Path Integral

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1 The axioms of time evolution

Let us consider the axioms of quantum mechanical time evolution:

1. States are described by kets at some starting time t_0: $|\alpha\rangle = |\alpha, t_0\rangle$;
2. their time evolution is described by a linear operator $U(t; t_0)$ as $|\alpha, t_0; t\rangle = U(t, t_0) |\alpha\rangle$;
3. this time evolution obeys $\lim_{t\to t_0} |\alpha, t; t_0\rangle = |\alpha; t_0\rangle$.

If we have an observable A, we can express our states with respect to its eigenbasis $|\alpha'\rangle$:

$$|\alpha, t_0\rangle = \sum_{\alpha'} c_{\alpha'}(t_0) \left|\alpha'\right\rangle , \tag{1}$$

and do the same for their evolved counterparts, with evolved coefficients $c_{\alpha'}(t)$. If $[A, H] = 0$ then $|c_{\alpha'}(t)| = |c_{\alpha'}(t_0)|$, while in general this does not hold.

We impose the normalization of kets: $1 = \langle\alpha|\alpha\rangle = \sum_{\alpha'} |c_{\alpha'}(t)|^2$ for all times. This directly implies that the linear operator U must be unitary: $U^\dagger U = \mathbb{1}$.

Also, we impose the composition law: if $t_2 \geq t_1 \geq t_0$, then $U(t_2; t_0) \stackrel{!}{=} U(t_2; t_1)U(t_1; t_0)$.

Condition 3 means that we can expand:

$$U(t_0 + \mathrm{d}t\,, t_0) = \mathbb{1} + \frac{H\,\mathrm{d}t}{i\hbar} \tag{2}$$

with some self-adjoint operator H. Manipulating this, for a generic time t we get:

$$\frac{\mathrm{d}}{\mathrm{d}t} U(t; t_0) = \frac{HU}{i\hbar} , \tag{3}$$

which directly implies the Schrödinger equation

$$i\hbar\partial_t |\alpha, t_0; t\rangle = H |\alpha, t_0; t\rangle \tag{4}$$

1.1 Time-independent Hamiltonians

We can Taylor-expand the evolution operator as such:

$$U(t, t_0) = \exp\left(\frac{H(t - t_0)}{i\hbar}\right) \tag{5a}$$

$$= \mathbb{1} + \frac{H(t - t_0)}{i\hbar} + \frac{1}{2}\frac{H^2(t - t_0)^2}{(i\hbar^2)^2} + o(|t - t_0|^2)\,, \tag{5b}$$

and also its derivative:

$$\partial_t U(t, t_0) = \frac{H}{i\hbar} + \frac{1}{2}\frac{H^2}{(i\hbar)^2}2t + O(|t - t_0|^2) \tag{6a}$$

$$= \frac{HU}{i\hbar}\,, \tag{6b}$$

which is consistent with the Schrödinger equation.

Alternatively, we can look at the limit of infinitesimal time evolutions:

$$\left(\mathbb{1} + \frac{H}{i\hbar}\frac{t}{N}\right)^N \xrightarrow{N\to\infty} \exp\left(\frac{Ht}{i\hbar}\right) \tag{7}$$

In general, continuous symmetries have representations in a Hilbert space: say we have the time translation symmetry $P(\xi)t = t + \xi$; its representation is generally in the form $\exp(-i\Omega t)$ for a self-adjoint Ω.

The fact that the generator of the time-translation symmetry is the Hamiltonian: $\Omega = H/\hbar$ is a postulate.

1.1.1 Time-dependent commuting Hamiltonians

We assume that $H = H(t)$, but $[H(t_1), H(t_2)] = 0$ for any $t_{1,2}$. Then:

$$U(t, t_0) = \exp\left(\frac{1}{i\hbar}\int_{t_0}^{t} H(\tau)\,\mathrm{d}\tau\right)\,, \tag{8}$$

which can be proved like before, substituting $Ht \to \int^t H(\tau)\,\mathrm{d}\tau$.

1.1.2 Time-dependent non-commuting Hamiltonians

In general, if $[H(t_1), H(t_2)] \neq 0$, we have the following expression by Dyson:

$$U(t, t_0) = \mathbb{1} + \sum_{N}^{\infty} \frac{1}{(i\hbar)^N} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \cdots \int_{t_0}^{t_{n-1}} \mathrm{d}t_n\, \pi_i H(t_i)\,. \tag{9}$$

A concrete Hamiltonian for which we'd need this is something in the form $H = -\mu \cdot B(t)$, where the magnetic field $B(t)$ changes directions. Since $\mu \cdot B \propto$

$s \cdot B$ and the s_j do not commute, this does not commute with itself at different times.

