Feynman path integral

1. Real-time path integrals

2. Imaginary-time path integrals

3. Stationary phase approximation

Refs. : 1. R. Shankar, Principles of quantum mechanics
(See Chap. 8 and 21) : Suggested ref. !

2. R. P. Feynman and A. R. Hibbs, Quantum mechanics and path integrals

3. L. S. Schulman, Techniques and applications of path integrals

. Alternative formulation Q.M.,

Schrödinger : Hamiltonian formalism

Feynman : Lagrangian formalism

· Useful :

- discussion Aharonov - Bohm effect (next chapter)
- semiclassical limit quantum theory
- nonperturbative approaches
- prototype to field theory (1-particle -> N-particles)

· Recall :

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$$

in the coordinate representation (1-D)

$$\psi(x,t) = \langle x|\psi(t)\rangle = \langle x|U(t,t_0)\underset{\substack{\uparrow\\ 1}}{|}\psi(t_0)\rangle$$

$$= \int_{-\infty}^{+\infty} dx' \; \langle x|U(t,t_0)|x'\rangle \, \psi(x',t_0)$$

Definition :

$$K(x,t\,;\,x',t'_0) = \langle x|U(t,t_0)|x'\rangle \quad : \text{ propagator} \tag{201.1}$$

in particular, if $H \neq H(t)$,

$$K(x,t\,;\,x',t'_0) = \langle x|e^{-iH(t-t_0)/\hbar}|x'\rangle \tag{201.2}$$

idea (201.1) :

$|K(x,t\,;\,x',t'_0)|^2$ = probability finding particle around position $\underline{\underline{x}}$ at time $t > t_0$ if particle around position $\underline{\underline{x'}}$ at initial time t_0.

note : if (201.1) is determined → Q.M. problem is solved !

Exercise : Show that (201.1) is the Green's function of the time-dependent Schrödinger equation,

$$\underbrace{(H - i\hbar\partial_t)}_{\text{differential operator.}} K(x,t;x',t'_0) = -i\hbar\,\delta(x-x_0)\,\delta(t-t')$$

Ex. : Free particle, 1-D.

$$K(x,t\,;\,x',0) = \langle x|\,\underset{\substack{\uparrow\\1}}{}\,e^{-iHt/\hbar}\,\underset{\substack{\uparrow\\1}}{}\,|x'\rangle$$

$$= \int dp'dp'' \,\langle x|p'\rangle \underbrace{\langle p'|e^{-ip^2t/2m}|p''\rangle}_{e^{-ip''^2t/2m}\langle p'|p''\rangle} \langle p''|x'\rangle$$

$$= \int dp' \,\frac{1}{2\pi\hbar}\, e^{ip'(x-x')/\hbar}\, e^{-ip'^2t/2m\hbar}$$: Gaussian integral

$$= \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \exp\left(im(x-x')^2/2\hbar t\right) \qquad (202.1)$$: propagator free particle (1-D)

Recall : Gaussian integral :

$$\int_{-\infty}^{+\infty} du\; e^{-au^2+bu} = \left(\frac{\pi}{a}\right)^{1/2} e^{+b^2/4a} \qquad (202.2)$$

Ex. : 1-D harmonic oscillator.

It's possible to show that

$$K(x,t\,;\,x',0) = \left(\frac{m\omega}{2\pi i\hbar \sin\omega t}\right)^{1/2} \exp\left(i\,\frac{m\omega}{2\hbar}\left((x^2+x'^2)\cot\omega t - \frac{2xx'}{\sin\omega t}\right)\right)$$

(202.3)

· Feynman,

idea : direct calculation (201.1), <u>without</u> operators

Recall classical mechanics :

$$S = \int_{t_0}^{t} dt' \, L(\dot{x}, x, t') \quad : \text{action}$$

where $L = \frac{1}{2} m \dot{x}^2 - V(x)$: Lagrangian

$$\delta S = 0 \rightarrow \underbrace{\frac{\partial L}{\partial x} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = 0}_{\text{Euler-Lagrange equation}} \longrightarrow \text{solution : } x = x_c(t)$$

(1 path)

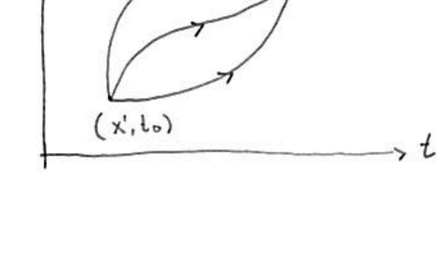
· in Q.M. (Feynman)

procedure to determine the propagator (201.1) :

- consider all paths $x(t)$ such that $(x', t_0) \longrightarrow (x, t)$
- determine the action $S[x]$ associated with $x(t)$
-

$$K(x, t; x', t_0) = A \sum_{\text{all paths } x(t)} e^{iS[x]/\hbar} \qquad (203.1)$$

$$= \int_{x(t_0) = x'}^{x(t) = x} \mathcal{D}x \; e^{iS[x]/\hbar} \quad ; \quad A : \text{cte}$$



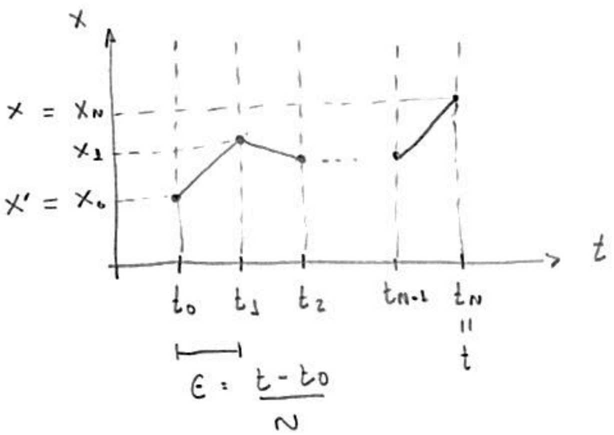
note : - not only the classical path $x_c(t)$ is included in (203.1)

- all paths $x(t)$ contribute with the same magnitude but different phases $S[x]/\hbar$.

idea evaluation $\sum\limits_{\text{all paths}}$:

usual integral $I = \int_a^b dx\, f(x) = \lim\limits_{\Delta x \to 0} \sum\limits_i \Delta x\, f(x_i)$
↳ discrete set of points

consider a discrete approximation for a path $x(t)$



↳ $$K(x,t;x',t_0) = \lim_{\epsilon \to 0} \frac{1}{A} \int_{-\infty}^{+\infty} \frac{dx_1}{A} \int_{-\infty}^{+\infty} \frac{dx_2}{A} \cdots \int_{-\infty}^{+\infty} \frac{dx_{N-1}}{A}\, e^{iS[x]/\hbar}$$

with A : normalization cte

. So far, we follow Ref. 2.

Let's now follow Ref. 3 and derive (203.1) from quantum theory.

1. Real-time path integral.

consider: particle mass m under potential $V = V(q)$ (1-D),

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

assumption: $t_0 = 0$.

↳ $K(x,t;x',0) = \langle x | e^{-iHt/\hbar} | x' \rangle$ (204.1)

- Let's devide the time interval $[0,t]$ in N-parts:

note identification: $t_0 = 0$ and $t_N = t$.

$$K(x,t;x',0) = \langle x | e^{-iH(t_N - t_{N-1})/\hbar} \, e^{-iH(t_{N-1} - t_{N-2})/\hbar} \cdots$$

$$\cdots e^{-iH(t_{K-1} - t_{K-2})/\hbar} \cdots e^{-iH(t_1 - t_0)/\hbar} | x' \rangle$$

note: $K = \langle x |$ N-exponentials $| x' \rangle$

- Let's introduce

$$1 = \int_{-\infty}^{+\infty} dx_k \, | x_k \rangle \langle x_k | \quad ; \quad 1 \leq k \leq N-1$$

between the exponentials:

Obs.: short notation: $K \equiv K(x,t;x',0)$

$$K = \int_{-\infty}^{+\infty} dx_1\, dx_2 \dots dx_{N-1}\ \langle x | e^{-iH(t_N - t_{N-1})/\hbar} | x_{N-1}\rangle \,\cdot$$

$$\cdot\, \langle x_{N-1} | e^{-iH(t_{N-1} - t_{N-2})/\hbar} | x_{N-2}\rangle \dots$$

$$\dots \underbrace{\langle x_k | e^{-iH(t_k - t_{k-1})/\hbar} | x_{k-1}\rangle}_{\equiv K_k} \dots$$

$$\dots \langle x_1 | e^{-iH(t_1 - t_0)/\hbar} | x'\rangle \tag{205.1}$$

- we define : $t_k - t_{k-1} \equiv \epsilon = t/N$

in the limit $N \to \infty$, we have

$$K_k \approx \langle x_k | 1 - iH\epsilon/\hbar | x_{k-1}\rangle$$

$$\approx \underset{\substack{\uparrow \\ 1}}{\langle x_k | x_{k-1}\rangle} - \frac{i\epsilon}{\hbar} \langle x_k | \underset{\substack{\uparrow \\ 1}}{\frac{p^2}{2m}} | x_{k-1}\rangle - \frac{i\epsilon}{\hbar} \underbrace{\langle x_k | V(q) | x_{k-1}\rangle}_{V(x_k)\, \underset{\substack{\uparrow \\ 1}}{\langle x_k | x_{k-1}\rangle}}$$

where

$$1 = \int_{-\infty}^{+\infty} dp_k\, |p_k\rangle\langle p_k|$$

since $\langle x_k | p_k\rangle = \dfrac{1}{\sqrt{2\pi\hbar}}\, e^{ip_k x_k/\hbar}$

$$\hookrightarrow \quad K_k \approx \int \frac{dp_k}{2\pi\hbar}\, e^{i p_k (x_k - x_{k-1})/\hbar} \left[1 - \frac{i\epsilon}{\hbar} \left(\frac{p_k^2}{2m} + V(x_k) \right) \right]$$

$$= \int \frac{dp_k}{2\pi\hbar}\, e^{i p_k (x_k - x_{k-1})/\hbar} \exp\left[\frac{-i\epsilon}{\hbar} \left(\frac{p_k^2}{2m} + V(x_k) \right) \right]$$

performing the Gaussian integral,

$$K_k = \sqrt{\frac{m}{2\pi i \hbar \epsilon}} \exp\left[\frac{i\epsilon}{\hbar} \left(\frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} - V(x_k) \right) \right]$$

Thus,

$$K(x,t;x',0) = \lim_{\substack{N\to\infty \\ (\epsilon\to 0)}} \int_{-\infty}^{+\infty} dx_1 \dots dx_{N-1} \left[\prod_{k=1}^{N} \sqrt{\frac{m}{2\pi i \hbar \epsilon}} \right] *$$

$$* \exp\left[\sum_{k=1}^{N} \frac{i\epsilon}{\hbar} \left(\frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} - V(x_k) \right) \right] \qquad (206.1)$$

Formally, we can write

$$K(x,t;x',0) = \int_{x(0)=x'}^{x(t)=x} \mathcal{D}x \; e^{iS[x]/\hbar} \qquad (206.2)$$

where

$$S = \int_0^t dt' \left(\frac{1}{2} m \dot{x}^2 - V(x) \right) \quad : \text{classical action of the particle}$$

$$\int_{x(0)=x'}^{x(t)=x} \mathcal{D}x = \lim_{\substack{\epsilon \to 0 \\ (N \to +\infty)}} \left[\prod_{k=1}^{N} \frac{m}{2\pi i \hbar \epsilon} \right] \int_{-\infty}^{+\infty} dx_1 \, dx_2 \ldots dx_{N-1} :$$

measure of the integral.

