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Comment on ‘Approximate bound states solution of the Hellmann potential’

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Abstract

We analyse the eigenvalues of the Schrödinger equation with the Hellmann potential obtained by means of the generalized parametric Nikiforov–Uvarov (NU) method under the Greene–Aldrich approximation. We show that the NU eigenvalues yield the correct result when the screening parameter δ vanishes but their slope at $\delta = 0$ differs considerably from the exact one. In addition, the NU eigenvalues behave pathologically at large values of the radial quantum number n and it is necessary to restrict its values to $0 \leqslant n < n_{\max}$.

Keywords: Hellmann potential, Hellmann–Faynman theorem, Schrödinger equation, Nikiforov–Uvarov method, slope at origin

1. Introduction

In a paper published in this journal, Hamzavi *et al* [1] solved the Schrödinger equation with the Hellmann potential by means of the generalized parametric Nikiforov–Uvarov (NU) method and obtained analytical expressions for the eigenvalues and eigenfunctions. They compared their results with those coming from the amplitude phase method and also with a perturbation expansion [2] and concluded that the agreement was good. The purpose of this Comment is the analysis of the eigenvalues derived by Hamzavi *et al.*

In section 2 we analyze and discuss the results derived by Hamzavi *et al* and in section 3 we summarize our main results and draw conclusions.

2. Analysis of the expressions

Hamzavi *et al* [1] tried to solve the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi,$$
$$V(r) = -\frac{a}{r} + \frac{b}{r}\mathrm{e}^{-\delta r}, \qquad (1)$$

where m is the mass of the particle, $a > 0$, $\delta > 0$ and b can have any real value. This eigenvalue equation is separable in spherical coordinates. If we choose $\psi(r, \theta.\phi) = \frac{R(r)}{r} Y_l^m(\theta, \phi)$, where $Y_l^m(\theta, \phi)$ are the spherical harmonics and $l = 0, 1, \ldots, m = 0, \pm 1, \ldots \pm l$ are the angular-momentum quantum numbers, then the problem reduces to the radial equation

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right]R(r) = ER(r). \qquad (2)$$

It is worth noting that the authors omitted $\hbar$ in all their equations. The eigenvalues and eigenfunctions are commonly written as E_{nl} and $\psi_{nl}(r, \theta.\phi) = \frac{R_{nl}(r)}{r} Y_l^m(\theta, \phi)$, respectively, where $n = 0, 1, \ldots$ is the radial quantum number (the number of zeros of $R_{nl}(r)$ in the interval $0 < r < \infty$).

In order to apply the NU method the authors resorted to the Greene–Aldrich approximation

$$\frac{1}{r} \approx \frac{\delta}{1 - \mathrm{e}^{-\delta r}}, \quad \frac{1}{r^2} \approx \frac{\delta^2}{(1 - \mathrm{e}^{-\delta r})^2}, \qquad (3)$$

that is valid for $\delta r \ll 1$. In this way, they obtained the eigenvalues

$$E_{nl}^{\mathrm{NU}}(a, b, \delta) = -\delta^2 \left\{ \left[\frac{\frac{a-b}{\delta} - (n+l+1)^2 - l(l+1)}{2(n+l+1)} \right]^2 - l(l+1) + \frac{a}{\delta} \right\}, \qquad (4)$$

where we have set $2m = 1$ because in their calculations the

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authors claimed to have chosen units such that $\hbar = 2m = 1$ (although, as mentioned above, the authors omitted $\hbar$ from the very beginning). As expected, this expression yields the correct limit

$$\lim_{\delta\to 0} E_{nl}^{\mathrm{NU}}(a, b, \delta) = -\frac{(a-b)^2}{4(n+l+1)^2}. \tag{5}$$

Note that when $\delta = 0$ the Schrödinger equation with the potential $V(r) = -\frac{a-b}{r}$ supports bound states provided that $a > b$.

