❦ Quantum Mechanics Assignment #1 part 5 ❦ TIF290

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Feynman propagator

Take $\hbar = 1$.

The Schrödinger equation,

$$i\frac{\partial}{\partial t}\left|\alpha\right\rangle = H\left|\alpha\right\rangle, \tag{SE}$$

has the solution

$$\left|\alpha(t)\right\rangle = \mathrm{e}^{-iHt}\left|\alpha(0)\right\rangle = \sum_a \left|a\right\rangle \left\langle a|\alpha(0)\right\rangle \mathrm{e}^{-iE_a t} \tag{1}$$

for an H-eigenbasis $\{\left|a\right\rangle\}$. We can project (1) onto the position basis by

$$\psi(\mathbf{x}, t) = \left\langle \mathbf{x}|\alpha(t)\right\rangle = \sum_a \left\langle \mathbf{x}|a\right\rangle \left\langle a|\alpha(0)\right\rangle \mathrm{e}^{-iE_a t}. \tag{2}$$

Denote $\left\langle \mathbf{x}|a\right\rangle$ by $u_a(\mathbf{x})$ & $\left\langle a|\alpha(0)\right\rangle$ by $c_a(0)$. Using resolution of identity

$$1 = \int \mathrm{d}^3x \left|\mathbf{x}\right\rangle \left\langle \mathbf{x}\right|, \tag{RES}$$

we can express

$$c_a(0) = \int \mathrm{d}^3x \left\langle a|\mathbf{x}\right\rangle \left\langle \mathbf{x}|\alpha(0)\right\rangle = \int \mathrm{d}^3x\; u_a^*(\mathbf{x})\psi(\mathbf{x}, 0).$$

Using (RES) again on (2) we get that

$$\begin{aligned}\psi(\mathbf{x}, t) &= \int \mathrm{d}^3x' \sum_a \left\langle \mathbf{x}|a\right\rangle \left\langle a|\mathbf{x}'\right\rangle \left\langle \mathbf{x}'|\alpha(0)\right\rangle \mathrm{e}^{-iE_a t} \\ &= \int \mathrm{d}^3x' K(\mathbf{x}, \mathbf{x}', t)\psi(\mathbf{x}', 0) \qquad (3)\end{aligned}$$

where

$$K(\mathbf{x}, \mathbf{x}', t) = \sum_a \langle \mathbf{x}|a\rangle \langle a|\mathbf{x}'\rangle \, \mathrm{e}^{-iE_a t} = \langle \mathbf{x}| \, \mathrm{e}^{-iHt} \, |\mathbf{x}'\rangle \, . \tag{4}$$

K is called *propagator* and is the Green's function for (SE) in the position basis.

Transition amplitudes

Switching to the Heisenberg picture:

$$\begin{aligned} |\alpha(t)\rangle &\mapsto |\alpha\rangle \\ \mathbf{x} &\mapsto \mathbf{x}(t) \\ \mathrm{e}^{iHt} \, |\mathbf{x}\rangle &\mapsto |\mathbf{x}(t)\rangle \, . \end{aligned} \tag{5}$$

The last mapping follows from that operators time-evolve according to

$$\mathcal{O}(t) = \mathrm{e}^{iHt}\mathcal{O}(0)\mathrm{e}^{-iHt},$$

so $|\mathbf{x}\rangle$ being an eigenvector to $\mathbf{x}$ implies $\mathrm{e}^{iHt} \, |\mathbf{x}\rangle$ being an eigenvector of $\mathbf{x}(t)$. [1]

We now have, by (5), that

$$K(\mathbf{x}, \mathbf{x}', t) = \langle \mathbf{x}(t)|\mathbf{x}'(0)\rangle \tag{6}$$

which is the probability amplitude of a particle starting at position $\mathbf{x}(0)$ at time 0 being observed at position $\mathbf{x}(t)$ at time t.

Path integrals

Since, for any t, $\{|x(t)\rangle\}$ form a complete eigenbasis of the state space, we can decompose K as

$$K(\mathbf{x}, \mathbf{x}'', t) = \langle \mathbf{x}(t)|\mathbf{x}'(0)\rangle = \int \mathrm{d}^3\mathbf{x}' \, \langle \mathbf{x}(t)|\mathbf{x}'(t')\rangle \, \langle \mathbf{x}'(t')|\mathbf{x}''(0)\rangle \, . \tag{7}$$

Dividing some time interval $[t_1, t_N]$ into N equal parts, we can inductively use (7) to obtain

$$K(\mathbf{x}_1, \mathbf{x}_N, t_N - t_1) = \tag{8}$$

$$\int \mathrm{d}^3\mathbf{x}_{N-1} \int \mathrm{d}^3\mathbf{x}_{N-2} \cdots \int \mathrm{d}^3\mathbf{x}_2 \, \langle \mathbf{x}_N(t_N)|\mathbf{x}_{N-1}(t_{N-1})\rangle \, \langle \mathbf{x}_{N-1}(t_{N-1})|\mathbf{x}_{N-2}(t_{N-2})\rangle \cdots \langle \mathbf{x}_2(t_2)|\mathbf{x}_1(t_1)\rangle \, .$$

This is an integral over all possible paths from $\mathbf{x}_1$ to $\mathbf{x}_N$.