Ex. 1 : Free particle (1-D).

Let's determine the propagator from Eq. (206.1).

Since $V(q) = 0$,

$$\hookrightarrow K(x,t;x',0) = \lim_{N \to \infty} \underbrace{\int_{-\infty}^{+\infty} dx_1 \, dx_2 \ldots dx_{N-1} \prod_{k=1}^{N} \sqrt{\frac{m}{2\pi i \hbar \epsilon}} \exp\left(\frac{im}{2\hbar\epsilon} (x_k - x_{k-1})^2 \right)}_{\text{Gaussian integrals}}$$

identity:

$$\int_{-\infty}^{+\infty} du \, e^{-a(x-u)^2 - b(u-y)^2} = \sqrt{\frac{\pi}{a+b}} \, e^{-ab(x-y)^2/(a+b)} \qquad (207.1)$$

we have, e.g.,

$$\left(\frac{m}{2\pi i \hbar \epsilon} \right) \int dx_1 \exp\left(\frac{im}{2\hbar\epsilon} (x_1 - \underset{\substack{\parallel \\ x'}}{x_0})^2 + \frac{im}{2\hbar\epsilon} (x_2 - x_1)^2 \right)$$

$$\underset{\substack{\uparrow \\ \text{exercise}}}{=} \sqrt{\frac{m}{2\pi i \hbar (2\epsilon)}} \exp\left(\frac{im}{2\hbar(2\epsilon)} (x_2 - x_0)^2 \right)$$

next,

$$\frac{m}{2\pi i\hbar}\frac{1}{\sqrt{2\epsilon\cdot\epsilon}}\int dx_2 \exp\left(\frac{im}{2\hbar(2\epsilon)}(x_2-x_0)^2+\frac{im}{2\hbar\epsilon}(x_3-x_2)^2\right)$$

$$= \sqrt{\frac{m}{2\pi i\hbar(3\epsilon)}}\exp\left(\frac{im}{2\hbar(3\epsilon)}(x_3-x_0)^2\right)$$

exercise

after $N-1$ steps,

$$K(x,t;x',0) = \lim_{N\to\infty}\sqrt{\frac{m}{2\pi i\hbar\underbrace{(N\epsilon)}_{t}}}\exp\left(\frac{im}{2\hbar\underbrace{(N\epsilon)}_{t}}(x-x')^2\right) : (202.1)!$$

Ex. 2 : Quadratic Lagrangian

idea : determine the propagator (204.1) for a system described by the Lagrangian

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

initial : Euler-Lagrange equation

$$\left(\frac{\partial L}{\partial x}\right) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = 0$$

$$\xrightarrow[\text{exercise}]{} m\ddot{x} + (\dot{b}+c)x + e = 0 \quad \oplus \quad \text{boundary conditions: } x(0)=x', \; x(t)=x$$

solution : $x = x_c(t')$ (208.1)

$\hookrightarrow$ classical !

change of variables:

$$y(t') \equiv x(t') - x_c(t')$$

since $x(0) = x_c(0) = x'$ and $x(t) = x_c(t) = x \;\to\; y(0) = y(t) = 0$ (*)

$$S = \int_0^t dt'\, L \longrightarrow \int_0^t dt' \left[\frac{1}{2} m (\dot{y} + \dot{x}_c)^2 + b(y + x_c)(\dot{y} + \dot{x}_c) - \frac{1}{2} c (y + x_c)^2 - e(y + x_c)^2 \right]$$

$$= S[x_c] + S[y] + \underbrace{\underbrace{\int_0^t dt'\, \dot{y}(m\dot{x}_c + b x_c)}_{\underbrace{y(m\dot{x}_c + b x_c)\Big|_{t'=0}^{t'=t}}_{=0,\ (*)} - \int_0^t dt'\, y(m\ddot{x}_c + b\dot{x}_c + \dot{b} x_c)} + y(b\dot{x}_c - c x_c)}_{\int_0^t dt'\, e y \;:\; \text{using } (208.1)}$$

$$= S[x_c] + \int_0^t dt'\, \frac{1}{2} m \dot{y}^2 - \frac{1}{2} \bar{c}(t') y^2 \quad ; \quad \bar{c}(t) = c + \dot{b}$$

obs.: in the last step, we use the fact that

$$\int dt'\, b y \dot{y} = -\frac{1}{2} \int dt'\, \dot{b} y^2 .$$

Thus,

$$K(x,t\,;\,x',0) = \int_{x(0)=x'}^{x(t)=x} \mathcal{D}x \; e^{iS[x]/\hbar}$$

$$= \underbrace{\int_{y(0)=0}^{y(t)=0} \mathcal{D}y \; \exp\left(\frac{i}{\hbar} \int_0^t dt' \; \frac{1}{2} m \dot{y}^2 - \frac{1}{2} \bar{c}\, y^2 \right)}_{\equiv G(t)} * e^{iS_c/\hbar} \qquad (210.1)$$

where

$$S_c = S[x_c]$$

Obs.: about the limits of the integral, see (*) on pg. 209.

. Next step: evaluate $G(t)$.

Let's consider the discrete form, similar to (206.1),

$$G(t) = \lim_{N\to\infty} \int_{-\infty}^{+\infty} dy_1\, dy_2 \ldots dy_{N-1} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{N/2} *$$

$$* \exp\left(\frac{i}{\hbar} \sum_{k=1}^{N} \frac{m}{2} \frac{(y_k - y_{k-1})^2}{\epsilon} - \frac{1}{2} \epsilon\, \bar{c}_{k-1}\, y_{k-1}^2 \right)$$

with $\bar{c}_k \equiv c(t_k)$

Defining,

$$\eta = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \end{pmatrix}$$

and the matrix,

$$\hat{\sigma} = \frac{m}{2i\hbar\epsilon}\begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \vdots & & \ddots & & & \vdots \\ & & & & 2 & -1 \\ 0 & & \cdots & & -1 & 2 \end{pmatrix} + \frac{i\epsilon}{2\hbar}\begin{pmatrix} \bar{c}_1 & 0 & 0 & \cdots & & 0 \\ 0 & \bar{c}_2 & 0 & & & \vdots \\ \vdots & & \ddots & & & \\ & & & & \bar{c}_{N-2} & 0 \\ 0 & & \cdots & & 0 & \bar{c}_{N-1} \end{pmatrix}$$

$\hookrightarrow$ $$G(t) = \lim_{N\to+\infty}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\int d\eta^{N-1}\, e^{-\eta^t\hat{\sigma}\eta}$$

σ can be diagonalized via an unitary transformation U,

$$\hat{\sigma} = U^+\hat{\sigma}_D U \quad ; \quad U^+U = 1$$

if $\zeta = U\eta$, we have

$$\int d\eta^{N-1}\, e^{-\eta^t\hat{\sigma}\eta} = \int d\zeta^{N-1}\, e^{-\zeta^t\hat{\sigma}_D\zeta} = \prod_{\alpha=1}^{N-1}\int d\zeta_\alpha\, e^{-\zeta_\alpha\sigma_{D,\alpha\alpha}\zeta_\alpha}$$

$$= \prod_{\alpha=1}^{N-1}\sqrt{\frac{\pi}{\sigma_{D,\alpha\alpha}}} = \frac{\pi^{N-1/2}}{\sqrt{\det\hat{\sigma}}}$$

condition: $\det\sigma \neq 0$!

$\hookrightarrow$ $$G(t) = \lim_{\substack{N\to\infty \\ (\epsilon\to 0)}}\left(\frac{m}{2\pi i\hbar f(t)}\right)^{1/2}$$

where

$$f(t) = \lim_{\substack{N\to\infty \\ (\epsilon\to 0)}}\epsilon\left(\frac{2i\hbar\epsilon}{m}\right)^{N-1}\det\hat{\sigma}.$$

It's possible to show (see below) that $f(t)$ is a solution of

$$\frac{d^2 f}{dt^2} + \frac{\bar{c}(t)}{m} f = 0 \qquad (212.1)$$

⊕ initial conditions : $f(0) = 0$ and $\dot{f}(0) = 1$

Thus,

$$K(x,t;x',0) = \sqrt{\frac{m}{2\pi i \hbar f(t)}}\; e^{+iS_c/\hbar} \qquad (212.2)$$

Ex. : 1-D harmonic oscillator.

$\bar{c}(t) = c = m\omega^2$

in (212.1) : $\ddot{f} + \omega^2 f = 0 \;\; \rightarrow \;\; f(t) = \frac{1}{\omega} \sin \omega t$: compare with Eq. (202.3)

Exercises:

(a) Derive the propagator for a free particle (1-D) from (212.2).

(b) Calculate S_c for the harmonic oscillator.

