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Quantum states of a particle in a box via unilateral Fourier transform

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The quantum problem of stationary states of a particle in a box is revisited by means of the unilateral Fourier transform. Homogeneous Dirichlet boundary conditions demand a finite Fourier sine transform which is actually the Fourier sine series.

Keywords: Particle in a box, Infinite square-well potential, Unilateral Fourier transform.

1. Introduction

In quantum theory, a particle confined by impenetrable walls is usually called a particle in box. For one-dimensional cases that kind of system is modeled by an infinite square-well potential. This is one of the easiest problems in quantum mechanics exhibiting many characteristics of the quantum physics and for this reason it appears in a plethora of introductory textbooks on quantum mechanics (see, e.g. [1]- [12]). Although it is not a realistic system, it serves as an idealization of complex systems occurring in the nature and, in some circumstances, reflects the properties of certain real systems. Unremarkably, the possible nonrelativistic bound-state solutions of a particle in a one-dimensional box are found by a straight and short resolution of the time-independent Schrödinger equation by imposing the continuity of the eigenfunctions on the confining walls. By contrast, in a recent paper diffused in the literature, the quantum problem of a particle in an infinite square-well potential was claimed to be solved via Laplace transform [13]. While emphatically refuted due to an erroneous inversion of the Laplace transform [14], Ref. [13] awakens interest in applying over a finite interval other kinds of integral transforms usually defined over an infinite or a semi-infinite range of integration.

In this work we approach the quantum problem of a particle in an infinite square-well potential with the unilateral Fourier transform. Ordinarily the unilateral Fourier transform is a useful tool for absolutely integrable functions defined over a semi-infinite interval depending on the homogeneous Dirichlet or the homogeneous Neumann boundary conditions at the origin. The way we are going to approach this problem, though, results in a finite Fourier sine transform. That kind of finite unilateral Fourier transform, and its close connection with Fourier series, can be of interest of teachers and students of mathematical methods applied to physics and quantum mechanics of undergraduate courses.

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2. Unilateral Fourier transform

The Fourier sine and cosine transforms of $f(x)$ are denoted by $\mathcal{F}_s\{f(x)\} = F_s(k)$ and $\mathcal{F}_c\{f(x)\} = F_c(k)$, respectively, and are defined by the integrals (see, e.g. [15]- [17])

$$F_s(k) = \mathcal{F}_s\{f(x)\} = \sqrt{\frac{2}{\pi}}\int_0^\infty dx\, f(x)\sin kx, \qquad (1)$$

$$F_c(k) = \mathcal{F}_c\{f(x)\} = \sqrt{\frac{2}{\pi}}\int_0^\infty dx\, f(x)\cos kx, \qquad (2)$$

where $k >= 0$. The original function $f(x)$, based on certain conditions, can be retrieved by the inverse unilateral Fourier transforms $\mathcal{F}_s^{-1}\{F_s(k)\}$ and $\mathcal{F}_c^{-1}\{F_c(k)\}$ expressed as

$$f(x) = \sqrt{\frac{2}{\pi}}\int_0^\infty dk\, F_s(k)\sin kx, \qquad (3)$$

and

$$f(x) = \sqrt{\frac{2}{\pi}}\int_0^\infty dk\, F_c(k)\cos kx. \qquad (4)$$

Sufficient conditions for the existence of the above integrals are ensured if $f(x)$, $F_s(k)$ and $F_c(k)$ are absolutely integrable. The choice of sine or cosine transform is decided by the homogeneous boundary conditions at the origin: Dirichlet condition $\left(f(x)|_{x=0} = 0\right)$ or Neumann condition $\left(df(x)/dx|_{x=0} = 0\right)$.

3. The particle in a box

The time-independent Schrödinger equation (for the stationary states) reads

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi_E(x) = E\psi_E(x). \qquad (5)$$

The quantity $|\psi_E(x)|^2$ is the position probability density, meaning that $|\psi_E(x)|^2 dx$ is the probability of finding the particle in the region dx about its point x. Then,

$$\int_{-\infty}^{+\infty} dx\, |\psi_E(x)|^2 = 1. \tag{6}$$

The desired solution of this eigenvalue problem is the characteristic pair (E, ψ_E) with $E \in \mathbb{R}$ and $\psi_E(x)$ is single valued, finite and continuous everywhere.

The infinite square-well potential

$$V(x) = \begin{cases} 0, & 0 \leq x \leq L \\ \infty, & x < 0 \quad \text{and} \quad x > L \end{cases} \tag{7}$$

emulates a particle constrained to move between two impenetrable walls at a distance L in such a way that one can write

$$\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + E\right)\psi_E(x) = 0, \quad 0 \leq x \leq L, \tag{8}$$

and

$$\psi_E(x) = 0, \quad x < 0 \quad \text{and} \quad x > L. \tag{9}$$

Continuity of the eigenfunction at the walls requires $\psi_E(0) = \psi_E(L) = 0$. Therefore, the eigenfunction $\psi_E(x)$ can be compactly written as

$$\psi_E(x) = \theta(x)\,\theta(L-x)\, f_E(x), \tag{10}$$

where $\theta(x)$ is is the step function

$$\theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0, \end{cases} \tag{11}$$

and $f_E(x)$ satisfies the equation

$$\left(\frac{d^2}{dx^2} + k^2\right) f_E(x) = 0, \quad 0 \leq x \leq L, \tag{12}$$

subject to the homogeneous Dirichlet boundary conditions $f_E(0) = f_E(L) = 0$, and

