Lec. 1

A primer on Quantum Mechanics

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Time evolution operator transforms the quantum mechanical state at an earlier time t_1 to a future time t_2 as

$$|\psi(t_2)\rangle = \hat{U}(t_2, t_1)\,|\psi(t_1)\rangle, \quad t_2 > t_1.$$

Clearly, for a time independent Hamiltonian, $\hat{U}(t_2, t_1) = e^{-\frac{i}{\hbar}\hat{H}(t_2 - t_1)}$, $t_2 > t_1$.

One can also write

$$\boxed{\hat{U}(t_2, t_1) = \theta(t_2 - t_1)\, e^{-\frac{i}{\hbar}\hat{H}(t_2 - t_1)}}.$$

This follows from the Schrödinger equation

$$i\hbar\,\partial_t |\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle,$$

$\hat{H}$ being time independent.

$$i\hbar\, \partial_{t_2} \hat{U}(t_2, t_1)$$

$$= i\hbar \Big[\partial_{t_2} \theta(t_2 - t_1)\, e^{-\frac{i}{\hbar}\hat{H}(t_2-t_1)} + \theta(t_2 - t_1)\left(-\frac{i}{\hbar}\hat{H}\right) e^{-\frac{i}{\hbar}\hat{H}(t_2-t_1)} \Big]$$

$$= i\hbar \Big[\delta(t_2 - t_1)\, e^{-\frac{i}{\hbar}\hat{H}(t_2-t_1)} - \frac{i}{\hbar}\, \theta(t_2 - t_1)\, \hat{H}\, e^{-\frac{i}{\hbar}\hat{H}(t_2-t_1)} \Big]$$

$$= i\hbar\, \delta(t_2 - t_1) + \theta(t_2 - t_1)\, \hat{H}.\, e^{-\frac{i}{\hbar}\hat{H}(t_2-t_1)}$$

$$= i\hbar\, \delta(t_2 - t_1) + \hat{H}\, \hat{U}(t_2, t_1).$$

$$\Rightarrow \left(i\hbar\, \partial_{t_2} - \hat{H}\right) \hat{U}(t_2, t_1) = i\hbar\, \delta(t_2 - t_1).$$

$\Rightarrow$ Time evolution operator is the Green's function.

Determining the operator is equivalent to finding its matrix elements in a given basis.

For example in the coordinate basis $\hat{q}\,|q\rangle = q\,|q\rangle$, one can write $\langle q_2 |\, \hat{U}(t_2, t_1)\, | q_1 \rangle$

$$\equiv U(q_2, t_2 ; q_1, t_1)$$

Knowing this function $U(q_2, t_2; q_1, t_1)$ completely gives the time evolution of the wave function as

$$\psi(q_2, t_2) = \int_{-\infty}^{+\infty} dq_1\, U(q_2, t_2 ; q_1, t_1)\, \psi(q_1, t_1)$$

kernel or Green's function

Path integrals in QM & QFT

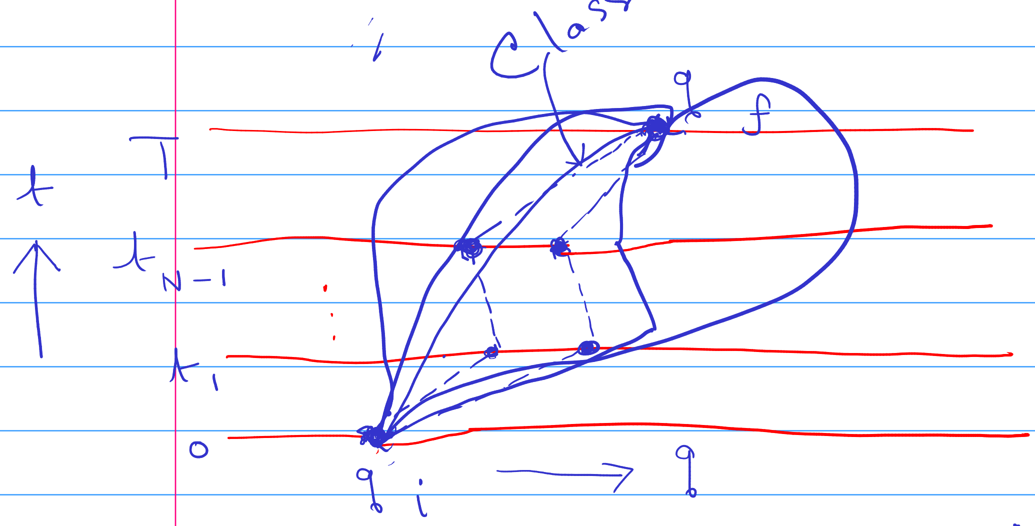
A basic quantity of interest in QM is the probability amplitude of transition to evolve from one q eigenstate to another in a time T.

