Revisiting the quantum harmonic oscillator via unilateral Fourier transforms

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Abstract

The literature on the exponential Fourier approach to the one-dimensional quantum harmonic oscillator problem is revised and criticized. It is shown that the solution of this problem has been built on faulty premises. The problem is revisited via the Fourier sine and cosine transform method and the stationary states are properly determined by requiring definite parity and square-integrable eigenfunctions.

Keywords: Fourier transform, harmonic oscillator, Fourier sine and cosine transform

1. Introduction

The integral transform methods are useful and powerful methods of solving ordinary linear differential equations because they can convert the original equation into a simpler differential equation or into an algebraic equation. Nevertheless, the inversion of the transform for reconstructing the original function may be a rather complicated calculation. If this is the case and one does not find the integral in tables, the method will be worthless.

The harmonic oscillator is ubiquitous in the literature on quantum mechanics because it can be solved in closed form with a variety of methods and its solution can be useful for approximations or exact solutions of various problems. The quantum harmonic oscillator is usually solved with the help of the power series method [1], by the algebraic method based on the algebra of operators [2], or by the path integral approach [3]. In recent times, the one-dimensional harmonic oscillator has also been approached by the exponential Fourier transform [4–7] and Laplace transform [8] methods. However, all of the accounts of the quantum harmonic oscillator via the exponential Fourier transform present calculations which are based on false basic assertions.

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The observation that the eigenfunction and its Fourier transform satisfy formally identical differential equations and identical boundary conditions at infinity led Muñoz [4] to conclude that the eigenfunction and its corresponding Fourier-transformed function differ at most by a proportionality constant. His critical flaw was not to consider that the eigenfunction and its corresponding Fourier transform are functions of different but interrelated variables and that there is a definite scaling property involving the pair of Fourier transforms: \( \mathcal{F}[f(cx)] = F(k/c)/|c| \). Ponomarenko [5] stated that the necessary and sufficient condition for the eigenfunction to have a definite parity can be expressed in terms of the solution of \((-1)^z = \pm 1\), but he missed the fact that this equation has many more solutions than those which have \(z\) expressed by integer numbers. Engel [6] came to the conclusion that Ponomarenko’s method may be used ‘if the requirement of definite parity of the eigenstates is replaced by that of normalization’. In addition, he argued that Ponomarenko failed to consider a Fourier-transformed function valid on the whole axis because the origin is a singular point of the corresponding Fourier-transformed equation. However, he himself apparently failed to observe that the transformed equation allows Fourier-transformed solutions with definite parities despite the mentioned singularity, and that the changing \(k\) to \(-k\) makes \(k^z\) even (odd) when \(a\) is an even (odd) integer. It should be mentioned, though, that Engel perceived that the relation between the \(n\)th moment of a function and the \(n\)th derivative of its transform at the origin plays an indispensable role for determining the bound-state solutions. Palma and Raff [7] developed a strategy for approaching the stationary states of the time-independent Schrödinger equation with a large class of potentials, but they erroneously returned to single valuedness of the eigenfunction in order to eliminate irrelevant overall phase factors.

In view of the fact that there are significant confusions regarding the quantum harmonic oscillator via the exponential Fourier transform method, we will revise the problem with the closely related unilateral Fourier (sine and cosine) transform method. Except for the one-dimensional double \( \delta \)-function potential [9], this method does not seem to have been directly applied to the Schrödinger equation. We will show that the unilateral Fourier transform is a straightforward and efficient manner in which bound-state solutions in nonrelativistic quantum mechanics can be treated by applying it to the harmonic oscillator. We will show that the relation between the convergence of the \(n\)th moment of the eigenfunction (in the sense of a conveniently weighted integral) and the derivatives of the corresponding Fourier-transformed function at the origin, already perceived by Engel in connection with the exponential Fourier transform [6], is inept at finding the unique solution of the problem. We will also show that both definite parity and square integrability of the eigenfunctions are requisites just sufficient to determine the proper solution. To prepare the ground, we will first give a short review of a few relevant properties of the Fourier sine and cosine transforms.