(c) Calculate the propagator for a forced harmonic oscillator.

$$L = \frac{1}{2} m \dot{x}^2 - \frac{m\omega^2}{2} x^2 - e(t)\, x \,.$$

· About eq. (212.1),

$$\epsilon \left(\frac{2i\hbar\epsilon}{m}\right)^{N-1} \det \hat{\sigma} \equiv \det \tilde{\sigma}_{N-1} \equiv p_{N-1}$$

where

$$\tilde{\sigma}_{N-1} = \begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \vdots & & & & & \vdots \\ & & & & 2 & -1 \\ 0 & \cdots & & & -1 & 2 \end{pmatrix} - \frac{\epsilon^2}{M} \begin{pmatrix} \vec{c}_1 & \cdots & & 0 \\ & \vec{c}_2 & & \vdots \\ & & \ddots & \\ 0 & \cdots & & \vec{c}_{N-1} \end{pmatrix}$$

using the expansion of $\tilde{\sigma}_{N-1}$ in first minors, we can show that

$$p_{j+1} = \left(2 - \frac{\epsilon^2}{M}\vec{c}_{j+1}\right) p_j - p_{j-1} \quad ; \quad j = 1, 2, \ldots, N-2$$

$$p_1 = 2 - \frac{\epsilon^2 \bar{c}_1}{M} \quad , \text{ and } \quad p_0 = 1$$

or

$$\frac{1}{\epsilon^2}\left(p_{j+1} - 2p_j + p_{j-1}\right) = -\frac{1}{M}\bar{c}_{j+1} p_j$$

$$\xrightarrow[\epsilon \to 0]{} \qquad \frac{d^2\varphi(t)}{dt^2} = -\frac{1}{M}\bar{c}(t)\varphi(t) \qquad (212.3)$$

with $\varphi(t) \equiv \epsilon p_j \; ; \; t = \epsilon j$

⊕ initial conditions:

$$\varphi(0) = \epsilon p_0 \xrightarrow[\epsilon \to 0]{} 0$$

$$\left.\frac{d\varphi(t)}{dt}\right|_{t=0} = \epsilon\left(\frac{p_1 - p_0}{\epsilon}\right) = 2 - \frac{\epsilon^2 c_1}{M} - 1 \xrightarrow[\epsilon \to 0]{} 1$$

note: $f(t) = \lim\limits_{\epsilon \to 0} \epsilon p_j = \varphi(t) \longrightarrow (212.3) \longrightarrow (212.2)$

2. Imaginary - time path integrals.

Let's consider the imaginary - time propagator

$$K(x, \tau ; x', 0) = \langle x | e^{-H\tau/\hbar} | x' \rangle \qquad (213.1)$$

note : (213.1) is equal to (201.2) with

$$t = -i\tau$$

Following the same procedure used to study the real time propagator [Eqs. (204.1) - (206.2)], it's possible to show that

$$K(x, \tau ; x', 0) = \int_{x(0) = x'}^{x(\tau) = x} \mathcal{D}x \; e^{-S_E[x]/\hbar} \qquad (213.2)$$

where

$$S_E = \int_0^\tau d\tau' \, L_E(\dot{x}, x, \tau) = \int_0^\tau d\tau' \left(\frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2 + V(x) \right) \; : \text{ Euclidean action}$$

$$\int_{x(0) = x'}^{x(\tau) = x} \mathcal{D}x = \lim_{N \to +\infty} \left[\prod_{k=1}^{N} \frac{m}{2\pi\hbar\epsilon} \right] \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_{N-1}$$

$$\epsilon = \frac{\tau}{N}$$

$$L_E = L_E(\dot{x}, x, \tau) \; : \text{ Euclidean action}$$

Recall :

$x^2 - c^2 t^2$: invariant in Minkowski space

$\xrightarrow[t=-i\tau]{}$ $x^2 + c^2\tau^2$: invariant in Euclidean space.

Exercises :

(a) Calculate the Euler-Lagrange equation for L_E and show that it corresponds to a particle moving in the potential $-V(x)$.

(b) Show that

$$iS \xrightarrow[t=-i\tau]{} -S_E$$

We can proceed as before and determine the propagator (213.2) for a free particle. We have

$$K(x,\tau;x',0) = \sqrt{\frac{m}{2\pi\hbar\tau}} \exp\left(-\frac{m(x-x')^2}{2\hbar\tau}\right) \qquad (214.1)$$

note : we can derive (202.1) by setting $\tau = it$ in (214.1).

This procedure is called <u>analytic</u> <u>continuation</u> !

Obs. : the imaginary-time propagator (213.1) is not an unitary operator but a Hermitian one.

↳ norm is not preserved in time.

$$K(x,\tau;x',0) = \sum_n \langle x|n\rangle\langle n|x'\rangle\, e^{-E_n\tau/\hbar}$$

$$\xrightarrow[\tau\to+\infty]{} \simeq \underbrace{\langle x|0\rangle\langle 0|x'\rangle}_{\text{ground state !}}\, e^{-E_0\tau/\hbar} = \psi_0^*(x')\psi_0(x)\, e^{-E_0\tau/\hbar}$$

2.1. Relation with quantum statistical mechanics.

Consider the partition function

$$Z = \sum_n e^{-\beta E_n}$$

where $\beta = 1/K_B T$; K_B : Boltzmann's cte

If $H|n\rangle = E_n|n\rangle$, we can write

$$Z = \mathrm{Tr}\, e^{-\beta H}$$

Considering the $\{|x\rangle\}$ basis,

$$Z = \int_{-\infty}^{+\infty} dx \langle x|e^{-\beta H}|x\rangle \underset{\text{Eq. (213.1)}}{=} \int_{-\infty}^{+\infty} dx\, K(x,\beta\hbar;x,0) \qquad (215.1)$$

Recall that the non-normalized density op. of a system in thermodynamic equilibrium is given by [Eq. (77.1)]

$$\hat{\rho} = e^{-\beta H}$$

if

$$\rho(x, x', \beta\hbar) = \langle x | e^{-\beta H} | x' \rangle, \qquad (\tau = \beta\hbar)$$

we can write a path integral representation for the density operator, i.e.,

$$\rho(x, x', \beta\hbar) = \int_{x(0)=x'}^{x(\beta\hbar)=x} \mathcal{D}x \quad \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \ \tfrac{1}{2}m\dot{x}^2 + V(x)\right) \qquad (216.1)$$

Thus, the partition function reads

$$Z = \int_{-\infty}^{+\infty} dx \ \rho(x, x, \beta\hbar)$$

$$= \int_{-\infty}^{+\infty} dx \int_{x(0)=x}^{x(\beta\hbar)=x} \mathcal{D}x \ \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \ \tfrac{1}{2}m\dot{x}^2 + V(x)\right) \qquad (216.2)$$

Exercise:

(a) Calculate $\rho(x, x', \beta\hbar)$ for the 1-D harmonic oscillator.

(b) Show that the free energy is given by

$$F = k_B T \ln\left(2\sinh\frac{\hbar\omega}{2k_BT}\right)$$

Recall: $Z = e^{-\beta F}$

3. Stationary phase approximation
(semiclassical approximation)

Consider a system such that

$$S[q] = \int_0^t dt' \, L(\dot{q}, q, t')$$

In the limit $\hbar \to 0$, the integrand of (206.2) oscillates very rapidly $\longrightarrow$ the most important contribution =
= stationary paths (classical path).

It's possible to show that, in this limit,

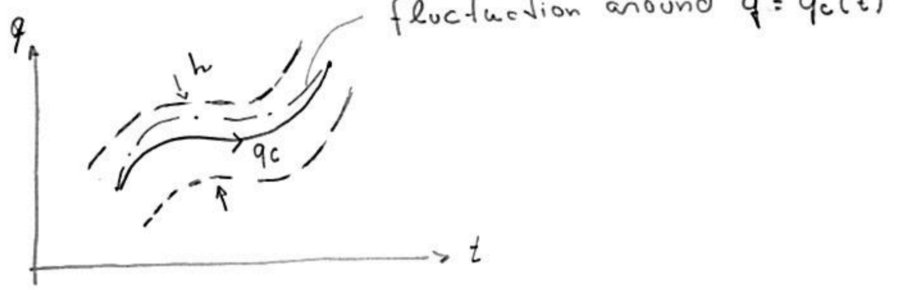
$$K(x,t\,;\,x',0) \simeq F(t)\, e^{-iS_c/\hbar} \qquad (217.1)$$

where

$$S_c = S[q_c]$$

i.e. the main contribution to the propagator is the classical path around $q = q_c(t)$)
$\oplus$ quantum fluctuations (associated with paths
which are encoded in $F(t)$.

idea :



· Let's define

$$\eta(t') \equiv q(t') - q_c(t')$$

Since $q(0) = q_c(0)$ and $q(t) = q_c(t)$ $\rightarrow$ $\eta(0) = \eta(t) = 0$

· Expanding the action around $q_c(t')$ up to second order in η.

$$S[q] \simeq \left[S[q_c] + \int_0^t dt' \, \delta q(t') \frac{\delta S}{\delta q(t')}\bigg|_{q_c} + \frac{1}{2}\int_0^t dt' \, dt'' \, \delta q(t') \, \delta q(t'') \frac{\delta^2 S}{\delta q(t') \, \delta q(t'')}\bigg|_{q_c} + \ldots \right] \qquad (218.1)$$

$$\simeq S[q_c] + \delta S + \delta^2 S + \ldots$$

· Note that (1) = 0.

$$\delta S = \int_0^t dt' \; \frac{\partial L}{\partial q}\bigg|_{q_c} \eta(t') + \frac{\partial L}{\partial \dot q}\bigg|_{q_c} \dot\eta(t')$$

$$= \underbrace{\frac{\partial L}{\partial \dot q} \, \eta(t') \bigg|_{t'=0}^{t'=t}}_{=0,\ \text{since } \eta(0) = \eta(t) = 0} + \int_0^t dt' \underbrace{\left[\frac{\partial L}{\partial q}\bigg|_{q_c} - \frac{d}{dt'}\left(\frac{\partial L}{\partial \dot q}\bigg|_{q_c} \right) \right]}_{=0,\ \text{because } q = q_c(t') \text{ is a solution of the Euler-Lagrange equation.}} \eta(t') = 0$$

integrating by parts.

. About (II),

~~Since the action S is instantaneous~~ $\cancel{\Rightarrow \frac{\delta^2 S}{\delta q(t')\,\delta q(t'')} \propto \delta(t'-t'')}$

we have

$$\delta^2 S = \frac{1}{2!}\int_0^t dt' \left[\left.\frac{\partial^2 L}{\partial q^2}\right|_{q_c} \eta(t')\,\eta(t') + 2\left.\frac{\partial^2 L}{\partial q\,\partial \dot q}\right|_{q_c} \eta(t')\,\dot\eta(t') \right.$$

$$\left. + \left.\frac{\partial^2 L}{\partial \dot q^2}\right|_{q_c} \dot\eta(t')\,\dot\eta(t') \right]$$

integrating by parts (exercise),

$$\delta^2 S = \frac{1}{2!}\int_0^t dt' \;\eta(t') \left[\left.\frac{\partial^2 L}{\partial q^2}\right|_{q_c} - \frac{d}{dt'}\left(\left.\frac{\partial^2 L}{\partial q\,\partial \dot q}\right|_{q_c} \right) - \right.$$

$$\left. - \frac{d}{dt'}\left(\left.\frac{\partial^2 L}{\partial \dot q^2}\right|_{q_c} \frac{d}{dt'} \right) \right] \delta\eta(t') \qquad (219.1)$$

[~~note that the integrand in (219.1) defines an eigenvalue/eigenvector problem:~~

$$\cancel{[\quad]\,\delta q(t') = \lambda\,\delta q(t')}$$

] Later

In particular, if

$$L = \frac{1}{2} m \dot q^2 - V(q)$$

we have (exercise)

$$-m\frac{d^2}{dt'^2}\delta q(t') - V''(q_c)\,\delta q(t') = \lambda\,\delta q(t') \qquad (220.1)$$

~~note that (220.1) is a Schrödinger-like equation of a fictitious particle under a potential $-V''(q_c)$. $\delta q(t')$ is a "wave function" with boundary conditions:~~ Later

$$\delta q(0) = \delta q(t) = 0$$

↳ The propagator then needs

$$K(x,t;x',0) \simeq e^{iS_c/\hbar}\int_{\eta(0)=0}^{\eta(t)=0}\mathcal{D}\eta \;\; *$$

$$* \exp\Bigg(\underbrace{\frac{-i}{2\hbar}\int_0^t dt'\,\eta(t')\left(m\frac{d^2}{dt'^2} + V''(q_c)\right)\eta(t')}_{\frac{i}{2\hbar}\int_0^t dt'\, m\dot{\eta}^2 - V''(q_c)\,\eta^2}\Bigg)$$

using Eq. (212.2)

$$\simeq \sqrt{\frac{m}{2\pi i\hbar f(t)}}\; e^{iS_c/\hbar} = G(t)\,e^{iS_c/\hbar}$$

with $m\dfrac{d^2 f}{dt^2} + V''(q_c)\,f = 0$; $f(0) = 0$ and $\dot{f}(0) = 1$

Obs.: In sec 4, we consider a different method to evaluate $\delta^2 S$!

