On the singular harmonic oscillator

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Abstract

We obtain the eigenvalues and eigenfunctions of the singular harmonic oscillator $V(x) = \alpha/(2x^2) + x^2/2$ by means of the simple and straightforward Frobenius (power-series) method. From the behaviour of the eigenfunctions at origin we derive two branches for the eigenvalues for negative values of $\alpha$. We discuss the well known fact that there are square-integrable solutions only for some allowed discrete values of the energy.

1 Introduction

Exactly solvable models are most useful for teaching some of the subtleties of quantum mechanics in introductory courses. For this reason most textbooks on quantum mechanics [1] and quantum chemistry [2] discuss at least the harmonic oscillator and the hydrogen atom. The former is useful for the analysis of the vibrational spectra of diatomic molecules and the latter for an introduction to atomic physics. The Schrödinger equation for these simple models can be solved in many different ways, one of them being the power-series method (also called Frobenius method [3]). From time to time teachers propose other quantum-mechanical models that exhibit particular features that may not appear in the problems just mentioned. For example, Palma and Raff [4] suggested

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the one-dimensional harmonic oscillator in the presence of a dipole-like interaction. This model is also called singular harmonic oscillator and has been treated by Pimentel and de Castro [5] with somewhat more detail.

Palma and Raff [4] and Pimentel and de Castro [5] wrote the potential-energy function of the singular harmonic oscillator as

\[ V(x) = \frac{m\omega^2 x^2}{2} + \frac{\hbar^2}{2m} \frac{\alpha}{(2mx^2)} \]

where \(\alpha\) is a dimensionless parameter related to the strength of the singular term. The former authors considered only the case \(\alpha > 0\) and the latter also negative values of this parameter. Since the discussion of the behaviour of the eigenfunctions at origin for this quantum-mechanical model appears to be of great pedagogical interest, a further analysis may be worthwhile.

In this paper we discuss the singular harmonic oscillator with somewhat more detail. In section 2 we outline the model and the behaviour of the eigenfunctions at origin. In section 3 we apply the power-series method and obtain the eigenvalues and eigenfunctions. A discussion about the existence of allowed values of the energy is given in appendix A. Finally in section 4 we summarize the main results and draw conclusions.

2 The model

In this paper we consider the time-independent Schrödinger equation with the Hamiltonian operator

\[ H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{V_{-2}}{2x^2} + \frac{V_2}{2} x^2, \quad x > 0, \]

(1)

where \(m\) is the mass of the particle (or a reduced mass) and \(V_2 > 0\). We will discuss possible values of \(V_{-2}\) later on. It is convenient for present purposes to restrict the domain to positive values of the coordinate \(x\). If we choose the units of length \(L = \hbar^{1/2} / (mV_2)^{1/4}\) and energy \(\hbar \sqrt{V_2/m} = \hbar \omega\) then we obtain the dimensionless Hamiltonian operator

\[ \hat{H} = \frac{1}{\hbar \omega} H = -\frac{1}{2} \frac{d^2}{d\tilde{x}^2} + \frac{\alpha}{2\tilde{x}^2} + \frac{1}{2} \tilde{x}^2, \quad \alpha = \frac{mV_{-2}}{\hbar^2}, \quad \tilde{x} = \frac{x}{L}. \]

(2)

Note that the Hamiltonian operator in equation (2) is identical to that of Palma and Raff [4] and Pimentel and de Castro [5] because \(V_{-2} = \hbar^2 \alpha/m\) and \(V_2 = \ldots\)
\(m \omega^2\) as shown by equation (2). However, it is more practical to carry out the calculation with the dimensionless expression (2). From now on, we omit the tilde over the dimensionless observables \(\tilde{H}\) and \(\tilde{x}\).

We first consider the behaviour of the eigenfunctions at origin that is dominated by the singular term \(\alpha/(2x^2)\); therefore, we focus on the operator

\[H_s = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{\alpha}{2x^2}.\]  

(3)

If we choose \(\phi(x) = x^s\) then we have \(H_s \phi = 0\) provided that \(\alpha = s(s - 1)\). The two roots of this equation are

\[s_\pm = \frac{1}{2} \left(1 \pm \sqrt{1 + 4\alpha}\right).\]  

(4)

\(\phi(x)\) is regular at origin if \(s > 0\); therefore, \(\alpha \geq -1/4\). If \(-1/4 < \alpha \leq 0\) then \(1 \geq s_+ > 1/2 > s_- \geq 0\) and both roots are suitable from a physical point of view if we only require that \(\phi(0^+)\) be finite. If \(\alpha > 0\) then \(s_+ > 0 > s_-\) and only \(s_+\) is acceptable. When \(\alpha = -1/4\) the two exponential solutions are identical because \(s_\pm = 1/2\). In order to obtain the second solution we proceed as follows:

\[
\frac{\partial}{\partial s} (H_s \phi) = H_s \frac{\partial}{\partial s} \phi + \frac{2s - 1}{2} x^{s-2} = 0, \\
\left.\frac{\partial}{\partial s} (H_s \phi)\right|_{s = 1/2} = \left.\frac{\partial}{\partial s} \phi\right|_{s = 1/2} = 0,
\]

