}{\hbar}\right)[H, X(0)] + \left(\frac{i^2 t^2}{2!\hbar^2}\right)[H[H, X(0)]] + \cdots$$

Using: $\quad [H, X(0)] = \dfrac{-i\hbar P(0)}{m}$ and $[H, P(0)] = i\hbar m\omega^2 X(0)$

$$\rightarrow X(t) = e^{\frac{iHt}{\hbar}} X(0)\, e^{-\frac{iHt}{\hbar}} = X(0) + \frac{P(0)}{m}t - \left(\frac{1}{2!}\right)t^2\omega^2 X(0)$$
$$+\left(\frac{1}{3!}\right)\frac{t^3\omega^2 P(0)}{m} + \cdots$$

$$= X(0)\cos\omega t + \frac{P(0)}{m\omega}\sin\omega t$$

Note also that;

$$\langle n | X(t) | n \rangle = 0 \quad , \quad \langle n | P(t) | n \rangle = 0 \quad \text{(because of orthogonality)}$$

This point is also obvious from our earlier conclusion, that;

$$\langle B \rangle_{|stationary\rangle} = \text{time-indep} \qquad (B: \text{observable})$$

i.e. Since $\langle X^{(S)} \rangle = 0 \longrightarrow \langle X^{(H)} \rangle = 0$

similarly $\langle P^{(S)} \rangle = 0 \longrightarrow \langle P^{(H)} \rangle = 0$

To observe oscillations reminiscent of the classical oscillation we must look at a superposition of energy eigenstates such as:

$$|\alpha\rangle = C_0 |0\rangle + C_1 |1\rangle$$

$$\langle X^{(H)}(t) \rangle_\alpha = \text{t-dep. (oscillates)}$$

We have seen that an energy eigenstate does not behave like the classical osc. — in the sense of oscillating expectation value for x and p — no matter how large n may be.

How can we construct a superposition of energy eigenstates that most closely imitates the classical osc.?

i.e., a wave packet that bounces back and forth without spreading in shape?

Answer $\longrightarrow$ The coherent state $|\lambda\rangle$ defined by

$$a|\lambda\rangle = \lambda|\lambda\rangle \qquad (a: \text{annihilation op})$$

does the desired job. $\qquad \lambda$: complex in general

The coherent state has many other remarkable properties:

1 — When expressed as a superposition of energy or N eigenstates,

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)\,|n\rangle$$

The distribution of $|f(n)|^2$ with respect to n is of the Poisson-type about some mean value $\bar{n}$

$$|f(n)|^2 = \left(\frac{\bar{n}^n}{n!}\right) e^{-\bar{n}}$$

2 - It can be obtained by translating the oscillator ground-state by some finite distance.

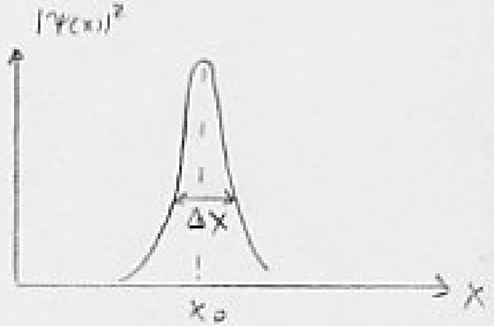
3 - It satisfies the minimum uncertainty product relation at all times.

The Motion of Wave Packets (Gottfried P260)

In the classical case;

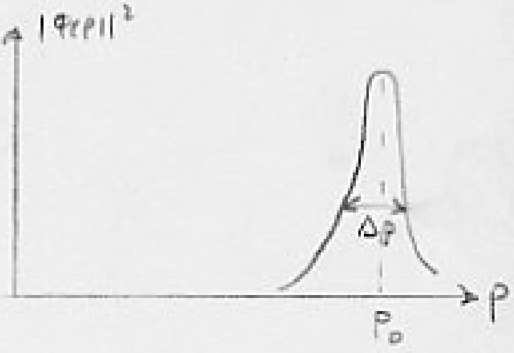
let; $\begin{cases} p_0 : \text{initial momentum} \\ x_0 : \quad " \quad \text{coord.} \end{cases}$ (at $t=0$)

$$\begin{cases} x(t) = x_0 \cos\omega t + \dfrac{p_0}{m\omega} \sin\omega t \\ p(t) = m\dot{x}(t) \end{cases} \qquad t > 0$$



Analogous situation in Q.M. is described by;

A wave packet localized within Δx about x_0 and Δp about p_0, at $t=0$



Assume $v_0 = \frac{p_0}{m} = 0$

If $\begin{cases} \text{i) } |x_0| >> \Delta x \\ \text{ii) } V(x) \text{ varies slowly within } \Delta x \end{cases}$

$\longrightarrow$ one would expect the packet to adhere to the classical trajectory for a considerable length of time.

For an oscillator pot. a stronger result actually holds, because the sols. of Heisenberg's equs. coinside in form with the classical sols..

$\xrightarrow{\text{consequently}}$ $\langle p \rangle$ and $\langle x \rangle$ for an arbitrary packet will follow the classical trajectory.

In general the shape of the packet will change with t, and for sufficiently pathological initial state (e.g. δ-func.) the motion will bear no resemblance to a classical motion

There is however a very special and interesting class of nonstationary states that do not spread in t. With appropriate choice of initial conds. these can be arranged to look very classical indeed.

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

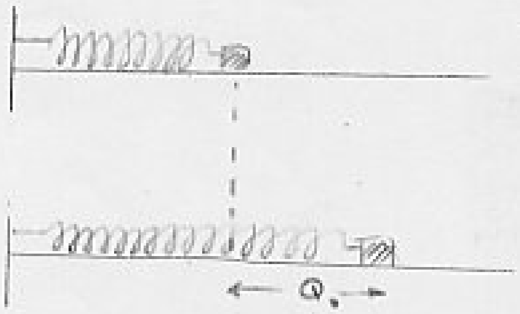
For simplification, let's introduce dimensionless variables;

$$\hat{H} \equiv H/_{\hbar\omega} = \frac{1}{2}(\underline{P}^2 + Q^2)$$

$$\underline{P} = \frac{P}{\sqrt{m\hbar\omega}}, \quad Q = \sqrt{\frac{m\omega}{\hbar}}\, x$$

let, $|\tilde{n}\rangle = e^{-i\underline{P}Q_0} |n\rangle$ — nth state of osc. displaced through the distance Q_0

with $Q_0 \neq 0$, this is no longer a stationary state



Classical analog

$$|\tilde{n};t\rangle = e^{-i\frac{Ht}{\hbar}} |\tilde{n}\rangle = e^{-i\hat{H}\omega t} |\tilde{n}\rangle$$

$$= e^{-i\hat{H}\omega t} e^{-i\underline{P}Q_0} |n\rangle$$

Now,

$$\langle \overset{(S)}{\underline{P}} \rangle_{\tilde{n}t} = \langle \overset{(H)}{\underline{P}(t)} \rangle_{\tilde{n}} = ?, \quad \langle \overset{(S)}{\underline{P}} \rangle_{\tilde{n}t} = \langle n | e^{i\underline{P}Q_0} \overset{(H)}{\underline{P}(t)} e^{-i\underline{P}Q_0} |n\rangle$$

$$p(t) = -m\omega x(0) \sin\omega t + p(0) \cos\omega t$$

$$\rightarrow \underline{P}(t) = -Q \sin\omega t + \underline{P} \cos\omega t$$

$$\langle \overset{(S)}{\underline{P}} \rangle_{\tilde{n}t} = -\sin\omega t \langle n | e^{i\underline{P}Q_0} Q e^{-i\underline{P}Q_0} |n\rangle + \cos\omega t \langle n | \underline{P} | n\rangle$$

Remark: $[x_i, F(\vec{p})] = i\hbar \frac{\partial F}{\partial p_i}$

$$\langle P^{(S)} \rangle_{\tilde{n}t} = -\sin\omega t \, \cancel{\langle n|(Q+Q_0)|n\rangle} + \cos\omega t \, \cancel{\langle n|P|n\rangle}$$

$$= -\sin\omega t \left[\cancel{\langle n|Q|n\rangle} + \langle n|Q_0|n\rangle \right] = -Q_0 \sin\omega t \qquad (1)$$

$\longrightarrow$ Expectation value follows the classical trajectory.

Similarly: $\langle Q^{(S)} \rangle_{\tilde{n}t} = \langle Q^{(H)}(t) \rangle_{\tilde{n}} = \langle n| e^{iPQ_0} Q^{(H)}(t) e^{-iPQ_0} |n\rangle$

$$= Q_0 \cos\omega t \qquad (2)$$

Also,

$$\langle P^{2\,(S)} \rangle_{\tilde{n}t} = \langle P^{2\,(H)}(t) \rangle_{\tilde{n}} = \langle P^2 \cos^2\omega t + Q^2 \sin^2\omega t - (PQ+QP)\cos\omega t \sin\omega t \rangle_{\tilde{n}}$$

$$= \langle n| e^{iPQ_0} \left(P^2 \cos^2\omega t + Q^2 \sin^2\omega t - (PQ+QP)\cos\omega t \sin\omega t \right) e^{-iPQ_0} |n\rangle$$

$$= \langle P^2 \rangle_n \cos^2\omega t + (Q_0^2 + \langle Q^2 \rangle_n) \sin^2\omega t - \langle PQ+QP \rangle_n \sin\omega t \cos\omega t$$

$$\langle n|(PQ+QP)|n\rangle = 0 \qquad (\text{using } a \text{ and } a^\dagger \text{ ops.})$$

$$\langle (\Delta P)^2 \rangle_t = \langle P^{2\,(S)} \rangle_{\tilde{n}t} - \langle P^{(S)} \rangle^2_{\tilde{n}t} = \langle P^2 \rangle_n \cos^2\omega t + \langle Q^2 \rangle_n \sin^2\omega t$$

By following the same route;

$$\langle (\Delta Q)^2 \rangle_t = \langle Q^{2\,(S)} \rangle_{\tilde{n}t} - \langle Q^{(S)} \rangle^2_{\tilde{n}t} = \langle Q^{2\,(S)} \rangle_n \cos^2\omega t + \langle P^{2\,(S)} \rangle_n \sin^2\omega t$$

But

$$\langle x^2 \rangle_n = \frac{\hbar}{2m\omega} \langle a^2 + a^{+2} + a^+a + aa^+ \rangle_n = \frac{\hbar}{2m\omega} \langle a^+a + aa^+ \rangle_n$$

$$\langle P^2 \rangle_n = -\frac{m\hbar\omega}{2} \langle a^2 + a^{+2} - a^+a - aa^+ \rangle_n = \frac{m\hbar\omega}{2} \langle a^+a + aa^+ \rangle_n$$

Since $a^+a + aa^+ = a^+a + (1 + a^+a) = 2a^+a + 1 = 2N + 1$

$$\rightarrow \begin{cases} \langle x^2 \rangle_n = \frac{\hbar}{2m\omega}(2n+1) = \frac{\hbar}{m\omega}(n+\frac{1}{2}) \\ \langle P^2 \rangle_n = \frac{m\hbar\omega}{2}(2n+1) = m\hbar\omega(n+\frac{1}{2}) \end{cases}$$

$$\rightarrow \begin{cases} \langle Q^2 \rangle_n = n + \frac{1}{2} \\ \langle P^2 \rangle_n = n + \frac{1}{2} \end{cases}$$ for stationary state $|n\rangle$

$$\longrightarrow \begin{cases} \langle (\Delta P)^2 \rangle_t = n + \frac{1}{2} \\ \langle (\Delta Q)^2 \rangle_t = n + \frac{1}{2} \end{cases}$$

Remark: Since $\langle Q \rangle_n = \langle P \rangle_n = 0$ for stationary states

$$\longrightarrow \begin{cases} \langle (\Delta P)^2 \rangle = n + \frac{1}{2} \\ \langle (\Delta Q)^2 \rangle = n + \frac{1}{2} \end{cases}$$ "

Therefore $\rightarrow$ We have shown that the packets $|\tilde{n}, t\rangle$ retain their shape.

One may therefore prepare a state $e^{-iPQ_0}|n\rangle$, with $Q_0 >> 1$, which will oscillate back and forth in accordance with the classical laws. (Equs. (1)(2) P 129)

The spread of this packet in Q-space $\dfrac{\text{will remain}}{\text{always}}$ small $\begin{cases}\text{compared to } Q_0 \\ \text{oscillation amplitude}\end{cases}$

The momentum spread $\overset{\text{Also}}{=}$ small $\begin{cases}\text{compared to } \langle P(t)\rangle_{\tilde{n}} \\ \text{except in the} \\ \text{neighborhood of the} \\ \text{classical turning} \\ \text{points}\end{cases}$

Wave packet formed by displacing the ground state $|0\rangle$:

Take $P_0 \neq 0$ initial mom.

If we want the initial mom. to be P_0, we append the momentum displacement op. $e^{iP_0 Q}$ (P_0 → number, Q → op) to $|\tilde{n}\rangle$.

$$|0, Q_0, P_0; t\rangle = e^{-i\hat{H}\omega t} e^{iP_0 Q} e^{-iPQ_0} |0\rangle$$

We shall use the identity:

$$e^{A+B} = e^{A} e^{B} e^{-\frac{1}{2}[A,B]}$$

$\forall A, B$ that $[A,[A,B]] = 0$ and $[B,[A,B]] = 0$

What is the probability of finding the state $|n\rangle$ in the wave packet at t?

i.e. $P_n \equiv |\langle n|0, Q_0, P_0; t\rangle|^2 = ?$

Using the above identity: $e^{iP_0 Q} e^{-iPQ_0} = e^{i(P_0 Q - PQ_0)} e^{\frac{1}{2} i P_0 Q_0}$

$= e^{\frac{1}{2} i P_0 Q_0} e^{i(P_0 Q - PQ_0)}$

Note that: $[iP_0 Q, -iPQ_0] =$
$= + P_0 Q_0 [Q, P] =$
$= + P_0 Q_0 \left(i\hbar \frac{1}{\sqrt{\hbar\omega}} \sqrt{\frac{\hbar\omega}{\hbar}}\right) = iP_0 Q_0$

Now

$X = \sqrt{\frac{\hbar}{2m\omega}} (a + a^+) \rightarrow Q = \frac{1}{\sqrt{2}} (a + a^+)$

$P = i\sqrt{\frac{m\hbar\omega}{2}} (-a + a^+) \rightarrow P = \frac{i}{\sqrt{2}} (-a + a^+)$

$\rightarrow i(P_0 Q - PQ_0) = a^+ \lambda - a\lambda^*$ $\qquad \lambda = \frac{1}{\sqrt{2}} (Q_0 + iP_0)$

Remark: $\hat{E} = \frac{1}{2}(P_0^2 + Q_0^2) = |\lambda|^2$ in units of $\hbar\omega$ of a classical particle with momentum P_0 through point Q_0

λ: the phase of motion in the classical sense.

$$\longrightarrow |0, Q_0, P_0, t\rangle = e^{\frac{1}{2} i P_0 Q_0} e^{-i\hat{H}\omega t} e^{(a^+\lambda - a\lambda^*)} |0\rangle$$

Employing the identity once more;

$$e^{(a^+\lambda - a\lambda^*)} = e^{a^+\lambda} e^{-a\lambda^*} e^{-\frac{1}{2}\hat{E}}$$

$$e^{-a\lambda^*} |0\rangle = |0\rangle \qquad (\text{because } a|0\rangle = 0)$$

$$\rightarrow |0, Q_0, P_0; t\rangle = e^{\frac{1}{2} i P_0 Q_0} e^{-\frac{1}{2}\hat{E}} e^{-i\hat{H}\omega t} e^{a^+\lambda} |0\rangle$$

Since $|n\rangle = \dfrac{(a^+)^n}{\sqrt{n!}} |0\rangle$

$$\longrightarrow |0, Q_0, P_0; t\rangle = e^{\frac{1}{2} i P_0 Q_0} e^{-\frac{1}{2}\hat{E}} \sum_{n=0}^{\infty} \frac{\overbrace{e^{-i(n+1)\omega t}}^{\text{oscillatory term}} \lambda^n}{\sqrt{n!}} |n\rangle$$

$$\longrightarrow P_n \equiv |\langle n|0, Q_0, P_0; t\rangle|^2 = \frac{\hat{E}^n}{n!} e^{-\hat{E}}$$ Poisson distribution in the variable $\hat{E}$

The most probable value for n (i.e. $|n\rangle$), is determined by finding the $(P_n)_{max}$.

When the <u>classical</u> energy is <u>large</u>, i.e., $\hat{E} \gg 1$,

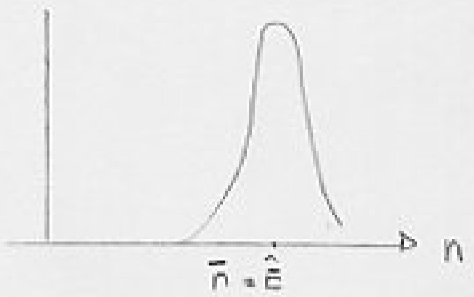
we can treat $P_n = f(n)$ ← continuous

$$\frac{P_n'}{P_n} = 0 \qquad (\text{logarithmic derivative})$$

$$P_n = \frac{\hat{E}^n}{n!} e^{-\hat{E}} \simeq \frac{\hat{E}^n}{\sqrt{2\pi n}\left(\frac{n}{e}\right)^n} e^{-\hat{E}}$$

($n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$)
stirling's formula
n: large

$$\frac{P_n'}{P_n} = 0 \rightarrow n = \hat{E} \quad (P_n : \text{max.})$$



2.4- Schrödinger Wave Equ.:

Time-Dep. Wave Equ.

We examine the time evolution of $|\alpha, t_0; t\rangle$ in x-rep.

i.e. $\psi(x', t) = \langle x' | \alpha, t_0, t\rangle$

Note that $\psi(x', t)$: a func. of t

where $|\alpha, t_0; t\rangle$: a state ket in the schrödinger picture at t.

and $\langle x'|$: a time-indep position eigenbra with eigenvalue x'.

The Hamiltonian, $H = \frac{p^2}{2m} + V(x)$

$V(x)$: local, in the sense that in x-rep.

$$\langle x'' | V(x) | x' \rangle = V(x') \delta(x' - x'')$$

We may have also other type of pots.;

$V(x, t)$: time-dep.

Non local but separable pot. : $\langle x'' | V(x) | x' \rangle = V_1(x') V_2(x'')$

Mom.-dep. Pot : $\begin{cases} P \cdot A + A \cdot P \\ A\text{: Vector pot.} \end{cases}$ with $V(x) = V_2(x) e^{\frac{-iP(x''-x')}{\hbar}} V_1(x)$

and so on...

$$i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t\rangle = H |\alpha, t_0; t\rangle$$

$$\rightarrow \quad i\hbar \frac{\partial}{\partial t} \langle x' | \alpha, t_0; t\rangle = \langle x' | H | \alpha, t_0; t\rangle$$

$$\langle x' | P^n | \alpha\rangle = (-i\hbar)^n \frac{\partial^n}{\partial x'^n} \langle x' | \alpha\rangle$$

$$\rightarrow \langle x' | \frac{P^2}{2m} | \alpha, t_0; t\rangle = -\left(\frac{\hbar^2}{2m}\right) \nabla'^2 \langle x' | \alpha, t_0; t\rangle$$

and $\langle x' | V(x) = \langle x' | V(x')$

↑ Hermitian

$$\rightarrow \quad i\hbar \frac{\partial}{\partial t} \langle x' | \alpha, t_0; t\rangle = \left(-\frac{\hbar^2}{2m}\right) \nabla'^2 \langle x' | \alpha, t_0; t\rangle + V(x') \langle x' | \alpha, t_0; t\rangle \qquad (1)$$

or;

$$i\hbar \frac{\partial}{\partial t} \Psi(x', t) = \left(-\frac{\hbar^2}{2m}\right) \nabla'^2 \Psi(x', t) + V(x') \Psi(x', t) \qquad (2)$$

The Q.M. based on the mentioned wave equ. is known as <u>Wave Mechanics</u>.

The Time-indep. Wave Equ.:

We have seen;

$$\langle x' | a', t_0; t\rangle = \langle x' | a'\rangle e^{-\frac{i E_{a'} t}{\hbar}}$$

time-dep. of a stationary state

where it is understood that; $[A, H] = 0$ (3)

$A|a'\rangle = a'|a'\rangle$, $\quad H|a'\rangle = E_{a'}|a'\rangle$

(3) in (1) $\rightarrow$ $$-\left(\frac{\hbar^2}{2m}\right)\nabla'^2 \langle x'|a'\rangle + V(x')\langle x'|a'\rangle = E_{a'}\langle x'|a'\rangle$$

(Partial diff. equ.)

