บทความวิจัย

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Path Integral for a Semi-Harmonic Oscillator

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บทคัดย่อ

ปัญหากึ่งฮาร์มอนิกออสซิลเลเตอร์เป็นปัญหาของอนุภาคเคลื่อนที่ในหนึ่งมิติภายใต้อิทธิพลของศักย์แบบฮาร์มอนิกออสซิลเลเตอร์ในย่าน $\chi > 0$ แต่ในย่าน $\chi \le 0$ ศักย์กลับกลายเป็นอนันต์ จุดประสงค์ของงานวิจัยนี้ต้องการหาฟังก์ชันคลื่นและระดับพลังงานที่เป็นไปได้ของอนุภาคโดยอาศัยทฤษฎีอินทิกรัลตามเส้นทาง หลังจากการประยุกต์ใช้วิธีจุดภาพกระจกเงากับทฤษฎีอินทิกรัลตามเส้นทาง พบว่าตัวแผ่กระจายสามารถเขียนอยู่ในรูปแบบเชิงวิเคราะห์ดังนี้

$$K(b,a)=\left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\times\exp\left(\frac{im\omega}{2\hbar\sin\omega T}(x_a^2+x_b^2)\cos\omega T\right)\left\{e^{\frac{-im\omega x_a x_b}{\hbar\sin\omega T}}-e^{\frac{im\omega x_a x_b}{\hbar\sin\omega T}}\right\},$$

โดยที่ $T=t_b-t_a$ จากตัวแผ่กระจายดังกล่าวสามารถนำมาคำนวณหาฟังก์ชันคลื่นและระดับพลังงานที่เป็นไปได้ของกึ่งฮาร์มอนิกออสซิลเลเตอร์ เราได้ฟังก์ชันคลื่น

$$\psi_n(x)=A_n e^{-m\omega x^2/2\hbar}H_n(\sqrt{\tfrac{m\omega}{\hbar}}x),\quad n=1,3,5,..,$$

เมื่อค่าคงตัวของการเป็นคลื่นปกติ

$$A_n=\left[\frac{1}{2^{n-1}n!}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\right]^{1/2},$$

ในที่นี้ $H_n(x)$ คือพหุนามแฮร์มิตอันดับที่ n และระดับพลังงานที่เป็นไปได้คือ

$$E_n=(n+1/2)\hbar\omega,\quad n=1,3,5,\dots .$$

หากไม่พิจารณาถึงเลขควอนตัม n รูปแบบเชิงคณิตศาสตร์ของผลลัพธ์ที่ได้นั้นเหมือนกับของฮาร์มอนิกออสซิลเลเตอร์ทุกประการ

Abstract

The propagator for a semi-harmonic oscillator(half-space harmonic oscillator) is evaluated exactly using the application of image-point method to path integral theory, we find that the propagator can be written in an analytical form :

$$K(b,a)=\left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\times\exp\left(\frac{im\omega}{2\hbar\sin\omega T}(x_a^2+x_b^2)\cos\omega T\right)\left\{e^{\frac{-im\omega x_a x_b}{\hbar\sin\omega T}}-e^{\frac{im\omega x_a x_b}{\hbar\sin\omega T}}\right\},$$

where $T=t_b-t_a$ From the propagator, the wave functions and the possible energy levels are derived. We obtain the wave functions :

$$\psi_n(x)=A_n e^{-m\omega x^2/2\hbar}H_n(\sqrt{\tfrac{m\omega}{\hbar}}x),\quad n=1,3,5,..,$$

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where the normalization constant :

$$A_n = \left[\frac{1}{2^{n-1} n!} \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} \right]^{1/2},$$

here $H_n(x)$ is Hermite polynomial of order n, and we obtain the energy level :

$$E_n = (n + 1/2)\hbar\omega, \quad n = 1,3,5,\ldots .$$

If we do not consider the quantum number n, the mathematical form of our results are the same as that of an harmonic oscillator.

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, 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 apply the image-point method to path integral of a semi-harmonic oscillator.

METHODOLOGY

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, the evolution of a wave function is determined by the equation (Messiah, 1961)

$$|\psi(t)\rangle = U(t,t')|\psi(t')\rangle \qquad (1)$$

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

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

In the configuration representation, Eq.(1) becomes

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

where we use the normalization condition

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

We can writes Eq.(3) as

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

where

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

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.