According to the Hellmann–Feynman theorem (HFT) [3, 4] we have

$$\frac{\partial E_{nl}}{\partial \delta} = -b\langle \mathrm{e}^{-\delta r}\rangle \begin{cases} <0 \text{ if } b > 0 \\ >0 \text{ if } b < 0 \end{cases}. \tag{6}$$

Hamzavi *et al* [1] did not pay attention (or forgot to mention) that in their table 2 $E_{nl}^{\mathrm{NU}}(a, b, \delta)$ decreases with δ in several cases with $b < 0$. This behavior can be considered to be pathological because it does not agree with the HFT (6) and it is probably caused by the Greene–Aldrich approximation

In particular,

$$\left.\frac{\partial E_{nl}}{\partial \delta}\right|_{\delta=0} = -b, \tag{7}$$

that we will call the slope at origin from now on. It is not difficult to verify that the slope at origin of the NU eigenvalues (4) is given by

$$\left.\frac{\partial E_{nl}^{\mathrm{NU}}}{\partial \delta}\right|_{\delta=0} = -\frac{a[l(2n+1)+n^2+2n+1]+b[2l^2+l(2n+3)+n^2+2n+1]}{2(l+n+1)^2}. \tag{8}$$

All the exact eigenvalues E_{nl} have the same slope at origin (7) but this quantity depends on n and l in the case of the NU eigenvalues (8). For example,

$$\begin{aligned} \lim_{\delta\to 0} \frac{\partial E_{n0}^{\mathrm{NU}}(2, -1, \delta)}{\partial \delta} &= -\frac{1}{2}, \\ \lim_{\delta\to 0} \frac{\partial E_{n0}^{\mathrm{NU}}(2, -2, \delta)}{\partial \delta} &= 0, \\ \lim_{\delta\to 0} \frac{\partial E_{n0}^{\mathrm{NU}}(2, -4, \delta)}{\partial \delta} &= 1. \end{aligned} \tag{9}$$

Although the NU eigenvalues yield the exact result when $\delta \to 0$ [because the Greene–Aldrich approximation (3) is exact] the slope at origin (8) differs considerably from the exact one (7).

When $b = 0$ the problem is exactly solvable and we can easily obtain the well known results for the Coulomb interaction. However, the authors' results in their table 3 are incorrect because of the use of the Greene–Aldrich approximation on $-a/r$.

The Schrödinger equation (1) has an infinite number of eigenvalues that satisfy

$$\lim_{n\to\infty} E_{nl} = 0, \tag{10}$$

but the NU eigenvalues behave in a completely different way

$$\lim_{n\to\infty} E_{nl}^{\mathrm{NU}} = -\infty. \tag{11}$$

It is clear that in the NU approximation we have to restrict the possible values of the radial quantum number to $0 \leqslant n < n_{\max}$, where $n_{\max}$ is given by

$$\left.\frac{\partial E_{nl}^{\mathrm{NU}}}{\partial n}\right|_{n=n_{\max}} = 0. \tag{12}$$

For a given set of values of a, b and δ, $n_{\max}$ depends on l.

The authors set $\hbar = 2m = 1$ and chose dimensionless values for a, b and δ but claimed that their results were given in units of $\mathrm{f\,m}^{-1}$ which is obviously nonsensical. Note that they compared their results with those of Ikhdair and Sever [2] who stated that their results were given in units of $\mu a^2/(2\hbar^2)$.

3. Conclusions

In the conclusions of their article Hamzavi *et al* [1] stated that 'the comparison with accurate numerical values clearly indicates the success of the analytic formalism'. However, they did not pay attention to the pathological behavior of E_{nl}^{NU} with respect to the screening parameter δ. Although the NU eigenvalues yield the correct result at $\delta = 0$ the slope at this point differs considerably from the exact one. In some cases the NU slope at origin exhibits a wrong sign. For this reason, the NU eigenvalues do not only exhibit the expected inaccuracy at large values of δ, due to the Greene–Aldrich approximation, but also their qualitative behavior is also incorrect at small values of δ. This fact limits considerably the range of applicability of the analytical expression (4). The authors also omitted a discussion about the number of bound states and we may add a comment about the surprising appearance of energy units $\mathrm{f\,m}^{-1}$.

References

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