In the wave mechanics,

$$H = f(x,p) \qquad \left(\text{like, } H = \frac{p^2}{2m} + V(x)\right)$$

and there is no need to refer explicitly to observable A that $[A,H]=0$, because we can always choose

$A = f(x,p)$ which $A \xrightarrow[\text{with}]{\text{coincides}} H$ itself

$\longrightarrow$ We may omit reference to a':

$$\longrightarrow \left(-\frac{\hbar^2}{2m}\right)\nabla'^2 u_E(x') + V(x')\,u_E(x') = E\,u_E(x') \qquad (4)$$

Time-indep. Wave equ.

To solve (4) some boundary conds. has to be imposed.

Suppose we seek a solution to (4) with

$$E < \lim_{|x'|\to\infty} V(x') \qquad (\text{i.e. } E - \underset{|x'|\to\infty}{V(x')} < 0\ )$$

$\longrightarrow$ eigenfunc. will be damped $\longrightarrow$ $u_E(x') \rightarrow 0$ as $|x'| \rightarrow \infty$

$\longrightarrow$ Physically: The particle is bound.

$\longrightarrow$ There are nontrivial sol. only for E = discrete

Interpretation of Wave Equ.;

$$|\alpha, t_0; t\rangle = \int d^3x' \, |x'\rangle \langle x'|\alpha, t_0; t\rangle$$

Define; $\rho(x', t) = |\psi_\alpha(x', t)|^2 = |\langle x'|\alpha, t_0; t\rangle|^2$

Probability density

$\rho(x', t)\, d^3x'$: the probability of recording a positive result at time t, by a detector

Using Schrödinger's time-dep. equ.;

$$i\hbar \psi^* \frac{\partial}{\partial t}\psi = (\psi^*)\left(-\frac{\hbar^2}{2m}\right)\nabla^2\psi + \psi^*(V\psi)$$

$$-i\hbar\left(\frac{\partial}{\partial t}\psi^*\right)\psi = \left(-\frac{\hbar^2}{2m}\right)(\nabla^2\psi^*)\psi + \underbrace{(V\psi^*)\psi}_{\text{They are equal since } V \text{ is Hermitian}}$$

subtract

$$\frac{\partial}{\partial t}(\psi^*\psi) + \frac{\hbar}{2mi}\nabla\cdot\left[\psi^*\nabla\psi - (\nabla\psi^*)\psi\right] = 0$$

$$J(x', t) = -\frac{i\hbar}{2m}\left[\psi^*\nabla\psi - (\nabla\psi^*)\psi\right] = \frac{\hbar}{m} I(\psi^*\nabla\psi)$$

$$\rho(x', t) = \psi^*\psi$$

$$\rightarrow \frac{\partial\rho}{\partial t} + \nabla\cdot J = 0$$ continuity equ.

(in source-free, sink free region)

$$\frac{\partial}{\partial t}\int \rho(x',t)\,d^3x' = -\int \nabla\cdot J(x',t)\,d^3x'$$

If $J(x',t) \longrightarrow 0$ faster than $\frac{1}{r^2}$ as $r \to \infty$

and if $\int \rho(x',t)\,d^3x'$ exists (Ψ: quadratically integrable)

then acc. to Gauss' theorem;

$$\frac{\partial}{\partial t}\int \rho(x',t)\,d^3x' = 0 \qquad \text{conservation of normalization}$$

The reality of pot. V (or the Hermicity of V op.) has curical role (in cancelation of the last terms).

A complex pot. can phenomenologically account for the disappearance of a particle.

Such pot. is often used for nuclear reactions when incident particles get absorbed by nuclei

Now;

$$\int d^3x' j(x',t) = \frac{\hbar}{2mi}\int [\psi^*\nabla\psi - (\nabla\psi^*)\psi]\, d^3x'$$

$$= \frac{\hbar}{2mi}\left\{ -\psi^*\psi\Big|_{-\infty}^{\infty} + \int [\psi^*\nabla\psi + \psi^*\nabla\psi]\, d^3x' \right\}$$

$$= \frac{\hbar}{mi}\int \psi^*\nabla\psi\, d^3x' = \frac{1}{m}\int \psi^*\left(\frac{\hbar}{i}\right)\nabla\psi\, d^3x'$$

$$= \frac{\langle p\rangle_t}{m}$$

Remark: For quadratically integrable wave func., we have

$$\int \psi^*\psi\, d\tau < \infty$$

or equivalently for normalized case $\int \psi^*\psi\, d\tau = 1$

Cond.: $\psi \xrightarrow[\text{as } x\to\infty]{} 0$ at least as fast as $\frac{1}{r^{\frac{1}{2}+\epsilon}}$ $(\epsilon > 0)$

Physical Significance of the wave func.:

Let us write it as

$$\psi(x,t) = \sqrt{\rho(x,t)}\, e^{\frac{iS(x,t)}{\hbar}}$$

ρ, S : real

which can always be done for any complex func. of x and t.

What is the physical interpretation of S ?

Noting,

$$\psi^* \nabla \psi = \sqrt{\rho}\, e^{-\frac{iS}{\hbar}} \left(\sqrt{\rho} \cdot \frac{i}{\hbar}(\nabla S) e^{\frac{iS}{\hbar}} + (\nabla \sqrt{\rho})\, e^{\frac{iS}{\hbar}} \right)$$

$$= \frac{i}{\hbar} \rho \nabla S + \sqrt{\rho}\, \nabla \sqrt{\rho}$$

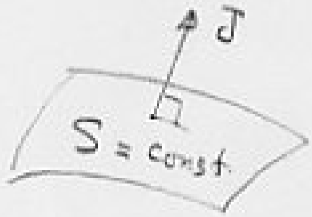
and $J = \frac{\hbar}{m} \mathrm{Im}(\psi^* \nabla \psi) = \frac{\rho \nabla S}{m}$

→ The spatial variation of phase $\left(\frac{\nabla S}{\hbar}\right)$ of the wave func.

characterizes the probability flux J.

→ The stronger phase variation (i.e. $\nabla S \to$ large)

→ the more intense the flux.



A simple example:

$$\psi(x,t) \sim e^{\left(\frac{i p \cdot x}{\hbar} - \frac{i E t}{\hbar}\right)}$$

Plane wave

p: eigenvalue of moment op.

$$S = \frac{i p \cdot x}{\hbar} - \frac{i E t}{\hbar} \quad \to \nabla S = p$$

we may regard $\frac{\nabla S}{m}$ as some kind of velocity;

$$V = \frac{\nabla S}{m}$$

Continuity equ. $\Rightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0$

just as in fluid dynamics.

Caution: One must be careful to interpret of J

as ρV defined at every point in space,

because a simultaneous precision measurement of x and V

would necessarily violate the uncertainty principle.

The classical limit: (of wave mechanics)

Substituting $\psi(x,t) = \sqrt{\rho(x,t)}\, e^{\left(\frac{iS(x,t)}{\hbar}\right)}$ in time-dep. Schrödinger equ;

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi$$

$$i\hbar \left[\frac{\partial}{\partial t}\sqrt{\rho} + \frac{i}{\hbar}\sqrt{\rho}\frac{\partial}{\partial t} S\right] = -\frac{\hbar^2}{2m}\left[\nabla^2\sqrt{\rho} + \frac{2i}{\hbar}(\nabla\sqrt{\rho})\cdot(\nabla S) - \frac{1}{\hbar^2}\sqrt{\rho}\,|\nabla S|^2 + \frac{i}{\hbar}\sqrt{\rho}\,\nabla^2 S\right] + \sqrt{\rho}\, V$$

Let us suppose:

$\hbar$: small quantity in some sense

let's assume $\begin{cases} \hbar\, |\nabla^2 S| \ll |\nabla S|^2 \\ \text{or } \hbar\, |\nabla \cdot P| \ll |P|^2 \end{cases}$ and so forth

Remark: The inequality is much more better satisfied if $\nabla \cdot P \to 0$ (compared to P) (the variation in P) i.e. If $V(x)$ varies slowly.

Neglecting the terms containing $\hbar$ and $\hbar^2$;

$$\to \frac{1}{2m} |\nabla S(x,t)|^2 + V(x) + \frac{\partial S(x,t)}{\partial t} \simeq 0$$

This is Hamilton-Jacobi equ. in classical mechanics,

$$H\left(q_1, \cdots q_n\, \frac{\partial S}{\partial q_1} \cdots \frac{\partial S}{\partial q_n}, t\right) + \frac{\partial S}{\partial t} = 0$$

$S(x,t)$: Hamilton's principal func.

So, in the $\hbar \to 0$ limit Cl.M. is contained in Schrödinger's wave mechanics.

$\hbar \underset{\text{phase}}{\left(\frac{S}{\hbar}\right)}$: Hamilton's principal func. (semiclassical interpretation)

Provided $\hbar$ can be regarded as a small quantity

Let us now look at a stationary state with time dependence,

$$e^{-i\frac{Et}{\hbar}}$$

This time dependence is <u>anticipated</u> from the fact that; for a classical system;

$H = \text{const}$ time-indep

S is <u>separable</u>, $S(x,t) = W(x) - Et$

$\downarrow$

Hamilton's characteristic func.

As t goes $\rightarrow$ a surface of const. S <u>advances</u> in much the same way as a surface of a const. phase in the wave optics — a <u>wave front advances</u>.

In classical Hamilton-Jacobi theory;

$$p_i = \frac{\partial S}{\partial q_i} \longrightarrow p_{cl} = \nabla S = \nabla W$$

which is consistent with our earlier identification of $\frac{\nabla S}{m}$ with some kind of velocity.

classical trajectory

cl. M.

Q. M.

- Ref.: 1) Q.M., V.K. Thankappan QC174.12.T48
2) Int. to Q.M. B.H. Bransden and C.J. Joachain QC174.12.B74

The WKB Approximation (Wentzel, Kramers, Brillouin)

or (Semi Classical ")

or (Phase Integral Method)

The method is suitable only to poblems that can be decomposed into $\left\{ \begin{array}{l} \text{one -} \\ \text{or} \\ \text{more one -} \end{array} \right.$ dimensional ones.

Now, the action,

$$S((q,p,t)_2, (q,p,t)_1) = \int_{t_1}^{t_2} L\,dt = \int_1^2 p\,dq - \int_1^2 H\,dt$$

$\delta S = 0$ for classical path

Remark: $L = T - V = 2T - H$

$T = \frac{1}{2}mv^2 = \frac{1}{2}p\dot{q}$

Using the Hamilton-Jacobi equs.

$$\left\{ \begin{array}{l} \frac{\partial S}{\partial t} = -H \\ \nabla S = p \end{array} \right.$$

in $H = \frac{p^2}{2m} + V(x)$

$$\rightarrow -\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V(x) \qquad (1)$$

t-dep. Hamilton-Jacobi equ. of cl. M.

The corresponding equ. of motion in Q.M.

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = H\,\Psi(x,t) \qquad (2)$$

$$\rightarrow \quad i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\Psi(x,t) \qquad (3)$$

Also from (2) $\rightarrow$ $\frac{\partial}{\partial t}\left(\frac{\hbar}{i}\ln\Psi\right) + H(t) = 0$ $\quad\left\{\begin{array}{l}\text{Remark:}\\ \frac{\partial}{\partial t}\ln\Psi(x,t) = \frac{\frac{\partial}{\partial t}\Psi}{\Psi}\end{array}\right.$

This equ. is the analogue of the Hamilton-Jacobi equ. in cl. M. with the <u>action</u> given by

$$S(x,t) \equiv \frac{\hbar}{i}\ln\Psi \longrightarrow \Psi = e^{\frac{i}{\hbar}S(x,t)} \qquad (4)$$

(4) in (3) $\rightarrow$ $\left(-\frac{\partial S}{\partial t}\right)\Psi = \left[\frac{(\nabla S\cdot\nabla S)}{2m} - \frac{i\hbar}{2m}\nabla^2 S + V(x)\right]\Psi \quad (5)$

where we have used $\nabla\cdot(A\varphi) = A\cdot\nabla\varphi + \varphi\,\nabla\cdot A$

in evaluating $\nabla^2\Psi = \nabla\cdot(\nabla\Psi) = \nabla\left(\underbrace{\frac{i}{\hbar}\nabla S}_{A}\ \underbrace{e^{i/\hbar S}}_{\varphi}\right)$

$$(5) \longrightarrow -\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V(x) - \frac{i\hbar}{2m}\nabla^2 S \qquad (6)$$

Comparing (1) and (6);

Q.M $\longrightarrow$ cl. M. $\qquad$ as $\hbar \to 0$

But $\hbar$ being universal const. cannot be equal zero

What is possible and is in effect equivalent to $\hbar \to 0$

is that the term containing $\hbar$ can be negligible compared with the term containing $(\nabla S)^2$.

$$\longrightarrow \quad |\nabla^2 S|\hbar \ll |\nabla S|^2 \quad \to \hbar \ll \frac{|\nabla S|^2}{|\nabla^2 S|} \qquad (7)$$

or $$|\nabla \cdot P|\hbar \ll |P|^2$$

If this cond. is satisfied, an approximation method based on a power series expansion of S in $\hbar$ is possible,

$$S = S_0 + \frac{\hbar}{i} S_1 + \left(\frac{\hbar}{i}\right)^2 S_2 + \cdots \qquad (8)$$

where

$$S \longrightarrow S_0 \qquad \text{in cl. limit}$$

$$S \longrightarrow S_0 + \frac{\hbar}{i} S_1 \qquad \text{in WKB approx.} \qquad (9)$$

The WKB wave func.

This method is limited to $\left\{ \begin{array}{l} \text{t-indep.} \\ \text{one-dim.} \end{array} \right.$ problems

In the case of stationary probs.

$$\psi(x,t) = \varphi(x)\, e^{-\frac{i}{\hbar}Et}$$

$$(4) \rightarrow \quad \varphi(x) = e^{\frac{i}{\hbar}W(x)}$$

where $\quad S(x,t) = W(x) - Et \qquad (10)$

For one-dim. case ;

$$(1) \longrightarrow \quad \left(\frac{dW_0}{dx}\right)^2 - 2m\left[E - V(x)\right] = 0 \qquad (11)$$

(Remember $(6) \xrightarrow[\hbar \to 0]{} (1)$ So the only $W_0(x)$ will contribute)

$$(6) \longrightarrow \quad \left(\frac{dW}{dx}\right)^2 - 2m\left[E - V(x)\right] - i\hbar\frac{d^2W}{dx^2} = 0 \qquad (12)$$

where

$$(8) \longrightarrow \quad W(x) = W_0(x) + \frac{\hbar}{i}W_1(x) + \left(\frac{\hbar}{i}\right)^2 W_2(x) + \cdots \qquad (13)$$

While the Schrödinger equ. (3) reduces,

$$\frac{d^2\varphi}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\varphi = 0 \qquad (14)$$

$$\text{with } \varphi(x) = e^{\frac{i}{\hbar}W(x)} \qquad (14')$$

Now

$$\begin{cases} \left\{2m\left[E - V(x)\right]\right\}^{\frac{1}{2}} = p(x) \quad \text{or} \quad \left\{\frac{2m}{\hbar^2}\left[E - V(x)\right]\right\}^{\frac{1}{2}} = k(x) & (E > V) \\ -i\left\{2m\left[V(x) - E\right]\right\}^{\frac{1}{2}} = p(x) = -i\bar{p}(x) \quad \text{or} \quad -i\left\{\frac{2m}{\hbar^2}\left[V(x) - E\right]\right\}^{\frac{1}{2}} = k(x) = -i\bar{k}(x) & (15) \end{cases}$$

$(E < V)$ classically forbidden region

Then

$$(14) \longrightarrow \quad \frac{d^2\varphi}{dx^2} + \frac{p^2}{\hbar^2}\varphi = 0 \qquad (16)$$

We are interested to solve this eqn. within the WKB approx.

This is obtained by substituting

$$W \approx W_0 + \frac{\hbar}{i} W_1$$

in (14').

Now let, $\quad u(x) = \frac{dW(x)}{dx} \quad$ for convenience $\quad$ (17)

(17)(15) in (12) $\rightarrow \frac{\hbar}{i}\frac{du}{dx} = P^2 - u^2 \quad$ (18)

Also,

(13) $\rightarrow \quad u(x) = u_0(x) + \frac{\hbar}{i} u_1(x) + \left(\frac{\hbar}{i}\right)^2 u_2(x) + \cdots \quad$ (19)

In terms of u, $\varphi(x)$ is given by

$$\varphi(x) = e^{\frac{i}{\hbar}\int^x \frac{dW}{dx'}dx'} = e^{\frac{i}{\hbar}\int u(x')dx'} \qquad (20)$$

(19) in (18) $\rightarrow \frac{\hbar}{i}\frac{du_0}{dx} + \left(\frac{\hbar}{i}\right)^2 \frac{du_1}{dx} + \cdots =$

$$= (P^2 - u_0^2) - 2\left(\frac{\hbar}{i}\right) u_0 u_1 - \left(\frac{\hbar}{i}\right)^2 \left[u_1^2 + 2u_0 u_2\right] + \cdots \qquad (21)$$

Equating the coeffs. of like powers of $\left(\frac{\hbar}{i}\right)$ on either side of (21),

$\rightarrow \quad u_0 = \pm P$

$u_1 = -\frac{1}{2u_0}\left(\frac{du_0}{dx}\right) = -\frac{1}{2P}\left(\frac{dP}{dx}\right) \quad$ for both sign

$- - - - \quad$ (22)

$$\rightarrow \begin{cases} u_+ = p - \frac{\hbar}{i}\frac{1}{2p}\left(\frac{dp}{dx}\right) = p - \frac{\hbar}{i}\frac{d}{dx}\left(\ln p^{1/2}\right) \\ u_- = -p - \frac{\hbar}{i}\frac{1}{2p}\left(\frac{dp}{dx}\right) = -p - \frac{\hbar}{i}\frac{d}{dx}\left(\ln p^{1/2}\right) \end{cases} \qquad (23)$$

(23) in (20) $\longrightarrow$ $$\begin{cases} \varphi_+(x) = \frac{1}{\sqrt{p}}\, e^{\frac{i}{\hbar}\int^x p\,dx'} \\ \varphi_-(x) = \frac{1}{\sqrt{p}}\, e^{-\frac{i}{\hbar}\int^x p\,dx'} \end{cases} \qquad (23)$$ two indep. sol. of (16)

$$\rightarrow \varphi_{WKB}(x) = \frac{A}{\sqrt{p}}\, e^{\frac{i}{\hbar}\int^x p(x')dx'} + \frac{B}{\sqrt{p}}\, e^{-\frac{i}{\hbar}\int^x p(x')dx'} \qquad (24)$$

Alternative approach;

(13) in (12) and equating to <u>zero</u> the coeffs. of each power of $\hbar$,

$$\longrightarrow \frac{1}{2m}\left(\frac{dW_0(x)}{dx}\right)^2 + V(x) - E = 0 \qquad (25)$$

$$\frac{dW_0(x)}{dx}\frac{dW_1(x)}{dx} - \frac{i}{2}\frac{d^2W_0(x)}{dx^2} = 0 \qquad (26)$$

$$\frac{dW_0(x)}{dx}\frac{dW_2(x)}{dx} + \left(\frac{dW_1(x)}{dx}\right)^2 - i\frac{d^2W_1(x)}{dx^2} = 0 \qquad (27)$$

which must be solved successively to find $W_0, W_1, W_2 \ldots$

Assuming $E > V(x)$ (like in scatt.) Classically allowed region of positive kinetic energy

$$(25) \longrightarrow W_0(x) = \pm\int^x p(x')\,dx' \qquad (28)$$

$$(28) \text{ in } (26) \longrightarrow W_1(x) = \frac{i}{2}\ln p(x) \qquad (29)$$

$$(28)(29) \text{ in } (27) \rightarrow W_2(x) = \frac{m}{2}\left(p(x)\right)^{-3}\frac{dV(x)}{dx} - \frac{m^2}{4}\int^x \left(p(x')\right)^{-5}\left(\frac{dV(x')}{dx'}\right)^2 dx' \qquad (30)$$

From this expression and that of $p(x)$

i.e. $p(x) = \left[2m\left(E - V(x)\right)\right]^{1/2}$

it is clear that W_2 will be small whenever;

$\begin{cases} \text{(i)} \ \frac{dV(x)}{dx} \to \text{small} \\ \text{(ii)} \ E-V \text{ not too close to zero} \end{cases}$ (i.e P not too close to zero)

If in addition all $\frac{d^nV(x)}{dx^n}$ $n \geq 2$ are small

$\longrightarrow$ $S_3, S_4 ---$ will also be small.