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

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 (6) can be written as

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

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.(6) 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. However, in real practice Eq.(9) is too complicate to perform. To simplify the path integral for handling, Feynman introduced some additional mathematical techniques which help us to sum over paths in some certain situation, by representing any possible path $\chi(t)$ by the classical path $\chi_{cl}(t)$ and the deviation from the classical path $y(t)$, i.e. $\chi(t) = \chi_{cl}(t) + y(t)$ then the propagator can be written as

$$K(\vec{x}'',t'';\vec{x}',t') = F(t'',t')e^{\frac{i}{\hbar}S_{cl}(\vec{x}'',\vec{x}')}, \tag{13}$$

where $F(t'',t')$ and $S_{cl}(\vec{x}'',\vec{x}')$ are the pre-factor and the classical action respectively. However, for a quadratic Lagrangian, van Vleck(1978) and Pauli(1952) had verified that $F(t'',t')$ can be evaluated exactly by using the formula

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

COMPUTATION PROCEDURE

The 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

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

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''). Geometrically, this second path can be constructed by first reflecting (x'',t'') about the line $x=0$, then constructing the free-particle path $x(t)$ from (x',t') to this image point $(-x'',t'')$ and finally reflecting the path back to (x',t') so that $x(t)\geq 0$ everywhere.

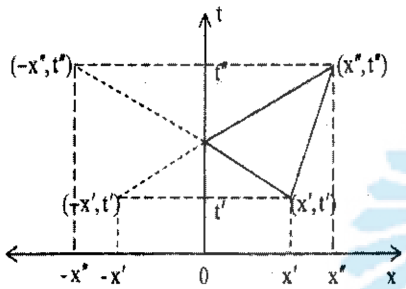

Figure 1 : Two classical paths connecting and and their corresponding image points.

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

$$\begin{aligned}&\langle x'',t''|x',t'\rangle\\&=\langle x'',t''|x',t'\rangle_F-\langle -x'',t''|x',t'\rangle_F\\&=\left(\frac{m}{2\pi i\hbar(t''-t')}\right)^{1/2}\times\left[\exp\left(\frac{im(x''-x')^2}{2\hbar(t''-t')}\right)\right.\\&\left.-\exp\left(\frac{im(-x''-x')^2}{2\hbar(t''-t')}\right)\right]\end{aligned}\qquad(16)$$

where the subscript F denote the propagator for a free particle. The phase factor -1 in the second term of the right of (16) can be thought of arising from the bound end reflection of the wave function at the barrier.

Momentum Eigenstates and Possible Allowed Energy Levels of an Infinite Potential Barrier

We now examine the momentum eigenstates and energy levels of an infinite potential barrier from the propagator of Eq.(16). By using the formula (Gradshteyn and Ryzhik, 1965)

$$\int_{-\infty}^{\infty}e^{-ax^2+ibx}dx=\sqrt{\frac{\pi}{a}}e^{-b^2/4a},\qquad(17)$$

we can transform the exponential factors of Eq.(16) into the integral form :

$$\begin{aligned}&\exp\left(\frac{im}{2\hbar(t''-t')}(\pm x''-x')^2\right)\\&=\left(\frac{i\hbar(t''-t')}{2m\pi}\right)^{1/2}\int_{-\infty}^{\infty}e^{-\frac{i\hbar}{2m}(t''-t')k^2+i(\pm x''-x')k}dk,\end{aligned}\qquad(18)$$

where k is a wave number of a particle which relates to the momentum as $p=\hbar k$. Substituting Eq.(18) into (16) we obtain

$$\begin{aligned}\langle x'',t''|x',t'\rangle&=\left(\frac{m}{2\pi i\hbar(t''-t')}\right)^{1/2}\left(\frac{i\hbar(t''-t')}{2m\pi}\right)^{1/2}\\&\times\int_{-\infty}^{\infty}e^{-\frac{i\hbar}{2m}(t''-t')k^2}(e^{i(x''-x')k}-e^{i(-x''-x')k})dk\\&=\frac{1}{\pi}\int_{-\infty}^{\infty}e^{-\frac{i\hbar}{2m}(t''-t')k^2}\sin(kx'')\sin(kx')dk.\end{aligned}\qquad(19)$$

