A Laplace transform approach to the quantum harmonic oscillator

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Received 8 August 2012, in final form 13 November 2012
Published 7 December 2012
Online at stacks.iop.org/EJP/34/199

Abstract
The one-dimensional quantum harmonic oscillator problem is examined via the Laplace transform method. The stationary states are determined by requiring definite parity and good behaviour of the eigenfunction at the origin and at infinity.

1. Introduction

The quantum harmonic oscillator is one of the most important systems in quantum mechanics because it can be solved in closed form and this can be useful for generating approximate or exact solutions to various problems. The harmonic oscillator is usually solved with the help of the power series method [1], by using the algebraic method based on the algebra of operators [2] or by employing the path integral approach [3]. In recent times, the one-dimensional harmonic oscillator has also been approached using the Fourier transform method [4–7]. Another operational method useful in quantum mechanics is the Laplace transform method. This last method was used during the first years of quantum mechanics by Schrödinger when discussing the radial eigenfunction of the hydrogen atom [8], and more than forty years later Englefield approached the Schrödinger equation with the Coulomb, oscillator, exponential and Yamaguchi potentials [9]. More than twenty years went by and the hydrogen atom was again examined using the Laplace transform method [10]. Later, the $1/x$ [11], Morse [12], $N$-dimensional harmonic oscillator [13], pseudoharmonic and Mie-type [14], and Dirac delta [15] potentials were solved for the Laplace transform some years ago.

In [9], Englefield found the spectrum of the three-dimensional harmonic oscillator by imposing that the radial eigenfunction vanishes at the origin and by using the closed-form solution for the Laplace transform. This paper approaches the one-dimensional Schrödinger equation for the harmonic oscillator with the Laplace transform method, following the recipe proposed by Englefield [9]. Nevertheless, we do not use the closed-form solution for the
Laplace transform. In addition, we enlarge the class of problems to include eigenfunctions satisfying the homogeneous Neumann condition at the origin. The main features of our approach are as follows. After factorizing the behaviour at infinity, the second-order differential equation for the eigenfunction \( \psi(x) \) transmutes in a nonhomogeneous first-order equation for the Laplace transform \( \Phi_1(s) \). The closed-form solution for \( \Phi_1(s) \) is not necessary. After inspecting the singularities of the differential equation for \( \Phi_1(s) \), we make a series expansion about the appropriate singular point, related to the proper behaviour of \( \psi(x) \) near infinity. The behaviour of the eigenfunction near the origin, related to the behaviour of \( \Phi_1(s) \) near infinity, implies truncation of the series. The root of the indicial equation is the quantization condition. The recurrence relation for the coefficients of the truncated series for \( \Phi_1(s) \) is solved and the inverse Laplace transform is identified with the Hermite polynomials. This procedure should be helpful for students on a mathematical physics course.

2. The Laplace transform applied to the harmonic oscillator

Let us begin with a brief description of the Laplace transform and a few of its properties [16]. The Laplace transform of a function \( f(t) \) is defined by

\[
F(s) = \mathcal{L}\{f(t)\} = \int_0^\infty dt \, e^{-st} f(t).
\]  

(1)

If there is some constant \( \sigma \in \mathbb{R} \) such that

\[
|e^{-\sigma t} f(t)| \leq M,
\]

(2)

for sufficiently large \( t \), the integral in equation (1) will exist for \( \text{Re} \, s > \sigma \) and \( f(t) \) is said to be of exponential order. The Laplace transform may fail to exist because of a sufficiently strong singularity in the function \( f(t) \) as \( t \rightarrow 0 \). In particular

\[
\mathcal{L}\left\{ \frac{t^\alpha}{\Gamma(\alpha + 1)} \right\} = \frac{1}{s^{\alpha+1}}, \quad \alpha > -1.
\]

(3)

The Laplace transform has the derivative properties

\[
\mathcal{L}\{f^{(n)}(t)\} = s^n \mathcal{L}\{f(t)\} - \sum_{k=0}^{n-1} s^{n-1-k} f^{(k)}(0),
\]

\[
\mathcal{L}\{t^n f(t)\} = (-1)^n \frac{d^n}{ds^n} F(s),
\]

