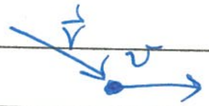
Particles in E.M. fields

Classically:



$$\vec{F} = q\left(\vec{E} + \frac{1}{c}\vec{v}\times\vec{B}\right) \quad \Big| \; \vec{E}, \vec{B} \text{ evaluate at } \vec{r}(t)$$

$$= q\left(-\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} + \frac{1}{c}\vec{v}\times(\vec{\nabla}\times\vec{A})\right)$$

$\vec{A}\times(\vec{B}\times\vec{C}) = B(\vec{A}\cdot\vec{C}) - (\vec{A}\cdot\vec{B})C \Rightarrow$

$$= \frac{1}{c}\vec{\nabla}(\vec{v}\cdot\vec{A}) - \frac{1}{c}(\vec{v}\cdot\vec{\nabla})\vec{A}$$

$$= +q\left[-\nabla\left(\phi - \frac{1}{c}\vec{v}\cdot\vec{A}\right) - \frac{1}{c}\left(\frac{\partial\vec{A}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{A}\right)\right]$$

L ①

following particle . $\bullet\longrightarrow\vec{v}$

$\vec{A}(\vec{r}(t), t)$

$$\frac{d\vec{A}}{dt} = \frac{\partial\vec{A}}{\partial\vec{r}}\cdot\dot{\vec{r}} + \frac{\partial\vec{A}}{\partial t} = (\vec{v}\cdot\vec{\nabla})\vec{A} + \frac{\partial\vec{A}}{\partial t}$$

$$\frac{d}{dt}A_x = \frac{d}{dt}\frac{\partial}{\partial v_x}(\vec{A}\cdot\vec{v})$$

$$\therefore F_x = q\left[-\partial_x U + \frac{d}{dt}\left(\frac{\partial U}{\partial v_x}\right)\right] \qquad U = \phi - \frac{1}{c}\vec{v}\cdot\vec{A}$$

$\uparrow$ potential is velocity dependent!

$$F_x = \frac{d}{dt}\frac{\partial\,\frac{1}{2}mv^2}{\partial v_x}$$

$$\frac{\partial L}{\partial x} = \frac{d}{dt}\left(\frac{\partial L}{\partial v_x}\right) \Rightarrow \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

Angel

11/21 $\Leftrightarrow \delta\left[\int_{t_1}^{t_2} L\,dt\right]=0$, i.e., $\delta S = 0$

$\therefore\ L = \underbrace{\frac{m}{2}v^2}_{T} - U = \frac{1}{2}mv^2 - q\phi + \frac{q}{c}\vec{A}\cdot\vec{v}$

$\vec{\pi} \equiv m\vec{v}$: mechanical momentum (Kinematic momentum)

$\vec{p}$ = Canonical momentum $\equiv \frac{\partial L}{\partial \dot{\vec{r}}} = m\vec{v} + \frac{q}{c}\vec{A}$

$H = \vec{p}\cdot\vec{v} - L$

mechanical momentum

$= \frac{1}{2}mv^2 + q\phi = \frac{(mv)^2}{2m} + q\phi = \frac{1}{2m}\left(p - \frac{q}{c}A\right)^2 + q\phi$

$\left(\frac{\partial H}{\partial q}\right)_p = \frac{\partial q\phi}{\partial q} + \frac{1}{m}\left(p - \frac{q}{c}A\right)\frac{-q}{c}\frac{\partial A}{\partial q} = q\frac{\partial \phi}{\partial q} - \frac{q}{c}\vec{v}\cdot\frac{\partial \vec{A}}{\partial q}$

In Quantum Mechanics, it is the canonical momentum $\vec{p}$ replaced by $\frac{\hbar}{i}\vec{\nabla}$!

$$\therefore\ \hat{H} = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{q}{c}\vec{A}\right)^2 + q\phi(\vec{r}) \qquad i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$$

$$\equiv \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi(\vec{r})$$

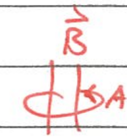
Feynman's heuristic arguement for replacing $\vec{p}$ by $\frac{\hbar}{i}\vec{\nabla}$ in $\hat{H}$.

(i) whatever $\hat{H}$ is, it only influences $i\hbar\frac{\partial \psi}{\partial t}$, not ψ itself!

$\therefore$ As we suddenly change $\vec{A}$, ψ is not changed! but only the rate of the change of ψ is changed!

$\therefore\ \frac{\hbar}{i}\vec{\nabla}\psi$ is not changed

(ii) Suppose we turn on $\vec{A}$ from 0 to $\vec{A}$.



$\vec{E} = \frac{-1}{c}\frac{\partial \vec{A}}{\partial t}$ is built up around $\vec{B}$!

Force $= q\vec{E} = -\frac{\partial q\vec{A}}{c\,\partial t}$. $\Rightarrow \int_0^t F\,dt' =$ total impulse

$\therefore$ The total impulse (changed) $= \frac{-q\vec{A}}{c} = m\vec{v}$ - - - ①

$\therefore\ m\vec{v} + \frac{q\vec{A}}{c}$ is not changed

$\because\ \frac{\hbar}{i}\nabla$ is not changed ⇒ see over important!

$\therefore\ \frac{\hbar}{i}\nabla = m\vec{v} + \frac{q\vec{A}}{c}$

One can't assign $m\vec{v} \to \frac{\hbar}{i}\nabla$ which would be inconsistent with ① (i.e. $\vec{p}$ is the generator of translation)

Correspondence principle

Classical : $\{A, B\} = \sum_i \left(\frac{\partial A(p,q)}{\partial q_i} \frac{\partial B(p,q)}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right)$

$\{q, p\} = 1$, $P =$ canonical momentum

$\dot{q}_i = \{q_i, H\}$ $[m\dot{q} = \vec{p} - q\vec{A}]$

$\dot{p}_i = \{p_i, H\}$ $\left[\frac{d}{dt} p = -\frac{\partial H}{\partial q} = -q\nabla\phi + \frac{q}{c}\nabla(\vec{v}\cdot\vec{A})\right]$

$\Leftrightarrow$ Q.M. $[q, p] = i\hbar$ $\quad \overset{\text{0}}{\shortparallel} \quad \overset{\shortparallel}{-\nabla(qU)}$

$\dot{p} = \frac{-i}{\hbar}[p, H]$ $\therefore$ should be the canonical momentum replaced by $\frac{\hbar}{i}\frac{\partial}{\partial q}$

$\dot{q} = \frac{-i}{\hbar}[q, H]$

Note : in $\hat{H}\psi \Rightarrow \left(\frac{\hbar}{i}\nabla - \frac{q\vec{A}}{c}\right)\cdot\left(\frac{\hbar}{i}\nabla - \frac{q\vec{A}}{c}\right)\psi$

also acting on this $\frac{q\vec{A}}{c}$!

$\left(p - \frac{q\vec{A}}{c}\right)^2 = p^2 - \frac{q}{c}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + \left(\frac{q}{c}\right)^2 A^2$ Hermitian !

11/21

Gauge invariance of the Aharonov – Bohm effect

Classically : real things $\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$, $\vec{B} = \nabla\times\vec{A}$

$\phi, \vec{A}$ not real can't show up in experiments : gauge invariance !

This is reflected in gauge invariance of $\vec{E}$ & $\vec{B}$:

$\vec{A} \to \vec{A} + \nabla\Lambda$ $\qquad \vec{B} = \nabla\times\vec{A}$

$\phi \to \phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}$ $\qquad \vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t}$ > not changed

the particle's equation of motion is gauge invariant !

$m\frac{d\vec{v}}{dt} = q(\vec{E} + \frac{1}{c}\vec{v}\times\vec{B})$ is also unchanged !

$\vec{p} = m\vec{v} + \frac{q}{c}\vec{A}$ is changed but not observable !

Q.M.

not gauge invariant

$$\frac{1}{2m}\left(\vec{p} - \frac{q\vec{A}}{c}\right)^2\Psi(x,t) + q\phi\,\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$\vec{A} \to \vec{A} + \nabla\Lambda(\vec{x},t) = \hat{A}$ $\qquad \frac{1}{2m}(\vec{p} - \frac{q}{c}\hat{A})^2\hat{\Psi} + q\hat{\Phi}\hat{\Psi}$

$\phi \to \phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t} = \hat{\Phi}$ $\qquad = i\hbar\frac{\partial\hat{\Psi}}{\partial t}$

$$\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A} - \frac{q}{c}\nabla\Lambda\right)^2\hat{\Psi}(x,t) + q\left(\Phi(x,t) - \frac{1}{c}\frac{\partial\Lambda}{\partial t}\right)\hat{\Psi}(x,t)$$
$$= i\hbar\frac{\partial\hat{\Psi}(x,t)}{\partial t}$$

Gauge transformation: $\hat{\Psi}(x,t) = e^{i\frac{q}{\hbar c}\Lambda(x,t)}\Psi(x,t)$

$|\hat{\Psi}(x,t)|^2 = |\Psi(x,t)|^2$: gauge invariant

probability current : gauge invariant !

* Q.M. $\vec{p}$ is no longer an observable

$\vec{\pi} = \vec{p} - \frac{q}{c}\vec{A}$ is gauge invariant & is an observable

Angel

$$\vec{J} = \frac{1}{2}\left[\psi(\hat{v}\psi)^* + \psi^*\hat{v}\psi\right] = \frac{1}{2}\left[\tilde{\psi}(\hat{v}'\tilde{\psi})^* + \tilde{\psi}^*(\hat{v}'\tilde{\psi})\right]$$

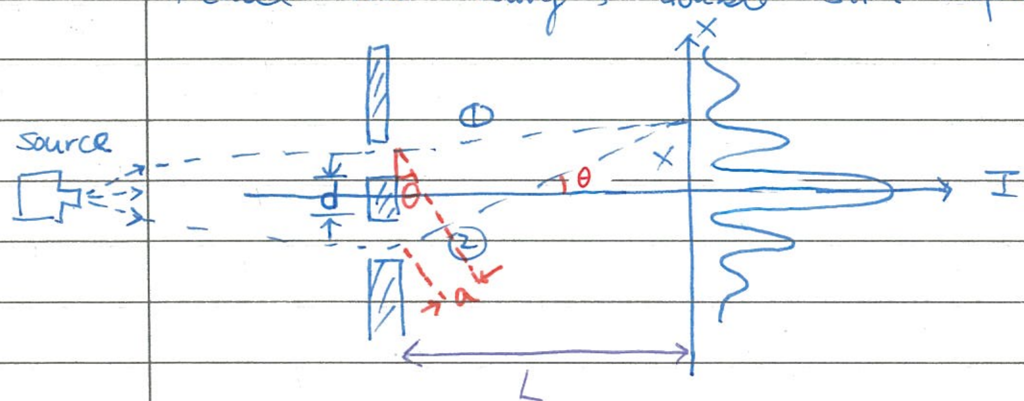
$$\hat{v} = \frac{\hat{p} - \frac{q}{c}\vec{A}}{m} \qquad \hat{v}' = \frac{\hat{p} - \frac{q}{c}\vec{A} - \frac{q}{c}\nabla\Lambda}{m}$$

$$\left(\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{J} = 0. \quad \rho = |\psi|^2\right)$$

But, does this mean $\vec{A}$ & ϕ are not real as they are in classical mechanics?
No!. They are real things

$\Rightarrow$ Aharonov–Bohm (AB) effect :
dual effect: Aharonov–Casher effect (AC effect)

Recall the Young's double-slit expt.



