The truncated Coulomb potential revisited

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Abstract
We apply the Frobenius method to the Schrödinger equation with a truncated Coulomb potential. By means of the tree-term recurrence relation for the expansion coefficients we truncate the series and obtain exact eigenfunctions and eigenvalues. From a judicious arrangement of the exact eigenvalues we derive useful information about the whole spectrum of the problem and can obtain other eigenvalues by simple and straightforward interpolation.

Keywords Truncated Coulomb potential · Frobenius method · Three-term recurrence relation · Exact eigenvalues and eigenfunctions

1 Introduction
The family of truncated Coulomb potentials $V(r) = -Ze^2/(β^k + r^k)^{1/k}$, $k = 1, 2, \ldots$, has received considerable attention [1–11]. In particular, the case $k = 2$ proved to be suitable as an approximation to the laser-dressed binding potential [2], in the UV and X-ray absorption cross section by hydrogen in the presence of an intense IR laser field [4] and in the discussion of the atomic states of hydrogen in the presence of intense laser fields [5]. The Schrödinger equation has been solved in many different ways, for example, Patil [3] described some analytic properties of the scattering phase shifts of a variety of potentials, including the cases $k = 1$ and $k = 2$. Dutt et al [6] applied $1/N$ expansion to the model with $k = 2$. Singh et al [7] obtained accurate eigenvalues for the cases $k = 1$ and $k = 2$ by means of a transformation of the radial equation followed by some iterative method. Ray and Mahata [8] calculated the energies of several states for the case $k = 1$ by means of the $1/N$ expansion. De Meyer and Vanden Berghe [9] calculated eigenvalues of the model with $k = 1$ from a secular equation derived by means of the Lie algebra SO(2,1) and a scaling parameter introduced by means
of a canonical transformation. Fernández [10] applied the Frobenius method, derived a three-term recurrence relation for the expansion coefficients and obtained exact eigenvalues and eigenfunctions of the model with $k = 1$ by suitable truncation of the series. By means of supersymmetry Drigo Filho [11] obtained the same three-term recurrence relation derived earlier by Fernández for the case $k = 1$ and discussed some eigenvalues and eigenfunctions.

The purpose of this paper is a more detailed analysis of the Frobenius method. In Sect. 2 we derive a suitable dimensionless eigenvalue equation for the radial part of the Schrödinger equation with the truncated Coulomb potential. In Sect. 3 we discuss and interpret the distribution of the eigenvalues stemming from the truncation of the Frobenius series. Finally, in Sect. 4 we summarize the main results and draw conclusions.

2 The model

Throughout this paper we restrict ourselves to the case $k = 1$ and focus on the model given by Hamiltonian operator

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 (r + r_0)}, \quad (1)$$

where $m$ is a reduced mass, $e$ is the electron charge, $Z$ the atomic number, $\varepsilon_0$ is the vacuum permittivity and $r_0$ a suitable cut-off radius. It is convenient to work with dimensionless equations [12]; for example, if, in the present case, we define the dimensionless coordinate $\tilde{r} = r/r_0$ and the Laplacian $\tilde{\nabla}^2 = r_0^2 \nabla^2$ the Hamiltonian operator (1) becomes

$$\tilde{H} = \frac{mr_0^2}{\hbar^2} H = -\frac{1}{2} \tilde{\nabla}^2 - \frac{\beta}{\tilde{r} + 1}, \quad \beta = \frac{mr_0 Ze^2}{4\pi\varepsilon_0 \hbar^2}, \quad (2)$$

where the eigenvalues $E$ of $H$ and $\tilde{E}$ of $\tilde{H}$ are related by $\tilde{E} = mr_0^2 E / \hbar^2$.