(4)

where the superscript \( (n) \) stands for the \( n \)th derivative with respect to \( t \) for \( f^{(n)}(t) \), and with respect to \( s \) for \( F^{(n)}(s) \). If near a singular point \( s_0 \) the Laplace transform behaves as

\[
F(s) \sim \frac{1}{(s - s_0)^\nu}
\]

(5)

then

\[
f(t) \sim \frac{1}{\Gamma(\nu)} \frac{1}{t^{\nu-1}} e^{s_0 t},
\]

(6)

where \( \Gamma(\nu) \) is the gamma function. On the other hand, if near the origin \( f(t) \) behaves like \( t^\alpha \), with \( \alpha > -1 \), then \( F(s) \) behaves near infinity as

\[
F(s) \sim \frac{\Gamma(\alpha + 1)}{s^{\alpha + 1}}.
\]

(7)
We are now ready to address the quantum harmonic oscillator problem. The one-dimensional Schrödinger equation for the harmonic oscillator reads

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 - E \psi(x) = 0.
\]

Because the harmonic oscillator potential is invariant under reflection through the origin \((x \rightarrow -x)\), eigenfunctions with well-defined parities can be built. Thus, it suffices to concentrate attention on the positive half-line and impose boundary conditions on \(\psi\) at the origin and at infinity. Normalizability demands \(\psi \rightarrow 0\) as \(x \rightarrow \infty\). 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. As \(x \rightarrow 0\), the solution varies as \(x^\delta\), where \(\delta\) is 0 or 1. 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 \((\psi(0)=0)\) 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,

\[
\psi(x) \sim x^\delta, \quad \delta = \begin{cases} 0, & \text{for } \psi \text{ even,} \\ 1, & \text{for } \psi \text{ odd.} \end{cases}
\]

On the other hand, the normalizable asymptotic form of the solution as \(x \rightarrow \infty\) is given by

\[
\psi(x) \sim e^{-m\omega x^2/(2\hbar)}.
\]

This behaviour invites us to define \(\xi = m\omega x^2/\hbar\) in such a way that equation (8) is written as

\[
\left(\xi \frac{d^2}{d\xi^2} + \frac{1}{2} \frac{d}{d\xi} + \frac{k-\xi}{4}\right)\psi(\xi) = 0,
\]

where \(k = 2E/(\hbar\omega)\). The solution for all \(\xi\) can now be written as

\[
\psi(\xi) = \phi(\xi) e^{-\xi/2},
\]

where the unknown \(\phi(\xi)\) is the solution to the confluent hypergeometric equation [17]

\[
\xi \frac{d^2\phi(\xi)}{d\xi^2} + (b-\xi) \frac{d\phi(\xi)}{d\xi} - a \phi(\xi) = 0,
\]

with \(a = (1-k)/4\) and \(b = 1/2\). Because the asymptotic behaviour of \(\psi(\xi)\) is given by \(\exp(-\xi/2)\) as \(\xi \rightarrow \infty\), one has to find a particular solution of (13) in such a way that \(\phi(\xi)\) tends to infinity no more rapidly than \(\exp(\alpha \xi^\beta)\), with \(\beta<1\) and arbitrary \(\alpha\), for sufficiently large \(\xi\). This occurs because \(a \xi^\beta - \xi/2 \rightarrow -\xi/2\) as \(\xi \rightarrow \infty\). This condition, in combination with the fact that \(\phi(\xi)\) varies near the origin as \(\xi^{k/2}\), ensures the existence of the Laplace transform of \(\phi(\xi)\).

Denoting \(\Phi(s) = \mathcal{L}\{\phi(\xi)\}\) and using the derivative properties of the Laplace transform given by equation (4), the transform of equation (13) furnishes the nonhomogeneous first-order differential equation for \(\Phi(s)\):

\[
s(s-1) \frac{d\Phi(s)}{ds} + \left(\frac{3}{2} s - \frac{k+3}{4}\right) \Phi(s) = \frac{\phi(0)}{2}.
\]

Note that \(s = 0\) and \(s = 1\) are singular points of this differential equation. To make use of the property of the Laplace transform near a singular point (equations (5) and (6)) and taking into
account the asymptotic behaviour of $\phi(\xi)$ near infinity, we try a series expansion of $\Phi(s)$ about $s = 0$:  

$$\Phi_v(s) = s^{-v} \sum_{j=0}^{\infty} c_j^{(v)} s^j, \quad c_0^{(v)} \neq 0.$$  

(15)

