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COMMENT

Comment on ‘shape invariance and the supersymmetry WKB approximation for a diatomic molecule potential’

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Abstract

We comment on several incorrect results given in a recent paper by Jia and co-workers. In particular, it is pointed out that their discussion with the help of the shape invariance approach and the supersymmetry WKB approximation is wrong, since the superpotential $W(r) = -\frac{\hbar}{\sqrt{2\mu}}\left(\frac{P}{e^{\eta r} - \lambda} + Q\right)$ of the four-parameter diatomic molecule potential employed in their calculation is not suitable in the case where the deformation parameter λ is $\lambda < 0$ or $0 < \lambda < 1$. The correct results for the energy levels and wavefunctions can be obtained in standard quantum mechanics through resolution of Schrödinger’s equation by taking into account the different ranges of the shape parameter λ of the potential.

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In a recent paper, Jia and co-workers [1] have discussed by means of the shape-invariance approach and the supersymmetry WKB approximation the problem of a diatomic molecule subjected to a four-parameter potential $V(r)$ defined by

$$v(r) = \frac{2m}{\hbar^2} V(r) = \frac{a}{(e^{\eta r} - \lambda)^2} - \frac{b}{e^{\eta r} - \lambda}, \quad (1)$$

with a , b and η as the real positive constants given by $a = \frac{2m}{\hbar^2} D_e (e^\alpha - \lambda)^2$, $b = \frac{4m}{\hbar^2} D_e (e^\alpha - \lambda)$ and $\eta = \frac{\alpha}{r_e}$. D_e , r_e and λ are the depth of the potential well, the equilibrium distance of the two nuclei and the dimensionless deformation parameter, respectively, and α is a positive dimensionless parameter, m being the reduced mass of the molecule.

In this comment, we would like to point out numerous errors in the paper of Jia and co-workers cited above. On the one hand, by expecting the first equation in (10) of [1], we have two solutions for the parameter P without any condition on the sign of the deformation parameter λ . Therefore, the conditions on the sign of λ in their solutions are not necessary.

The radial wavefunction (11) in [1] defined by

$$R(r) = \frac{N}{r} (e^{\eta r} - \lambda)^{P/\eta\lambda} e^{(Q-P/\lambda)r} \quad (2)$$

is a physically acceptable solution for the ground state problem only if the boundary condition,

$$\lim_{r \rightarrow \infty} r R(r) = 0, \quad (3)$$

is satisfied. We see that solution (2) fulfils condition (3) when $Q < 0$. Then, if $P < 0$ and $Q < 0$, the second equation in (10) of [1] cannot be verified. In others words, the nonlinear Riccati equation (3) in [1] is not satisfied. In this case, one cannot cast the potential (1) into a supersymmetric form. Consequently, the solution

$$P = \frac{\eta\lambda - \sqrt{\eta^2\lambda^2 + 4a}}{2} \quad (4)$$

in (12) of [1] must be discarded.

On the other hand, in order to check the hermiticity of the radial momentum operator $P_r = \frac{\hbar}{i} \frac{\partial}{r \partial r} r$, let us suppose that r lies in the range (r_0, ∞) with $r_0 \geq 0$. Then

$$\begin{aligned} 0 &= \langle R, P_r R \rangle - \langle R, P_r R \rangle^* \\ &= 4\pi \int_{r_0}^{\infty} [R^*(r)(P_r R(r)) - (P_r R(r))^* R(r)] r^2 dr \\ &= 4\pi \frac{\hbar}{i} \int_{r_0}^{\infty} \left[\frac{\partial}{\partial r} |r R(r)|^2 \right] dr. \end{aligned} \quad (5)$$

Since $Q < 0$, $r R(r)$ vanishes as $r \rightarrow \infty$, the integral with respect to r is equal to its value at the point $r = r_0$. The operator P_r is not therefore Hermitian that if one restricts oneself to the wavefunction $R(r)$ which fulfils the condition

$$\lim_{r \rightarrow r_0} r R(r) = 0. \quad (6)$$

From this condition, it follows that

$$r_0 = \frac{1}{\eta} \ln \lambda \geq 0, \quad (7)$$

and consequently

$$\lambda \geq 1. \quad (8)$$

On the basis of the above remarks, it is clear that one can cast the potential (1) into a supersymmetric form only for $P > 0$, $Q < 0$ and $\lambda \geq 1$ contrary to the statement of the authors of [1].