Let $\mathcal{L}$ be the classical Lagrangian & denote by Δt the difference between t_n & t_{n-1}. Then, by what Feynman discovered,

$$\langle \mathbf{x}_n(t_n)|\mathbf{x}_{n-1}(t_{n-1})\rangle = \frac{1}{w(\Delta t)} \exp\left\{ i \int_{t_{n-1}}^{t_n} \mathcal{L}(\mathbf{x}, \dot{\mathbf{x}}) \mathrm{d}t \right\} \tag{9}$$

[1] I am here implicitly using the fact that exponents of operators can be added like $\mathrm{e}^A\mathrm{e}^B = \mathrm{e}^{A+B}$ if A & B commute. Since any operator commutes with itself, this is clearly allowed here.

where $\int_{t_{n-1}}^{t_n} \mathcal{L}(\mathbf{x}, \dot{\mathbf{x}})\mathrm{d}t$ is an integral taken over some specific path, thus it depends implicitly on $\mathbf{x}_n$ & $\mathbf{x}_{n-1}$. If we apply (9) to (8) we get

$$K(\mathbf{x}_1, \mathbf{x}_N, t_N - t_1) = \left(\frac{1}{w(\Delta t)}\right)^{N-1} \int \mathrm{d}^3\mathbf{x}_{N-1} \int \mathrm{d}^3\mathbf{x}_{N-2} \cdots \int \mathrm{d}^3\mathbf{x}_2 \exp\left\{ i \int_{t_1}^{t_N} \mathcal{L}(\mathbf{x}, \dot{\mathbf{x}})\mathrm{d}t \right\}. \tag{10}$$

Defining

$$\int_{\mathbf{x}_1}^{\mathbf{x}_N} \mathcal{D}[\mathbf{x}(t)] = \lim_{N\to\infty} \left(\frac{1}{w(\Delta t)}\right)^{N-1} \int \mathrm{d}^3\mathbf{x}_{N-1} \int \mathrm{d}^3\mathbf{x}_{N-2} \cdots \int \mathrm{d}^3\mathbf{x}_2$$

we have

$$K(\mathbf{x}_1, \mathbf{x}_N, t_N - t_1) = \int_{\mathbf{x}_1}^{\mathbf{x}_N} \mathcal{D}[\mathbf{x}(t)] \exp\left\{ i \int_{t_1}^{t_N} \mathcal{L}(\mathbf{x}, \dot{\mathbf{x}})\mathrm{d}t \right\}. \tag{11}$$

which is know as *Fenyman's path integral.*

By dimensional analysis, we see that there must be a $\frac{1}{\hbar}$ factor in the exponent in (11). As $\hbar \to 0$ we can then see that any path not satisfying

$$\delta \left(\int_{t_1}^{t_N} \mathcal{L}(\mathbf{x}, \dot{\mathbf{x}})\mathrm{d}t \right)$$

will not have a significant contribution to K due to interference. This implies that classical mechanics is retrieved in the limit of (11) as $\hbar \to 0$.

Putting K back into SE

We are now in a position to check whether Feynman's discovery is consistent with (SE). First, consider a short time interval $[t_{n-1}, t_n]$, then (taking $m = 1$)

$$\int_{t_{n-1}}^{t_n} \mathcal{L}(\mathbf{x}, \dot{\mathbf{x}})\mathrm{d}t = \int_{t_{n-1}}^{t_n} \frac{1}{2}\dot{\mathbf{x}}^2 - V(\mathbf{x})\mathrm{d}t = \Delta t \left[\frac{1}{2} \left(\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\Delta t} \right)^2 - V(\mathbf{x}_n) \right].$$

Now

$$\langle \mathbf{x}_n(t_n) | \mathbf{x}_{n-1}(t_{n-1}) \rangle = \frac{1}{w(\Delta t)} \exp\left\{ i\Delta t \left[\frac{1}{2} \left(\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\Delta t} \right)^2 - V(\mathbf{x}_n) \right] \right\}. \tag{12}$$

Using $\langle \mathbf{x}_n(t_n) | \mathbf{x}_{n-1}(t_{n-1}) \rangle = \delta^3(\mathbf{x}_n - \mathbf{x}_{n-1})$ & letting $V(\mathbf{x}) = 0$ momentarily, we can integrate (12) over $\mathbb{R}^3$ to obtain

$$1 = \int_{\mathbb{R}^3} \mathrm{d}^3\mathbf{x}_n \frac{1}{w(\Delta t)} \exp\left\{ i \frac{(\mathbf{x}_n - \mathbf{x}_{n-1})^2}{2\Delta t} \right\} = \frac{1}{w(\Delta t)} (2\pi i \Delta t)^{\frac{3}{2}} \tag{13}$$

$$w(\Delta t) = (2\pi i \Delta t)^{\frac{3}{2}}. \tag{14}$$

Assuming w is independent of V, we restate (12) as

$$\langle \mathbf{x}_n(t_n) | \mathbf{x}_{n-1}(t_{n-1}) \rangle = \frac{1}{(2\pi i \Delta t)^{\frac{3}{2}}} \exp\left\{ i \frac{(\mathbf{x}_n - \mathbf{x}_{n-1})^2}{2\Delta t} - i\Delta t V(\mathbf{x}_n) \right\}. \tag{15}$$

