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# Shape-invariance approach and Hamiltonian hierarchy method on the Woods–Saxon potential for $\ell \neq 0$ states

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**Abstract**    An analytically solvable Woods–Saxon potential for $\ell \neq 0$ states is presented within the framework of Supersymmetric Quantum Mechanics formalism. The shape-invariance approach and Hamiltonian hierarchy method are included in calculations by means of a translation of parameters. The approximate energy spectrum of this potential is obtained for $\ell \neq 0$ states, applying the Woods–Saxon square approximation to the centrifugal barrier term of the Schrödinger equation.

**Keywords**    Supersymmetric quantum mechanics · Hamiltonian hierarchy method ·
Woods–Saxon potential · Diatomic molecules

## 1 Introduction

Introductory courses in quantum chemistry have been refrained from dealing with more than single particle considerations, since the molecular problems have been considerably complex in chemical structures. A systematic method which is used for fitting Rydberg-Klein-Rees (RKR) data with polynomial expressions for instance has been introduced to study the potential energy curve of a diatomic molecule in large internuclear distances [1]. In addition, the Hill determinant method has been developed for constructing potential energy curves of diatomic molecules [2]. In this method, the

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Dunham and the perturbed Morse oscillator potentials have been used to fit spectro-scopic data. An algebraic procedure based on a Bogoliubov transformation has been derived to generalize anharmonic oscillator wave functions [3]. The dynamical Lie algebraic approach has been applied to investigate the energy transfer in the collinear collision between an atom and an anharmonic oscillator [4]. Recently, the number of exact solutions presented on these types of topics have been increased by using various methods and potentials [5–9]. The supersymmetric quantum mechanics (SQM) is one of the best frameworks used to determine energy eigenvalues and eigenfunctions of quantum mechanical problems. The SQM has been appeared about 25 years ago and has been considering as a new field of research, providing not only a supersymmetric interpretation of the Schrödinger equation but also important contributions to a vari-ety of non-relativistic quantum mechanical problems [10]. One of the most important approaches in the SQM has been presented by Gendenshtein who was introduced a discrete parametrization approach which was labelled "shape-invariance" approach [11]. The validity of this approach has been attempted by using the shape-invariance potentials and their exact energy levels have been found analytically by making use of the shape-invariance approach [12,13].

The association of factorization and hierarchy of Hamiltonian methods with the SQM formalism is applied to obtain the approximate energy spectra of non-exactly solvable [14,15], the isospectral [16], the periodic [17] and the exponential types of potentials [18,19]. Using the physical arguments, it is possible to make an *ansatz* for the superpotential which satisfies the Riccati equation. Therefore, the Riccati equation is solved to create a superpotential. These steps are successfully used to obtain the energy spectra of the chemical systems which are well-fitted by exponential types of potentials.

In this article, an analytically solvable effective potential model through the SQM formalism is presented by using the shape-invariance approach and the hierarchy of Hamiltonian method. The potential is selected as the Woods–Saxon which is one of the exponential types of potentials. After having introduced the SQM formalism briefly in the Sect. 2, the Woods–Saxon potential and its shape-invariance properties are inves-tigated for a general situation. The Woods–Saxon square approximation is applied to the centrifugal barrier term of the Schrödinger equation under the condition of the first-term approximation. The obtained results are compared with those of the shape-invariance approach. A set of the energy eigenvalues is obtained for $\ell \neq 0$ states. Finally, the energy spectrum obtained by means of the SQM formalism is discussed at the end of paper.

