Path Integrals and Quantum Mechanics

Consider a quantum mechanical system in the Heisenberg picture. Let us denote by $\hat{Q}(t)$ the coordinate operator and $|q,t\rangle$ its eigenstate

$$\hat{Q}\,|q,t\rangle = q\,|q,t\rangle$$

in the Schrödinger picture the associated $\hat{Q}_S$ is time independent

$$\hat{Q}(t) = e^{i\hat{H}t/\hbar}\,\hat{Q}_S\,e^{-i\hat{H}t/\hbar}$$

and its eigenstates are

$$\hat{Q}_S\,|q\rangle = q\,|q\rangle \qquad (\text{time-independent})$$

$$\Rightarrow \quad |q\rangle = e^{-i\hat{H}t/\hbar}\,|q,t\rangle$$

These states are complete

$$I = \sum_q |q\rangle\langle q|$$

$$\Rightarrow \quad F(q't'|qt) = \langle q't'|qt\rangle = \langle q'|\,e^{-\frac{i}{\hbar}H(t'-t)}\,|q\rangle$$

If H is time-independent $\Rightarrow$

$$e^{(a+b)H} = e^{aH}\,e^{bH} \qquad \text{since } [H,H]=0$$

$\Rightarrow$ we can always do the following

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

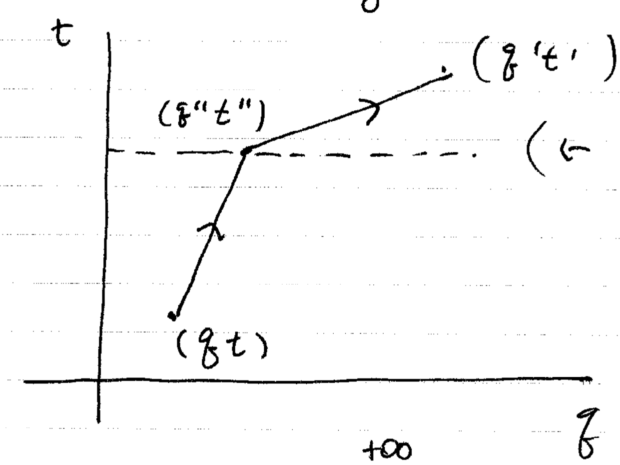
for any t'' / $t < t'' < t'$

By inserting I between the exponentials we get

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

$$\Rightarrow \quad F(q't'|qt) = \sum_{q''} F(q't'|q''t'') F(q''t''|qt)$$

This is nothing but the superposition pple.



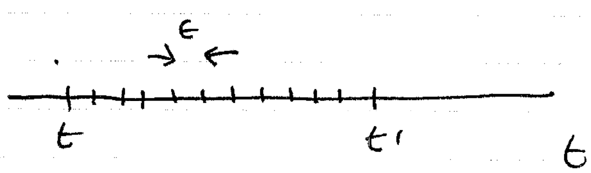
(← sum over all states $|q''\rangle$)

$$\Rightarrow \quad F(q't'|qt) = \int_{-\infty}^{+\infty} dq'' \, F(q't'|q''t'') \, F(q''t''|qt)$$

We can obviously repeat this process indefinitely.

Let us split the interval $[t, t']$ into n intervals of length $\epsilon = \frac{t'-t}{n} = \Delta t$ and define the sequence of times $\{t_j\}$ $(j = 0, \dots, n+1)$ where

$$t_0 \equiv t \leq t_1 \leq t_2 \leq \cdots \leq t_n \leq t_{n+1} \equiv t'$$



$$\Rightarrow \quad t_j = t_0 + \epsilon j$$

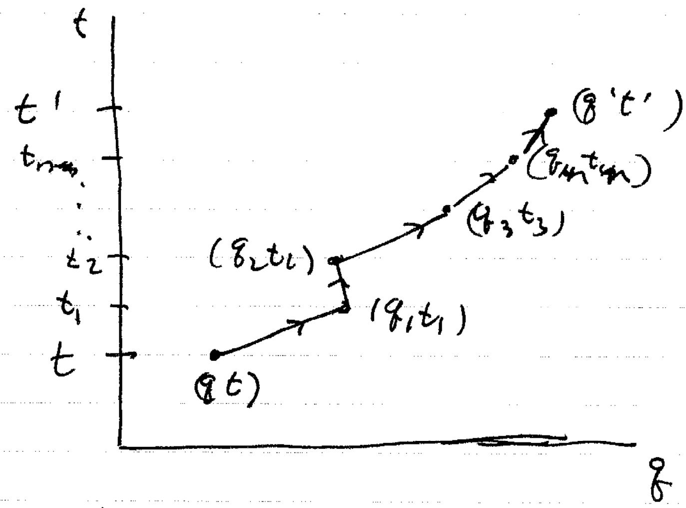
L11

We can then write

$$F(q't'|qt) = \int_{-\infty}^{+\infty} dq_1 \cdots \int_{-\infty}^{+\infty} dq_n \; \langle q't'|q_n t_n\rangle \langle q_n t_n | q_{n-1} t_{n-1}\rangle \cdots$$
$$\cdots \langle q_1 t_1 | q t\rangle$$

We will use the notation

$$q_j = q(t_j)$$



The product inside the integral can be regarded as a sequence of states (a history) $|\{q(t_j)\}\rangle$

Our formula says that we must sum over all histories with a weight $\prod_{j=0}^{n} \langle q(t_{j+1}) | q(t_j)\rangle$

Each factor is

$$\langle q(t_{j+1}) | q(t_j)\rangle \equiv \langle q_{j+1}| \, e^{-\frac{i}{\hbar}(t_{j+1}-t_j)H} \, |q_j\rangle$$
$$\equiv \langle q_{j+1}| \, e^{-\frac{i}{\hbar}\epsilon H} \, |q_j\rangle$$

If ϵ is small we can expand

$$e^{-i\frac{\epsilon H}{\hbar}} \simeq I - i\frac{\epsilon}{\hbar} H + O(\epsilon^2)$$

$$\Rightarrow \langle q(t_{j+1}) | q(t_j)\rangle \approx \langle q_{j+1}| \left[I - i\frac{\epsilon}{\hbar} H + O(\epsilon^2)\right] |q_j\rangle$$

$$= \langle q_{j+1} | q_j \rangle - \frac{i\epsilon}{\hbar} \langle q_{j+1} | \hat{H} | q_j \rangle + O(\epsilon^2)$$

Since the states $\{|q\rangle\}$ are orthonormal $\Rightarrow$

$$\langle q_{j+1} | q_j \rangle = \delta(q_{j+1} - q_j)$$

Let us consider Hamiltonians of the form

$$H = \frac{\hat{P}^2}{2M} + V(\hat{Q})$$

The momentum operator also defines a complete set of eigenstates $\{|p\rangle\}$

$$\hat{P} |p\rangle = p |p\rangle$$

These states are complete and orthonormal. The overlap $\langle q | p \rangle$ is

$$\langle q | p \rangle = \frac{1}{\sqrt{L}} e^{i p q / \hbar} \qquad \left(\Delta p = \frac{2\pi\hbar}{L} \right)$$

Furthermore

$$2\pi\hbar\, \delta(p - p') = \int_{-\infty}^{+\infty} dq\, e^{i q (p - p') / \hbar}$$

and

$$\hat{I} = \sum_p |p\rangle \langle p| = \int \frac{dp}{2\pi\hbar} L\, |p\rangle \langle p|$$

$$\Rightarrow \langle q_{j+1} | q_j \rangle = \langle q_{j+1} | \hat{I} | q_j \rangle = \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \langle q_{j+1} | p_j \rangle \langle p_j | q_j \rangle$$

$$= L \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \left(\frac{1}{\sqrt{L}} \right)^2 e^{i (q_{j+1} - q_j) p_j / \hbar}$$

Likewise

$$\langle q_{j+1} | \hat{P}^2 | q_j \rangle = \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} L \; \langle q_{j+1} | p_j \rangle \; p_j^2 \langle p_j | q_j \rangle$$