In the previous lessons we introduced the Dirac representation, where we defined:

$$\begin{aligned}
\left|\alpha t_0 t\right\rangle &= U(t-t_0)\left|\alpha t_0\right\rangle &\text{(10a)}\\
&= e^{-\frac{iH(t-t_0)}{\hbar}}\left|\alpha\right\rangle &\text{(10b)}\\
&= \sum_{a'} e^{-\frac{iE_{a'}(t-t_0)}{\hbar}}\left|a'\right\rangle\left\langle a'\middle|a t_0\right\rangle &\text{(10c)}\\
&= \sum c_a'(t_0) e^{-\frac{iE_{a'}(t-t_0)}{\hbar}}\left|a'\right\rangle &\text{(10d)}\\
&= \sum c_a'(t)\left|a'\right\rangle &\text{(10e)}
\end{aligned}$$

and

$$\left\langle \bar{x'}\middle|a' t_0 t\right\rangle = \sum c_a'(t_0) e^{-\frac{iE_{a'}(t-t_0)}{\hbar}}\left\langle \bar{x'}\middle|a'\right\rangle, \tag{11}$$

such that $\psi(\bar{x'},t) = \sum c_a'(t_0) e^{-\frac{iE_{a'}(t-t_0)}{\hbar}} u_{a'}(\bar{x'})$. Than from Dirac completeness relation,

$$c_{a'}(t_0) = \left\langle a'\middle|\alpha t_0\right\rangle = \int d^3x' \left\langle a'\middle|\bar{x'}\right\rangle\left\langle \bar{x'}\middle|\alpha t_0\right\rangle, \tag{12}$$

and for this reason

$$\begin{aligned}
\left\langle x''\middle|\alpha t_0 t\right\rangle &= \sum e^{-\frac{iE_{a'}(t-t_0)}{\hbar}}\left\langle x''\middle|a'\right\rangle \int d^3x' \left\langle a'\middle|x'\right\rangle\left\langle x'\middle|a t_0\right\rangle &\text{(13a)}\\
&= \int d^3x' \sum \left\langle x''\middle|a'\right\rangle\left\langle a'\middle|x'\right\rangle e^{-\frac{iE_{a'}(t-t_0)}{\hbar}}\left\langle x'\middle|a t_0\right\rangle &\text{(13b)}\\
&= \int d^3x' K \left\langle x'\middle|a t_0\right\rangle &\text{(13c)}
\end{aligned}$$

where we defined the propagator K. We write otherwise $\psi(x'',t) = \int d^3x' K(x'',t,x',t_0)\psi(x',t_0)$, such that the propagator satisfies:

- K respects Schrodinger equation, since $i\hbar\left\langle x'\middle|\alpha \dot{t_0} t\right\rangle = \left\langle x'\right| H \left|\alpha t_0 t\right\rangle$ and $\left\langle x'\middle|a' t_0 t\right\rangle = e^{-\frac{iE_{a'}(t-t_0)}{\hbar}}\left\langle x''\middle|a'\right\rangle$
- $\lim_{t\to t_0} K = \delta^3(x''-x')$, i.e. the evolution of a particle which was in x' at $t=0$

1.2 Free particle propagator

Now we want to obtain the propagator K aforementioned for the particular case of a free particle hamiltonian. In the space of momenta we have

$$P\left|p'\right\rangle = p'\left|p'\right\rangle, \left\langle x'\middle|p'\right\rangle = \frac{e^{\frac{ip'x'}{\hbar}}}{\sqrt{2\pi\hbar}}, \qquad H\left|p'\right\rangle = \frac{p'^2}{2m}\left|p'\right\rangle. \tag{14}$$

In this case we have

$$K = \int dp' \left\langle x''\middle|p'\right\rangle \left\langle p'\middle|x'\right\rangle e^{-\frac{ip^2(t-t_0)}{\hbar 2m}} = \int_{-\infty}^{+\infty} dp' \frac{e^{\frac{i}{\hbar}\left(p'(x''-x')-\frac{p'^2}{2m}(t-t_0)\right)}}{2\pi\hbar} \tag{15}$$

Considering that

$$\frac{i}{\hbar}\left(p'(x''-x') - \frac{p'^2}{2m}(t-t_0)\right) = -\frac{i(t-t_0)}{2m\hbar}\left(p'^2 - \frac{2mp'(x''-x')}{t-t_0}\right) = -\frac{i(t-t_0)}{2m\hbar}\left(p' - \frac{m(x''-x')}{t-t_0}\right)^2 + \frac{i(t \tag{16}$$