2. Fourier transforms and their main properties

The exponential Fourier transform pair is defined by [10–17]

\[
\mathcal{F}\{\phi(x)\} = \Phi(\kappa) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \phi(x) e^{i\kappa x},
\]

\[
\mathcal{F}^{-1}\{\Phi(\kappa)\} = \phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\kappa \, \Phi(\kappa) e^{-i\kappa x}.
\]

For odd \((\phi_0(-x) = -\phi_0(+x))\) and even \((\phi_0(-x) = +\phi_0(+x))\) functions there are two modifications of the exponential Fourier transform. Defining \(\zeta = |x|\) and \(k = |\kappa|\), the Fourier sine and cosine transforms of the functions \(\phi_0(\zeta)\) and \(\phi_0(\zeta)\) are expressed by
Given $\phi_s$ and $\phi_c$, a sufficient condition for the existence of the unilateral Fourier transforms (and their inverses) is ensured if $\phi_s$ and $\phi_c$ are absolutely integrable on $[0, \infty)$. In particular, $\phi_s$ and $\phi_c$ must vanish as $\zeta \to \infty$ ($k \to \infty$). Furthermore, the unilateral Fourier transform pairs satisfy Parseval’s formulas

$$
\int_0^\infty d\zeta |\phi_s(\zeta)|^2 = \int_0^\infty dk |\Phi_s(k)|^2
$$

and

$$
\int_0^\infty d\zeta |\phi_c(\zeta)|^2 = \int_0^\infty dk |\Phi_c(k)|^2.
$$

It is instructive to note that the inversion of the unilateral Fourier transforms requires that $\phi_s$ and $\phi_c$ satisfy different boundary conditions at the origin, namely $\lim_{\zeta \to 0} \phi_s(\zeta) = 0$ and $\lim_{\zeta \to 0} d\phi_c/d\zeta = 0$. The convenience of using the sine or cosine transform is dictated by these boundary conditions. Note also that

$$
\lim_{\zeta \to 0} \frac{d^{2n+1} \phi_s(\zeta)}{d\zeta^{2n+1}} = (-1)^n \sqrt{\frac{2}{\pi}} \int_0^\infty dk k^{2n+1} \Phi_s(k)
$$

and

$$
\lim_{\zeta \to 0} \frac{d^{2n+1} \phi_c(\zeta)}{d\zeta^{2n+1}} = (-1)^n \sqrt{\frac{2}{\pi}} \int_0^\infty dk k^{2n+1} \Phi_c(k)
$$

In applications to differential equations, it is necessary to know how to express the transforms of functions involving the derivatives of $\phi(\zeta)$ in terms of $\Phi(k)$. The unilateral Fourier transforms have the derivative properties

$$
\lim_{k \to 0} \frac{d^{2n+1} \Phi_s(k)}{dk^{2n+1}} = (-1)^n \sqrt{\frac{2}{\pi}} \int_0^\infty d\zeta \zeta^{2n+1} \phi_s(\zeta)
$$

and

$$
\lim_{k \to 0} \frac{d^{2n+1} \Phi_c(k)}{dk^{2n+1}} = (-1)^n \sqrt{\frac{2}{\pi}} \int_0^\infty d\zeta \zeta^{2n+1} \phi_c(\zeta)
$$

In applications to differential equations, it is necessary to know how to express the transforms of functions involving the derivatives of $\phi(\zeta)$ in terms of $\Phi(k)$. The unilateral Fourier transforms have the derivative properties
\[ \mathcal{F} \left\{ \frac{d\phi(\zeta)}{d\zeta} \right\} = -\Phi(k) - k \frac{d\Phi(k)}{dk} \]
\[ \mathcal{F} \left\{ \frac{d^2\phi(\zeta)}{d\zeta^2} \right\} = -k^2\Phi(k), \]

where the operator \( \mathcal{F} \) and the function \( \Phi(k) \) refer either to the Fourier sine or to the Fourier cosine transform of the functions satisfying the proper boundary conditions for ensuring the existence of inverse transforms.

