The rotating harmonic oscillator revisited

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Abstract

We analyze the distribution of the eigenvalues of the quantum-mechanical rotating harmonic oscillator by means of the Frobenius method. A suitable ansatz leads to a three-term recurrence relation for the expansion coefficients. Truncation of the series yields some particular eigenvalues and eigenfunctions in exact analytical form. The former can be organized in such a way that one obtains suitable information about the whole spectrum of the model.

1 Introduction

For several years there has been great interest in the quantum-mechanical rotating harmonic oscillator. Langer [1] resorted to this model in his analysis of the mathematical difficulties in the application of WKB to vibration-rotation spectroscopy and derived an asymptotic expression for the eigenvalues in terms of the interaction parameter α. Fröman and Fröman [2] derived an improved asymptotic expression for the eigenvalues of this model. Flessas [3] applied the Frobenius method and derived a three-term recurrence relation for the coefficients of the expansion. He conjectured that the eigenvalues are integer numbers and independent of α. Fröman et al [4] argued that the conclusions drawn by

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Flessas are wrong and calculated the eigenvalues by numerical integration and from the confluent hypergeometric function to prove the point. Apparently unaware of the latter paper Flessas extended his previous analysis and confirmed that the eigenvalues of the rotating harmonic oscillator are given by integer numbers and are independent of $\alpha$. He analyzed the asymptotic behaviour of the coefficients of the expansion in order to prove the point. By a judicious analysis of the asymptotic behaviour of the expansion coefficients given by the three-term recurrence relation Karlsson et al. concluded that the arguments given by Flessas contain serious mistakes and, consequently, his conclusions are incorrect. Based on the three-term recurrence relation for the coefficients of the Frobenius expansion Singh et al. proved that there is a convergent continued fraction representation of the Green’s function and showed that one can obtain exact eigenvalues and eigenfunctions from suitable truncation of the series. Nieto and Gutschick obtained asymptotic expansions for small and large values of the equilibrium distance. Masson derived the three-term recurrence relation and examined the continued fraction in detail. He showed that one can obtain information about the eigenvalues from the analytic continuation of the continued fraction. In a sequel paper Mason applied the theory of self-adjoint analytic families to the rotating harmonic oscillator, obtained weak and strong coupling expansions for the eigenvalues and estimated the radius of convergence of the former series. Gangopadhyay et al. applied $1/N$ perturbation expansion to the $N$-dimensional rotating harmonic oscillator. Leute and Marcilhacy examined the rotating harmonic oscillator, among other quantum-mechanical problems, by means of the biconfluent Heun equation. They derived a three-term recurrence relation, truncated the series expansion and showed that the roots are all real and distinct. Killingbeck argued that the three-term recurrence relations may lead to false eigenvalues and concluded that it is not surprising that Flessas and Singh et al. reached erroneous conclusions; he obtained some eigenvalues numerically. Roychoudhury and Varshni applied the $1/N$-expansion approach to the three-dimensional rotating harmonic oscillator and compared such approximate results with the
exact ones obtained by means of supersymmetric quantum mechanics for particular values of the model parameter $\alpha$. Lay et al. [15] constructed asymptotic solutions of a Schrödinger equation in the vicinity of a second order pole by means of the comparison equation method and obtained the expansion of the eigenvalues of the rotating oscillator for large equilibrium distances.

The purpose of this paper is a more careful analysis of the exact results provided by the truncation of the Frobenius series by means of the three-term recurrence relation. In section 2 we present the model and transform the Schrödinger equation into a suitable dimensionless eigenvalue equation. In section 3 we apply the Frobenius method, derive a three-term recurrence relation for the expansion coefficients that enables one to truncate the expansion series and obtain exact eigenvalues and eigenfunctions. We analyze the distribution of the eigenvalues and organize them in order to derive information about the spectrum of the problem. Finally, in section 4 we summarize the main results and draw conclusions.

2 The rotating oscillator

The Schrödinger equation for the rotating oscillator is

$$H\psi = E\psi, \quad H = -\frac{\hbar^2}{2m} \nabla^2 + \frac{k}{2} (r - r_e)^2,$$

(1)

where $m$ is the reduced mass of the diatomic molecule, $k$ the force constant of the bond and $r_e$ the equilibrium distance. If we define dimensionless coordinates $\tilde{r} = r/r_e$ we obtain the dimensionless equation [16]

$$\tilde{H}\tilde{\psi} = \tilde{E}\tilde{\psi}, \quad \tilde{H} = -\tilde{\nabla}^2 + \frac{(\tilde{r} - 1)^2}{4\alpha^2},$$

$$\alpha^2 = \frac{\hbar^2}{4mk r_e^2}, \quad \tilde{E} = \frac{2mr_e^2}{\hbar^2} E.$$  

(2)

