The Feynman-Dirac Path Integral

Schrödinger: $i\hbar\,\partial_t|\psi\rangle = \hat{H}|\psi\rangle$

Formal sol$^{\underline{n}}$: $|\psi(t')\rangle = \hat{U}(t',t)|\psi(t)\rangle$

For a time-indep. $\hat{H}$: $\hat{U}(t',t) = e^{-\frac{i}{\hbar}\hat{H}(t'-t)}$

Consider a real-~~space~~ set of ~~states~~ $|q\rangle$ ← particle at position q

$$\psi(q',t') = \langle q'|\psi(t')\rangle = \langle q'|\hat{U}(t',t)\overset{\mathbb{1}=\int dq\,|q\rangle\langle q|}{\downarrow}|\psi(t)\rangle = \int dq\, U(q',t';q,t)\,\psi(q,t)$$

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

is known as the propagator of the theory with $\hat{H}$

From now on: let $t \to 0$, $t' \to t$ so $U(q';t;q,0)$

Need to study $e^{-\frac{i}{\hbar}\hat{H}t}$. Strategy: let $t = \Delta t \cdot N$, $N \to \infty$

so $e^{-\frac{i}{\hbar}\hat{H}t} = \left[e^{-\frac{i}{\hbar}\hat{H}\Delta t} \right]^N$ Assume $\hat{H} = \hat{T} + \hat{V}$

Then:
$$e^{-\frac{i}{\hbar}\hat{H}\Delta t} = e^{-\frac{i}{\hbar}(\hat{T}+\hat{V})\Delta t} = 1 - \frac{i}{\hbar}(\hat{T}+\hat{V})\Delta t + \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2(\hat{T}+\hat{V})^2\Delta t^2 + \dots$$

$$= \left[1 - \frac{i}{\hbar}\hat{T}\Delta t + O(\Delta t^2)\right]\left[1 - \frac{i}{\hbar}\hat{V}\Delta t + O(\Delta t^2)\right] + O(\Delta t^2)$$

$$= e^{-\frac{i}{\hbar}\hat{T}\Delta t}\, e^{-\frac{i}{\hbar}\hat{V}\Delta t} + O(\Delta t^2)$$

$\sim [\hat{T}, \hat{V}]\Delta t^2$ dropped

If $[a,b]=0$, then
$$e^{a+b} = e^a e^b$$

<u>BUT</u>: if $[a,b] \neq 0$, then $e^{a+b} \neq e^a e^b$

The propagator can be approximated as

$$\mathbb{1}_i \equiv \mathbb{1}_{q_i} \mathbb{1}_{p_i}$$

$$\langle q_f | \left[e^{-\frac{i}{\hbar}\hat{H}\Delta t} \right]^N | q_i \rangle = \langle q_f | \underbrace{\mathbb{1}_N e^{-\frac{i}{\hbar}\hat{T}\Delta t} e^{-\frac{i}{\hbar}\hat{V}\Delta t} \mathbb{1}_{N-1} e^{-\frac{i}{\hbar}\hat{T}\Delta t} e^{-\frac{i}{\hbar}\hat{V}\Delta t} \cdots e^{-\frac{i}{\hbar}\hat{T}\Delta t} e^{-\frac{i}{\hbar}\hat{V}\Delta t}}_{N \text{ time steps}} | q_i \rangle$$

Insert useful resolutions of identity

$$\mathbb{1}_q = \int dq \, |q\rangle\langle q| \qquad \mathbb{1}_p = \int dp \, |p\rangle\langle p|$$

"coordinate" variable

"momentum"

Typical sub-product:
$$\ldots e^{-\frac{i}{\hbar}\hat{V}\Delta t} \int dq_n |q_n\rangle\langle q_n| \int dp_n |p_n\rangle\langle p_n| e^{-\frac{i}{\hbar}\hat{T}\Delta t} \ldots$$

Now: assume that

$$\hat{V} = V(\hat{q}) \quad \& \quad \hat{T} = T(\hat{p}),$$

Now: $\hat{q}|q_n\rangle = q_n|q_n\rangle$

& $\hat{p}|p_n\rangle = p_n|p_n\rangle$

Thus:
$$e^{-\frac{i}{\hbar}V(\hat{q})\Delta t}|q_n\rangle = e^{-\frac{i}{\hbar}V(q_n)\Delta t}|q_n\rangle \quad \& \quad \langle p_n|e^{-\frac{i}{\hbar}T(\hat{p})\Delta t} = e^{-\frac{i}{\hbar}T(p_n)\Delta t}\langle p_n|$$