①: $c_1 e^{i\phi_1}$ ②: $c_2 e^{i\phi_2}$

$\delta = \phi_1 - \phi_2$ = phase difference $\qquad a = d\sin\theta = d\frac{x}{L}$

$$\delta = -\frac{a}{\lambda}\cdot 2\pi = -\frac{2\pi}{\lambda}\frac{x}{L}d \qquad (x \ll L,\ a$$

$\delta = \pi(2n+1) \Rightarrow$ out of phase $\Rightarrow$ min $\therefore x_n = \frac{L}{d}\left(\frac{2n+1}{2}\right)\lambda$

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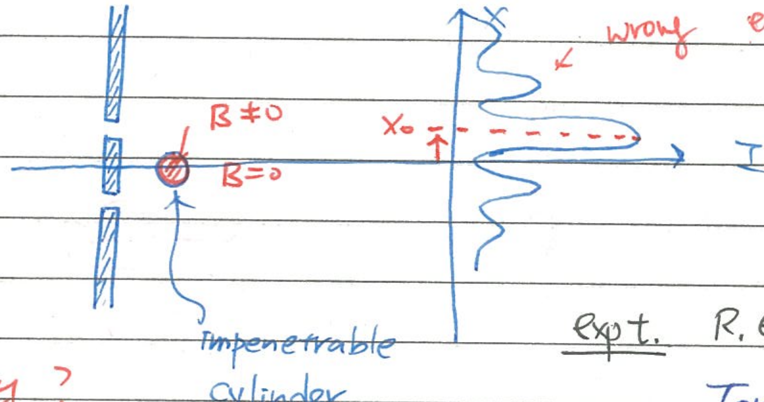
What about if we put a solenoid?



wrong envelope shape is fixed! no net momentum exchange! see over

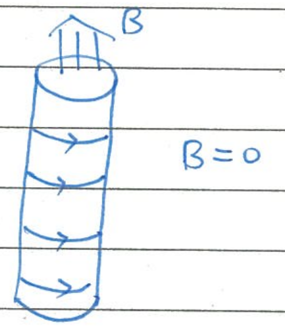
$\Rightarrow$ AB effect!

Why?

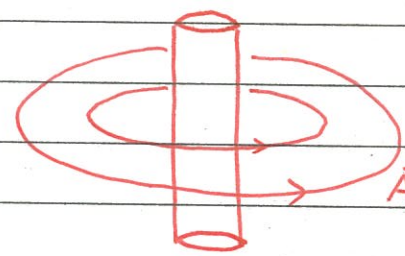
~~expt.~~ R. G. Chambers, PRL 5, 3, 1960

Tonomura et. al PRL 48, 1443 (1982)

Ideal solenoid:



$\vec{A} \neq 0 \quad \because \oint \vec{A} \cdot d\vec{\ell} = \int \vec{B} \cdot d\vec{S} \neq 0$



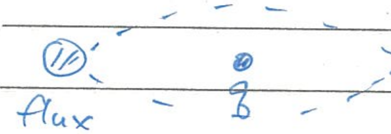
It is the $\vec{A}$ field that causes the shift!!

A is real!!

Note that gauge invariance is still obeyed!

the shift turns out to depend only the total flux of $\vec{B}$ inside the solenoid.

AC effect:



interference.

natural flux: fluxons in superconductors $\Phi_0 = \frac{h}{2e}$

or particles (neutral) carrying magnetic momentum

Before we dive into more appropriate formulation for the AB effect, let's examine the effect of $\vec{A}$ more closely in the Schrödinger equation; see how special is the setup of Young's expt.

(i) Since $\vec{A} \to \vec{A} + \nabla\Lambda$, $\phi \to \phi - \frac{1}{c}\frac{\partial \Lambda}{\partial t}$

& $\psi \to e^{\frac{ie\Lambda}{\hbar c}}\psi$, the Schrödinger eq. is invariant.

Can we choose appropriate gauge, Λ, to make $\vec{A} = 0$?

When this happens, $\Rightarrow \vec{A} + \nabla\Lambda = 0$, $\vec{A} = -\nabla\Lambda$, $\nabla\times\vec{A} = \vec{B} = 0$

On the contrary, if $\vec{B} = \nabla\times\vec{A} = 0$, only when the domain we consider is simply-connected, one can say $\vec{A} = -\nabla\Lambda$ (i.e., $\Lambda = -\int^{r} \vec{A}(\vec{r}')\cdot d\vec{r}'$)

In this case, if no $\vec{B}$ is present, the Schrödinger equation reduces to free-particle case!

(ii) Obviously, one sees that the set up of Young's expt. breaks the requirement "simply-connected"!

$\therefore$ $\vec{A}$ can't be made vanishing!

In this case, Λ becomes path dependent

$\Lambda_1 = -\int_{\Gamma_1}^{r} \vec{A}(\vec{r}')\cdot d\vec{r}'$, $\Lambda_2 = -\int_{\Gamma_2}^{r} \vec{A}(\vec{r}')\cdot d\vec{r}'$ are different.

Along 1, $\underset{\substack{\Uparrow \\ \text{free}}}{\tilde{\psi}} = e^{\frac{ig}{\hbar c}\Lambda_1}\psi_0$

$$\psi_{\Gamma_1} = e^{+\frac{ig}{\hbar c}\int_{\Gamma_1}^{r} \vec{A}(\vec{r}\,')\,d\vec{r}\,'} \qquad \psi_0 = \psi(r_0)$$

Along 2, $\tilde{\psi} = e^{\frac{ig}{\hbar c}\Lambda_2}\psi_0$

$$\psi_{\Gamma_2} = e^{\frac{ig}{\hbar c}\int_{\Gamma_2}^{r} \vec{A}(\vec{r}\,')\cdot d\vec{r}\,'}\psi_0$$

∴ At O', we have a phase difference

$$= \frac{g}{\hbar c}\oint \vec{A}\cdot d\vec{l} = \frac{g}{\hbar c}\phi_B$$

not single-value at O' ?

⇒ need the path integral formula

for clearer explanation

何以要以 $\vec{p}-\frac{q}{c}\vec{A}$ 之形式出現？

由p.13-4可知 $m\frac{d\vec{x}}{dt} = \vec{p}-\frac{q}{c}\vec{A}$

即 $m\vec{v} = \vec{p} - q/c\,\vec{A}$

$m\vec{v}$ 為直接牽涉到 velocity 之量，稱為 mechanical momentum ($\vec{\pi}$)

$\vec{p}$ 則是 "generalized momentum".

$\therefore \vec{p} = \underbrace{m\vec{v}}_{\vec{\pi}} + q/c\,\vec{A}$,

注意：$\vec{\pi}$ 是 直接可測之量，而 $\vec{A}$ 則沒有絕對物理意義，因此，$\vec{p}$ 的絕對值沒有意義。

不過，$\vec{p}$ 的引入卻是必要的！

原因是在有磁場下，mechanical momentum 並不守恆。
我們將發現，引入 $\vec{p}$ 可以維持動量守恆

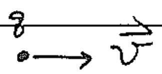
例：Biot-Savart law 告訴我們一段電流

$$\vec{B} = \frac{1}{c}\frac{i\,d\vec{l}\times\vec{r}}{r^3}$$

$\therefore$ 一個以 $\vec{v}$ 運動之電荷 q，取 $dl = v\,dt$

則 $i\,dl = \frac{q}{dt}v\,dt = qv$

$\therefore \vec{B} = \frac{1}{c}\frac{q\vec{v}\times\vec{r}}{r^3}$



NO.
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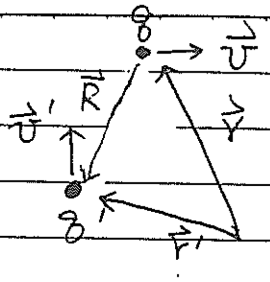
∴若有另一個电荷 q'，則所受之力為

$$\vec{F}_{q'} = \frac{1}{c} q' \vec{v}' \times \left(\frac{1}{c} \frac{q \vec{v} \times \vec{R}}{R^3} \right)$$



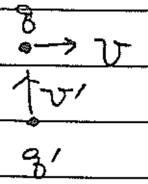
而 q 所受之力

$$\vec{F}_q = \frac{1}{c} q \vec{v} \times \left(\frac{1}{c} \frac{q' \vec{v}' \times (-\vec{R})}{R^3} \right) \qquad \vec{R} = \vec{r}' - \vec{r}$$

$$= -\frac{q q'}{c} \frac{\vec{v} \times (\vec{v}' \times \vec{R})}{R^3}$$

由此可見，$\vec{F}_q + \vec{F}_{q'}$ 一般 $\neq 0$

特例



$\vec{F}_{q'} \neq 0$，$\vec{F}_q = 0$

因此 $\frac{d}{dt} m' \vec{v}' + \frac{d}{dt} m \vec{v} \neq 0$

Why? 這是因為磁場也帶有動量。

要說明此點，首先，我們有

$$\vec{v} \times (\vec{v}' \times \vec{R}) = \vec{v}' (\vec{v} \cdot \vec{R}) - (\vec{v} \cdot \vec{v}') \vec{R} \qquad \times (-1)$$

$$\vec{v}' \times (\vec{v} \times \vec{R}) = \vec{v} (\vec{v}' \cdot \vec{R}) - (\vec{v} \cdot \vec{v}') \vec{R} \qquad \times (+1)$$

$$\therefore \vec{F}_q + \vec{F}_{q'} = \frac{q q'}{c^2} \left[\vec{v}' \frac{\vec{v} \cdot (\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|^3} + \frac{\vec{v} (\vec{v}' \cdot (\vec{r}' - \vec{r}))}{R^3} \right]$$

$$\because \frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|^3} = -\nabla \frac{1}{|\vec{r} - \vec{r}'|} = \nabla' \frac{1}{|\vec{r} - \vec{r}'|}$$

$$\therefore\ \frac{qq'}{c^2}\vec{v}'\left[\frac{\vec{v}\cdot(\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|^3}\right] = -\frac{q}{c}\left(\vec{v}\cdot\nabla\frac{1}{|\vec{r}-\vec{r}'|}\right)\frac{q'\vec{v}'}{c}$$

$$= -\frac{q}{c}(\vec{v}\cdot\vec{\nabla})\underbrace{\left[\frac{q'\vec{v}'}{c|\vec{r}-\vec{r}'|}\right]}_{\text{此為}q'\text{所產生之}A\text{（在}q\text{之位置上）}} = -\frac{q}{c}(\vec{v}\cdot\vec{\nabla})\vec{A}(\vec{r})$$

同理 $\frac{qq'}{c^2}\vec{v}\,\frac{\vec{v}'\cdot(\vec{r}'-\vec{r})}{|\vec{r}-\vec{r}'|^3} = -\frac{q'}{c}(\vec{v}'\cdot\vec{\nabla}')\vec{A}(\vec{r}')$

而 $\vec{r},\vec{r}'$ 皆為 t 之函數

$$\therefore\ (\vec{v}\cdot\vec{\nabla})\vec{A}(\vec{r}(t)) = \frac{d}{dt}\vec{A}(\vec{r}(t))$$

$$(\vec{v}'\cdot\vec{\nabla}')\vec{A}(\vec{r}'(t)) = \frac{d}{dt}\vec{A}(\vec{r}'(t))$$

$$\therefore\ \vec{F}_q+\vec{F}_{q'} = -\frac{d}{dt}\left(\frac{q}{c}\vec{A}(\vec{r}(t))+\frac{q'}{c}\vec{A}(\vec{r}'(t))\right)$$

$$\therefore\ \frac{d}{dt}\left(mv+\frac{q}{c}A(r)\right)+\frac{d}{dt}\left(m'v'+\frac{q'}{c}A(r')\right)=0$$

即 generalized momentum $\vec{p}$ 是守恆的.

