An ubiquitous three-term recurrence relation

Paolo Amore∗
Facultad de Ciencias, CUICBAS, Universidad de Colima,
Bernal Díaz del Castillo 340, Colima, Colima, Mexico
and
Francisco M. Fernández†
INIFTA, División Química Teórica,
Blvd. 113 y 64 (S/N), Sucursal 4, Casilla de Correo 16,
1900 La Plata, Argentina

Abstract

We solve an eigenvalue equation that appears in several papers about a wide range of physical problems. The Frobenius method leads to a three-term recurrence relation for the coefficients of the power series that, under suitable truncation, yields exact analytical eigenvalues and eigenfunctions for particular values of a model parameter. From these solutions some researchers have derived a variety of predictions like allowed angular frequencies, allowed field intensities and the like. We also solve the eigenvalue equation numerically by means of the variational Rayleigh-Ritz method and compare the resulting eigenvalues with those provided by the truncation condition. In this way we prove that those physical predictions are merely artifacts of the truncation condition.

∗e-mail: paolo@ucol.mx
†e-mail: fernande@quimica.unlp.edu.ar
1 Introduction

In a series of papers, several authors discuss a wide variety of physical models in cylindrical coordinates that, after some suitable transformations of the main dynamical (or eigenvalue) equation, can be reduced to an eigenvalue equation in the radial variable with Coulomb (or Coulomb–like) and harmonic (or harmonic-like) interactions. Through further application of the Frobenius (power-series) method they obtain a three-term recurrence relation. They state that in order to have finite solutions (or normalizable ones) the power series should terminate and they place a suitable truncation condition for that purpose. As a result of this truncation those authors invariably draw the conclusion that some model parameters, like the intensity of a magnetic field or the oscillator frequency, for example, should be discrete. In other words, they claim that the eigenvalue equation has square-integrable solutions for some particular values (allowed values) of such parameters. For example, Verçin [1] derives an exact solution to the problem of two identical charged anyons moving in a plane under the influence of a static uniform magnetic field perpendicular to that plane. He argues that there are bound states if and only if the series terminates, which occurs only for certain discrete values of the magnetic field. Later, Myrheim et al [2] discussed Verçin’s results with more detail. Furtado et al [3] discuss the influence of a disclination on the spectrum of an electron or a hole in a magnetic field in the framework of the theory of defects and three-dimensional gravity of Katanaev and Volovich [4]. In this case the cyclotron frequency and the magnetic field should depend on the quantum numbers. Bakke and Moraes [5] introduce a geometric model to explain the origin of the observed shallow levels in semiconductors threaded by a dislocation density and find allowed values of the oscillator frequency or of the constant $k$ associated to the momentum along the $z$-axis. Bakke and Beilish [6] obtain the bound states for a non-relativistic spin-half neutral particle under the influence of a Coulomb-like potential induced by the Lorentz symmetry breaking effects. They claim to present a new
possible scenario of studying the Lorentz symmetry breaking effects on a non-relativistic quantum system defined by a fixed space-like vector field parallel to the radial direction interacting with a uniform magnetic field along the z-axis. They also discuss the influence of a Coulomb-like potential induced by Lorentz symmetry violation effects on a two-dimensional harmonic oscillator and find allowed values of the cyclotron frequency. Bakke [7] discusses a model that consists of the interaction between a moving electric quadrupole moment and a magnetic field and also adds a two-dimensional harmonic-oscillator potential thus obtaining allowed values of the oscillator frequency. Bakke [8] studies the bound states of a quantum-mechanical model given by the interaction between the electric quadrupole of a moving particle and an electric field. In two other models the author adds a harmonic potential and a linear plus harmonic potential and also finds allowed oscillator frequencies. Bakke and Belich [9] study the effects of the Lorentz symmetry violation in the non-relativistic quantum dynamics of a spin-1/2 neutral particle interacting with external fields confined to a two-dimensional quantum ring and also finds oscillator frequencies that depend on the quantum numbers. Fonseca and Bakke [10] propose a model for the interaction of a magnetic quadrupole moment with electric and magnetic fields and in a second model they add a harmonic-oscillator potential finding that the angular frequency depends on the quantum numbers. Bakke and Furtado [11] study the influence of a Coulomb-type potential on the Klein-Gordon oscillator and find that the angular frequency should depend on the quantum numbers.

