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Comment

Comment on: ‘PT-/non-PT-symmetric and non-Hermitian Hellmann potential: approximate bound and scattering states with any ℓ -values’

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Abstract

We carry out an analysis of the paper published in Arda and Sever (2014 *Phys. Scr.* **89** 105204) and reveal several unclear points. In the first place, the derivation of the main equations does not appear to be correct. In the second place, the expression for the energy does not appear to yield the results reported by the authors. In the third place, they failed to indicate the references reporting the eigenvalues chosen for comparison. In the fourth place the eigenvalues reported by the authors do not show the same order as those of the Hellmann potential thus leading to a different underlying physics. What is more: the spectrum of the modified model is qualitatively different from the one supported by the Hellmann potential.

Keywords: Hellmann potential, energies, analytical expression

Some time ago, Hellmann [1] proposed an approximation to the study of atoms in which the atomic kernel is treated by means of the Thomas–Fermi equation and the valence electrons by means of the Schrödinger one. In this way the author derived a simple potential for the valence electrons of the form $V(r) = -1/r + (A/r)e^{-2kr}$ in atomic units. This potential also proved suitable for the study of metallic binding [2].

In a recent paper Arda and Server [3] obtained approximate expressions for the eigenvalues and eigenfunctions of the Hellmann potential as well as for a non-Hermitian variant. They resorted to a suitable modification of the Coulomb interaction and the centrifugal part of the radial eigenvalue

equation in order to obtain an exactly solvable equation. Since the authors did not discuss the range of validity of the substitutions carried out we tried to fill this gap. However, when trying to reproduce their results we found several inconsistencies that we want to discuss in this comment.

The authors studied the Schrödinger equation with the Hellmann potential

$$V(r) = \frac{-a + be^{-\lambda r}}{r}. \quad (1)$$

The behaviour near the origin is given by $V(r) \approx (b - a)r^{-1}$ and at a great distance from the origin by $V(r) \approx -a/r$. Therefore, if $a > 0$ the attractive Coulomb tail at sufficiently large r supports an infinite number of bound states.

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The radial part of the Schrödinger equation is

$$\left\{ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} [E - V(r)] \right\} R(r) = 0, \quad (2)$$

where $l = 0, 1, \dots$ is the angular-momentum quantum number and the boundary conditions

$$\begin{aligned} R(0) &= 0 \\ \lim_{r \rightarrow \infty} R(r) &= 0 \end{aligned} \quad (3)$$

apply to the bound states.

In order to solve the equation analytically the authors carried out the following substitutions

$$\frac{1}{r} \rightarrow \frac{\lambda}{1 - e^{-\lambda r}}, \quad \frac{1}{r^2} \rightarrow \frac{\lambda^2}{(1 - e^{-\lambda r})^2} \quad (4)$$

that have already been used by other authors in the past [4–6]. It follows from the Taylor expansions

$$\begin{aligned} \frac{\lambda}{1 - e^{-\lambda r}} &= \frac{1}{r} + \frac{\lambda}{2} + \frac{\lambda^2 r}{12} - \dots \\ \frac{\lambda^2}{(1 - e^{-\lambda r})^2} &= \frac{1}{r^2} + \frac{\lambda}{r} + \frac{5\lambda^2}{12} + \frac{\lambda^3 r}{12} + \dots \end{aligned} \quad (5)$$

that the errors increase with λ .

By means of the ansatz

$$\psi(u) = R(-\ln(u)/\lambda) = u^{\lambda_1} (1 - u)^{\lambda_2} F(u) \quad (6)$$

Arda and Sever obtained a differential equation for $F(u)$. Since the transformation $u = e^{-\lambda r}$ maps $0 \leq r < \infty$ onto $1 \geq u > 0$ the exponents λ_1 and λ_2 should be positive in order to have a solution that satisfies both boundary conditions. In order to obtain a suitable differential equation the authors chose

$$\begin{aligned} \lambda_1^2 &= \frac{2m}{\lambda^2 \hbar^2} (E + a\lambda) + l(l+1) \\ \lambda_2 &= \frac{1}{2} \left[1 \pm \sqrt{1 + 4l(l+1)} \right] \end{aligned} \quad (7)$$

but, curiously, did not specify the sign of these parameters. As argued previously both should be positive.