Note that for $V(x) = V_0$ const. pot.

$\rightarrow W = W_0 + W_1 = \pm P_0 X + \frac{i}{2} \ln P_0$ (exact)

$\cancel{S = S_0 = \pm P_0 X}$, $\cancel{S_1 = S_2 = \cdots} = 0$

exact

$\longrightarrow \varphi(x) = A \, e^{\pm \frac{i}{\hbar} P_0 X}$ plane wave sol.

Note also that;

if $\frac{d^nV(x)}{dx^n} \longrightarrow$ small $\forall n$

$\longrightarrow$ pot. is slowly varing func. of x

i.e. $V(x)$ change slightly over de Brogli wave lengh

$$\lambda(x) = \frac{h}{P(x)}$$ (remember $P(x)$ must not be small) $\rightarrow \lambda \rightarrow$ small

So we retain only the first two terms of equ. (8);

Using (28)(29) in (14');

$$\varphi(x) = A \frac{1}{\sqrt{P(x)}} e^{\pm \frac{i}{\hbar} \int^x P(x')dx'} \qquad (E > V)$$

Criterion for the Validity of the Approx.;

WKB approx. is valid if;

$$\left| \frac{\hbar}{2} W_2(x) \right| \ll 1 \qquad (31)$$

{ this approx is leading to (33) / is consistent with (34)

Taking into account that both terms in (30) are of the same order of mag. (because of integration) → { For example assume $V(x)=x^2$ and evaluate both terms

Mag. of $S_2 \approx$ Mag. of first term.

$$\longrightarrow \left| \frac{\hbar m \,(dV(x)/dx)}{[2m(E-V(x))]^{3/2}} \right| \ll 1 \qquad (32)$$

This is satisfied if $\begin{cases} \dfrac{dV(x)}{dx} \to \text{small} & \text{(slow varring Pot.)} \\ E-V \longrightarrow \text{large} & \text{(Kinetic energy)} \end{cases}$

An alternative way of writing (32);

$$(32) \longrightarrow \left| \frac{\hbar m\,(dV(x)/dx)}{P^3_{(x)}} \right| = \left| \frac{\hbar}{P^2_{(x)}} \frac{dP(x)}{dx} \right| = \left| \frac{1}{P(x)} \frac{dP(x)}{dx} \lambda\!\!\!^{-}(x) \right| \ll 1 \qquad (33)$$

where $\lambda\!\!\!^{-}(x) = \dfrac{\hbar}{P(x)} = \dfrac{\lambda(x)}{2\pi}$

and we have used $\dfrac{dP(x)}{dx} = \dfrac{d}{dx}\left[2m(E-V(x))\right]^{1/2} = -\dfrac{m}{P(x)} \dfrac{dV(x)}{dx}$

(33) means that! The fractional change in $P(x)$ must be small in a wave length.

In other words:

The pot. must change slowly that the momentum of the particle is nearly const. over many wavelength.

Inequality (33) is evident also from (7).

$$\hbar\,|\nabla.P| << |P^2| \rightarrow \hbar\left|\frac{dP}{dx}\right| << |P^2|$$

$$\rightarrow \left|\frac{1}{P}\frac{dP}{dx}\,\lambda\!\!\!^-\right| << 1 \qquad (34)$$

(33) can be written as: $\left|\frac{d\lambda\!\!\!^-(x)}{dx}\right| << 1$ (34')

$\lambda\!\!\!^- = \frac{\hbar}{P}$

$\frac{d\lambda\!\!\!^-}{dx} = \hbar\,\frac{-\frac{dP}{dx}}{P^2}$

Now, $\delta\lambda\!\!\!^-(x) = \frac{d\lambda\!\!\!^-}{dx}\,\delta x$ the change occuring in $\lambda\!\!\!^-$ in the distance δx

Upon setting $\delta x = \lambda\!\!\!^-$

$$|\delta\lambda\!\!\!^-(x)| = \left|\frac{d\lambda\!\!\!^-(x)}{dx}\,\lambda\!\!\!^-(x)\right| << \lambda\!\!\!^-(x) \qquad (35)$$

Showing $\lambda\!\!\!^-$ must only change by a small fraction of itself over a distance of order of $\lambda\!\!\!^-$.

For classically forbiden regions of negative kinetic energy $(E<V) \longrightarrow p(x)$: purely imaginary

Solving (25) (26);

$$\psi'(x) = \frac{A}{\sqrt{|p(x)|}} e^{\pm\frac{1}{\hbar}\int^x |p(x')|dx'} \qquad E<V$$

$$\psi'_{WKB} = \frac{1}{\sqrt{|p(x)|}}\left[C e^{-\frac{1}{\hbar}\int^x |p(x')|dx'} + D e^{+\frac{1}{\hbar}\int^x |p(x')|dx'}\right]$$

$E<V$

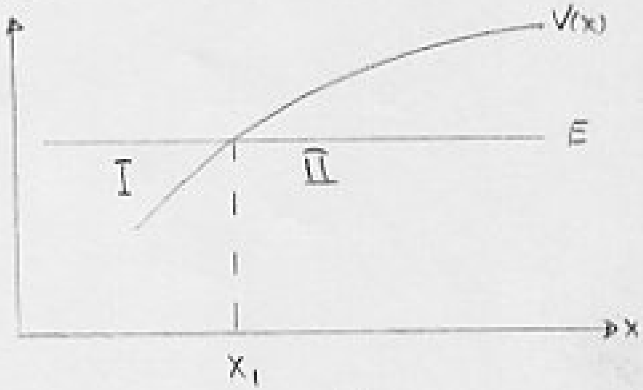
(36)

Connection Formulae

At classical turning point the cond. (32) or (33) <u>is not</u> satisfied

At this point $\begin{cases} p(x) = 0 \\ \text{but } \dfrac{dp(x)}{dx} \neq 0 \end{cases}$

$\rightarrow$ Ψ_{WKB} or Ψ'_{WKB} <u>is not</u> the <u>true</u> sol. <u>near</u> this point.



I : classical allowed region

II : Non-classical region

x_1 : Turning point

We have to <u>find</u> a way to <u>connect</u> the two sols.

i.e. To <u>extend</u> the WKB sol. from one region to the other <u>through</u> the <u>turning</u> point.

The Procedure;

i) Solving the Schrodinger equ (16) <u>exactly</u> near the Turning Point

ii) And <u>extra-polating</u> the sol. for regions <u>far</u> away from the turning point.

The extrapolated (or asymptotic) sols. will resemble the WKB sols.

Classically;

A particle would be turned back at $x = x_1$, when

$T = E - V(x) = 0$ kinetic energy

Quantum mechanically;

Since the force $-\frac{dV(x)}{dx}$ is finite at $x = x_1$

$\longrightarrow$ $V(x)$ represents a translusent wall rather than opaque one (i.e. $V(x_1) \to \infty$)

$\longrightarrow$ There is a leakage from region I to region II (tunneling).

For $E > V(x)$, (I-region)

$$(24) \to \varphi_I(x) = \frac{A_1}{\sqrt{P}} e^{\frac{i}{\hbar}\int_{x_1}^{x} P\,dx'} + \frac{B_1}{\sqrt{P}} e^{-\frac{i}{\hbar}\int_{x_1}^{x} P\,dx'}$$

$$= \frac{A}{\sqrt{P}} \sin\left[-\frac{1}{\hbar}\int_{x_1}^{x} P\,dx' + \frac{\pi}{4}\right] + \frac{B}{\sqrt{P}} \cos\left[-\frac{1}{\hbar}\int_{x_1}^{x} P\,dx' + \frac{\pi}{4}\right] \quad (1)$$

Where $$A = (A_1 - iB_1)\, e^{i\pi/4}$$
$$B = -(A_1 + iB_1)\, e^{-i\pi/4} \qquad (2)$$

For $E < V(x)$, (II-region)

$$p(x) = i\,|p(x)|$$

$$\varphi_{\mathrm{II}}(x) = \frac{A_2}{\sqrt{p}}\, e^{-\frac{1}{\hbar}\int_{x_1}^{x} p\, dx'} + \frac{B_2}{\sqrt{p}}\, e^{\frac{1}{\hbar}\int_{x_1}^{x} p\, dx'} \qquad (3)$$

Now φ_{I} and φ_{II} are appox. to the same func. φ.

$$\rightarrow A_1, B_1 \xleftrightarrow{\text{are related}} A_2, B_2$$

The sol. of Schrödinger equ. near the turning point:

Assume, $$V(x) \simeq V(x_1) + (x - x_1)\left(\frac{dV}{dx}\right)_{x=x_1}$$ (linear near x_1)

$$\simeq E + C(x - x_1) \qquad (4)$$

$C = \left(\frac{dV}{dx}\right)_{x=x_1} > 0$ increasing func. (Fig. P 156)

Note that $V(x)|_{x=x_1} = E$

$$p^2 = 2m(E - V) \underset{x \sim x_1}{\simeq} -2mC(x - x_1) \qquad (5)$$

Substituting p^2 in;

$$(16P148) \rightarrow \frac{d^2\varphi}{dx^2} + \frac{p^2}{\hbar^2}\varphi = 0 \longrightarrow \frac{d^2\psi}{d\xi^2} - \xi\psi = 0 \qquad (6)$$

when $\xi = \left(2m\frac{c}{\hbar^2}\right)^{1/3}(x - x_1)$

$$\psi(\xi) = \varphi(x) \qquad (7)$$

$$\rightarrow \begin{cases} \xi < 0 & : \text{region - I} \\ \xi > 0 & : \quad " \quad \text{- II} \\ \text{Turning point: } \xi = 0 \end{cases}$$

The sols. are known as Airy Funcs.;

$$Ai(\xi) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{s^3}{3} + s\xi\right)ds$$

$$Bi(\xi) = \frac{1}{\pi}\int_0^\infty \left[e^{-s\xi - \frac{s^3}{3}} + \sin\left(\frac{s^3}{3} + s\xi\right)\right]ds \qquad (8)$$

The sol. is a combination of these two;

$$\psi(\xi) = Ai(\xi) + Bi(\xi) \qquad (9)$$

We are interested only in the asymptotic forms of Ai and Bi;

$$\mathrm{Ai}(\xi) \sim (-\pi^2 \xi)^{-\frac{1}{4}} \sin\left[\tfrac{2}{3}(-\xi)^{\frac{3}{2}} + \tfrac{\pi}{4}\right] \qquad \xi << 0$$

$$\sim \tfrac{1}{2}(\pi^2 \xi)^{-\frac{1}{4}} \, e^{-\frac{2}{3}\xi^{3/2}} \qquad \xi >> 0$$

$$\mathrm{Bi}(\xi) \sim (-\pi^2 \xi)^{-\frac{1}{4}} \cos\left[\tfrac{2}{3}(-\xi)^{\frac{3}{2}} + \tfrac{\pi}{4}\right] \qquad \xi << 0$$

$$\sim (\pi^2 \xi)^{-\frac{1}{4}} \, e^{\frac{2}{3}\xi^{\frac{3}{2}}} \qquad \xi >> 0$$

(10)

Now for $\xi < 0$ (i.e. $x < x_1$);

$$\frac{2}{3}(-\xi)^{3/2} = \int_0^{+\xi} \sqrt{-\xi'}\, d(-\xi') = -\int_0^{\xi} \sqrt{-\xi'}\, d\xi'$$

$$= -\int_{x_1}^{x} \left(2m\frac{c}{\hbar^2}\right)^{\frac{1}{2}} (x_1 - x')^{\frac{1}{2}} dx' = -\frac{1}{\hbar}\int_{x_1}^{x} p(x')\, dx' \qquad (11)$$

where we have used equs (5) and (7).

Also;

$$(-\xi)^{1/4} = (2mc)^{1/12}\, \hbar^{-1/6} (x_1 - x)^{1/4} = (2mc\hbar)^{-\frac{1}{6}} \left[2mc(x_1 - x)\right]^{1/4}$$

$$= (2mc\hbar)^{-1/6} \sqrt{p(x)} \qquad (12)$$

Similarly for $\xi > 0$ (i.e $x > x_1$)

$$\frac{2}{3}\xi^{2/3} = \frac{1}{\hbar}\int_{x_1}^{x} |p(x')|\, dx' \qquad (13)$$

and $(\xi)^{1/4} = (2mC\hbar)^{-1/6}\sqrt{|P(x)|}$ (14)

$$\rightarrow \quad Ai(\xi) = \varphi_1^{osc}(x) \sim \frac{\alpha}{\sqrt{p}} \sin\left[\frac{1}{\hbar}\int_x^{x_1} p(x')\,dx' + \frac{\pi}{4}\right] \qquad \xi \ll 0 \text{ or } x \ll x_1$$

$$Ai(\xi) = \varphi_1^{exp}(x) \sim \frac{\alpha}{2\sqrt{|P|}} e^{-\frac{1}{\hbar}\int_{x_1}^{x} |P|\,dx'} \qquad \xi \gg 0 \text{ or } x \gg x_1$$

$$Bi(\xi) = \varphi_2^{osc}(x) \sim \frac{\alpha}{\sqrt{p}} \cos\left[\frac{1}{\hbar}\int_x^{x_1} p(x')\,dx' + \frac{\pi}{4}\right] \qquad \xi \ll 0 \text{ or } x \ll x_1$$

$$Bi(\xi) = \varphi_2^{exp}(x) \sim \frac{\alpha}{\sqrt{|P|}} e^{\frac{1}{\hbar}\int_{x_1}^{x} |P|\,dx'} \qquad \xi \gg 0 \text{ or } x \gg x_1$$

(15)

where $\alpha = (2mC\hbar/\pi^3)^{1/6}$

φ_k^{osc} : The wave fuc. in Classical region

φ_k^{exp} : Continuation of φ_k^{osc} in the non-classical region

The connection;

cl.-region | non-cl. region

$\varphi_1^{osc}(x) \longleftrightarrow \varphi_1^{exp}$ ⤳ decreasing func.

$\varphi_2^{osc}(x) \longleftrightarrow \varphi_2^{exp}$ ⤳ increasing func.

Connection formulae (16)

The general sol.;

$$\varphi^{osc}(x) \sim \frac{\alpha}{\sqrt{P}} \left[\sin\left[\frac{1}{\hbar}\int_x^{x_1} P(x')dx' + \frac{\pi}{4}\right] + \cos\left[\frac{1}{\hbar}\int_x^{x_1} P(x')dx' + \frac{\pi}{4}\right]\right] \quad x \ll x_1$$

$$\varphi^{exp}(x) \sim \frac{\alpha}{\sqrt{|P|}} \left[\frac{1}{2} e^{-\frac{1}{\hbar}\int_{x_1}^{x} |P(x')|dx'} + e^{\frac{1}{\hbar}\int_{x_1}^{x} |P(x')|dx'}\right] \quad (17)$$

$$x \gg x_1 \qquad (18)$$

Comparing (1)(3) with (17)(18);

We see that;

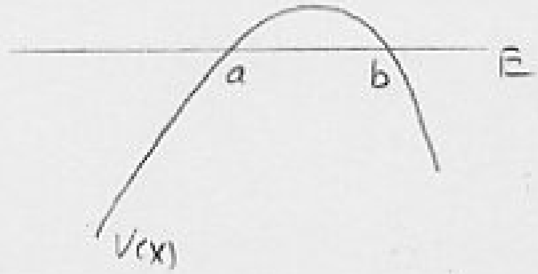
φ^{osc} is φ_{WKB} (region I)

φ^{exp} is φ'_{WKB} (" II)

$$\begin{cases} A_2 = \frac{\alpha}{2} = \frac{A}{2} \\ B_2 = \alpha = B \end{cases} \qquad (19)$$

where $\alpha = \left(\frac{2m\hbar}{\pi^3} \left(\frac{dV}{dx}\right)_{x=x_1} \right)^{1/6}$

Since the approxs. (15) are valid for regions far away from the turning points, this method cannot be applied when there are two turning points close to each other.



In fact substituting

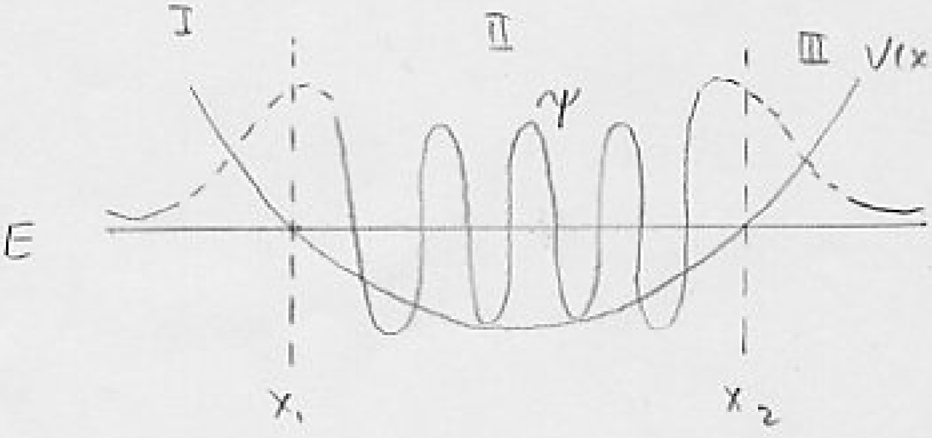
$$P^2 \cong -2mC(x-x_1) \qquad (x \sim x_1)$$

in $\left|\frac{1}{P}\frac{dP}{dx}\lambda\right| \ll 1$ we get;

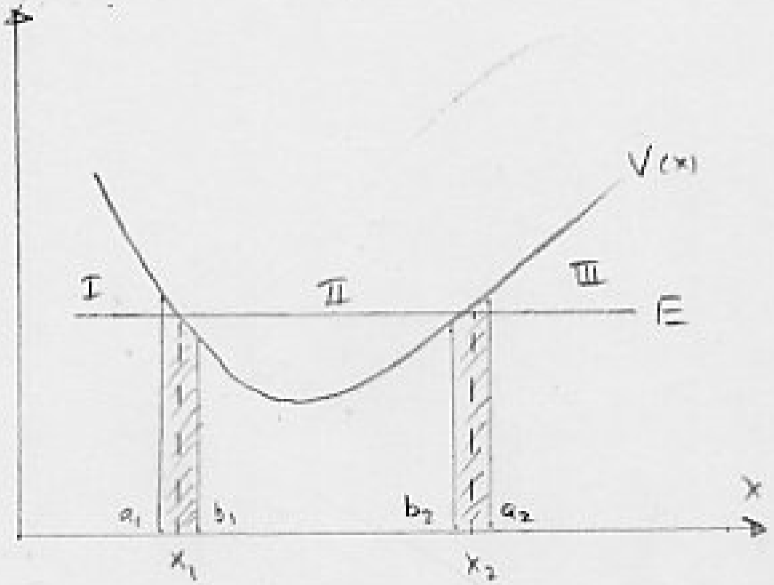
$$\longrightarrow \quad |x-x_1| \gg \lambda \qquad (20)$$

as the cond. for the validity of WKB approx at x

$\longrightarrow$ For the applicability of WKB method it is necessary that $|x_a - x_b| \gg \lambda$ (at least several times)



Applications:



Bound States:

The energy levels of one-dim. bound system?