This equation is separable in spherical coordinates and the radial part $R(\tilde{r})$ is a solution to

$$\left[ -\frac{1}{\tilde{r}^2} \frac{d}{d\tilde{r}} \tilde{r}^2 \frac{d}{d\tilde{r}} + \frac{l(l+1)}{\tilde{r}^2} + \frac{(\tilde{r} - 1)^2}{4\alpha^2} \right] R(\tilde{r}) = \tilde{E} R(\tilde{r}).$$

(3)
where $l = 0, 1, \ldots$ is the rotational quantum number. The function $f(\tilde{r}) = \tilde{r} R(\tilde{r})$ satisfies the eigenvalue equation

$$\left[ -\frac{d^2}{d\tilde{r}^2} + \frac{l(l+1)}{\tilde{r}^2} + \frac{(\tilde{r} - 1)^2}{4\alpha^2} \right] f(\tilde{r}) = \tilde{E} f(\tilde{r}),$$

that is the one used in most of the papers mentioned above provided that $\tilde{E} = \alpha^{-1} (\lambda + 1/2)$, where $\lambda$ is the eigenvalue chosen by those authors [1][7][9][10][12][15].

In this paper we prefer an alternative form of this equation that we obtain by means of the change of variables $q = \tilde{r}/\sqrt{2\alpha}$:

$$\left[ -\frac{d^2}{dq^2} + \frac{l(l+1)}{q^2} - aq + q^2 \right] f(q) = W f(q),$$

$$a = \sqrt{\frac{2}{\alpha}}, W = 2\alpha \tilde{E} - \frac{1}{2\alpha}.$$  \hspace{1cm} (5)

In the case of the rotating oscillator $a > 0$, but here we allow all real values of $a$ for generality. According to the Hellmann-Feynman theorem the eigenvalues are decreasing functions of $a$

$$\frac{dW}{da} = - \langle q \rangle.$$  \hspace{1cm} (6)

We label the eigenvalues in the usual way as $W_{\nu,l}$, $\nu = 0, 1, \ldots$ so that $W_{\nu,l} < W_{\nu+1,l}$.

### 3 The three-term recurrence relation

In what follows we apply the Frobenius method to the eigenvalue equation (5). If we try the ansatz

$$f(q) = q^{l+1} P(q) \exp\left(\frac{a}{2}q - \frac{q^2}{2}\right), \quad P(q) = \sum_{j=0}^{\infty} c_j q^j,$$

we obtain a three-term recurrence relation for the expansion coefficients $c_j$

\begin{align*}
  c_{j+2} &= A_j c_{j+1} + B_j c_j, \quad j = -1, 0, 1, \ldots, c_{-1} = 0, c_0 = 1, \\
  A_j &= -\frac{a(j+l+2)}{(j+2)(j+2l+3)}, \\
  B_j &= \frac{4(2j+2l+3-W) - a^2}{4(j+2)(j+2l+3)}. \hspace{1cm} (8)
\end{align*}
If we require that \( c_n \neq 0, \ c_{n+1} = c_{n+2} = 0 \) then \( P(q) \) reduces to a polynomial of degree \( n \) because \( c_j = 0 \) for all \( j > n \). It follows from this condition that \( B_n = 0 \). Therefore, we have exact solutions with polynomial factors \( P(q) \) if
\[
W = W_i^{(n)} = 2n + 2l + 3 - \frac{a^2}{4}, \ c_{n+1} \ (W, a) = 0.
\] (9)

It can be proved that all the roots of the nonlinear equation \( c_{n+1} \left( W_i^{(n)}, a \right) = 0 \) are real \[12, 17, 18\]. Since \( c_1 = -a/2 \) the truncation condition with \( n = 0 \) yields the ground state of the harmonic oscillator. The other cases are more interesting.

When \( n = 1 \) we obtain
\[
W_i^{(1)} = 5 + 2l - \frac{a^2}{4}, \ \ a_i^{(1,1)} = -\frac{2}{\sqrt{l+2}}, \ \ a_i^{(1,2)} = \frac{2}{\sqrt{l+2}}, \ \ a_i^{(1,3)} = \frac{2}{\sqrt{l+2}}
\] (10)

and
\[
c_i^{(1,1)} = \frac{1}{\sqrt{l+2}}, \ c_i^{(1,2)} = -\frac{1}{\sqrt{l+2}}
\] (11)

It is clear that \( P_i^{(1,1)}(q) \) does not have nodes and \( P_i^{(1,2)}(q) \) has one node.

When \( n = 2 \) we obtain
\[
W_i^{(2)} = 7 + 2l - \frac{a^2}{4}, \ a_i^{(2,1)} = -2\sqrt{\frac{4l + 9}{(l+2)(l+3)}}, \ a_i^{(2,2)} = 0, \ a_i^{(2,3)} = 2\sqrt{\frac{4l + 9}{(l+2)(l+3)}}
\] (12)

and the corresponding coefficients are
\[
c_i^{(2,1)} = \sqrt{\frac{4l + 9}{(l+2)(l+3)}}, \ c_i^{(2,2)} = \frac{1}{l+3}, \ c_i^{(2,3)} = \frac{1}{l+3}
\] (13)

The polynomial \( P_i^{(2,1)}(q) \) has no nodes, while \( P_i^{(2,2)}(q) \) and \( P_i^{(2,3)}(q) \) have one node each in \( 0 < q < \infty \).