Now, defining the new variable $\xi = p' - \frac{m(x''-x')}{t-t_0}$, we finally obtain

$$K = \frac{e^{\frac{im(x''-x')^2}{2m\hbar}}}{2\pi\hbar}\int_{-\infty}^{+\infty} d\xi e^{-\frac{i(t-t_0)\xi^2}{2m\hbar}} = \frac{e^{\frac{im(x''-x')^2}{2m\hbar}}}{2\pi\hbar}\sqrt{\frac{2m\pi\hbar}{i(t-t_0)}} \tag{17}$$

1.3 Harmonic oscillator

In the same way we studied the free particle problem, we want to obtain the propagator for the harmonic oscillator, i.e. a single particle system under the evolution with the hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \tag{18}$$

where we know that defining the operator distruction $a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right)$, we obtain an explicit writing for the eigenvalues $E_N = \hbar\omega(N + \frac{1}{2})$ and the eigenfunctions respect the relations $|n+1\rangle = \frac{a^+}{\sqrt{n+1}|n\rangle}$, in such a way that

$$\left\langle x'\right| a\left|0\right\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left\langle x'\right|\left(x + \frac{ip}{m\omega}\right)\left|0\right\rangle. \tag{19}$$

It follows that $\left(x' + \frac{i}{m\omega}(-i\hbar\frac{d}{dx'})\right)\left\langle x' \middle| 0 \right\rangle$ and, defining $x_0 = \sqrt{\frac{\hbar}{m\omega}}$, we have $\left\langle x' \middle| 0 \right\rangle = \eta e^{-\frac{x'^2}{2x_0^2}}$ with $\eta = \frac{1}{(x_0\pi)^{\frac{1}{4}}}$. In this case we obtain

$$\left\langle x' \middle| n \right\rangle = \frac{1}{\pi^{\frac{1}{4}}\sqrt{2^n n}} \frac{\left(x' - x_0^2\frac{d}{dx'}\right)^n}{x_0^{n+\frac{1}{2}}} e^{-\frac{x'^2}{2x_0^2}} = \frac{1}{\pi^{\frac{1}{4}}\sqrt{2^n n!}} H_n(y) e^{-\frac{x'^2}{2x_0^2}}, \tag{20}$$

where we defined $y = \frac{x'}{x_0}$, and the propagator

$$K = \sum_{n=0}^{\infty} \left\langle x' \middle| n \right\rangle \left\langle n \middle| x'' \right\rangle e^{-i\omega(n+\frac{1}{2})(t-t_0)} = \frac{e^{-\frac{i\omega\delta t}{2}}}{\sqrt{\pi}x_0} e^{-\frac{1}{2}\left(\frac{x''^2}{x_0^2}+\frac{x'^2}{x_0^2}\right)} \sum \frac{e^{-i\omega\delta t n}}{2^n n!} H_n(\frac{x''}{x_0}) H_n(\frac{x'}{x_0}). \tag{21}$$

Now, considering that, for $\zeta = e^{-i\omega\delta t}$, $\xi = \frac{x''}{x_0}$ and $\eta = \frac{x'}{x_0}$

$$e^{-(\xi^2+\eta^2)} \sum \frac{\zeta^n}{2^n n!} H_n \xi H_n \eta = \frac{e^{-\frac{\xi^2+\eta^2-2\xi\eta\zeta}{1-\zeta^2}}}{\sqrt{i-\zeta^2}}, \tag{22}$$

we have

$$K = \frac{e^{-\frac{i\omega\delta t}{2}}}{\sqrt{\pi}x_0} e^{\frac{1}{2}(\xi^2+\eta^2)} \frac{e^{-\frac{\xi^2+\eta^2-2\xi\eta\zeta}{1-\zeta^2}}}{\sqrt{i-\zeta^2}} = \frac{e^{\left(-\frac{(\xi^2+\eta^2)e^{i\omega\delta t}-2\xi\eta}{e^{i\omega\delta t}-e^{-i\omega\delta t}}+\frac{\xi^2+\eta^2}{2}\right)}}{x_0\sqrt{2\pi i \sin(\omega\delta t)}} = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega\delta t)}} e^{-\frac{(\xi^2+\eta^2)(\cos(\omega\delta t)+i\sin(\omega\delta t))-2\xi\eta-is(\xi^2+}{2i\sin(\omega\delta t)}} \tag{23}$$