Last detail: $\mathbb{1}_n = \mathbb{1}_{q_n}\mathbb{1}_{p_n} = \int dq_n dp_n |q_n\rangle \underbrace{\langle q_n|p_n\rangle}_{\text{Fourier: } = e^{\frac{i}{\hbar}q_n p_n}/\sqrt{2\pi\hbar}} \langle p_n|$ → (135 in notes)

Collecting everything:

$$\langle q_f | e^{-\frac{i}{\hbar}\hat{H}t} | q_i \rangle \simeq \int \prod_{n=1}^{N} \frac{dq_n\, dp_n}{\sqrt{2\pi\hbar}}\, e^{\frac{i}{\hbar} q_n p_n} \langle q_f | q_N \rangle \underbrace{\langle p_N | q_{N-1} \rangle}_{\frac{e^{-\frac{i}{\hbar} p_N q_{N-1}}}{\sqrt{2\pi\hbar}}} \langle p_{N-1} | \dots | q_i \rangle \times$$

$$\times\, e^{-\frac{i}{\hbar} T(p_N)\Delta t}\, e^{-\frac{i}{\hbar} V(q_{N-1})\Delta t} \cdots$$

Remarkable fact: no more quantum operators here!

$$\langle q_f | e^{-\frac{i}{\hbar}Ht} | q_i \rangle = \int \prod_{n=1}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar}\, e^{-\frac{i\Delta t}{\hbar} \sum_{n=0}^{N-1} \underbrace{\left[T(p_{n+1}) + V(q_n) - p_{n+1} \frac{q_{n+1}-q_n}{\Delta t} \right]}_{\sim T + V - p\dot{q}}}$$

In limit $N \to \infty$ $\quad \Delta t \sum_n \ldots \to \int_0^t dt' \ldots \quad \underbrace{q_{n+1} - q_n}_{\Delta t} \to \dot{q}$

so we get

$$\boxed{\langle q_f | e^{-\frac{i}{\hbar}\hat{H}t} | q_i \rangle = \int \mathcal{D}x \; e^{\frac{i}{\hbar}\int_0^t dt' \left[p\dot{q} - \overbrace{H(p,q)}^{T+V}\right]}}$$

$q_f = q(t)$

$q_i = q(0)$

$$\lim_{N\to\infty} \int \prod_{n=1}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar}$$

$$\langle q_f | U | q_i \rangle = \int \mathcal{D}x \, e^{\frac{i}{\hbar}S}$$

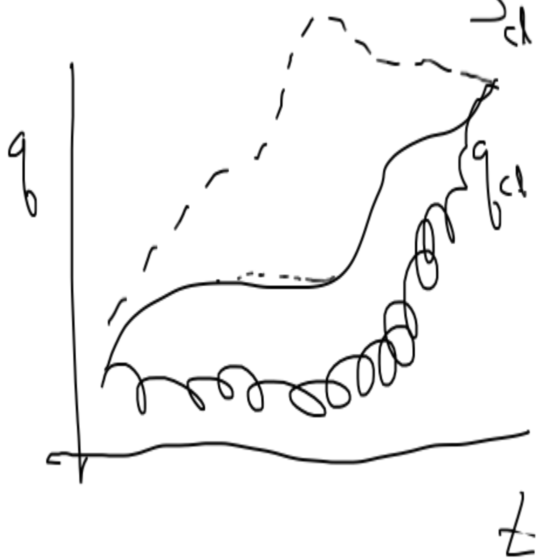
Special case: free dynamics $\hat{T} = \frac{\hat{p}^2}{2m}$

→ integral over momentum variables p_n is Gaussian & can be performed

$$\langle q_f | e^{-\frac{i}{\hbar}\hat{H}t} | q_i \rangle = \int \mathcal{D}q \, e^{\frac{i}{\hbar} S[q,\dot{q}]} \Big|_{\substack{q(t)=q_f \\ q(0)=q_i}}$$

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

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



$$\mathcal{D}q = \lim_{N\to\infty} \left(\frac{Nm}{2\pi\hbar i t}\right)^{N/2} \prod_{n=1}^{N-1} dq_n$$

The path integral for a free particle $\hat{H} = \frac{\hat{p}^2}{2m}$

2 derivations given in notes: – direct integration (p. 29)
à la Feynman
– using matrices (p. 30)

Result: $\langle q_f | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t} | q_i \rangle = \left(\frac{m}{2\pi i \hbar t}\right)^{1/2} \exp\left\{ \frac{i m (q_f - q_i)^2}{2\hbar t} \right\} \equiv U_{free}(q_f, q_i; t)$