It's possible to show that (see cap. 13, Schulman)

$$G(t) = \sqrt{\frac{i}{2\pi\hbar} \frac{\partial^2 S_c(x,x',t)}{\partial x \partial x'}} ,$$

which can be generalized to d dimensions

$$G(t) = \left[\det \left(\frac{i}{2\pi\hbar} \frac{\partial^2 S_c(\vec{x},\vec{x}',t)}{\partial x_i \partial x'_j} \right) \right]^{1/2}$$

. References:

. Lecture notes based on:

A. O. Caldeira, an introduction to macroscopic quantum phenomena and quantum dissipation.

- Introduction and aplications:

A. Altland and B. Simons, Condensed matter field theory.

4.- Euclidean functional integrals,

Ref. : - Appendix D, A.O. Caldeira

- Aspects of symmetry, S. Coleman (see Chap. 7)

Consider : particle mass $\underline{\underline{m}}$ in 1-D.

Hamiltonian :

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

idea : Derive well-known results via a rather awkward method and get familiar with it.
This method is useful in quantum field theory.

Our fundamental tool is the imaginary-time path integral representation for the density operator, Eq. (216.1),

$$\rho(x_f, x_i, \hbar\beta) = \langle x_f | e^{-\beta H} | x_i \rangle = \int_{q(0)=x_i}^{q(\hbar\beta)=x_f} \mathcal{D}q \; e^{-S_E[q]/\hbar} , \qquad (221.1)$$

where

$$S_E[q] = \int_0^{\hbar\beta} d\tau \underbrace{\frac{1}{2} m\dot{q}^2 + V(q)}_{L_E(q,\dot{q})} \quad : \text{Euclidean action} \qquad (221.2)$$

and $\dot{q} = \partial q / \partial \tau$

note : L_E corresponds to the Lagrangian of a particle mass $\underline{\underline{m}}$ under potential $-V(q)$!

inserting,

$$1 = \sum_n |\psi_n\rangle\langle\psi_n|,$$

where $H|\psi_n\rangle = E_n|\psi_n\rangle$, in the L.H.S. of (221.1), we have

$$\rho(x_f, x_i, \hbar\beta) = \sum_n e^{-\beta E_n} \underbrace{\langle x_f|\psi_n\rangle\langle\psi_n|x_i\rangle}_{\psi_n^*(x_i)\,\psi_n(x_f)} \xrightarrow[\substack{\beta \to \infty \\ (T\to 0)}]{} \psi_0^*(x_i)\,\psi_0(x_f)\,e^{-\beta E_0},$$

(221.2.a)

i.e., $$\lim_{\beta \to +\infty} \int_{q(0)=x_i}^{q(\hbar\beta)=x_f} \mathcal{D}q \, e^{-S_E[q]/\hbar} \longrightarrow$$ energy and wave function of the ground state of the system!

Since the evaluation of (221.1) is nontrivial, it's necessary to consider approximated schemes. We employ the stationary phase approximation (SPA).

- Let's recall the SPA and apply it to the Euclidean formalism,

Within the SPA, we have

$$S_E[q] \simeq S_E[q_c] + \delta^2 S,$$

where $q_c = q_c(\tau)$ is the solution of

$$\delta S_E = 0 \;\rightarrow\; -m\ddot{q}_c + V'(q_c) = 0 \qquad (221.3)$$

with boundary conditions: $q_c(0) = x_i$

$q_c(\hbar\beta) = x_f$

It's possible to show that [see Eq. (219.1)]

$$\delta^2 S = \frac{1}{2!}\int_0^{\hbar\beta} d\tau\, \eta(\tau) \underbrace{\left[\frac{\partial^2 L_E}{\partial^2 q}\bigg|_{q_c} - \frac{d}{d\tau}\left(\frac{\partial^2 L_E}{\partial q\,\partial \dot q}\bigg|_{q_c}\right) - \frac{d}{d\tau}\left(\frac{\partial^2 L_E}{\partial^2 \dot q}\bigg|_{q_c}\frac{d}{d\tau}\right)\right]}_{(*)} \eta(\tau), \tag{221.4}$$

where $\eta(\tau) = q(\tau) - q_c(\tau)$

note : the boundary conditions for $q_c(\tau) \to \eta(0) = \eta(\hbar\beta) = 0$.

If $\quad L_E = \frac{1}{2} m \dot q^2 + V(q)$

$$\xrightarrow[\text{exercise}]{} \quad (*) = -m\frac{d^2}{d\tau^2} + V''(q_c).$$

In order to evaluate $\delta^2 S$, we consider a method $\neq$ from the one employed in pg. 220.

- Let's consider the eigenvalue problem defined by $(*)$:

$$\left[-m\frac{d^2}{d\tau^2} + V''(q_c)\right] q_n(\tau) = \lambda_n q_n(\tau) \tag{221.5}$$

with the boundary conditions $q_n(0) = q_n(\hbar\beta) = 0$.

Since $\{q_n(\tau)\}$ is an orthonormal set,

$$\int_0^{\hbar\beta} d\tau\, q_n(\tau)\, q_m(\tau) = \delta_{nm},$$

we can write

$$\eta(\tau) = \sum_{n=0}^{\infty} c_n q_n(\tau). \qquad (221.6)$$

Note : $\eta(0) = \eta(\hbar\beta) = 0$ since $q_n(0) = q_n(\hbar\beta) = 0$.

(221.6) in (221.4),

$$\delta^2 S = \frac{1}{2}\sum_{nm}\int_0^{\hbar\beta} d\tau \, c_n c_m \, q_n(\tau)\underbrace{\left[-m\partial_\tau^2 + V''(q_c)\right] q_m(\tau)}_{\lambda_m q_m(\tau)}$$

$$= \frac{1}{2}\sum_{n=0}^{\infty}\lambda_n c_n^2 .$$

↳ Eq. (221.1) :

$$\rho(x_f, x_i, \hbar\beta) \approx e^{-S_E[q_c]/\hbar} \underbrace{\int \frac{\mathcal{J}}{\mathcal{N}} \, dc_0 \, dc_1 \ldots dc_n \ldots \exp\left(-\frac{1}{2\hbar}\sum_n \lambda_n c_n^2\right)}_{\frac{\mathcal{J}}{\mathcal{N}}\prod_{n=0}^{\infty} \underbrace{\int dc_n \exp\left(-\frac{\lambda_n}{2\hbar}c_n^2\right)}_{\sqrt{\frac{2\pi\hbar}{\lambda_n}}}}$$

where : $\mathcal{N}$: normalization cte [see Eq. (206.1)],

$\mathcal{J}$: Jacobian of the transformation $\prod dq \rightarrow \prod dc_n$.

note : the functional integral in (221.1) is reduced to a product of discrete (Gaussian) integrals !

we write

$$\frac{1}{N}\prod_{n=0}^{\infty}\sqrt{\frac{2\pi\hbar}{\lambda_n}} = \underbrace{\left[\frac{1}{N}\prod_n (2\pi\hbar)^{1/2}\right]}_{\equiv \frac{1}{N_R}} \frac{1}{\sqrt{\prod_n \lambda_n}}$$

notation: $\prod_n \lambda_n = \det\left(-m\partial_\tau^2 + V''(q_c)\right)$

$$\hookrightarrow \rho(x_f, x_i, \hbar\beta) \approx \frac{1}{N_R}\left[\det\left(-m\partial_\tau^2 + V''(q_c)\right)\right]^{-1/2} e^{-S_E[q_c]/\hbar} \qquad (221.7)$$

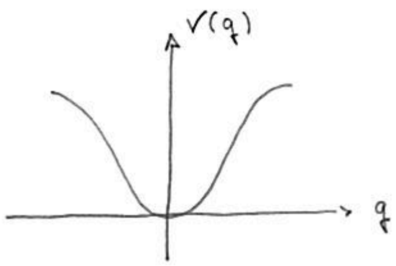
Eq. (221.7): "density op" with the SPA!

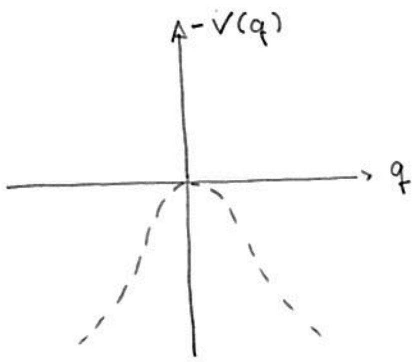
Obs.: the equation of motion (221.3) corresponds to the Euclidean energy

$$E = \frac{1}{2}m\dot{q}_c^2 - V(q_c), \qquad (221.8)$$

which is a cte of motion.

Ex. 1: particle (1-D) under $V(q)$:





Assumption: $x_i = x_f = 0$.

"potential within Euclidean formalism".

- Let's determine the "density op" within SPA, Eq. (221.1)

2 steps:

(1) Solution eq. of motion (221.3) with the boundary conditions $q_c(0) = q_c(\hbar\beta) = 0$:

$$q_c(\tau) = 0$$

$\hookrightarrow$ $S_E[q_c] = 0$.

(2) Pre-factor. It's possible to show that (see pg. 221.12) in the limit $\hbar\beta \to +\infty$,

$$\frac{1}{N_R}\left[\det\left(-m\partial_\tau^2 + V''(q_c)\right)\right]^{-1/2} \approx \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\hbar\omega\beta/2},$$

where $V''(q_c) = V''(0) \equiv m\omega^2$.