Referring to equations (7) and (9), we find

$$\Phi(s) \sim \begin{cases} \frac{\Gamma(1)}{\sqrt{s}}, & \text{for } \psi \text{ even,} \\ \frac{\Gamma(1/2)}{s^{1/2}}, & \text{for } \psi \text{ odd.} \end{cases}$$  

(16)

Thus, the series terminates at $j = n$ in such a way that

$$v = \begin{cases} n + 1, & \text{for } \psi \text{ even,} \\ n + 3/2, & \text{for } \psi \text{ odd,} \end{cases}$$  

(17)

and

$$c_n^{(n)} = \begin{cases} \phi(0), & \text{for } \psi \text{ even,} \\ \text{arbitrary, for } \psi \text{ odd.} \end{cases}$$  

(18)

Beyond making $\phi(\xi)$ behave as $\xi^{-1}$ as $\xi \to \infty$, another important consequence of the term $s^{-v} c_0^{(v)}$ in equation (15) is to give rise to the quantization condition $v = (k + 3)/4$. Thus,

$$E_n = \hbar \omega \begin{cases} 2n + 1/2, & \text{for } \psi \text{ even,} \\ 2n + 1 + 1/2, & \text{for } \psi \text{ odd.} \end{cases}$$  

(19)

Inserting equation (15) into equation (14), we obtain the recurrence relation

$$c_{j+1}^{(n)} = -\frac{c_j^{(n)}}{j+1} \begin{cases} n - j + 1/2, & \text{for } \psi \text{ even,} \\ n - j, & \text{for } \psi \text{ odd.} \end{cases}$$  

(20)

Inspection and induction yields

$$c_j^{(n)} = c_0^{(n)} \frac{(-1)^j}{j!} \begin{cases} \frac{\Gamma(n+1/2)}{\Gamma(n+1/2)} & \text{for } \psi \text{ even,} \\ \frac{n!}{(n-j)!} & \text{for } \psi \text{ odd,} \end{cases}$$  

(21)

so that

$$\Phi_v(s) = c_0^{(n)} \begin{cases} \Gamma(n + 1/2) \sum_{j=0}^{n} \frac{(-1)^j}{\Gamma(n-j+1/2) \Gamma(n+1/2)} s^{j}, & \text{for } \psi \text{ even,} \\ n! \sum_{j=0}^{n} \frac{(-1)^j}{\Gamma(n-j+1/2) \Gamma(n+1/2)}, & \text{for } \psi \text{ odd.} \end{cases}$$  

(22)

Using equation (3) and inverting the Laplace transform term by term, we can reconstruct $\phi_n(\xi)$:

$$\phi_n(\xi) = c_0^{(n)} \begin{cases} \Gamma(n + 1/2) \sum_{j=0}^{n} \frac{(-1)^j \xi^{-j}}{\Gamma(n-j+1/2) \Gamma(n+1/2)} s^{j}, & \text{for } \psi \text{ even,} \\ n! \sum_{j=0}^{n} \frac{(-1)^j \xi^{-j+1/2}}{\Gamma(n-j+1/2) \Gamma(n+1/2)}, & \text{for } \psi \text{ odd.} \end{cases}$$  

(23)

Using Legendre’s duplication formula [17]

$$\Gamma(z+1)\Gamma(z+1/2) = 2^{-2z}\sqrt{\pi}\Gamma(2z+1),$$  

(24)

The series expansion about $s = 1$ would ruin the good behaviour of $\phi(\xi)$ as $\xi \to \infty$.

The quantization condition is the root of the indicial condition.
$\phi_n(\xi)$ turns out to be

$$\phi_n(\xi) = \frac{e^{(n+\frac{1}{2})}}{\sqrt{\pi}} \left\{ \Gamma(n+1/2) \sum_{j=0}^{n} (-1)^j (2\sqrt{\xi})^{2j} \right\}, \text{ for } \psi \text{ even},$$

$$n! \sum_{j=0}^{n} \frac{(-1)^j (2\sqrt{\xi})^{2j}}{j((2n+1-2j)!)}, \text{ for } \psi \text{ odd}.$$  \hspace{1cm} (25)

