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More on the quantum harmonic oscillator via unilateral Fourier transform

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The stationary states of the quantum harmonic oscillator are properly determined by means of the unilateral Fourier transform without having to recourse to the properties of the confluent hypergeometric functions. This simpler procedure is reminiscent of the algebraic method based on the ladder operators and depends on the value of just one tabulated definite integral related to the ground state.

Keywords: Fourier transform, Harmonic oscillator, Unilateral Fourier transform.

1. Introduction

Ordinarily the unilateral Fourier transform is a useful tool for solving problems involving absolutely integrable functions defined over a semi-infinite interval. A proper use of the unilateral Fourier transform, though, takes into account the adequate homogeneous boundary conditions at the origin. The convenience of using the Fourier sine transform or the Fourier cosine transform is dictated by the Dirichlet boundary condition or Neumann boundary condition, respectively. Those small details have been many times overlooked in the literature [1–10] (see Ref. [11] for criticisms).

The unilateral Fourier transform has proved to be a straightforward and efficient manner to deal with a few bound-state solution problems in nonrelativistic quantum mechanics [12–14]. In recent times, the quantum harmonic oscillator has also been approached by the Laplace transform [15–18], by the exponential Fourier transform [19–22], and also by the unilateral Fourier transform [12]. In Ref. [12], the quantum harmonic oscillator was approached by the unilateral Fourier transform method and the eigenfunctions were obtained by recurring to a few properties of the sometimes clumsy confluent hypergeometric function (Kummer's function). In the present paper we will show that the eigenfunctions can be obtained by an unlimited sequence of functions generated by that one related to the ground state. This process is reminiscent of the algebraic method based on the ladder operators (see, e.g. [23]), and depends on the calculation of just one definite integral easily found in math tables.

2. The Unilateral Fourier Transform

Let us begin with a brief description of the unilateral Fourier transform and a few of its properties. The unilateral Fourier transform can be obtained from the real form of the Fourier integral theorem [24]. It is worthwhile to note that once the unilateral Fourier transform and their inverse are established, the behaviour of $f(\zeta)$ and its transform on the other side of the axis does not matter. The direct Fourier sine and cosine transforms of $f(\xi)$ are denoted by $\mathcal{F}_s\{f(\xi)\} = F_s(k)$ and $\mathcal{F}_c\{f(\xi)\} = F_c(k)$, respectively, and are defined by the integrals (see, e.g. [24–26])

$$\begin{aligned} F_s(k) &= \mathcal{F}_s\{f(\xi)\} = \sqrt{\frac{2}{\pi}}\int_0^\infty d\xi\, f(\xi)\sin k\xi, \\ F_c(k) &= \mathcal{F}_c\{f(\xi)\} = \sqrt{\frac{2}{\pi}}\int_0^\infty d\xi\, f(\xi)\cos k\xi. \end{aligned} \tag{1}$$

The original function $f(\xi)$ can be recovered by the inverse unilateral Fourier transforms $\mathcal{F}_s^{-1}\{F_s(k)\}$ and $\mathcal{F}_c^{-1}\{F_c(k)\}$ expressed as

$$\begin{aligned} f(\xi) &= \mathcal{F}_s^{-1}\{F_s(k)\} = \sqrt{\frac{2}{\pi}}\int_0^\infty dk\, F_s(k)\sin k\xi, \\ f(\xi) &= \mathcal{F}_c^{-1}\{F_c(k)\} = \sqrt{\frac{2}{\pi}}\int_0^\infty dk\, F_c(k)\cos k\xi. \end{aligned} \tag{2}$$

We now observe that $f(\xi)$ retrieved by $F_s(k)$ must satisfy the homogeneous Dirichlet boundary condition at the origin, whereas $f(\xi)$ retrieved by $F_c(k)$ must satisfy the homogeneous Neumann boundary condition at the origin:

$$\begin{aligned} F_s(k) &\Rightarrow \quad f(\xi)|_{\xi=0} = 0, \\ F_c(k) &\Rightarrow \quad \frac{df(\xi)}{d\xi}|_{\xi=0} = 0. \end{aligned} \tag{3}$$