說明： $\because \vec{A}$ 與 t 無關，由 page 13-4 的式

$$\nabla^2\vec{A} = -\frac{4\pi}{c}\vec{J} \iff \nabla^2\phi = -4\pi\rho$$

可見 $\vec{A}(\vec{r}) = \int\frac{\vec{J}(r')}{|\vec{r}-\vec{r}'|}d^3r' \iff \phi(\vec{r}) = \int\frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3r'$

點电荷 $\vec{J}(r) = q\vec{v}\,\delta(\vec{r}-\vec{r}_0(t))$

$$\therefore\ \vec{A}(\vec{r}\ ) = \frac{q\vec{v}}{|\vec{r}-\vec{r}_0(t)|}$$

Formal statement of Gauge invariance

I. Covariant derivatives : $\underbrace{i\hbar\frac{\partial}{\partial t}-q\phi}$, $\vec{D}=\vec{p}-\frac{e}{c}\vec{A}$

2. Classical

$$\frac{d\vec{r}}{dt}=\frac{\partial H}{\partial\vec{p}}=\frac{\vec{p}-\frac{q}{c}\vec{A}(\vec{r})}{m},\quad H=\frac{1}{2m}(\vec{p}-\frac{q}{c}\vec{A})^2+q\phi(\vec{r})$$

$$\frac{d\vec{p}}{dt}=-\frac{\partial H}{\partial\vec{r}}=-q\nabla\phi+\underbrace{\frac{\vec{p}-\frac{q}{c}\vec{A}}{m}\cdot\frac{q}{c}\nabla\vec{A}}_{\frac{q}{c}\nabla\vec{v}\cdot\vec{A}}=-\nabla U$$

$$\phi\to\phi-\frac{1}{c}\frac{\partial\Lambda}{\partial t},\quad \vec{A}\to\vec{A}+\nabla\Lambda,\quad \vec{r}'=\vec{r},\quad \vec{\pi}'=\vec{\pi}$$

$$\vec{p}'=\vec{p}+q/c\,(\nabla\Lambda)$$

not gauge invariant, ∴ not true physical quantity

3. Quantum

Let g denotes the gauge

$$|\psi_{g'}\rangle=G(g',g)\,|\psi_g\rangle$$

$$\hat{O}_{g'}=G(g',g)\,\hat{O}_g\,G^{\dagger}(g',g)$$

> gauge transformation

invariance $\langle\psi_{g'}|\psi_{g'}\rangle=\langle\psi_g|\psi_g\rangle$ ∴ $G^{\dagger}(g',g)G(g',g)=1$

$$\langle\psi_{g'}|\hat{O}_{g'}|\psi_{g'}\rangle=\langle\psi_g|G^{\dagger}(g',g)\,\hat{O}_{g'}\,G(g',g)|\psi_g\rangle$$

$$=\langle\psi_g|\hat{O}_g|\psi_g\rangle$$

Example $g = \{\vec{A}, \phi\}$

$$g' = \{\vec{A} + \nabla\Lambda,\ \phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}\}$$

$$\hat{O}_{g'} = \frac{1}{2m}\left(\vec{p} - \frac{q\vec{A}}{c} - \frac{q}{c}\nabla\Lambda\right)^2$$

$$G(g',g) = e^{\frac{iq}{\hbar c}\Lambda}$$

$$\therefore\ G^{+} O_{g'} G = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 = O_g$$

$\Rightarrow$ invariance.

11/27 /95

How do we understand the AB effect? (Shakar's Chapt 2.8)

Feyman's path integral formulation: Ref. ① Quantum Mechanics and Path Integrals Feynman & Hibbs. ② Path Integrals in Q.M. Statistics and Polymer Physic Hagen Kleinert

(i) evolution operators (propagator)

$$|\psi(t)\rangle = e^{\frac{-i\hat{H}(t-t_0)}{\hbar}} |\psi(t_0)\rangle \quad t>t_0$$

$$\psi(x,t) = \int d^3x' \underbrace{\langle x| e^{\frac{-iH(t-t_0)}{\hbar}} |x'\rangle}_{\text{III}} \underset{\langle x'|\psi(t_0)\rangle}{\psi(x', t_0)} \quad \cdots ①$$

Let's define $K^+(xt;x't_0) = \theta(t-t_0) \langle x| e^{-\frac{iH}{\hbar}(t-t_0)} |x'\rangle$ $\quad K(xt;x',t_0)$ (propagator) (Causality, $t>t_0$)

Important properties:

(a) $\lim_{t\to t_0^+} K^+(xt;x't_0) = \delta(x-x')$

(b) Analogy: $\phi(x) = \int d^3x' \frac{\rho(x')}{\underbrace{|x-x'|}_{\text{Green's function}}}$

$$\nabla^2 \frac{1}{|r-r'|} = -4\pi\delta(r-r')$$

What about $K^+(xt;x't_0)$?

$$i\hbar \frac{\partial K^+(xt;x't_0)}{\partial t} = i\hbar\delta(t-t_0) \langle x| e^{-\frac{iH}{\hbar}(t-t_0)} |x'\rangle$$

$$+ \langle x| H e^{\frac{-iH}{\hbar}(t-t_0)} |x'\rangle \theta(t-t_0)$$

$$= i\hbar\delta(t-t_0)\langle x|x'\rangle + \left(\frac{-\hbar^2}{2m}\nabla^2 + V(x)\right) K^+(xt;x't_0)$$

$$\therefore \left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2 - V(r)\right] K^+(rt;r't_0) = i\hbar\delta(t-t_0)\delta(\vec{r}-\vec{r}')$$

Once $K^+(rt;r't_0)$ is known, given any $\psi(r',t_0)$, we know $\psi(r,t)$ by equation ①

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Free particle $\hat{H} = \frac{p^2}{2m}$

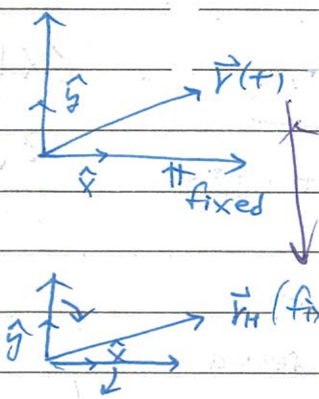
$$K^+(rt, r't_0) = \theta(t-t_0)\sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\ \exp\left[\frac{im(r-r')^2}{2\hbar(t-t_0)}\right]$$

(1D)

(c) $\overset{+}{K}(rt; r't_0)$ as a transition amplitude:

Interpretation by Heisenberg-picture:

Recall that
$$\langle A \rangle = \langle \psi(t) | A | \psi(t) \rangle = \underbrace{\langle \psi(0) |}_{\psi_H} \underbrace{e^{\frac{i}{\hbar}Ht} A\, e^{-\frac{i}{\hbar}Ht}}_{A_H} | \psi(0) \rangle$$



Schrödinger picture

analogous to state

Heisenberg picture

$\hat{x}, \hat{y}$ rotate oppositely!

$\therefore\ |\psi(t)\rangle_S = e^{-\frac{iHt}{\hbar}} |\psi(0)\rangle_S$

$e^{\frac{iHt}{\hbar}} |x\rangle = |x, t\rangle \equiv |x\rangle_H$

basis

$$\boxed{\begin{aligned} &{}_H\langle \psi | x \rangle_H \\ &= \langle \psi(0) | e^{\frac{i}{\hbar}Ht} | x \rangle \\ &= \langle \psi(t) | x \rangle \end{aligned}}$$

not only ⟨ ⟩ same but only components are the same

$$\therefore\ \overset{+}{K}(xt; x't_0) = \langle x | e^{-i\frac{H}{\hbar}t} e^{\frac{iH}{\hbar}t_0} | x' \rangle$$
$$= \langle x t | x' t_0 \rangle \quad (t > t_0)$$

= the amplitude to find the particle at x when $t = t$; which was located at x' when $t = t_0$

⇒ see over

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(d) Composition rule :

Firstly, we note : $\int d^3x \, |x\rangle\langle x| = \mathbb{I}$

$$\int d^3x \; e^{\frac{iH}{\hbar}t} |x\rangle\langle x| \, e^{\frac{-iHt}{\hbar}} = \mathbb{I}$$

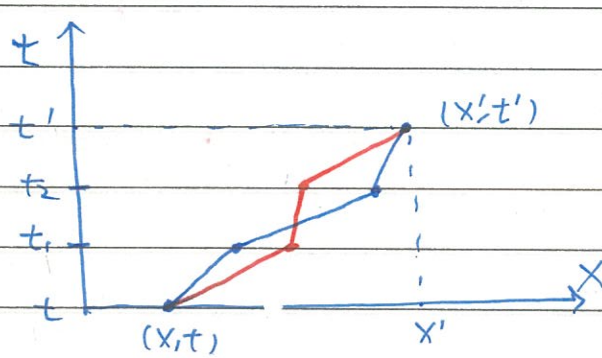
$$\Rightarrow \int d^3x \; |x,t\rangle\langle x,t| = \mathbb{I}$$

$$\langle x'\, t' | x\, t\rangle = \int d^3x_1 \;\; \langle x'\, t' | x_1\, t_1\rangle\langle x_1\, t_1 | x\, t\rangle$$

$$t' > t_1 > t$$

Similarly $\langle x' t' | x t\rangle = \int d^3x_2 \int d^3x_1 \; \langle x' t' | x_2 t_2\rangle\langle x_2 t_2 | x_1 t_1\rangle\langle x_1 t_1 | x t\rangle$

$$t' > t_2 > t_1 > t$$



(ii) Feyman's formulation : Calculating $\langle x' t' | x t\rangle$ is enough !

$t_1 = \Delta t + t$

$t_2 = 2\Delta t + t$

$\vdots$

$t_N = N\Delta t + t$

$\Delta t = \frac{t' - t}{N+1}$

$$\langle x' t' | x t\rangle$$
$$= \int dx_N \int dx_{N-1} \cdots \int dx_1$$
$$\langle x' t' | x_N t_N\rangle\langle x_N t_N | x_{N-1} t_{N-1}\rangle$$
$$\cdots \;\; \langle x_1 t_1 | x t\rangle$$

As $N \to \infty$, $\Delta t \to 0$

$$\langle x_n t_n | x_{n-1} t_{n-1} \rangle = \langle x_n | e^{-\frac{i}{\hbar} H (t_n - t_{n-1})} | x_{n-1} \rangle$$

$$= \langle x_n | e^{-\frac{i}{\hbar} H \Delta t} | x_{n-1} \rangle$$

$$e^{-\frac{i}{\hbar} H \Delta t} = e^{-\frac{i}{\hbar} \Delta t \left[\frac{p^2}{2m} + V(x) \right]}$$

$$\left[\frac{p^2}{2m}, V(x) \right] = \frac{1}{2m} \left\{ p \left[p, V(x) \right] + \left[p, V(x) \right] p \right\}$$

$$= \frac{1}{m} \frac{\hbar}{i} V'(x) p \quad \text{non commute !}$$

but $$e^{-\frac{i}{\hbar} H \Delta t} = 1 - \frac{i}{\hbar} \Delta t (H) + O(\Delta t^2)$$

$$\Rightarrow \quad = e^{-\frac{i}{\hbar} \Delta t \frac{p^2}{2m}} e^{-\frac{i}{\hbar} \Delta t V(x)} + O(\Delta t^2)$$

(Trotter formula)

$$\therefore \langle x_n | e^{-\frac{i}{\hbar} H \Delta t} | x_{n-1} \rangle$$

$$= \langle x_n | e^{-\frac{i}{\hbar} \Delta t \frac{p^2}{2m}} e^{-\frac{i}{\hbar} \Delta t V(x)} | x_{n-1} \rangle + O(\Delta t^2)$$

$$= \underbrace{\langle x_n | e^{-\frac{i}{\hbar} \Delta t \frac{p^2}{2m}} | x_{n-1} \rangle}_{\text{free particle propagator (or using midterm result)}} e^{-\frac{i}{\hbar} \Delta t V(x_{n-1})} + O(\Delta t^2)$$

$$= \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \, e^{\frac{i m (x_n - x_{n-1})^2}{2\hbar \Delta t}} e^{-\frac{i}{\hbar} \Delta t V(x_{n-1})} + O(\Delta t^2)$$

As $\Delta t \to 0$. x_{n-1}, x_n & $\frac{x_n + x_{n-1}}{2}$ have no much difference.