[where I used that

$$\hat{P}^2 = \Sigma_p \; p^2 \; |p\rangle\langle p| \equiv \int_{-\infty} \frac{dp}{2\pi\hbar} L \; p^2 \; |p\rangle\langle p| \;]$$

$$\Rightarrow \langle q_{j+1} | \frac{\hat{P}^2}{2m} | q_j \rangle = \frac{L}{2\pi\hbar} \int_{-\infty}^{+\infty} dp_j \; \frac{1}{L} \; e^{+i (q_{j+1} - q_j) \frac{p_j}{\hbar}} \; p_j^2$$

$$\langle q_{j+1} | V(\hat{Q}) | q_j \rangle = \delta(q_{j+1} - q_j) \; V(q_j)$$

$$= \frac{L}{2\pi\hbar} \int_{-\infty}^{+\infty} dp_j \; \frac{1}{L} \; e^{+i (q_{j+1} - q_j) \frac{p_j}{\hbar}} \; V(q_j)$$

$$\Rightarrow \langle q_{j+1} | H | q_j \rangle = \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \; e^{+\frac{i}{\hbar} p_j (q_{j+1} - q_j)} \left[\frac{p_j^2}{2m} + V(q_j) \right]$$

and

(within approx)

$$\langle q_{j+1} t_{j+1} | q_j t_j \rangle \approx \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \; e^{+\frac{i}{\hbar} p_j (q_{j+1} - q_j)} \left[1 + \frac{i\epsilon}{\hbar} \left\{ \frac{p_j^2}{2m} + V\left(\frac{q_j + q_{j+1}}{2} \right) \right\} \right]$$

$$\approx \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \; e^{+\frac{i}{\hbar} p_j (q_{j+1} - q_j) + \frac{i\epsilon}{\hbar} \left[\frac{p_j^2}{2m} + V\left(\frac{q_j + q_{j+1}}{2} \right) \right]}$$

The total amplitude is then

$$\langle q't' | q t \rangle = \int_{-\infty}^{+\infty} dq_1 \ldots \int_{-\infty}^{+\infty} dq_n \prod_{j=0}^{n} \langle q(t_{j+1}) | q(t_j) \rangle$$

$$\equiv \left(\prod_{j=0}^{n} \int_{-\infty}^{+\infty} \frac{dq_j \, dp_j}{2\pi\hbar} \right) e^{\frac{i}{\hbar} \sum_{j=0}^{n} p_j (q_{j+1} - q_j) - \frac{i}{\hbar} \sum_{j=0}^{n} H[q_j, p_j] \epsilon}$$

$$q(t_{j+1}) - q(t_j) \approx \left.\frac{dq}{dt}\right|_{t_j} (t_{j+1} - t_j) = \left.\frac{dq}{dt}\right|_{t_j} \epsilon$$

The expression

$$\sum_{j=0}^{n} p_j (q_{j+1} - q_j) - \sum_{j=0}^{n} \epsilon \, H[p_j, q_j] =$$

$$= \sum_{j=0}^{n} \epsilon \left[p(t_j) \left.\frac{dq}{dt}\right|_{t_j} - H[p(t_j), q(t_j)] \right]$$ Riemann sum!

$$\underset{\substack{n \to \infty \\ \epsilon \to 0}}{\equiv} \int_{t_i}^{t_f} dt \left[p(t) \frac{dq}{dt} - H(p(t), q(t)) \right]$$

$t_i = t$, $t_f = t'$ and $\left. \begin{array}{l} q(t_i) = q \\ q(t_f) = q' \end{array} \right]$ initial and final conditions

while $p(t)$ is unrestricted

$\Rightarrow$

$$\langle q't' | q t\rangle \equiv \int \mathcal{D}p\, \mathcal{D}q \quad e^{+\frac{i}{\hbar} S(p,q)}$$

$S(p,q)$ is the <u>classical action</u>

$$S(p,q) = \int_{t_i}^{t_f} dt \; \left[p\dot{q} - H(p,q) \right]$$

and the measure

$$\mathcal{D}p\, \mathcal{D}q \equiv \lim_{\substack{n\to\infty \\ \epsilon\to 0}} \prod_{j=1}^{n} \frac{dp(t_j)\, dq(t_j)}{2\pi\hbar}$$

It is an integral over histories in phase space, i.e.

<u>all</u> possible functions $p(t)$, $q(t)$

[note: $p \neq m\dot{q}$]

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

We can integrate p out at every intermediate time to get

$$\int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \; e^{-i\frac{\epsilon}{\hbar}\frac{p_j^2}{2m} + \frac{i}{\hbar}\epsilon\, p_j \dot{q}_j} = \sqrt{\frac{m\hbar}{2\pi\epsilon}} \; e^{+i\frac{\epsilon}{\hbar} m \dot{q}_j^2}$$

$$\left[\frac{p_j^2}{2m} - p_j\dot{q}_j = \frac{1}{2}\left[\left(\frac{p_j}{\sqrt{m}}\right)^2 - 2\frac{p_j}{\sqrt{m}}\dot{q}_j\sqrt{m}\right] = \frac{1}{2}\left(\frac{p_j}{\sqrt{m}} - \dot{q}_j\sqrt{m}\right)^2 - \frac{1}{2}\left(\dot{q}_j\sqrt{m}\right)^2 \right]$$

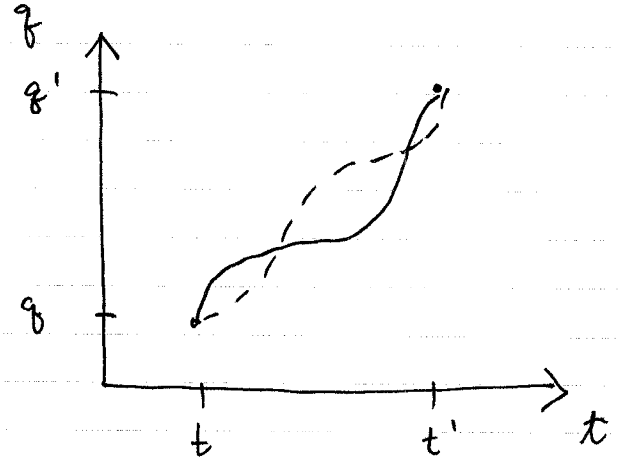
$$\Rightarrow \quad \langle q't' | q t \rangle = \int \mathcal{D}q \; e^{+\frac{i}{\hbar}\int_{t_i}^{t_f} dt \left[\frac{m}{2}\dot{q}^2 - V(q)\right]}$$

$$\left[\mathcal{D}q = \lim_{\substack{\epsilon \to 0 \\ n \to \infty}} \prod_j dq(t_j) \sqrt{\frac{m\hbar}{2\pi\epsilon}} \right] \qquad \begin{array}{l} q(t_i) = q \\ q(t_f) = q' \end{array}$$

and we recognize the action (in Lagrangian form)

$$S(q) = \int_{t_i}^{t_f} dt \left[\frac{1}{2} m \left(\frac{dq}{dt}\right)^2 - V(q)\right] = \int_{t_i}^{t_f} dt \; L\left(q, \frac{dq}{dt}\right)$$

This is a very interesting expression. It means that the amplitude $\langle q't' | q t \rangle$ can be viewed as a sum over the histories of the particle $q(t)$ with a weight $e^{\frac{i}{\hbar} S(q)}$ with $S(q)$ being the classical action for <u>that</u> history.



Matrix Elements

Let us choose some intermediate time t_0, $\quad t \leq t_0 \leq t'$

Let us compute the matrix element

$$\langle q' t' | \hat{Q}(t_0) | q t \rangle$$

By repeating the construction of the Feynman Path Integral one finds

$$\langle q' t' | \hat{Q}(t_0) | q t \rangle = \int \mathcal{D}p \, \mathcal{D}q \quad q(t_0) \, e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \, [p \dot{q} - H]}$$

Let us consider two times t_1 and t_2, $\quad t \leq t_1 \leq t_2 \leq t'$

$$\Rightarrow \langle q' t' | \hat{Q}(t_1) \hat{Q}(t_2) | q t \rangle = \int \mathcal{D}p \, \mathcal{D}q \; q(t_1) \, q(t_2) \, e^{\frac{i}{\hbar} S}$$

For the reverse ordering $\quad t_2 < t_1$

$$\langle q' t' | \hat{Q}(t_2) \hat{Q}(t_1) | q t \rangle = \int \mathcal{D}p \, \mathcal{D}q \; q(t_2) \, q(t_1) \, e^{\frac{i}{\hbar} S}$$

which is the same expression.

$$\Rightarrow \quad \langle q' t' | T [\hat{Q}(t_1) \hat{Q}(t_2)] | q t \rangle = \int \mathcal{D}p \, \mathcal{D}q \; q(t_1) \, q(t_2) \, e^{\frac{i}{\hbar} S}$$

i.e. the P.I. ~~gives~~ yields time ordered products.