It immediately follows that

$$F_s(k)|_{k=0} = \left.\frac{dF_c(k)}{dk}\right|_{k=0} = 0. \tag{4}$$

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Those often overlooked boundary conditions are essential in applications that include the origin as an implicit boundary condition [1–10]. Moreover, they allow that the direct and the inverse unilateral Fourier transform can be extended continuously to the other side of the semiaxis. It is clear from (1) and (2) that the only difference between the direct and the inverse unilateral Fourier transform is the exchange of ξ by k. In addition, the functions and their respective transforms, if they are square integrables, are related by the Parseval's formulas:

$$\begin{aligned} \int_0^\infty d\xi\,|f(\xi)|^2 &= \int_0^\infty dk\,|F_s(k)|^2, \\ \int_0^\infty d\xi\,|f(\xi)|^2 &= \int_0^\infty dk\,|F_c(k)|^2. \end{aligned} \tag{5}$$

The usefulness of the unilateral transform method for solving problems depends of course on the mutual inversion process for the pairs $(f(\xi), F_s(k))$ and $(f(\xi), F_c(k))$ with the proper boundary conditions at the origin. In the following development we assume that the conditions for the existence of the inverses are satisfied in all the circumstances. The unilateral Fourier transforms have the following derivative properties

$$\begin{aligned} \mathcal{F}_s\left\{\frac{d^2f(\xi)}{d\xi^2}\right\} &= -k^2F_s(k), \\ \mathcal{F}_c\left\{\frac{d^2f(\xi)}{d\xi^2}\right\} &= -k^2F_c(k), \end{aligned} \tag{6}$$

and

$$\begin{aligned} \mathcal{F}_s\left\{\xi\frac{df(\xi)}{d\xi}\right\} &= -F_s(k) - k\frac{dF_s(k)}{dk}, \\ \mathcal{F}_c\left\{\xi\frac{df(\xi)}{d\xi}\right\} &= -F_c(k) - k\frac{dF_c(k)}{dk}. \end{aligned} \tag{7}$$

Differentiating $F_s(k)$ and $F_c(k)$ and assuming that $\xi^n f(\xi)$, with $n = 0, 1, 2, \ldots$, is well behaved, one obtains

$$\begin{aligned} \frac{d^{2n}F_s(k)}{dk^{2n}} &= (-1)^n\mathcal{F}_s\{\xi^{2n}f(\xi)\}, \\ \frac{d^{2n+1}F_s(k)}{dk^{2n+1}} &= (-1)^n\mathcal{F}_c\{\xi^{2n+1}f(\xi)\}, \\ \frac{d^{2n}F_c(k)}{dk^{2n}} &= (-1)^n\mathcal{F}_c\{\xi^{2n}f(\xi)\}, \\ \frac{d^{2n+1}F_c(k)}{dk^{2n+1}} &= (-1)^{n+1}\mathcal{F}_s\{\xi^{2n+1}f(\xi)\}. \end{aligned} \tag{8}$$

This last group of formulas establishes a connection between the existence of the unilateral Fourier transform of $\xi^n f(\xi)$ and the existence of the n-th derivatives of $\mathcal{F}_s\{f(\xi)\}$ and $\mathcal{F}_c\{f(\xi)\}$.

3. The Unilateral Fourier Transform Applied to the Harmonic Oscillator

We are now ready to address the one-dimensional quantum harmonic oscillator delineated by the boundary problem for the characteristic pair (ε, ψ):

$$\begin{aligned} &\frac{d^2\psi(x)}{dx^2} + (2\varepsilon - x^2)\psi(x) = 0, \\ &\int_{-\infty}^{+\infty} dx\,|\psi(x)|^2 < \infty. \end{aligned} \tag{9}$$

The differential equation in this eigenvalue problem is nothing more than the time-independent Schrödinger equation. The normalization condition is there for consistency of the probability interpretation of quantum mechanics. As a matter of fact, the normalization condition demands $\psi(x) \to 0$ as $|x| \to \infty$ in such a way that $\psi(x)$ tends to $e^{-x^2/2}$ for sufficiently large $|x|$. Because the differential equation is invariant under reflection through the origin ($x \to -x$) and $x = 0$ is a regular point, eigenfunctions and their first derivatives continuous on the whole line with well-defined parities can be constructed by taking symmetric and antisymmetric linear combinations of ψ defined on the positive side of the x-axis, by imposing additional boundary conditions on ψ at the origin: the homogeneous Dirichlet boundary condition ($\psi(x)|_{x=0} = 0$) for odd-parity eigenfunctions, and the homogeneous Neumann condition ($d\psi(x)/dx|_{x=0} = 0$) for even-parity eigenfunctions. Thus, it suffices to concentrate attention on the positive half-line ($\xi = |x|$). The imposed behaviour of $\psi(\xi)$ and $d\psi(\xi)/d\xi$ at the origin, besides the behaviour at infinity, allows us to use the unilateral Fourier transform like a shot into (9). However, this is an ineffective action because the transformed equation and transformed boundary conditions have the same form. In other words, the eigenvalue problem for $\psi(x)$ is invariant with respect to the unilateral Fourier transform. Indeed, using (6) and the first and the third lines of (8), one finds

