บทความวิจัย

อินทิกรัลตามเส้นทางสำหรับกำแพงศักย์อนันต์

Path Integral for an Infinite Potential Barrier

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บทคัดย่อ

บทความนี้ศึกษาปัญหากำแพงศักย์อนันต์ในหนึ่งมิติโดยอาศัยวิธีอินทิกรัลตามเส้นทางของฟายน์แมน ได้คำนวณตัวแผ่กระจายสำหรับกำแพงศักย์อนันต์โดยวิธีอินทิกรัลตามเส้นทางแบบลากรางเกียน ผลเฉลยที่ได้อาศัยวิธีจุดภาพกระจกเงาซึ่งสมมูลกับการรวมเส้นทางแบบฉบับ ตัวแผ่กระจายที่ได้อยู่ในรูปแบบที่กระชับ และจากตัวแผ่กระจายดังกล่าวสามารถนำไปคำนวณหาสถานะเจาะจงโมเมนตัมและระดับพลังงานที่เป็นไปได้ของอนุภาคที่อยู่ภายใต้อิทธิพลของกำแพงศักย์อนันต์ได้

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Abstract

In this paper we study an infinite potential barrier problem in one dimension using Feynman path integral approach. The propagator for the infinite potential barrier is calculated by means of the Lagrangian path integral. This solution uses an image-point method equivalent to a sum over classical paths. The propagator is evaluated in a closed form, and from this propagator we obtained the momentum eigenstates and possible energy levels of a particle under the influence of an infinite potential barrier.

Introduction

In 1948, Feynman proposed a new approach to quantum mechanics which provides the propagator of a particle as a path integral over all possible histories of the system(Feynman and Hibbs, 1965). Since then the path integral approach has attracted much attention and has proven useful in many areas of physics. A strange fact is that Feynman's theory has been powerless in solving some problems such as an electron in a Coulomb potential, an infinite potential barrier, and an infinite square well, etc. Historically, for a Coulomb potential problem, Ho an Inomata(1982)succeeded in performing the configuration space path integration for the Hydrogen atom and they obtained Green's function of an electron in a closed form. From this Green's function, Choosiri and Sayakanit(1984) derived the energy levels and wave functions of the hydrogen atom in three dimensions. In 1981, Goodman proposed an image-point method, after applying this method to path integral of an infinite potential barrier problem he obtained the propagator of a particle under this potential. Here we will show how to examine the wave functions and energy levels of the particle from this propagator.

The Propagator and Feynman's Path Integral

In quantum mechanics, the dynamical information of a quantum mechanical system is contained in the wave function. It is a function that determines the wave associated with a particle. In practice we can obtain this wave function by solving Schrodinger's equation. In Schrodinger's picture, there exists a state vector $|\psi(t)\rangle$ whose evolution is determined by the equation(Messiah, 1961)

$$|\psi(t)\rangle = U(t,t')|\psi(t')\rangle \tag{1}$$

where $U(t,t')$ is the time evolution operator. If the Hamiltonian operator of the system is not an explicit function of time then the evolution operator is of the form

$$U(t'',t') = \exp\left\{-\frac{i}{\hbar}(t''-t')H\right\}. \tag{2}$$

In the configuration representation, Eq.(1) becomes

$$\langle\vec{x}''|\psi(t'')\rangle = \int_{-\infty}^{\infty}\langle\vec{x}''|U(t'',t')|\vec{x}'\rangle\langle\vec{x}'|\psi(t')\rangle d^3x' , \tag{3}$$

where we use the normalization condition

$$\int_{-\infty}^{\infty} |\vec{x}'\rangle\langle\vec{x}'| d^3x' = 1. \tag{4}$$

We can writes Eq.(3) as

$$\psi(\vec{x}'',t'') = \int_{-\infty}^{\infty} K(\vec{x}'',t'';x',t')\psi(\vec{x}',t')d^3x' , \tag{5}$$

where

$$K(\vec{x}'',t'';\vec{x}',t') = \langle\vec{x}''|U(t'',t')|\vec{x}'\rangle = \langle\vec{x}'',t''|\vec{x}',t'\rangle \tag{6}$$

and is called the propagator or probability amplitude of a particle going from $\vec{x}'$ at time t' to $\vec{x}''$ at time t'' .

According to Feynman's ideas there are infinitely many paths that a particle can travel going from $\vec{x}'$ at t' to $\vec{x}''$ at t''. The amplitude is the sum of the contribution from each path i.e.

$$K(\vec{x}'',t'';\vec{x}',t') = \sum_{\substack{\text{over all paths} \\ \text{from } \vec{x}' \text{ to } \vec{x}''}} \Phi[\vec{x}(t)] . \tag{7}$$