## 2 Supersymmetric quantum mechanics

The simplest way of generating a new exactly solvable Hamiltonian is to consider an invertible bounded operator. In this case, a given Hamiltonian and its supersymmetric partner possess an identical spectra which is excepted the zero energy of ground state. In the SQM formalism, we have two nilpotent operators, $Q$ and $Q^+$, satisfying the following algebras

$$\{Q, Q^+\} = H_S, \quad \{Q, Q\} = \{Q^+, Q^+\} = 0, \tag{1}$$

where $H_S$ is the supersymmetric Hamiltonian. Therefore, the supercharges $Q$ and $Q^+$ commute with $H_S$ which is responsible for the degeneracy. This algebra can be realized as follows

$$Q = \begin{pmatrix} 0 & 0 \\ A^- & 0 \end{pmatrix}, \quad Q^+ = \begin{pmatrix} 0 & A^+ \\ 0 & 0 \end{pmatrix}, \tag{2}$$

where $A^\pm$ are bosonic operators. Beginning with this realization, the supersymmetric Hamiltonian $H_S$ is given by

$$H_S = \begin{pmatrix} A^+ A^- & 0 \\ 0 & A^- A^+ \end{pmatrix} = \begin{pmatrix} H^- & 0 \\ 0 & H^+ \end{pmatrix}. \tag{3}$$

$H^\pm$ are called supersymmetric partner Hamiltonians (see Ref. [10] for a review),

$$E_\nu^{(+)} = E_{\nu+1}^{(-)}. \tag{4}$$

In the case of the non-spontaneously broken supersymmetry, this lowest level is of the zero energy, $E_1^{(-)} = 0$. The Schrödinger equation for a particle of mass $m$ in a spherically symmetric potential is written

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) \right] \Psi(r) = E\Psi(r), \tag{5}$$

where $\Psi(r)$ is the wave function, $V(r)$ is the potential and $E$ is the energy. In the Hamiltonian form, this equation is given as

$$H^\pm = -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_\pm(r) = A^\mp A^\pm, \tag{6}$$

where $V_\pm(r)$ are called partner potentials. The operators $A^\pm$ are defined in terms of the superpotential $W(r)$

$$A^\pm = \mp \frac{\hbar}{\sqrt{2m}} \frac{d}{dr} + W(r), \tag{7}$$

which satisfies the Riccati equation as a consequence of the factorization of the Hamiltonians $H^\pm$;

$$W^2 \pm \frac{\hbar}{\sqrt{2m}} W' = V_\pm(r). \tag{8}$$

If $V_+(r)$ and $V_-(r)$ have similar shapes, they are said to be shape-invariant, and they satisfy the following relation

$$V_+(r, a_1) = V_-(r, a_2) + R(a_2), \tag{9}$$

where $a_1$ denotes a set of parameters and $a_2$ is a function of $a_1$ ($a_2 = f(a_1)$). Moreover, $R(a_2)$ is independent of $r$. For a given Hamiltonian $H_1$, it is possible to construct its hierarchy of Hamiltonians. In this case, we have

$$H_1 = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_1(r) = A_1^+ A_1^- + E_0^{(1)}, \tag{10}$$

where $E_0^{(1)}$ is the ground state eigenvalue of $V_1(r)$. The bosonic operators are defined by Eq. 7 whereas the superpotential $W_1(r)$ satisfies the Riccati equation as follows

$$W_1^2 - \frac{\hbar}{\sqrt{2m}}W_1' = V_1(r) - E_0^{(1)}. \tag{11}$$

The unnormalized energy eigenfunction for the lowest state is related to the superpotential $W_1$;

$$\Psi_0^{(1)}(r) = N \exp\left(-\frac{\sqrt{2m}}{\hbar}\int_0^r W_1(\bar{r})d\bar{r}\right), \tag{12}$$

where $N$ is the normalization constant. On the other hand, the supersymmetric partner Hamiltonian is given by

$$H_2 = A_1^- A_1^+ + E_0^{(1)} = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \left(W_1^2 + \frac{\hbar}{\sqrt{2m}}W_1'\right) + E_0^{(1)}. \tag{13}$$

