Boundary Condition and the Auxiliary Phase in Feynman Path Integral

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When employing Feynman path integrals to compute propagators in quantum physics, the concept of summing over the set of all paths is not always naïve. In fact, an auxiliary phase often has to be included as a weight for each summand. In this article we discuss the nature of this auxiliary phase when the classical path involved is reflected through the instance of a free particle confined to a line segment.

I. INTRODUCTION

The wave function of a free particle trapped in an infinite potential well has been studied thoroughly using both the Schrödinger equation and Feynman path integral [1].

Fix some $L > 0$ and let

$$H = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x),$$

where $V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases}$. The corresponding (time-independent) Schrödinger equation is the eigenvalue problem

$$H\psi = E\psi$$

subject to the Dirichlet boundary condition $\psi(0) = \psi(L) = 0$.

On the spectral end, the arising eigenvalues $E$ are discrete. One simply label them as $E_n$ (each with multiplicity one) and the corresponding eigenfunctions as $\psi_n = |n\rangle$. In fact, after normalization

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin(k_n x),$$

where $k_n = \frac{n\pi}{L}$ and therefore $E_n = \frac{\hbar^2}{2m} k_n^2 = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$ for $n = 1, 2, 3, \ldots$.

Decomposed by the spectrum of $H$, the propagator can then be computed by

$$K(y, t_1; x, t_0) = \frac{2}{L} \sum_{n=1}^{\infty} e^{\frac{\pi}{L} E_n (t_1 - t_0)} \sin(k_n x) \sin(k_n y).$$

On the other hand, since this is a case with a quadratic Laplacian, it suffices to consider only the contribution from all classical paths [2–6]. The expansion along the momentum $p$ gives an expression for $K(y, t_1; x, t_0)$:

$$\sum_{r=-\infty}^{\infty} \epsilon_r \frac{\hbar}{2\pi} \int_{\mathbb{R}} e^{-\frac{i\pi}{\hbar} (t_1 - t_0)} e^{i p (y_r - x)} dp,$$

where the sum over $r$ is the sum indexed by possible classical paths, and $\epsilon_r$ is a unitary phase factor associated to the path to $y_r$. Detail of these derivation can be found in [1, 7, 8], where they pointed out that the $\epsilon_r$ above should be $(-1)^r$. Under such ansatz, the results derived from the two ways of computing the propagator match.

One disparity between the two approaches lies within the assignment of phases. Since Schrödinger equation deals with wave functions, it is by construction that phases are included when considering the interaction between states. On the other hand, even though path integral taken all paths into account, so far it does not seem to exist an intrinsic way of associating phases to each path in general. Related discussion can be found in [2, 4].

To further study this auxiliary phase factor, certain modification on the model has to be made. Instead of considering the infinite potential well, one consider the wave function of an 1-dimensional free
particle confined to a line segment \([0, L]\). This interpretation makes it sensible to discuss other boundary conditions such as the Neumann boundary condition and so on.

In particular, the original problem of an infinite potential well can be regarded as the special case of imposing the Dirichlet boundary condition on both ends.

The main conclusion of this article goes as follows:

**Ansatz.** When the boundary condition on each boundary point is assigned as Dirichlet or Neumann type, the phase \(\epsilon\) associated to a classical path \(\gamma : [t_0, t_1] \to [0, L]\) can be computed by multiplying \(-1\) (resp. \(1\)) each time the path reflects upon touching any boundary point with Dirichlet (resp. Neumann) boundary condition.

**II. NEUMANN BOUNDARY CONDITIONS**

In this section we consider \([4]\) with the boundary condition \(\psi'(0) = \psi(L) = 0\). Once again, the eigenvalues in this case are discrete multiplicity-free and will be labelled as \(E_n\). The corresponding eigenfunctions are

\[
\psi_n(x) = \sqrt{\frac{2}{L}} \cos(k_n x)
\]

with \(k_n = \frac{n\pi}{L}\), \(E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}\) for \(n = 1, 2, \ldots\). Note that here the case \(n = 0\) also contributes a nontrivial solution \(\psi_0 = \sqrt{\frac{1}{L}}\).