Consider $\langle \mathbf{x}(t+\Delta t)|\mathbf{x}_1(t_1)\rangle$, using decomposition we can write this as

$$\langle \mathbf{x}(t+\Delta t)|\mathbf{x}_1(t_1)\rangle = \int \mathrm{d}^3(\Delta\mathbf{x}) \frac{1}{(2\pi i\Delta t)^{\frac{3}{2}}} \exp\left\{ i\frac{(\Delta\mathbf{x})^2}{2\Delta t} - i\Delta t V(\mathbf{x}) \right\} \langle (\mathbf{x}-\Delta\mathbf{x})(t)|\mathbf{x}_1(t_1)\rangle \,. \tag{16}$$

Expanding (16) in power series in $\Delta\mathbf{x} = (\Delta x, \Delta y, \Delta z)$ & Δt we get

$$\begin{aligned}
&\langle (\mathbf{x})(t)|\mathbf{x}_1(t_1)\rangle + \Delta t\frac{\partial}{\partial t}\langle (\mathbf{x})(t)|\mathbf{x}_1(t_1)\rangle + \mathcal{O}((\Delta t)^2) \\
&= \int \mathrm{d}^3(\Delta\mathbf{x}) \frac{1}{(2\pi i\Delta t)^{\frac{3}{2}}} \exp\left\{ i\frac{(\Delta\mathbf{x})^2}{2\Delta t} \right\} \left[1 - i\Delta t V(\mathbf{x}) + \mathcal{O}((\Delta t)^2) \right] \langle (\mathbf{x}-\Delta\mathbf{x})(t)|\mathbf{x}_1(t_1)\rangle \\
&= \int \mathrm{d}^3(\Delta\mathbf{x}) \frac{1}{(2\pi i\Delta t)^{\frac{3}{2}}} \exp\left\{ i\frac{(\Delta\mathbf{x})^2}{2\Delta t} \right\} \left[1 - i\Delta t V(\mathbf{x}) + \mathcal{O}((\Delta t)^2) \right] \left[1 + \frac{(\Delta\mathbf{x})^2}{2}\frac{\partial^2}{\partial\mathbf{x}^2} + \mathcal{O}(|\Delta\mathbf{x}|^3) \right] \langle \mathbf{x}(t)|\mathbf{x}_1(t_1)\rangle \,.
\end{aligned} \tag{17}$$

Here, in the last parentheses, we have neglected any odd power of Δx, Δy, or Δz which vanishes when integrated over $\mathbb{R}^3$ due to symmetry (all other factors are even in $\Delta\mathbf{x}$). By $\frac{\partial^2}{\partial\mathbf{x}^2}$, we mean the Laplacian.

Using

$$\int \mathrm{d}^3(\Delta\mathbf{x})(\Delta\mathbf{x})^2 \exp\left\{ i\frac{(\Delta\mathbf{x})^2}{2\Delta t} \right\} = 6\sqrt{2}\pi^{3/2}(i\Delta t)^{5/2} \tag{18}$$

& pairing the first order Δt terms, we have

$$\begin{aligned}
\Delta t\frac{\partial}{\partial t}\langle \mathbf{x}(t)|\mathbf{x}_1(t_1)\rangle &= \left[-\frac{(2\pi i\Delta t)^{\frac{3}{2}}}{(2\pi i\Delta t)^{\frac{3}{2}}} i\Delta t V(\mathbf{x}) + \frac{6\sqrt{2}\pi^{3/2}(i\Delta t)^{5/2}}{2(2\pi i\Delta t)^{\frac{3}{2}}}\frac{\partial^2}{\partial\mathbf{x}^2} \right] \langle \mathbf{x}(t)|\mathbf{x}_1(t_1)\rangle \\
&= \left[-i\Delta t V(\mathbf{x}) + \frac{3}{2} i\Delta t\frac{\partial^2}{\partial\mathbf{x}^2} \right] \langle \mathbf{x}(t)|\mathbf{x}_1(t_1)\rangle \,.
\end{aligned} \tag{19}$$

Multiplying (19) by $-\frac{i}{\Delta t}$ on each side, we get

$$i\frac{\partial}{\partial t}\langle \mathbf{x}(t)|\mathbf{x}_1(t_1)\rangle = \left[V(\mathbf{x}) - \frac{3}{2}\frac{\partial^2}{\partial\mathbf{x}^2} \right] \langle \mathbf{x}(t)|\mathbf{x}_1(t_1)\rangle \,, \tag{20}$$

which is the (SE) in positional basis.

Remarks

When evaluating integrals such as (13) & (18), we have pushed Δt down into the lower half of the complex plane by some amount ϵ in order to achieve convergence. After having evaluated such a convergent integral, we can let $\epsilon \to 0$ to retrieve an ϵ-independet expression.