Then, using the formula for the Hermite polynomial [17]

$$H_n(y) = n! \sum_{j=0}^{[n/2]} (-1)^j (2y)^{n-2j} j! (n-2j)!,$$  \hspace{1cm} (26)

where $[n/2]$ denotes the largest integer $\leq n/2$, the eigenfunction is found to be

$$\psi_n(x) = \frac{e^{(n+\frac{1}{2})}}{\sqrt{\pi}} \exp\left(-\frac{m\omega}{2\hbar} x^2\right) \left\{ \Gamma(n+1/2) \right\} H_{2n} \left(\sqrt{\frac{m\omega}{\hbar}} x\right), \text{ for } \psi \text{ even},$$

$$n! \sum_{j=0}^{[n/2]} \frac{n!}{j!(n-2j)!} H_{2n+1} \left(\sqrt{\frac{m\omega}{\hbar}} x\right), \text{ for } \psi \text{ odd}.$$  \hspace{1cm} (27)

Because $H_n(-y) = (-1)^n H_n(y)$, the solution can also be expressed as

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega, \quad n = 0, 1, 2, \ldots,$$  \hspace{1cm} (28)

$$\psi_n(x) = A_n \cdot e^{-m\omega x^2/(2\hbar)} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x\right),$$

where $A_n$ are normalization constants.

### 3. Conclusion

We have shown that the complete solution of the one-dimensional quantum harmonic oscillator can be approached via the Laplace transform method with simplicity and elegance, even if the eigenfunction does not vanish at the origin. Englefield’s recipe allows exploration of the asymptotic expansions of the eigenfunction and its Laplace transform to gain information from the Schrödinger equation even if it is not possible to solve it in closed form. The discussion presented here may apply to any other problem that, after factorization of the behaviour at the origin and at infinity, reduces to the confluent hypergeometric equation, such as the pseudoharmonic, Coulomb and Kratzer potentials.

### Acknowledgments

This work was supported in part by means of funds provided by CNPq and FAPESP.

### References

[1] Sommerfeld A 1930 Wave Mechanics (London: Methuen) (Engl. transl.)
[2] Sakurai J J 1967 Modern Quantum Mechanics (Reading, MA: Addison-Wesley)
[3] Feynman R P and Hibbs A R 1965 Quantum Mechanics and Path Integrals (New York: McGraw-Hill)
[4] Muñoz G 1998 Integral equations and the simple harmonic oscillator Am. J. Phys. 66 254–6
[5] Ponomarenko S A 2004 Quantum harmonic oscillator revisited: a Fourier transform approach Am. J. Phys. 72 1259–60
[6] Engel A 2006 Comment on ‘Quantum harmonic oscillator revisited: a Fourier transform approach’ Am. J. Phys. 74 837

Ponomarenko A A 2004 Quantum harmonic oscillator revisited: a Fourier transform approach Am. J. Phys. 72 1259–60
[7] Palma G and Raff U 2011 A novel application of a Fourier integral representation of bound states in quantum mechanics Am. J. Phys. 79 201–5
[8] Schrödinger E 1926 Quantisierung als eigenwertproblem Ann. Phys. 384 361–76
[9] Englefield MJ 1968 Solution of the Schrödinger equation by Laplace transform J. Aust. Math. Soc. 8 557–67
[10] Swainson RA and Drake GWF 1991 A unified treatment of the non-relativistic and relativistic hydrogen atom: I. The wavefunctions J. Phys. A: Math. Gen. 24 79–94
[11] Ran Y, Xue L, Hu S and Su R-K 2000 On the Coulomb-type potential of the one-dimensional Schrödinger equation J. Phys. A: Math. Gen. 33 9265–72
[12] Chen G 2004 The exact solution of the Schrödinger equation with the Morse potential via Laplace transforms Phys. Lett. A 326 55–7
[13] Chen G 2005 Exact solutions of the N-dimensional harmonic oscillator via Laplace transformation Chin. Phys. 14 1075
[14] Arda A and Server R 2012 Exact solutions of the Schrödinger equation via Laplace transform approach: pseudoharmonic potential and Mie-type potentials J. Math. Chem. 50 971–80
[15] de Castro AS 2012 Bound states in a double delta potential via Laplace transform Rev. Bras. Ens. Fis. 34 4301
[16] Doetsch G 1974 Introduction to the Theory and Application of the Laplace Transformation (New York: Springer)
[17] Lebedev NN 1965 Special Functions and Their Applications (Englewood Cliffs, NJ: Prentice-Hall)