Decompose by the spectrum of \(H\), the propagator can \(K(y, t_1; x, t_0)\) thereby be computed by

\[
\frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}E_n(t_1-t_0)} \cos(k_n x) \cos(k_n y).
\]

Performing the path integral calculation gives another expression for \(K(y, t_1; x, t_0)\):

\[
\frac{1}{2\pi\hbar} \sum_{r=-\infty}^{\infty} \epsilon_r \int_{\mathbb{R}} e^{-\frac{i}{\hbar}E_n(t_1-t_0)} e^{\frac{i}{\hbar}p(y_n-x)} dp.
\]

The Ansatz indicates that \(\epsilon_r = 1\) in this case. Notice that

\[
y_r = \begin{cases} rL + y & \text{for even } r \\ (r+1)L - y & \text{for odd } r \end{cases}
\]

Reset the parameter modulo 2 as \(r = 2l\) for even \(r\) or \(2l - 1\) for odd \(r\) with \(l \in \mathbb{Z}\) and plugging into \([3]\), \(K(y, t_1; x, t_0)\) is then

\[
\frac{1}{\pi\hbar} \int_{-\infty}^{\infty} \sum_{l=-\infty}^{\infty} e^{\frac{i}{\hbar}L(l^2+2l+1)} e^{-\frac{i}{\hbar}\pi x} \cos(py/h) dp
\]

By Poisson summation formula,

\[
\int_{-\infty}^{\infty} \sum_{l=-\infty}^{\infty} e^{2i\pi lp/h} f(p) dp = \frac{\pi\hbar}{L} \sum_{n=-\infty}^{\infty} f(n\pi h/L).
\]

Thus \(K(y, t_1; x, t_0)\) equals

\[
\frac{1}{L} \sum_{n=-\infty}^{\infty} e^{-\frac{i}{\hbar}E_n(t_1-t_0)} e^{-ik_n x} \cos(k_n y)
\]

\[
= \frac{2}{L} \left( \frac{1}{2} + \sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}E_n(t_1-t_0)} \cos(k_n x) \cos(k_n y) \right).
\]

The last equation \([4]\) follows from writing \(e^{-ik_n x} = \cos(k_n x) - i \sin(k_n x)\) and observe the parity of the functions. The formula above matches the result of the spectral decomposition.

**III. MIXED BOUNDARY CONDITIONS**

We now consider \([4]\) with the boundary condition \(\psi'(0) = \psi(L) = 0\). Then the eigenfunctions, again labelled as \(\psi_n\) are given by

\[
\psi_n(x) = \sqrt{\frac{2}{L}} \cos(k_n x)
\]

with \(k_n = (n - \frac{1}{2})\frac{\pi}{L}\) and \(E_n = (n - \frac{1}{2})^2 \frac{\pi^2\hbar^2}{2mL^2}\) for \(n = 1, 2, \ldots\). The spectral decomposition tells us that \(K(y, t_1; x, t_0)\) equals

\[
\frac{2}{L} \sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}E_n(t_1-t_0)} \cos(k_n x) \cos(k_n y).
\]

The path integral approach considers the (weighted) sum over classical paths

\[
\frac{1}{2\pi\hbar} \sum_{r=-\infty}^{\infty} \epsilon_r \int_{\mathbb{R}} e^{-\frac{i}{\hbar}E_n(t_1-t_0)} e^{\frac{i}{\hbar}p(y_n-x)} dp.
\]

The Ansatz indicates that \(\epsilon_r = 1\) if \(r = -1, 0\) modulo 4 and \(\epsilon_r = -1\) if \(r = 1, 2\) modulo 4. We can therefore
rewriting the sum as
\[
\frac{1}{\pi \hbar} \int_{-\infty}^{\infty} \sum_{l = -\infty}^{\infty} e^{4iLp/\hbar} e^{-iLp/2} (t_1 - t_0) e^{-i\hbar p x} e^{i\hbar p y} (1 - e^{2iLp/\hbar}) dp
\]

Employing the Poisson summation formula,
\[
\int_{-\infty}^{\infty} \sum_{l = -\infty}^{\infty} e^{4iLp/\hbar} f(p) dp = \pi \hbar \sum_{b = -\infty}^{\infty} f(b \pi \hbar/2L).
\]

Thus \( K(y,t_1;x,t_0) \) equals
\[
\frac{1}{2L} \sum_{b = -\infty}^{\infty} \sum_{n = -\infty}^{\infty} e^{-i\pi b(2n+1)/2L} (t_1 - t_0) e^{-ib\pi x/2L} \cos(b\pi y/2L)(1 - e^{ib\pi}).
\]