The purpose of this paper is to study the radial eigenvalue equation derived in those papers and investigate to which extent the truncation of the power series by means of the tree-term recurrence relation affects the physical conclusions drawn by their authors. In section 2 we outline the main equation solved in the papers mentioned above. In section 3 we solve the radial eigenvalue equation by means of the Frobenius method and truncation through a three-term recurrence relation for the series coefficients in order to derive analytical solutions. By means of a reliable variational method we also obtain accurate numerical eigenvalues that are compared with the analytical ones. Finally, in section 4 we
summarize the main results and draw conclusions.

2 The time-dependent equation

In several of the papers discussed here the starting point is a time-dependent quantum-mechanical equation of the form [5–10]

\[ i \frac{\partial \psi}{\partial t} = H \psi, \]  

(1)

where the Hamiltonian operator \( H = H (\rho, \partial_\rho, \partial_\varphi, \partial_z), \partial_q = \partial / \partial q, \) is given in cylindrical coordinates \( 0 < \rho < \infty, \ 0 \leq \varphi \leq 2\pi, \ -\infty < z < \infty. \) Upon choosing the particular solution

\[ \psi(t, \rho, \varphi, z) = e^{-iEt} e^{ij\varphi} e^{ikz} R(\rho), \]  

(2)

where \( j = l = 0 \pm 1 \pm 2, \ldots \) in some cases [7,8,10,11], \( j = l+1/2 \) in others [5,6,9] and \( -\infty < k < \infty \) the authors derive a eigenvalue equation for \( R(\rho): \)

\[ H_{jk} (\rho, \partial_\rho) R(\rho) = E R(\rho). \]  

(3)

In most of those papers the authors state that they are looking for bound states although it is plain that their models do not support such kind of solutions. As a matter of fact, a bound state requires that

\[ \int \int \int |\psi(t, \rho, \varphi, z)|^2 \rho d\rho d\varphi dz < \infty, \]  

(4)

but in the general example outlined above the improper integral over \( z \) is divergent. Besides, the energy depends on \( -\infty < k < \infty \) which clearly shows that the spectrum is continuous. This is one of the conceptual errors in those papers. Other authors consider a motion in a plane where there are truly bound states [1,2,11]. In what follows we assume that the motion of the particle in the three-dimensional space can be restricted to a fictitious motion in the \( x-y \) plane so that we can truly speak of bound states.

As an illustrative example we consider the influence of a disclination on the spectrum of an electron or a hole in a magnetic field in the framework of the
theory of defects and three-dimensional gravity of Katanaev and Volovich [4] discussed by Furtado et al [3]. The model Hamiltonian derived from the metric

\[ ds^2 = dz^2 + d\rho^2 + \alpha^2 \rho^2 d\phi^2, \]  

in cylindrical coordinates and the interaction between the charge of the particle \( q \) and the magnetic field \( B \) is

\[ H = -\frac{\hbar^2}{2m^*} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{1}{\alpha^2 \rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{i\hbar q B}{2\alpha^2 m^* c} \frac{\partial}{\partial \phi} + \frac{q^2 B^2}{8m^* c^2 \alpha^2} \rho^2, \]  

where the precise meaning of each parameter is given in the authors’ paper [3]. The authors also add the self-interaction term

\[ \tilde{U} = \frac{q^2}{4\pi \epsilon} \frac{\kappa(p)}{\rho}, \]  

to the Hamiltonian operator in the Schrödinger equation \( H\psi = E\psi \).