$\hookrightarrow$ Eqs. (221.2.a) and (221.7):

$$\rho(0,0,\hbar\beta) \approx |\psi_0(0)|^2 e^{-\beta E_0} \approx \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\hbar\omega\beta/2}$$

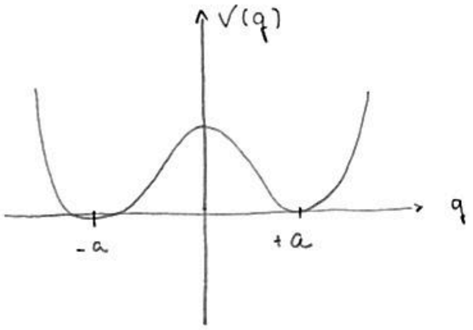
$\hookrightarrow$ $E_0 = \frac{1}{2}\hbar\omega$: ground state energy

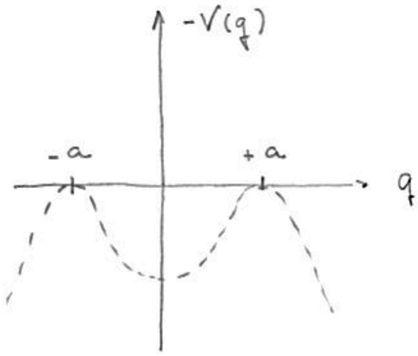
$|\psi_0(0)|^2 = |\langle x=0|n=0\rangle|^2 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}$: harmonic oscillator results!

As expected since the SPA corresponds to a harmonic approximation for $V(q)$!

Ex. 2 : Double well and instantons.

Consider particle under the potential





. $\pm a$: minima $V(q)$

. definition : $V''(\pm a) \equiv m\omega^2$

. idea : calculate the matrix elements

$$\langle -a| e^{-\beta H} |-a\rangle = \langle a| e^{-\beta H} |a\rangle,$$

$$\langle a| e^{-\beta H} |-a\rangle = \langle -a| e^{-\beta H} |a\rangle$$

using Eq. (221.7).

Obs. : Instead of $[0, \hbar\beta]$, we consider the time interval $[-\hbar\beta, +\hbar\beta]$.

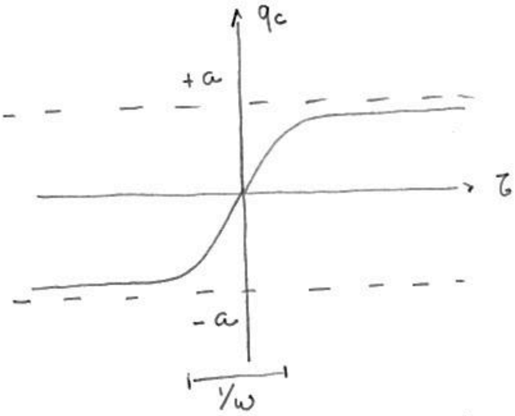
Again : we are interested in the limit $\beta \to +\infty$.

First step : solution eq. of motion (221.3) consistent with boundary conditions.

3 solutions : (1) : $q_c(\tau) = +a$ ~ boundary conditions $q_c(-\frac{\hbar\beta}{2}) = q_c(+\frac{\hbar\beta}{2}) = +a$

(2) : $q_c(\tau) = -a$ ~ " $q_c(-\frac{\hbar\beta}{2}) = q_c(+\frac{\hbar\beta}{2}) = -$

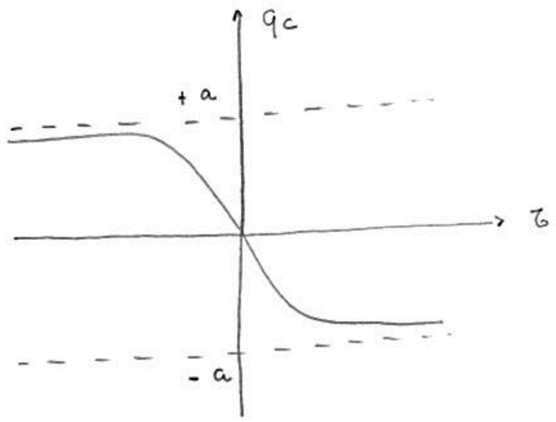
(3) : instanton/ anti-instanton (see figure) " $q_c(-\frac{\hbar\beta}{2}) = \mp\, q_c(+\frac{\hbar\beta}{2}) = \mp a$



: such a solution is called an <u>instanton</u>

note : - particle rests a long time at $q = -a$, it quickly moves to $q = +a$, where it rests.

. consistent with boundary conditions $q_c(-\hbar\beta/2) = -a$,
$q_c(+\hbar\beta/2) = +a$.



: <u>anti</u> - <u>instanton</u>.

. characteristic instanton solution:

(1) solution with Euclidean energy $E = 0$.

Since the Euclidean energy is a cte of motion,

Eq. (221.8) limit $\beta \to +\infty$:

$$\left.\begin{array}{l} q_c(-\hbar\beta/2) \to -a \to \dot{q}_c = 0 \\ V(q_c) = V(-a) = 0 \end{array}\right\} \to E = 0.$$

(2) localized objects in time.

limit $\beta \to +\infty$: $q_c(+\hbar\beta/2) \simeq +a$

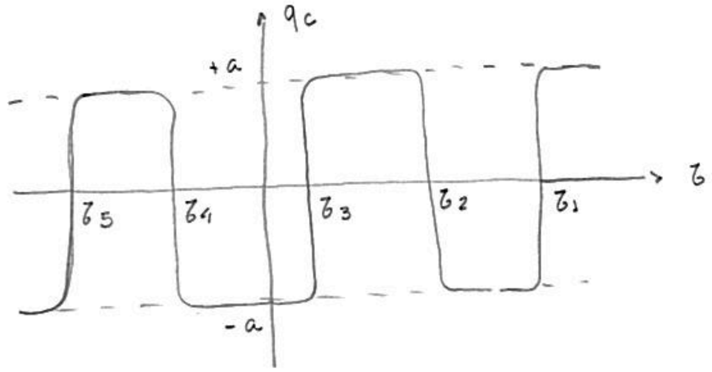
$V(q) \simeq \frac{1}{2} m (q-a)^2 \omega^2$: consistent with $V''(q_c) = m\omega^2$!

Eq. (221.8) : $E = 0 = \frac{1}{2} m \dot{q}^2 - \frac{1}{2} m (q-a)^2 \omega^2$

↳ $\dot{q} \simeq m\omega (q-a) \to (q(\tau) - a) \simeq e^{-\omega\tau}$

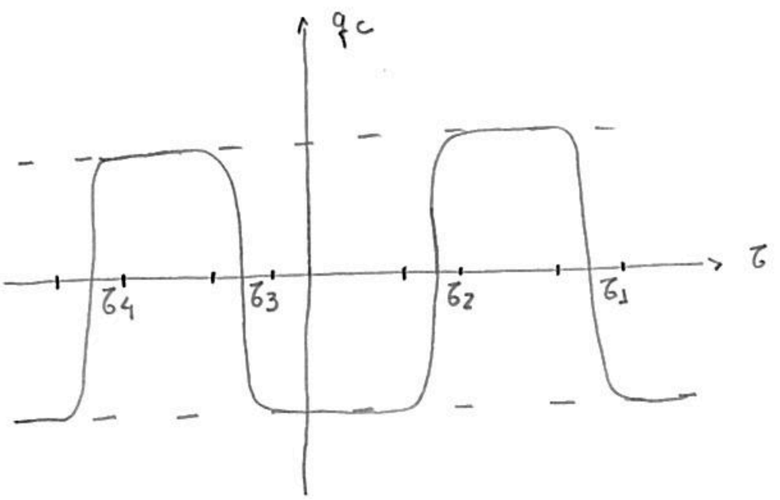
↳ "size of the instanton" ~ $1/\omega$!

. Since an instanton is a well-localized object, we should also consider the solutions to the eq. of motion (221.3) :



: N (odd) instantons/anti-instantons centered at $\tau_1, \tau_2, \ldots \tau_N$.

(consistent with boundary conditions $q_c(-\hbar\beta/2) = \mp q_c(+\frac{\hbar\beta}{2}) = \mp a$.)



: N (even) instantons/anti-instantons centered at $\tau_1, \tau_2, \ldots, \tau_N$.

(consistent with boundary conditions $q_c(-\hbar\beta/2) = q_c(+\hbar\beta/2) = -a$.)

· Evaluation (221.7), 3 steps:

(1) (221.8) with $E = 0 \rightarrow \frac{1}{2} m \dot{q}_c^2 = V(q_c)$

↳ $S_E[q_c] = \int_{-\infty}^{+\infty} d\tau \; \frac{1}{2} m \dot{q}_c^2 + V(q_c) = \int_{-\infty}^{+\infty} d\tau \; m \dot{q}_c^2 \equiv S_0$: action for a instanton

lim $\beta \rightarrow +\infty$

↳ for N "noninteracting objects": $S_E[q_c] = N S_0$

"Dilute instanton gas approximation"

(2) about the prefactor.

recall : instantons are well-localized objects

↳ apart from the small time intervals τ_i

around τ_i (see fig. pg. 221.8) we have $q_c = \pm a \;\; \forall \tau$!

↳ harmonic approximation should be valid (previous example)

$$↳ \frac{1}{N_R} \left[\det\left(-m \partial_\tau^2 + V''(q_c)\right) \right]^{-1/2} \approx \left(\frac{m\omega}{\pi \hbar} \right)^{1/2} e^{-\hbar\omega\beta/2}$$

$$= K^N \left(\frac{m\omega}{\pi \hbar} \right)^{1/2} e^{-\hbar\omega\beta/2}$$

cte K, to be calculated latter.

Requirement: it should provide the right answer for one instanton.