$\frac{|||}{x_n}$

In deed, as shown in $e^{\frac{i m (x_n - x_{n-1})^2}{2\hbar \Delta t}} \Rightarrow \langle (x_n - x_{n-1}) \rangle_{\text{free}} \sim \sqrt{\Delta t}$

Replacing x_{n-1} by $\frac{x_n+x_{n-1}}{2}$ (difference $= \frac{x_n-x_{n-1}}{2} \sim \sqrt{\Delta t}$)

will cause $(\Delta t)^{\frac{3}{2}}$ error which can be neglected!

$\Rightarrow \Delta t \to 0$, $\langle x_n | e^{-\frac{i}{\hbar} H \Delta t} | x_{n-1} \rangle$

$$= \sqrt{\frac{m}{2\pi i \hbar \Delta t}}\, e^{\frac{i m (x_n - x_{n-1})^2}{2\hbar \Delta t} - \frac{i}{\hbar}\Delta t\, V(\bar{x}_n)} + O\left(\frac{\Delta t^{3/2}}{\sqrt{\Delta t}}\right)$$

$$= \sqrt{\frac{m}{2\pi i \hbar \Delta t}}\, e^{\frac{i}{\hbar}\left[\frac{m}{2}\left(\frac{x_n - x_{n-1}}{\Delta t}\right)^2 - U(\bar{x}_n)\right]\Delta t} + O\left(\frac{\Delta t^{3/2}}{\sqrt{\Delta t}}\right)$$

$\therefore \langle x' t' | x t \rangle$

$$= \int dx_N \int dx_{N-1} \ldots \int dx_1 \left(\sqrt{\frac{m}{2\pi i \hbar \Delta t}}\right)^{N+1} e^{\frac{i}{\hbar} S[x(t)]}$$

$$S[x(t)] = \Delta t \sum_{n=1}^{N+1} \left[\frac{m}{2}\left(\frac{x_n - x_{n-1}}{\Delta t}\right)^2 - U(\bar{x}_n)\right], \quad x_0 = x,\ x_{N+1} = x'$$

$$= \int_t^{t'} dt\, \frac{1}{2} m (\dot{x})^2 - U(x)$$

$$= \int_x^{x'} \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}\int_t^{t'} dt\, L(x,\dot{x})} \quad \text{--- ①}$$

$\leftarrow$ Lagrangian

functional integral!! : Configuration space path integral

$$\int_x^{x'} \mathcal{D}[x(t)] \equiv \lim_{\substack{N\to\infty \\ (\Delta t \to 0)}} \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{\frac{N+1}{2}} \int dx_N \int dx_{N-1} \ldots \int dx_1$$

Always remember eq.① is only a concise way to write $\langle x' t' | x t \rangle$!! One has to write it out to calculate!!

Problem of rigorness :

1.
Baker – Campbell – Hausdorff formula

$$e^{\frac{-i\epsilon}{\hbar}(\hat{V}+\hat{T})} = e^{-i\epsilon\hat{V}/\hbar}\, e^{-i\epsilon\hat{T}/\hbar}\, e^{-i\epsilon^2\hat{X}/\hbar^2} \cdots$$

$$\hat{X} \equiv \frac{i}{2}[\hat{V},\hat{T}] - \frac{\epsilon}{\hbar}\left(\frac{1}{6}[\hat{V},[\hat{V},\hat{T}]] - \frac{1}{3}[[\hat{V},\hat{T}],\hat{T}]\right) + \cdots$$

exercise, $\hat{T} = \hat{p}^2$, $V = \hat{x}$

Trotter formula :

$$e^{\frac{-i}{\hbar}(t_a - t_b)\hat{H}} = \lim_{N\to\infty}\left[e^{-\frac{i\epsilon\hat{V}}{\hbar}}\, e^{-\frac{i\epsilon\hat{T}}{\hbar}}\right]^{N+1}$$

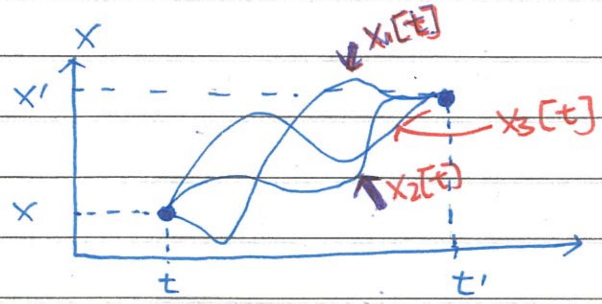
i.e. $\hat{X}$ does not contribute when $N\to\infty$
($\hat{T}$, $\hat{V}$ have to be bounded from below !)

2. The Feynman path has difficulties for singular potentials such as $V = \frac{-1}{|x|}$.

we shall not go into this problem.

see Kleinert's book chapter. 12.

Picture : Sum over all possible paths



$\Longleftrightarrow$ multi-slit expts.

action

each path contributes $e^{\frac{i}{\hbar}S[x(t)]}$

Thus, the classical Hamilton principle: $\delta S = 0$ for $x(t) = x_{cl}(t)$, finds a natural explanation here!

When $x = x_{cl}(t)$, nearby paths (x') have the same S ($\Leftarrow \because \delta S = 0$), thus, they are in phase, they contribute coherently!

(to first order in $\delta x \equiv x' - x_{cl}$).

In the classical scale; typical scale ~ 1 erg sec ~ $10^{27}\hbar$

When $x \neq x_{cl}(t)$, nearby paths will not have the same S, since $\hbar = 1.05 \times 10^{-27}$ erg-sec is a small number, a small difference in S will normally cause enormous change in the phase. As a result, $e^{\frac{iS}{\hbar}}$ will oscillate exceedingly rapidly!

If we look at, say, $\sin(\frac{S}{\hbar})$ or $\cos\frac{S}{\hbar}$, they are equally possible at peak or valley! Hence, they cancel each other. Therefore, effectively, only S_{cl} survives!

No.

Date

10/27/96

Saddle point approximation

The survival of S_{cl} may be understood by the saddle point approximation :

Consider $I = \int \frac{dx}{\sqrt{2\pi i\hbar}} e^{\frac{i a(x)}{\hbar}}$

When $\hbar \to 0$, the integral is dominated by the extremum of $a(x)$ with the smallest absolute value (denoted as X_{cl}) : $a'(X_{cl}) = 0$

expand, $a(x) = a(X_{cl}) + \frac{1}{2} a''(X_{cl}) (\underbrace{\delta x}_{y})^2 + \frac{1}{3!} a^{(3)}(X_{cl}) (\delta x)^3 + \cdots$

$$\therefore I = e^{\frac{i a(X_{cl})}{\hbar}} \int \frac{dy}{\sqrt{2\pi i\hbar}} e^{\frac{i}{\hbar} a''(X_{cl}) y^2} \, e^{\frac{i}{\hbar}\left[\frac{1}{3!} a^{(3)}(X_{cl}) y^3 + \frac{1}{4!} a^{(4)}(X_{cl}) y^4 + \cdots\right]}$$

$$\qquad\qquad = 1 + \frac{i}{\hbar}[\quad " \quad] - \frac{1}{\hbar^2}[\quad]^2 + \cdots$$

$$\int \frac{dy}{\sqrt{2\pi i\hbar}} e^{\frac{i}{\hbar} a''(X_{cl}) y^2} y^n = \begin{cases} \dfrac{(n-1)!!}{[a''(X_{cl})]^{\frac{n+1}{2}}} (i\hbar)^{n/2}, & n = \text{even} \\ 0 & n = \text{odd} \end{cases}$$

$$= e^{\frac{i}{\hbar} a(X_{cl})} \left[\frac{1}{\sqrt{a''(X_{cl})}} + O(\hbar) \right]$$

~~Fixed Energy Amplitude & classical limit~~

~~To get the classical limit, one has to fix the energy first:~~

$$\delta S = S[x(t)+\delta x(t)] - S[x(t)]$$

$$= \int_{t_1}^{t_2} \left[\tfrac{1}{2}m(\dot{x}+\delta\dot{x})^2 - U(x+\delta x) - \tfrac{1}{2}m\dot{x}^2 + U(x)\right] dt$$

$$= \int_{t_1}^{t_2} m\dot{x}\,\delta\dot{x} + \cancel{\tfrac{1}{2}m(\delta\dot{x})^2} - \frac{\partial U}{\partial x}\delta x \; dt + O(\delta x^2)$$

$$= \int_{t_1}^{t_2} \frac{d}{dt}[m\dot{x}\,\delta x] - \underbrace{m\ddot{x}\,\delta x}_{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right)} - \underbrace{\frac{\partial U}{\partial x}\delta x}_{\frac{\partial L}{\partial x}} \; dt$$

$$\frac{\partial L}{\partial \dot{x}}$$

$$= \overbrace{m v_2}^{P_2}\,\delta x(t_2) - \overbrace{m v_1}^{P_1}\,\delta x(t_1)$$

$$+ \int_{t_1}^{t_2} dt\, \delta x\left[-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) + \frac{\partial L}{\partial x}\right] + O(\delta x^2, \delta\dot{x}^2)$$

$\delta x(t_2) = 0, \quad \delta x(t_1) = 0$

$$\therefore \delta S = \int_{t_1}^{t_2} dt\, \delta x\left[\frac{\partial L}{\partial x} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right)\right] + O(\delta x^2, \delta\dot{x}^2)$$

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

$$\frac{\delta S}{\delta x} = 0 \quad \therefore \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \frac{\partial L}{\partial x}, \quad x = x_{cl}$$

For classical paths, one has

$$\delta S = P_2\,\delta x(t_2) - P_1\,\delta x(t_1)$$

$$\therefore \frac{\partial S_{cl}}{\partial x(t_2)} = p_2^{cl}$$

$$\frac{\partial S_{cl}}{\partial x(t_1)} = -p_1^{cl}$$

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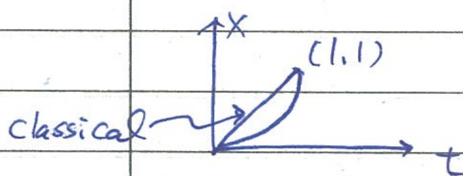
⇓ ~~but the above is only~~ correct to $O(\delta x)$ & beyond $O(\delta x)$ interference shows up ∴ rough measurement of precision of classical path

$\Delta S = S[x'] - S[x_{cl}] \simeq \hbar$, δx is the "width" of x_{cl}!
(not δS!)
($\delta x = x' - x_{cl}$)

In the classical scale, this is usually very small. On the other hand, if it's an electron ($m \sim 10^{-27} g$), this could be large! ⇒ Saddle point Approximation.

Example 1.