We can easily derive a dimensionless equation by means of a well-known systematic procedure [12]. We define the dimensionless coordinates

\[ \tilde{\rho} = \rho \frac{L}{L}, \tilde{z} = \frac{z}{L}, L = \sqrt{\frac{2c\alpha h}{|q| B}}, \]  

in terms of the unit of length \( L \) and the dimensionless Hamiltonian operator

\[ \tilde{H} = \frac{2m^* L^2}{\hbar^2} H = -\left( \frac{1}{\tilde{\rho}} \frac{\partial}{\partial \tilde{\rho}} \tilde{\rho} \frac{\partial}{\partial \tilde{\rho}} + \frac{1}{\alpha^2 \tilde{\rho}^2} \frac{\partial^2}{\partial \tilde{\phi}^2} + \frac{\partial^2}{\partial \tilde{z}^2} \right) + \frac{2i\hbar q}{\alpha |q|} \frac{\partial}{\partial \tilde{\phi}} + \tilde{\rho}^2 + \frac{a}{\tilde{\rho}} \]  

\[ a = \frac{m^* q^2 \kappa}{\pi \epsilon \hbar^2} \sqrt{\frac{c\alpha h}{2|q| B}}, \]  

where \( \hbar^2 / (2m^* L^2) \) is a natural unit of energy. If we propose the particular solution

\[ \psi(\tilde{\rho}, \tilde{\varphi}, \tilde{z}) = e^{il\tilde{\varphi}} e^{ik\tilde{z}} R(\tilde{\rho}), \]  

the resulting differential equation for \( R(\tilde{\rho}) \) is

\[ -\left( \frac{1}{\tilde{\rho}} \frac{\partial}{\partial \tilde{\rho}} \tilde{\rho} \frac{\partial}{\partial \tilde{\rho}} - \frac{l^2}{\alpha^2 \tilde{\rho}^2} \right) R + \tilde{\rho}^2 R + \frac{a}{\tilde{\rho}} R = W R, \]  

\[ W = \frac{4m c \alpha E}{\hbar |q| B} - k^2 + \frac{2gl}{\alpha |q|}. \]
Notice that present parameter $a$ is exactly the parameter $b$ in Furtado et al’s paper [3]. In other articles the authors simply state that they resort to units such that $\hbar = c = 1$ [5–11] but this non-rigorous way of choosing suitable units was recently criticized in a pedagogical paper [12].

3 The three-term recurrence relation

By means of suitable transformations of the eigenvalue equation (3) the authors mentioned above derive an eigenvalue equation of the form [1–3, 5–11]

\[ \hat{L} R = W R, \]
\[ \hat{L} \equiv -\frac{d^2}{d\xi^2} - \frac{1}{\xi} \frac{d}{d\xi} + \frac{\gamma^2}{\xi^2} - \frac{a}{\xi} + \xi^2, \]  

(12)

where $\gamma$ and $a$ are real constants and, in general, $\gamma$ depends on the rotational quantum number $l$. A particular example was derived in the preceding section.

By means of the ansatz

\[ R(\xi) = \xi^{|\gamma|} e^{-\frac{\xi^2}{2}} P(\xi), \quad P(\xi) = \sum_{j=0}^{\infty} c_j \xi^j, \]  

(13)

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

\[ c_{j+2} = -\frac{a}{(j+2)(j+2|\gamma|+2)} c_{j+1} + \frac{2j+2|\gamma|+2 - W}{(j+2)(j+2|\gamma|+2)} c_j, \]

\[ j = -1, 0, 1, \ldots, \ c_{-1} = 0, \ c_0 = 1. \]  

(14)

In the papers just mentioned the authors state, in one way or another, that in order to obtain bound states one has to force the termination conditions

\[ W = 2n + 2|\gamma| + 2, \ c_{n+1} = 0, \ n = 1, 2, \ldots \]  

(15)

Clearly, under such conditions $c_j = 0$ for all $j > n$ and $P(\xi)$ reduces to a polynomial of degree $n$. In this way, they obtain analytical expressions for the eigenvalues $W_{n,l} = 2n + 2|\gamma| + 2$ and the radial eigenfunctions $R_{n,l}(\xi)$ [1–3, 5–11].

For the sake of clarity and generality, in this section we use $\gamma$ instead of $l$ as an effective quantum number because the form of $\gamma$ is not the same in all those
papers. Besides, we will also include the truncation condition for \( n = 0 \) although in this case the only solution is \( a = 0 \) and the problem reduces to the exactly solvable harmonic oscillator.