(3) From figs on pg. 221.8, we have

$$-\frac{\hbar\beta}{2} < \tau_N < \tau_{N-1} < \dots < \tau_2 < \tau_1 < +\frac{\hbar\beta}{2}.$$

Since there is no restriction about the position of the centre of the instanton, we should integrate over τ_i:

$$\lim_{\beta\to+\infty} \int_{-\hbar\beta/2}^{+\hbar\beta/2} d\tau_1 \int_{-\hbar\beta/2}^{\tau_1} d\tau_2 \dots \int_{-\hbar\beta/2}^{\tau_{N-1}} d\tau_N = \lim_{\beta\to+\infty} \frac{(\hbar\beta)^N}{N!}$$

Thus, Eq. (221.7):

$$\cdot\ \rho(a,a,\hbar\beta) = \sum_{N\ \text{even}} \int_{-\hbar\beta/2}^{+\hbar\beta/2} d\tau_1 \dots \int_{-\hbar\beta/2}^{\tau_{N-1}} d\tau \ \underbrace{K^N \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\hbar\omega\beta/2}}_{\text{pre factor}} e^{-NS_0/\hbar}$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\hbar\omega\beta/2} \sum_{N\ \text{even}} \frac{1}{N!} \left(K\hbar\beta\, e^{-S_0/\hbar}\right)^N$$

$$= \rho(-a,-a,\hbar\beta)$$

Similarly

$$\cdot\ \rho(-a,+a,\hbar\beta) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\hbar\omega\beta/2} \sum_{N\ \text{odd}} \frac{1}{N!} \left(K\hbar\beta\, e^{-S_0/\hbar}\right)^N$$

$$= \rho(+a,-a,\hbar\beta)$$

$$\hookrightarrow \quad \rho(a,a,\hbar\beta) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\hbar\omega\beta/2}\ \frac{1}{2}\left(\exp\left(\kappa\hbar\beta e^{-S_0/\hbar}\right) + \exp\left(-\kappa\hbar\beta e^{-S_0/\hbar}\right)\right)$$

$$\rho(-a,a,\hbar\beta) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\hbar\omega\beta/2}\ \frac{1}{2}\left(\exp\left(\kappa\hbar\beta e^{-S_0/\hbar}\right) - \exp\left(-\kappa\hbar\beta e^{-S_0/\hbar}\right)\right)$$

(221.9)

Reccle eq. (221.2.a), ($\lim \beta \to +\infty$)

$$\rho(a,a,\hbar\beta) \simeq \underbrace{\langle a|S\rangle\langle S|a\rangle}_{|\psi_S(a)|^2} e^{-\beta E_S} + \underbrace{\langle a|A\rangle\langle A|a\rangle}_{|\psi_A(a)|^2} e^{-\beta E_A}$$

$$\rho(-a,a,\hbar\beta) \simeq \underbrace{\langle -a|S\rangle\langle S|a\rangle}_{\psi_S(-a)\,\psi_S^*(a)} e^{-\beta E_S} + \underbrace{\langle -a|A\rangle\langle A|a\rangle}_{\psi_A(-a)\,\psi_A^*(a)} e^{-\beta E_A} \qquad (221.10)$$

where:

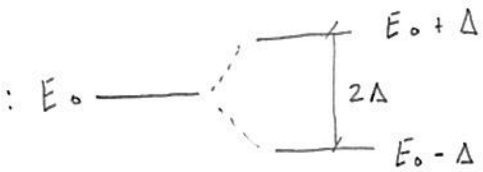
$|S\rangle$: ground state (symmetric state)

$|A\rangle$: first excited state (antisymmetric state)

Comparing Eqs. (221.9) and (221.10): Energy g.s. h.o.

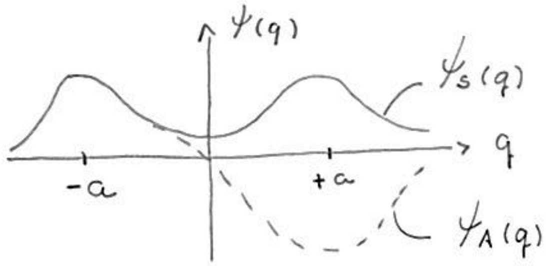
$$E_S = \frac{1}{2}\hbar\omega - \hbar\kappa e^{-S_0/\hbar} \equiv E_0 - \Delta$$

$$E_A = \frac{1}{2}\hbar\omega + \hbar\kappa e^{-S_0/\hbar} \equiv E_0 + \Delta$$



$$|\psi_S(a)|^2 = |\psi_A(a)|^2 = \psi_S(-a)\,\psi_S^*(a) = -\psi_A(-a)\,\psi_A(a) = \frac{1}{2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}$$

$\hookrightarrow$



· About the prefactor on pg. 221.6,

since $V''(q_c) = V''(0) = m\omega^2$

$\hookrightarrow \det(-m\partial_\tau^2 + m\omega^2) \sim$ harmonic oscilator.

Eq. (202.3) with $t = -i\tau = -i\hbar\beta$,

$$\rho(0,0,\hbar\beta) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\hbar\beta)}}$$

$$\xrightarrow[\beta\to+\infty]{} \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\hbar\omega\beta/2} .$$

Obs.:

1. For a $\neq$ procedure, see Appendix I, chap. 7, Coleman.

2. About the cte K (pg. 221.9), see chap. 7, Coleman.

Obs.: The results derived in this subsection are the starting point to understand the <u>quantum</u> <u>Hall</u> <u>effect</u>!

see, e.g., Stormer et al., Rev. Mod. Phys. <u>71</u>, S298 (1999).

Stormer, Rev. Mod. Phys. <u>71</u>, 875 (1999).

5. The Aharonov-Bohm effect.

Ref.: Aharonov and Bohm, Phys. Rev. <u>115</u>, 485 (1959)

. Recall classical electrodynamics:

- vector $\vec{A}$ and scalar ϕ potentials are <u>only</u> math tools to calculate $\vec{E}$ and $\vec{B}$.
- only $\vec{E}$ and $\vec{B}$ have physical significance
- eqs. of motion invariant under gauge transf. (222.2)

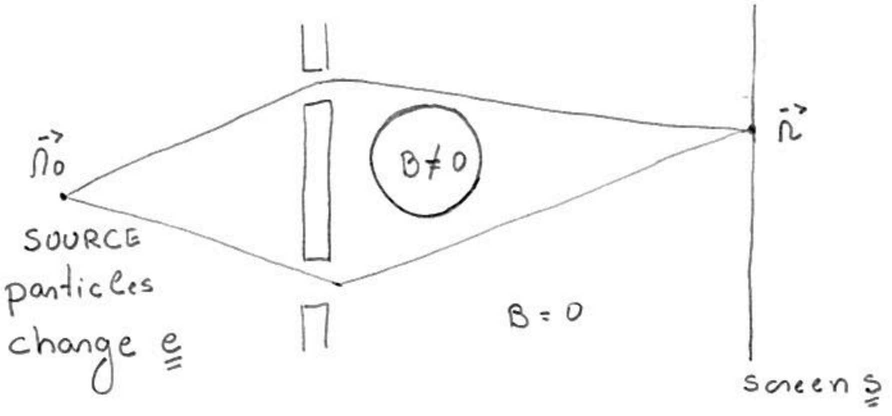
. in quantum mechanics:

- eq. of motion (49.1) for $|\psi(t)\rangle$ is invariant under gauge transformation (228.1): not only $\vec{A}$ and ϕ changes, but the phase of $|\psi(t)\rangle$ is also modified.
- since (228.1) comes from the classical analog (222.2)

  $\longrightarrow$ in principle, only $\vec{E}$ and $\vec{B}$ have physical significance.

However, this is not the case!

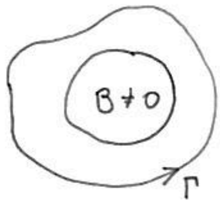
Let's consider the double slit experiment



Obs.: $\vec{B} \neq 0$ only inside the impenetrable cylinder.

note: although $\vec{\nabla} \times \vec{A} = \vec{B} = 0$ outside the cylinder, $\vec{A} \neq 0$ in this region.

Consider, e.g., a path surrounding the cylinder:



$$\oint_\Gamma \vec{A} \cdot d\vec{\ell} = \int_S (\vec{\nabla} \times \vec{A}) \cdot d\vec{S} = \int_S \vec{B} \cdot d\vec{S} = \Phi_B \qquad (244.1)$$

$$\text{if } \Phi_B \neq 0 \rightarrow \vec{A} \neq 0 \text{ along } \Gamma \text{ !}$$

Let's determine the interference pattern in the screen S

Recall path integral formalism:

$$\psi(\vec{r}, t) = \int d^3 r' \, K(\vec{r}, t ; \vec{r}', 0) \, \psi(\vec{r}', 0)$$

$$\text{where } K(r, t ; \vec{r}', 0) = \int_{\vec{q}(0) = \vec{r}'}^{\vec{q}(t) = \vec{r}} \mathcal{D}\vec{q} \; e^{i S[\vec{q}]/\hbar} \qquad (244.2)$$

S_0 : action with $\vec{A} = 0$

S : action with $\vec{A} \neq 0$

Recall the Lagrangian (223.1). We can write

$$S = S_0 + \frac{e}{c}\int_0^t dt' \frac{d\vec{q}}{dt'} \cdot \vec{A} = S_0 + \frac{e}{c}\int_{\vec{r}'}^{\vec{r}} \vec{A}\cdot d\vec{\ell}$$

The integral in (244.2) can be separated in two parts

$$K = \underset{\substack{\text{paths above}\\\text{cylinder}}}{\int} \mathcal{D}\vec{q}\,(\dots) + \underset{\substack{\text{paths below}\\\text{cylinder}}}{\int} \mathcal{D}\vec{q}\,(\dots)$$

in details,

$$K = \underset{\text{(paths above)}}{\int_{\vec{q}(0)=\vec{r}'}^{\vec{q}(t)=\vec{r}}} \mathcal{D}\vec{q}\; e^{iS_0/\hbar} \exp\left(\frac{ie}{\hbar c}\int_{\vec{r}'}^{\vec{r}} \vec{A}\cdot d\vec{\ell}\right) +$$

$$+ \underset{\text{(paths below)}}{\int_{\vec{q}(0)=\vec{r}'}^{\vec{q}(t)=\vec{r}}} \mathcal{D}\vec{q}\; e^{iS_0/\hbar} \underbrace{\exp\left(\frac{ie}{\hbar c}\int_{\vec{r}'}^{\vec{r}} \vec{A}\cdot d\vec{\ell}\right)}_{(*)}$$

Since $\vec{\nabla}\times\vec{A} = 0 \rightarrow (*)$ is path independent.
It's a common factor and
it can be put outside the integral!

if $\psi(\vec{r}',0) = \delta(\vec{r}'-\vec{r}_0)$

↳ $\psi(\vec{r},t) = K_{Above}(\vec{r},t;\vec{r}_0,0)\exp\left(\frac{ie}{\hbar c}\int_{Above}\vec{A}\cdot d\vec{l}\right)$

$$+ K_{below}(\vec{r},t;\vec{r}_0,0)\exp\left(\frac{ie}{\hbar c}\int_{below}\vec{A}\cdot d\vec{l}\right)$$

$$\equiv \psi_{Above}(\vec{r},t) + \psi_{below}(\vec{r},t)$$

↳ $|\psi(\vec{r},t)|^2 = |\psi_{Above}|^2 + |\psi_{below}|^2 + \underbrace{2\,\mathrm{Re}\,(\psi_{Above}\psi^*_{below})}_{(*)}$

note: Comparing with the case $\vec{B}=0$ inside the cylinder, (∗) has an extra phase factor given by

$$\exp\left(\frac{ie}{\hbar c}\underset{(\text{Above})}{\int_{\vec{r}_0}^{\vec{r}}}\vec{A}\cdot d\vec{l} - \frac{ie}{\hbar c}\underset{(\text{below})}{\int_{\vec{r}_0}^{\vec{r}}}\vec{A}\cdot d\vec{l}\right) = \exp\frac{ie}{\hbar c}\oint_\Gamma \vec{A}\cdot d\vec{l}$$

↳ surrounding the cylinder

$$\underset{(244.1)}{=} e^{ie\Phi_B/\hbar c} = e^{2\pi i\,\Phi_B/\Phi_0} \qquad (246.1)$$

where $\Phi_0 = \frac{hc}{e}$: magnetic flux quantum (see pg. 238)

↳ the interference pattern depends on the B-flux inside the cylinder, even though the particles never goes inside the cylinder!