$$\int_0^L dx\, |f_E(x)|^2 = 1. \tag{13}$$

4. The solution of the problem

To begin with, we discard the Fourier cosine transform due to the homogeneous Dirichlet boundary condition at the origin. Rather, we suppose that $f_E(x)$ can be expressed by a Fourier sine transform as

$$f_E(x) = \int_0^\infty dk\, F^{(E)}(k) \sin kx. \tag{14}$$

Furthermore, the remaining homogeneous Dirichlet boundary condition at $x = L$ enforces that k is restricted to discrete values

$$k = \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots, \tag{15}$$

so that the function $F^{(E)}(k)$ can be regarded as an infinite set of numbers $F_n^{(E)}$. Moreover, instead of an integral over the continuous variable k, we have a sum over n:

$$f_E(x) = \sum_{n=1}^{\infty} F_n^{(E)} \sin\frac{n\pi x}{L}. \tag{16}$$

The alert reader can see that (16) is just a Fourier sine series as has been already suggested in Ref. [14]. Substitution of this Fourier sine series into Eq. (12) furnishes

$$\sum_{n=1}^{\infty}\left(\frac{\hbar^2\pi^2 n^2}{2mL^2} - E\right) F_n^{(E)} \sin\frac{n\pi x}{L} = 0. \tag{17}$$

Multiplying this series by

$$\sin\frac{\tilde{n}\pi x}{L}, \quad \tilde{n} = 1, 2, 3, \ldots, \tag{18}$$

and integrating from 0 to L, we find

$$\sum_{n=1}^{\infty}\left(\frac{\hbar^2\pi^2 n^2}{2mL^2} - E\right) F_n^{(E)} \int_0^L dx\, \sin\frac{n\pi x}{L}\sin\frac{\tilde{n}\pi x}{L} = 0. \tag{19}$$

Taking advantage of the orthonormality relation

$$\int_0^L dx\, \sin\frac{n\pi x}{L}\sin\frac{\tilde{n}\pi x}{L} = \frac{L}{2}\delta_{n\tilde{n}}, \tag{20}$$

where $\delta_{n\tilde{n}}$ is the Kronecker delta symbol

$$\delta_{n\tilde{n}} = \begin{cases} 1, & \tilde{n} = n \\ 0, & \tilde{n} \neq n, \end{cases} \tag{21}$$

we find

$$\sum_{n=1}^{\infty}\left(\frac{\hbar^2\pi^2 n^2}{2mL^2} - E\right) F_n^{(E)} \delta_{n\tilde{n}} = 0, \tag{22}$$

in such a way that the Kronecker delta symbol kills every term in the sum except the one for which $n = \tilde{n}$. Then, the left-hand side of (22) reduces to one term:

$$\left(\frac{\hbar^2\pi^2 n^2}{2mL^2} - E\right) F_n^{(E)} = 0. \tag{23}$$

Taking one and only one $F_n^{(E)} \neq 0$ we find

$$f_n(x) = F_n^{(n)} \sin\frac{n\pi x}{L}, \tag{24}$$

with

$$E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}, \tag{25}$$

and the eigenfunctions are finally expressed as

$$\psi_n(x) = \theta(x)\,\theta(L-x)\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}, \tag{26}$$

where $F_n^{(n)} = \sqrt{2/L}$ was determined by (13). This characteristic par (E_n, ψ_n), given by (25) and (26), is in agreement with that one found by usual methods.

5. Final remarks

We have shown that the stationary states of the particle in a box via unilateral Fourier transform can be found with simplicity because it is a tool that favors compliance with boundary conditions from the start. Regarding the Laplace transform used in Ref. [13]

$$\mathcal{L}\left\{\psi_E\left(x\right)\right\} = \int_0^L dx\, e^{-sx} f_E\left(x\right), \qquad (27)$$

it was shown in Ref. [14] that

$$\begin{aligned}\mathcal{L}\left\{\frac{d^2\psi_E\left(x\right)}{dx^2}\right\} &= s^2\mathcal{L}\left\{\psi_E\left(x\right)\right\} - \left.\frac{df_E\left(x\right)}{dx}\right|_{x=0} \\ &+ e^{-sL}\left.\frac{df_E\left(x\right)}{dx}\right|_{x=L}, \end{aligned} \qquad (28)$$

so that all the inconvenience of the finite Laplace transform is due to the border term proportional to e^{-sL} that vanishes only when Re $s > 0$ and $L \to \infty$. On the other hand, it can be shown that

$$\mathcal{F}_s\left\{\frac{d^2\psi_E\left(x\right)}{dx^2}\right\} = -k^2\mathcal{F}_s\left\{\psi_E\left(x\right)\right\}, \qquad (29)$$

without border terms in such a way that

$$\mathcal{F}_s^{(n)}\left\{\psi_E\left(x\right)\right\} = \sqrt{\frac{2}{\pi}}\int_0^L dx\, f_E\left(x\right)\sin\frac{n\pi x}{L}, \qquad (30)$$

furnishes

$$\left(\frac{\hbar^2\pi^2 n^2}{2mL^2} - E\right)\mathcal{F}_s^{(n)}\left\{\psi_E\left(x\right)\right\} = 0. \qquad (31)$$

As a matter of fact, the homogeneous Dirichlet boundary condition at $x = L$ has allowed to change by reversal the usual transition from a Fourier series to a Fourier transform (see, e.g. [15]- [16]). The problem of a particle in a box symmetric about $x = 0$, and the related Fourier sine transform and Fourier cosine transform, is left for the readers.

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