$S_{cl} = \frac{1}{2} m \int_0^1 dt = \frac{1}{2} m \qquad v = \frac{dx}{dt} = 1$

Consider the path $x = t^2$

$v = 2t$

$\therefore S = \frac{1}{2} m \int_0^1 4t^2 dt = \frac{4}{6} m = \frac{2}{3} m$

$\therefore \delta S = \frac{1}{6} m$

For a classical particle, $m \sim 1g$. $\delta S \sim 1 \sec \mathrm{erg} \sim 10^{27} \hbar$

For an electron, $m \sim 10^{-27} g$. $\delta S \sim \frac{1}{6} \hbar$!!

(also contributes
can't be neglected!)

∴ One can't assume electrons follow a well-defined ~~path~~ trajectory, x_{cl}.

Example 2. Free particle:

$(x, t) \qquad (x' t')$

$$x_{cl}(t'') = x' + \frac{x - x'}{t - t'}(t'' - t')$$

$$S_{cl} = \int_{t'}^{t} L \, dt'' = \frac{1}{2} m \frac{(x-x')^2}{t - t'}$$

$\frac{1}{2} \left(\frac{x - x'}{t - t'}\right)^2 m$

$$\therefore \quad e^{\frac{i}{\hbar} S_{cl}} = e^{\frac{im(x-x')^2}{2\hbar(t-t')}} \sim K(xt; x't')$$

$\uparrow$ exact!

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

$K(xt; x't') \sim e^{\frac{iS_{cl}}{\hbar}}$! (see, p 231, Chapt. 8)

Verify the Equivalence to Schröding eq. $\hookrightarrow$ see next page

Consider $\varepsilon \ll 1$

$$\psi(x,\varepsilon) = \int_{-\infty}^{\infty} K^{+}(x\varepsilon; x')\, \psi(x',0)\, dx'$$

$$= \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left\{\frac{i}{\hbar}\left[\frac{m(x-x')^2}{2\varepsilon} - \varepsilon V\left(\frac{x+x'}{2}\right)\right]\right\} \psi(x',0)\, dx'$$

$$= \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \exp\left[\frac{-i}{\hbar}\varepsilon V\left(x+\frac{\eta}{2}\right)\right] \psi(x+\eta,0)\, d\eta$$

$$\psi(x+\eta,0) = \psi(x,0) + \eta\frac{d\psi}{dx} + \frac{\eta^2}{2}\frac{d^2\psi}{dx^2} + \cdots$$

$$\exp\left[\frac{-i}{\hbar}\varepsilon V\left(x+\frac{\eta}{2}\right)\right] = 1 - \frac{i\varepsilon}{\hbar}V\left(x+\frac{\eta}{2}\right) + \cdots$$

$$= 1 - \frac{i\varepsilon}{\hbar}V(x) + \cdots$$

can rescale $\frac{\eta}{\sqrt{\varepsilon}} \equiv X$

Now, the factor $e^{\frac{im\eta^2}{2\hbar\varepsilon}}$ basically restricts $\frac{m\eta^2}{2\hbar\varepsilon} \lesssim \pi$! For η larger than this region, $e^{\frac{im\eta^2}{2\hbar\varepsilon}}$ oscillates a lot and thus has little contribution

$\therefore\ \eta \lesssim \sqrt{\varepsilon}$ $\therefore$ to $O(\varepsilon)$, we collect terms such as $O(1)$, ε, η, η^2 !

$\therefore\ \psi(x+\eta, 0)\exp\left[\frac{-i}{\hbar}\varepsilon V\left(x+\frac{\eta}{2}\right)\right]$

$$\simeq \psi(x,0) - \frac{i\varepsilon}{\hbar}V(x)\psi(x,0) + \eta\frac{\partial\psi}{\partial x} + \frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2} + O(\varepsilon^{3/2})$$

$$\therefore\ \psi(x,\varepsilon) = \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty}\exp\left[\frac{im\eta^2}{2\hbar\varepsilon}\right]\left[\psi(x,0) - \frac{i\varepsilon}{\hbar}V(x)\psi(x,0)\right.$$

$$\left. + \cancel{\eta\frac{\partial\psi}{\partial x}} + \frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right]d\eta$$

$\to 0$ (odd in η)

$$\int_{-\infty}^{\infty} e^{\frac{im\eta^2}{2\hbar\varepsilon}}d\eta = \left(\frac{2\pi\hbar i\varepsilon}{m}\right)^{\frac{1}{2}}$$

$$\int_{-\infty}^{\infty}\eta^2 e^{\frac{im\eta^2}{2\hbar\varepsilon}}d\eta = -i\frac{d}{d\alpha}\int_{-\infty}^{\infty}e^{i\alpha\eta^2}d\eta = -i\frac{d}{d\alpha}\sqrt{\frac{i\pi}{\alpha}} = \frac{1}{2}\sqrt{\frac{i\pi}{\alpha^2}}\ \frac{1}{\alpha} = \frac{1}{2\alpha}\sqrt{\frac{2\pi\hbar i\varepsilon}{m}}$$

$\alpha = \frac{m}{2\hbar\varepsilon}$

$$\Rightarrow\ \psi(x,\varepsilon) = \psi(x,0) - \frac{i\varepsilon}{\hbar}V(x)\psi(x,0)$$

$$-\frac{i\varepsilon}{\hbar}\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,0) + O(\varepsilon^{3/2})$$

$$\Rightarrow\ i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

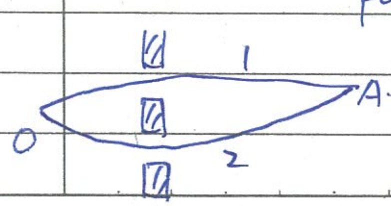
* Back to <u>AB effect</u>

When $\vec{A}$ presents, one has $L = \underbrace{\frac{1}{2}m\dot{x}^2 - V(x)}_{L_0} + \frac{q}{c}\vec{A}\cdot\dot{\vec{x}}$

$$\therefore\ S = \int_t^{t'}L\,dt = S_0 + \int_t^{t'} q/c\,\vec{A}\cdot\dot{\vec{x}}\,dt = S_0 + \frac{q}{c}\int_x^{x'}\vec{A}\cdot d\vec{x}$$

need to be careful

$\therefore$ In the presence of a $\vec{B}$ field, the phase for a given path is shifted: $\phi = \phi_0\ (B=0) + \frac{q}{\hbar c}\int_{path}\vec{A}\cdot d\vec{\ell}$



Therefore, $\phi_1 = \phi_{10} + \frac{q}{\hbar c}\int_1\vec{A}\cdot d\vec{\ell}$

$\phi_2 = \phi_{20} + \frac{q}{\hbar c}\int_2\vec{A}\cdot d\vec{\ell}$

↳ see over

$V = a + bx + cx^2 + d\dot{x} + ex\dot{x}$ most general form of quadratic in x & $\dot{x}$

($\dot{x}^2 \to$ Kinetic)

$$S[x] = S[x_{cl}] + \int_t^{t'} dt \underbrace{\frac{\delta S}{\delta x(t)}}_{0} \delta x(t)$$

$$+ \frac{1}{2} \int_t^{t'} dt_1 dt_2 \frac{\delta S}{\delta x(t_1)\, \delta x(t_2)} \delta x(t_1)\, \delta x(t_2) + \cdots$$

$\therefore$ One expects $S[x] = \frac{1}{2} m \dot{x}^2 - V$ $y \equiv \delta x$

$$= S_{cl} + \underbrace{\int_0^t dt' \left(\frac{1}{2} m \dot{y}^2 - c y^2 - e y \dot{y}\right)}_{\text{must be } O(y^2)}$$

$\because x_{cl}(0) = x$, $x_{cl}(t) = x'$

$\therefore y(0) = y(t') = 0$

$$\therefore U(xt; x') = e^{\frac{iS_{cl}}{\hbar}} \underbrace{\int_0^0 \mathcal{D}[y(t)]\, e^{\frac{i}{\hbar}\int_0^t \left(\frac{m}{2}\dot{y}^2 - c y^2 - e y \dot{y}\right) dt'}}_{\substack{||| \\ A(t)}}$$

$\therefore$ up to a time-dependant factor $A(t)$,

$$U \sim e^{\frac{i}{\hbar} S_{cl}}.$$

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$$\delta = \Phi_1 - \Phi_2 = \delta_0 + \frac{q}{\hbar c}\left(\int_1 \vec{A}\cdot d\vec{\ell} - \int_2 \vec{A}\cdot d\vec{\ell}\right)$$

same for any path starting at 0 arriving at A

$$= \delta_0 - \frac{q}{\hbar c}\oint \vec{A}\cdot d\vec{\ell}$$

$$= \delta_0 - \frac{q}{\hbar c}\Phi_B \qquad \Phi_B = B\cdot a > 0$$

if B is pointing out of the paper

$=$ flux passing through the solenoid

gauge invariant

$\because \quad \vec{A} \to \vec{A} + \nabla\Lambda$

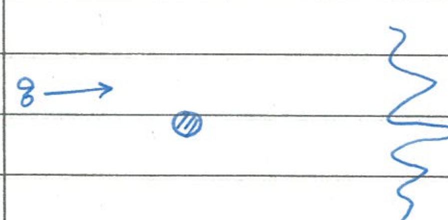
$\oint \vec{A}\cdot d\vec{\ell}$ is the same!!

Now, $\because \quad \delta_0 = -\frac{2\pi}{\lambda}\frac{x}{L}d$

$$\therefore \delta = -\frac{2\pi}{\lambda}\frac{x}{L}d - \frac{q}{\hbar c}\Phi_B$$

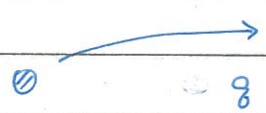
$$x_0 = -\frac{\lambda q L}{hcd}\Phi_B > 0 \quad \text{if B is pointing outwards!} \ (q<0)$$

* Aharonov – Casher effect : (Physical Review Letters 53, 319, 1984)



AB effect

What about



? AC effect.

neutral flux line : vortices in superconductors (type II)

magnetic moment for $\oslash$ $\neq 0$

$$\vec{m} = \frac{1}{2c}\int \vec{r}\times\vec{j}(\vec{r})\, d^3\vec{r} = \frac{i}{2c}\oint \vec{r}\times d\vec{r} = \frac{iA}{c}\hat{z}$$

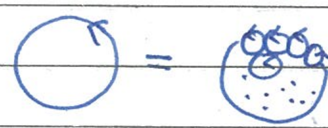
solenoid $\quad \vec{j}\,d^3\vec{r} = i\,d\vec{r} \quad aj = i$

∴ One may replace solenoids by particles with magnetic moment : neutron (no charge to be attracted to or repelled from q).

(note : neutrons have non-zero magnetic moment.)

Now, ∵ $\nabla\cdot\vec{J}=0$ $\left(\frac{\partial\rho}{\partial t}+\nabla\cdot\vec{J}=0,\ \frac{\partial\rho}{\partial t}=0\right)$

$\therefore \vec{J}=\nabla\times\vec{u}(\vec{r})$



$\Rightarrow \vec{m}=\frac{1}{c}\int d^3\vec{r}\,\vec{u}(\vec{r})$

$$\vec{m}=\frac{1}{2c}\int \underbrace{\vec{r}\times(\nabla\times\vec{u}(\vec{r}))}\,d^3\vec{r}$$

$$\nabla(\vec{r}\cdot\vec{u}(r))-\underbrace{(\vec{r}\cdot\vec{\nabla})\,\vec{u}(\vec{r})}-(\vec{u}(\vec{r})\cdot\vec{\nabla})\,\vec{r}-\vec{u}(\vec{r})\times\cancel{(\vec{\nabla}\times\vec{r})}^{\,0}$$

$(\vec{u}(\vec{r})\cdot\vec{\nabla})\,\vec{r} \to \vec{u}$

$(\vec{r}\cdot\vec{\nabla})\,\vec{u}(\vec{r}) = \nabla\cdot(\vec{r}\,\vec{u}(\vec{r})) - (\nabla\cdot\vec{r})\,\vec{u}(\vec{r})$

$\nabla\cdot(\vec{r}\,\vec{u}(\vec{r}))$ → integrated out

$$=\frac{1}{2c}\int\left[\nabla(\vec{r}\cdot\vec{u}(r))+2\vec{u}(\vec{r})\right]d^3\vec{r}$$

$$\int\nabla\phi\,d^3\vec{r}=\int\phi\,d\vec{S}\to 0 \qquad \phi=\vec{r}\cdot\vec{u}(\vec{r})$$

$$\therefore\ \vec{m}=\frac{1}{c}\int\vec{u}(\vec{r})\,d^3\vec{r}$$ magnetic moment density

In the rest frame of the solenoid (or flux, neutrons), one has $\rho_0=0,\ \vec{J}=\nabla\times\vec{u}(\vec{r})$.