Meaning of $\langle q't'|T\,\hat{Q}(t_1)\,\hat{Q}(t_2)|q t\rangle$:

$$|q,t\rangle = e^{iHt/\hbar}\,|q\rangle$$

$$\Rightarrow \langle q't'|T\,\hat{Q}(t_1)\,\hat{Q}(t_2)|q t\rangle =$$

$$= \langle q'|\, e^{-\frac{i}{\hbar}\hat{H}t'}\, e^{\frac{i}{\hbar}\hat{H}t_2}\,\hat{Q}\, e^{-\frac{i}{\hbar}\hat{H}t_2}\, e^{\frac{i}{\hbar}\hat{H}t_1}\,\hat{Q}\, e^{-\frac{i}{\hbar}\hat{H}t_1}\, e^{\frac{i}{\hbar}\hat{H}t}\,|q\rangle$$

$t_2 > t_1$

$$= \langle q'|\, e^{\frac{i}{\hbar}\hat{H}(t_2-t')}\,\hat{Q}\, e^{\frac{i}{\hbar}\hat{H}(t_1-t_2)}\,\hat{Q}\, e^{\frac{i}{\hbar}\hat{H}(t-t_1)}\,|q\rangle$$

$$= \sum_{n,m,r} e^{-\frac{i}{\hbar}E_n(t'-t_2)}\,\langle q'|n\rangle\langle n|\hat{Q}|m\rangle\, e^{-\frac{i}{\hbar}E_m(t_2-t_1)}\,\langle m|\hat{Q}|r\rangle \times e^{-\frac{i}{\hbar}E_r(t_1-t)}\,\langle r|q\rangle$$

Analytic continuation: same as adiabatic switching off and on

$t \to iT \to i\infty$

$t' \to iT' \to -i\infty$

$\Rightarrow$ Only the ground state contributes

$$\Rightarrow \langle q't'|\hat{T}\,\hat{Q}(t_1)\,\hat{Q}(t_2)|q t\rangle =$$

$$= \sum_m e^{-\frac{i}{\hbar}E_0(t'-t_2)}\,\varphi_0(q')\,\varphi_0^*(q)\, e^{-\frac{i}{\hbar}E_0(t_1-t)}$$

$$\times\, |\langle 0|\hat{Q}|m\rangle|^2\, e^{-\frac{i}{\hbar}E_m(t_2-t_1)}$$

$$= e^{-\frac{i}{\hbar}E_0(t'-t)}\,\varphi_0(q')\,\varphi_0^*(q)\sum_m |\langle 0|\hat{Q}|m\rangle|^2\, e^{-\frac{i}{\hbar}(E_m-E_0)(t_2-t_1)}$$

$$\Rightarrow \frac{\langle q''t'' | T\, Q(t_1)\, Q(t_2) | q t\rangle}{\langle q't' | q t\rangle} \xrightarrow[t_2>t_1]{} \sum_m |\langle 0|\hat{Q}|m\rangle|^2 e^{-\frac{i}{\hbar}(E_m - E_0)(t_2 - t_1)}$$

(L12) Thus if we compute such T-ordered products we can compute both excitation energies $(E_m - E_0)$ and matrix elements.

In order to compute these matrix elements the simplest thing to do is to add an extra term to H of the form

$$H_{ext} = - J(t)\, Q(t)$$

where $J(t)$ is a "Source" which vanishes for both $t \to \pm\infty$

$$\frac{d}{dJ} e^{\frac{i}{\hbar} J q}\Big|_{J=0} = \frac{i}{\hbar} q\, e^{\frac{i}{\hbar} J q}\Big|_{J=0} = \frac{i}{\hbar} q$$

$$\Rightarrow q(t_1) \cdots q(t_n) = \frac{d}{dJ(t_1)} \cdots \frac{d}{dJ(t_n)} e^{i\int dt\, J(t)\, q(t)}\Big|_{J=0} \left(\frac{\hbar}{i}\right)^n$$

$\Rightarrow$ The action is now

$$S = \int (p\dot{q} - H)\, dt + \int dt\, J(t)\, q(t)$$

Same as $\hat{H} \to \hat{H} - J(t)\, \hat{Q}(t)$

Alternatively, we can ask for an arbitrary matrix element

$$\langle \psi_f, t_f | \psi_0, t_f \rangle$$

where $|\psi_i\rangle$ and $|\psi_f\rangle$ are two arb. states. For example they could be the ground state of a time indep. system. These states can be decomposed in terms of their amplitudes in the coord. rep.

$$|\psi\rangle = \int_{-\infty}^{+\infty} dq \; |q\rangle \; \psi(q)$$

$$\langle \psi | = \int_{-\infty}^{+\infty} dq \; \psi^*(q) \; \langle q|$$

$$\Rightarrow \langle \psi_f, t_f | \psi_i, t_i \rangle = \int_{-\infty}^{+\infty} dq_f \int_{-\infty}^{+\infty} dq_i \; \psi_f^*(q_f) \; \psi_i(q_i) \; \langle q_f \, t_f | q_i \, t_i \rangle$$

we have an expression for this

For instance we may want to compute $|\psi\rangle = |0\rangle$ (Gnd state.)

$t_1 > t_2$ $\quad \langle 0, t_f | \hat{Q}(t_1) \, \hat{Q}(t_2) | 0, t_0 \rangle =$

$$= e^{-\frac{i}{\hbar} E_0 (t_f - t_i)} \sum_n e^{-\frac{i}{\hbar}(E_n - E_0)(t_1 - t_2)} \; |\langle 0 | \hat{Q} | n \rangle|^2$$

$$\Rightarrow \frac{\langle 0, t_f | T[\hat{Q}(t_1) \hat{Q}(t_2)] | 0, t_i \rangle}{\langle 0, t_f | 0, t_i \rangle} = \sum_n |\langle 0 | \hat{Q} | n \rangle|^2 \; e^{-\frac{i}{\hbar}(E_n - E_0)|t_2 - t_1|}$$

wave functions. excitation energies info about

(12)

Analytic Continuation and the relation with Statistical Mechanics

As we saw before, the time evolution of (pure) quantum states in the Schrödinger picture is generated by the evolution operator

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle \equiv \hat{U}(t)|\psi(0)\rangle$$

A quantum system in thermodynamic equilibrium with a heat bath at temperature T is not described by a pure state but by the density matrix of the canonical ensemble

$$\hat{\rho} = \frac{1}{Z}e^{-\hat{H}/k_BT}, \qquad Z = \mathrm{tr}\, e^{-\hat{H}/k_BT} \equiv \sum_n \langle n|e^{-\hat{H}/k_BT}|n\rangle$$

[The time evolution of $\hat{\rho}$, is $\hat{\rho}(t) = \hat{U}(t)\,\hat{\rho}\,\hat{U}^{-1}(t)$]

Define $\beta = \frac{1}{k_BT}$

$\Rightarrow$ there is a formal analogy between $e^{-\beta\hat{H}}$ and the evolution operator $e^{-\frac{i}{\hbar}\hat{H}t}$. Indeed, if we perform the analytic continuation $t \to -i\tau$

we have $\qquad \beta = \tau/\hbar$

$$e^{-\frac{i}{\hbar}\hat{H}t} \rightarrow e^{-\beta\hat{H}}$$

In particular

$$\langle q'|\, e^{-\frac{i}{\hbar} t \hat{H}} |q\rangle \longrightarrow \langle q'|\, e^{-\frac{\tau}{\hbar}\hat{H}} |q\rangle$$
$$= \langle q'|\, e^{-\beta \hat{H}} |q\rangle$$

In practice we want to consider long time evolution,
$\Rightarrow t \to \infty \Rightarrow$ we also want $\beta \to \infty$ $(T \to 0)$

In particular

$$\langle 0|\, \hat{Q}(t)\, \hat{Q}(t')\,|0\rangle \to \langle 0|\, \hat{Q}(\tau)\, \hat{Q}(\tau')\,|0\rangle$$

$$\hat{Q}(\tau) = e^{\frac{\tau \hat{H}}{\hbar}}\, \hat{Q}\, e^{-\frac{\tau \hat{H}}{\hbar}} \qquad (\tau \leftrightarrow \tau')$$

$$\Rightarrow \langle 0|\, T\, \hat{Q}(\tau)\, \hat{Q}(\tau')\,|0\rangle =$$
$$= \langle 0|\, T\, e^{\frac{\tau \hat{H}}{\hbar}}\, \hat{Q}\, e^{-\frac{\tau \hat{H}}{\hbar}}\, e^{\frac{\tau' \hat{H}}{\hbar}}\, \hat{Q}\, e^{-\frac{\tau' \hat{H}}{\hbar}}\,|0\rangle$$
$$= e^{+\frac{|\tau-\tau'|}{\hbar} E_0} \sum_n |\langle 0|Q|n\rangle|^2\, e^{-|\tau-\tau'|\frac{E_n}{\hbar}}$$
$$= \sum_n |\langle 0|Q|n\rangle|^2\, e^{-|\tau-\tau'|\frac{E_n - E_0}{\hbar}}$$

At long imaginary times only the term with the smallest $E_n - E_0$ survives $\Rightarrow$

$$\lim_{\tau\to\infty} \langle 0|T\, \hat{Q}(\tau)\, \hat{Q}(\tau')\,|0\rangle \approx |\langle 0|\hat{Q}|n^*\rangle|^2\, e^{-(E_{n^*}-E_0)\frac{|\tau-\tau'|}{\hbar}}$$

where $|n^*\rangle$ is the lowest energy state that mixed with $|0\rangle$ through the op. $\hat{Q}$.