$$\langle q_f | \, e^{-\frac{i}{\hbar}\hat{H} T} \, | q_i \rangle$$

basic ket

$$= \langle q_f, T | q_i, 0 \rangle \quad \ldots \quad (1)$$

$$| q, t \rangle = e^{\frac{i}{\hbar}\hat{H} t} | q \rangle \quad \ldots \quad (2)$$



$$| q, t \rangle \;\cancel{=}\; e^{\frac{i}{\hbar}\int^t H(t')\, dt'} | q \rangle$$

$$\hat{H}\left(\hat{p}(t), \hat{q}(t), \cancel{t}\right)$$

$$\int_{-\infty}^{+\infty} dq \, |q, t\rangle \langle q, t| = 1 \quad \ldots \; (3)$$

Ex. 1 Using $\int dq \, |q\rangle\langle q| = 1$,

prove eq. (3).

Hint: Use eq. (2).

Divide the time interval into N equal steps:

$$t_m = m\varepsilon \quad , \quad \varepsilon = T/N$$

$$N \to \infty \quad , \quad \varepsilon \to 0$$

$$t_N \equiv T = N\varepsilon$$

$$t_0 = 0$$

$$\langle q_f, T | q_i, 0 \rangle$$

$$= \int_{-\infty}^{+\infty} dq_{N-1} \ldots dq_1 \, \langle q_f, T | q_{N-1}, t_{N-1} \rangle \langle q_{N-1}, t_{N-1} | \ldots \ldots | q_1, t_1 \rangle \langle q_1, t_1 | q_i, 0 \rangle$$

$$= \int_{-\infty}^{+\infty} dq_{N-1} \cdots dq_1$$

$$\prod_{m=0}^{N-1} \langle q_{m+1}, \underline{t_{m+1}} | q_m, t_m \rangle$$

Translate back to Schrödinger picture

$$\langle q_{m+1}, t_{m+1} | q_m, t_m \rangle$$

$$= \langle q_{m+1} | e^{-\frac{i}{\hbar}\hat{H} t_{m+1}} e^{\frac{i}{\hbar}\hat{H} t_m} | q_m \rangle$$

$$= \langle q_{m+1} | e^{-\frac{i}{\hbar}\hat{H}(t_{m+1} - t_m)} | q_m \rangle$$

$$= \langle q_{m+1} | \mathbb{1} e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | q_m \rangle$$

$$= \int_{-\infty}^{+\infty} dp_m \langle q_{m+1} | p_m \rangle \langle p_m | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | q_m \rangle .$$

$$\int dp_m \, |p_m\rangle\langle p_m| = \mathbb{1}$$

Evaluation of the matrix element

$$\langle p_m | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | q_m \rangle$$

$$= \langle p_m | \mathbb{1} - \frac{i}{\hbar}\hat{H}\varepsilon + O(\varepsilon^2) | q_m \rangle$$