In what follows we will focus on solving the radial Schrödinger equation associated to the dimensionless operator $\tilde{H}$; however, for comparison purposes it is convenient to show the connection between this operator and those studied in earlier papers. For example, if we now define $\tilde{r} = \beta \tilde{r}$ and $\tilde{\nabla}^2 = \beta^{-2} \nabla^2$ we obtain an alternative expression for the dimensionles Hamiltonian operator

$$\tilde{H} = \beta^{-2} H = -\frac{1}{2} \tilde{\nabla}^2 - \frac{1}{\tilde{r} + \beta}, \quad (3)$$

where the energy eigenvalues $\tilde{E}$ of $\tilde{H}$ and $\tilde{E}$ of $\tilde{H}$ are related by $\tilde{E} = \beta^2 \tilde{E}$.
3 Exact solutions

The radial part of the Schrödinger equation with the Hamiltonian (2) can be written as

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{\beta}{r+1}\right]f(r) = Ef(r), \quad f(0) = 0, \quad \lim_{r \to \infty} f(r) = 0,$$

where $l = 0, 1, \ldots$ is the angular momentum quantum number and we have omitted the tilde over the radial variable.

In order to solve the eigenvalue equation (4) we resort to the well known Frobenius method and instead of the ansatz used earlier [10] here we try

$$f(r) = r^{l+1}(1 + r)e^{-\alpha r} \sum_{j=0}^{\infty} c_j r^j, \quad \alpha = \sqrt{-2E}.$$  \hspace{1cm} (5)

A straightforward calculation shows that the expansion coefficients $c_j$ satisfy the recurrence relation

$$c_{j+2} = A_j(\alpha)c_{j+1} + B_j(\alpha, \beta)c_j, \quad j = -1, 0, 1, 2, \ldots, \quad c_{-1} = 0, \quad c_0 = 1,$$

$$A_j(\alpha) = \frac{2\alpha(j + l + 2) - j^2 - j(2l + 5) - 2(2l + 3)}{(j + 2)(j + 2l + 3)},$$

$$B_j(\alpha, \beta) = \frac{2\alpha(j + l + 2) - \beta}{(j + 2)(j + 2l + 3)}.$$  \hspace{1cm} (6)

We obtain exact eigenvalues and eigenfunctions if the truncation conditions $c_n \neq 0$, $c_{n+1} = c_{n+2} = 0$, $n = 0, 1, \ldots$, are satisfied by real positive values of $\alpha$ and $\beta$ because, in such a case, $c_j = 0$ for all $j > n$ and the series in Eq. (5) becomes a polynomial of degree $n$. These truncation conditions are equivalent to $B_n = 0$, $c_{n+1} = 0$, $n = 0, 1, \ldots$. The former gives us a simple relationship between $\alpha$ and $\beta$ and from the latter we obtain $\alpha$. The truncation conditions then reduce to

$$\beta = \alpha(n + l + 2), \quad c_{n+1} = 0, \quad n = 0, 1, \ldots,$$

and the coefficient $B_j(\alpha, \beta)$ takes a simpler form

$$B_j(\alpha, \beta) = B_j(\alpha) = \frac{2\alpha(j - n)}{(j + 2)(j + 2l + 3)}.  \hspace{1cm} (7)$$

For example, for $n = 0$ we obtain $\beta = l + 2$ and $\alpha = 1$ and the corresponding eigenfunction does not have nodes because $c_j = 0$ for all $j > 0$.

For $n = 1$ we have

$$\beta_i^{(1,i)} = \alpha_i^{(1,i)}(l + 3), \quad i = 1, 2,$$

$$\alpha_i^{(1,1)} = \frac{3\sqrt{l + 2} - \sqrt{l + 6}}{2\sqrt{l + 2}} < \alpha_i^{(1,2)} = \frac{\sqrt{l + 6} + 3\sqrt{l + 2}}{2\sqrt{l + 2}}.$$  \hspace{1cm} (8)
From the coefficients 

\[ c_{1,j}^{(1,1)} = \frac{\sqrt{l+2} - \sqrt{l+6}}{2\sqrt{l+2}}, \quad c_{1,j}^{(1,2)} = \frac{\sqrt{l+6} + \sqrt{l+2}}{2\sqrt{l+2}}, \]

we conclude that the ansatz \( f_1^{(1,1)}(r) \) has one node and \( f_1^{(1,2)}(r) \) is nodeless. This result is consistent with the fact that \( E_1^{(1,1)} > E_1^{(1,2)} \), where \( E_i^{(n,i)} = -\left[ \alpha_i^{(n,i)} \right]^2/2 \).