Reminder: diffusion $P(r_f, \tau | r_i, 0) = \left(\frac{1}{4\pi D \tau}\right)^{1/2} \exp\left\{ -\frac{(r_f - r_i)^2}{4 D \tau} \right\}$

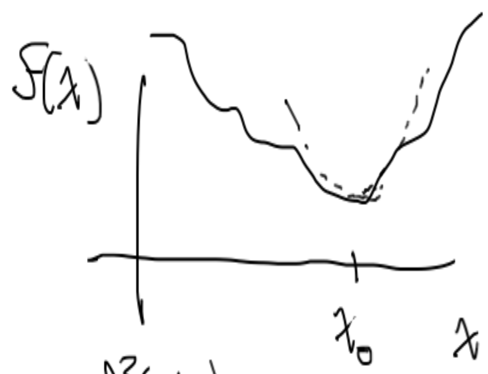
Same if $\tau = i t \times \left(\frac{\hbar}{2 D m}\right)$

Diffusion eq$^{\underline{n}}$ $\quad \frac{\partial}{\partial t} \rho = D \nabla^2 \rho$

Schrödinger eq$^{\underline{n}}$ $\quad i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2 \nabla^2}{2m} \psi$

Approximation method for generic integrals

Let $f(x)$ be some fⁿ on the real axis, which is assumed to be bounded from below & asymptotes to ∞ at $x \to \pm\infty$.



Want to know $I[f] = \int_{-\infty}^{\infty} dx\, e^{-f(x)}$

$\left.\frac{d^2 f}{dx^2}\right|_{x_0}$

Strategy: approx $f(x)$ around its minimum: $f(x) = f(x_0) + \frac{a}{2}(x-x_0)^2 + \dots$

Then, $I[f] = \int_{-\infty}^{\infty} dx\, e^{-f(x_0) - \frac{a}{2}(x-x_0)^2 - O(3)} = e^{-f(x_0)} \int_{-\infty}^{\infty} dx\, e^{-\frac{a}{2}(x-x_0)^2} (1+\dots) = e^{-f(x_0)} \sqrt{\frac{2\pi}{a}} (1+\dots)$

Nice example: The Gamma f^{n} $\Gamma(z+1) = \int_0^\infty dx\, \underbrace{x^z e^{-x}}_{e^{-f(x)}}$ $\quad f(x) = x - z\ln x$

Blind application of our tricks

Min pt of $f(x)$: $\quad \frac{df}{dx} = 1 - \frac{z}{x} \rightarrow x_0 = z \qquad f(x_0) = z(1 - \ln z)$

$$a = \left.\frac{d^2 f}{dx^2}\right|_{x_0} = \frac{1}{z} \rightarrow \sqrt{\frac{2\pi}{a}} = \sqrt{2\pi z}$$

So: $\Gamma(z+1) = e^{z(\ln z - 1)} \sqrt{2\pi z}\,(1 + \ldots) \rightarrow$ Stirling's approx^{n}

Stationary phase approx$^{\underline{n}}$ of path integrals

Q: what is the expected dominant path?

A: the classical one, defined by the cond$^{\underline{n}}$

$$q_{cl}(t): \quad \left.\frac{\delta S[q]}{\delta q(t)}\right| = 0$$

Functions, functionals, functional derivatives $\quad q(t)\ t\in(0,t[$

$f(q) \quad q\in\mathbb{R} \qquad F_{t,g}[q]=\int_0^t dt'\, g(t')\,q(t')$

Functional derivative:

$$\frac{\delta F[q]}{\delta q(t'')}=\lim_{\varepsilon\to 0}\frac{F[q+\varepsilon\delta(t-t'')]-F[q]}{\varepsilon}$$

for our example, $\displaystyle \frac{\delta F}{\delta q(t')}=\frac{1}{\varepsilon}\int_0^t dt'\, g(t')\left[\cancel{q(t')}+\varepsilon\delta(t'-t'')-\cancel{q(t')}\right]=g(t'')$

"Taylor series" for functionals:

some chosen base f^{n}

$$F[x] = F[\bar{x} + y] = F[\bar{x}] + \int dt\, y(t) \left.\frac{\delta F}{\delta x(t)}\right|_{\bar{x}}$$

$$+ \frac{1}{2} \int dt_1\, dt_2\, y(t_1)\, y(t_2) \left.\frac{\delta^2 F}{\delta y(t_1)\, \delta y(t_2)}\right|_{\bar{x}} + \dots$$