$$= \langle p_m | q_m \rangle - \frac{i}{\hbar}\varepsilon \langle p_m | \hat{H}(\hat{p}, \hat{q}) | q_m \rangle + O(\varepsilon^2)$$

$$= \langle p_m | q_m \rangle - \frac{i}{\hbar} \varepsilon H(p_m, q_m) \langle p_m | q_m \rangle + O(\varepsilon^2).$$

$$\Rightarrow \langle q_{m+1}, t_{m+1} | q_m, t_m \rangle$$

$$= \int dp_m \langle q_{m+1} | p_m \rangle \Big[\langle p_m | q_m \rangle - \frac{i}{\varepsilon} H(p_m, q_m) \langle p_m | q_m \rangle + O(\varepsilon^2) \Big]$$

$$= \int dp_m \langle q_{m+1} | p_m \rangle \langle p_m | q_m \rangle \Big[1 - \frac{i}{\hbar} \varepsilon H(p_m, q_m) + O(\varepsilon^2) \Big].$$

$$\simeq \int dp_m \, e^{-\frac{i}{\hbar} H(p_m, q_m)\varepsilon} \langle q_{m+1} | p_m \rangle \langle p_m | q_m \rangle$$

$$= \int \frac{dp_m}{2\pi\hbar} e^{-\frac{i}{\hbar}\left[H(p_m, q_m)\varepsilon - p_m(q_{m+1} - q_m) \right]}$$

Dirac - δ normalization

$$\langle p_m | q_m \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar} p_m q_m}$$

$$\langle q_{m+1} | p_m \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p_m q_{m+1}} .$$

$$\langle q_f, T | q_i, 0 \rangle = \int_{-\infty}^{+\infty} \prod_{i=1}^{N-1} dq_i \prod_{m=0}^{N-1} \int_{-\infty}^{+\infty} \frac{dp_m}{2\pi\hbar} \times e^{-\frac{i}{\hbar}\left[H(p_m, q_m)\varepsilon - p_m(q_{m+1} - q_m) + O(\varepsilon^2)\right]}$$

$$= \int \frac{dp_{N-1}}{2\pi\hbar} dq_{N-1} \cdots \frac{dp_1}{2\pi\hbar} dq_1 \frac{dp_0}{2\pi\hbar} \times e^{-\frac{i}{\hbar} \sum_{m=0}^{N-1} \underbrace{\left[H(p_m, q_m)\varepsilon - p_m(q_{m+1} - q_m) + O(\varepsilon^2)\right]}}$$

$$= \varepsilon \left[H(p_m, q_m) - p_m \frac{(q_{m+1} - q_m)}{\varepsilon} + O(\varepsilon)\right]$$

$\lim \varepsilon \to 0$

$$= \int_{q_{i,0}}^{q_{f,T}} [\mathcal{D}p \, \mathcal{D}q] \, e^{\frac{i}{\hbar} \int_0^T dt \left[p\dot{q} - H(p,q) \right]} .$$

Phase - space path integral

$$\langle q_f, T | q_i, 0 \rangle = \int [\mathcal{D}p \, \mathcal{D}q]_{q_i,0}^{q_f,T} \, e^{\frac{i}{\hbar}\int_0^T dt \left[p\dot{q} - H(p,q) \right]} . \quad \ldots \quad (4)$$

The integral runs over all paths $p(t)$ and $q(t)$ in phase-space with given $q(T)$ and $q(0)$ in the $\varepsilon \to 0$ limit.

This is the Hamiltonian path integral or functional integral, the sum over phase-space paths weighted by $e^{\frac{i}{\hbar}S}$ with S being the action in the Hamiltonian form.