As the shape-invariance approach and the supersymmetry WKB approximation are not convenient for handling the potential (1) whatever the signs of the parameters P and λ may be, we propose to deal with this diatomic molecule potential through the Schrödinger equation approach by considering all potential shapes determined by the parameter λ . If $\lambda = 0$, we have the ordinary Morse potential. In the case where $\lambda < 0$, the potential (1) may be called 'generalized Woods–Saxon potential' and 'generalized Hulthén potential' if $\lambda > 0$. Therefore, the potential function (1) represents three kinds of potentials according to the choice of λ . As the features of these potentials are quite different, it is clear that their treatment does not enable us to obtain their solutions in a unified manner. In what follows, we will be concerned in solving the Schrödinger equation

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \frac{2m}{\hbar^2} E - v(r) \right] R(r) = 0, \quad (9)$$

when the deformation parameter λ is positive or negative, separately.

First, for $\lambda < 0$, and $r \in \mathbb{R}^+$, the diatomic molecule potential (1) is a generalization of the Woods–Saxon potential. Substituting λ for $(-\lambda)$ in (1), that is to say the new parameter λ becomes positive, and introducing the new variable

$$y = \frac{\lambda}{e^{\eta r} + \lambda}, \tag{10}$$

the radial differential equation for $u(r) = rR(r)$ may be written as

$$\left[y(1-y) \frac{d^2}{dy^2} + (1-2y) \frac{d}{dy} + \frac{2mE}{\hbar^2 \eta^2} \frac{1}{y(1-y)} - \frac{a}{\lambda^2 \eta^2} \frac{y}{1-y} + \frac{b}{\lambda \eta^2} \frac{1}{1-y} \right] u(r) = 0. \tag{11}$$

To solve this differential equation, we introduce a new function $\varphi(y)$ through the relation

$$u(r) = y^{\nu}(1-y)^{\mu} \varphi(y). \tag{12}$$

If we impose on ν and μ the conditions

$$\nu = \sqrt{-\frac{2mE}{\hbar^2 \eta^2}}, \tag{13}$$

and

$$\mu = \sqrt{\frac{a}{\lambda^2 \eta^2} - \frac{b}{\lambda \eta^2} - \frac{2mE}{\hbar^2 \eta^2}}, \tag{14}$$

the following hypergeometric equation for $\varphi(y)$ is obtained:

$$\left[y(1-y) \frac{d^2}{dy^2} + [2\nu + 1 - (\alpha + \beta + 1)y] \frac{d}{dy} - \alpha\beta \right] \varphi(y) = 0, \tag{15}$$

where

$$\alpha = \nu + \mu + \frac{P}{\lambda \eta}, \quad \beta = \nu + \mu - \frac{P}{\lambda \eta} + 1, \tag{16}$$

and

$$\frac{P}{\lambda \eta} = \frac{1}{2} \left(1 + \sqrt{1 + \frac{4a}{\lambda^2 \eta^2}} \right). \tag{17}$$

The general solution of the differential equation (15) is then given by

$$\begin{aligned} \varphi(y) = & A_{12} F_1 \left(\nu + \mu + \frac{P}{\lambda \eta}, \nu + \mu - \frac{P}{\lambda \eta} + 1, 2\nu + 1; y \right) \\ & + A_2 y^{-2\nu} {}_2F_1 \left(\mu - \nu + \frac{P}{\lambda \eta}, \mu - \nu - \frac{P}{\lambda \eta} + 1, 1 - 2\nu; y \right). \end{aligned} \tag{18}$$

So

$$\begin{aligned} u(r) = & A_1 y^{\nu} (1-y)^{\mu} {}_2F_1 \left(\nu + \mu + \frac{P}{\lambda \eta}, \nu + \mu - \frac{P}{\lambda \eta} + 1, 2\nu + 1; y \right) \\ & + A_2 y^{-\nu} (1-y)^{\mu} {}_2F_1 \left(\mu - \nu + \frac{P}{\lambda \eta}, \mu - \nu - \frac{P}{\lambda \eta} + 1, 1 - 2\nu; y \right). \end{aligned} \tag{19}$$