Note that \( e^{ib\pi} = (-1)^b \), so
\[
1 - e^{ib\pi} = \begin{cases} 2 & \text{for odd } b \\ 0 & \text{for even } b \end{cases}.
\]

Writing the odd \( b \) as \( 2n - 1 \), we have \( \frac{1}{2L} (b \pi \hbar)^2 = \frac{n}{2L} (n - \frac{1}{2})^2 = E_n \) and \( \frac{b \pi}{2L} = \frac{n}{2L} (n - \frac{1}{2}) = k_n \). That is, \( K(y,t_1;x,t_0) \) equals
\[
\frac{1}{L} \sum_{n = -\infty}^{\infty} e^{-iE_n(t_1-t_0)} e^{-ik_n x} \cos(k_n y)
\]
\[
= \frac{2}{L} \sum_{n = -\infty}^{\infty} e^{-iE_n(t_1-t_0)} \cos(k_n x) \cos(k_n y).
\]

Again, this matches the result from spectral decomposition.

### IV. REMARKS

Using the terminology of this article, in \( \square \) it was stated that for Dirichlet boundary condition, \( \epsilon_r = (-1)^r \). This is a result of a phase change by \(-1\) each time the classical path reflects along the boundaries.

From a classical point of view, this phase change should be a local factor and is dependent only upon the condition around the boundary point.

**Conjecture.** The phase factor associated to each reflection can be determined using either the model of a free particle on a ray with suitable boundary condition imposed, or a finite potential barrier model (details in the following passage). The auxiliary phase that occurs as the weight for each classical path in the sum equals the product over all reflections of that path.

In this article we discussed the auxiliary phase that is associated to the boundary point, depending on the boundary condition on the equation imposing on that point being of Dirichlet or Neumann type. We also proved that the resulting formulae on the propagator matches those arising from the Schrödinger equation, with a trivial normalization factor.

There are several generalizations of this result that should be worth investigating:

1. In this article, we interpret the infinite potential well problem as the Schrödinger equation on a line segment with Dirichlet boundary condition and verified that the auxiliary phase is
\(-1 = e^{i\pi}\). It can be shown that for a potential barrier of finite height \(h\), the phase factor associated to the reflection should be \(e^{-i\theta}\), where

\[
\theta = \cot^{-1}\left(\frac{k^2 - q^2}{2kq}\right)
\]

with \(k, q\) determined by \(h\) (refer to appendix for detail).

Assuming the Conjecture, the phase factor computed above can then be applied to the problem of a finite potential well. In fact, by doing so, one can obtain its bound states spectra through the sum over classical paths weighted by the corresponding auxiliary phase (which are computed by \(\epsilon_r = e^{-i\theta} \)).

2. To study whether the Ansatz holds in computing the auxiliary phase on a higher dimensional model when reflecting along the boundary. It would be particularly interesting to know if the geometry (shape) of the boundary plays a part.

3. Deriving a formula for the phase factor in this model under other boundary conditions such as the Robin boundary condition.

**APPENDIX: AUXILIARY PHASE FOR A FINITE POTENTIAL WELL**

Consider the Schrödinger equation with a (finite) constant step barrier:

\[
H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)
\]

where \(V(x) = \begin{cases} 0 & x \leq 0 \\ h & \text{otherwise} \end{cases}\).

It is a standard calculation for scattering problem that can be found in, say [12, 13]. Defining the wave function \(\psi(x) = \begin{cases} \psi_0(x) & \text{for } x < 0 \\ \psi_1(x) & \text{for } x \geq 0 \end{cases}\). We consider an incoming wave with energy \(E < h\). It turns out that

\[
\psi_0(x) = e^{ikx} + Re^{-ikx} \quad \text{and} \quad \psi_1(x) = Te^{-qx}.
\]

with \(R = \frac{k-q}{k+q}\), where \(k = \sqrt{\frac{2m}{\hbar^2}E}\) and \(q = \sqrt{\frac{2m}{\hbar^2}(h - E)}\). The physical interpretation here is that \(R = e^{-i\theta}\) is the phase change in the reflected wave (moving toward the negative direction). It is where we easily see that the phase factor \(e^{-i\theta} \rightarrow -1\) as \(h \to \infty\).

Furthermore, writing \(e^{-i\theta} = \cos(\theta) - i\sin(\theta)\) gives the formula \(\theta = \cot^{-1}\left(\frac{k^2 - q^2}{2kq}\right)\).
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