Stationary phase approximation

The integral is dominated by the point of stationary phase.

$$0 = \frac{\partial}{\partial p}\left[p\dot{q} - H(p, q) \right]$$

$$= \dot{q} - \frac{\partial H(p, q)}{\partial p}$$

$$= \dot{q} - f(p, q)$$

$$\Rightarrow \dot{q} = f(p, q)$$

$$\Rightarrow p = g(q, \dot{q})$$

$$\Rightarrow p\dot{q} - H(p, q)$$

$$= g(q, \dot{q})\,\dot{q} - H(g(q, \dot{q}), q)$$

$$= L(q, \dot{q}) \ldots$$

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Lagrangian Path Integral

$$\langle q_f, T | q_i, 0 \rangle = \int [\mathcal{D}p\,\mathcal{D}q]_{q_{i,0}}^{q_{f,T}} e^{\frac{i}{\hbar}\int_0^T dt[p\dot{q} - H(p,q)]}$$

$$\simeq \int [\mathcal{D}p\,\mathcal{D}q]_{q_{i,0}}^{q_{f,T}} \delta[p - g(q,\dot{q})] \times e^{\frac{i}{\hbar}\int_0^T dt\,[p\dot{q} - H(p,q)]}$$

$$= \int [\mathcal{D}q]_{q_{i,0}}^{q_{f,T}} e^{\frac{i}{\hbar}\int_0^T dt[g(q,\dot{q})\dot{q} - H(g(q,\dot{q}),q)]}$$

$$= \int [\mathcal{D}q]_{q_{i,0}}^{q_{f,T}} e^{\frac{i}{\hbar}\int_0^T dt\, L(q,\dot{q})}$$

$$= \int [\mathcal{D}q]_{q_{i,0}}^{q_{f,T}} e^{\frac{i}{\hbar}S[q]} \quad \ldots\ldots \quad (6)$$

This is the Lagrangian path integral, the integral over all paths $q(t)$ in configuration space weighted by $e^{\frac{i}{\hbar}S}$, where now S is the Lagrangian action.

CLASSICAL LIMIT

As $\hbar \to 0$, the integral is dominated by the paths of stationary phase,

$$\frac{\delta S}{\delta q(t)} = 0,$$ which is indeed the classical equation of motion.

NON-RELATIVISTIC HAMILTONIAN

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

Lets write down the phase-space path integral once more.

$$\langle q_f, T | q_i, 0\rangle = \int [\mathcal{D}p\, \mathcal{D}q]_{q_{i,0}}^{q_{f,T}}\, e^{\frac{i}{\hbar}\int_0^T dt\,[p\dot{q} - H(p,q)]}$$

$$= \int_{-\infty}^{+\infty} dq_{N-1} \frac{dp_{N-1}}{2\pi\hbar} \cdots dq_1 \frac{dp_1}{2\pi\hbar} \frac{dp_0}{2\pi\hbar} \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \times e^{\frac{i}{\hbar}\varepsilon \sum_{m=0}^{N-1} \left[p_m\left(\frac{q_{m+1}-q_m}{\varepsilon}\right) - H(p_m, q_m)\right]}.$$

with the non-relativistic Hamiltonian, the p-integrals are Gaussian.

Carrying out the m^{th} p - integral

$$\int_{-\infty}^{+\infty} \frac{dp_m}{2\pi\hbar}\, e^{-\frac{i}{\hbar}\varepsilon\left[\frac{p_m^2}{2m} - \frac{(q_{m+1}-q_m)}{\varepsilon}p_m\right]}$$

$$= \int_{-\infty}^{+\infty} \frac{dp_m}{2\pi\hbar}\, e^{-\frac{i\varepsilon}{2m\hbar}\left[\left\{p_m - \frac{m(q_{m+1}-q_m)}{\varepsilon}\right\}^2 - 4m^2\frac{(q_{m+1}-q_m)^2}{4\varepsilon^2}\right]}$$

$$\int_{-\infty}^{+\infty} e^{-ax^2}\,dx = \sqrt{\frac{\pi}{a}} \quad Re(a) > 0$$

$$= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\, e^{\frac{im}{2\hbar\varepsilon}(q_{m+1}-q_m)^2}.$$