Thus, $H_2$ is obtained in terms of a new pair of bosonic operators, $A_2^\pm$,

$$H_2 = A_2^+ A_2^- + E_0^{(2)} = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \left(W_2^2 - \frac{\hbar}{\sqrt{2m}}W_2'\right) + E_0^{(2)}, \tag{14}$$

where $E_0^{(2)}$ is the lowest eigenvalue of $H_2$ and $W_2$ satisfy the Riccati equation

$$W_2^2 - \frac{\hbar}{\sqrt{2m}}W_2' = V_2(r) - E_0^{(2)}. \tag{15}$$

The hierarchy of Hamiltonians is constructed with a simple relation, connecting the eigenvalues and eigenfunctions of the $\nu$-members [10],

$$E_\nu^{(1)} = E_0^{(\nu+1)}, \tag{16}$$

$$H_\nu = A_\nu^+ A_\nu^- + E_0^{(\nu)}, \tag{17}$$

$$A_\nu^\pm = \mp \frac{\hbar}{\sqrt{2m}} \frac{d}{dr} + W_\nu(r), \tag{18}$$

$$\Psi_\nu^{(1)} = A_1^+ A_2^+ \ldots A_\nu^+ \psi_0^{(\nu+1)} \tag{19}$$

where $\Psi_0^{(1)}(r)$ is given by Eq. 12. With the help of Eqs. 16–19, we can work out the energy eigenvalues and eigenfunctions for the shape-invariance potentials. To clarify the shape-invariance approach, we will explicitly compute the energy eigenvalues for the Woods–Saxon potential ($\ell \neq 0$ states).

## 3 Woods–Saxon potential and its shape-invariance property

We consider the following potential which consists of the well-known Woods–Saxon and its square form

$$V(r) = -\frac{V_0}{1 + e^{\left(\frac{r-R_0}{a}\right)}} + \frac{C}{\left(1 + e^{\left(\frac{r-R_0}{a}\right)}\right)^2}. \tag{20}$$

As a definition of the potential, the first term on the right-hand side of Eq. 20 denotes the volume Woods–Saxon potential and the second one represents a potential which corresponds to the square of first term, where $r$ is the center-of-mass distance. $R_0$ is the width of the potential, $V_0$ is the potential depth, $a$ is the diffuseness parameter and lastly $C$ is the setting parameter which is proposed by us ($C > 0$). In our calculations, we used a different form of the potential that the numerators and denominators of Eq. 20 are multiplicand by $exp[-(r - R_0)/a]$;

$$V_1(r) \equiv V(r) = -\frac{V_0 e^{-\left(\frac{r-R_0}{a}\right)}}{1 + e^{-\left(\frac{r-R_0}{a}\right)}} + \frac{C\, e^{-2\left(\frac{r-R_0}{a}\right)}}{\left(1 + e^{-\left(\frac{r-R_0}{a}\right)}\right)^2}. \tag{21}$$

The Schrödinger equation for diatomic molecules with the Woods–Saxon potential and its squared form is written as

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi_{n\ell m}(\mathbf{r}) + V(r)\Psi_{n\ell m}(\mathbf{r}) = E\Psi_{n\ell m}(\mathbf{r}), \tag{22}$$

and the Hamiltonian hierarch method is used to find a solution of Eq. 22. As a wave equation with spherically symmetric potential, Eq. 22 can be separated in spherical coordinates to give

$$\Psi_{n\ell m}(\mathbf{r}) = \frac{1}{r}\chi_{n\ell}(r)Y_{\ell m}(\theta, \phi), \tag{23}$$

where $\chi_{n\ell}(r)$ is a radial wave function whereas $Y_{\ell m}(\theta, \phi)$ is a spherical harmonics with angular momentum quantum numbers $\ell$ and $m$ ($n$ is commonly called the principle quantum number). We can then obtain the radial Schrödinger equation for all of the angular momentum states

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\chi_{nl}(r) + \left(V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right)\chi_{n\ell}(r) = E\chi_{n\ell}(r) \tag{24}$$

by putting Eq. 23 into Eq. 22. As a generalization of the potential given in Eq. 21, it is substituted into the Schrödinger equation for the zero angular momentum states;