Now, for $u(r)$ to be a physically acceptable solution of equation (11), it has to satisfy the boundary conditions

$$\lim_{r \rightarrow \infty} u(r) = 0, \tag{20}$$

and

$$u(0) = 0. \tag{21}$$

Also as $r \rightarrow \infty$, $y \rightarrow 0$ and $y^{-\nu} \rightarrow \infty$, the boundary condition (20) requires that $A_2 = 0$. Thus, according to (10), the solution of the radial Schrödinger equation (11) can be written as

$$u(r) = A_1 \left(\frac{e^{\eta r}}{\lambda} \right)^\mu \left(\frac{\lambda}{e^{\eta r} + \lambda} \right)^{\mu+\nu} {}_2F_1 \left(\nu + \mu + \frac{P}{\lambda\eta}, 1 + \nu + \mu - \frac{P}{\lambda\eta}, 2\nu + 1; \frac{\lambda}{e^{\eta r} + \lambda} \right), \quad (22)$$

where A_1 is a constant factor. Using the fact that the hypergeometric function in equation (22) tends to unity when $r \rightarrow \infty$, we obtain

$$u(r) \sim A_1 \lambda \sqrt{\frac{-2mE}{\hbar^2 \eta^2}} e^{-\sqrt{\frac{-2mE}{\hbar^2}} r}. \quad (23)$$

Thus, we have obtained the correct asymptotic behaviour. In order to get the possible energies for the bound states, we use the boundary condition (21). We realize that the solution (22) fulfils condition (21) when

$${}_2F_1 \left(\nu + \mu + \frac{P}{\lambda\eta}, 1 + \nu + \mu - \frac{P}{\lambda\eta}, 2\nu + 1; \frac{\lambda}{1 + \lambda} \right) = 0. \quad (24)$$

It follows that the energy levels can be found from a numerical solution of the transcendental equation (24).

On making the substitution $\lambda = q e^{\eta R}$ with $q > 0$ in expression (1), we obtain the following potential which is a special form of the deformed Woods–Saxon potential:

$$v_{WS}(r) = \frac{W_0}{(e^{\eta(r-R)} + q)^2} - \frac{V_0}{e^{\eta(r-R)} + q}, \quad (25)$$

where $V_0 = b e^{-\eta R}$, $W_0 = a e^{-2\eta R}$ and $\eta R \gg 1$. The parameter R is the nuclear radius and η^{-1} is the thickness of the surface layer.

In this case, we note that $\frac{\lambda}{1+\lambda} \simeq 1$ for $\eta R \gg 1$. Then, thanks to Gauss's transformation formula [2]

$$\begin{aligned} {}_2F_1(a, b, c; z) &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} {}_2F_1(a, b, a+b-c+1; 1-z) + (1-z)^{c-a-b} \\ &\times \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} {}_2F_1(c-a, c-b, c-a-b+1; 1-z), \end{aligned} \quad (26)$$

it is easy to show that the quantization condition for the bound states (24) takes the following form:

$$\frac{\Gamma(2\mu)\Gamma(1+\nu-\frac{P}{\lambda\eta}-\mu)\Gamma(\nu+\frac{P}{\lambda\eta}-\mu)}{\Gamma(-2\mu)\Gamma(1+\nu-\frac{P}{\lambda\eta}+\mu)\Gamma(\nu+\frac{P}{\lambda\eta}+\mu)} \left(\frac{e^{-\eta R}}{q} \right)^{-2\mu} = -1. \quad (27)$$

To simplify the discussion of this equation (27), we only consider the case where $\mu^2 < 0$, so that according to equation (14), μ turns out to be imaginary. Writing

$$\mu = i\beta, \quad (28)$$

and defining ϕ_1 , ϕ_2 and ψ as

$$\begin{cases} \phi_1 = \arg \Gamma \left(\nu + \frac{P}{\lambda\eta} + i\beta \right), \\ \phi_2 = \arg \Gamma \left(\nu - \frac{P}{\lambda\eta} + i\beta \right), \\ \psi = \arg \Gamma(2i\beta), \end{cases} \quad (29)$$

we can also express (27) in the form

$$\exp \left[2i\psi - 2i\phi_1 - 2i\phi_2 - 2i \arctan \left(\frac{\beta}{\nu - \frac{P}{\eta\lambda}} \right) \right] \left(\frac{e^{-\eta R}}{q} \right)^{-2i\beta} = -1. \quad (30)$$