What is the path-integral form for $\langle q'| e^{-\beta H}|q\rangle$?

$$\langle q'| e^{-\beta \hat{H}} |q\rangle \equiv \int \mathcal{D}q[\tau] \; e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{1}{2}m\left(\frac{dq}{d\tau}\right)^2 + V(q)\right]}$$

(analytic continuation)

$$\frac{i}{\hbar}\int_{t_i}^{t_f} dt \left[\frac{1}{2} m \left(\frac{dq}{dt}\right)^2 - V(q)\right] \longrightarrow -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{1}{2}m\left(\frac{dq}{d\tau}\right)^2 + V(q)\right]$$

$$\tau_i = 0, \quad \tau_f = \beta\hbar$$

$$Z = \operatorname{tr} e^{-\beta \hat{H}} = \int \mathcal{D}q[\tau] \; e^{-\int_0^{\beta} d\tau \left[\frac{1}{2\hbar^2}m\left(\frac{dq}{d\tau}\right)^2 + V(q)\right]} \qquad \left(\frac{\tau}{\hbar} \to \tau\right)$$

with $q(0) = q(\beta)$ (PBC's)

The formula on the r.h.s. looks like a problem in Classical Statistical mechanics on a <u>line</u> of length <u>β</u> and classical Hamiltonian

$$E\left(q, \frac{dq}{d\tau}\right) = \frac{1}{2\hbar^2} m \left(\frac{dq}{d\tau}\right)^2 + V(q)$$

$$Z = \operatorname{tr} e^{-\beta \hat{H}} = \sum_n e^{-\beta E_n} = e^{-\beta E_0} \sum_n e^{-\beta(E_n - E_0)}$$

$$\beta \to \infty \; (T \to 0) \qquad Z \simeq e^{-\beta E_0} + \cdots$$

$$E_0 = \lim_{\beta\to\infty} -\frac{1}{\beta} \ln Z = \lim_{\beta\to\infty} -\frac{1}{\beta} \ln \int_{\text{PBC's}} \mathcal{D}q \; e^{-\int_0^{\beta} d\tau \, E\left(q, \frac{dq}{d\tau}\right)}$$

Classical Limit

Let us consider the correspondence limit $\hbar \to 0$. The path integral (or functional integral) is a sum of rapidly oscillating functions. We can estimate its behavior as $\hbar \to 0$ by a steepest descent (or saddle point) approximation. For a conventional integral

$$\int_{-\infty}^{+\infty} dx \quad e^{-z f(x)} \underset{z\to\infty}{\approx} \int_{-\infty}^{+\infty} dx \quad e^{-z f(x_0) - \frac{z}{2} f''(x_0)(x-x_0)^2 + \dots}$$

if x_0 is a stationary point of $f(x)$

$$f'(x_0) = 0 \qquad \text{(extremum)}$$

$$\approx \sqrt{\frac{2\pi}{z f''(x_0)}} \quad e^{-z f(x_0)} \left\{ 1 + O\left(\frac{1}{z}\right) \right\}$$

The Saddle points of $S(q, \dot{q})$ are the extrema

$$\delta S = 0$$

$$\delta S = \int_{t_0}^{t_f} dt \left[\frac{\partial L}{\partial \dot{q}} \delta\dot{q} + \frac{\partial L}{\partial q} \delta q \right]$$

$$= \int_{t_i}^{t_f} dt \left[\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) \right] \delta q + \int_{t_i}^{t_f} dt \, \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{q}} \delta q \right]$$

Thus if we fix the initial and final condition

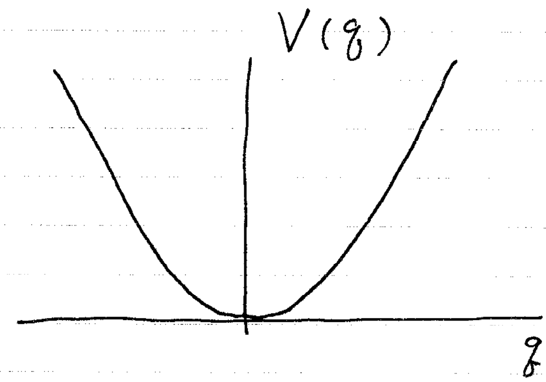
$$q(t_i) = q \quad , \quad q(t_f) = q'$$

$$\Rightarrow \quad \delta q(t_i) = 0 \quad \text{and} \quad \delta q(t_f) = 0$$

$\Rightarrow$ The condition for the extremum is the Least Action Principle $\delta S = 0 \Rightarrow$ Classical Equation of Motion.

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0$$

Example: Harmonic Oscillator



$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$$

$$L = \frac{1}{2} m \left(\frac{dq}{dt}\right)^2 - \frac{1}{2} m\omega^2 q^2$$

Classical Path: $\bar{q}(t)$

$$\bar{q}(t) = q \quad , \quad \bar{q}(t') = q'$$

and $\bar{q}(t)$ satisfies

$$0 = \frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = -m\omega^2 \bar{q} - m\frac{d^2\bar{q}}{dt^2}$$

$$\Rightarrow \quad \frac{d^2\bar{q}}{dt^2} + \omega^2 \bar{q} = 0$$

subject to the initial and final conditions.

An arbitrary path is not equal to the Classical path but only those paths $q(t)$ close enough to $\bar{q}(t)$ will contribute $\Rightarrow$

$$q(t) = \bar{q}(t) + \xi(t)$$

Since $q(t_i) = \bar{q}(t_i) = q$ and $q(t_f) = \bar{q}(t_f) = q'$

$\Rightarrow \xi(t_i) = 0$ and $\xi(t_f) = 0$

$$L(q, \dot{q}) = L(\bar{q} + \xi, \dot{\bar{q}} + \dot{\xi})$$

For a H.O. we have

$$L(\bar{q} + \xi, \dot{\bar{q}} + \dot{\xi}) = L(\bar{q}, \dot{\bar{q}}) + L(\xi, \dot{\xi}) +$$
$$+ m \frac{d\bar{q}}{dt}\frac{d\xi}{dt} - m\omega^2 \bar{q}\xi$$

$$\Rightarrow S(q) = S(\bar{q}) + S(\xi) + \int_{t_i}^{t_f} dt \left[m \frac{d\bar{q}}{dt}\frac{d\xi}{dt} - m\omega^2 \bar{q}\xi\right]$$

$$\Rightarrow S(q) = S(\bar{q}) + S(\xi) + m\, \xi(t) \frac{d\bar{q}}{dt}\Big|_{t_i}^{t_f}$$
$$- m\int_{t_i}^{t_f} dt\, \xi(t) \left(\frac{d^2\bar{q}}{dt^2} + \omega^2 \bar{q}\right)$$

but $\xi(t_i) = \xi(t_f) = 0$ and $\frac{d^2\bar{q}}{dt^2} + \omega^2\bar{q} = 0$

$$\Rightarrow S(q) = \underbrace{S(\bar{q})}_{\text{action of classical path}} + S(\xi)$$

or $$S(q) = \underbrace{S_c(\bar{q}, \dot{\bar{q}})}_{\text{classical action}} + \underbrace{\int_{t_i}^{t_f} dt \; L(\xi, \dot{\xi})}_{\text{quantum fluctuations}}.$$

For a general potential $V(q)$ we get

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

$$\bar{q} / \quad m\frac{d^2\bar{q}}{dt^2} = -V'(\bar{q}) = F(\bar{q}) \qquad (\text{Force} = ma)$$

$$L(\bar{q}+\xi, \dot{\bar{q}}+\dot{\xi}) = \frac{m}{2}\dot{\bar{q}}^2 + \frac{m}{2}\dot{\xi}^2 + m\dot{\bar{q}}\dot{\xi} - V(\bar{q}+\xi)$$