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\chi_n(r) + V(r)\chi_n(r) = E\chi_n(r). \tag{25}$$

Substituting the ground state eigenfunction $\chi_0(r)$ ($n = 0$) into Eq. 25, we obtain

$$W_1^2 - \frac{\hbar}{\sqrt{2m}}\frac{dW_1}{dr} = V(r) - E_0^{(1)}, \tag{26}$$

where $E_0^{(1)}$ is the lowest energy-eigenvalue or the ground state energy. Through the superalgebra, we take superpotential

$$W_1 = -\frac{\hbar}{\sqrt{2m}}\left(S_1 + S_2\frac{e^{-\alpha(r-R_0)}}{1 + e^{-\alpha(r-R_0)}}\right), \tag{27}$$

satisfies the associated Riccati equation (Eq. 11) and substituting this expression into Eq. 26, we find the following identity

$$\frac{\hbar^2 S_1^2}{2m} + \frac{\hbar^2(2S_1S_2 - \alpha S_2)}{2m\left(1 + e^{\alpha(r-R_0)}\right)} + \frac{\hbar^2(S_2^2 + \alpha S_2)}{2m\left(1 + e^{\alpha(r-R_0)}\right)^2}$$
$$= -\frac{V_0}{1 + e^{\left(\frac{r-R_0}{a}\right)}} + \frac{C}{\left(1 + e^{\left(\frac{r-R_0}{a}\right)}\right)^2} - E_0^{(1)}. \tag{28}$$

With the comparison of the each side of the Eq. 28, we obtain

$$\alpha = 1/a,$$
$$\frac{\hbar^2 S_1^2}{2m} = -E_0^{(1)},$$
$$\frac{\hbar^2}{2m}(2S_1 S_2 - \alpha S_2) = -V_0,$$
$$\frac{\hbar^2}{2m}(S_2^2 + \alpha S_2) = C. \tag{29}$$

The solution of Eq. 29 yields

$$S_1 = \frac{U}{2S_2} - \frac{S_2}{2}, \tag{30}$$

$$S_2 = -\frac{\alpha}{2} \pm \sqrt{\left(\frac{\alpha}{2}\right)^2 + \frac{2mC}{\hbar^2}}, \tag{31}$$

where $U = \frac{2m}{\hbar^2}(C - V_0)$. It is seen from Eq. 31 that $S_2$ has two roots because of the sign in front of the square root term in the second part of the expression. We selected however the positive-sign one in calculations because this selection would of course be a right choice to ensure the well-behaved nature of the eigenfunction at the origin and the infinity. After from this point, the supersymmetric partner potentials can be expressed by using Eq. 27. First, we substituted Eqs. 30 and 31 into Eq. 27, and then solved Eq. 8 for both $V_+(r)$ and $V_-(r)$. Consequently, these partner potentials are obtained as follows

$$V_+(r) = \frac{\hbar^2}{2m}\left[S_1^2 + \frac{U - S_2^2}{1 + e^{\alpha(r-R_0)}} + \frac{S_2^2}{\left(1 + e^{\alpha(r-R_0)}\right)^2} + \frac{\alpha S_2}{1 + e^{\alpha(r-R_0)}}\right.$$
$$\left. - \frac{\alpha S_2}{\left(1 + e^{\alpha(r-R_0)}\right)^2}\right], \tag{32}$$

$$V_-(r) = \frac{\hbar^2}{2m}\left[S_1^2 + \frac{U - S_2^2}{1 + e^{\alpha(r-R_0)}} + \frac{S_2^2}{\left(1 + e^{\alpha(r-R_0)}\right)^2} - \frac{\alpha S_2}{1 + e^{\alpha(r-R_0)}}\right.$$
$$\left. + \frac{\alpha S_2}{\left(1 + e^{\alpha(r-R_0)}\right)^2}\right]. \tag{33}$$