This leads on to the quantization condition

$$\beta(\eta R + \ln q) + \psi - \phi_1 - \phi_2 - \arctan\left(\frac{\beta}{v - \frac{P}{\eta\lambda}}\right) = (2n + 1)\frac{\pi}{2}, \tag{31}$$

with $n = 0, 1, 2, 3, \dots$

If we make the replacements $a = 0$ and $q = 1$, the potential (25) turns to the standard Woods–Saxon potential [3]. The quantization condition can be deduced from equation (27),

$$\beta\eta R + \psi - 2\phi - \arctan\left(\frac{\beta}{v}\right) = (2n + 1)\frac{\pi}{2}, \tag{32}$$

where

$$\begin{cases} \beta = \frac{1}{\eta}\sqrt{V_0 + \frac{2mE}{\hbar^2}} \\ \phi = \arg \Gamma(v + i\beta), \\ \psi = \arg \Gamma(2i\beta), \end{cases} \tag{33}$$

and $n = 0, 1, 2, 3, \dots$. This last result is in agreement with that of the literature [3].

Now, for $\lambda > 0$, we have to inspect the variation of the potential $v(r)$ according to the values of the parameter λ . We must distinguish two cases. If $0 < \lambda < 1$, $v(r)$ is continuous on the whole interval \mathbb{R}^+ . But, if $\lambda \geq 1$, $v(r)$ has a strong singularity at the point $r = r_0 = \frac{1}{\eta} \ln \lambda$, and in this case, we have two distinct regions, one is defined by the interval $]0, r_0[$ and the other by the interval $]r_0, \infty[$. This leads us to deal with the Schrödinger equation for this potential in each case.

Consider first the case in which $\lambda \geq 1$. In this case, we will discuss the potential (1) only in the interval $]r_0, \infty[$ since, in the other interval, the solution cannot be analytically found.

Changing the independent variable r in (9) to y given by

$$y = \lambda e^{-\eta r},$$

the radial differential equation for $u(r) = rR(r)$ becomes

$$\left[y^2 \frac{d^2}{dy^2} + y \frac{d}{dy} + \frac{2mE}{\hbar^2 \eta^2} - \frac{a}{\eta^2 \lambda^2} \frac{y^2}{(1-y)^2} + \frac{b}{\eta^2 \lambda} \frac{y}{1-y} \right] u(r) = 0. \tag{34}$$

Introducing a new function $\varphi(y)$ defined by the relation

$$u(r) = y^\nu (1-y)^\mu \varphi(y), \tag{35}$$

and using the notation

$$\begin{cases} \nu = \sqrt{-\frac{2mE}{\hbar^2 \eta^2}}, & \mu = \frac{P}{\eta\lambda} = \frac{1}{2} \left(1 + \sqrt{1 + \frac{4a}{\eta^2 \lambda^2}} \right), \\ \varepsilon = \sqrt{\nu^2 + \frac{a}{\eta^2 \lambda^2} + \frac{b}{\eta^2 \lambda}}, & \alpha' = \nu + \frac{P}{\eta\lambda} + \varepsilon, & \beta' = \nu + \frac{P}{\eta\lambda} - \varepsilon, \end{cases} \tag{36}$$

we obtain from (34) the hypergeometric differential equation

$$\left[y(1-y) \frac{d^2}{dy^2} + [2\nu + 1 - (\alpha' + \beta' + 1)y] \frac{d}{dy} - \alpha' \beta' \right] \varphi(y) = 0. \tag{37}$$

The general solution of this equation can be written in the form

$$\begin{aligned} \varphi(y) = & B_1 {}_2F_1\left(\frac{P}{\lambda\eta} + \nu + \varepsilon, \frac{P}{\lambda\eta} + \nu - \varepsilon, 2\nu + 1; y\right) \\ & + B_2 y^{-2\nu} {}_2F_1\left(\frac{P}{\lambda\eta} - \nu + \varepsilon, \frac{P}{\lambda\eta} - \nu - \varepsilon, 1 - 2\nu; y\right). \end{aligned} \tag{38}$$