The authors stated that the function $F(u)$ reduces to a polynomial when

$$\begin{aligned} -n &= \lambda_1 + \lambda_2 + \frac{1}{2} \sqrt{-\frac{8m}{\lambda^2 \hbar^2} (E + b\lambda)} \\ n &= 0, 1, \dots \end{aligned} \quad (8)$$

Since the left- and right-hand sides of this equation have opposite signs one concludes that there is no possible solution. However, from this equation the authors derived

Table 1. Eigenvalues of the radial equation (14) with $\lambda = 0.01$ and $b = 1$.

State	Present	[8]	[3]
1s	−0.2598520035	−0.25985	−0.26502
2s	−0.07192801595	−0.07193	−0.07760
2p	−0.07202032438	−0.07202	−0.07502
3s	−0.03656400027	−0.03656	−0.04300
3p	−0.03664789365	−0.03664	−0.04180
3d	−0.03681429863	−0.03681	−0.03947
4s	−0.02363657974	−0.02364	−0.03102
4p	−0.02371070818	−0.02371	−0.03031
4d	−0.02385702542	−0.02386	−0.02891
4f	−0.02407191089	−0.02407	−0.02690

the following expression for the energy

$$\begin{aligned} E &= -\frac{m}{8\hbar^2(n+l+1)^2} \left\{ 4(a^2 + b^2) \right. \\ &\quad + 4\frac{\hbar^2}{m}\lambda b \left[2l^2 + (n+l)^2 + l(3+2n) \right] \\ &\quad + \frac{\lambda^2 \hbar^4}{m^2} \left[l(1+2n) + (n+l)^2 \right]^2 \\ &\quad \left. + 4a \left[-2b + \frac{\lambda \hbar^2}{m} \left[l(1+2n) + (n+l)^2 \right] \right] \right\} \end{aligned} \quad (9)$$

that we rewrote in such a way that m and \hbar always appear in the ratio \hbar^2/m . In their table 1 the authors gave dimensionless values to the potential parameters a , b , and λ but did not specify the ratio \hbar^2/m . In order to test this expression they chose $\lambda = 0$, $\hbar = 1$ and obtained the hydrogenic energy levels

$$E = -\frac{ma^2}{2(n+l+1)^2} \quad (10)$$

but never specified the value of m . The authors made their paper even more unclear when in their table 1 chose $n \geq l+1$ instead of the quantum number indicated above in equation (9). When $n = l = 0$ the energy given by equation (9) becomes independent of λ in disagreement with the results in their table 1.

We could not reproduce the authors' results in the third column of their table 1 by trying some reasonable choices of \hbar^2/m in their expression (9). To make any analysis even more difficult the authors claimed to compare their results in table 1 with those of the references [11] and [28] of their paper (present references [1] and [7]). However, those references do not show any result for the eigenvalues of the Hellmann potential.

Some time ago Adamowski [8] calculated the eigenvalues of the Hamiltonian with the Hellmann potential

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{A}{r} + \frac{Be^{-Cr}}{r}, \quad (11)$$

where $A, C > 0$. This paper, which is useful for present purposes as shown below, was omitted by Arda and Sever [3].

It follows from the Hellmann–Feynman theorem

$$\frac{\partial E}{\partial C} = -B \langle e^{-Cr} \rangle \quad (12)$$

that

$$\begin{aligned} E(C \rightarrow \infty) < E < E(C = 0), \quad B > 0 \\ E(C = 0) < E < E(C \rightarrow \infty), \quad B < 0, \end{aligned} \quad (13)$$

where E is the energy of any bound-state solution to $H\psi = E\psi$. These bounds can be calculated exactly because the potential is Coulombic at both limits [8].