3. The quantum harmonic oscillator

3.1. The eigenvalue problem

We are now prepared to address the quantum harmonic oscillator problem. The one-dimensional time-independent Schrödinger equation for the harmonic oscillator in dimensionless variables can be written as

\[ \frac{d^2\psi(x)}{dx^2} + (2\varepsilon - x^2)\psi(x) = 0, \quad x \in (-\infty, +\infty). \tag{8} \]

Equation (8) is an eigenvalue equation for the characteristic pair \((\varepsilon, \psi)\) with \( \varepsilon \in \mathbb{R} \) and

\[ \int_{-\infty}^{+\infty} dx \left| \psi(x) \right|^2 < \infty. \tag{9} \]

Because \( x = 0 \) is a regular point of equation (8), \( \psi \) is analytic at the origin, i.e. \( |d^n \psi/dx^n|_{x=0} < \infty \) for all \( n \in \mathbb{N} \). Because \( \psi(-x) \) is also a solution of equation (8), the linear combinations \( \psi(x) \pm \psi(-x) \) are also solutions, so two different eigenfunctions with well defined parities can be built. Thus, it suffices to concentrate attention on the positive half-line and use boundary conditions on \( \psi \) at the origin and at infinity. 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 \( \psi \) defined on the positive side of the \( x \)-axis. Incidentally, the combinations \( \psi(x) \pm \psi(-x) \) share the same eigenvalue so that at first glance one would expect a twofold degeneracy, but we will show that the requirement of continuity of the eigenfunctions and their first derivatives invalidates one of the two combinations for a given eigenvalue, in accordance with the nondegeneracy theorem (a general result valid for bound states in one-dimensional nonsingular potentials) [18]. As \( x \to 0 \), the solution with definite parity varies as \( x^\delta \), where \( \delta = 0 \) or \( 1 \) regardless the magnitude of \( \varepsilon \). The homogeneous Neumann condition \( (d\psi/dx)|_{x=0} = 0 \) develops for \( \delta = 0 \) but not for \( \delta = 1 \), whereas the homogeneous Dirichlet boundary condition \( (\psi)|_{x=0} = 0 \) develops for \( \delta = 1 \) but not for \( \delta = 0 \). The continuity of \( \psi \) at the origin excludes the possibility of an odd-parity eigenfunction for \( \delta = 0 \), and the continuity of \( d\psi/dx \) at the origin excludes the possibility of an even-parity eigenfunction for \( \delta = 1 \). Thus, \( \delta = 0 \) for even solutions, and \( \delta = 1 \) for odd solutions. On the other hand, the square-integrable asymptotic form of the solution as \( |x| \to \infty \) is given by \( \psi(x) \sim x^\alpha e^{-x^2/2} \) with arbitrary \( \alpha \).

We write \( \psi(x) = \phi(x)e^{ix^2/2} \) in such a way that \( \phi \) is a solution of the equation

\[ \frac{d^2\phi(x)}{dx^2} + 2\alpha \frac{d\phi(x)}{dx} + (2\varepsilon + 1) \phi(x) = 0. \tag{10} \]

Notice that the parity of \( \phi \) is the same as that of \( \psi \) and that \( x = 0 \) is a regular point of (10). As a matter of fact, \( \phi \) varies in the neighbourhood of the origin as \( x^\delta \). Notice also that one has to
find a particular solution of (10) in such a way that \( \phi \) behaves like \( x^a e^{-x^2} \) for sufficiently large \( |x| \). This condition, added by the regularity at \( x = 0 \) ensures the existence of the Fourier sine (cosine) transform for \( \phi \) odd (even).

