Journal of Mathematical Chemistry
https://doi.org/10.1007/s10910-021-01308-5

LETTER TO THE EDITOR

Comment on "a new approach to solve the Schrödinger equation with an anharmonic sextic potential"

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Received: 2 November 2021 / Accepted: 9 November 2021

Abstract
We analyze a recent application of the Nikiforov-Uvarov (NU) method to an N -dimensional anharmonic oscillator with a central-field sextic potential-energy function. We show that most of the equations derived by the author exhibit errors (or typos) and that his interpretation of the results may not be correct. By means of the Frobenius (power-series) method we derive exact particular solutions to the Schrödinger equation and compare them with those coming from the NU method.

Keywords Sextic oscillator · NU method · Frobenius method · Conditionally-solvable model

1 Introduction

In a recent paper publish in this journal, Nanni[1] solved the Schr ödinger equation for an anharmonic oscillator with a central-field sextic potential by means of the Nikiforov-Uvarov (NU) method (which the author called Nikirov-Uvarov). According to the autor such a potential has been of interest for its role in the spectra of complex molecules as well as in chemical kinetics. The purpose of this Comment is the analysis of Nanni's results.

In Sect. 2 we outline Nanni's results and discuss their validity by means of well known theorems in applied mathematics and quantum physics and chemistry. In Sect. 3 we solve the problem by means of the well known power-series method of Frobenius[2]. Finally, in Sect. 4 we provide further comments and draw conclusions.

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Published online: 25 November 2021

2 Nanni's NU results

Nanni chose the Schrödinger equation

$$\left[-\frac{1}{2}\nabla^2 + U(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{1}$$

in N dimensions with the central-field sextic anharmonic potential

$$U(\alpha, \beta, \gamma, r) = \alpha r^6 + \beta r^4 + \gamma r^2, \tag{2}$$

and stated that "the requirement of constraint $\alpha > 0$ will be clarified below". It is clear that if $\alpha > 0$ there are bound states for all real values of β and γ. If $\alpha = 0$ there are bound states for all values of γ provided that $\beta > 0$. If $\alpha = \beta = 0$ there are bound states for all $\gamma > 0$. Nanni resorted to natural units such that $\hbar = 1$, $e = 1$ and $\mu = 1$, where μ is the reduced mass. Unfortunately, he did not explain the meaning of a reduced mass in the case of a complex molecule. Besides, we have recently criticized this unclear way of developing dimensionless Schrödinger equations[3].

We can obtain some valuable information about the behaviour of the eigenvalues of the Schrödinger equation (1) with the potential (2) without solving such equation. For example, the Hellmann-Feynman theorem[4, 5] states that

$$\frac{\partial E}{\partial \alpha} = \left\langle r^6 \right\rangle > 0, \ \frac{\partial E}{\partial \beta} = \left\langle r^4 \right\rangle > 0, \ \frac{\partial E}{\partial \gamma} = \left\langle r^2 \right\rangle > 0. \tag{3}$$

If we are not considering the case $\alpha = 0$ we can set $\alpha = 1$ without loss of generality[3]. However, we will keep this model parameter in our calculations in order to compare present results with those of Nanni.

The Schrödinger equation (1) with the central-field potential (2) is separable in hyperspherical coordinates and Nanni arrived at the eigenvalue equation

$$\begin{aligned} &\left[\frac{d^2}{dr^2} - \frac{4\delta^2 - 1}{4r^2} + 2\left(E - \alpha r^6 - \beta r^4 - \gamma r^2\right)\right] R(r) = 0, \\ &\delta = (l - 1 + N/2), \end{aligned} \tag{4}$$

for the radial factor $R(r)$, where l is the angular-momentum quantum number. Note that there is a missing factor 2 before the potential-energy function in Nanni's equation (16).

In order to apply the NU method Nanni resorted to the change of variables $s = (\alpha/2)^{1/4} r^2$ and derived his equation (17) that does not look correct because the term coming from γr^2 is missing. Besides, the β term also appears to be incorrect. After applying the NU method Nanni derived two equations, one that restricts the possible values of the model parameters

$$l - 1 + N/2 = \frac{\gamma}{(2\alpha)^{1/2}} + 2(n + 1) - \frac{\beta^2}{2(2\alpha)^{3/2}}, \tag{5}$$

and another one for the energy levels

$$E(n,l) = -\frac{\beta}{(2\alpha)^{1/2}}\left[n - (l - 1 + N/2) + 1\right]. \tag{6}$$

He concluded that "two consecutive energy levels are evenly spaced by $\Delta E(n+1,n) = \beta/(2\alpha)^{1/2}$". We may assume that n stands for the radial quantum number with values $n = 0, 1, \ldots$. First, Nanni's results do not apply to the case $\alpha = 0$ and, consequently, are not general (note that there are only two independent parameters because of equation (5)). Second, $\lim_{n\to\infty} E(n,l) = -\infty$ which is inconsistent with the fact that the potential $U(\alpha,\beta,\gamma,r)$ is bounded from below. Third, it is well known that the eigenvalues of the sextic potential behave asymptotically as $n^{3/2}$ for large n[6] (paper already cited by Nanni).

Nanni stated that the NU method "is simpler and more elegant than the wavefunction ansatz method" which attributed to Dong[7, 8]. The fact is that the latter approach is the well known Frobenius power-series method[2] that can be introduced in two or three lines while Nanni required a whole section to develop the main equations of the NU method. Of course, the use of adjectives like *simple* and *elegant* is a matter of taste.