(5)

where we substituted \(s(s - 1)\) for \(\alpha\) in \(H_s\). In this way, we realize that the two solutions for \(\alpha = -1/4\) are \(\phi_1 = x^{1/2}\) and \(\phi_2 = x^{1/2} \ln x\) [5]. It is clear that \(\phi'(x)\) diverges as \(x \to 0^+\) when \(-1/4 \leq \alpha < 0\) but we do not reject this kind of solutions.

### 3 Frobenius method

Many textbooks on quantum mechanics and quantum chemistry solve the Schrödinger equation for the harmonic oscillator and hydrogen atom (among other exactly-solvable problems) by means of the power-series method [12]. It is probably the simplest and most intuitive approach for introductory courses on quantum me-
chanics and quantum chemistry and in what follows we apply it to the singular harmonic oscillator.

If we assume that $\alpha > -1/4$ we can try solutions of the form

$$
\psi(x) = x^s e^{-x^2/2} u(x), \quad u(x) = \sum_{j=0}^{\infty} c_j x^{2j},
$$

and require that

$$
\int_0^\infty |\psi(x)|^2 \, dx < \infty.
$$

Upon substituting the ansatz (6) into the dimensionless Schrödinger equation $H\psi = E\psi$ we can easily verify that the coefficients $c_j$ satisfy the two-term recurrence relation

$$
c_{j+1} = A_j c_j, \quad j = 0, 1, \ldots, c_0 \neq 0,
$$

$$
A_j = \frac{4j + 2s + 1 - 2E}{2(j + 1)(2j + 2s + 1)}.
$$

It is not difficult to prove that $A_j > \beta/(j + 1)$, $1/2 < \beta < 1$, when $j > \frac{E}{2(1-\beta)} + \frac{(2s+1)(2\beta-1)}{4(1-\beta)}$. Therefore, it follows from the results of the appendix A that $u(x) > C \exp(\beta x^2) + P_k(x^2)$, where $C > 0$ and $P_k(x^2)$ is a polynomial function of $x^2$ of degree $k$. We thus conclude that $\psi(x)$ is not square integrable unless

$$
E = E_{n,s} = 2n + s + \frac{1}{2}, \quad n = 0, 1, \ldots,
$$

from which it follows that

$$
A_j = \frac{2(j - n)}{(j + 1)(2j + 2s + 1)}.
$$

Note that $c_j = 0$ for all $j > n$ when $E$ is one of the allowed values $E_{n,s}$ of the energy and the series $u(x)$ reduces to a polynomial of degree $2n$. In other words, the eigenfunctions are square integrable because they are of the form

$$
\psi_{n,s}(x) = x^s e^{-x^2/2} \sum_{j=0}^{n} c_{j,s} x^{2j}.
$$

Figure 1 shows the first four eigenvalues $E_{n,s}$ for some values of $\alpha$. We appreciate that the number of eigenvalues and eigenfunctions for $-1/4 < \alpha \leq 0$
is twice the number of those for $\alpha > 0$. The reason is that the solution with $s = s_- < 0$ for $\alpha > 0$ is not regular at origin and, consequently, it is not acceptable from a physical point of view. Palma and Raff [4] did not consider the case $\alpha < 0$ and Pimentel and de Castro [5] only showed those solutions with $s = s_+$ in their figures. For this reason, we think that our figure 1 may be revealing from a pedagogical point of view. For $\alpha = 0$ we can consider the variable interval $-\infty < x < \infty$ in which case the solutions with $s_- = 0$ and $s_+ = 1$ give rise to the well known even and odd states, respectively, of the harmonic oscillator [1,2]. Present figure 1 shows that the eigenvalue $s$ for these even and odd states come from the two branches $E_{n,s_+}$ and $E_{n,s_-}$ as $\alpha \to 0^-$. Pimentel and de Castro explicitly indicated the eigenvalues for the even and odd states in their figure 4 but did not show where the former come from.

The behaviour of the eigenvalues for $-1/4 < \alpha \leq 0$ is most interesting. According to the Hellmann-Feynman theorem (HFT) [7,8] (see [1,2] for a more pedagogical introduction) we have

$$\frac{\partial E}{\partial \alpha} = \left\langle \frac{1}{x^2} \right\rangle > 0,$$

which is obviously satisfied by the solutions with $s = s_+$ (blue lines) but not by those with $s = s_-$ (red lines). The reason is that this theorem does not apply to the latter solutions because $0 < s_- < 1/2$ and, consequently, the expectation value in equation (12) is divergent.