In the lab frame, the solenoid moves with velocity $\vec{v}$. By Lorentz transformation : $\vec{v}\parallel\hat{x}$

$$\rho=\gamma\left(\rho_0+\frac{v}{c^2}J_x\right)=\gamma\frac{v}{c^2}J_x$$

$$=\frac{\gamma}{c^2}\vec{v}\cdot\vec{J},\qquad \gamma=\frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$$

∴ To the leading term $\rho=\frac{1}{c^2}\vec{v}\cdot\vec{J}$ (see over)

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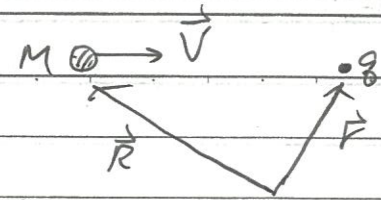


$$L = \frac{1}{2}MV^2 - \int \rho\, \Phi(\vec R' - \vec r)\, d^3\vec R'$$

$$= \frac{1}{2}MV^2 - \int \frac{1}{c^2}\, \vec V \cdot \vec J\, \Phi(\vec R' - \vec r)\, d^3\vec R'$$

$$= \frac{1}{2}MV^2 - \int \frac{1}{c^2}\, \vec V \cdot \underbrace{(\nabla_{R'} \times \vec \mu)\, \Phi(\vec R' - \vec r)}_{\parallel}\, d^3\vec R'$$

$$\nabla_{R'} \times \left(\Phi(\vec R' - \vec r)\, \vec \mu(\vec R') \right)$$

$$- \left(\nabla_{R'} \Phi(\vec R' - \vec r) \right) \times \vec \mu(\vec R')$$

$$= \frac{1}{2}MV^2 - \int \frac{1}{c^2}\, \vec V \cdot \vec E(\vec R' - \vec r) \times \vec \mu(\vec R')\, d^3\vec R'$$

$$= \frac{1}{2}MV^2 - \frac{1}{c}\, \vec V \cdot \vec E(\vec R - \vec r) \times \vec m \quad \text{--- ①}$$

(11) ↑
is small

direct from Lorentz!

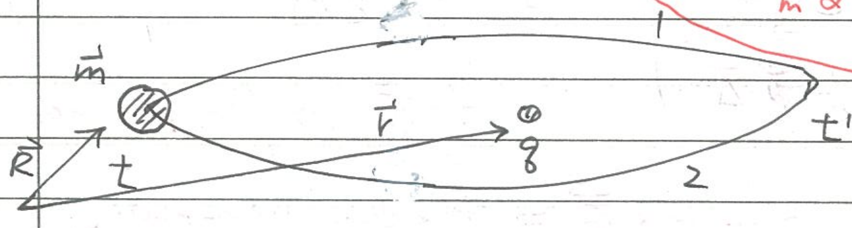
$\Leftrightarrow$ S, L interaction

$-\frac{1}{c}(\vec U \times \vec E) \cdot \vec m = -\underline{\vec B \cdot \vec m}$!

$\vec m \propto \vec S$, $\vec U \times \vec E \propto \vec U \times \vec r \propto \vec L$

(not including Thomas precession!)

AC effect:



$$\phi_1 - \phi_2 = \frac{-1}{c} \int_1 dt\, \vec V \cdot \vec E(\vec R - \vec r) \times \vec m$$

$$+ \frac{1}{c} \int_2 dt\, \vec V \cdot \vec E(\vec R - \vec r) \times \vec m$$

$$= \frac{1}{c} \oint d\vec R \cdot \vec E(\vec R - \vec r) \times \vec m$$

$\Uparrow$
electric field at $\vec R$ due to q

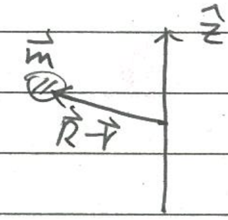
Consider extending $q \rightarrow$ to a line charge

(so that the space is no longer simple connected, nontrivial topology !)

$\overset{\odot}{q} \rightarrow \quad \Big| \quad \lambda$ = charge density per length

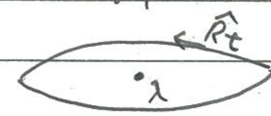
$$\vec{E}(\vec{R}-\vec{r}) = \frac{2\lambda}{|\vec{R}-\vec{r}|^2}(\vec{R}-\vec{r})$$

$\uparrow\ \uparrow$ 2D vectors



Let $\vec{m} = m\hat{z}$

top view



$$\vec{m} \times \vec{E}(\vec{R}-\vec{r})$$

$$= \frac{2\lambda}{|\vec{R}-\vec{r}|}\hat{R}_t$$

$$\therefore \quad \oint d\vec{R}\cdot\vec{E}(\vec{R}-\vec{r})\times\vec{m} = m\underbrace{\oint d\vec{R}\cdot\frac{2\lambda}{|\vec{R}-\vec{r}|}\hat{R}_t}_{\text{solenoid with } \Phi_B = 4\pi\lambda}$$

$$= m\, 4\pi\lambda$$

$\uparrow$ flux

$$\therefore \quad \phi_1 - \phi_2 = \frac{4\pi}{c}m\lambda$$

$\rightarrow$ expt. for example W.J. Elion etc. PRL 71, 2311 (1993)

In general, if charge & magnetic moment are moving simultaneously, it's better to use vector potential to describe :

Firstly, one realizes in ①, $\vec{E}(\vec{R}-\vec{r})\times\vec{m} = \dfrac{q(\vec{R}-\vec{r})\times\vec{m}}{4\pi|\vec{R}-\vec{r}|^3}$

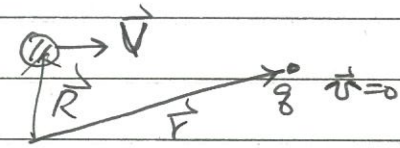
$$= \frac{q\,\vec{m}\times(\vec{r}-\vec{R})}{4\pi|\vec{r}-\vec{R}|^3}$$

$$= q\,\underbrace{\vec{A}(\vec{r}-\vec{R})}_{\text{II}}$$

the vector potential at $\vec{r}$ produced by $\vec{m}$ at $\vec{R}$

$$\therefore\ L = \frac{1}{2}MV^2 - \frac{q}{c}\vec{A}(\vec{r}-\vec{R})\cdot\vec{V}$$

This is a special case when the charge is fixed in space:



The AB effect is another extreme: $\vec{V}=0$, $\vec{v}\neq 0$

one has $\quad L = \frac{1}{2}mv^2 + \frac{q}{c}\vec{A}(\vec{r}-\vec{R})\cdot\vec{v}$

Adding these two gives the general form when both $\vec{V}$ & $\vec{v}$ $\neq 0$:

$$L = \frac{1}{2}MV^2 + \frac{1}{2}mv^2 + \frac{q}{c}\vec{A}(\vec{r}-\vec{R})\cdot(\vec{v}-\vec{V})$$

* Example : How to do path integrals

Free particles:

$$\langle x't'|xt\rangle = \lim_{\substack{N\to\infty\\ \Delta t\to 0}} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N+1}{2}} \int dx_N \int dx_{N-1}\cdots\int dx_1$$

$$\times \exp\left\{\frac{i}{\hbar}\frac{m}{2\varepsilon}\left[(x'-x_N)^2+(x_N-x_{N-1})^2+\cdots(x_2-x_1)^2+(x_1-x)^2\right]\right\}$$

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The integrals we need to do are

$$\int_{-\infty}^{\infty} \exp\left\{\frac{im}{2\hbar\varepsilon}\left[(x_2-x_1)^2+(x_1-x)^2\right]\right\} dx_1 \quad , \quad \varepsilon = \Delta t$$

$$= \sqrt{\frac{2\pi i\hbar\varepsilon}{m}\frac{1}{2}} \quad e^{\frac{im}{2\hbar\varepsilon}\frac{(x_2-x)^2}{2}}$$

$$\int_{-\infty}^{\infty} \exp\left\{\frac{im}{2\hbar\varepsilon}\left[(x_3-x_2)^2+\frac{(x_2-x)^2}{2}\right]\right\} dx_2$$

$$= \sqrt{\frac{2\pi i\hbar\varepsilon}{m}\frac{2}{3}} \quad \exp\left\{\frac{im}{2\hbar\varepsilon}\frac{(x_3-x)^2}{3}\right\}$$

$$\int_{-\infty}^{\infty} \exp\left\{\frac{im}{2\hbar\varepsilon}\left[(x_4-x_3)^2+\frac{(x_3-x)^2}{3}\right]\right\} dx_3$$

$$= \sqrt{\frac{2\pi i\hbar\varepsilon}{m}\frac{3}{4}} \quad e^{\frac{im}{2\hbar\varepsilon}\frac{(x_4-x)^2}{4}}$$

$$\therefore \langle x't'|xt\rangle = \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{N+1}{2}} \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{\frac{N}{2}} \sqrt{\frac{1}{2}\cdot\frac{2}{3}\cdot\frac{3}{4}\cdots\frac{N}{N+1}}$$

$$\times\, e^{\frac{im}{2\hbar\varepsilon}\frac{(x'-x)^2}{N+1}}$$

$$(N+1)\,\varepsilon = t'-t$$

$$= \left[\frac{m}{2\pi i\hbar(t'-t)}\right]^{\frac{1}{2}} e^{\frac{im(x'-x)^2}{2\hbar(t'-t)}}$$

$\Rightarrow$ matrix point of view

~~[illegible]~~

☆ Useful integral : $\int_{-\infty}^{\infty} dx \quad e^{ia\left[(y-x)^2+\frac{(x-y')^2}{b}\right]}$

$$= \sqrt{\frac{i\pi b}{a(1+b)}} \quad e^{\frac{ia}{1+b}(y-y')^2}$$

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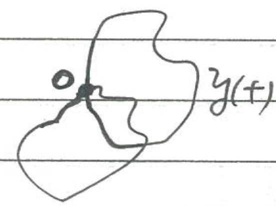
The case when $\langle x't'|xt\rangle = A(t)\, e^{\frac{i}{\hbar}S_{cl}}$: $V = a + bx + cx^2 + d\dot{x} + ex\dot{x}$

$$\langle x't'|xt\rangle = \int_x^{x'} \mathcal{D}x(t'')\, e^{\frac{i}{\hbar}S[x(t'')]}$$

Change variable : $x(t'') = x_{cl}(t'') + y(t'')$, $x_i = x_{cl}^i + y_i$

$$\because \int dx_i = \int dy_i \ , \quad \mathcal{D}x(t'') = \mathcal{D}y(t'')$$

$$\int_x^{x'} \mathcal{D}x(t'') = \int_0^0 \mathcal{D}y(t'')$$



$$S[x_{cl}+y] = \int_t^{t'} L(x_{cl}+y, \dot{x}_{cl}+\dot{y})\, dt'' \ , \quad L = \tfrac{1}{2}m\dot{x}^2 - V(x,\dot{x})$$

is quadratic !