For a bound system

$\psi \longrightarrow 0$ as $x \to \pm\infty$

WKB approx. not valid in the dashed points

II - Cl. -region

i.e. $\varphi_{I\,WKB}$: decreasing

$\varphi_{III\,WKB}$: "

$$\longrightarrow \begin{cases} \varphi_I(x) \approx \dfrac{A_1}{\sqrt{|P|}}\, e^{-\frac{1}{\hbar}\int_x^{x_1} |P(x')|\,dx'} & x < a_1 \\ \varphi_{III}(x) \approx \dfrac{A_3}{\sqrt{|P|}}\, e^{-\frac{1}{\hbar}\int_{x_2}^{x} |P(x')|\,dx'} & x > a_2 \end{cases} \qquad (A_i(\xi)\ \text{sol.}) \tag{21}$$

Acc. to connection formulae:

$$\varphi_{II}(x) \approx \frac{2A_1}{\sqrt{P}} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x} P(x')\,dx' + \frac{\pi}{4}\right]$$
$$\approx \frac{2A_3}{\sqrt{P}} \sin\left[\frac{1}{\hbar}\int_{x}^{x_2} P(x')\,dx' + \frac{\pi}{4}\right] \tag{22}$$

But $$\int_{x_1}^{x} p(x')dx' = \int_{x_1}^{x_2} p\,dx' - \int_{x}^{x_2} p\,dx'$$

$$\to \sin\left[\frac{1}{\hbar}\int_{x_1}^{x} p\,dx' + \frac{\pi}{4}\right] = \sin\left[\left(\frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx' + \frac{\pi}{2}\right) - \left(\frac{1}{\hbar}\int_{x}^{x_2} p\,dx' + \frac{\pi}{4}\right)\right] \quad (23)$$

(23) in (22) $\to$

$$A_1 \sin\left[\left(\frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx' + \frac{\pi}{2}\right) - \left(\frac{1}{\hbar}\int_{x}^{x_2} p\,dx' + \frac{\pi}{4}\right)\right] = A_3 \sin\left(\frac{1}{\hbar}\int_{x}^{x_2} p\,dx' + \frac{\pi}{4}\right) \quad (24)$$

Comparing with the identity;

$$\sin(n\pi - \theta) = (-)^{n-1} \sin\theta \qquad n = 1, 2, 3, \ldots$$

$$\to \begin{cases} \dfrac{1}{\hbar}\displaystyle\int_{x_1}^{x_2} p(x)\,dx + \dfrac{\pi}{2} = (n+1)\pi \\ \dfrac{A_3}{A_1} = (-)^n \end{cases} \qquad n = 0, 1, 2 \ldots \quad (25)$$

Remark: $\int_{x_1}^{x_2} p(x)\,dx \geqslant 0$

Now; $$2\int_{x_1}^{x_2} p\,dx = \int_{x_1}^{x_2} p\,dx - \int_{x_2}^{x_1} p\,dx = \oint p\,dx$$

$$\to \oint p\,dx = \left(n + \frac{1}{2}\right)h \qquad (n = 0, 1, 2, \ldots) \qquad (26)$$

We recall the Bohr–Sommerfeld quantization rule of the old quantum Theory,

$$\oint P\,dq = nh$$

But (26) is in <u>better agreement</u> with the <u>exact</u> result.

The approximate wave func. is given by (22) and <u>A_1</u> is determined by the normalization requirement.

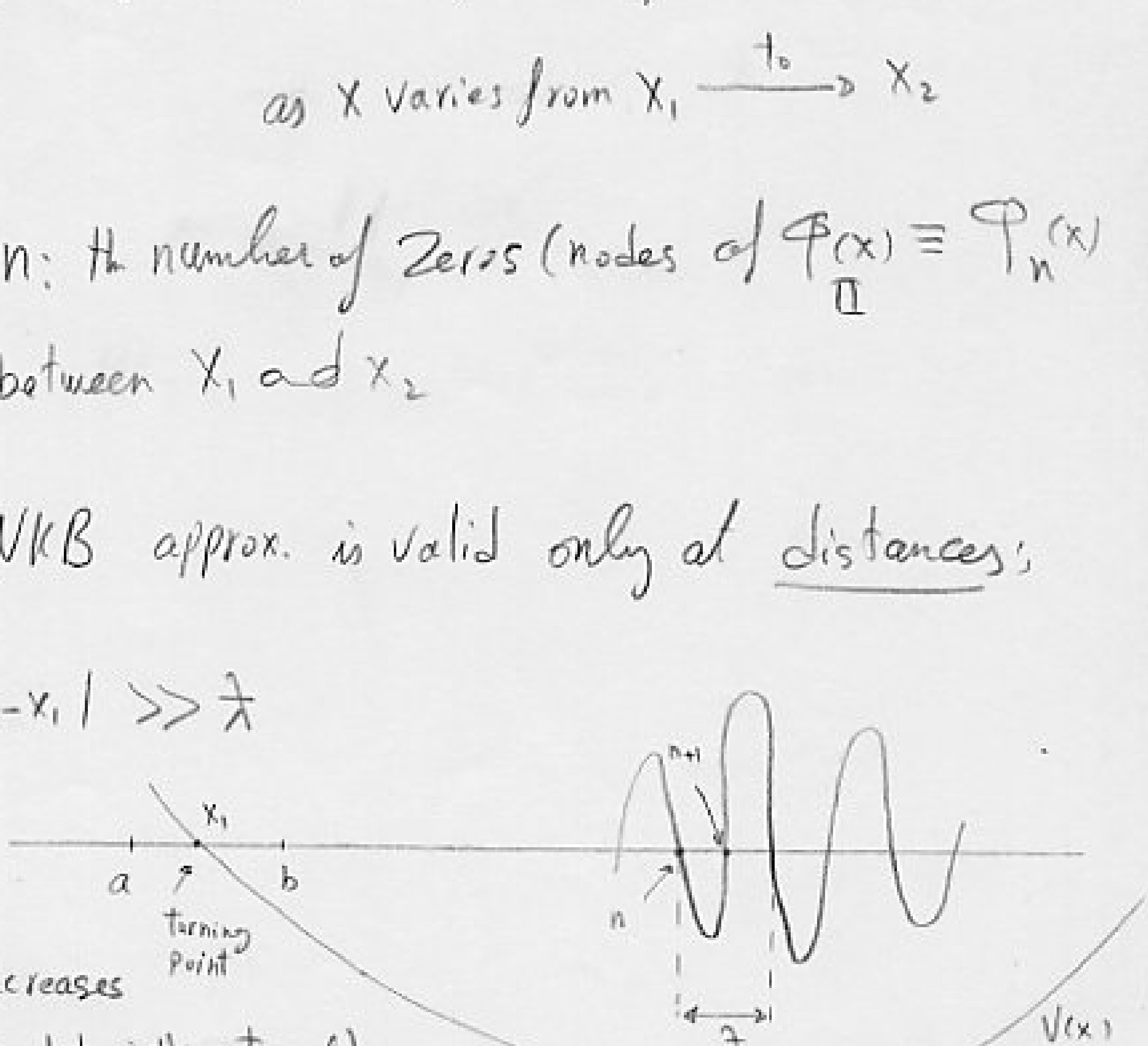
Acc. to (25);

The phase of Sine func. in (22) Varies from $\pi/4 \xrightarrow{\text{to}} (n+\frac{3}{4})\pi$

as x varies from $x_1 \xrightarrow{\text{to}} x_2$

<u>Thus</u> $\rightarrow$ n: the number of Zeros (nodes of $\phi_{\boxed{\text{II}}}(x) \equiv \phi_n(x)$ between x_1 and x_2

But the WKB approx. is valid only at <u>distances</u>; that; $|x - x_1| \gg \lambda\!\!\!^{-}$



For large n;
(a – b) interval decreases
(WKB approx. is <u>not</u> valid in this interval)

$\longrightarrow$ Equ(22) is good approx. for large n.

In that case the sine-func. oscillates rapidly in the interval $x_1 < x < x_2$

For rapid oscillation; $\int |\sin(\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' + \frac{\pi}{4})|^2 dx' \simeq \frac{1}{2}$

Thus the normalization;

$$1 = \int_{-\infty}^{\infty} |\varphi_n(x)|^2 dx \simeq \int_{x_1}^{x_2} |\varphi_n(x)|^2 dx$$

$$\simeq 4|A_1|^2 \int_{x_1}^{x_2} \frac{1}{2} \frac{dx}{p(x)} = 4|A_1|^2 \frac{\tau_n}{4m} = |2A_1|^2 \frac{\pi}{2m\omega_n} \quad (27)$$

where $\tau_n = \dfrac{2\pi}{\omega_n} = 2m \displaystyle\int_{x_1}^{x_2} \frac{dx}{p(x)}$ the period on the n-th mode

Remark; $p(x) = mv(x) = m\dfrac{dx}{dt}$

(the time required for the particle to mome from x_1 to x_2 and x_2 to x_1)

(27) in (22);

$$\varphi_n(x) \simeq \left(\frac{2m\omega_n}{\pi p(x)}\right)^{1/2} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' + \frac{\pi}{4}\right]$$

Ex. A ball bouncing up and down over a hard surface;

$$V = \begin{cases} mgx & x>0 \\ \infty & x<0 \end{cases} \qquad (1)$$

One might be temped to use (25) directly with;

$$x_1 = 0 \ , \ x_2 = \frac{E}{mg}$$

which are classical turning points.

But in derivation of (25) we have assumed the WKB wave func. has leakage into $x < x_1$ region,

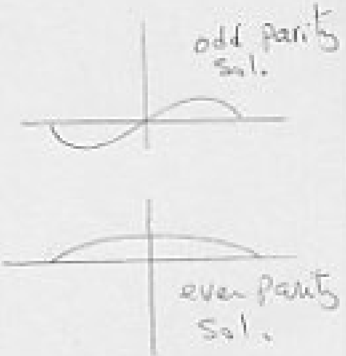
While in our prob. the wave func. must strictly vanish for $x \leq x_1 = 0$

A much more satisfactory approach;

We consider odd-parity sols. — guaranteed to vanish at $x = 0$ of a modified prob. defined by;

$$V(x) = mg|x| \qquad (-\infty < x < \infty)$$

with turning points $\begin{cases} x_1 = -\dfrac{E}{mg} \\ x_2 = +\dfrac{E}{mg} \end{cases}$



Remark: The mentioned pot. produces odd-parity sols.
even- "

The energy spectrum of odd-parity states for this modified prob. $\underline{\underline{\text{must be}}}$ same as that of original prob.

$$\int_{x_1}^{x_2} p(x)\,dx = (n_{odd} + \tfrac{1}{2})\pi\hbar$$

n_{odd}: because of odd-parity sols.

$$\int_{-\frac{E}{mg}}^{+\frac{E}{mg}} \sqrt{2m(E - mg|x|)}\,dx = (n_{odd} + \tfrac{1}{2})\pi\hbar \qquad (n_{odd} = 1, 3, 5, \ldots)$$

$$\int_0^{E/mg} \sqrt{2m(E - mgx)}\,dx = (\tfrac{n_{odd}}{2} + \tfrac{1}{4})\pi\hbar = (n - \tfrac{1}{4})\pi\hbar \quad (n = 1, 2, 3, \ldots)$$

$$\rightarrow E_n = \frac{[3(n-\frac{1}{4})\pi]^{2/3}}{2} (mg^2\hbar^2)^{1/3}$$

quantized energy levels for the bouncing ball

This prob. is soluble analitically without any approx. The energy eigenvalues can be expressed in terms of the Zeros of the Airy func.

$$Ai(-\lambda_n) = 0$$

as $\quad E_n = \left(\frac{\lambda_n}{2^{1/3}}\right)\left(mg^2\hbar^2\right)^{1/3}$

The agreement is excellent (see Table) even for small n, and essentially exact for $n \simeq 10$

n	WKB	Exact
1	2.320	2.338
2	4.082	4.088
⋮	⋮	⋮
10	12.828	12.829

The pot. of the type (1) is of interest in studying the energy spectrum of a quark-antiquark bound system (quarkonium)

$$V = ar$$

The force is estimated to be $\sim 1\,\text{Gev}/\text{fm} \simeq 1.6\times10^{3}\ \text{N}$

~ 1.6 Tons

2-5 Propagators and Feynman Path Integrals:

Propagators in Wave Mechanics

We remember;

$$|\alpha, t_0; t\rangle = e^{-\frac{i}{\hbar}H(t-t_0)}\,|\alpha, t_0\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha, t_0\rangle\, e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} \qquad (1)$$

<u>for t-indep. H</u>

$$\rightarrow \langle x'|\alpha, t_0; t\rangle = \sum_{a'} \langle x'|a'\rangle\langle a'|\alpha, t_0\rangle\, e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} \qquad (2)$$

In the language of wave mechanics;

$$\psi(x', t) = \sum_{a'} c_{a'}(t_0)\, u_{a'}(x')\, e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} \qquad (3)$$

with $\quad u_{a'}(x') = \langle x'|a'\rangle$

Note also that;

$$\langle a'|\alpha, t_0\rangle = \int d^3x'\, \langle a'|x'\rangle\langle x'|\alpha, t_0\rangle$$

or

$$c_{a'}(t_0) = \int d^3x'\, u^*_{a'}(x')\,\psi(x', t_0) \qquad (4)$$

(4) in (2) $\rightarrow$ $\langle x''|\alpha, t_0; t\rangle = \sum_{a'} \langle x''|a'\rangle \int d^3x'\, \langle a'|x'\rangle\langle x'|\alpha, t_0\rangle\, e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}$

$$= \int d^3x' \sum_{a'} \langle x''|a'\rangle\langle a'|x'\rangle\, e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}\, \langle x'|\alpha, t_0\rangle \qquad (5)$$

$$\rightarrow \psi(\vec{x},t) = \underbrace{\int d^3x' \, K(\vec{x},t;\vec{x}',t_0)}_{\text{integral op.}} \psi(\vec{x}',t_0) \qquad (6)$$

Where

$$K(\vec{x},t;\vec{x}',t_0) = \sum_{a'} \underbrace{\langle \vec{x}|a'\rangle}_{u_{a'}(\vec{x})} \langle a'|\vec{x}'\rangle \, e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} \qquad (7)$$

the Kernel of the integral op. Known as Propagator in wave mechanics.

K is pot.-dep. (see equ. (8))

but it is indep. of the initial $\psi(\vec{x}',t_0)$.

If $\begin{cases} K(\vec{x},t;\vec{x}',t_0) \\ \psi(\vec{x}',t_0) \end{cases}$ are known $\longrightarrow$ The time evolution of the wave func. is completely predicted.

In this sence Schrödinger wave mechanichs is a perfectly causal theory.

The time development of a wave func. subjected to some pot. is as deterministic as anything else in Cl. M. provided that the system is left undisturbed.

The only peculiar feature, if any, is that when a measurement intervences, the wave func. changes abruptly, in an uncontrollable way, into one of the eigenfuncs., of the observable being measured.

The properties of the Propagator:

i) For $\underline{t > t_0}$ it satisfies Schrödinger t-dep equ. in the variables of x'' and t; with x' and t_0 fixed.

This is evident from (7); because $\langle x''|a'\rangle e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}$ being the wave func. corresponding to $U(t,t_0)|a'\rangle$ satisfies the wave equ.

Calling $|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|x'\rangle e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}$

$$\langle x''|\left(i\hbar\frac{\partial}{\partial t}\right)|\alpha\rangle \overset{?}{=} \langle x''|H|\alpha\rangle$$

$$i\hbar\frac{\partial}{\partial t}\sum_{a'}\langle x''|a'\rangle\langle a'|x'\rangle e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} \overset{?}{=} \sum_{a'}\langle x''|H(x'')|a'\rangle\langle a'|x'\rangle e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}$$

$$\sum_{a'} E_{a'}\langle x''|a'\rangle\langle a'|x'\rangle e^{-\frac{i}{\hbar}E_{a'}(t-t_0)} \underset{(ok)}{=} \sum_{a'} E_{a'}\langle x''|a'\rangle\langle a'|x'\rangle e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}$$

ii) $\lim_{t\to t_0} K(x'',t;x',t_0) = \delta^3(x''-x')$

$$\lim_{t\to t_0} K(x'',t;x',t_0) = \sum_{a'}\langle x''|a'\rangle\langle a'|x'\rangle(1) = \langle x''|x'\rangle = \delta^3(x''-x')$$

Because of these $\underline{\text{two}}$ properties; $K(x'',t;x',t_0)$ regarded as a func. of x'', is simply the wave func at t of a particle which was localized $\underline{\text{precisely}}$ at x' at t_0.

This interpretation follows, more elegantly, from,

$$(7) \rightarrow \quad K(x'',t;x',t_0) = \langle x''| \underbrace{e^{-\frac{i}{\hbar}H(t-t_0)} |x'\rangle}_{\substack{\text{The state ket at } t \text{ of a system that was} \\ \text{localized precisely at } t_0 (<t). \\ (\text{i.e. eigenket } |x'\rangle)}} \quad (8)$$

Remark: Analogue case in <u>electrostatic</u>:

$$\psi(x'',t) = \int d^3x' \, K(x'',t;x',t_0)\, \psi(x',t_0)$$

$$\Phi(x'') = \int d^3x' \, \frac{1}{|x''-x'|} \rho(x') \qquad (\text{electrostatic pot.})$$

$$\begin{cases} K(x'',t;x',t_0) : \text{ sol. for eigenket } |x'\rangle \\ \psi(x',t_0) : \text{ particle wave func.} \end{cases}$$

$$\begin{cases} \dfrac{1}{|x''-x'|} : \text{ sol. for point charge} \\ \rho(x') : \text{ charge dist.} \end{cases}$$

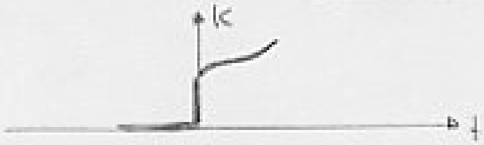
The propagator $K(x'',t;x',t_0)$ is simply the Green's func for the time-dep. wave equ. satisfying:

$$\left[-\frac{\hbar^2}{2m}\nabla''^2 + V(x'') - i\hbar\frac{\partial}{\partial t}\right] K(x'',t;x',t_0) = -i\hbar\,\delta^3(x''-x')\,\delta(t-t_0)$$

(when $t \lessgtr t_0$ situation is also included) with the boundary cond.:

$$K(\vec{x}, t; \vec{x}', t_0) = 0 \quad \text{for} \quad t < t_0$$

The δ-func. $\delta(t-t_0)$ is needed, because K varies discontinuously at $t = t_0$.



Or; $\quad (H - i\hbar \frac{\partial}{\partial t})\, G(\vec{x}, t; \vec{x}', t_0) = -i\hbar\, \delta^3(\vec{x} - \vec{x}')\, \delta(t - t_0)$

where $\quad G(\vec{x}, t; \vec{x}', t_0) = \theta(t - t_0)\, K(\vec{x}, t; \vec{x}', t_0)$

Ref.: R.P. Feynman and A.R. Hibbs, Q.M. and Path Integrals, McGraw-Hill book Co., New york. 1965

Remark:

$$(\nabla^2 + k^2)\,\psi(r) = U(r)\,\psi(r) \qquad E = \frac{\hbar^2 k^2}{2m} \qquad U(r) = \frac{2m}{\hbar^2} V(r)$$

The standard way of incorporating boundary conds. into a differential equ. is to convert the equ. into an integral equ.. Consider,

$(\nabla^2 + k^2)\, G_k(r, r') = \delta(r - r')$ $\quad$ Green's func. for the Helmholtz equ.

By construction $\quad \psi(r) = \int G_k(r, r')\, U(r')\, \psi(r')\, d^3 r'$

If we wish, we may add to this any sol. of the homogeneous equ.

$(\nabla^2 + k^2)\, \varphi = 0$

$$\psi(r) = \varphi(r) + \int G_k(r, r')\, U(r')\, \psi(r')\, d^3 r'$$

Inhomogeneous integral equ.
(General sol. for Schrödinger equ.)

$K(x'',t;x',t_0)$ depends on the pot.

Ex. Free particle in one-dim.

$$[H,P]=0$$

$$\to P|p'\rangle = p'|p'\rangle \quad , \quad H|p'\rangle = \frac{p'^2}{2m}|p'\rangle$$

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{i}{\hbar}p'x'}$$ momentum eigenfunc.

$$(7) \to K(x'',t;x',t_0) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp'\, e^{\frac{i}{\hbar}p'(x''-x') - \frac{i}{\hbar}\frac{p'^2}{2m}(t-t_0)}$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp'\, e^{-\frac{i(t-t_0)}{2m\hbar}\left(p'-\frac{m}{(t-t_0)}(x''-x')\right)^2} \cdot e^{\frac{im}{2\hbar(t-t_0)}(x''-x')^2}$$

$$= \frac{e^{\frac{im}{2\hbar}\frac{(x''-x')^2}{(t-t_0)}}}{2\pi\hbar}\int_{-\infty}^{\infty} dq\, e^{-\frac{i(t-t_0)}{2m\hbar}q^2}$$

Now since, $\int_{-\infty}^{\infty} e^{-ax^2}\,dx = \sqrt{\frac{\pi}{a}}$

$$\to K(x'',t;x',t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\; e^{\frac{im(x''-x')^2}{2\hbar(t-t_0)}}$$

Ex. A system is initially represented by the minimum uncertainty wave packet (Gaussian wave). How does it spread out as a func. of t ?

$$\psi(x, t_0=0) = \frac{1}{(2\pi(\Delta x)_0^2)^{1/4}} e^{-\frac{x^2}{4(\Delta x_0)^2} + ik_0 x}$$

$$\psi(x,t) = \int d_x^{3'} K(x,t;x',t_0)\, \psi(x',t_0)$$

$$\psi(x,t) = \left(\frac{m}{2\pi i \hbar (t-t_0)}\right)^{1/2} \frac{1}{(2\pi(\Delta x)_0^2)^{1/4}} \cdot$$

$$\int_{-\infty}^{\infty} \exp\left[-\frac{m(x-x')^2}{2i\hbar(t-t_0)} - \frac{[x'-2ik_0(\Delta x)_0^2]^2}{4(\Delta x)_0^2} - k_0^2(\Delta x)_0^2\right] dx'$$

with the help of $\int_{-\infty}^{\infty} e^{-ax^2} dx = \left(\frac{\pi}{a}\right)^{1/2}$

$$\psi(x,t) = \frac{1}{(2\pi(\Delta x)_0^2)^{1/4}} \left[1 + \frac{i\hbar(t-t_0)}{2(\Delta x)_0^2 m}\right]^{-\frac{1}{2}} \cdot$$

$$\cdot \exp\left[\frac{-\frac{x^2}{4(\Delta x)_0^2} + ik_0 x - ik_0^2 \frac{\hbar(t-t_0)}{2m}}{1 + \frac{i\hbar(t-t_0)}{2(\Delta x)_0^2 m}}\right]$$

The wave packet advances acc. to the classical laws, but spreads in time.