The contribution of a path has a phase proportional to the action

$$\Phi[\vec{x}(t)] = \text{const}.e^{\frac{i}{\hbar}S[\vec{x}(t)]}, \tag{8}$$

where the action

$$S = \int_{t'}^{t''} L(\vec{x},\dot{\vec{x}})dt$$

and the Lagrangian

$$L(\vec{x},\dot{\vec{x}}) = \frac{1}{2}m\dot{\vec{x}}^2 - V(\vec{x}).$$

On a polygonal basis, the propagator (7) can be written as

$$K(\vec{x}'',t'';\vec{x}',t') = \lim_{\substack{N\to\infty \\ \varepsilon\to 0}}\left(\frac{2\pi\hbar i\varepsilon}{m}\right)^{-3N/2} \int\int ... \int \exp\left\{\frac{i}{\hbar}\sum_{i=1}^{N}\left[\frac{m}{2\varepsilon}(\vec{x}_i - \vec{x}_{i-1})^2 - \varepsilon V(\vec{x}_i)\right]\right\} d^3x_1 d^3x_2 ... d^3x_{N-1} . \tag{9}$$

Feynman wrote this sum over paths in a less restrictive notation as

$$K(\vec{x}'',t'';\vec{x}',t') = \int_{\vec{x}'}^{\vec{x}''} e^{\frac{i}{\hbar}S[\vec{x}'',\vec{x}']} D[\vec{x}(t)] \tag{10}$$

which he called "a path integral". In addition, when the energy spectrum of a particle is discrete, the propagator of Eq.(10) can be written in a form

$$K(\vec{x}'',t'';\vec{x}',t') = \sum_n \psi_n(\vec{x}'')\psi_n^*(\vec{x}')e^{-\frac{iE_n}{\hbar}(t''-t')} \tag{11}$$

and for a continuous spectrum Eq.(11) becomes

$$K(\vec{x}'',t'';\vec{x}',t') = \int_{-\infty}^{\infty} \psi_k(\vec{x}'')\psi_k^*(\vec{x}')e^{-\frac{iE(k)}{\hbar}(t''-t')}d^3k\,. \tag{12}$$

From Eq.(11) and (12) we realize that the propagator contains information both eigenstates and energy levels of a particle in quantum mechanical system. Furthermore, for any particle whose Lagrangian is quadratic in position and velocity, the propagator has the form $Fe^{\frac{i}{\hbar}S_{cl}}$, where F is a pre-factor or normalizing factor and S_{cl} is the classical action, the integral of the Lagrangian along the classical path. The pre-factor can be evaluated by using the formula (van Vleck, 1978; Pauli, 1952)

$$F(t'',t') = \det\left[\frac{i}{2\pi\hbar}\frac{\partial^2}{\partial\vec{x}'\partial\vec{x}''}S_{cl}(\vec{x}'',\vec{x}')\right]^{1/2}. \tag{13}$$

So that for a quadratic Lagrangian, th propagator becomes

$$\langle\vec{x}'',t''|\vec{x}',t'\rangle = \det\left[\frac{i}{2\pi\hbar}\frac{\partial^2}{\partial\vec{x}'\partial\vec{x}''}S_{cl}(\vec{x}'',\vec{x}')\right]^{1/2} e^{\frac{i}{\hbar}S_{cl}(\vec{x}'',\vec{x}')}. \tag{14}$$

Infinite Potential Barrier

The infinite potential barrier is one of the simplest unbounded-state problem in wave mechanics; it is usually one of the first example given in any introductory quantum mechanics course. The problem is to solve for the motion in one dimension of a particle under the influence of the potential

$$V(x) = \begin{cases} 0 & \text{for} \quad x > 0 \\ \infty & \text{for} \quad x \le 0. \end{cases} \tag{15}$$

The momentum eigenstates for the potential are not of a free particle, but rather

$$\psi_p(x) = \begin{cases} \frac{1}{\sqrt{\pi\hbar}}\sin\left(\frac{px}{\hbar}\right) & \text{for} \quad x > 0 \\ 0 & \text{for} \quad x \le . \end{cases} \tag{16}$$

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According to Goodman's ideas for the infinite potential barrier, there are two classical paths(see Fig. 1). The first is that of a free particle, while the second is that of a particle that bounces off the wall on it way from (x',t') to (x'',t'). However, this second path is equivalent to the path of a free particle going directly from (x',t') to $(-x'',t'')$.

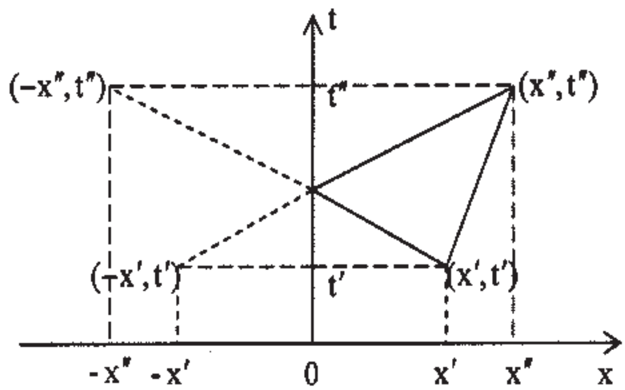

Fig.1 Two classical paths connecting (x',t') and (x'',t'') and their corresponding image points.