### 3.2. Fourier sine and cosine transforms

Restricting our attention on the positive half-line \( (x > 0) \), the unilateral Fourier transform establishes a mapping of the second-order equation for \( \phi \) into an integrable first-order equation for \( \Phi \)

\[
\frac{d^2 \Phi(k)}{dk^2} + \left( \frac{k}{2} + \frac{1 - 2 \varepsilon}{2k} \right) \Phi(k) = 0,
\]

where \( \Phi \) denotes \( \Phi_k \) or \( \Phi_0 \). The solution of (11) is expressed as

\[
\Phi(k) = A^{(\alpha)} k^a e^{-k^2/4},
\]

where \( A^{(\alpha)} \) is an arbitrary constant of integration and \( a = \varepsilon - 1/2 \in \mathbb{R} \) is as yet undetermined. Due to the fact that \( k^a = e^{\alpha \log k} \) and \( \log k \) is multivalued, this solution can be cast into the form

\[
\Phi(k) = A^{(\alpha)} \left| k^a \right| e^{-k^2/4} e^{i2\pi m}, \quad m \in \mathbb{Z}.
\]

This form explicitly shows that \( \Phi(k) \) has infinite branches if \( a \) is an irrational number, and \( q \) branches if \( a = p/q \), where \( p \) and \( q \) are integers with \( q \neq 0 \).

It is true that when \( a \) is not an integer number \( \Phi(k) \) is a multivalued function but their dissimilar branches differ by \( k \)-independent phase factors \( (e^{i2\pi ma}) \) without physical consequences thanks to the normalization condition expressed by (9) and to Parseval’s formulas.

Notice that \( k = 0 \) is itself a singular point of equation (11) and so the neighbourhood of \( k = 0 \) needs careful handling because \( \Phi \) may exhibit a singularity at the origin. The point of danger lies in the exponent of \( k \).

Parseval’s formulas expressed by (4), related to square-integrable eigenfunctions, demand \( a > -1/2 \) to guarantee convergence.

The derivatives of \( \Phi_k \) and \( \phi \) tend to finite limits as \( \zeta \) approaches the origin. Thus, the two first lines of equation (5) demand that the \( 2n \)th moment of \( \Phi_k \) and the \( (2n + 1) \)th moment of \( \Phi_0 \) are finite numbers so that \( a > -1 \). Note that this condition is weaker than that originating from Parseval’s formulas. It is a pity that the last line of equation (5) proves clumsy to impose restrictions on \( a \).

The derivatives of \( \Phi \) near the origin impose more restrictions on the allowed values for \( a \). Using the property of the gamma function \( \Gamma(z + 1) = z\Gamma(z) \) (see, e.g., [19], [20]), one finds

\[
\lim_{k \to 0} \frac{d^n \Phi(k)}{dk^n} = A^{(\alpha)} \frac{\Gamma(a + 1)}{\Gamma(a + 1 - n)} \lim_{k \to 0} k^{a-n}
\]

for any branch of \( \Phi(k) \).

Because \( \Gamma(z) \) has no zeros but has simple poles at \( z = -n \), with \( n \in \mathbb{N} \), equation (14) is equal to zero when \( a = n - 1 - n \), so \( a \leq n - 1 \) with \( a \in \mathbb{Z} \). Taking into account the restriction resulting from Parseval’s formulas, one can say that
\[
\lim_{k \to 0} \frac{d^{2n}\Phi(k)}{dk^{2n}} = 0 \text{ if } a \leq 2n - 1, \text{ with } a \in \mathbb{N} \text{ and } n \neq 0.
\]
\[
\lim_{k \to 0} \frac{d^{2n+1}\Phi(k)}{dk^{2n+1}} = 0 \text{ if } a \leq 2n, \text{ with } a \in \mathbb{N}.
\]  

(15)

At large $\zeta$ the exponentially decreasing factors in $\phi_\zeta^1$ and $\phi_\zeta^2$ always predominate over any power increasing factor and so the $2n$th moment of $\phi_\zeta^1$ and the $(2n + 1)$th moment of $\phi_\zeta^2$ are finite numbers. In this case, the properties of the unilateral Fourier transforms expressed by the first two lines of (6) imply that

\[
\left| \lim_{k \to 0} \frac{d^{2n}\Phi_0(k)}{dk^{2n}} \right| < \infty, \quad \left| \lim_{k \to 0} \frac{d^{2n+1}\Phi_0(k)}{dk^{2n+1}} \right| < \infty.
\]