Exercise - Calculate $|\psi(x,t)|^2$ for above mentioned prob., and show that the wave packet moves uniformly and at the same time spreads so that:

$$(\Delta X)_t^2 = (\Delta X)_0^2 \left[1 + \frac{\hbar^2 (t-t_0)^2}{4 (\Delta X)_0^4 m^2}\right]$$

$(\Delta x)^2 \equiv \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x^2 \rangle$

Ex.

The linear harmonic osc., is another example:

The wave func is given by:

$$u_n(x')\, e^{-\frac{iE_n t}{\hbar}} = \frac{1}{2^{n/2}\sqrt{n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega^2 x^2}{2\hbar}} \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) \cdot e^{-i\omega(n+\frac{1}{2})t}$$

The Green's func. sol. of the eqn.

$$i\hbar \frac{\partial K(x'', t; x', t_0)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 K(x'', t; x', t_0)}{\partial x''^2} + \frac{1}{2} m\omega^2 x''^2 K(x'', t; x', t_0)$$

is to be found

$$K(x'', t; x', t_0) = \left(\frac{m\omega}{2\pi i\hbar \sin[\omega(t-t_0)]}\right)^{\frac{1}{2}} e^{\frac{im\omega}{2\hbar \sin[\omega(t-t_0)]}\left[(x''^2 + x'^2)\cos[\omega(t-t_0)] - 2x''x'\right]} \tag{1}$$

This may, for instance, be obtained from the Harmonic osc. eigenfuncs. by the use of Mehler's formula, P. M. Morse and H. Feshbach, Methods of Theoretical Physics, McGraw-Hill book Co., New York, 1953, P 781, Problem 6.21.

$$\left(\frac{1}{\sqrt{1-\zeta^2}}\right) e^{-\frac{\xi^2+\eta^2-2\xi\eta\zeta}{1-\zeta^2}} = e^{-(\xi^2+\eta^2)} \sum_{n=0} \left(\frac{\zeta^n}{2^n n!}\right) H_n(\xi) H_n(\eta)$$

may be used (P 786 of the mentioned book).

Another way to prove is to use the $a, a^\dagger$ op method (Saxon 1968 144-45), or alternatively, the Path integral method.

(1) is a periodic func. of t with angular frequency ω.

This means that a particle initially localized precisely at $\underline{x'}$ will return to its original position with certainty at $\frac{2\pi}{\omega}, \frac{4\pi}{\omega}, \ldots$ later

Some integrals derivable from $K(x'', t; x', t_0)$;

Let $t_0 = 0$, $x'' = x'$

$$G(t) \equiv \int d^3x' \, K(x', t; x', 0) = \int d^3x' \sum_{a'} |\langle x'|a'\rangle|^2 \, e^{\frac{-iE_{a'}t}{\hbar}}$$

This is the trace of time evolution op. in x-representation. But

$$\sum_{a''} \langle a''| e^{\frac{-iHt}{\hbar}} |a''\rangle = \sum_{a''} \langle a''| \left(\sum_{a'} |a'\rangle e^{\frac{-iE_{a'}t}{\hbar}} \langle a'| \right) |a''\rangle$$

$$= \sum_{a'} e^{\frac{-iE_{a'}t}{\hbar}}$$

trace of time-evolution op in a'-representation

Since the trace is indep. of representation.

$$\longrightarrow G(t) = \sum_{a'} e^{\frac{-iE_{a'}t}{\hbar}}$$

Now, we see that the eqn for $G(t)$ is just sum over states, reminiscent of the position func. in statistical mechanics.

In fact, if we analytically continue in the t variable and make t purely imaginary, with β defined by

$$\beta = \frac{it}{\hbar} \qquad \beta : \text{real, positive}$$

$$G(t) \to Z \quad , \quad Z = \sum_{a'} e^{-\beta E_{a'}} \quad \text{partition func.}$$

For this reason some of the techniques encountered in studying propagators in Q.M. are also useful in statistical mechanics.

Laplace-Fourier transform of $G(t)$:

$$\tilde{G}(t) \equiv -i \int_0^\infty dt\, G(t)\, e^{iEt} = -i \int_0^\infty dt \sum_{a'} e^{-iE_{a'}t}\, e^{iEt}$$

The integrand oscillates indefinetly. But we can make the integral meaningful by

$$E \to E + i\epsilon \qquad \epsilon > 0$$

$$\tilde{G}(E) = \sum_{a'} \frac{1}{E - E_{a'}}$$

$\epsilon \to 0$

We observe that, the complete energy <u>spectrum</u> is exhibited as <u>simple poles</u> of $\bar{G}(E)$ in the complex E-plane

If we wish to know the energy spectrum of a physical system, it is sufficient to study the analytic properties of $\bar{G}(E)$.

Propagator as a Transition Amplitude:

Note that;

$$\psi_\alpha(x',t) = \underbrace{\langle x'|}_{\substack{\text{fixed}\\ \text{bra}}}\underbrace{\alpha,t_0,t\rangle}_{\substack{\text{moving}\\ \text{ket}}}$$ (see P113) Schrödinger

This can also be regarded as

$$\psi_\alpha(x',t) = \underbrace{\langle x',t|}_{\substack{\text{moving}\\ \text{oppositely}\\ \text{bra}}}\underbrace{\alpha,t_0\rangle}_{\text{fixed ket}}$$ Heisenberg

Likewise;

$$K(x'',t;x',t_0) = \sum_{a'} \langle x''|a'\rangle\langle a'|x'\rangle\, e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}$$

$$= \sum_{a'} \langle x''|\, e^{-\frac{i}{\hbar}Ht}\,|a'\rangle\langle a'|\, e^{\frac{i}{\hbar}Ht_0}\,|x'\rangle = {}_H\langle x'',t|x',t_0\rangle_H$$

when $|x',t_0\rangle$ and $\langle x'',t|$ are eigenket and eigenbra in Heisenberg pict.

In Section (2.1) we showed that; (in Heisenberg pict. notation)

$\langle b',t|a'\rangle$: The probability amplitude for a system (initially prepared to be in $|a'\rangle$, an eigenstate of A at $t_0=0$) to be found in $|b'\rangle$, an eigenstate of B at a later time t.

(see P114)

Thus $\longrightarrow$ $\langle x'', t | x', t_0 \rangle$: the probability amplitude for a particle prepared at t_0 with position x', to be found at a later time t at x''

Roughly speaking;

$$(x', t_0) \xrightarrow{\langle x'' t | x', t_0 \rangle \text{ (the amplitude for this tr.)}} (x'', t)$$

So, $\langle x'', t | x', t_0 \rangle$: transition amplitude

Alternative Interpretation;

$| x', t_0 \rangle$: The position eigenket at t_0 with the eigenvalue x' in the Heisenberg pict.

Because at any given time, the Heisenberg pict. eigenkets of an observable (like X) can be chosen as base kets, we can regard

$\langle x'', t | x', t_0 \rangle$ as the transformation func. that connects the two sets of the base kets at different times

$$\underbrace{\{ | x', t_0 \rangle \}}_{\text{the base at } t_0} \xrightarrow[\text{(time evolution)}]{\text{unitary tr}} \underbrace{\{ | x'', t \rangle \}}_{\text{the base ket at } t} \quad \text{in the Heisenberg pict.}$$

This is reminiscent of classical physics in which the time-development of classical dynamic variable such as $x(t)$ is viewed as a canonical (or contact) tr. generated by the classical Hamiltonian.

$$\xi = \eta + \delta\eta \qquad \delta\eta = \epsilon J \frac{\partial G(\eta)}{\partial \eta} \qquad \left(J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \right)$$

$$[\eta, u] = J \frac{\partial u}{\partial \eta} \qquad \delta\eta = \epsilon [\eta, G]$$

$$\epsilon \equiv dt, \quad G \equiv H \longrightarrow \delta\eta = dt\,[\eta, H] = \dot{\eta}\,dt = d\eta$$

η: initial coord. at t $\qquad$ ξ: the coord. at $t+dt$

Notation:

$$\langle x'', t \mid x', t_0 \rangle \longrightarrow \langle x'', t'' \mid x', t' \rangle \quad \text{for convenience}$$

$$\int d^3x'' \, |x'', t''\rangle\langle x'', t''| = I \qquad (\text{since } \{|x'', t''\rangle\} \text{ is complete})$$

Using this identity,

$$\langle x''', t''' \mid x', t' \rangle = \int d^3x'' \langle x''', t''' \mid x'', t'' \rangle \langle x'', t'' \mid x', t' \rangle$$

$$t''' > t'' > t'$$

This is <u>composition property</u> of the tr. amplitude.

clearly we can divide the time interval as many smaller subintervals as we wish.

$$\langle \vec{x}'''', t'''' | \vec{x}', t' \rangle = \int d^3x''' \int d^3x'' \, \langle \vec{x}'''', t'''' | \vec{x}''', t''' \rangle \langle \vec{x}''', t''' | \vec{x}'', t'' \rangle \langle \vec{x}'', t'' | \vec{x}', t' \rangle$$

$$t'''' > t''' > t'' > t' \qquad (1)$$

and so on.

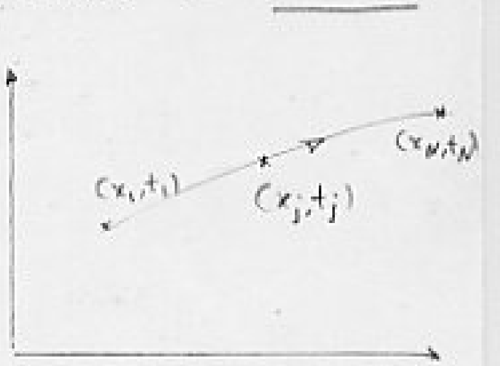
If we somehow guess the form of $\langle \vec{x}'', t'' | \vec{x}', t' \rangle$ for an infinitesimal time interval between t' and $t'' = t' + dt'$

$\longrightarrow$ We should be able to obtain the amplitude $\langle \vec{x}'', t'' | \vec{x}', t' \rangle$ for a finite time interval by compounding the appropriate tr. amplitudes for infinitesimal time intervals in a manner analogous to (1).

Path Integrals as the Sum Over Paths

Without loss of generality we restrict ourselves to one-dim. problems.

$\langle x_1, t_1 | x_N, t_N \rangle = ?$ tr. amp.



$$t_j - t_{j-1} = \Delta t = \frac{(t_N - t_1)}{N-1}$$

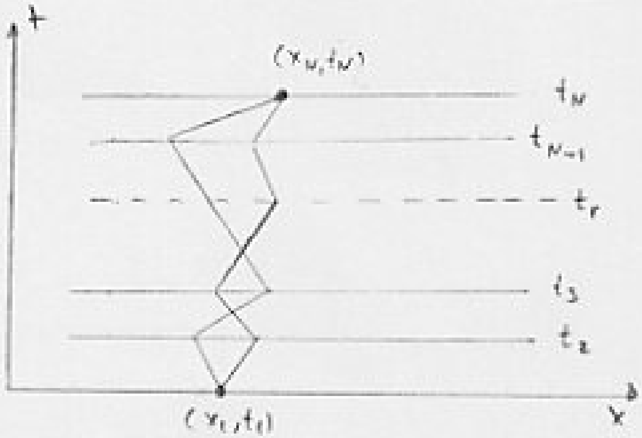
i.e. $t_N - t_1 = (N-1)\Delta t$ $\qquad 1 < j < N$

Exploiting the composition property;

$$\langle x_N, t_N | x_1, t_1 \rangle = \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \ \langle x_N, t_N | x_{N-1}, t_{N-1} \rangle$$

$$\cdot \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \cdots \langle x_2, t_2 | x_1, t_1 \rangle$$

For each <u>time segment</u> say between t_j and t_{j-1} we consider the <u>tr. amp.</u> to go from (x_{j-1}, t_{j-1}) to (x_j, t_j) and then integrate over $x_2, x_3 \cdots x_{N-1}$.



This means that we must <u>sum</u> over all possible paths in the space-time plane with the end points <u>fixed</u>.

Classical Path;

$$\mathcal{L}_{cl.}(x, \dot{x}) = \frac{m\dot{x}^2}{2} - V(x)$$

Given the end points (x_1, t_1) and (x_N, t_N) there exists a <u>unique</u> path that corresponds to the <u>actual motion</u> of the <u>classical</u> path.

$$\delta \int_{t_1}^{t_2} dt \, \mathcal{L}_{cl.}(x, \dot{x}) = 0$$

Acc. to the Hamilton's <u>principle</u>

i.e. Any arbitrary path <u>is not</u> allowed in Cl. M.

Ex. $V(x) = mgx$

$$\begin{cases} (x_1, t_1) = (h, 0) \\ (x_N, t_N) = \left(0 \ \sqrt{\frac{2h}{g}}\right) \end{cases} \longrightarrow x = h - \frac{gt^2}{2} \quad \text{cl. path}$$

Feynman's Formulation

$$\begin{cases} \text{In cl. M.: A definite path is allowed} \\ \text{In Q.M.: All possible paths must play roles including those} \\ \qquad \text{which do not bear any resemblance to the cl. path.} \end{cases}$$

Yet $\quad$ Q.M $\xrightarrow[\text{reduced}]{\text{must be}}$ cl. M. $\quad$ in the limit $\hbar \to 0$

Dirac in his book had the following remark;

$$e^{\frac{i}{\hbar}\int_{t_1}^{t_2} dt\, \mathcal{L}_{cl.}(x, \dot{x})} \xrightarrow{\text{Corresponds to}} \langle x_2, t_2 | x_1, t_1 \rangle$$

A young graduate student at Princeton Univ. R.P. Feynman attempted to make sense out of this remark.

Is "Corresponds to" the same thing as $\begin{cases} \text{is equal to} \\ \text{or is proportional to} \end{cases}$?

In so doing he was led to formulate a space-time approach to Q.M. based on path Integrals.

For compactness, we introduce a new notation;

$$S(n,n-1) \equiv \int_{t_{n-1}}^{t_n} dt \, \mathcal{L}_{cl.}(x,\dot{x}) \qquad \text{for any particular path}$$

Acc. to Dirac we associate $e^{\frac{i}{\hbar}S(n,n-1)}$ with a segment between (x_{n-1}, t_{n-1}) and (x_n, t_n).

(The segment is infinitesimally small)

For a definite path;

$$\prod_{n=2}^{N} e^{\frac{i}{\hbar}S(n,n-1)} = e^{\frac{i}{\hbar}\sum_{n=2}^{N} S(n,n-1)} = e^{\frac{i}{\hbar}S(N,1)}$$

Still $e^{\frac{i}{\hbar}S(N,1)} \sim \langle x_N, t_N | x_1, t_1 \rangle$

Because $e^{\frac{i}{\hbar}S(N,1)}$ is only for a particular path.

→ We must integrate over $x_2, x_3 - - x_{N-1}$.

$$\langle x_N, t_N | x_1, t_1 \rangle \sim \sum_{\text{all paths}} e^{\frac{i}{\hbar}S(N,1)} \qquad (1)$$

(innumerably infinite set of paths!)

The cl. limit: $(\hbar \to 0)$

As $\hbar \to 0$ $\longrightarrow$ the exponential in (1) oscillates violently

So $\longrightarrow$ there is a tendency for cancellation among various contributions from neighboring paths.

The reason:

$\left\{ \begin{array}{l} e^{\frac{i}{\hbar}S} \text{ for some definite path} \\ \text{and} \\ \text{" " a slightly different path} \end{array} \right.$ $\longrightarrow$ have a very different phases, because of smallness of $\hbar$.

$\longrightarrow$ So most paths do not contribute when $\hbar \to 0$

However there is an important exception;

Consider we consider a path that satisfies;

$$\delta S(N,1) = 0 \qquad (2)$$

i.e. $\delta S = \left(\frac{dS}{d\alpha}\right)_0 d\alpha$ $\quad$ α: Variation (deformation) Parameter (infinitesimal)

For exaple if $S \equiv S(y(x,\alpha), \dot{y}(x,\alpha), x)$

$$y(x,\alpha) = y(x,0) + \alpha\eta(x)$$

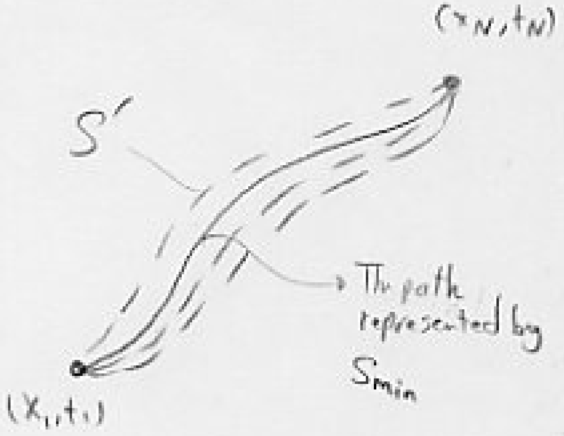
where $\eta(x_1) = \eta(x_2) = 0$

This is precisely the classical path by virtue of <u>Hamilton's</u> principle.

Denote the S satisfying (2) by <u>S_{min}</u>.

Now

S': The action of a deformed path very <u>close</u> to <u>S_{min}</u>



$S' \approx S_{min}$ to first order

(even $\hbar$ = small)

→ As long as we stay <u>near</u> the classical path, <u>constructive</u> interference between neighboring paths is <u>possible</u>.

→ In the $\hbar \to 0$ limit → the major contributions must arrise from a very <u>narrow strip</u> (or a tube in higher dims.) containing the cl. path.

Formulation of the Feynman Conjecture:

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \left(\frac{1}{W(\Delta t)}\right) e^{\frac{iS(n,n-1)}{\hbar}}$$

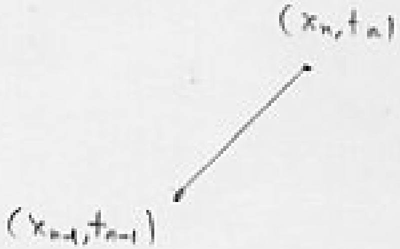
$t_n - t_{n-1} \longrightarrow$ infinitesimally small

We evaluate $S(n, n-1)$ in a moment in the $\Delta t \to 0$ limit.

$\frac{1}{W(\Delta t)}$: weight factor

$W = W(\Delta t)$ but $W \neq W(V(x))$ (assumption)

Now when $\Delta t \to 0$, we may make a straight-line approx. to the path jointing (x_{n-1}, t_{n-1}) and (x_n, t_n):



Then $\begin{cases} \frac{dx}{dt} \simeq \frac{x_n - x_{n-1}}{\Delta t} & \text{near } x_n \\ \frac{dx}{dt} \simeq \text{const} & \text{"} \end{cases}$

and $\begin{cases} V(x) \simeq V\left(\frac{x_n + x_{n-1}}{2}\right) & \text{"} \\ V(x) \simeq \text{const} & \text{"} \end{cases}$

$$S(n,n-1) = \int_{t_{n-1}}^{t_n} dt \left[\frac{m\dot{x}^2}{2} - V(x) \right]$$

$$= \Delta t \left\{ \frac{m}{2} \left[\frac{(x_n - x_{n-1})}{\Delta t} \right]^2 - V\left(\frac{x_n + x_{n-1}}{2} \right) \right\}$$

<u>Ex.</u> Free particle $V = 0$

$$\rightarrow \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \frac{1}{W(\Delta t)} e^{\frac{i m (x_n - x_{n-1})^2}{2\hbar \Delta t}} \qquad (1)$$

The exponent appearing here is completely <u>identical</u> to the one in the expression for the free-particle propagator (P176).

A similar comparison may be worked out for a <u>simple</u> Harmonic Osc.