For small ξ, $V(\bar{q}+\xi) \approx V(\bar{q}) + V'(\bar{q})\xi + \frac{1}{2}V''(\bar{q})\xi^2 + \cdots$

$$L(\bar{q}+\xi, \dot{\bar{q}}+\dot{\xi}) \approx \frac{m}{2}\dot{\bar{q}}^2 + \frac{m}{2}\dot{\xi}^2 + m\dot{\bar{q}}\dot{\xi} - V(\bar{q}) - V'(\bar{q})\xi - \frac{1}{2}V''(\bar{q})\xi^2 + \cdots$$

[where $\bar{q} = \bar{q}(t)$ in general]

$\Rightarrow$ collecting terms we get

$$L(q) = \left[\frac{1}{2}m\dot{\bar{q}}^2 - V(\bar{q})\right] + \left[m\dot{\bar{q}}\dot{\xi} - V'(\bar{q})\xi\right] + \left[\frac{1}{2}m\dot{\xi}^2 - \frac{1}{2}V''(\bar{q})\xi^2\right] + \cdots$$

$$S(q) = S_c(\bar{q}) + \cancel{\int_{t_i}^{t_f} dt \frac{d}{dt}(m\dot{\bar{q}}\xi)}^{\,0} - \int_{t_i}^{t_f} dt \left[m\frac{d^2\bar{q}}{dt^2} + V'(\bar{q})\right]\xi(t)$$
$$+ \int_{t_i}^{t_f} dt \left[\frac{1}{2}m\dot{\xi}^2 - \frac{1}{2}V''(\bar{q})\xi(t)^2\right] + O(\xi^3)$$

L13

$$\Rightarrow \quad \langle q't' | q t \rangle = e^{\frac{i}{\hbar} S_c(\bar{q}, \dot{\bar{q}})} \times \int \mathcal{D}\xi(t)\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt \left[\frac{1}{2} m \dot{\xi}^2 - \frac{1}{2} V''(\bar{q})\xi^2\right]} \left[1 + O(\hbar)\right]$$

In WKB we neglect $O(\hbar) = O(\xi^3)$

$\Rightarrow$ at the semiclassical level we need to compute path integrals of quadratic forms.

$$Z = \int_{\xi(t_i)=\xi(t_f)=0} \mathcal{D}\xi[t]\; e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\left[\frac{1}{2} m \left(\frac{d\xi}{dt}\right)^2 - \frac{1}{2} V''(\bar{q})\xi^2\right]}$$

$$\equiv \int \mathcal{D}\xi[t]\; e^{\frac{i}{2\hbar}\int_{t_i}^{t_f} dt\, \xi(t)\left[-m\frac{d^2}{dt^2} - V''(\bar{q})\right]\xi(t)}$$

$$\equiv \langle 0, t_f | 0, t_i \rangle$$

$$\left[\int_{t_i}^{t_f} dt \left(\frac{d\xi}{dt}\right)^2 = \int_{t_i}^{t_f} dt \left[\frac{d}{dt}\left(\xi \frac{d\xi}{dt}\right) - \xi\frac{d^2}{dt^2}\xi\right] = \underbrace{\xi\frac{d\xi}{dt}\Big|_{t_i}^{t_f}}_{=0} - \int_{t_i}^{t_f} dt\, \xi \frac{d^2}{dt^2}\xi\right]$$

L14

<u>How do we compute these integrals?</u>

Consider the diff. operator $\hat{A} = -m\frac{d^2}{dt^2} - V''(\bar{q})$

[where $\bar{q}(t)$ is the classical solution]

Let $\{\psi_n(t)\}$ be a complete set of eigenstates of $\hat{A}$,

$$\hat{A}\,\psi_n(t) = A_n\ \psi_n(t)$$

satisfying $\psi_n(t_i) = 0 \qquad \psi_n(t_f) = 0$

$$\Rightarrow \quad \Sigma_n\ \psi_n^*(t)\ \psi_n(t') = \delta(t-t') \qquad \text{(completeness)}$$

$$\int_{t_i}^{t_f} dt\ \psi_n^*(t)\ \psi_m(t) = \delta_{n,m}$$

$$\int_{t_i}^{t_f} dt\ |\psi_n(t)|^2 = 1 \qquad \text{(orthonormal real basis)}$$

Let us expand $\xi(t)$ in that basis

$$\xi(t) = \Sigma_n\ c_n\ \psi_n(t) \qquad \text{[orthogonal transf. of Jacobian 1]}$$

and the coeffs parametrize $\xi(t)$ (since $\{\psi_n(t)\}$ is complete)

$$\Rightarrow \int_{t_i}^{t_f} dt\ \xi(t)\ \hat{A}\ \xi(t) =$$

$$= \int_{t_i}^{t_f} dt \sum_{n,m} c_n\ \psi_n(t)\ \hat{A}\ c_m\ \psi_m(t)$$

$$= \int_{t_i}^{t_f} dt\ \Sigma_{n,m}\ c_n\, c_m\ A_m\ \psi_n(t)\psi_m(t)$$

$$= \Sigma_{n,m}\ c_n\, c_m\ A_m\ \delta_{n,m}$$

$$= \Sigma_n\ c_n^2\ a_n$$

$$Z = \int \left(\prod_n dc_n\right) e^{\frac{i}{2\hbar}\Sigma_n c_n^2 a_n} = \prod_n \left(\frac{-i\,A_n}{2\pi\hbar}\right)^{-1/2}$$

$$Z = \text{const} \times \left[\prod_n A_n\right]^{-1/2}$$

the determinant of a matrix M is

$\det M = \prod_n M_n$ (i.e. the product of the eigenvalues of M)

$\Rightarrow$ For an operator, the determinant is also the product of its eigenvalues

$$\mathrm{Det}\,\hat{A} = \prod_n A_n$$

$$\Rightarrow \quad Z = \text{const} \times \underline{\left[\mathrm{Det}\,\hat{A}\right]^{-1/2}} = \langle 0, t_f | 0, t_i \rangle$$

How to compute $\mathrm{Det}\,\hat{A}$

We first go to imaginary time and write

$$\hat{A} = -\frac{m}{\hbar^2}\frac{d^2}{d\tau^2} + V''(q)$$ [notice the change of the sign of V'']

Consider the following operator:

$$-\frac{\partial^2}{\partial x^2} + W(x) \qquad \text{with } x \in [0, L]$$

$$x = \frac{\hbar}{\sqrt{m}}\tau \qquad L = \frac{\beta\hbar}{\sqrt{m}}$$

Let $\psi(x)$ be an eigenvector of $-\frac{\partial^2}{\partial x^2} + W(x)$ with e.v. λ

$$-\frac{\partial^2}{\partial x^2}\psi + W(x)\psi = \lambda\psi$$

with $\psi(0) = \psi(L) = 0$

Define the function $\psi_\lambda(x)$ which

(1) is an eigenvector $-\frac{\partial^2}{\partial x^2}\psi_\lambda + W(x)\,\psi_\lambda = \lambda\,\psi_\lambda$

(2) it obeys initial conditions $\psi_\lambda(0) = 0$

$\partial_x \psi(0) = 1$ (slope)

$\Rightarrow$ $-\partial^2 + W$ has an e.v. λ_n iff $\psi_{\lambda_n}(L) = 0$

and $\mathrm{Det}\,(-\partial^2 + W) = \prod_n \lambda_n$

where λ_n are the zeroes of $\psi_\lambda(x)$ at $x = L$.

Consider two potentials W_1 and W_2 and the corresponding functions are ψ_1 and ψ_2.

$\Rightarrow$ we can show that

$$\frac{\mathrm{Det}\,(-\partial^2 + W_1 - \lambda)}{\mathrm{Det}\,(-\partial^2 + W_2 - \lambda)} = \frac{\psi_\lambda^{(1)}(L)}{\psi_\lambda^{(2)}(L)}$$

indeed, the l.h.s. is a meromorphic function of λ (in the complex λ plane) that has zeros (simple) at the e.v's of $-\partial^2 + W_1$ and poles at the e.v's of $-\partial^2 + W_2$ and it approaches 1 as $\lambda \to \infty$ everywhere except along the pos. real axis (spectrum).