To find the physically acceptable solution of (34), we have to impose the boundary conditions

$$\lim_{r \rightarrow r_0} u(r) = 0, \quad (39)$$

and

$$\lim_{r \rightarrow \infty} u(r) = 0. \quad (40)$$

Also as $r \rightarrow \infty$, $y \rightarrow 0$ and $y^{-\nu} \rightarrow \infty$, the boundary condition (40) requires that $B_2 = 0$. Thus both boundary conditions will be satisfied if we choose $B_2 = 0$ and $\frac{P}{\lambda\eta} + \nu + \varepsilon = -n_r$ ($n_r = 0, 1, 2, \dots$). The possible energies for the bound states are then given by

$$E_{n_r} = -\frac{\hbar^2}{2m} Q^2, \quad (41)$$

and by using (26) the corresponding normalized wavefunctions can be expressed in the form

$$u_{n_r}^{\lambda \geq 1}(r) = \left[-\frac{2Q(P + n_r\lambda\eta - \lambda Q)}{(P + n_r\lambda\eta)} \frac{\Gamma(n_r + \frac{2P}{\eta\lambda})\Gamma(n_r + \frac{2P}{\eta\lambda} - \frac{2Q}{\eta})}{n_r!\Gamma(n_r - \frac{2Q}{\eta} + 1)} \right]^{\frac{1}{2}} \\ \times \frac{1}{\Gamma(\frac{2P}{\eta\lambda})} (1 - \lambda e^{-\eta r})^{\frac{P}{\eta\lambda}} (\lambda e^{-\eta r})^{-\frac{Q}{\eta}} {}_2F_1\left(-n_r, n_r + \frac{2P}{\eta\lambda} - \frac{2Q}{\eta}, \frac{2P}{\eta\lambda}; 1 - \lambda e^{-\eta r}\right), \quad (42)$$

with

$$Q = \frac{(P + n_r\lambda\eta)^2 - a - \lambda b}{2\lambda(P + n_r\lambda\eta)}. \quad (43)$$

We realize that (42) fulfils condition (40) when

$$Q < 0. \quad (44)$$

Therefore, it is seen from (43) and (44) that

$$n_r < \left\lfloor \frac{\sqrt{a + \lambda b} - P}{\eta\lambda} \right\rfloor. \quad (45)$$

Here $\{k\}$ denotes the largest integer inferior to k .

Consider now the case in which $0 < \lambda < 1$. The analysis presented above holds; but in this case, we prefer to introduce the new variable $y = 1 - \lambda e^{-\eta r}$. Similarly, by using the boundary conditions $u(0) = 0$ and $\lim_{r \rightarrow \infty} u(r) = 0$, we show that the solution of the radial differential equation has the form

$$u(r) = C_1 (1 - \lambda e^{-\eta r})^{\frac{P}{\eta\lambda}} (\lambda e^{-\eta r})^\nu {}_2F_1\left(\frac{P}{\lambda\eta} + \nu + \varepsilon, \frac{P}{\lambda\eta} + \nu - \varepsilon; 2\frac{P}{\lambda\eta}; 1 - \lambda e^{-\eta r}\right), \quad (46)$$

where C_1 is a constant factor. Then, the energy spectrum can be found from a numerical solution of the transcendental equation

$${}_2F_1\left(\frac{P}{\lambda\eta} + \nu + \varepsilon, \frac{P}{\lambda\eta} + \nu - \varepsilon, 2\frac{P}{\lambda\eta}; 1 - \lambda\right) = 0. \quad (47)$$

In conclusion, the shape-invariance approach and the supersymmetry WKB approximation employed by Jia and co-workers are shown inappropriate since only one of their solutions remains valid when $\lambda \geq 1$ and in the interval $\left[\frac{1}{\eta} \ln \lambda, \infty\right]$. The previous analysis reveals that the diatomic molecule potential cannot be cast in the supersymmetric quantum mechanics formalism whatever the parameter λ may be.

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