(16)

Due to the exponent of $k$, equation (16) is satisfied if $a \geq 2n$ for $\Phi_0^1$ and $a \geq 2n + 1$ for $\Phi_0^2$ with $a \in \mathbb{R}$. Thus, with the aid of (15) one finds $a = n$ for both $\Phi_0^1$ and $\Phi_0^2$. In principle, the spectrum has been determined: $\varepsilon_n = n + 1/2$.

3.3. The inversion of the Fourier sine and cosine transforms

In order to reconstruct $\phi_\zeta^1$ and $\phi_\zeta^2$ on the half-line one needs to calculate the integrals related to the inverse Fourier transforms. It follows that

\[
\phi_\zeta^1(a) = A_0 \sqrt{\frac{2}{\pi}} \int_0^\infty dk \ k^a e^{-k^2/4} \cos k\zeta.
\]
\[
\phi_\zeta^2(a) = A_0 \sqrt{\frac{2}{\pi}} \int_0^\infty dk \ k^a e^{-k^2/4} \sin k\zeta.
\]

(17)

From (3.952.7) and (3.952.8) of [16], one finds

\[
\phi_\zeta^1(a) = A_0 e^{-\zeta^2/4} \ _1F_1\left(-\frac{n}{2}, \frac{1}{2}, \zeta^2\right),
\]
\[
\phi_\zeta^2(a) = A_0 e^{-\zeta^2/4} \ _1F_1\left(-\frac{n}{2} + 1, \frac{3}{2}, \zeta^2\right).
\]

(18)

The confluent hypergeometric function or Kummer’s function, $\_1F_1(a_1, b_1, z)$, also denoted $M(a_1, b_1, z)$, is defined by the series (see, e.g. [19, 20])

\[
\_1F_1(a, b_1, z) = \frac{\Gamma(b_1)}{\Gamma(a)} \sum_{j=0}^\infty \frac{\Gamma(a + j)}{\Gamma(b_1 + j)} \frac{z^j}{j!} \quad \text{for } b_1 > a_1 > 0, \quad a_1 = -1, -1, \ldots.
\]

(19)

This series converges for all $z \in \mathbb{C}$ and has asymptotic behaviour prescribed by

\[
\_1F_1(a_1, b_1, z) \sim \frac{\Gamma(b_1)}{\Gamma(a)} \sum_{j=0}^\infty \frac{\Gamma(a + j)}{\Gamma(b_1 + j)} \frac{z^j}{j!}, \quad z \to \pm \infty.
\]

(20)

The presence of $e^z$ in (20) ruins the asymptotic behaviour of $\phi_\zeta^1(a)$ and $\phi_\zeta^2(a)$ decided before beyond doubt ($e^z e^{-\zeta^2}$). This unfavourable situation can be remedied by considering the poles of $\Gamma(a_1)$ and demanding $a_1 = -\bar{n}$. In this case, $\_1F_1(-\bar{n}, b_1, z)$ behaves asymptotically as $z^\bar{n}$ and the series (19) is truncated at $j = \bar{n}$ in such a way that the confluent hypergeometric function results in polynomial in $z$ of degree not exceeding $\bar{n}$. Therefore, $n$ is even for $\phi_\zeta^1$ and $\phi_\zeta^2$ is odd for $\phi_\zeta^2$. As a matter of fact, $\_1F_1(-\bar{n}, b_1, z)$ is proportional to the generalized Laguerre polynomial $L_{\bar{n}}^{(b_1-1)}(z)$ with $z \in [0, \infty)$, and $L_{\bar{n}}^{(-1/2)}(z)$ and $L_{\bar{n}}^{(1/2)}(z)$ are proportional to $H_{2\bar{n}}(z^{1/2})$ and $z^{-1/2}H_{2\bar{n}+1}(z^{1/2})$ respectively, where $H_{\bar{n}}(z^{1/2})$ is the Hermite polynomial.
Therefore, \( F_1(-n/2, 1/2, \zeta^2) \) with \( n \) even and \( F_1(-n/2 + 1/2, 3/2, \zeta^2) \) with \( n \) odd are proportional to \( H_n(\zeta) \), with the desired properties \( dH_{2n}/d\zeta|_{\zeta=0} = 0 \) and \( H_{2n+1}|_{\zeta=0} = 0 \). Hence, \( \phi_c \) and \( \phi_s \) take the form