The fact is that with the above-mentioned change of variables Nanni should have obtained an eigenvalue equation with Coulomb-like, linear and harmonic terms. Such quantum-mechanical models have been widely discussed, and also misinterpreted, as shown in recent papers[9–11] (and references therein). Nanni also misinterpreted equations (5) and (6). We are dealing with a conditionally-solvable quantum-mechanical model as shown by the following fact: from equation (5) you obtain, for example, $\gamma = \gamma_{n,l}(\alpha,\beta)$. Therefore, for given values of α and β the third parameter γ is completely determined in such a way that it depends on the integer number n and the angular momentum quantum number l. Consequently, the eigenvalues $E(n,\, l)$ are associated to different quantum mechanical problems $U(\alpha,\beta,\gamma_{n,l},r)$. This fact is characteristic of conditionally-solvable or quasi-solvable quantum-mechanical models (see, for example, the remarkable review by Turbiner[12], and the references therein, for more examples)

In what follows we apply the Frobenius method to the sextic oscillator outlined above.

3 Frobenius method

For simplicity we define

$$\xi^2 = \frac{4\delta^2 - 1}{4} = \frac{(2l + N - 1)(2l + N - 3)}{4}, \tag{7}$$

and write the radial equation as

$$
\begin{aligned}
R(r) =& r^s \exp\left(-ar^2 - br^4\right) \sum_{j=0}^{\infty} c_j r^{2j}, \\
s =& \frac{\sqrt{4\xi^2 + 1} + 1}{2},\ a = \frac{\beta}{2\sqrt{2\alpha}},\ b = \frac{\sqrt{2\alpha}}{4}.
\end{aligned}
\tag{8}
$$

A straightforward calculation shows that the expansion coefficients c_j satisfy the three-term recurrence relation

$$
\begin{aligned}
c_{j+2} =& A_j c_{j+1} + B_j c_j,\ j = 0, 1, \ldots,\ c_0 = 1, \\
A_j =& \frac{\beta(4j + 2s + 5) - 2\sqrt{2\alpha}E}{2\sqrt{2\alpha}(j + 2)(2j + 2s + 3)}, \\
B_j =& \frac{(2\alpha)^{3/2}(4j + 2s + 3) + 4\alpha\gamma - \beta^2}{4\alpha(j + 2)(2j + 2s + 3)}.
\end{aligned}
\tag{9}
$$

If $c_n \neq 0$, $c_{n+1} = c_{n+2} = 0$, $n = 0, 1, \ldots$, the infinite series in equation (8) reduces to a polynomial of degree n . These conditions require that $B_n = 0$ from which we obtain

$$
(2\alpha)^{3/2}(4n + 2s + 3) + 4\alpha\gamma - \beta^2 = 0, \tag{10}
$$

that resembles Nanni's equation (25) (or equation (5) above). Solving for γ and substituting the result into the expression for B_j we obtain

$$
B_j = \frac{2\sqrt{\alpha}(n - j)}{(j + 2)(2j + 2s + 3)}. \tag{11}
$$

For $n = 0$ we have

$$
\begin{aligned}
\gamma_{0,l} =& \frac{\beta^2}{4\alpha} - \frac{\sqrt{2\alpha}(2s + 3)}{2}, \\
E_l^{(0)} =& \frac{\beta(2s + 1)}{2\sqrt{2\alpha}}.
\end{aligned}
\tag{12}
$$

For a given set of values of α and β and l the truncation method yields an eigenvalue $E_l^{(0)}$ provided that $\gamma = \gamma_{0,l}$. Note that a change in the angular-momentum quantum number l gives rise to a different potential-energy function $U(\alpha, \beta, \gamma_{0,l}, r)$.

For $n = 1$ we obtain

$$\begin{aligned}
\gamma_{1,l} =& \frac{\beta^2}{4\alpha} - \frac{\sqrt{2\alpha}(2s+7)}{2}, \\
E_l^{(1,1)} =& \frac{\Delta + 2\sqrt{2\alpha^2(2s+1)^2 - \sqrt{2}\alpha\beta(2s+1)(2s+3) + \beta^2}}{2\sqrt{2\alpha}}, \\
E_l^{(1,2)} =& \frac{\Delta - 2\sqrt{2\alpha^2(2s+1)^2 + \sqrt{2}\alpha\beta(2s+1)(2s+3) + \beta^2}}{2\sqrt{2\alpha}}, \\
\Delta =& \beta(2s+3) - 2\sqrt{2}\alpha(2s+1).
\end{aligned} \tag{13}$$

For a given set of values of α, β and l the potential $U(\alpha, \beta, \gamma_{1,l}, r)$ supports two states with polynomial radial factors $R(r)$. In general, we obtain $\gamma_{n,l}$ from equation (10) and $n+1$ roots of $c_{n+1} = 0$: $E_l^{(n,i)}$, $i = 1, 2, \ldots, n+1$. It is worth stressing the fact that $E_l^{(n,i)}$ and $E_{l'}^{(n,i)}$ are eigenvalues of two different quantum-mechanical Hamiltonian operators with potentials $U(\alpha, \beta, \gamma_{n,l}, r)$ and $U(\alpha, \beta, \gamma_{n,l'}, r)$, respectively. We do not discuss this kind of solutions any longer because they have been studied in detail in two earlier papers for the case $N = 1$ [9] and $N = 2$[13] (see also [12] and references therein).

4 Conclusions

It is not clear whether the N-dimensional anharmonic oscillator with a central-field sextic potential-energy function exhibits any actual physical or chemical application. The results derived by Nanni and the conclusions drawn from them do not appear to be correct. The NU solutions resemble those that one obtains by other methods (like the Frobenius one) for conditionally-solvable or quasi-solvable quantum-mechanical problems. Such results are useful provided that one is able to arrange and connect them properly[9–11]. The misinterpretation of the exact polynomial solutions to quasi-solvable quantum-mechanical problems is not uncommon[9–11].

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