The r.h.s. is also meromorphic and, by construction, it has the same zeros and poles and it also approaches 1 at ∞ (again except along $\mathrm{Re}\,\lambda > 0$)

$\Rightarrow$ $\dfrac{\text{l.h.s.}}{\text{r.h.s.}}$ is analytic everywhere and goes to 1 as $|\lambda| \to \infty$ (except ...) $\Rightarrow$ by the fundamental thm. of complex functions it is equal to 1 everywhere (and can be extended to 1 on $\mathrm{Re}\,\lambda > 0$)

$$\Rightarrow \frac{\mathrm{Det}\,(-\partial^2 + W_1 - \lambda)}{\psi_\lambda^{(1)}(L)} = \frac{\mathrm{Det}\,(-\partial^2 + W_2 - \lambda)}{\psi_\lambda^{(2)}(L)} = \text{const.}$$

indep. of W!

L15

$$\Rightarrow N \cdot \left[\mathrm{Det}\,(-\partial^2 + W)\right]^{-1} = \left[2\pi\hbar\, \psi_0(L)\right]^{-1} \qquad = \pi\hbar^2 N$$

normalization of P.I.

All we need is the "zero mode" $\psi_0(x)$ at $x = L$.

H.O. $\quad W = \omega^2$

$$\left[-\partial^2 + m\omega^2\right]\psi_0 = 0$$

$$\psi_0(0) = 0 \qquad \partial_x \psi_0\big|_0 = 1$$

$$\psi_0 = a\, e^{\sqrt{m}\,\omega x} + b\, e^{-\sqrt{m}\,\omega x} \Rightarrow a = -b = \frac{1}{2\omega\sqrt{m}}$$

$$\varphi_0(x) = \frac{\sinh \sqrt{m}\,\omega x}{\sqrt{m}\,\omega}$$

$$\Rightarrow \quad N\left[\mathrm{Det}\left(-\frac{\partial^2}{\partial x^2} + m\omega^2\right)\right]^{-1/2} = \left[\frac{\pi\hbar}{\sqrt{m}\,\omega}\sinh\sqrt{m}\,\omega L\right]^{-1/2}$$

$$Z = \left[\frac{\pi\hbar}{\sqrt{m}\,\omega}\sinh\omega\beta\hbar\right]^{-1/2}$$

For large β ($\beta\hbar\omega \gg 1$) we get

$$Z \simeq \left[\frac{\pi\hbar}{\sqrt{m}\,2\omega}e^{\beta\hbar\omega}\right]^{1/2}$$

or, at real (large) times $T = t_f - t_i$

$$Z \approx \left[\frac{\pi\hbar}{\sqrt{m}\,2\omega}e^{i\cancel{\hbar}\omega T/\cancel{\hbar}}\right]^{1/2}$$

$$Z(T) \simeq \left(\frac{\pi\hbar}{2\omega\sqrt{m}}\right)^{1/2} e^{\frac{i}{2}\omega T}$$

(a) Probab. of return after a long time T

$$|\langle 0,T|0,0\rangle|^2 = |Z(T)|^2 = \frac{\pi\hbar}{2\sqrt{m}\,\omega}$$

(b) <u>Gnd. State Energy:</u>

$$E_0 = -\lim_{\beta\to\infty}\frac{1}{\beta}\ln Z = \lim_{\beta\to\infty}\frac{1}{2\beta}\ln\left[\frac{\pi\hbar}{\sqrt{m}\,\omega}\sinh\beta\hbar\omega\right]$$

$$= \lim_{\beta\to\infty}\frac{1}{2\beta}\ln\left[\frac{\pi\hbar}{\sqrt{m}\,\omega}\frac{e^{\beta\hbar\omega}}{2}\left(1-\cancel{e^{-2\beta\hbar\omega}}\right)\right]$$

$$\simeq \frac{\hbar\omega}{2} + \frac{1}{2\beta}\ln\frac{\pi\hbar}{2\omega\sqrt{m}} + \cdots \longrightarrow \frac{\hbar\omega}{2} \quad \text{(as it should)}$$

L 15

Examples

(a) Free particle propagation $\langle q_f t_f | q_i t_i \rangle$

for $H = \dfrac{\hat{p}^2}{2m}$

$$q(t) = \bar{q}(t) + \xi(t)$$

/ $q(t_f) = q_f \qquad q(t_i) = q_i$

$$\Rightarrow \quad \bar{q}(t_f) = q_f \qquad \bar{q}(t_i) = q_i$$

while $\xi(t_f) = \xi(t_i) = 0$

$$\frac{i}{\hbar}\int_{t_i}^{t_f} dt \ \frac{m}{2}\left(\frac{dq}{dt}\right)^2 =$$

$$= \frac{i}{\hbar}\int_{t_i}^{t_f} dt \ \frac{m}{2}\left(\frac{d\bar{q}}{dt}\right)^2 + \frac{i}{\hbar}\int_{t_i}^{t_f} dt \ \frac{m}{2}\left(\frac{d\xi}{dt}\right)^2$$

where $\dfrac{d^2\bar{q}}{dt^2} = 0$ (free particle)

$$\frac{d\bar{q}}{dt} = v = \text{const.}$$

$$\bar{q}(t) = v(t - t_i) + q_i$$

$$v = \frac{q_f - q_i}{t_f - t_i} \qquad \Delta t = t_f - t_i$$

$$\frac{i}{\hbar}\int_{t_i}^{t_f} dt \ \frac{1}{2} m v^2 = \frac{i}{\hbar}\frac{m}{2} v^2 \Delta t = \frac{i}{\hbar}\frac{m}{2}\frac{(\Delta q)^2}{(\Delta t)^{\cancel{2}}}\cancel{\Delta t}$$

$$= \frac{i}{2\hbar} m \frac{(\Delta q)^2}{\Delta t}$$

$$\Rightarrow \quad \langle q_f\, t_f | q_i, t_0 \rangle = e^{\frac{i}{2\hbar} m \frac{(\Delta q)^2}{\Delta t}} \langle 0, t_f | 0, t_i \rangle$$

$$\langle 0, t_f | 0, t_0 \rangle = \lim_{\omega \to 0} Z\,[\text{Harmonic Oscillator}]$$

$$= \lim_{\omega \to 0} \left(\frac{2\pi \hbar i}{\sqrt{m}\, \omega} \sin \omega \Delta t \right)^{-1/2}$$

$$= \left(\frac{2\pi \hbar i}{\sqrt{m}} \Delta t \right)^{-1/2} \qquad \begin{bmatrix} \Delta q = q_f - q_i \\ \Delta t = t_f - t_i \end{bmatrix}$$

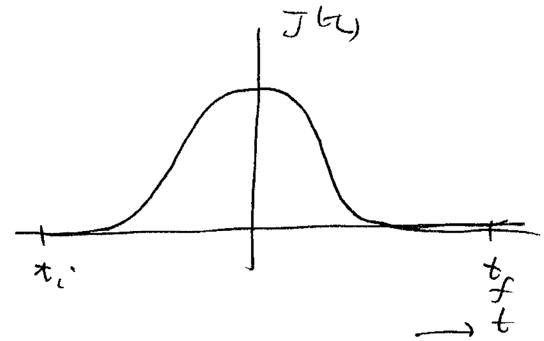
$$\Rightarrow \quad \langle q_f\, t_f | q_i\, t_0 \rangle = \left(\frac{2\pi \hbar i}{\sqrt{m}} \Delta t \right)^{-1/2} e^{\frac{i}{2\hbar} m (\Delta q)^2 / \Delta t}$$

(Imaginary time $\Delta t \to -i\tau$

$$\Rightarrow \quad \langle q_f, \tau | q_i, 0 \rangle = \left(\frac{2\pi \hbar \tau}{\sqrt{m}} \right)^{-1/2} e^{-\frac{m}{2\hbar} \frac{(\Delta q)^2}{\tau}} \Bigg]$$

$$|\langle q_f, T | 0, q_i \rangle|^2 \sim \frac{\sqrt{m}}{\pi \hbar |\Delta t|}$$

(b) Forced Harmonic Oscillator



$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{Q}^2 - \hat{J} \hat{Q}$$

where $\hat{J}(t) \longrightarrow 0$ as $t \to \pm\infty$

I want to compute $\langle q_f\, t_f | q_i\, t_i \rangle_J$ with $t_i \to -\infty$, $t_f \to +\infty$

$$\langle q_f\, t_f | q_i\, t_i \rangle_J = \int_{\substack{q(t_i)=q_i \\ q(t_f)=q_f}} \mathcal{D}q \; e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt \left\{ \frac{1}{2} m \left(\frac{dq}{dt}\right)^2 - \frac{1}{2} m\omega^2 q^2 + Jq \right\}}$$