$$\frac{d^2\Psi(k)}{dk^2} + (2\varepsilon - k^2)\Psi(k) = 0, \tag{10}$$

where $\Psi(k)$ is the unilateral transform of $\psi(\xi)$. Furthermore,

$$\int_0^\infty d\xi\,|\psi(x)|^2 = \int_0^\infty dk\,|\Psi(k)|^2. \tag{11}$$

Nevertheless, Ponomarenko's trick [20]

$$\psi(\xi) = \phi(\xi)e^{\xi^2/2}, \tag{12}$$

is able to accomplish the purpose. The factorization prescribed by (12) dictates that $\phi(\xi)$ obeys the equation

$$\frac{d^2\phi(\xi)}{d\xi^2} + 2\xi\frac{d\phi(\xi)}{d\xi} + (2\varepsilon + 1)\phi(\xi) = 0. \tag{13}$$

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Note that Ponomarenko's trick [20] is nothing more than the elimination of the first-derivative term of a second-order differential equation in reverse gear. Notice that $\phi(\xi)$ and $d\phi(\xi)/d\xi$ have the same behaviour as $\psi(\xi)$ and $d\psi(\xi)/d\xi$ at the origin, and tend to $e^{-\xi^2}$ for sufficiently large ξ. Therefore, $\phi(\xi)$ is amenable to unilateral Fourier transforms and is also square integrable. Using (6) and (7), with $\Phi(k)$ denoting the unilateral Fourier transform of $\phi(\xi)$, one obtains

$$\frac{d\Phi(k)}{dk}+\left(\frac{k}{2}-\frac{\varepsilon-1/2}{k}\right)\Phi(k)=0, \tag{14}$$

with

$$\int_0^\infty d\xi\,|\phi(\xi)|^2=\int_0^\infty dk\,|\Phi(k)|^2. \tag{15}$$

The boundary conditions on $\phi(\xi)$ and $\Phi(k)$ plus (15) establish the equivalence of the eigenvalue problem for $\phi(\xi)$ and that one for $\Phi(k)$. The transformed first-order differential equation (14) has a singularity at $k=0$ so that the solution could exhibit some pathological behaviour at the singular point. The general solution of Eq. (14) is expressed as

$$\Phi(k)=Ak^{\varepsilon-1/2}e^{-k^2/4}, \tag{16}$$

where A is an arbitrary constant and ε is as yet undetermined. From the definition of the unilateral Fourier transform, one sees that the acceptable behaviour at the origin restricts ε to $\varepsilon>1/2$ if one considers the sine Fourier transform, and to $\varepsilon=1/2$ or $\varepsilon>3/2$ if one considers the cosine Fourier transform. Parseval's formula (15) only requires $\varepsilon>0$. A more strong condition on ε follows from the existence of the unilateral Fourier transform of $\xi^n\phi(\xi)$, with $n=0,1,2,\ldots$, requiring in this way infinitely differentiable unilateral Fourier transforms for all values of k as can be seen from (8). Coming back to (16), one observes that $\Phi(k)$ is infinitely differentiable at $k=0$ only if $\varepsilon-1/2=n$ in such a way that

$$\varepsilon_n=n+\frac{1}{2}. \tag{17}$$

We now proceed to the inversion of the unilateral Fourier transform. Let $\phi_n^{(+)}(\xi)$ and $\phi_n^{(-)}(\xi)$ denote $\mathcal{F}_c^{-1}\{\Phi(k)\}$ and $\mathcal{F}_s^{-1}\{\Phi(k)\}$, respectively. They are expressed as

$$\begin{aligned}\phi_n^{(+)}(\xi) &= A_n^{(+)}\int_0^\infty dk\,k^n e^{-k^2/4}\cos k\xi,\\ \phi_n^{(-)}(\xi) &= A_n^{(-)}\int_0^\infty dk\,k^n e^{-k^2/4}\sin k\xi,\end{aligned} \tag{18}$$

with

$$\phi_{n+1}^{(\mp)}(\xi)=\mp\frac{A_{n+1}^{(\mp)}}{A_n^{(\pm)}}\frac{d}{d\xi}\phi_n^{(\pm)}(\xi). \tag{19}$$