For example, when \( n = 1 \) the truncation condition (15) yields

\[
W_{1,\gamma} = 2 (|\gamma| + 2), \quad a_{1,\gamma}^{(1)} = -\sqrt{2 (2|\gamma| + 1)}, \quad a_{1,\gamma}^{(2)} = \sqrt{2 (2|\gamma| + 1)}.
\] (16)

There is no doubt that we have obtained only one eigenvalue \( W = W_{1,\gamma} \) for two particular values of \( a = a_{1,\gamma}^{(i)}, \ i = 1, 2, \) that depend on the chosen value of \( \gamma \).

In the general case, we obtain the same value \( W_{n,\gamma} \) for each of the particular roots \( a_{n,\gamma}^{(k)}, \ k = 1, 2, \ldots, n + 1, \ a_{n,\gamma}^{(k)} < a_{n,\gamma}^{(k+1)} \), of \( c_{n+1} = 0 \) (including \( a = 0 \) as a possible solution). For example, we have three real roots for \( n = 2 \)

\[
\begin{align*}
W_{2,\gamma} &= 2\gamma + 6, \\
a_{2,\gamma}^{(1)} &= -2\sqrt{4\gamma + 3}, \ a_{2,\gamma}^{(2)} = 0, \ a_{2,\gamma}^{(3)} = 2\sqrt{4\gamma + 3},
\end{align*}
\] (17)

and four for \( n = 3 \)

\[
\begin{align*}
W_{3,\gamma} &= 2\gamma + 8, \\
a_{2,\gamma}^{(1)} &= -\sqrt{2}\sqrt{10 (\gamma + 1) + 64\gamma^2 + 128\gamma + 73}, \\
a_{2,\gamma}^{(2)} &= -\sqrt{2}\sqrt{10 (\gamma + 1) - 64\gamma^2 + 128\gamma + 73} \\
a_{2,\gamma}^{(3)} &= \sqrt{2}\sqrt{10 (\gamma + 1) - 64\gamma^2 + 128\gamma + 73}, \\
a_{2,\gamma}^{(4)} &= \sqrt{2}\sqrt{10 (\gamma + 1) + 64\gamma^2 + 128\gamma + 73}.
\end{align*}
\] (18)

It is obvious to anybody familiar with conditionally solvable quantum-mechanical models \cite{[15]} (and references therein) that the approach just described does not produce all the eigenvalues of the operator \( \hat{L} \) for a given set of values of \( \gamma \) and \( a \) but only those states with polynomial solutions for \( P(\xi) \). These particular eigenvalues \( W_{n,\gamma} = 2n + 2|\gamma| + 2, \ n = 0, 1, \ldots \) are related to the harmonic oscillator ones and each of them corresponds to a set of particular values of \( a \), namely \( a_{n,\gamma}^{(k)} \). On the other hand, if we solve the eigenvalue equation (12) in a proper way we obtain an infinite set of eigenvalues \( W_{\nu,\gamma}(a), \ \nu = 0, 1, 2, \ldots \) for each set of real values of \( a \) and \( \gamma \). The condition that determines these allowed
values of $W$ is that the corresponding radial eigenfunctions $R(\xi)$ are square integrable
\[ \int_0^{\infty} |R(\xi)|^2 \xi \, d\xi < \infty, \] as shown in any textbook on quantum mechanics [13]. Notice that $\nu$ is the actual radial quantum number (that labels the eigenvalues in increasing order of magnitude) whereas $n$ is just a positive integer that labels some particular solutions with polynomial factors $P(\xi)$. In other words: $n$ is a fictitious quantum number used in those earlier papers [1–3, 5–11].

The true eigenvalues $W_{\nu,\gamma}(a)$ of equation (12) are decreasing functions of $a$ as follows from the Hellmann-Feynman theorem [13, 16]
\[ \frac{\partial W}{\partial a} = -\left\langle \frac{1}{\xi} \right\rangle < 0. \] (20)
From this expression we can draw a simple conclusion: for a given value of $n$ the pair $\left(a_{n,\gamma}^{(1)}, W_{n,\gamma}\right)$ is a point on the true ground-state curve, $W_{0,\gamma}(a)$, $\left(a_{n,\gamma}^{(2)}, W_{n,\gamma}\right)$ is a point on the true first-excited-state curve $W_{1,\gamma}(a)$, and so on.