In the general case we obtain \( n+1 \) real distinct roots \( a_i^{(n,i)}, i = 1, 2, \ldots, n+1 \) for the same energy \( W_i^{(n)} \) and the corresponding eigenfunctions
\[
f_i^{(n,i)}(q) = q_i^{n+1} P_i^{(n,i)}(q) \exp \left( \frac{a_i^{(n,i)}}{2} q - \frac{q^2}{2} \right), \ P_i^{(n,i)}(q) = \sum_{j=0}^{n} c_{j,i}^{(n,i)} q^j.
\] (14)
Notice that all these functions are square-integrable solutions to the radial equation (5) and, consequently, represent bound states of some quantum-mechanical systems. Therefore, Killingbeck’s criticism of the three-term recurrence relation is not entirely correct [13].

A most important question arises as to the precise meaning of those eigenvalues and eigenfunctions. Taking into account the results above for \( n = 1, 2 \) and the Hellmann-Feynman theorem [3] we conclude that \( (a^{(n,i)}_l, W^{(n)}_l) \) is a point of the curve \( W_{l-1,i}(a) \), \( i = 1, 2, \ldots, n + 1 \). The reason is that the number of nodes of \( P^{(n,i)}_l(q) \) increases with \( i \) and \( W_{\nu,l}(a) \) is a decreasing function of \( a \) for every \( \nu \) and \( l \). Figure 1 shows pairs of points \( (a^{(n,i)}_0, W^{(n)}_0) \) for \( n = 1, 2, \ldots, 30, i = 1, 2, \ldots, n + 1 \) (red circles) and blue lines that join some points on the curves \( W_{\nu,0}(a) \), \( \nu = 0, 1, \ldots, 8 \). The two green curves are the inverted parabolas \( W^{(n)}_0(a) \) for \( n = 1 \) and \( n = 30 \) that limit the region considered by present calculation. Figure 2 shows those points of the previous figure joined by blue lines and the eigenvalues calculated numerically by means of the Rayleigh-Ritz variational method with the basis set of non-orthogonal functions \( \{ u_{i,l}(q) = q^{i+l+1} \exp \left( -q^2/2 \right), i = 0, 1, \ldots \} \) (blue squares). The variational results that coincide with those given by the truncation method are marked by blue circumferences (empty circles). The fact that the variational results appear on the blue lines (or on continuations of them) confirms the conclusion drawn above about the meaning of the points \( (a^{(n,i)}_l, W^{(n)}_l) \).

When \( W = W^{(n)}_l \) the eigenvalues \( \lambda = \frac{W}{2} + \frac{1}{2n} - \frac{i}{2} = \frac{W}{2} + \frac{1}{2} - \frac{i}{2} \) are integer numbers \( \lambda^{(n)}_l = n + l + 1 \) as argued by Flessas [3,5]; however, it is not true that the eigenvalues \( \lambda \) are independent of \( a \) as shown in figures 1 and 2. Besides, there are some eigenvalues \( \lambda_{\nu,l} \) that are not integer numbers (for example the blue squares that are not on the blue lines). In other words, only the values of \( \lambda \) given by the truncation condition are integer numbers.
4 Conclusions

In this paper we have re-examined the three-term recurrence relation stemming from the application of the Frobenius method to the Schrödinger equation for the rotating harmonic oscillator. Although such recurrence relation was already discussed in the past we think that present analysis casts light about some aspects of this approach that was overlooked in those earlier studies [1–15].

It is clear that the truncation method provides useful information about the distribution of the eigenvalues of the quantum-mechanical model from which one may obtain part of its spectrum from suitable interpolation of the points \( (n,i), W_l(n) \). This fact is clearly shown by Figure 2 where we see that the blue lines give us the position of eigenvalues that do not stem from the truncation condition. In this paper we have not attempted to obtain a suitable fit and merely joined the points \( (n,i), W_l(n) \) stemming from the truncation condition. As far as we know this utility of the exact solutions to conditionally solvable quantum-mechanical models has not been discussed before.

In addition to what has just been said we have shown that the conclusions drawn by Flessas [3,5] about the eigenvalues of the rotating harmonic oscillator and those drawn by Killingbeck [13] about the three-term recurrence relations are not entirely correct.

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Figure 1: Eigenvalues $W_0^{(n)}$, $n = 1, 2, \ldots, 30$

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Figure 2: Eigenvalues $W_{\nu,0}(a)$ obtained from the truncation condition (red circles) and from a variational calculation (blue squares)