\[
\phi_c^{(2n)}(\zeta) = A_{2n} e^{-\zeta^2} H_{2n}(\zeta) \\
\phi_s^{(2n+1)}(\zeta) = A_{2n+1} e^{-\zeta^2} H_{2n+1}(\zeta).
\]

It is worthwhile to note that the last line of (6) imposes severe restrictions on the allowed values for \( a \) without postulating the convergence of the moments of \( \phi \). Now the exponent of \( k \) makes equation (14) vanish for real values of \( a \) subject to the conditions \( a > 2n + 1 \) for \( \phi_c \), and \( a > 2n \) for \( \phi_s \). Additional restrictions arising from (15) and (16) make \( a = n \) for both \( \phi_c \) and \( \phi_s \). The formulas (3.952.9) and (3.952.10) of [16] allow us to obtain the integrals for \( \phi_c \) and \( \phi_s \) expressed by (17) at once in terms of confluent hypergeometric functions. Eventually, the good asymptotic behaviour of \( \phi_c \) and \( \phi_s \) prescribed by the normalization condition establishes \( a = 2n \) for \( \phi_c \) and \( a = 2n + 1 \) for \( \phi_s \), with \( \phi_c \) and \( \phi_s \) realized in terms of Hermite polynomials. The only remaining question is how to write the eigenfunctions.

3.4. Complete solution of the problem

Following up our earlier comments about eigenfunctions of definite parity, one could think about antisymmetric and symmetric extensions of \( \phi_c^{(2n)}(\zeta) \) and \( \phi_s^{(2n+1)}(\zeta) \). Nevertheless, antisymmetric (symmetric) extensions of \( \phi_c^{(2n)}(\zeta) \) (\( \phi_s^{(2n+1)}(\zeta) \)) are not allowed because the solution of (10) is infinitely differentiable at the origin. This further constraint makes \( \psi_n \) even (odd) parity for \( n \) even (odd), namely

\[
\psi_{2n}(x) = e^{\zeta^2/2 \sigma^2} \left[ \phi_c^{(2n)}(\zeta) + \phi_c^{(2n)}(-\zeta) \right] \\
\psi_{2n+1}(x) = e^{\zeta^2/2 \sigma^2} \left[ \phi_s^{(2n+1)}(\zeta) - \phi_s^{(2n+1)}(-\zeta) \right]
\]

so that the spectrum is nondegenerate, in agreement with the nondegeneracy theorem [18]. Finally, using the property \( H_n(-x) = (-1)^n H_n(x) \), the solution of the original problem is expressed as

\[
\varepsilon_n = n + 1/2 \\
\psi_n(x) = N_n e^{-x^2/2} H_n(x),
\]

where \( N_n \) are normalization constants.

4. Conclusion

In conclusion, we have shown that the complete solution of the one-dimensional quantum harmonic oscillator can be approached via the unilateral Fourier transform method. Single-valuedness of the eigenfunction is not a fair request. The convergence of the moments of the unilateral Fourier transform is not enough to do the job and the convergence of the moments of \( e^{-\zeta^2/2 \sigma^2}\psi(\zeta) \) is difficult to handle, especially because one has to appeal to the properties of the confluent hypergeometric function. Fortunately, the inversion of the Fourier sine and cosine transforms results in tabulated integrals and the proper bound-state solutions can be straightforwardly determined, just requiring definite parity and square-integrable eigenfunctions.
Acknowledgments

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