$$\langle q_f, T \,|\, q_i, 0\rangle = \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2}$$

$$\times \int_{-\infty}^{+\infty} dq_{N-1}\ldots dq_1\, e^{\frac{i}{\hbar}\varepsilon\sum_{m=0}^{N-1}\left[\frac{m}{2}\left(\frac{q_{m+1}-q_m}{\varepsilon}\right)^2 - V(q_m)\right]}$$

$$= \int [\mathcal{D}q]_{q_{i,0}}^{q_{f,T}}\, e^{\frac{i}{\hbar}\int_0^T L\,dt}$$

$$= \int [\mathcal{D}q]_{q_{i,0}}^{q_{f,T}}\, e^{\frac{i}{\hbar}S[q]}.$$

Free particle path integral

$V(q) = 0$

$\langle q_f, T | q_i, 0 \rangle$

$$= \lim_{\substack{\varepsilon \to 0 \\ N \to \infty}} A \int_{-\infty}^{+\infty} dq_{N-1} \ldots dq_1 \, e^{\frac{i\varepsilon}{\hbar} \sum_{m=0}^{N-1} \frac{m}{2} \left(\frac{q_{m+1} - q_m}{\varepsilon} \right)^2},$$

$$A = \left(\frac{m}{2\pi i \hbar \varepsilon} \right)^{N/2}.$$

One of the ways to work with this integral is to work a few lower ones and then derive a pattern.

Let us perform the q_1- integral first.

$$\int_{-\infty}^{+\infty} dq_1 \, e^{\frac{i\varepsilon}{\hbar} \frac{m}{2\varepsilon^2} \left[(q_1 - q_0)^2 + (q_2 - q_1)^2 \right]}$$

$$= \sqrt{\frac{2 i \pi \hbar \varepsilon}{m}} \frac{1}{\sqrt{2}} \, e^{\frac{i m}{2\hbar\varepsilon} \frac{1}{2} (q_2 - q_0)^2}.$$

q_2 - integral

$$\int_{-\infty}^{+\infty} dq_2 \, e^{\frac{i}{\hbar}\frac{m}{2\varepsilon}(q_3-q_2)^2} \, e^{\frac{im}{4\hbar\varepsilon}(q_2-q_0)^2}$$

$$= \sqrt{\frac{2\pi i\hbar\varepsilon}{m}} \sqrt{\frac{2}{3}} \, e^{\frac{im}{2\hbar\varepsilon}\frac{1}{3}(q_3-q_0)^2}$$

$$\langle q_f, T \mid q_i, 0\rangle = \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2}$$

$$\times \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{(N-1)/2} \frac{1}{\sqrt{N}} \, e^{\frac{im}{2\hbar\varepsilon}\frac{1}{N}(q_N-q_0)^2}$$

$$= \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \frac{1}{\sqrt{N}} \, e^{\frac{im}{2\hbar\varepsilon N}(q_N-q_0)^2}$$

$$= \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \sqrt{\frac{m}{2\pi i\hbar N\varepsilon}} \, e^{\frac{im}{2\hbar N\varepsilon}(q_N-q_0)^2}$$

$$= \sqrt{\frac{m}{2\pi i\hbar T}} \, e^{\frac{im}{2\hbar T}(q_f-q_i)^2} \quad ; \; q_N \equiv q_f, \; q_0 \equiv q_i$$

NOTE: As $T \to 0$, $\langle q_f, T | q_i, 0 \rangle \to \delta(q_f - q_i)$

which is the orthonormality relation for states in the Heisenberg picture.

• Imaginary time formalism

Let us consider the time evolution operator $\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}$.

Set $t = -i\tau \Rightarrow \hat{U}(\tau = it) = e^{-\frac{1}{\hbar}\hat{H}\tau}$.