Now by the orthonormality;

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle \Big|_{t_n = t_{n-1}} = \delta(x_n - x_{n-1}) \qquad (2)$$

$$\rightarrow \frac{1}{W(\Delta t)} = \sqrt{\frac{m}{2\pi i \hbar \Delta t}}$$

$$\left\{ \begin{aligned} &(1)(2) \rightarrow \int \frac{1}{W(\Delta t)} e^{\frac{i m (x_n - x_{n-1})^2}{2\hbar \Delta t}} d(x_n - x_{n-1}) \\ &= \int \delta(x_n - x_{n-1})\, d(x_n - x_{n-1}) \\ &\quad \Delta t = t_n - t_{n-1} \rightarrow 0 \\ &\frac{1}{W(\Delta t)} \sqrt{\frac{2\pi i \hbar \Delta t}{m}} = 1 \end{aligned} \right.$$

Where we have used

$$\int_{-\infty}^{\infty} d\xi \, e^{\frac{im\xi^2}{2\hbar\Delta t}} = \sqrt{\frac{2\pi i\hbar\Delta t}{m}}$$

and $$\lim_{\Delta t\to 0} \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \; e^{\frac{im\xi^2}{2\hbar\Delta t}} = \delta(\xi)$$

This weight factor is, of course, anticipated from the expression for the free-particle propagator (P176).

To summarize;

$$\langle x_n,t_n | x_{n-1},t_{n-1}\rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \; e^{\frac{i}{\hbar}S(n,n-1)} \qquad \text{as } \Delta t\to 0$$

$$\langle x_N,t_N | x_1,t_1\rangle = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{(N-1)/2} \int dx_{N-1}\int dx_{N-2}\cdots\int dx_2 \cdot \prod_{n=2}^{N} e^{\frac{i}{\hbar}S(n,n-1)}$$

where the $N\to\infty$ limit is taken with x_N, t_N <u>fixed</u>.

Define multidimensional (infinite-dimentional) integral op.;

$$\int_{x_1}^{x_N} \mathcal{D}[x(t)] \equiv \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{(N-1)/2} \int dx_{N-1}\int dx_{N-2}\cdots\int dx_2$$

$$\langle x_N, t_N | x_1, t_1 \rangle = \int_{x_1}^{x_N} \mathcal{D}[x(t)] \; e^{i\int_{t_1}^{t_N} dt \, \frac{L_{cl}(x,\dot{x})}{\hbar}}$$

Feynman path integral

Our steps leading to this equ. are not meant to be a derivation.

Rather we (or Feynman) have attemped a new formulation of Q.M based on the concept of paths, motivated by Dirac's mysterious remark.

In this formulation we used:

i) The superposition principle (contributions from various paths)

ii) The composition property of the tr. amp.

iii) Classical correspondence in the $\hbar \to 0$ limit.

Feynman's formulation is completely equivalent to the Schrödinger wave mechanics. (for free particle we showed it)

Now we prove the Feynman's expression for $\langle x_N, t_N | x_1, t_1 \rangle$ indeed satisfies Schrödinger Time-dep. wave equ. in the variables x_N, t_N just as the propogator $K(x'', t, x', t_0)$.

We start with:

$$\langle x_N, t_N | x_1, t_1 \rangle = \int dx_{N-1} \langle x_N, t_N | x_{N-1}, t_{N-1} \rangle \langle x_{N-1}, t_{N-1} | x_1, t_1 \rangle$$

$$= \int_{-\infty}^{\infty} dx_{N-1} \sqrt{\frac{m}{2\pi i\hbar \Delta t}}\, e^{\left(\frac{im}{2\hbar}\right)\frac{(x_N - x_{N-1})^2}{\Delta t} - \frac{i}{\hbar} V\left(\frac{x_N + x_{N-1}}{2}\right)\Delta t} \cdot \langle x_{N-1}, t_{N-1} | x_1, t_1 \rangle$$

where $t_N - t_{N-1}$: infinitesimal

Introducing $\xi = x_N - x_{N-1}$

and letting $x_N \to x$ and $t_N \to t + \Delta t$

$$\rightarrow \langle x, t+\Delta t | x_1, t_1 \rangle = \sqrt{\frac{m}{2\pi i\hbar \Delta t}} \int_{-\infty}^{\infty} d\xi\, e^{\frac{im\xi^2}{2\hbar \Delta t} - \frac{iV\Delta t}{\hbar}} \langle x - \xi, t | x_1, t_1 \rangle$$

Recalling again

$$\lim_{\Delta t \to 0} \sqrt{\frac{m}{2\pi i\hbar \Delta t}}\, e^{\frac{im\xi^2}{2\hbar \Delta t}} = \delta(\xi)$$

→ In the limit $\Delta t \to 0$, the major contribution to this integral comes from the $\xi \simeq 0$ region.

→ It is legitimate to expand $\langle x - \xi, t | x_1, t_1 \rangle$ in powers of ξ.

We also expand $\langle x,t+\Delta t|x_i,t_i\rangle$ and $e^{-\frac{i}{\hbar}V\Delta t}$ in powers of Δt, so

$$\langle x,t|x_i,t_i\rangle + \Delta t \frac{\partial}{\partial t}\langle x,t|x_i,t_i\rangle =$$

$$= \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\int_{-\infty}^{\infty} d\xi\, e^{\frac{im\xi^2}{2\hbar\Delta t}} \left(1-\frac{iV\Delta t}{\hbar}+\dots\right)\Big[\langle x,t|x_i,t_i\rangle + \underbrace{\cancel{\xi\frac{\partial}{\partial x}\langle x,t|x_i,t_i\rangle}}_{}$$

$\emptyset$ when integrated w.r.t. ξ

$$+\frac{\xi^2}{2!}\frac{\partial^2}{\partial x^2}\langle x,t|x_i,t_i\rangle + \dots\Big]$$

Since $$\int_{-\infty}^{\infty} d\xi\, e^{\frac{im\xi^2}{2\hbar\Delta t}} = \sqrt{\frac{2\pi i\hbar\Delta t}{m}} \qquad (1)$$

The $\langle x,t|x_i,t_i\rangle$ term on the left-hand side just matches the leading term on the right-hand side.

Collecting terms first order in Δt;

$$\Delta t\frac{\partial}{\partial t}\langle x,t|x_i,t_i\rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\,(\sqrt{2\pi})\left(\frac{i\hbar\Delta t}{m}\right)^{3/2}\frac{1}{2}\frac{\partial^2}{\partial x^2}\langle x,t|x_i,t_i\rangle$$

$$-\frac{i}{\hbar}\Delta t\, V\,\langle x,t|x_i,t_i\rangle$$

where we have used;

$$\int_{-\infty}^{\infty} d\xi\,\xi^2\, e^{\frac{im\xi^2}{2\hbar\Delta t}} = \sqrt{2\pi}\left(\frac{i\hbar\Delta t}{m}\right)^{3/2}$$

Obtained by differentiating (1) w.r.t. Δt

In this manner we see that $\langle x,t|x_1,t_1\rangle$ satisfies Schrödinger time-dep. wave equ.;

$$i\hbar\frac{\partial}{\partial t}\langle x,t|x_1,t_1\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\langle x,t|x_1,t_1\rangle + V\langle x,t|x_1,t_1\rangle$$

Conclusion:

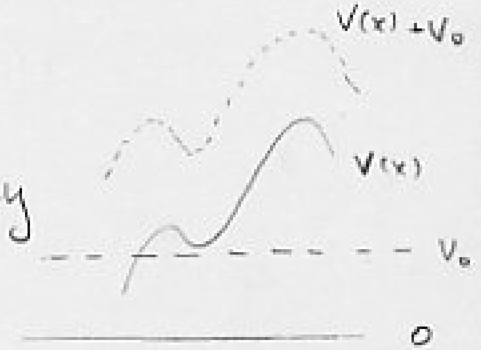
$\langle x,t|x_1,t_1\rangle$ constructed acc. to Feynman's prescription is the same as the propagator in Schrödinger's wave mechanics.

Feynman's path integral approach is not too convenient for attacking practical probs. in nonrelativistic Q.M.

But it is very powerful in quantum field theory and statistical mechanics.

2.6. Potentials and Gauge Transformation

Constant potentials



In classical M., the zero point of the pot. energy is of no significance.

The time development of dynamic variables such as $X(t)$ and $L(t)$ is indep. of whether we use $V(x)$ or $V(x)+V_0$,

where V_0: const in space and time

$F = ma$ Newton's Second law

$F = -\nabla V \longrightarrow V_0$ does not affect the force

What about in Q.M.

In Schrödinger pict.:

$|\alpha, t_0, t\rangle$ the state ket in the presence of $V(x)$

$|\widetilde{\alpha, t_0, t}\rangle$ the corresponding " " " $\tilde{V}(x) = V(x) + V_0$

To be precise let us agree that the initial conds. are such that both kets coincide with $|\alpha\rangle$ at $t = t_0$.

This can be done by a <u>suitable</u> choice of the phase.

$$\widetilde{|\alpha,t_0,t\rangle} = e^{-i\left(\frac{p^2}{2m}+V(x)+V_0\right)\frac{(t-t_0)}{\hbar}}|\alpha\rangle = \underbrace{e^{\frac{-iV_0(t-t_0)}{\hbar}}}_{\varphi}|\alpha,t_0,t\rangle$$

The influence of V_0

For stationary states:

If the time-dependence computed with $V(x)$ is: $e^{-\frac{i}{\hbar}E(t-t_0)}$

The corresponding " " " : $V(x)+V_0$ will be: $e^{-\frac{i}{\hbar}(E+V_0)(t-t_0)}$

In other words:

$$V(x) \longrightarrow \hat{V}(x)$$

$$\longrightarrow \quad E \longrightarrow E+V_0$$

Acc. to

$$\langle B\rangle = \sum_{a'}\sum_{a''} C_{a'}^{*} C_{a''} \langle a'|B|a''\rangle e^{-\frac{i}{\hbar}(E_{a''}-E_{a'})t}$$

$$\omega_{a''a'} = \frac{E_{a''}-E_{a'}}{\hbar}$$ the Bohr frequency

$\omega_{a''a'}$ are the <u>same</u> whether we use $V(x)$ or $V(x)+V_0$

$\longrightarrow$ $\langle x\rangle_t$, $\langle S\rangle_t$, ... are the same in <u>both</u> cases.

$$V(x) \longrightarrow V(x) + V_0$$

is an example of a class of <u>Gauge</u> transformations.

This change in the <u>zero</u> point energy of the Pot.; yeids;

$$\longrightarrow \quad |\alpha, t_0, t\rangle \longrightarrow e^{-\frac{i}{\hbar} V_0 (t - t_0)} |\alpha, t_0, t\rangle$$

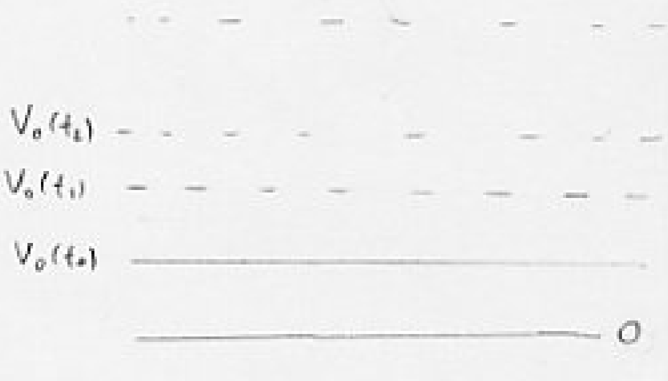
$$\psi(x', t) \longrightarrow e^{-\frac{i}{\hbar} V_0 (t - t_0)} \psi(x', t)$$

Second example: $V_0 = V_0(t)$ time-dep. but spatially uniform

So, $$|\alpha, t_0, t\rangle \longrightarrow e^{-i \int_{t_0}^{t} dt' \frac{V_0(t')}{\hbar}} |\alpha, t_0, t\rangle$$

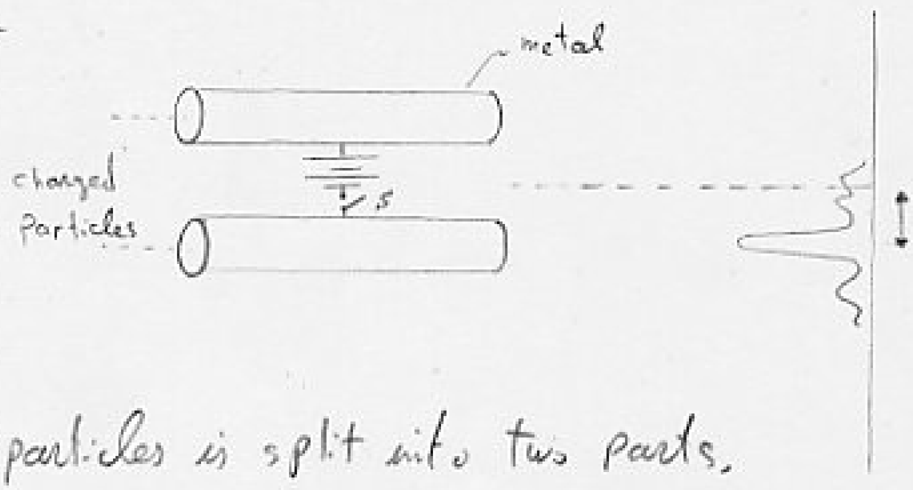
Physically:

We are choosing a <u>new</u> zero point of the energy scale at each <u>instant</u> of time.



Gedanken Experiment:

Even though the choice of the absolute scale of the pot. is arbitrary, pot. differences (ΔV) are of nontrivial physical significance.



i) A beam of charged particles is split into two parts, each of which enters a metallic cage.

A particle in the beam $\dfrac{\text{can be}}{\text{visualized}}$ as a wave packet

such that; Dim. of the wave packet $<<$ Dim. of cage

ii) We switch on the S after the wave packet enter the cage and switch it off before the wave packets leave the cage.

iii) In this way the cages are brought in different potentials.

$$V_{cage_1} = V_{10} = \text{const} \qquad V_{cage_2} = V_{20} = \text{const}$$

Since $\nabla V_{10} = 0$, $\nabla V_{20} = 0$ $\longrightarrow$ No force on the particles (i.e. No $\bar{E}$ inside the cages)

Remark: Note that from $F = -\nabla V$, F is non-zero

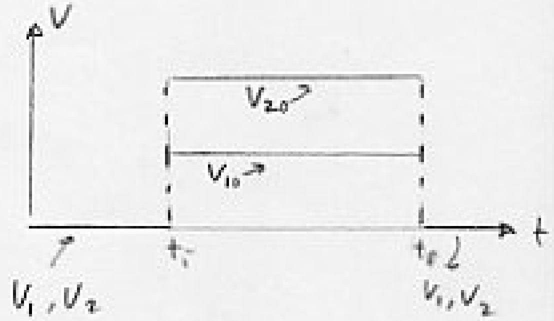
if there exists spatial variation in V.

Switching on and off the S only cause t-dependent

variation in V.

Now, because of

$$|\alpha, t_0, t\rangle \longrightarrow e^{-i\int_{t_0}^{t} dt' \frac{V_0(t')}{\hbar}} |\alpha, t_0, t\rangle$$



since $V_{10} \neq V_{20}$

→ the particles in different cages

suffer different phases.

→ As a result there is an observable interference in the

beam intensity in the interference region;

$$\varphi_1 - \varphi_2 = \frac{1}{\hbar} \int_{t_i}^{t_f} dt \, [V_2(t) - V_1(t)]$$

Conclusion: Despite $F = 0$, there is an observable

effect that depends on ΔV

This effect is purely quantum mechanical.

In the limit $\hbar \to 0$, the interesting interference effect gets washed out (because of infinitely rapid oscillation).

Gravity in Q.M.

The role of gravity in Cl.M. and Q.M.

For a falling body;

$$m\ddot{\vec{x}} = -m\nabla\varphi_{grav.} = -mg\hat{z} \qquad (1)$$

inertial mass

gravitational mass

Since $m_{in} = m_{gr} \longrightarrow \ddot{\vec{x}} = -\nabla\varphi = -g\hat{z}$

$\longrightarrow$ A feather and a stone behave in same way.

This is the consequence of the Einstein's Equivalence principle

Since the mass does not appear in the equ. of the particle's trajectory $\longrightarrow$ Gravity in Cl. M. is often said to be a purely geometric theory.

The situation is rather <u>different</u> in Q.M.;

The analogue equ. of (1) in Q.M.;

$$\left[-\left(\frac{\hbar^2}{2m}\right)\nabla^2 + m\Phi_{grav.}\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t} \qquad (2)$$

The mass <u>no longer</u> cancels.

$$(2) \longrightarrow \left[-\frac{1}{2}\left(\frac{\hbar}{m}\right)\nabla^2 + \frac{m}{\hbar}\Phi_{grav.}\right]\Psi = i\frac{\partial\Psi}{\partial t} \qquad (3)$$

$\rightarrow$ The mass appears in the combination $\frac{\hbar}{m}$

$\rightarrow$ where $\hbar$ appears, m is also expected to appear.

This is also <u>evident</u> from Feynman Path int. for a falling body:

$$\langle x_n, t_n | x_{n-1}, t_{n-1}\rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\; e^{i\int_{t_{n-1}}^{t_n} dt \frac{(m\dot{x}^2/2 - mgz)}{\hbar}} \qquad (4)$$

$$t_n - t_{n-1} = \Delta t \rightarrow 0$$

This is in sharp contrast with Hamilton's classical approach based on;

$$\delta\int_{t_1}^{t_2} dt\left(\frac{m\dot{x}^2}{2} - mgz\right) = 0 \qquad (5)$$

$$\longrightarrow \int_{t_1}^{t_2} dt\left(\frac{\dot{x}^2}{2} - gz\right) = 0 \qquad (m \text{ is eliminated})$$

By the Ehrenfest's Theorem;

$$m \frac{d^2}{dt^2} \langle x \rangle = \frac{d}{dt} \langle p \rangle = -\langle \nabla V(x) \rangle$$

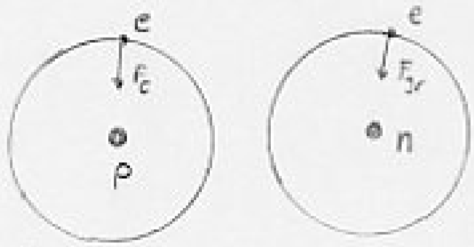
$$\rightarrow \frac{d^2}{dt^2} \langle x \rangle = -g \hat{z} \qquad (6)$$

Here $\hbar$ does not appear, nor m.

To see nontrivial quantum mechanical effect of gravity we must study effects in which $\hbar$ appear explicitly.

For a falling elementary particle classical equ. (1) or quantum mechanical equ. (6) suffice, but $\hbar$ does not appear. (compatible with the observations).

On the microscopic scale gravitational forces are too weak to be readily observable.



$$F_C \sim 2 \times 10^{39} F_{gr}$$

For an electron-proton bound by Coulomb force,

$$a_0 = \frac{\hbar^2}{e^2 m_e} \quad \text{Bohr radius}$$

For an electron-neutron bound by Gravitational force

$$a_0' = \frac{\hbar^2}{G_N m_e^2 m_n}$$

G_N: Newton's gravitational const.

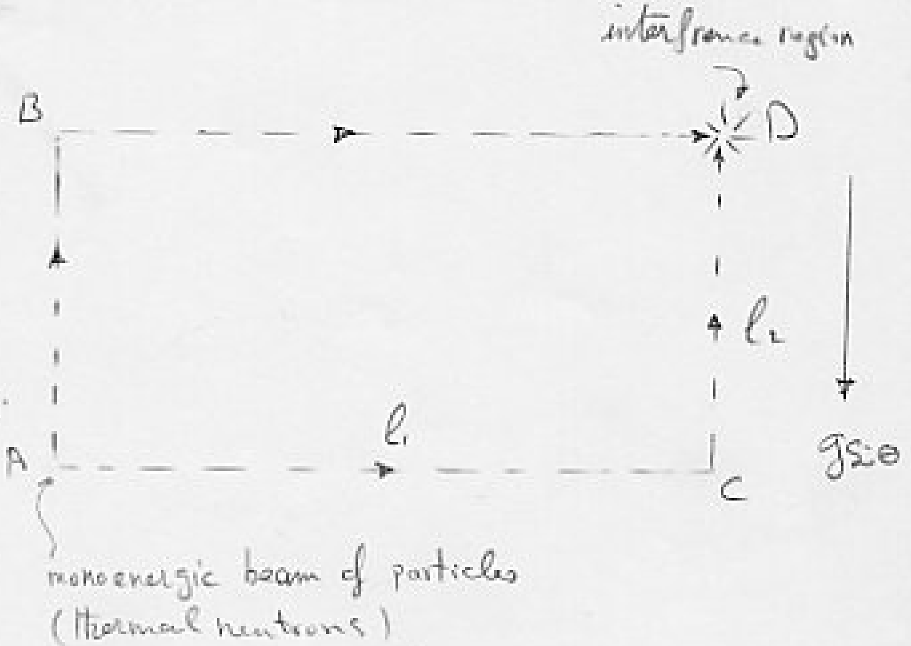
$a' \sim 10^{31}$ cm (10^{13} light yr)

Gravity-induced Q. interference:

In this experiment the effect of gravity can be observed.

