The propagator of a particle in an infinite well

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The problem:

(a) Find the propagator of a particle in an infinite well by direct calculation.

(b) Repeat (a) but now use Feynman path integral method.

(c) Verify that the results are identical.

The solution:

(a) The hamiltonian for this problem is

$$\mathcal{H} = \frac{p^2}{2m} + V(x) \qquad , V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & otherwise \end{cases}$$

As is well known, the spatial parts of the normalized energy eigenfunctions and eigenvalues are given by

$$\varphi_n(x) = \sqrt{\frac{2}{L}} sin(\frac{n\pi x}{L}) \qquad , n = 1, 2, ...$$

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2$$

Where m is the mass of the particle. We will use $\hbar = 1$.

The propagator by direcet calculation (§ 25.2 in the lecture notes) is:

$$U(x|x_0) = \langle x, t|x_0, 0\rangle = \langle x|e^{-i\mathcal{H}t}|x_0\rangle = \sum_{n=1}^{\infty} \langle x|e^{-i\mathcal{H}t}|n\rangle\langle n|x_0\rangle = \sum_{n=1}^{\infty} e^{-iE_n t}\langle x|n\rangle\langle n|x_0\rangle = \frac{2}{L}\sum_{n=1}^{\infty} e^{-i\omega n^2 t} sin(\frac{n\pi x}{L}) sin(\frac{n\pi x_0}{L})$$

where ω=E_1

(b) Path integral calculation:
Let us first clarify how the particle can travel from $(x_0, 0)$ to (x, t).
We have to allow all paths along which the particle can travel from $x_0 \rightarrow$ x. There is an infinite number of possibilities: the direct path (free propagation from $x_0 \rightarrow$ x), while on a second path, the particle bounces against the rigid wall one time before travelling on to the final point, and so on, i.e., bouncing off the wall an infinite number of times to the right and the left, while on its way from $x_0 \rightarrow$ x.
Thus we shall construct the propagator by forming the sum of all these infinitely many classical paths.
The contribution of each classical path is the free particle propagator, multiplied by (-1) for every collision against the wall.
It is natural to generalize the result we have already know for a reflecting wall (ex. 815):

$$U(x|x_0) = \sqrt{\frac{m}{2\pi i t}} [e^{\frac{im}{2t}(x-x_0)^2} - e^{\frac{im}{2t}(-x-x_0)^2}]$$

Geometrically, one can say that the end point (x, t) is reached via the image point (-x, t), starting at $(x_0, 0)$, and by the superposition principle, the propagator consists of the sum of the contributions of all the classical paths. Now, we have to add $2L$ at every turning point, i.e., twice the width L of the box.

The generalization of the above formula reads:

$$U_L(x|x_0) = \sqrt{\frac{m}{2\pi it}} \sum_{k=-\infty}^{\infty} [e^{\frac{im}{2t}(x-x_0-2Lk)^2} - e^{\frac{im}{2t}(x+x_0-2Lk)^2}]$$

(the subscript L on U_L reminds us that the particle is trapped between the walls of the box).

(c) Now we would like to verify that the two results are identical.
First, by using the identity -

$$sin(\frac{n\pi x}{L}) = \frac{1}{2i}(e^{\frac{in\pi x}{L}} - e^{\frac{-in\pi x}{L}})$$

We can write the propagator in (a) in the form

$$U(x|x_0) = \frac{1}{2L}[\sum_{n=-\infty}^{\infty} e^{-i\omega n^2 t} e^{\frac{in\pi}{L}(x-x_0)} - \sum_{n=-\infty}^{\infty} e^{-i\omega n^2 t} e^{\frac{in\pi}{L}(x+x_0)}]$$

Second, we use Poisson sumation formula:

$$\sum_n e^{-\pi a n^2 + 2\pi i b n} = \frac{1}{\sqrt{a}} \sum_k e^{-\pi \frac{(k-b)^2}{a}}$$

Remembering that $\omega = \frac{\pi^2}{2mL^2}$ and writing $a = \frac{i\omega t}{\pi}$ and $b = \frac{x-x_0}{2L}$ we get:

For the first sumation - $\frac{1}{2L} \sum_{n-\infty}^{\infty} e^{-i\omega n^2 t + i\frac{n\pi}{L}(x-x_0)} = \frac{1}{2L} \frac{1}{\sqrt{\frac{i\omega t}{\pi}}} \sum_{k-\infty}^{\infty} e^{\frac{-\pi^2(k-\frac{x-x_0}{2L})^2}{i\omega t}} = \sqrt{\frac{m}{2\pi it}} \sum_{k=-\infty}^{\infty} e^{\frac{im}{2t}(x-x_0-2Lk)^2}$
And similar result for the second sumation - $\sqrt{\frac{m}{2\pi it}} \sum_{k=-\infty}^{\infty} e^{\frac{im}{2t}(x+x_0-2Lk)^2}$.

Finaly, we can summarize:

$$U_L(x|x_0) = \sqrt{\frac{m}{2\pi it}} \sum_{k=-\infty}^{\infty} [e^{\frac{im}{2t}(x-x_0-2Lk)^2} - e^{\frac{im}{2t}(x+x_0-2Lk)^2}]$$

$$= \frac{2}{L} \sum_{n=1}^{\infty} e^{-i\omega n^2 t} sin(\frac{n\pi x}{L}) sin(\frac{n\pi x_0}{L})$$