By applying the image method to the path integral approach, the propagator of the infinite potential barrier can be written as

$$\langle x'',t''|x',t'\rangle = \left(\frac{m}{2\pi i\hbar(t''-t')}\right)^{1/2} \times \left[\exp\left(\frac{im(x''-x')^2}{2\hbar(t''-t')}\right) - \exp\left(\frac{im(-x''-x')^2}{2\hbar(t''-t')}\right)\right]$$

$$= \langle x'',t''|x',t'\rangle_F - \langle -x'',t''|x',t'\rangle_F , \tag{17}$$

where the subscript F denote the propagator for a free particle.

The results has an explanation using path integral concepts. Since the particle is essential free for x>0, it would seem that it behavior would be closely linked to that of a free particle. It is well known that for a free particle the propagator has the form $Fe^{\frac{i}{\hbar}S_{cl}}$, for the infinite potential barrier the key difference is that there are two classical paths (see Fig. 1). The first is that of a free particle, while the second term is that of a particle that bounces off the wall onits way from (x',t') to (x'',t''). Geometrically, this second path can be constructed by first reflecting (x'',t'') about the line $x = 0$, then constructing the free particle path from (x',t') to this image point $(-x'',t'')$, and finally reflecting the path back to (x'',t'') so that $x \geq 0$ everywhere. Alternatively, we may perform these reflections with (x',t') rather than (x'',t''), and obtain exactly the same results. This corresponds to the fact that the second term of Eq. (17) may also be written as $\langle x'',t''|-x',t'\rangle_F$. However, for simplicity we will consider from now on only reflection of the final point. Applying the superposition principle, we would expect the propagator to be the sum of contributions from this two classical paths, which should be the free-particle propagator from (x',t') to (x'',t'') and $(-x'',t'')$ respectively, except perhaps for some effect of the barrier on the reflect path. Equation (17) confirms these expectations and indicates that the effect of the barrier on the reflected path to multiply its propagator by the phase factor -1. This phase factor can be thought of arising from the bound end reflection of the wave function at the barrier.

Momentum Eigenstates and Possible Allowed Energy Levels

We now examine the momentum eigenstates and energy levels of an infinite potential barrier from the propagator of Eq.(17). By using the formula (Gradshteyn and Ryzhik, 1965)

$$\int_{-\infty}^{\infty} e^{-ax^2+ibx} dx = \sqrt{\frac{\pi}{a}} e^{-b^2/4a}, \tag{18}$$

we can transform the exponential factors of Eq.(17) into the integral form :

$$\exp\left(\frac{im}{2\hbar(t''-t')}(\pm x''-x')^2\right) = \left(\frac{i\hbar(t''-t')}{2m\pi}\right)^{1/2} \int_{-\infty}^{\infty} e^{-\frac{i\hbar}{2m}(t''-t')k^2+i(\pm x''-x')k} dk, \tag{19}$$

where k is a wave number of a particle which relates to the momentum as $p = .\ \hbar k$ Substituting Eq.(19) into (17) we obtain

$$\langle x'',t''|x',t'\rangle = \left(\frac{m}{2\pi i\hbar(t''-t')}\right)^{1/2} \left(\frac{i\hbar(t''-t')}{2m\pi}\right)^{1/2} \times \int_{-\infty}^{\infty} e^{-\frac{i\hbar}{2m}(t''-t')k^2} (e^{i(x''-x')k} - e^{i(-x''-x')k}) dk = \frac{1}{\pi} \int_{-\infty}^{\infty} e^{-\frac{i\hbar}{2m}(t''-t')k^2} \sin(kx'')\sin(kx') dk. \tag{20}$$

In momentum-space representation, Eq.(20) becomes

$$\langle x'',t''|x',t'\rangle = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t''-t')} \sin(\tfrac{p}{\hbar}x'')\sin(\tfrac{p}{\hbar}x') dp. \tag{21}$$

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Comparing Eq.(21) to Eq.(12) we get the momentum eigenstates

$$\left.\begin{aligned}\psi_p(x'') &= \frac{1}{\sqrt{\pi\hbar}}\sin(\tfrac{p}{\hbar}x'') \\ \psi_p^*(x') &= \frac{1}{\sqrt{\pi\hbar}}\sin(\tfrac{p}{\hbar}x')\end{aligned}\right\} \tag{22}$$

with possible continuous energy levels $E(p) = \frac{1}{2m}p^2$. This is the same as Eq.(16) which derived from the Schrodinger equation.

Discussion and Conclusion

The solution of an infinite potential barrier problem is already well known. Therefore the solution itself is not particularly important. The main problem is whether or not the path integration can be carried out for such a problem. The only path integrals known to be solvable are those of Gaussian with unbounded domain. What was done in this paper was to give the concept of image-point method for handling the path integral of an infinite potential barrier. The key concept is that there are two classical paths. The first is that of a free particle, while the second is that of a particle bounces off the wall on it way from (x',t') to (x'',t''). From the corresponding propagator, we can derive the momentum eigenstates and energy levels of a particle in this system.

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