The shape-invariance approach given in Eq. 9 can be written from Eqs. 32 and 33

$$V_+(r, S_2) = V_-(r, S_2 - \alpha) + \frac{\hbar^2}{2m} \left[ \left( \frac{U}{2S_2} - \frac{S_2}{2} \right)^2 - \left( \frac{U}{2(S_2 - \alpha)} - \frac{S_2 - \alpha}{2} \right)^2 \right].$$

$$(34)$$

The shape-invariance approach which was introduced by Gendenshtein [11] is therefore precisely provided by comparing Eq. 9 with Eq. 34 and using the transformation of parameters $S_2 \to a_1$, $S_2 - \alpha \to a_2$,

$$R(a_2) = \frac{\hbar^2}{2m} \left[ \left( \frac{U}{2a_1} - \frac{a_1}{2} \right)^2 - \left( \frac{U}{2a_2} - \frac{a_2}{2} \right)^2 \right]. \tag{35}$$

On repeatedly using the shape-invariance approach, it is then clear that we can form a set of Hamiltonians in terms of $k$,

$$H^{(k)} = -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_-(r; a_k) + \sum_{s=1}^{k} R(a_s), \tag{36}$$

where $H^{(k)}$ is a series of Hamiltonians, $k = 1, 2, 3, \ldots$, and $H^{(1)} \equiv H_-$. The bound state energy spectrum of $H^{(k)}$ is therefore obtained by

$$E_0^{(k)} = \sum_{s=1}^{k} R(a_s) \tag{37}$$

and its $n$th level is coincident with the ground state of the Hamiltonian $H_n$. The energy eigenvalues of Hamiltonian are given by $E_0^{(-)} = 0$ and

$$E_n^{(-)} = \frac{\hbar^2}{2m} \left[ \left( \frac{U}{2S_2} - \frac{S_2}{2} \right)^2 - \left( \frac{U}{2(S_2 - n\alpha)} - \frac{S_2 - n\alpha}{2} \right)^2 \right]. \tag{38}$$

Hence, the energy levels of Woods–Saxon potential plus its squared form are found from the relationship $E_n = E_n^{(-)} + E_0^{(1)}$. Recalling $E_0^{(1)}$ from Eq. 29, we can rearrange its value in terms of $S_2$,

$$E_0^{(1)} = -\frac{\hbar^2 S_1^2}{2m} = -\frac{\hbar^2}{2m} \left[ \frac{U}{2S_2} - \frac{S_2}{2} \right]^2 \tag{39}$$

using the equalities $S_1 = \frac{\alpha}{2} - \frac{2mV_0}{\hbar^2} \frac{1}{2S_2}$ and $\alpha = \frac{1}{S_2} \left( \frac{2mC}{\hbar^2} - S_2^2 \right)$. Therefore, the corresponding eigenvalue equation reads

$$E_n = E_n^{(-)} + E_0^{(1)} = -\frac{\hbar^2}{2m} \left[ \frac{U}{2(S_2 - n\alpha)} - \frac{S_2 - n\alpha}{2} \right]^2, \tag{40}$$

where it is note that one can write a relationship between $V(r)$ and $V_-(r)$.

The Hamiltonian of the Woods–Saxon potential for $\ell \neq 0$ cases is written as

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{V_0}{1 + e^{\left(\frac{r-R_0}{a}\right)}} + \frac{\hbar^2\ell(\ell+1)}{2mr^2}. \tag{41}$$

The second term on the right-hand side of Eq. 41 comes from the Woods–Saxon potential and third term in the same side comes from the centrifugal barrier. This last term is preventive to build the same superfamily as in $\ell \neq 0$ cases, since the full potential is not exactly solvable. However, several numerical approaches have been utilized in order to evaluate the spectra of energy eigenvalues and eigenfunctions [20]. Now, we introduce a new effective potential whose its functional form is given as follows

$$V_{eff} = -\frac{V_0}{1 + e^{\left(\frac{r-R_0}{a}\right)}} + \frac{\hbar^2\ell(\ell+1)}{2ma^2\left(1 + e^{\left(\frac{r-R_0}{a}\right)}\right)^2}. \tag{42}$$