This would have been the time evolution operator if the Schrödinger equation had been

$$-\hbar \frac{d}{d\tau} | \psi(\tau) \rangle = \hat{H} | \psi(\tau) \rangle .$$

A formula for $\hat{U}(\tau)$ can be written down at once

$$\hat{u}(\tau) = \sum_n |n\rangle\langle n|\, \hat{u}(\tau)$$

$$= \sum_n |n\rangle\langle n|\, e^{-\frac{1}{\hbar}\hat{H}\tau}$$

$$= \sum_n |n\rangle\langle n|\, e^{-\frac{1}{\hbar}E_n\tau},$$

$$\hat{H}|n\rangle = E_n|n\rangle.$$

The main point to note is that even though the time is now imaginary, the eigenvalues and eigenfunctions that enter into the formula for $\hat{u}(\tau)$ are the usual ones.

$$t = -i\,\underset{\sim}{t} \implies \underset{\sim}{t} = it$$

$$t = 0,\ \underset{\sim}{t} = 0\ ;\ t = T,\ \underset{\sim}{t} = iT = \tau.$$

$$u(x,\tau;x',0) = \langle x,\tau|x',0\rangle$$

$$= \int [\mathcal{D}x]_{x',0}^{x,\tau}\, e^{\frac{i}{\hbar}\int_0^\tau (-i\,d\underset{\sim}{t})\left[\frac{m}{2}\left(\frac{dx}{d\underset{\sim}{t}}\frac{d\underset{\sim}{t}}{dt}\right)^2 - V(x(\underset{\sim}{t}))\right]}$$

$$= \int [\mathcal{D}x]_{x',0}^{x,\tau} \, e^{-\frac{1}{\hbar}\int_0^\tau d\underset{\sim}{t} \left[\frac{m}{2}\left(\frac{dx}{d\underset{\sim}{t}}\right)^2 + V(x(\underset{\sim}{t}))\right]}$$

$$= \int [\mathcal{D}x]_{x',0}^{x,\tau} \, e^{-\frac{1}{\hbar} S_E} \longrightarrow \underline{\text{Euclidean path integral}}$$

$$S_E = \int_0^\tau dt \left[\frac{m}{2}\dot{x}(t)^2 + V(x(t))\right]$$

$$\equiv \int_0^\tau dt \, L_E(x(t), \dot{x}(t)) \longrightarrow \underline{\text{Euclidean action}}$$

- **Connection with Statistical mechanics**

$$Z = \mathrm{tr}\left(e^{-\beta \hat{H}}\right)$$

$$= \sum_n \langle n | e^{-\beta \hat{H}} | n \rangle, \quad \hat{H}|n\rangle = E_n |n\rangle$$

$$= \sum_n \langle n | e^{-\beta E_n} | n \rangle$$

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

Now we exploit the fact that the trace is invariant under a unitary change of basis and switch to the x-basis to obtain

$$Z = \int_{-\infty}^{+\infty} dx \, \langle x | e^{-\beta \hat{H}} | x \rangle$$

$$= \int_{-\infty}^{+\infty} \mathcal{U}(x, \beta\hbar \, ; x, 0) \, dx \, ,$$

$$\langle x | e^{-\beta \hat{H}} | x \rangle = \langle x | e^{-\frac{1}{\hbar} \beta \hbar \hat{H}} | x \rangle$$

$$= \mathcal{U}(x, \beta\hbar \, ; x, 0) .$$

Hence, the partition function Z is the sum over amplitudes to go from the point x back to the point x in imaginary time $\tau = \beta\hbar$.

$$Z(\beta) = \int_{-\infty}^{+\infty} dx \int [\mathcal{D}x]_{x,0}^{x,\beta\hbar} \, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar}\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x(\tau))\right] d\tau}$$

Periodic path integral

Remark: A $(D+1)$-dimensional Euclidean quantum field theory can be related to a D-dimensional quantum statistical system since the Euclidean time interval can be consistently identified with $\beta = \frac{1}{k_B T}$.