· Experimental measurement AB effect: see, e.g.,

Webb et al., Phys. Rev. Lett. 54, 2696 (1985).

· Bound state AB effect: see problem 2.38, Sakurai and Napolitano.

6. The adiabatic approximation and the Berry phase

(see, e.g., Sec. 5.6, Sakurai and Napolitano)

Consider $H = H(t)$

· assumption: $H = H(t) = H[\vec{R}(t)]$

where $\vec{R}(t) = (R_1(t), R_2(t), \dots)$: set of parameters

and functions $R_i(t)$ slowly varies with time

Ex.: spin-½ ⊕ magnetic field $\vec{B} = \vec{B}(t)$

Hamiltonian (see pg. 135):

$$H = -\frac{2\mu}{\hbar}\vec{S}\cdot\vec{B}(t) \qquad (247.1)$$

i.e., $\vec{R}(t) \equiv \vec{B}(t) = (B_1(t), B_2(t), B_3(t))$

characteristic time scale system: $\tau = \frac{\hbar}{\Delta E} = \frac{\hbar}{|E_- - E_+|}$

time scale variation $\vec{B}(t)$: T

"slowly varies" = $T \gg \tau$!

idea: to solve the eq. of motion (49.1) for $|\psi(t)\rangle$

within the <u>adiabatic approximation</u>.

· Definition : instantaneous basis $\{|\varphi_n(t)\rangle\}$,

$$H(t)|\varphi_n(t)\rangle = E_n(t)|\varphi_n(t)\rangle \tag{248.1}$$

with $\langle\varphi_n(t)|\varphi_m(t)\rangle = \delta_{n,m}$

note : $\underline{\underline{t}}$ is a parameter !

· Recall Eq. (49.1) :

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle \tag{248.2}$$

we can write

$$|\psi(t)\rangle = \sum_n c_n(t)|\varphi_n(t)\rangle \tag{248.3}$$

with $|\psi(0)\rangle = \sum_n c_n(0)|\varphi_n(0)\rangle$

· Eq. (248.3) in (248.2),

$$i\hbar\sum_n \dot{c}_n(t)|\varphi_n(t)\rangle + i\hbar\sum_n c_n(t)\frac{d}{dt}|\varphi_n(t)\rangle =$$

$$= \sum_n c_n(t)\underbrace{H(t)|\varphi_n(t)\rangle}_{E_n(t)|\varphi_n(t)\rangle}$$

$\langle\varphi_k(t)|$:

$$i\hbar\dot{c}_k(t) - E_k(t)c_k(t) = -i\hbar\sum_n c_n(t)\underbrace{\langle\varphi_k(t)|\frac{d}{dt}|\varphi_n(t)\rangle}_{(*)} \tag{248.4}$$

i.e., differential eq. for $c_k(t)$!

Let's determine (*).

Two cases,

(i) $k = n$

$$\langle \varphi_n(t) | \varphi_n(t) \rangle = 1$$

$$\hookrightarrow \underbrace{\left[\frac{d}{dt} \langle \varphi_n | \right]}_{\langle \Phi_n(t) |} | \varphi_n \rangle + \langle \varphi_n | \underbrace{\frac{d}{dt} | \varphi_n \rangle}_{\equiv | \Phi_n(t) \rangle} = 0$$

$$= \underbrace{\langle \Phi_n | \varphi_n \rangle}_{\langle \varphi_n | \Phi_n \rangle^*} + \langle \varphi_n | \Phi_n \rangle = 2 \,\mathrm{Re} \langle \varphi_n(t) | \frac{d}{dt} | \varphi_n(t) \rangle = 0$$

$$\hookrightarrow \underbrace{\langle \varphi_n(t) | \frac{d}{dt} | \varphi_n(t) \rangle}_{\text{pure imaginary number!}} \equiv i \alpha_n(t) \; ; \; \alpha_n(t) \in \mathbb{R} \qquad (249.1)$$

(ii) $k \neq n$

$$\frac{d}{dt} \text{ Eq. } (248.1) : \quad \frac{dH}{dt} | \varphi_n(t) \rangle + H(t) \frac{d | \varphi_n(t) \rangle}{dt} =$$

$$= \dot{E}_n(t) | \varphi_n(t) \rangle + E_n(t) \frac{d}{dt} | \varphi_n(t) \rangle$$

$$\langle \varphi_k(t) | : \quad \langle \varphi_k | \dot{H} | \varphi_n \rangle + \underbrace{\langle \varphi_k | H}_{E_k \langle \varphi_k |} \frac{d}{dt} | \varphi_n \rangle =$$

$$= \dot{E}_n(t) \underbrace{\langle \varphi_k | \varphi_n \rangle}_{=0} + E_n(t) \langle \varphi_k | \frac{d}{dt} | \varphi_n \rangle$$

$\hookrightarrow \langle \varphi_k(t) | \frac{d}{dt} | \varphi_n(t) \rangle = \dfrac{\langle \varphi_k(t) | \dot{H}(t) | \varphi_n(t) \rangle}{E_n(t) - E_k(t)}$ (250.1)

(249.1) and (250.1) in (248.4),

$$\dot{c}_k(t) + \frac{i}{\hbar}\left(E_k(t) + \hbar \alpha_k(t) \right) c_k(t) =$$

$$= - \sum_{n \neq k} c_n(t) \underbrace{\frac{\langle \varphi_k(t) | \dot{H}(t) | \varphi_n(t) \rangle}{E_n(t) - E_k(t)}}_{(*)} \simeq 0 \qquad (250.2)$$

adiabatic approximation !

note: $(*) \sim \frac{1}{T \Delta E} \sim \frac{\tau}{T} \ll 1$!

using assumption pg. 247.

solution (250.2):

$$c_k(t) = c_k(0) \exp\left(\frac{-i}{\hbar} \int_0^t dt' E_k(t') \right) \exp\left(\underbrace{-i \int_0^t \alpha_k(t') dt'}_{\equiv i \gamma_k(t)} \right) \qquad (250.3)$$

$$\hookrightarrow |\psi(t)\rangle = \sum_n c_n(0) \exp\left(\frac{-i}{\hbar} \int_0^t dt' E_n(t') \right) e^{i \gamma_n(t)} |\varphi_n(t)\rangle, \qquad (250.4)$$

i.e., solution $|\psi(t)\rangle$ within the adiabatic approximation !

note : if $C_n(0) = \delta_{k,n}$

$$\hookrightarrow \ |\psi_k(t)\rangle = \underbrace{\exp\left(\frac{-i}{\hbar}\int_0^t dt'\, E_k(t')\right)}_{\text{dynamical phase}} e^{i\gamma_k(t)} \, |\varphi_k(t)\rangle$$

dynamical phase
(it generalizes the time-independent case)

extra (non-dynamical) phase: Berry phase.

It follows from the adiabatic approx. for t-dependent problem!

· note : time evolution does not yield transition between instanteneous states.

· Obs. : the states

$$|\tilde{\varphi}_n(t)\rangle = \exp\left(\frac{-i}{\hbar}\int_0^t dt'\, E_n(t')\right) e^{i\gamma_n(t)} \, |\varphi_n(t)\rangle$$

are called adiabatic states.

6.1 - The Berry phase

Ref. : M.V. Berry. Proc. Roy. Soc. Lond. A 392, 45 (1984)

idea : to consider in details $\gamma_n(t)$.

It's possible to show that $\gamma_n(t)$ can be $\neq 0$.

Moreover, it's possible to measure $\gamma_n(t)$!

Recall : $H = H(t) = H[\vec{R}(t)]$
$\hookrightarrow$ set of parameters

notation : $|\varphi_n(t)\rangle \equiv |n(\vec{R}(t))\rangle = |n(\vec{R})\rangle$

Let's consider a path $\underline{C}$ in the parameter space such that $\vec{R}(0) = \vec{R}(t)$, i.e., $\underline{C}$ is a <u>closed</u> path.

Eq. (249.1) : $\alpha_n(t) = -i \langle \varphi_n(t) | \frac{d}{dt} | \varphi_n(t) \rangle \quad := -i \langle n(\vec{R}) | \vec{\nabla}_R | n(R) \rangle \cdot \frac{d\vec{R}}{dt}$

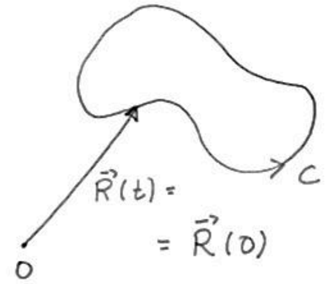
$$= -i \langle n(\vec{R}) | \underbrace{\frac{d}{dt} | n(\vec{R}) \rangle}_{\vec{\nabla}_R | n(\vec{R}) \rangle \cdot \frac{d\vec{R}}{dt}}$$

$$\hookrightarrow \quad \gamma_n(t) = -\int_0^t \alpha_n(t')\, dt' = i \int_0^t \langle n(\vec{R}) | \vec{\nabla}_R | n(\vec{R}) \rangle \cdot \frac{d\vec{R}}{dt}\, dt$$

$$= i \oint_C \underbrace{\langle n(\vec{R}) | \vec{\nabla}_R | n(\vec{R}) \rangle \cdot d\vec{R}}_{\text{pure imaginary number since } \alpha_n(t) \in \mathbb{R}\,!} \equiv \gamma_n(C) \ : \ \text{Berry phase}$$

note : $\gamma_n(C)$ is a <u>non-dynamical phase</u>.
It depends only on the path $\underline{C}$ the state $|n(\vec{R})\rangle$ "travels" within the parameter space.
$\gamma_n(C)$ is also called <u>geometric phase</u>.

. path $\underline{C}$:



· assumption : $\vec{R}(t) \in \mathbb{R}^3$.