The reflection symmetry of $W$ with respect to $a$ suggested by the analytical energy eigenvalues shown in those earlier papers [1–3, 5–11] is fictitious, the analysis above clearly shows, for example, that: $W_{0,0}(-\sqrt{2}) = W_{1,0}(\sqrt{2}) = 4$, $W_{0,1}(-\sqrt{6}) = W_{1,1}(\sqrt{6}) = 6$, $W_{0,0}(-\sqrt{12}) = W_{2,0}(\sqrt{12}) = 6$ (using the correct quantum number $\nu$). The fact that $W_{\nu,\gamma}(-|a_{n,\gamma}|) = W_{\nu',\gamma}(|a_{n,\gamma}|)$ for $\nu < \nu'$ is a consequence of the Hellmann-Feynman theorem (20) just mentioned.

The eigenvalue equation (12) cannot be solved exactly in the general case. In order to obtain sufficiently accurate eigenvalues of the operator $\hat{L}$ we resort to the reliable Rayleigh-Ritz variational method that is well known to yield increasingly accurate upper bounds to all the eigenvalues of the Schrödinger equation [16] (and references therein). For simplicity we choose the basis set of non-orthogonal functions $\{u_j(\xi) = \xi^{|\gamma|+j}e^{-\xi^2/2}, j = 0, 1, \ldots\}$. We test the accuracy of these results by means of the powerful Riccati-Padé method [17].

Figures 1, 2 and 3 show present numerical eigenvalues $W_{\nu,\gamma}$ for $\gamma = 0$, $\gamma = 1/2$, and $\gamma = 1$, respectively. Every blue, continuous, line is a curve
\( W_{\kappa,\gamma}(a) \) and the red circles indicate pairs \( (a_{n,\gamma}^{(k)}, W_{n,\gamma}) \) coming from the artificial truncation condition \([15]\). These figures clearly confirm the theoretical analysis carried above.

The quantization of the parameter \( a \) (allowed values of \( a \), or its dependence on the quantum numbers) is a mere artifact of the truncation condition \([15]\) and does not exhibit any physical meaning. This fact is more than evident in the light of present numerical calculations. In other words, the existence of allowed values of the field strength, oscillator frequency, etc, claimed in those earlier papers \([1,3,5,7,9,10]\) is merely an artifact of that unnecessary truncation condition. Consider, for example, the eigenvalue equation \([11]\) from which the artificial quantization of the parameter \( a = a_{n,l} \) may be interpreted, according to equation \([9]\), as the existence of allowed field strengths \( B = B_{n,l} \) \([3]\). Present numerical results clearly show that there are square-integrable solutions for any \( B \neq B_{n,l} \). To be clearer: the set of bound states produced by the truncation condition \([15]\) is contained in the set of all bound states. The majority of bound states do not satisfy such arbitrary, unnecessary condition.

4 Conclusions

Since 1991 several authors have been discussing a wide variety of physical models that lead to either dynamic or time-independent equations that can be reduced to a three-term recurrence relation by means of the Frobenius method \([1,3,5,7,9,11]\). By means of an unnecessary truncation condition they obtain particular solutions \([13]\) with factors \( P(\xi) \) that are polynomial functions of the radial coordinate. These particular solutions take place for particular values of one or another model parameter (\( a \) in the present case). Since the authors appear to believe that these particular solutions are the only ones allowed they conjecture that there are allowed angular frequencies or allowed field intensities and the like. In this paper we show that all those physical conclusions are mere artifacts of the unnecessary truncation condition that only produces some particular solutions without any physical relevance. The only interest in them is purely academic as
they are exact solutions of a problem that is not exactly solvable [14][15]. Present numerical calculations, illustrated by means of three figures, reveal that there are square-integrable solutions for any value of the dimensionless parameter $a$ (blue lines). Those figures also show the particular arbitrary eigenvalues (red circles) coming from the truncation condition that have been interpreted as if there were allowed angular frequencies, field intensities, etc. Those particular eigenvalues and their corresponding model parameters have no relevant role in the physics of the problem, except that they correspond to polynomial factors $P(\lambda)$.

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Figure 1: Eigenvalues for $\gamma = 0$

Figure 2: Eigenvalues for $\gamma = 1/2$
Figure 3: Eigenvalues for $\gamma = 1$