$$L(x_{cl}+y, \dot{x}_{cl}+\dot{y}) = L(x_{cl},\dot{x}_{cl}) + \frac{\partial L}{\partial x}\Big|_{x=x_{cl}} y + \frac{\partial L}{\partial \dot{x}}\Big|_{x=x_{cl}} \dot{y}$$

$$+ \frac{1}{2}\Big(\underbrace{\frac{\partial^2 L}{\partial x^2}\Big|_{x_{cl}}}_{\substack{\shortparallel \\ -2c}} y^2 + 2\underbrace{\frac{\partial^2 L}{\partial x \partial \dot{x}}\Big|_{x_{cl}}}_{-e} y\dot{y} + \underbrace{\frac{\partial^2 L}{\partial \dot{x}^2}\Big|_{x_{cl}}}_{m} \dot{y}^2 \Big)$$

$$\int_t^{t'} \Big(\frac{\partial L}{\partial x}\Big|_{x_{cl}} y + \frac{\partial L}{\partial \dot{x}}\Big|_{x_{cl}} \dot{y}\Big)\, dt$$

$$= \int_t^{t'} y \Big(\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}\Big)_{x_{cl}} dt + \underbrace{\frac{\partial L}{\partial \dot{x}}\Big|_{x_{cl}} y \Big|_t^{t'}}_{\to 0}$$

$$= 0$$

$$\therefore S[x_{cl}+y] = S_{cl} + \int_t^{t'} dt'' \Big[\tfrac{1}{2}m\dot{y}^2 - ey\dot{y} - cy^2\Big]$$

$$\langle x't'|xt\rangle = e^{\frac{i}{\hbar}S_{cl}} \underbrace{\int_0^0 \mathcal{D}y(t'')\, e^{\frac{i}{\hbar}\int_t^{t'} dt'' \left[\frac{1}{2}m\dot{y}^2 - ey\dot{y} - cy^2\right]}}_{A(t'-t)}$$

$\therefore \langle x't'|xt\rangle = A(t)\, e^{\frac{i}{\hbar}S_{cl}}$

Example : ① free particle $A(t) = \left(\frac{m}{2\pi\hbar i(t'-t)}\right)^{\frac{1}{2}}$

② $V = a + bx$ (linear potential)

$$A(t) = \int_0^0 \mathcal{D}y(t'')\, e^{\frac{i}{\hbar}\int_t^{t'} dt'' \frac{1}{2}m\dot{y}^2}$$

$$= A_{free}(t) = \sqrt{\frac{m}{2\pi\hbar i(t'-t)}} \;!$$

(In this case, Feynman's method is better!!

Conventional way : $\hat{H} = \frac{\hbar^2}{2m}p^2 + a + bx$, hard!)

Other examples such as $V = \frac{1}{2}m\omega^2 x^2$ (simple harmonic oscillator), see Feynman & Hibbs's Path Integral and Quantum Mechanics.

Phase space path integral :

The above form $\langle x't'|xt\rangle = \int_x^{x'} \mathcal{D}x(t'')\, e^{\frac{i}{\hbar}S[x(t'')]}$ is the Configuration Space path integral, i.e., involves only x & $\dot{x}$.

As we know, in classical mechanics, L can be expressed in terms $p\dot{x} - H(x,p)$, which involves p !

This is actually a Legendre transformation

: transform (x, p) into $(x, \dot{x})$ as the variables.

Can we do the same thing in the path integral formulation? After all, this seems odd because (x, p) are not commute in Q.M. But it turns out that this is possible in the path integral formulation:

Recall ~~our derivation~~:

$$\langle x't' | xt \rangle = \int dx_N \int dx_{N-1} \cdots \int dx_1 \, \langle x't' | x_N t_N \rangle \langle x_N t_N | x_{N-1} t_{N-1} \rangle \cdots \langle x_1 t_1 | x t \rangle$$

$$= \int dx_N \int dx_{N-1} \cdots \int dx_1 \, \langle x' | e^{-\frac{i}{\hbar} H \Delta t} | x_N \rangle \langle x_N | e^{-\frac{i}{\hbar} H \Delta t} | x_{N-1} \rangle \cdots \langle x_1 | e^{-\frac{i}{\hbar} H \Delta t} | x \rangle$$

$$\langle x't' | xt \rangle = \langle x' | e^{-\frac{i}{\hbar} H (t'-t)} | x \rangle$$

$$= \langle x' | \underbrace{e^{-\frac{i}{\hbar} H \Delta t} \overset{|x_N\rangle\langle x_N|}{} e^{-\frac{i}{\hbar} H \Delta t} \cdots \overset{|x_1\rangle\langle x_1|}{} e^{-\frac{i}{\hbar} H \Delta t}}_{(N+1) \text{ times}} | x \rangle$$

$(N+1) \Delta t = t' - t$, $t' > t$.

$$= \langle x' | e^{-\frac{i}{\hbar} \frac{\Delta t}{2m} p^2} e^{-\frac{i \Delta t}{\hbar} V(x)} e^{-\frac{i \Delta t}{2m\hbar} p^2} e^{-\frac{i \Delta t}{\hbar} V(x)} \cdots | x \rangle$$

$$+ O(\Delta t^2)$$

$\because \int_{-\infty}^{\infty} dx \, |x\rangle\langle x| = 1$, $\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} |p\rangle\langle p| = 1$

$$\langle x | p \rangle = e^{\frac{i}{\hbar} p x}$$

no $\int dx$!

$\int \frac{dp_{N+1}}{2\pi\hbar} \int \frac{dx_N}{2\pi\hbar}$

$$\therefore \langle x't'|xt\rangle = \int \frac{dp_N}{2\pi\hbar} \int dx_{N-1} \int \frac{dp_{N-1}}{2\pi} \int dx_{N-2} \cdots \int \frac{dp_1}{2\pi}$$

$$\langle x'| e^{\frac{-i\Delta t}{2m\hbar}p^2} |p_{N+1}\rangle\langle p_{N+1}| e^{-\frac{i\Delta t}{\hbar}V(x)} |x_N\rangle\langle x_N| e^{-\frac{i\Delta t}{2m\hbar}p^2} |p_N\rangle\langle p_N|$$

$$e^{-\frac{i\Delta t}{\hbar}V(x)} |x_{N-1}\rangle\langle x_{N-1}| e^{-\frac{i\Delta t}{2m\hbar}p^2} |p_{N-1}\rangle\langle p_{N-1}| e^{-\frac{i\Delta t}{\hbar}V(x)} |x_{N-2}\rangle$$

$$\cdots \langle x_1| e^{-\frac{i\Delta t}{2m\hbar}p^2} |p_1\rangle\langle p_1| e^{-\frac{i}{\hbar}\Delta t V(x)} |x\rangle$$

The integrand $= e^{-\frac{i\Delta t}{2m\hbar}p_{N+1}^2} e^{-\frac{i\Delta t}{\hbar}V(x_N)} e^{-\frac{i\Delta t}{2m\hbar}p_N^2} e^{-\frac{i\Delta t}{\hbar}V(x_{N-1})}$

$$\cdots e^{-\frac{i\Delta t}{2m\hbar}p_1^2} e^{-\frac{i}{\hbar}\Delta t V(x)}$$

$$\times \langle x'|p_{N+1}\rangle\langle p_{N+1}|x_N\rangle\langle x_N|p_N\rangle\langle p_N|x_{N-1}\rangle \cdots \langle x_1|p_1\rangle\langle p_1|\underset{\uparrow \atop x_0}{x}\rangle$$

$$= e^{\sum_{n=1}^{N+1} \frac{-i\Delta t}{2m\hbar}p_n^2 - \frac{i\Delta t}{\hbar}V(\underset{\uparrow \atop x_0 = x}{x_{n-1}})} \cdot e^{\frac{i}{\hbar}p_{N+1}x'} e^{-\frac{i}{\hbar}p_{N+1}x_N} e^{\frac{i}{\hbar}p_N x_N}$$

$$e^{-\frac{i}{\hbar}p_{N}x_{N-1}} \times \cdots \times e^{\frac{i}{\hbar}x_1 p_1} e^{-\frac{i}{\hbar}p_1 x}$$

$$= e^{\sum_{n=1}^{N+1} \frac{-i\Delta t}{2m\hbar}p_n^2 - \frac{i\Delta t}{\hbar}U(x_{n-1}) + \frac{i}{\hbar}p_n(x_n - x_{n-1})}, \quad x_0 = x,\ x_{N+1} = x'$$

$$\therefore \langle x't'|xt\rangle = \underbrace{\int \cdots \int \prod_{n=1}^{N+1} \frac{dp_n}{2\pi\hbar} \prod_{n=1}^{N} dx_n}_{2N+1 \text{ times}} \exp\left\{\frac{i}{\hbar}\int_t^{t'} p\dot{x} - H(x,p)\, dt''\right\}$$

$$\parallel$$

$$\int \mathcal{D}p\,\mathcal{D}x$$

Homework: verify that if we integrate out $p_n \Rightarrow$ configuration space path integral.

Angel

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3D.

$$\langle \vec{r}' t' | \vec{r} t \rangle = \int_{\vec{r}}^{\vec{r}'} \mathcal{D}x(\tau)\, \mathcal{D}y(\tau)\, \mathcal{D}z(\tau)$$

$$e^{\frac{i}{\hbar}\int_t^{t'} \left[\frac{m}{2}(\dot{x}^2+\dot{y}^2+\dot{z}^2) - U(x,y,z)\right] dt''}$$

$$= \int \mathcal{D}P_x\, \mathcal{D}x\, \mathcal{D}P_y\, \mathcal{D}y\, \mathcal{D}P_z\, \mathcal{D}z$$

$$\times\, e^{\frac{i}{\hbar}\int_t^{t'} \left[P_x\dot{x} + P_y\dot{y} + P_z\dot{z} - H(\vec{r},\vec{p})\right] dt''}$$

More on
Free particle

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From the matrix point of view.

$$A(t_b - t_a) = \lim_{N\to\infty} \int dx_1 \cdots \int dx_N \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N+1}{2}}$$

$$\times \exp\left\{\underbrace{\frac{i}{\hbar}\frac{m}{2\Delta t}\left[(0-x_N)^2 + (x_N - x_{N-1})^2 + \cdots + (x_2-x_1)^2 + (x_1-0)^2\right]}_{\parallel}\right.$$

$$-\psi^T A \psi$$

$$\psi \equiv \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} \qquad A = \frac{m}{2\Delta t\hbar i}\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & \\ -1 & 2 & -1 & 0 & 0 & \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & \\ & & & & & 0 \\ & & 0 & & -1 & 2 & -1 \\ & & & & & -1 & 2 \end{pmatrix}$$

$\Rightarrow$ multi-dimension gaussian integral.

$$\psi = U\eta. \qquad (\det U = 1)$$

$$-\psi^T A \psi = -\eta^T \underbrace{U^T A U}\eta$$

diagonalized with eigenvalue λ_i

$$A(t_b - t_a) = \lim_{N\to\infty} \int d\eta_1 \cdots \int d\eta_N \; e^{-\sum_i \lambda_i \eta_i^2} \cdot \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N+1}{2}}$$

$$= \prod_{i=1}^{N} \sqrt{\frac{\pi}{\lambda_i}} = \pi^{N/2} \prod_{i=1}^{N} \frac{1}{\sqrt{\lambda_i}}$$

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Supplement **Quantum Statistical Mechanics**

Energy eigenket's representations:

$$\langle x | e^{-\frac{iH}{\hbar}(t-t_0)} | x' \rangle$$

$$= \sum_j \langle x | \phi_j \rangle \langle \phi_j | x' \rangle \, e^{-\frac{i}{\hbar}E_j(t-t_0)}$$

$$= \sum_j \phi_j(x) \, \phi_j^*(x') \, e^{-\frac{i}{\hbar}E_j(t-t_0)} \quad \text{--- ①}$$

Statistical Mechanics

$$\bar{A} = \frac{\sum_i A_i \, e^{-\frac{E_i}{K_BT}}}{\sum_i e^{-E_i/K_BT}} \qquad A_i \equiv \langle i | A | i \rangle$$

$$= \frac{1}{Z} \sum_i \langle i | A \, e^{-\frac{H}{K_BT}} | i \rangle$$

$$= \frac{1}{Z} \mathrm{Tr}\left[A e^{-H/K_BT} \right] \equiv \mathrm{Tr}[A\rho] \qquad \hat{\rho} = \frac{1}{Z} e^{-H/K_BT}$$

$\hat{\rho}$ = density matrix

$\mathrm{Tr}\,\hat{\rho} = 1$, Z = partition function $\equiv \mathrm{tr}\, e^{-\hat{H}/K_BT} = \sum_j e^{-\frac{1}{K_BT}E_j}$

Knowing $Z \Rightarrow$ know $\bar{A}$!