Figure 2 shows the normalized eigenfunctions

$$\psi_{0,s} = \sqrt{\frac{2}{\Gamma(s + 1/2)}} x^s e^{-x^2/2},$$

for $\alpha = -0.0475$. Both solutions with $s = s_- = 0.05$ and $s = s_+ = 0.95$ are square integrable and, consequently, physically acceptable. This figure also shows the harmonic-oscillator eigenfunctions $\psi_{0,0}$ and $\psi_{0,1}$ ($\alpha = 0$, green dashed lines) for comparison. Since $|\alpha| \ll 1$ this figure shows that the eigenfunctions of the singular harmonic oscillator approach those of the well known harmonic oscillator as $\alpha \to 0^-$. 

5
4 Conclusions

In this paper we enlarged the results of Parma and Raff [4] and Pimentel and de Castro [5] by considering both solutions of the Schrödinger equation for the attractive singular potential. In this way we derived two branches of the eigenvalues in the range $-1/4 < \alpha < 0$ that were not considered in those papers. An interesting outcome of this analysis is that one of the branches $(s = s_+)$ satisfies the HFT (12) while the other $(s = s_-)$ does not. That the solution to a Schrödinger equation may not satisfy such celebrated theorem may be revealing in a course on quantum mechanics. This fact is most important for a discussion of the conditions under which a mathematical result is derived.

Another interesting feature of present discussion is that it shows that the even and odd eigenfunctions of the harmonic oscillator stem from the solutions of the singular harmonic oscillator with $s = s_+$ and $s = s_-$, respectively.

Both Parma and Raff [4] and Pimentel and de Castro [5] obtained the eigenvalues from the properties of the confluent hypergeometric function. In order to follow such an analysis the students should resort to suitable books or tables of functions and integrals in order to make use of the asymptotic behaviour of such solutions. In the present case, on the other hand, we resorted to the Frobenius (power-series) method that the students may probably find more intuitive, clearer and easier to follow from beginning to end. This approach can obviously be applied to any quantum-mechanical problem in which the solution of the Schrödinger equation can be reduced to a two-term recurrence relation for the coefficients of the series expansion. It is clear that a teacher should also encourage the students to resort to well known functions and polynomials that may be found in available literature on applied mathematics, but we think that the comparison of both strategies may be most fruitful.
Figure 1: First four eigenvalues of the dimensionless singular harmonic oscillator

Figure 2: Eigenfunctions $\psi_{0,s}$ for $\alpha = -0.0475$. The green, dashed lines correspond to the eigenfunctions for $\alpha = 0$
A On the behaviour of a class of power series

Suppose that we have two series of the form

\[ S(r) = \sum_{j=0}^{\infty} a_j r^j, \quad T(r) = \sum_{j=0}^{\infty} b_j r^j, \quad (A.1) \]

and that their coefficients satisfy the two-term recurrence relations

\[
\begin{align*}
    a_{j+1} &= A_j a_j, \quad j = 0, 1, \ldots, a_0 \neq 0, \\
    b_{j+1} &= B_j b_j, \quad j = 0, 1, \ldots, b_0 \neq 0.
\end{align*} \quad (A.2)
\]

We also assume that

\[
\lim_{j \to \infty} A_j = 0, \quad \lim_{j \to \infty} B_j = 0, \quad (A.3)
\]

so that both series converge for all \( r \).

If

\[ A_j \geq B_j > 0, \quad j > k, \quad (A.4) \]

then

\[ \frac{a_j}{a_k} = A_{j-1} A_{j-2} \cdots A_k \geq \frac{b_j}{b_k} = B_{j-1} B_{j-2} \cdots B_k, \quad j > k. \quad (A.5) \]

Without loss of generality we assume that \( a_k > 0 \) and \( b_k > 0 \) (note that, if necessary, we may multiply any one of the series by \(-1\) in order to satisfy these inequalities). Therefore, for \( r > 0 \) we have

\[
S(r) \geq \frac{a_k}{b_k} T(r) + \sum_{j=0}^{k} \left( a_j - \frac{a_k}{b_k} b_j \right) r^j. \quad (A.6)
\]

If \( 0 < \lim_{j \to \infty} j A_j = D < \infty \), then there exists \( 0 < \beta < D \) such that \( A_j > \beta/(j+1) \), \( j > k \), for some integer \( k \). Therefore, if we choose \( B_j = \beta/(j+1) \) then \( T(r) = e^{\beta r} \) and

\[
S(r) \geq Ce^{\beta r} + P_k(r), \quad (A.7)
\]

where \( C > 0 \) and \( P_k(r) \) is a polynomial function of \( r \) of degree \( k \). This result will prove useful for the analysis of the solutions of the singular harmonic oscillator in section 3.
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