Here, the operator $\frac{d}{d\xi}$ is seen as a raising operator because it brings into existence, from $\phi_n^{(\pm)}(\xi)$ associated with ε_n, new solutions associated with ε_{n+1}. Using the definite integral labelled as 3.896.4 in Ref. [26], viz.

$$I(\xi)=\int_0^\infty dk\,e^{-k^2/4}\cos k\xi=\sqrt{\pi}e^{-\xi^2}, \tag{20}$$

one finds

$$\begin{aligned}\int_0^\infty dk\,k^{2n}e^{-k^2/4}\cos k\xi &= (-1)^n\frac{d^{2n}I(\xi)}{d\xi^{2n}},\\ \int_0^\infty dk\,k^{2n+1}e^{-k^2/4}\sin k\xi &= (-1)^{n+1}\frac{d^{2n+1}I(\xi)}{d\xi^{2n+1}},\end{aligned} \tag{21}$$

so that

$$\begin{aligned}\phi_{2n}^{(+)}(\xi) &= A_{2n}\frac{d^{2n}}{d\xi^{2n}}e^{-\xi^2}, \quad \text{with}\\ &\qquad \left.\frac{d\phi_{2n}^{(+)}(\xi)}{d\xi}\right|_{\xi=0}=0,\\ \phi_{2n+1}^{(-)}(\xi) &= A_{2n+1}\frac{d^{2n+1}}{d\xi^{2n+1}}e^{-\xi^2}, \quad \text{with}\\ &\qquad \phi_{2n+1}^{(-)}(\xi)|_{\xi=0}=0.\end{aligned} \tag{22}$$

Then, combining these results with (12), one obtains $\psi_{2n}(\xi)=\phi_{2n}^{(+)}(\xi)e^{\xi^2/2}$ and $\psi_{2n+1}(\xi)=\phi_{2n+1}^{(-)}(\xi)e^{\xi^2/2}$. Explicitly, $\psi_{2n}(\xi)$ and $\psi_{2n+1}(\xi)$ are

$$\begin{aligned}\psi_{2n}(\xi) &= A_{2n}e^{\xi^2/2}\frac{d^{2n}}{d\xi^{2n}}e^{-\xi^2}, \quad \text{with}\\ &\qquad \left.\frac{d\psi_{2n}(\xi)}{d\xi}\right|_{\xi=0}=0,\\ \psi_{2n+1}(\xi) &= A_{2n+1}e^{\xi^2/2}\frac{d^{2n+1}}{d\xi^{2n+1}}e^{-\xi^2}, \quad \text{with}\\ &\qquad \psi_{2n+1}(\xi)|_{\xi=0}=0.\end{aligned} \tag{23}$$

Taking symmetric and antisymmetric linear combinations of $\psi(\xi)$, as discussed before, one finds the eigenfunctions defined on the whole x-axis:

$$\begin{aligned}\psi_{2n}(x) &= \frac{\psi_{2n}(\xi)+\psi_{2n}(-\xi)}{2}\\ &= A_{2n}e^{x^2/2}\frac{d^{2n}}{dx^{2n}}e^{-x^2},\\ \psi_{2n+1}(x) &= \frac{\psi_{2n+1}(\xi)-\psi_{2n+1}(-\xi)}{2}\\ &= A_{2n+1}e^{x^2/2}\frac{d^{2n+1}}{dx^{2n+1}}e^{-x^2}.\end{aligned} \tag{24}$$

Then, using Rodrigues's formula for the Hermite polynomial (see, e.g. 8.950.1 in Ref. [26])

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \tag{25}$$

one finds

$$\psi_n(x) = A_n e^{-x^2/2} H_n(x). \tag{26}$$

4. Final Remarks

We have shown that the complete solution of the one-dimensional quantum harmonic oscillator can be approached via the unilateral Fourier transform method without having to recourse to the properties of the confluent hypergeometric function as in Ref. [12]. Ponomarenko approached the quantum harmonic oscillator with the exponential Fourier transform grounded on the normalizability and parity of the eigenfunctions as necessary and sufficient conditions for solving the problem. Nevertheless, Ponomarenko used the solution of $(-1)^z = \pm 1$ without perceiving that this equation has many more solutions than those with z expressed by integer numbers. In the present work we have used Ponomarenko's trick [20] and the unilateral Fourier transform method including properly the boundary condition at the origin. Square-integrable eigenfunctions have been taken into account demanding the existence of the unilateral Fourier transform of $\xi^n e^{-\xi^2/2}\psi(\xi)$, with $n = 0, 1, 2, \ldots$, with the use of the unilateral Fourier transform properties grouped in (8).

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