The argument of the exponential (i.e. the action) is a quadratic functional of $q(t)$ and $\frac{dq}{dt}$. We will solve this problem by shifting $q(t)$ in such a way that we eliminate the term linear in q. That is we will write

$$q(t) = \bar{q}(t) + \xi(t) \quad / \quad \bar{q}(t_i) = q_i\,;\ \bar{q}(t_f) = q_f \qquad \xi(t_i) = \xi(t_f) = 0$$

and determine $\bar{q}(t)$ from the requirement that there are no terms linear in $\xi(t)$ or in $\frac{d\xi}{dt}$. [This is the same as completing squares).

$$\int_{t_i}^{t_f} dt \left\{ \frac{1}{2} m \left(\frac{dq}{dt}\right)^2 - \frac{1}{2} m\omega^2 q^2 + Jq \right\} =$$

$$= \int_{t_i}^{t_f} dt \left\{ \frac{1}{2} m \left(\frac{d\bar{q}}{dt}\right)^2 - \frac{1}{2} m\omega^2 \bar{q}^2 + J\bar{q} \; + \right.$$

$$+ \frac{1}{2} m \left(\frac{d\xi}{dt}\right)^2 - \frac{1}{2} m\omega^2 \xi^2$$

$$\left. + m \frac{d\bar{q}}{dt}\frac{d\xi}{dt} - m\omega^2 \bar{q}\xi + J\xi \right\}$$

$$= \int_{t_i}^{t_f} dt \left\{ \frac{1}{2} m \dot{\bar{q}}^2 - \frac{1}{2} m\omega^2 \bar{q}^2 + J\bar{q} \right\} + \int_{t_i}^{t_f} dt \left\{ \frac{1}{2} m \dot{\xi}^2 - \frac{1}{2} m\omega^2 \xi^2 \right\}$$

+ linear terms

$$\text{linear term} = \int_{t_i}^{t_f} dt \; \xi \left[-m \frac{d^2\bar{q}}{dt^2} - m\omega^2 \bar{q} + J \right] + m \xi \frac{d\bar{q}}{dt}\Big|_{t_i}^{t_f}$$

The linear terms vanish if we choose $\bar{q}$ /

$$m \frac{d^2\bar{q}}{dt^2} + m\omega^2 \bar{q} = J(t)$$

[the term $m \xi \frac{d\bar{q}}{dt}\Big|_{t_i}^{t_f} = 0$ with the BC's we chose for ξ]

Thus, we need to solve a diff. equation

$$\frac{d^2\bar{q}}{dt^2} + \omega^2 \bar{q} = \frac{1}{m} J(t)$$

$$\bar{q}(t_i) = q_i \, , \quad \bar{q}(t_f) = q_f$$

Before solving this equation, we notice that the amplitude we want to compute can be written in the much simpler form

$$\langle q_f t_f | q_i t_i \rangle_J = e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \left\{ \frac{1}{2} m \dot{\bar{q}}^2 - \frac{1}{2} m\omega^2 \bar{q}^2 + J\bar{q} \right\}} \times$$

$$\times \langle 0 t_f | 0 t_i \rangle_{J=0}$$

$$\langle 0 t_f | 0 t_i \rangle_{J=0} = \int_{\xi(t_i)=\xi(t_f)=0} \mathcal{D}\xi \; e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \left[\frac{1}{2} m \dot{\xi}^2 - \frac{1}{2} m\omega^2 \xi^2 \right]}$$

$$\int_{t_i}^{t_f} dt \left\{ \frac{1}{2} m \dot{\bar{q}}^2 - \frac{1}{2} m\omega^2 \bar{q}^2 + J \bar{q} \right\} =$$

$$= \frac{1}{2} m \bar{q} \dot{\bar{q}} \Big|_{t_i}^{t_f} + \int_{t_i}^{t_f} dt \left\{ - \frac{m}{2} \ddot{\bar{q}} - \omega^2 \frac{m}{2} \bar{q} + J \right\} \bar{q}$$

But $\quad m \ddot{\bar{q}} + m\omega^2 \bar{q} = J$

$$\Rightarrow \quad S = \frac{1}{2} m \bar{q} \dot{\bar{q}} \Big|_{t_i}^{t_f} + \int_{t_i}^{t_f} dt \; \frac{1}{2} \bar{q}(t) J(t)$$

$$\Rightarrow \langle q_f t_f | q_i t_i \rangle_J = e^{\frac{i}{\hbar}\left[\frac{1}{2} m \bar{q} \dot{\bar{q}} \Big|_{t_f}^{t_i} \right]} e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \; \frac{1}{2} \bar{q}(t) J(t)} \times$$

$$\times \quad \langle 0 t_f | 0 t_i \rangle_{J=0}$$

We will work with the simpler problem

$q_i = q_f = 0 \quad$ and $\quad t_i \to -\infty \, , \; t_f \to +\infty$

$$\Rightarrow \lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} \langle 0 t_f | 0 t_i \rangle = e^{\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \; \frac{1}{2} \bar{q}(t) J(t)}$$

$$\lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} \langle 0 t_f | 0 t_i \rangle_{J=0}$$

We now need to solve

$$\frac{d^2 \bar{q}}{dt^2} + \omega^2 \bar{q} = \frac{1}{m} J(t)$$

subject to the conditions $\quad \lim_{t \to -\infty} \bar{q}(t) = \lim_{t \to +\infty} \bar{q}(t) = 0$

[recall that $\quad J \to 0 \quad$ as $t \to \pm\infty$]

L14

Use the Green function:

$$\bar{q}(t) = \frac{1}{m}\int_{-\infty}^{+\infty} dt'\; G(t,t')\; J(t')$$

$$\Rightarrow \frac{d^2\bar{q}}{dt^2} + \omega^2 \bar{q} = \frac{1}{m} J(t) \Rightarrow$$

$$\frac{d^2}{dt^2} G(t,t') + \omega^2 G(t,t') = \delta(t-t')$$

Obviously $G(t,t') = G(t-t')$

and it must satisfy

$$\lim_{t\to\pm\infty} G(t,t') = 0$$

Since the expression

$$\int_{-\infty}^{+\infty} dt\; \bar{q}(t)\, J(t) = \frac{1}{m}\int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt'\; J(t)\; G(t,t')\; J(t')$$

$$= \frac{1}{m}\int_{-\infty}^{+\infty} dt' \int_{-\infty}^{+\infty} dt\; J(t')\; G(t',t)\; J(t)$$

$$\Rightarrow G(t,t') = G(t',t)$$

and $G(t,t') = G(t-t') \Rightarrow G(t,t') = G(|t-t'|)$

Solve $\dfrac{d^2}{dt^2} G(t) + \omega^2 G(t) = \delta(t)$

by Fourier transform

$$G(t) = \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi}\; e^{i\Omega t}\; \tilde{G}(\Omega)$$

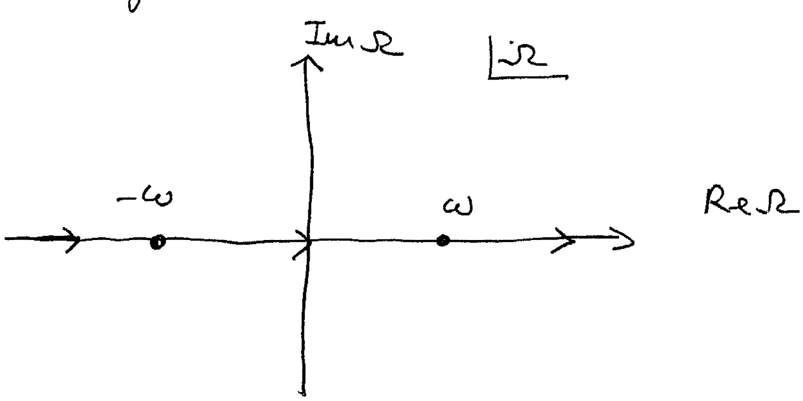
$$\Rightarrow \quad \delta(t) = \int \frac{d\Omega}{2\pi} \, e^{i\Omega t}$$

$$\Rightarrow \quad \int \frac{d\Omega}{2\pi} \, e^{i\Omega t} \left[-\Omega^2 + \omega^2 \right] \tilde{G}(\Omega) = \int \frac{d\Omega}{2\pi} \, e^{i\Omega t}$$