$\Rightarrow \therefore$

$$Z = \int dx \langle x | e^{-\hat{H}/K_BT} | x \rangle = \int dx \sum_j \phi_j(x) \, \phi_j^*(x) \, e^{-\frac{1}{K_BT}E_j}$$

$$\equiv \int dx \, Z(x,x) \, , \quad \text{where } Z(x,x') \equiv \sum_j \phi_j(x) \, \phi_j^*(x') \, e^{-\frac{1}{K_BT}E_j} \quad \text{--- ②}$$

In terms of $Z(x, x')$, we have

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$$\bar{A} = \frac{1}{Z}\int dx \sum_i \phi_i^*(x)\left(\hat{A}\phi_i(x)\right) e^{-\beta E_i}$$

$$A_i = \langle i|A|i\rangle = \int dx \int dx' \langle i|x\rangle\langle x|A|x'\rangle\langle x'|i\rangle$$

$$= \int dx \int dx' \, \phi_i^*(x) \, \underset{\uparrow \text{ acting on } x}{\hat{A}_{\underline{x}}} \, \delta(x-x')\phi_i(x')$$

$$= \int dx \, \phi_i^*(x) \, \hat{A} \, \phi_i(x)$$

$$\therefore \bar{A} = \frac{1}{Z}\int dx \, \hat{A}(x') \, Z(x',x)\Big|_{x'=x}$$

Comparing ① & ②, one knows that

quantum statistical mechanics

$\updownarrow$ $\quad t - t_0 = -\frac{i\hbar}{k_B T}$

Q.M. $\quad \Delta t \equiv -i\eta$, $\quad \eta = \frac{\hbar/k_B T}{(N+1)}$

$$Z(x',x) = \langle x'| e^{-\frac{H}{k_B T}} |x\rangle , \quad H = \frac{p^2}{2m} + V(x)$$

$$= \int \mathcal{D}x(u) \exp\{\cdots\}$$

$$\sqrt{\frac{m}{2\pi i\hbar\Delta t}} \rightarrow \sqrt{\frac{m}{2\pi\hbar\eta}} , \quad \therefore \int \mathcal{D}x(x) = \left(\frac{m}{2\pi\hbar\eta}\right)^{\frac{N+1}{2}} \int dx_N \cdots \int dx_1$$

$$\{\cdots\} = \frac{i}{\hbar} S = \frac{i}{\hbar}\Delta t \sum_{n=1}^{N+1}\left[\frac{m}{2}\left(\frac{x_n - x_{n-1}}{\Delta t}\right)^2 - V(\bar{x}_n)\right] , \quad x_0 = x, \; x_{N+1} = x'$$

$$\rightarrow -\sum_{n=1}^{N+1}\left[\frac{m}{2\hbar\eta}(x_n - x_{n-1})^2 + V(\bar{x}_n)\cdot\frac{\eta}{\hbar}\right] = \frac{-1}{\hbar}\int_0^{\beta\hbar} du\left[\frac{m}{2}\dot{x}^2(u) + V(x)\right]$$

$$\beta = 1/k_B T$$

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Perturbative expansion

$$\langle b\, t_b | a\, t_a \rangle = \int_a^b \mathcal{D}x(t) \exp \frac{i}{\hbar} \int_{t_a}^{t_b} \left[\frac{m}{2}\dot{x}^2 - V(x,t)\right] dt$$

$$\equiv K(b,a)$$

expand $e^{\frac{-i}{\hbar}\int_{t_a}^{t_b} V(x,t)\, dt}$

$$= 1 - \frac{i}{\hbar}\int_{t_a}^{t_b} V(x,t)\, dt + \frac{1}{2!}\left(\frac{i}{\hbar}\right)^2 \left[\int_{t_a}^{t_b} V(x,t)\, dt\right]^2 + \cdots$$

$$\therefore K(b,a) = K_0(b,a) + K_1(b,a) + K_2(b,a) + \cdots$$

$$K_0(b,a) = \int_a^b \mathcal{D}x(t)\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{m}{2}\dot{x}^2 dt} = \exp \frac{im(b-a)^2}{2\hbar(t_b-t_a)}$$

$$K_1(b,a) = \frac{-i}{\hbar}\int_a^b \mathcal{D}x(t) \int_{t_a}^{t_b} V(x(s),s)\, ds\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{m}{2}\dot{x}^2 dt}$$

$$= \frac{-i}{\hbar}\int_{t_a}^{t_b} F(s)\, ds$$

$$F(s) = \int_a^b \mathcal{D}x(t)\, V[x(s),s]\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{m}{2}\dot{x}^2 dt}$$

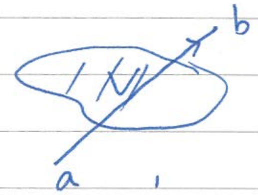
$$= \int_{-\infty}^{\infty} dx(s)\, K_0(b, x(s))\, V[x(s),s]\, K_0(x(s),a)$$

$$= \int_{-\infty}^{\infty} dx\, e^{\frac{im(b-x)^2}{2\hbar(t_b-s)}}\, V[x,s]\, e^{\frac{im(x-a)^2}{2\hbar(s-t_a)}}$$

$$\therefore K_1(b,a) = \frac{-i}{\hbar}\int_{t_a}^{t_b} \int_{-\infty}^{\infty} K_0(b,c)\, V(c)\, K_0(c,a)\, dx_c\, dt_c$$

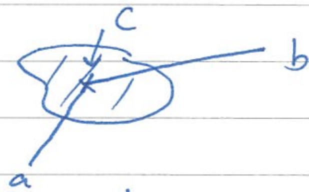
Diagram representation

$K_0(b,a)$



$\vdots$

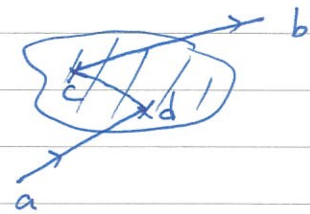
$K_1(b,a)$



"Feynman" diagram.

$\vdots$

$K_2(b,a)$



$\vdots$

Feynman rule : each —— $= K_0$

each $\underset{c}{\times}$ carries $-\frac{i}{\hbar}V$ and integration $\int dx_c \int_a^b dt_c$

example

$$K_2(b,a) = \left(-\frac{i}{\hbar}\right)^2 \iint K_0(b,c)\,V(c)\,K_0(c,d)\,V(d)\,K_0(d,a)\,dx_c\,dt_c\,dx_d\,dt_d$$

$$t_a < t_d < t_c < t_b$$

(built into K_0!)

See chapter 6 of Feynaman & Hibbs for more details.

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NO. 1.
DATE

Finding $K_0^+(xt;x't')$ by using (${K_0}^+$ is defined to be zero for $t<t'$)

$$\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)K_0^+(xt;x't') = i\hbar\,\delta(x-x')\,\delta(t-t')$$

with. B.C. $K_0^+(xt;x't')=0$ for $t<t'$

$$K_0^+(xt;x't') = \int\frac{dk}{2\pi}\int\frac{d\omega}{2\pi}\,K_0^+(k,\omega)\,e^{i[k(x-x')-\omega(t-t')]}$$

$$\delta(x-x')\,\delta(t-t') = \int\frac{dk}{2\pi}\int\frac{d\omega}{2\pi}\,e^{i[k(x-x')-\omega(t-t')]}$$

$$\therefore\ \left(\hbar\omega-\frac{\hbar^2k^2}{2m}\right)K_0^+(k,\omega) = i\hbar$$

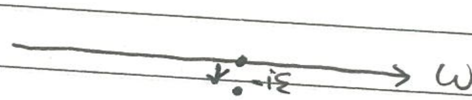
$$K_0^+(k,\omega) = \frac{i\hbar}{\hbar\omega-\hbar^2k^2/2m} = \frac{i}{\omega-E_k/\hbar}$$

$$\therefore\ K_0^+(xt;x't') = \int\frac{dk}{2\pi}\int\frac{d\omega}{2\pi}\,\frac{i}{\omega-E_k/\hbar}\,e^{i[k(x-x')-\omega(t-t')]}$$

There is a pole along the path of ω-integral if one takes $\int d\omega = \int_{-\infty}^{\infty}d\omega$

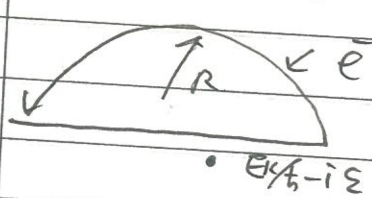
The Fourier transform actually doesn't restrict to integral along the real axis. One can deform the path which is equivalent to shift the pole.

Consider the shifting



i.e. $$\frac{1}{\omega-E_k/\hbar}\ \rightarrow\ \frac{1}{\omega-E_k/\hbar+i\varepsilon}\qquad \varepsilon\rightarrow 0^+$$

$t<t'$: $$\int\frac{d\omega}{2\pi}\,e^{-i\omega(t-t')}\,\frac{1}{\omega-E_k/\hbar+i\varepsilon} = 0$$



$\leftarrow e^{-i\omega(t-t')}\rightarrow 0$ as $R\rightarrow\infty$ for $t-t'<0$

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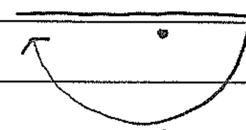
$t > t'$

$$\int \frac{d\omega}{2\pi} \frac{i}{\omega - E_k/\hbar + i\varepsilon} e^{-i\omega(t-t')}$$

$$= \frac{-2\pi i}{2\pi} i \; e^{\frac{-iE_k}{\hbar}(t-t')}$$



$$= e^{-\frac{i}{\hbar}E_k(t-t')}$$

$e^{-i\omega(t-t')} \to 0$
for $t > t'$

$\therefore$

$$K_0^+(xt; x't') = \theta(t-t') \int \frac{dk}{2\pi} e^{i\left[k(x-x') - \frac{E_k}{\hbar}(t-t')\right]}$$

$$= \theta(t-t') \int \frac{dp}{2\pi} e^{i\frac{p}{\hbar}(x-x') - \frac{iE_k}{\hbar}(t-t')}$$

$$= \theta(t-t') \langle x | e^{-\frac{i}{\hbar}H(t-t')} | x' \rangle$$