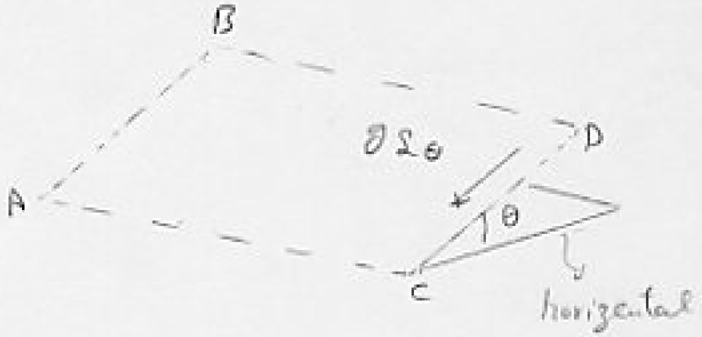
$\lambda_{\text{particles}} \ll l_1$ or l_2

$\longrightarrow$ we can apply the concept of classical trajectory.



If $\theta = 0$

we can set $V = 0$ for any fenomenon that take place in this plane.



In the case $\theta \neq 0$,

For AC-path $\quad V = 0$

For BD-path $\quad V = mg\, l_2 \sin\theta$

Acc. to $|\alpha, t_0, t\rangle \longrightarrow e^{-\frac{iV_0(t-t_0)}{\hbar}} |\alpha, t_0, t\rangle$

$$(ABD)_{\substack{\text{phase}\\\text{change}}} = (AB)_{ph.ch.} + (BD)_{ph.ch.}$$

$$(ACD)_{ph.ch.} = (AC)_{ph.ch.} + (CD)_{ph.ch.}$$

But, $(AB)_{ph.ch.} = (CD)_{ph.ch.}$

$$\frac{(ABD)_{ph.ch.}}{(ACD)_{ph.ch.}} = \frac{(DB)_{ph.ch.}}{(AC)_{ph.ch.}} = \frac{e^{-\frac{im_n g l_2 S\Theta T}{\hbar}}}{e^{-\frac{i(0)T}{\hbar}}} = e^{\overbrace{-\frac{im_n g l_2 S\Theta T}{\hbar}}^{\varphi}}$$

$$\varphi_{ABD} - \varphi_{ACD} = -\frac{m_n g l_2 S\Theta T}{\hbar}$$

but $T = \dfrac{l_1}{V_{\substack{\text{wave}\\\text{packet}}}} = \dfrac{l_1 m_n}{p} = \dfrac{l_1 m_n \lambda}{\hbar}$

$$\varphi_{ABD} - \varphi_{ACD} = -\frac{m_n^2 g l_1 l_2 \lambda S\Theta}{\hbar^2} \qquad \text{Phase diff.} \qquad (7)$$

This is an observable interference

By changing Θ. one may change this phase difference.

Alternative look;

Since V: t-indep. $\longrightarrow \frac{p^2}{2m} + mgz = E$ const.

A slight difference in height ($l_2 \sin\theta$) between level BD and AC

implies $\longrightarrow \Delta P = P_{AC} - P_{BD}$

$\longrightarrow \Delta\lambda = \lambda_{BD} - \lambda_{AC}$

This wave mechanical approach also leads to the same result for $\varphi_{ABD} - \varphi_{ACD}$

For $\lambda = 1.42\,\mathring{A}$ (comparable to interatomic spacing in silicon)

and $l_1 l_2 = 10\,cm^2$

$\longrightarrow m_n^2 g l_1 l_2 \lambda / \hbar^2 = 55.6$

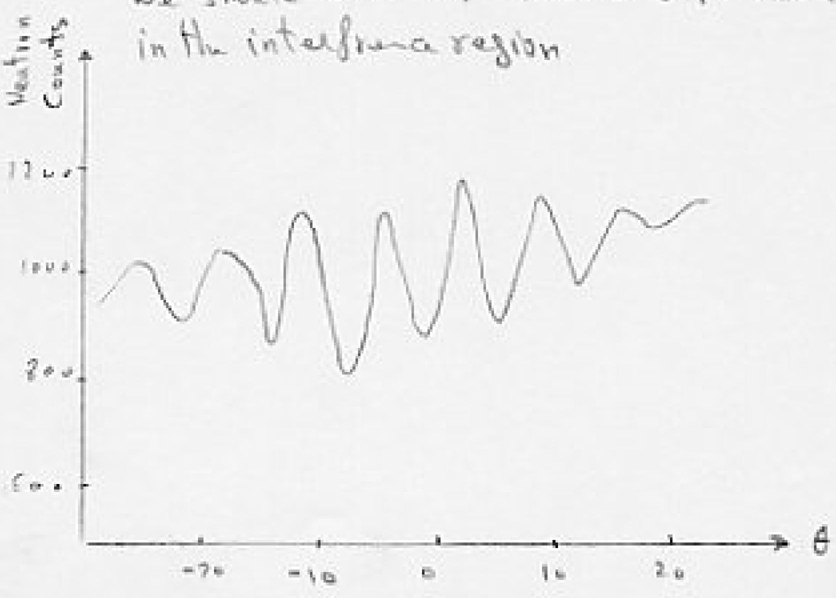
as $\theta = 0 \xrightarrow{to} \theta = \frac{\pi}{2}$ $\Longrightarrow \frac{55.6}{2\pi} \simeq 9$ oscillations

we should see 9 minima and 9 maxima in the interference region

This is <u>purely</u> Q. Mechanical because as $\hbar \to 0$

$\to \Delta\varphi \to \infty$

$\longrightarrow$ the interference pattern gets <u>washed</u> out.



We see that V_{gr} enters into the schrödinger equ. just as expected.

This experiment also shows that $\longrightarrow$ Gravity is not purely geometric at the quantum level, because the effect depends on $\left(\frac{m}{\hbar}\right)^2$ (in $\Delta\varphi$).

However, this does not imply that the equivalence principle is unimportant in understanding an effect of this sort.

If $m_{grav} \neq m_{inert}$

$\xrightarrow{\text{then}}$ we have to replace $\left(\frac{m}{\hbar}\right)^2 \xrightarrow{\text{to}} \dfrac{m_{grav} \cdot m_{inert}}{\hbar^2}$

The fact that we could correctly predict the interference pattern without making a distinction between m_{grav} and m_{inert}, shows some support for the equivalence principle at the Q. level.

Gauge Transformations in Electromagnetism:

$$E = -\nabla \varphi \quad , \quad B = \nabla \times A \qquad \begin{cases} \varphi(x) & : t\text{-indep} \\ A(x) & : \quad " \end{cases}$$

Classical Electromagnetism $\longrightarrow$ $H = \frac{1}{2m}\left(P - \frac{eA}{c}\right)^2 + e\varphi$ (e<0 for electron)

In Q.M. $\varphi \equiv \varphi(\bar{x})$, $A = A(\bar{x})$ $\qquad \bar{X}$: Position oP.

Since $[A(x), P] \neq 0$

$$\left(P - \frac{eA}{c}\right)^2 = P^2 - \left(\frac{e}{c}\right)(P \cdot A + A \cdot P) + \left(\frac{e}{c}\right)^2 A^2$$

Now $\frac{dx_i}{dt} = \frac{[x_i, H]}{i\hbar} = \frac{1}{m}\left(P_i - \frac{e}{c}A_i\right)$

Note that $P \neq m\frac{dx}{dt}$ $\qquad P$: generator of tr.

$$\Pi = m\frac{dx}{dt} = P - \frac{eA}{c}$$ Kinematical or mechanical momentum

P : canonical momentum

Even though $[P_i, P_j] = 0$

but $\qquad [\Pi_i, \Pi_j] = \left(\frac{i\hbar e}{c}\right)\epsilon_{ijk} B_k$

Rewriting H as $H = \frac{\Pi^2}{2m} + e\varphi$ and using the fundamental commutation relation of $[\Pi_i, \Pi_j]$,

$$\frac{d\Pi_i}{dt} = \frac{1}{i\hbar}[\Pi_i, H]$$

$$\longrightarrow m\frac{d^2 x}{dt^2} = \frac{d\Pi}{dt} = e\left[E + \frac{1}{2c}\left(\frac{dx}{dt}\times B - B\times\frac{dx}{dt}\right)\right]$$ Lorentz force in Q.M.

This is Ehrenfest's theorem, written in the Heisenberg pict. for the charged particle in the presence of E and B.

Now we study Schrödinger's wave equ. with φ and A;

$$\langle x'|\left(P - \frac{e}{c}A(x)\right)^2|\alpha, t_0, t\rangle =$$

$$= \int d^3x'' \langle x'|\left(P - \frac{e}{c}A(x)\right)|x''\rangle \cdot \langle x''|\left(P - \frac{e}{c}A(x)\right)|\alpha, t_0, t\rangle$$

$$= \int d^3x'' \left(-i\hbar\nabla' - \frac{e}{c}A(x')\right)\langle x'|x''\rangle \cdot \langle x''|\left(P - \frac{e}{c}A(x)\right)|\alpha, t_0, t\rangle$$

$$= \left(-i\hbar\nabla' - \frac{e}{c}A(x')\right)\cdot\left(-i\hbar\nabla' - \frac{e}{c}A(x')\right)\langle x'|\alpha, t_0, t\rangle$$

(see P71)

$$H\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

$$\rightarrow \frac{1}{2m}\left(-i\hbar\nabla' - \frac{e}{c}A(x')\right)\cdot\left(-i\hbar\nabla' - \frac{e}{c}A(x')\right)\langle x'|\alpha, t_0, t\rangle$$

$$+ e\varphi(x')\langle x'|\alpha, t_0, t\rangle = i\hbar\frac{\partial}{\partial t}\langle x'|\alpha, t_0, t\rangle$$

From this expression we readily obtain, the continuity equ.;

$$\frac{\partial \rho}{\partial t} + \nabla'\cdot J = 0$$

where $\psi = \langle x' | \alpha, t_0, t \rangle$, $\rho = |\psi|^2$

but; $\mathbf{j} = \left(\frac{\hbar}{m}\right) \mathrm{Im}(\psi^* \nabla \psi) - \frac{e}{mc} \mathbf{A} |\psi|^2$

which is just what we expect from the substitution;

$$\nabla' \longrightarrow \nabla' - \left(\frac{ie}{\hbar c}\right) \mathbf{A}$$

(equivalent to $\quad p \rightarrow (p - \frac{e}{c} \mathbf{A})$)

Now, with $\quad \psi(x,t) = \sqrt{\rho(x,t)}\, e^{\frac{i}{\hbar} S(x,t)}$

$$\rightarrow \mathbf{j} = \left(\frac{\rho}{m}\right)\left(\nabla S - \frac{e\mathbf{A}}{c}\right)$$

(compare with $\mathbf{j} = \frac{\rho}{m} \nabla S$ in the absence of $\mathbf{A}$)

We find this form to be more convenient in discussing superconductivity, flux quantization -- and so on.

Also $\displaystyle\int d^3x'\, \mathbf{j} = \frac{\langle \mathbf{p} - \frac{e}{c}\mathbf{A} \rangle}{m} = \frac{\Pi}{m}$

We now discuss the subject of Gauge tr.:

First consider, $\varphi \longrightarrow \varphi + \lambda$, $A \to A$ (1)

where λ = const. (x,t)-indep

Under this tr., $E \to E$, $B \to B$

This tr. just amounts to a change in the Zero point of the energy scale.

We have earlier discussed such a tr.;

i.e. $|\alpha, t_0, t\rangle \longrightarrow e^{-\frac{i V_0 (t-t_0)}{\hbar}} |\alpha, t_0, t\rangle$

with $e\varphi$ replaced by V_0.

Much more interesting tr.:

$\varphi \longrightarrow \varphi$, $A \to A + \nabla \Lambda$ (2)

where $\Lambda \equiv \Lambda(\bar{x})$ scalar func

Under this tr.:

$E \longrightarrow E$, $B \to B$

Both (1) and (2) are special cases of

$$\varphi \to \varphi - \frac{1}{c}\frac{\partial \Lambda}{\partial t} \quad , \quad A \to A + \nabla \Lambda$$

which leave E and B, given by

$$E = -\nabla\varphi - \frac{1}{c}\frac{\partial A}{\partial t} \qquad B = \nabla \times A$$

unchanged. But in the following we consider t-indep fields (A) and potentials (φ).

In classical Physics:

Observable effects such as the trajectory of a charged particle are indep. of the gauge used. (i.e. particular choice Λ)

Ex. A charged particle in a uniform mag. field in the z-dir.:

$$\bar{B} = B\hat{z}$$

$\bar{B}$ may be derived from:

$$A_x = -\frac{BY}{2} \quad A_y = \frac{BX}{2} \quad , A_z = 0 \qquad (3)$$

$$\bar{B} = \nabla \times A = \begin{vmatrix} i & j & k \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ -\frac{BY}{2} & \frac{BX}{2} & 0 \end{vmatrix} = B\hat{z}$$

or also from:

$$A_x = -BY \quad , \quad A_Y = 0 \quad , \quad A_z = 0 \qquad (4)$$

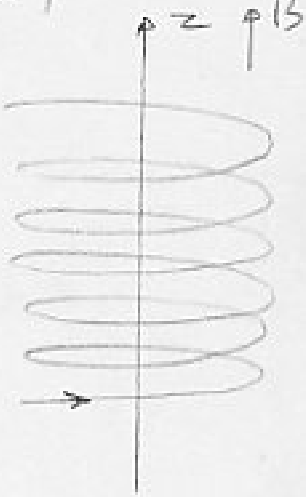
The second form is obtained from the first by

$$A \longrightarrow A - \nabla\left(\frac{BXY}{2}\right) \qquad (5)$$

which is of the form $\begin{cases} \varphi \longrightarrow \varphi \\ A \longrightarrow A + \nabla\Lambda \end{cases}$

Regardless of the form of A (i.e. (3) or (4)), the trajectory of a charged particle with a given set of initial conds. is the same.

It is a helix (when projected in the x-y plane)



Recalling the Hamilton's equs. of motion

$$\dot{p} = -\frac{\partial H}{\partial q} \rightarrow \frac{\partial P_x}{\partial t} = -\frac{\partial H}{\partial x} \cdots$$

with $A = -\frac{BY}{2}\hat{i} + \frac{BX}{2}\hat{j} + 0$ (eqn 3)

So $H = \frac{1}{2}\left(P - \frac{e}{c}\left(-\frac{BY}{2}\hat{i} + \frac{Bx}{2}\hat{j}\right)\right)^2 + 0$

Then $\longrightarrow \frac{\partial P_x}{\partial t} = 0$ const of motion

But with $A = -By\hat{i} + 0 + 0 \rightarrow H = \frac{1}{2}\left(P - \frac{e}{c}(-By\hat{i})\right)^2$

$$\longrightarrow \frac{\partial P_x}{\partial t} \neq 0 \longrightarrow$$ The canonical momentum is not a gauge invariant

But the kinematic momentum $\Pi = m\frac{dx}{dt}$ that traces the trajectory of the particle is a gauge invariant quantity.

Because of $\quad \Pi = m\frac{dx}{dt} = P - \frac{e}{c}A$

P must change to compensate for the change in A given by (5).

It is reasonable that to demand that:

$\langle \quad \rangle$ in Q.M behave in a manner similar to the corresponding cl. quantities

under gauge trs.

So, $\langle x \rangle$ and $\langle \Pi \rangle$ are not to change under gauge tr.

while $\langle P \rangle$ is expected to change.

Now

let $|\alpha\rangle$: state ket in the presence of A

$|\tilde{\alpha}\rangle$: " " for the same physical situation

when $\tilde{A} = A + \nabla\Lambda \qquad (\Lambda \equiv \Lambda(\vec{x}))$ position op.

Our basic requirement: $\langle\alpha|X|\alpha\rangle = \langle\tilde{\alpha}|X|\tilde{\alpha}\rangle \qquad (6)$

and $\langle\alpha|\Pi|\alpha\rangle = \langle\tilde{\alpha}|\Pi|\tilde{\alpha}\rangle \qquad (7)$

or $\langle\alpha|(P-\frac{e}{c}A)|\alpha\rangle = \langle\tilde\alpha|(P-\frac{e}{c}A')|\tilde\alpha\rangle$

In addition; $\langle\alpha|\alpha\rangle = \langle\tilde\alpha|\tilde\alpha\rangle$ (norm conservation)

We must construct $\mathcal{G}$ such that $|\tilde\alpha\rangle = \mathcal{G}|\alpha\rangle$

Invariance properties of (6) and (7) are gauranteed if:

i) $$g^{\dagger} x g = x \qquad (8)$$

and ii) $$g^{\dagger}\left(P-\frac{eA}{c}-\frac{e\nabla\Lambda}{c}\right)g = P-\frac{eA}{c} \qquad (9)$$

We assert: $$g = e^{\frac{ie\Lambda(x)}{\hbar c}} \qquad (10)$$

First, $g^{\dagger}g = I$ (unitary)

$\longrightarrow$ $\langle\alpha|\alpha\rangle = \langle\tilde\alpha|\tilde\alpha\rangle$ is all right.

Second, (8) is satisfied (because $[x, f(x)] = 0$)

Finally; since $[P_i, G(x)] = -i\hbar\frac{\partial G}{\partial x_i}$

$$e^{-\frac{ie\Lambda}{\hbar c}} P e^{\frac{ie\Lambda}{\hbar c}} = e^{-\frac{ie\Lambda}{\hbar c}}\left[P, e^{\frac{ie\Lambda}{\hbar c}}\right] + P$$

$$= -e^{-\frac{ie\Lambda}{\hbar c}}\left(i\hbar\nabla\left(e^{\frac{ie\Lambda}{\hbar c}}\right)\right) + P = P + \frac{e\nabla\Lambda}{c} \qquad (11)$$

$\longrightarrow$ So (9) is also satisfied.

The invariance of Q.M. under gauge trs. can also be demonstrated by looking directly at the Schrödinger equ.

Let, $|\alpha, t_0, t\rangle$: sol. to the Schrödinger equ in the presence A

$$\left[\frac{(P - \frac{eA}{c})^2}{2m} + e\varphi \right] |\alpha, t_0, t\rangle = i\hbar \frac{\partial}{\partial t} |\alpha, t_0, t\rangle \qquad (12)$$

The corresponding sol. in the presence of $\tilde{A}$ must satisfy;

$$\left[\frac{(P - \frac{e}{c}A - e\nabla\Lambda/c)^2}{2m} + e\varphi \right] \widetilde{|\alpha, t_0, t\rangle} = i\hbar \frac{\partial}{\partial t} \widetilde{|\alpha, t_0, t\rangle} \qquad (13)$$

We see that if the new ket is taken to be;

$$\widetilde{|\alpha, t_0, t\rangle} = e^{\frac{ie\Lambda}{\hbar c}} |\alpha, t_0, t\rangle \qquad (14)$$

in accordance with (10), the new Schrödinger equ. will be satisfied.

All we have to note (in this check) that;

$$e^{-\frac{ie\Lambda}{\hbar c}} \left(P - \frac{eA}{c} - \frac{e\nabla\Lambda}{c} \right)^2 e^{\frac{ie\Lambda}{\hbar c}} = \left(P - \frac{eA}{c} \right)^2$$

(by applying (11) twice)

$$(14) \rightarrow \quad \tilde{\Psi}(x',t) = e^{\frac{ie\Lambda(x')}{\hbar c}} \Psi(x',t) \qquad (15)$$

$\Lambda(x')$: real func. of position vector eigenvalue x'.

This can be verified by directly substituting (15) into the Schrödinger equ. with $A \xrightarrow[\text{by}]{\text{replaced}} A + \nabla\Lambda$

Under this tr. (in term ρ and S);

$$\rho \longrightarrow \rho$$

but $S \longrightarrow S + \frac{e\Lambda}{c}$

Recalling $J = \frac{\rho}{m}\left(\nabla S - \frac{eA}{c}\right)$

$$\rightarrow \quad J \longrightarrow J$$

The invariance under (10) is called <u>gauge invariance</u>.