Adamowski chose the length and energy units $a_0 = \hbar^2/(mA)$ and $mA^2/(2\hbar^2)$, respectively. After separation of the angular part of the Schrödinger equation the remaining radial equation becomes

$$\left\{ -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2}{r} + \frac{b}{r}e^{-\lambda r} \right\} R(r) = ER(r), \quad (14)$$

where $b = 2B/A$ and $\lambda = a_0 C$. In this case the bounds derived above are

$$\begin{aligned} E(\lambda = 0) &= -\frac{(2-b)^2}{4\nu^2}, \quad \nu = 1, 2, \dots \\ E(\lambda \rightarrow \infty) &= -\frac{1}{2\nu^2}. \end{aligned} \quad (15)$$

Now that we have an equation derived in a clear way we are able to calculate its eigenvalues. Table 1 shows the eigenvalues of the radial equation (14) with $\lambda = 0.01$ and $b = 1$. From left to right the four columns display the states labelled as in the hydrogen atom, present results obtained by means of the Riccati–Padé method [9], the results of Adamowski [8], and those of Arda and Sever [3]. Although we do not know the value of m/\hbar^2 chosen by the latter authors or how they calculated their eigenvalues the column of results labelled *present* in their table 1 seems to match the other two ones quite satisfactorily. At first sight the approximate eigenvalues reported by Arda and Sever appear to agree reasonably well with those calculated accurately for equation (14). However, the order of the almost degenerate energy levels appears to be incorrect. If we denote the energy levels by $E_{\nu l}$, where $\nu = n + l + 1 = 1, 2, \dots$ is the principal quantum number, then we appreciate that the eigenvalues of (14) exhibit the order $E_{\nu l+1} < E_{\nu l}$ whereas the substitution (4) leads to the opposite order (assuming that the results of Arda and Sever were already calculated for the Hellmann potential with the substitutions indicated by equation (4)).

The Riccati–Padé method enables us to calculate the eigenvalues with much more accuracy than the one in table 1. We do not show more accurate results here because it is obviously unnecessary for present purposes.

Our original purpose of determining the range of validity of the substitutions (4) was hindered by the fact that we could

not reproduce the results of the authors' table 1 with the authors' analytical expression (9). However, we can easily show that the approximation is bound to fail for sufficiently large values of λ . The reason is that the modified Coulomb potential $-\frac{2\lambda}{1-e^{-\lambda r}}$ does not longer support an infinite number of bound states and, what is more, this number shrinks to none at some critical value of λ . The addition of the Hulthen-like potential $\frac{b\lambda e^{-\lambda r}}{1-e^{-\lambda r}}$ does not change this fact.

In conclusion: present analysis of the paper by Arda and Sever [3] reveals a number of unclear points. In the first place, it is not clear to us how they derived their expression for the bound states. In the second place, this expression does not appear to yield the eigenvalues shown in their table 1. In the third place, they failed to indicate the references reporting the eigenvalues used for comparison. One may give the authors the benefit of the doubt and assume that all such obscurities are merely due to misprints and typos. However, even in this case there remains the fact that the eigenvalues obtained by the authors for a given ν and different l exhibit the wrong order; in other words: the analytical formula describes the underlying physics incorrectly. In addition to it, the discrepancy between the eigenvalues calculated with the left and right expressions in (4) should increase with λ . This is probably the reason why the authors only showed results for quite small values λ . Our analysis above shows that the substitution (4) transforms a problem with an infinite number of bound states into one with a finite number. As λ increases the bound states of the modified model disappear one by one until a critical value is obtained beyond which there is no eigenvalue. This drastic change introduced by the substitution (4) was entirely omitted by the authors.

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