In the cases of $a = R_0/2$ and the small value of $a$, the second term on the right-hand side of Eq. 42 behaves as a centrifugal barrier term of Eq. 41 in the first-term approximation. If we want to investigate this term, it should be expanded according to the exponential part;

$$\frac{\hbar^2\ell(\ell+1)}{2ma^2\left(1 + e^{\left(\frac{r-R_0}{a}\right)}\right)^2} = \frac{\hbar^2\ell(\ell+1)}{2ma^2\left[1 + \left(1 + \frac{r-R_0}{a} + \frac{1}{2!}\left(\frac{r-R_0}{a}\right)^2 + \cdots\right)\right]^2}$$

$$\approx \frac{\hbar^2\ell(\ell+1)}{2mr^2}. \tag{43}$$

The first-term approximation means that the second and higher order terms can be ignored in the expended exponential part of Eq. 43. Therefore, the effective potential given by Eq. 42 has the same functional form as the potential part of Eq. 41. Furthermore, we can solve the Schrödinger equation by the factorization method of the SQM because the Schrödinger equation for this potential is solvable analytically under the condition of the shape-invariance approach. In this case, if we can perform the parameter transformation $C \to \hbar^2\ell(\ell+1)/2ma^2$, comparing Eq. 42 with Eq. 20, the energy levels of the effective potential in Eq. 42 are approximately obtained as follows

$$E_{n\ell \neq 0} = -\frac{\hbar^2}{2ma^2} \times \left[\left(\frac{\frac{2mV_0a^2}{\hbar^2} - \ell(\ell+1)}{1 + 2n - \sqrt{1 + 4\ell(\ell+1)}}\right)^2 + \frac{1}{2}\left(\frac{2mV_0a^2}{\hbar^2} - \ell(\ell+1)\right)\right.$$

$$\left. + \frac{1}{16}\left(1 + 2n - \sqrt{1 + 4\ell(\ell+1)}\right)^2\right], \tag{44}$$

or in the closed form

$$
E_{n\ell \neq 0} = -\frac{\hbar^2}{32ma^2} \left[ 1 + 2n - \sqrt{1 + 4\ell(\ell+1)} + \frac{4\left(\frac{2mV_0a^2}{\hbar^2} - \ell(\ell+1)\right)}{1 + 2n - \sqrt{1 + 4\ell(\ell+1)}} \right]^2.
$$

(45)

It is well-known that the energy spectrum of actual diatomic molecules can be represented by the Morse, Kratzer, Coulomb, etc., potentials [21]. An alternative potential model suggested to use in the molecular science can be the Woods–Saxon potential. In order to study this type of potential in the SQM formalism, we need the shape-invariance approach with a translation of parameters. In addition, the hierarch of Hamiltonians method is necessary for obtaining explicit eigenvalues in all of the angular momentum quantum numbers [22,23]. Nevertheless, we can clearly say that the Woods–Saxon potential can not be applied for $\ell = 0$ state in the SQM formalism. The situation may be arisen from the Woods–Saxon potential which is finite at $r = 0$, and cannot satisfy the boundary condition in our approach.

## 4 Conclusions

We have applied the shape-invariance approach and hierarchy of Hamiltonian method in the context of SQM to obtain the energy spectra of the Woods–Saxon potential. We have used a new effective potential which consists of the Woods–Saxon and its square form. We have obtained an approximate analytical eigenvalue equation for $\ell \neq 0$ states. We would like to point out that although the SQM formalism works quite well for the effective Woods–Saxon potential, an extensive application to other effective Woods–Saxon-like potentials is needed to test the credibility of the method.

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