$$\Rightarrow \quad \tilde{G}(\Omega) = \frac{1}{\omega^2 - \Omega^2}$$

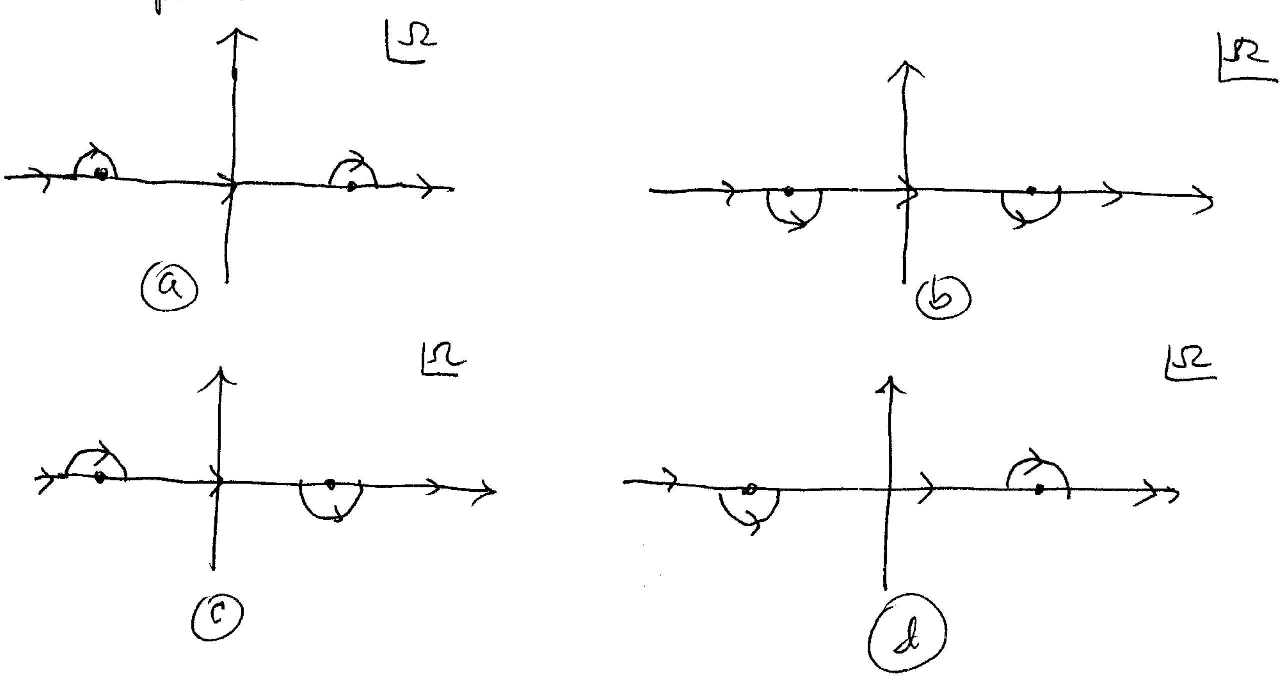
L16

Problem: $\tilde{G}(\Omega)$ has poles at $\Omega = \pm\omega$ which are on the real axis $\Rightarrow \int \frac{d\Omega}{2\pi} \tilde{G}(\Omega) e^{i\Omega t}$ is not well defined



I will choose the integration path s.t. the integral is well defined and the b.c.'s are satisfied

Four possibilities



We can do this integrals by residues since the $\int$ over large arcs $\Omega = Re^{i\phi}$ $(R \to \infty)$ converges in the following way

$$\frac{e^{i\Omega t}}{\omega^2 - \Omega^2} = \frac{e^{iRt\cos\phi - Rt\sin\phi}}{\omega^2 - R^2 e^{2i\phi}}$$

$\Rightarrow$ For $t>0$, it converges as $R\to\infty$ for $0 \leq \phi \leq \pi$

while for $t<0$, it converges as $R\to\infty$ for $-\pi \leq \phi \leq 0$

$\Rightarrow$ we must close the contour on the upper half plane for $t>0$ and on the lower half plane for $t<0$. The result (the ~~expression~~ of the integral) depends now on the choice of contour

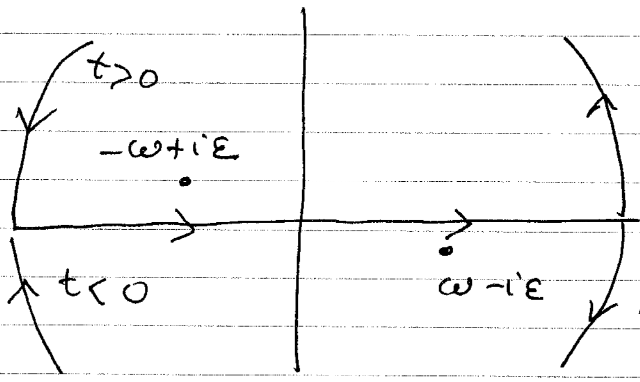
(a) $$\int_{(a)} \frac{d\Omega}{2\pi} \tilde{G}(\Omega)\, e^{i\Omega t} = \begin{cases} \frac{1}{2\pi} 2\pi i \sum_{res} G(\Omega) e^{i\Omega t} & t>0 \\ 0 & t<0 \end{cases}$$

$\Rightarrow$ $G(t) = 0$ for $t<0$ and $G(t) \neq 0$ for $t>0$

This is called the causal [retarded] GF and it does not obey $G(t) = G(-t)$

(b) is the same story but replacing $t>0$ with $t<0$ [advanced GF]

(c) and (d) are actually equivalent [(c) is anti-time ordered and (d) is time ordered]



$(\varepsilon \to 0)$

$$G(t) = \theta(t)\ \frac{2\pi i}{2\pi}\ \frac{e^{i(-\omega+i\varepsilon)t}}{-2(-\omega+i\varepsilon)} +$$

$$+\theta(-t)\ \frac{-2\pi i}{2\pi}\ \frac{e^{i(\omega-i\varepsilon)t}}{-2(\omega-i\varepsilon)}$$

$$G(t) = \theta(t)\ \frac{i}{2\omega}\ e^{-i\omega t-\varepsilon t} + \theta(-t)\ \frac{i}{2\omega}\ e^{i\omega t+\varepsilon t}$$

$$G(t) \underset{\varepsilon\to 0}{=} \frac{i}{2\omega}\ e^{-i\omega|t|-\varepsilon|t|}$$

$$G(t) = G(-t)$$

and $\lim_{t\to\pm\infty} G(t) = 0$

This is the G.F. we actually need.

$$\Rightarrow \lim_{\substack{t_i\to-\infty \\ t_f\to+\infty}} \langle 0 t_f | 0 t_i\rangle_J = e^{\frac{i}{2\hbar}\int_{-\infty}^{+\infty}dt\int_{-\infty}^{+\infty}dt'\ J(t)\ \frac{i}{2\omega m} e^{-i\omega|t-t'|-\varepsilon|t-t'|}\ J(t')}$$

$$\times \lim_{\substack{t_i\to-\infty \\ t_f\to+\infty}} \langle 0 t_f | 0 t_i\rangle_{J=0}$$

For example, for an impulsive force

$$J(t) = J\,\delta(t)$$

we get

$$\langle 0 t_f | 0 t_i \rangle_J = e^{-\frac{J^2}{4\hbar\omega m}} \langle 0 t_f | 0, t_i \rangle_{J=0}$$

$$\langle 0, t_f | 0, t_i \rangle_J = e^{-J^2/4\hbar\omega m} \left(\frac{\pi\hbar}{2\omega\sqrt{m}} \right)^{1/2} e^{i\omega T/2}$$

$$T = t_f - t_i$$

Notice that $[J(t)] = \frac{E}{L}$

and $J(t) = J\,\delta(t) \Rightarrow [J(t)] = [J]\,\frac{1}{T}$

$$\Rightarrow [J] = T\,\frac{E}{L}$$

$$\left[\frac{J^2}{m}\right] = \frac{T^2 E^2}{L^2}\,\frac{1}{[m]} = \frac{E^2}{[m v^2]} = E$$

$\Rightarrow \frac{J^2}{m}$ has units of energy: it is the kinetic energy acquired by the particle from the impulsive force.

$\Rightarrow \frac{J^2}{\hbar\omega m}$ is dimensionless.

$\Rightarrow$ Probab. of return $= |\langle 0, t_f | 0, t_i \rangle|^2 = e^{-\frac{1}{2}\frac{J^2/m}{\hbar\omega}}\,\frac{\pi\hbar}{2\omega\sqrt{m}}$

$\Rightarrow$ If $\frac{J^2}{m} \gg \hbar\omega \Rightarrow$ Probab. $\to 0$

$\frac{J^2}{m} \ll \hbar\omega \Rightarrow$ Probab $\to \frac{\pi\hbar}{2\sqrt{m}\,\omega}$ [same as probab. of return in gnd state]