Using Stokes theorem, we can write

$$\gamma_n(c) = -\mathrm{Im} \oint_c \langle n(\vec{R}) | \vec{\nabla}_R | n(\vec{R}) \rangle \cdot d\vec{R}$$

$$= -\mathrm{Im} \int_S \underbrace{\left[\vec{\nabla}_R \times \langle n(\vec{R}) | \vec{\nabla}_R | n(\vec{R}) \rangle \right]}_{\underbrace{\epsilon_{ijk}\, \partial_j \langle n | \partial_k | n \rangle\, ds_i}_{\epsilon_{ijk} \left(\langle \partial_j n | \partial_k n \rangle + \langle n | \cancel{\partial_j} \overset{\circ}{\partial_k} | n \rangle \right) ds_i}} \cdot d\vec{S}$$

$$= -\mathrm{Im} \int_S \underbrace{\langle \vec{\nabla}_R n(\vec{R}) | \times | \vec{\nabla}_R n(\vec{R}) \rangle}_{\epsilon_{ijk} \langle \partial_j n | \partial_k n \rangle\, ds_i} \cdot d\vec{S}$$

$$\uparrow$$

$$1 = \sum_m |m(\vec{R})\rangle \langle m(\vec{R})|$$

$$= -\mathrm{Im} \sum_{m \neq n} \int \left[\langle \nabla_R n(\vec{R}) | m(\vec{R}) \rangle \times \langle m(\vec{R}) | \nabla_R n(\vec{R}) \rangle \right] \cdot d\vec{S} \tag{253.1}$$

Obs. : $m = n$ is not included because

$$\langle n(\vec{R}) | n(\vec{R}) \rangle = 1 \rightarrow \langle \vec{\nabla}_R n | n \rangle + \langle n | \vec{\nabla}_R n \rangle = 0$$

$$\hookrightarrow \langle \vec{\nabla}_R n | n \rangle \times \langle n | \vec{\nabla}_R n \rangle = 0.$$

Let's determine $\langle \vec{\nabla}_R n | m \rangle$.

$\vec{\nabla}_R$ Eq. (248.1) : $(\vec{\nabla}_R H)|n\rangle + H|\vec{\nabla}_R n\rangle = (\vec{\nabla}_R E_n(\vec{R}))\,|n\rangle$

$$+ E_n(\vec{R})\,|\vec{\nabla}_R n\rangle$$

$\langle m(\vec{R})|: \quad \langle m|\vec{\nabla}_R H|n\rangle + \underbrace{\langle m|H}_{E_m(\vec{R})\langle m|}|\vec{\nabla}_R n\rangle = (\vec{\nabla}_R E_n)\underbrace{\langle m|n\rangle}_{0} + E_n\langle m|\vec{\nabla}_R n\rangle$

$$\hookrightarrow \langle m(\vec{R})|\vec{\nabla}_R n(\vec{R})\rangle = \frac{\langle m(\vec{R})|\vec{\nabla}_R H|n(\vec{R})\rangle}{E_n(\vec{R}) - E_m(\vec{R})}$$

in (253.1),

$$\gamma_n(c) = -\int \underbrace{\mathrm{Im}\sum_{m\neq n}\frac{\langle n|\vec{\nabla}_R H|m\rangle \times \langle m|\vec{\nabla}_R H|n\rangle}{(E_n - E_m)^2}}_{\equiv \vec{V}_n(\vec{R})} \cdot d\vec{s}$$

$$= -\int \vec{V}_n(\vec{R}) \cdot d\vec{s} \qquad (254.1)$$

Ex.: spin-1/2 $\oplus$ magnetic field $\vec{B} = \vec{B}(t)$

idea: to determine $\gamma_n(c)$ using (254.1).

Hamiltonian: Eq. (247.1),

$$H(t) = H(\vec{B}(t)) = -\frac{2\mu}{\hbar}\vec{S}\cdot\vec{B}(t) \qquad (254.2)$$

we identify $\vec{R} \longrightarrow \vec{B} = \vec{B}(t)$

eigenvalues (254.2) (see P.7, liste 1):

$E_+(t) = -\mu B(t) \longrightarrow |+(\vec{B})\rangle$

$E_-(t) = +\mu B(t) \qquad |-(\vec{B})\rangle$

Eq. (254.1):

$$\vec{V}_\sigma(c) = + \,\mathrm{Im}\, \frac{\langle \sigma(\vec{B}) |\, \vec{\nabla}_B H \,| -\sigma(\vec{B})\rangle \times \langle -\sigma(\vec{B}) |\, \vec{\nabla}_B H \,| \sigma(\vec{B})\rangle}{\left(E_\sigma(B) - E_{-\sigma}(B)\right)^2},$$

$$\sigma = \pm$$

we have,

$$[\,E_\sigma(B) - E_{-\sigma}(B)\,]^2 = 4\mu^2 B^2(t)$$

$$\vec{\nabla}_B H = -\frac{2\mu}{\hbar}\vec{S}$$

In order to evaluate $\langle \sigma | \vec{\nabla}_B H | -\sigma\rangle$, it's interesting to use the fact that the system has rotational symmetry.

- we assume $\vec{B} \parallel \hat{z}$

$\Rightarrow \vec{S} = \frac{1}{2}(S_+ + S_-)\hat{x} + \frac{1}{2i}(S_+ - S_-)\hat{y} + S_z\hat{z}$

$\xrightarrow[\text{exercise}]{}$ $\langle +(\vec{B}) | \nabla_B H | -(\vec{B})\rangle = -\frac{2\mu}{\hbar}\langle + | \vec{S} | -\rangle = \mu(\hat{x} - i\hat{y})$

$$\langle -(\vec{B}) | \nabla_B H | +(\vec{B})\rangle = \mu(\hat{x} + i\hat{y})$$

$\xrightarrow[\text{exercise}]{}$ $\langle + | \nabla_B H | -\rangle \times \langle - | \nabla_B H | +\rangle = 2\mu^2 i\,\hat{z}$

$$\langle - | \nabla_B H | +\rangle \times \langle + | \nabla_B H | -\rangle = -2\mu^2 i\,\hat{z}$$

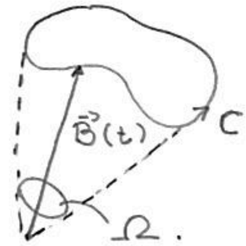
$\Rightarrow \vec{V}_\sigma(\vec{B}) = + \frac{\sigma}{2B^2(t)}\hat{z}$

· general case, i.e., $\vec{B}$ any direction

↳ $\vec{V}_\sigma(\vec{B}) = + \frac{\sigma}{2B^2(t)}\hat{B}$

↳ $\gamma_\pm(C) = \mp \frac{1}{2} \int \frac{\hat{B}\cdot d\vec{S}}{B^2(t)} = \mp \frac{1}{2}\Omega$

↳ solid angle



(256.1)

Eq. (256.1): it depends only on Ω, not the details path $\underline{C}$.

it does not depend on $\underline{\mu}$!

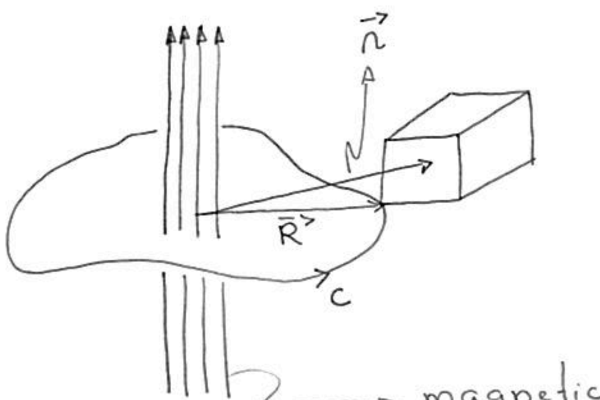
Ex.: The Aharonov-Bohm effect.

It's possible to show that the AB effect is related to the geometric phase $\gamma_n(C)$!

Consider: charged particle confined inside box, position op. $\vec{r}$.

$\vec{R}$: vector reference point in the box.

↳ external parameter.



· $\vec{B} = 0$ but $\vec{A} \neq 0$ inside box!

→ magnetic flux lines : Φ_B : total flux.

· Hamiltonian particle, case $\Phi_B = 0$ ($\vec{A} = 0$):

$$H = H(\vec{p}, \vec{r} - \vec{R})$$

$$\hookrightarrow \quad H \psi_n(\vec{r} - \vec{R}) = E_n \psi_n(\vec{r} - \vec{R})$$

· Hamiltonian particle, case $\Phi_B \neq 0$ ($\vec{A} \neq 0$):

$$H = H\left(\vec{p} - \frac{q}{c}\vec{A}(\vec{r}), \vec{r} - \vec{R}\right)$$

$$\hookrightarrow \quad H |n(\vec{R})\rangle = E_n |n(\vec{R})\rangle$$

· $\langle \vec{r} | n(\vec{R})\rangle$ and $\psi_n(\vec{r} - \vec{R})$ are related via a gauge transf. (228.1),

$$\langle \vec{r} | n(\vec{R})\rangle \sim e^{iq\chi/\hbar c} \psi_n(\vec{r} - \vec{R})$$

$$\vec{A} = \vec{\nabla}\chi \quad \rightarrow \quad \chi = \int \vec{A} \cdot d\vec{\ell}$$

in details, we can write

$$\langle \vec{r} | n(\vec{R})\rangle = \exp\left(\frac{iq}{\hbar c} \int_{\vec{R}}^{\vec{r}} \vec{A}(\vec{r}\,') \cdot d\vec{r}\,'\right) \psi_n(\vec{r} - \vec{R})$$

consider: (adiabatic) transport box along close path C

we have,

$$\langle \vec{r} | \vec{\nabla}_R n(\vec{R})\rangle = \exp\left(\frac{iq}{\hbar c} \int_{\vec{R}}^{\vec{r}} \vec{A}(\vec{r}\,') \cdot d\vec{r}\,'\right) *$$

$$* \left(\vec{\nabla}_R - \frac{iq}{\hbar c}\vec{A}(\vec{R})\right) \psi_n(\vec{r} - \vec{R})$$

$\hookrightarrow \langle n(\vec{R}) | \vec{\nabla}_R n(\vec{R}) \rangle = \int d^3r \, \psi_n^*(\vec{r}-\vec{R}) \, *$

$$* \left(\vec{\nabla}_R - \frac{iq}{\hbar c} \vec{A}(\vec{R}) \right) \psi_n(\vec{r}-\vec{R}) = -\frac{iq}{\hbar c} \vec{A}(\vec{R})$$

since $\nabla_R \underbrace{\int d^3r \, |\psi_n(\vec{r}-\vec{R})|^2}_{1} = 0$!

$\rightarrow \gamma_n(C) = -\mathrm{Im} \oint_C \left(\frac{-iq}{\hbar c} \right) \vec{A}(R) \cdot d\vec{R} = \frac{q}{\hbar c} \Phi_B$: in agreement with (246.1).

$\hookrightarrow$ the phase acquired by the wave function in the AB effect = geometric phase !

Obs. 1 : measurements $\gamma_n(C)$,
see, e.g., Richardson et al., Phys. Rev. Lett. 61, 2030 (1988).
Filipp et al., Phys. Rev. Lett. 102, 030404 (2009).

Obs. 2 : the Berry phase is an important ingredient to understand the so-called topological insulators.
see, e.g.,

Obs. 3 : Further reading : Magnetic monopole, Sec. 2.7, Sakurai and Napolitano.