In momentum-space representation, Eq. (19) becomes

$$\begin{aligned}&\langle x'',t''|x',t'\rangle\\&=\frac{1}{\pi\hbar}\int_{-\infty}^{\infty}e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t''-t')}\sin(\tfrac{p}{\hbar}x'')\sin(\tfrac{p}{\hbar}x')dp.\end{aligned}\qquad(20)$$

Comparing Eq.(20) to Eq.(12) we get the momentum eigenstates

$$\left.\begin{aligned}\psi_p(x'')&=\frac{1}{\sqrt{\pi\hbar}}\sin(\tfrac{p}{\hbar}x'')\\\psi_p^*(x')&=\frac{1}{\sqrt{\pi\hbar}}\sin(\tfrac{p}{\hbar}x')\end{aligned}\right\}\qquad(21)$$

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

The Semi-Harmonic Oscillator

The semi-harmonic oscillator or half-space harmonic oscillator is a particle moving in one dimension under the influence of the potential

$$V(x)=\begin{cases}\infty & \text{for } x\le 0\\ \frac{1}{2}m\omega^2x^2 & \text{for } x>0\,.\end{cases} \quad (22)$$

Similarly to that of the infinite potential barrier, after applying the image-point method to path integral of a semi-harmonic oscillator we obtain the propagator

$$\langle x_b,t_b|x_a,t_a\rangle=\left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\times \exp\left(\frac{im\omega}{2\hbar\sin\omega T}(x_a^2+x_b^2)\cos\omega T\right)\times \left\{e^{\frac{-im\omega x_a x_b}{\hbar\sin\omega T}}-e^{\frac{im\omega x_a x_b}{\hbar\sin\omega T}}\right\}. \quad (23)$$

where $T=t_b-t_a$. To obtain the wave functions and energy levels of a semi-harmonic oscillator we must expand the right of (23) into a series as in the form of (11) by using the formulas (Gradshteyn and Ryzhik, 1965)

$$\left.\begin{aligned} i\sin\omega T &= \tfrac{1}{2}e^{i\omega T}(1-e^{-2i\omega T})\\ \cos\omega T &= \tfrac{1}{2}e^{i\omega T}(1+e^{-2i\omega T})\end{aligned}\right\} ,(24)$$

$$\left.\begin{aligned}(1+x)^{-1/2} &= 1-\tfrac{1}{2}x+\tfrac{1\cdot 3}{2\cdot 4}x^2-\tfrac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}x^3+\ldots,-1<x<1\\ (1+x)^{-1} &= 1-x+x^2-x^3+\ldots,-1<x<1\end{aligned}\right\}, (25)$$

and

$$e^{\theta}=1+\theta+\tfrac{1}{2!}\theta^2+\tfrac{1}{3!}\theta^3+\ldots \quad . \quad (26)$$

RESULTS, DICUSSION AND CONCLUSIONS

After applying (24)-(26) to (23) , the propagator of a semi-harmonic oscillator becomes ,(27)

$$\langle x_b,t_b|x_a,t_a\rangle=\sum_n \psi_n(x_b)\psi_n^*(x_a)e^{-\frac{iE_nT}{\hbar}} ,(27)$$

where

$$\psi_n(x)=A_n e^{-m\omega x^2/2\hbar}H_n(\sqrt{\tfrac{m\omega}{\hbar}}x),\ n=1,3,5,.., \quad (28)$$

$$A_n=\left[\frac{1}{2^{n-1}n!}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\right]^{1/2},n=1,3,5,..., \quad (29)$$

and the possible energy levels

$$E_n=(n+1/2)\hbar\omega,\quad n=1,3,5,... \ .(30)$$

The solution of a semi-harmonic oscillator problem may be solved by using Schrodinger equation. 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 an unbounded domain. What was done in this paper was to give the concept of image- point method for handling the path integral of a semi-harmonic oscillator. The key concept is that there are two classical paths. The first is that of a particle going directly between the two points, while the second is that of a particle bounces off the wall on it way from (x_a,t_a) to (x_b,t_b). From the corresponding propagator, we can derive the eigenstates and energy levels of a particle in this system.

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