In general we obtain \( \beta_i^{(n,i)} = \alpha_i^{(n,i)}(n + l + 2), \quad n = 0, 1, \ldots, \quad i = 1, 2, \ldots, n + 1, \) which we arrange so that \( \alpha_i^{(n,i+1)} > \alpha_i^{(n,i)} \), and the corresponding eigenfunctions are given by

\[ f_1^{(n,i)}(r) = r^{l+1}(1 + r)e^{-\alpha_i^{(n,i)}r} \sum_{j=0}^{n} c_{j,l}^{(n,i)} r^j, \]

where \( f_1^{(n,i)}(r) \) has \( n + 1 - i \) nodes. It can be proved that all the roots of \( c_{n+1} = 0 \) are real, as was already done for other models [13–15].

The eigenvalues of the radial equation (4) are commonly labelled as \( E_{\nu,l} \), where \( \nu = 0, 1, \ldots \) in such a way that \( E_{\nu,l} < E_{\nu+1,l} \) from which we obtain the corresponding parameters \( \alpha_{\nu,l}(\beta) = \sqrt{-2E_{\nu,l}}. \) The question arises as to the relation between \( \alpha_l^{(n,i)} \) and \( \alpha_{\nu,l} \). It follows from the arguments given above that \( \left( \beta_l^{(n,i)}, \alpha_l^{(n,i)} \right) \) is a point on the curve \( \alpha_{\nu,l}(\beta) \) for \( \nu = n + 1 - i. \)

Figure 1 shows some values of \( \alpha \) calculated from the truncation condition with \( l = 0 \) (red circles) and suitable continuous lines that connect points on the curves \( \alpha_{\nu,0}, \nu = 0, 1, \ldots, 8. \) Numerical values of \( \alpha_{\nu,0} \), obtained by means of the Riccati-Padé method (RPM) [16] for \( \beta = 40 \), marked by crosses, appear on the blue lines between red circles confirming the argument put forward above. Notice that \( E_{\nu,l} \) decreases with \( \beta \) in agreement with the Hellmann-Feynman theorem [17].

![Fig. 1 Eigenvalues \( \alpha_{\nu,0}, \nu = 0, 1, \ldots, 8. \) obtained from the truncation condition (red circles) and numerically (blue crosses) (Color figure online)](image_url)
and, consequently, $\alpha_{l,j}$ increases with this parameter.

Figure 2 shows values of $a_{l,j}$ for $l = 0, 1, \ldots, 9$ connected by blue lines along every curve $a_{0,l}(\beta)$. For every value of $\beta$ $a_{0,l}$ decreases with $l$.

In the case of the Coulomb problem ($r_0 = 0$, or $\beta = 0$) all $\alpha_{v,k}$, $v = 0, 1, \ldots, k$ are identical because the energy depends on $v + l$. The curves $\alpha_{v,2-v}(\beta)$, $v = 0, 1, 2$ and $\alpha_{v,3-v}(\beta)$, $v = 0, 1, 2, 3$ in Fig. 3 shows how the cut off removes this degeneracy.

The continuous lines in Figs. 1, 2 and 3 are just straight lines that connect pairs of points given by the truncation condition (7). In principle, one can obtain

$$\frac{dE}{d\beta} = -\left\langle \frac{1}{r + 1} \right\rangle,$$

and

Figure 3 shows the relationship between $\alpha$ and $\beta$ for different values of $l$.
reasonably accurate values of \( \alpha \) between those points by suitable interpolation; for example Lagrange interpolation. Using 21 exact points of the curve \( \alpha_{0,0}(\beta) \) obtained from the truncation condition we estimate \( \alpha^{TC}_{0,0}(40) = 6.856 \) while the accurate numerical RPM result is \( \alpha^{RPM}_{0,0} = 6.854786377 \). This accuracy is obviously sufficient for any physical application of such a simple model.

4 Conclusions

The truncated Coulomb model (1) is quasi-sovable (or conditionally solvable) because we can only obtain eigenvalues and eigenfunctions exactly for some values of the model parameter \( \beta \). However, if we arrange the roots \( \beta^{(n,i)}_l, \alpha^{(n,i)}_l \), provided by the truncation condition, judiciously we derive useful information about the spectrum of the problem. For example, we can obtain sufficiently accurate curves \( \alpha_{r,j}(\beta) \) or \( E_{r,j}(\beta) \) by simple and straightforward interpolation of the points given by the truncation condition (7).

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