(in going from the gauge $A \xrightarrow{\text{to}} A + \nabla\Lambda$ gauge)

The Aharonov-Bohm Effect:

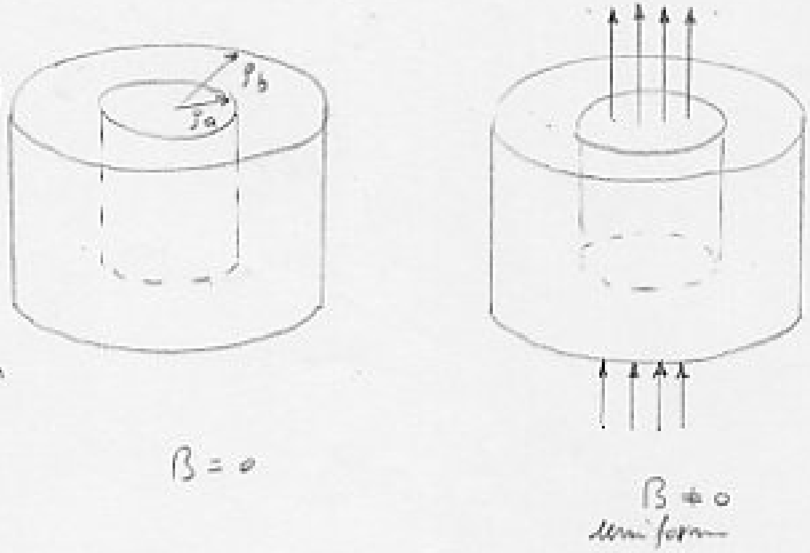
Consider a hollow cylinderical shell ($B = 0$)

Assume an electron $\underline{e}$ can be completely confined to the $\underline{\text{interior}}$ of the shell with $\underline{\text{rigid}}$ walls (example: ideal solenoid)

i.e. $\psi \to 0$ as $\rho \to \rho_a$

$\psi \to 0$ as $\rho \to \rho_b$

$\psi \to 0$ at the top and bottom



This boundary-value prob. can be solved in a straightforward manner to get the energy eigenvalues.

Modified arrangement:

The sylindrical shell encloses a uniform mag. field B.

$B \neq 0$ for $\rho < \rho_a$

$B = 0$ for $\rho \geq \rho_a$

The boundary conds. are taken to be as before.

Intuitively one may conjecture that

The energy spectrum with $B=0$ $\underset{?}{\overset{\text{the same as}}{=\!=}}$ The energy spectrum with $B \neq 0$

because the region with $B \neq 0$ is completely inaccessible to the charged particle trapped inside the shell.

But Q.M. tells us this conjecture is not correct.

Even though $B=0$ inside the shell, but $A \neq 0$ there

The vector pot. needed to produce $\bar{B} = B\hat{z}$ is

$$\bar{A} = \left(\frac{B \rho_a^2}{2\rho}\right)\hat{\varphi} \qquad \text{in the interior region}$$

Note that;

$$\nabla \times A = \left(\frac{1}{\rho}\frac{\partial A_z}{\partial \varphi} - \frac{\partial A_\varphi}{\partial z}\right)\hat{\rho} + \left(\frac{\partial A_\rho}{\partial z} - \frac{\partial A_z}{\partial \rho}\right)\hat{\varphi} + \frac{1}{\rho}\left(\frac{\partial}{\partial \rho}(\rho A_\varphi) - \frac{\partial A_\rho}{\partial \varphi}\right)\hat{z}$$

$\rightarrow B = \nabla \times A = 0$ in the interior region

Using Stoke's theorem;

$$\oint_C A \cdot dl = \int_S (\nabla \times A) \cdot n \, da$$

$$\rightarrow \Phi_B = \oint_C A \cdot dl = \oint_C \left(\frac{B\rho_a^2}{2\rho}\right) dl \cdot \hat{\varphi}$$

C: Take a circular path

$$\Phi_B = \frac{B\rho_a^2}{2\rho}\oint dl\, \zeta_0 = \frac{B\rho_a^2}{\rho}(2\pi\rho) = B(\pi\rho_a^2)$$

In attempting to solve the Schrödinger equ. (to find the energy eigenvalues) for this new prob.:

we need to replace $\nabla \longrightarrow \nabla - \frac{ie}{\hbar c}A$

Since $\nabla = \hat{\rho}\frac{\partial}{\partial\rho} + \hat{\varphi}\frac{1}{\rho}\frac{\partial}{\partial\varphi} + \hat{z}\frac{\partial}{\partial z}$

we need to replace $\frac{\partial}{\partial\varphi} \longrightarrow \frac{\partial}{\partial\varphi} - \frac{ie}{\hbar c}\left(\frac{B\rho_a^2}{2}\right)$

This replacement $\xrightarrow{\text{results}}$ in an observable change in the energy spectrum.

This is remarkable, because the particle never touches the mag. field.

i.e. $F_{\text{Lorentz}} = 0$

Yet, the energy spectrum $\xrightarrow{\text{depends on}}$ whether or not B is finite in the hole region inaccessible to the particle

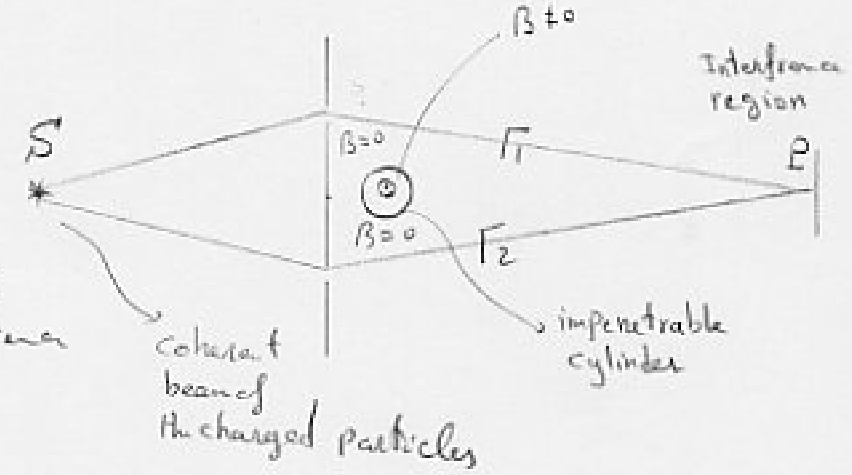
This prob. is the bound state version of what is commonly referred to as the Aharonov-Bohm effect.

Original Aharonov-Bohm Effect:

Our aim:

P (φ inside the cylinder) = ?

the Probability of finding the particle in the interference region.



We follow path int. method;

let x_1 and x_N be typical points in source region (S) and interference regione (P) respectively.

From the cl. mechanics;

$$L^{(0)}_{cl} = \frac{m}{2}\left(\frac{dx}{dt}\right)^2 \longrightarrow L^{(0)}_{cl} + \frac{e}{c}\frac{dx}{dt}\cdot A$$

in the absence of A

in the presence of A

The corresponding change in the action for some <u>definite</u> path segment going from $(x_{n-1}, t_{n-1}) \xrightarrow{\text{to}} (x_n, t_n)$

$$S^{(0)}(n, n-1) \longrightarrow S^{(0)}(n,n-1) + \frac{e}{c}\int_{t_{n-1}}^{t_n} dt \left(\frac{dx}{dt}\right)\cdot A$$

But;
$$\frac{e}{c}\int_{t_{n-1}}^{t_n} dt\left(\frac{dx}{dt}\right)\cdot A = \frac{e}{c}\int_{x_{n-1}}^{x_n} A\cdot ds$$

ds: the diff. line element along the path segment

For the entire contribution from x_1 to x_N, we have;

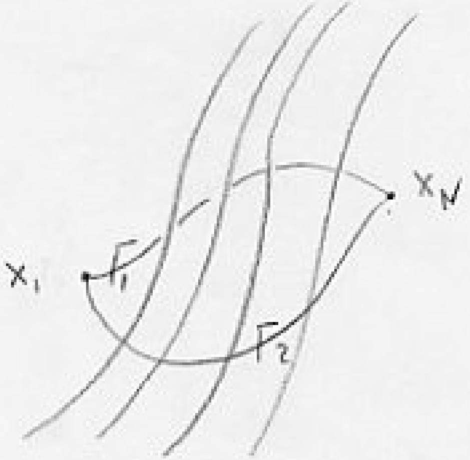
$$\prod e^{\frac{iS^{(0)}(n,n-1)}{\hbar}} \xrightarrow{A} \left\{\prod e^{\frac{iS^{(0)}(n,n-1)}{\hbar}}\right\} e^{\frac{ie}{\hbar c}\int_{x_1}^{x_N} A\cdot ds}$$

All this is for a particular path such as going above the cylinder.

We must still sum over all possible paths.

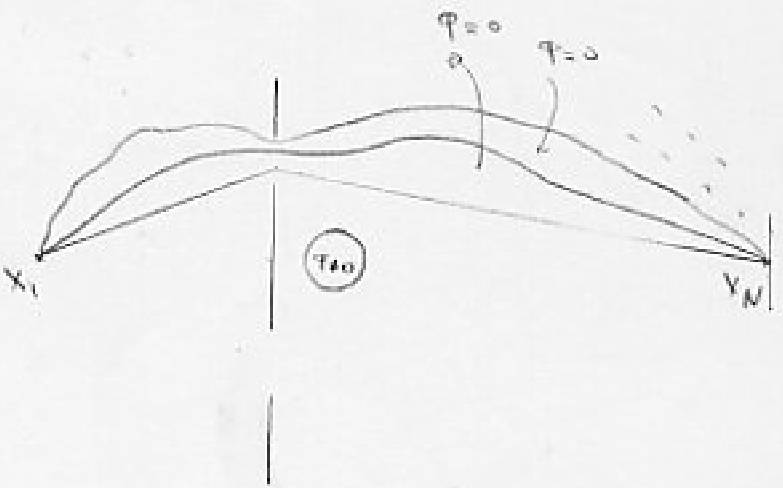
Now note that;

$$\int_{x_1, \Gamma_1}^{x_N} A\cdot dl - \int_{x_1, \Gamma_2}^{x_N} A\cdot dl = \oint A\cdot dl$$



$$= \int_S (\nabla\times A)\cdot ds = \int_S B\cdot ds = \varphi$$

So $\int_{\Gamma_1} A\cdot dl = \int_{\Gamma_2} A\cdot dl$ if $\varphi = 0$



→ All $\int_\Gamma A\cdot dl$ above are the same.

Also all $\int_\Gamma A\cdot dl$ below are the same.

$$\int_{\text{above}} \mathcal{D}[x(t)]\, e^{\frac{iS^{(0)}(N,1)}{\hbar}} + \int_{\text{below}} \mathcal{D}[x(t)]\, e^{\frac{iS^{(0)}(N,1)}{\hbar}}$$

$$\xrightarrow{A} \int_{\text{above}} \mathcal{D}[x(t)]\, e^{\frac{iS^{(0)}(N,1)}{\hbar}} \left\{ e^{\left[\frac{ie}{\hbar c}\int_{x_1}^{x_N} A\cdot ds\right]_{\text{above}}} \right\}$$

common factor for all paths above

$$+ \int_{\text{below}} \mathcal{D}[x(t)]\, e^{\frac{iS^{(0)}(N,1)}{\hbar}} \left\{ e^{\left[\frac{ie}{\hbar c}\int_{x_1}^{x_N} A\cdot ds\right]_{\text{below}}} \right\}$$

common factor for all paths below

$P \sim |\text{tr. amplitude}|^2 \longrightarrow \sim$ phase difference between the contribution from the paths going above and below.

$$\Delta\varphi = \left[\left(\frac{e}{\hbar c}\right)\int_{x_1}^{x_N} A\cdot ds\right]_{\text{above}} - \left[\left(\frac{e}{\hbar c}\right)\int_{x_1}^{x_N} A\cdot ds\right]_{\text{below}}$$

$$= \left(\frac{e}{\hbar c}\right)\oint A\cdot ds = \left(\frac{e}{\hbar c}\right)\Phi_B$$

phase difference due to the presence of B.

inside the impenetrable sylinder

This means:

As we change $B \longrightarrow P$ varries sinusoidaly with a period given by a fundamental unit of mag. flux;

$$T = \frac{2\pi\hbar c}{|e|} = 4.135\times10^{-7} \text{ Gauss-cm}^2$$

$\longrightarrow$ In Q.M. it is A rather B that is fundamental.

A is not just a mathematical tool to solve the problems.

However the observable effects in both examples depend only on Φ_B which is directly expressible in terms of B.

Alternative look:

In the presence of vector pot. A,

$$\psi^{(0)}(x) \xrightarrow{A} \psi(x) = \psi^{(0)}(x)\, e^{\frac{ie}{\hbar c}\int_\Gamma^x A(x')\cdot dx'}$$

$\int_\Gamma^x$: integration from some origin up to x on the Γ-path

$\psi^0(x)$: Sol. for the Schrödinger equ. in the absence of A.

$$\psi = \psi_1^0\, e^{\frac{ie}{\hbar c}\int_{\Gamma_1}^x A(x')\cdot dx'} + \psi_2^0\, e^{\frac{ie}{\hbar c}\int_{\Gamma_2}^x A(x')\cdot dx'}$$

$$\psi = e^{\frac{ie}{\hbar c}\int_{\Gamma_2}^{x} A(x')\cdot dx'} \left[\psi_2^\circ + \psi_1^\circ e^{\frac{ie}{\hbar c}\oint A(x')dx'}\right]$$

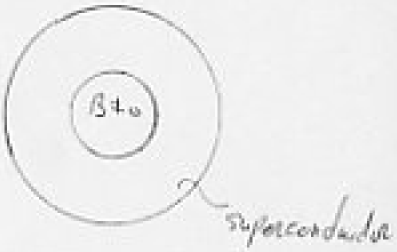
$$= e^{\frac{ie}{\hbar c}\int_{\Gamma_2}^{x} A(x')\cdot dx'} \left[\psi_2^\circ + \psi_1^\circ e^{\frac{ie}{\hbar c}\Phi}\right]$$

$\longrightarrow$ the interference is determined by Φ due to A

Φ: relative change in phase (due to the flux)

<u>Ex.</u> A Correlated Pair of electrons in a Superconductor ring:

The <u>absence</u> of the mag. field in a superconducting material is known as the <u>Meissner effect</u>.



The wave func. for <u>an electron pair</u> as a Q. mechanical quasi-particle,

$$\psi_{2e} = \psi^\circ e^{\frac{i(2e)}{\hbar c}\int_{\Gamma}^{x} A(x')\cdot dx'}$$

at the presence of A.

$q = 2e$ for quasi particle

This expression should be single-valued. The wave func. Ψ must be the same whether or not the path of integration encloses the flux. Otherwise the wave func. would be multivalued.

i.e. $\Psi_1 = \Psi_0 \, e^{\frac{i(2e)}{\hbar c}\int_{a\Gamma}^{a} A(x')\cdot dx'} = \Psi_0$

$\Psi_2 = \Psi_0 \, e^{\frac{i(2e)}{\hbar c}\oint_{a\Gamma}^{2\pi r} A(x')\cdot dx'}$

Since there is no force on the pair

$\rightarrow \Psi_1 \overset{must}{=} \Psi_2$

$\rightarrow \frac{2e}{\hbar c}\oint A(x')\cdot dx' = 2n\pi$

or $\Phi = \frac{\hbar\pi c}{e}\, n \quad n = 0, \pm 1, \pm 2, \cdots$

where $\frac{\pi\hbar c}{e} = 2.07 \times 10^{-7}$ gauss/cm²

$\longrightarrow$ The mag. field trapped by the superconductor ring must exhibit a step behavior in units of $\frac{\pi\hbar c}{e}$.

Magnetic Monopole:

One of the most remarkable predictions in Q. Phys, which has yet to be verified experimentally.

In Maxwell's eqns, we have

$$\nabla \cdot E = 4\pi \rho$$
$$\nabla \cdot B = 0 \qquad (\text{and not } \nabla \cdot B = 4\pi \rho_M)$$

The mag. charge commonly referred to as a mag. monopole analogous to electric charge is absent.

Q.M. does not predict that a mag. monopole must exist.

However it requires that if a mag monopole is ever found in nature, the magnitude of mag. charge must be quantized in terms of e, $\hbar$, and c.

Suppose a point mag. monopole at origin

$$\bar{B} = \frac{e_M}{r^2}\hat{r} \qquad (1)$$

This field can not be derived from the vector pot.

$$\bar{A} = \frac{e_m(1-\cos\theta)}{r\sin\theta}\hat{\varphi} \qquad (2)$$

because it is singular at $\theta = \pi$

Remark:

$$\nabla \times A = \hat{r}\left[\frac{1}{r S\theta}\frac{\partial}{\partial\theta}(A_\varphi S\theta) - \frac{\partial A_\theta}{\partial\varphi}\right] + \hat{\theta}\frac{1}{r}\left[\frac{1}{S\theta}\frac{\partial A_r}{\partial\varphi} - \frac{\partial}{\partial r}(r A_\varphi)\right]$$
$$+ \hat{\varphi}\frac{1}{r}\left[\frac{\partial}{\partial r}(r A_\theta - \frac{\partial A_r}{\partial\theta})\right]$$

In fact it turns out to be impossible to construct a singular-free pot. valid everywhere for this prob. .

To see this we first note Gauss's law;

$$\oint_{S'} B \cdot d\sigma = 4\pi \sigma_m \qquad (3)$$

For non-singular A $\longrightarrow \nabla \cdot (\nabla \times A) = 0$ everywhere

$$\oint_S B \cdot d\sigma = \int_V \nabla \cdot (\nabla \times A)\, d x^3 = 0$$

which is in contradition with (3)

$\longrightarrow$ must be singular.

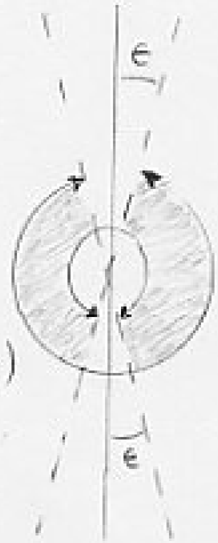
But since A is just a device for obtaining B, we need not insist on having a single expression fo A valid everywhere.

Suppose

$$\vec{A}^{(I)} = \frac{e_m(1-\cos\theta)}{r\sin\theta}\hat{\varphi} \qquad \theta < \pi - \epsilon$$

$$\vec{A}^{(II)} = \frac{-e_m(1+\cos\theta)}{r\sin\theta}\hat{\varphi} \qquad \theta > \epsilon$$

Now consider the overlap region $\epsilon < \theta < \pi - \epsilon$ where we may use either $\vec{A}^{(I)}$ or $\vec{A}^{(II)}$.



Because $\vec{A}^{(I)}, \vec{A}^{(II)} \xrightarrow{\text{lead}}$ The same $\vec{B}$

$\longrightarrow \quad \vec{A}^{(I)} \xleftrightarrow[\text{Gauge tr.}]{\text{are related by a}} \vec{A}^{(II)}$ (in the overlap region)

$$\vec{A}^{(II)} - \vec{A}^{(I)} = -\left(\frac{2e_m}{r\sin\theta}\right)\hat{\varphi}$$

and since $\nabla\Lambda = \hat{r}\frac{\partial\Lambda}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial\Lambda}{\partial\theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial\Lambda}{\partial\varphi}$

$\longrightarrow \quad \Lambda = -2e_m\varphi$ (will do the job)

Now, $\vec{A}^{(I)} \longrightarrow \psi^{(I)}$
$\vec{A}^{(II)} \longrightarrow \psi^{(II)}$

for a charged particle in the mag. field of $\vec{B} = \frac{e_m}{r^2}\hat{r}$

Acc. to $\tilde{\psi}(x,t) = e^{\frac{ie\Lambda(x')}{\hbar c}}\psi(x',t)$

$\rightarrow \psi^{(II)} = e^{\frac{-2iee_m\varphi}{\hbar c}}\psi^{(I)}$ in the overlap region

Wave funcs. $\psi^{(I)}$ and $\psi^{(II)}$ must each be single-valued.

For a certain θ and r,

$$\psi^{(I)}(r,\theta,\varphi) \overset{\text{must}}{=} \psi^{(I)}(r,\theta,\varphi+2\pi)$$

$$\psi^{(II)}(r,\theta,\varphi) \overset{''}{=} \psi^{(II)}(r,\theta,\varphi+2\pi)$$

$$\longrightarrow \quad \frac{2e\,e_m}{\hbar c} = n \qquad , \quad n = 0, \pm 1, \pm 2, \cdots$$

$$\longrightarrow \quad e_M = \frac{\hbar c}{2e}\, n \qquad\qquad ''$$

$$\frac{\hbar c}{2|e|} \simeq \left(\frac{137}{2}\right)|e| \qquad \text{unit of mag. charge}$$

Mag. charge quantization was first shown by P. A. M. Dirac.
The derivation given here is due to T. T. Wu and C. N. Yang.