

Deformed Schiöberg-Type Potential and Rotational-Vibrational Spectra for Some Diatomic Molecules

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ABSTRACT

This thesis aims to discuss the deformed Schiöberg-type potential for some diatomic molecules. The Varshni's conditions are used to show a common diatomic molecular potential model. It also aims to employ the radial spherically symmetric Schrödinger equation and convert our potential into a format that allows us to use supersymmetric quantization and find a closed form analytical solution for the rotational and vibrational energy levels. We talk about our findings by utilizing three diatomic molecules $H_2(x^1\Sigma_g^+)$, HF ($x^1\Sigma_g^+$) and $N_2(x^1\Sigma_g^+)$. The findings of the thesis showed that there is a great comparison with those from a generalized pseudospectral numerical method (GPS).

Keywords: rotational-vibrational energy spectra, deformed Schiöberg-type potential, diatomic molecules.

ÖZ

Bu tezin amacı iki-atomlu moleküllerde deforme edilmiş Schiöberg-tipi potansiyellerin incelenmesidir. Ortak iki-atomlu molekül potansiyelinin tesbitinde Varshni şartları kullanılmıştır. Ayrıca radyal simetrik Schrödinger denklemi potansiyeli supersimetrik Kuantum formatına sokulup dönme ve titreşimli enerji seviyeleri tam olarak bulunmuştur. Üç örnek seçilmiştir, bunlar $H_2(x^1\Sigma_g^+)$, $HF(x^1\Sigma_g^+)$ ve $N_2(x^1\Sigma_g^+)$ 'dir. Tezin bulguları genelleştirilmiş spektral gibi görünen nümerik yöntemlerle mukayese edilebildiğini göstermiştir.

Anahtar sözcükler: dönmeli – titreşimsel enerji spektrumu, deforme edilmiş Schiöberg-tipi potansiyel, iki-atomlu moleküller.

DEDICATION

This thesis is dedicated to

- My beloved son (Aran).
- My darling siblings.
- My dear wife.
- My nieces and nephews.

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Chapter 1

INTRODUCTION

Relevant information about a diatomic molecule is encoded in the energy-distant relation provided by empirical diatomic potential energy functions. Hence, a large number of diatomic empirical potentials was suggested and investigated [1-23]. The crucial test is represented by how good an empirical potential function is in the reproduction of the so called experimental Rydberg-Klein-Rees (RKR) energy curves, and the rotational- vibrational energy levels for diatomic molecules. In addition, the investigations on such potentials included the relations among the suggested potentials.

Hajigeorgiou [6], for example, has investigated an extended Lennard-Jones diatomic potential, Manning and Rosen [11] have studied the vibrational levels through the so called Manning-Rosen potential, Deng and Fan [3] have introduced the Deng-fan potential that is used, later on, by Mustafa [14] to study the rotational and vibrational energies, Schiöberg [18] has introduced a hyperbolic potential function, Mustafa [13] has suggested a deformed Schiöberg-type potential and obtained very accurate (compared with numerical as well as RKR results) rotational and vibrational energy levels for a number of diatomic molecules, Wang et al [23] have shown that a deformed and shifted Rosen-Morse [6] is equivalent to Tietz and Wei potentials [9], ... etc.

Here are some potential that are unavoidable in the process. The Morse [12] three-parameters empirical potential energy function,

$$U(r) = D_e \left(1 - e^{-\alpha(r-r_e)}\right)^2. \quad (1.1)$$

Where D_e is the dissociation energy, r_e is the equilibrium bond length, and α is the range of the potential. The Morse potential is still been used in molecular physics and quantum chemistry [23]. The Manning and Rosen [11] potential function for diatomic molecules,

$$U(r) = \frac{h^2}{8\mu\pi^2 b^2} \left[\frac{\beta(\beta-1)e^{-2\alpha r}}{(1-e^{-\alpha r})^2} - \frac{A e^{-\alpha r}}{1-e^{-\alpha r}} \right], \quad (1.2)$$

With β and A are two dimensionless parameters, and is sometimes called a generalize Morse potential [11]. The Deng and Fan [6] potential,

$$U(r) = D_e \left(1 - \frac{e^{-\alpha r} e - 1}{e^{-\alpha r} - 1}\right)^2, \quad (1.3)$$

which is suggested to be better than the Morse potential (1.1) in representing diatomic interaction for vibration of diatomic [3]. The Schiöberg [18] potential function,

$$U(r) = D(1 - \eta \coth \alpha r)^2, \quad (1.4)$$

Where D , η , α are three adjustable positive parameters, $\eta < 1$. Schiöberg [18] believed that this potential function (1.4) is more accurate than the Morse potential function for some diatomic molecules [23]. Moreover, the Schiöberg potential function, the Deng-Fan potential function and the Manning-Rosen potential function are the same empirical potential functions for diatomic molecules [13]. Also, Wang et al [22] generated improved expressions for two versions of the Schiöberg potential

function. Both versions of the Schiöberg potential function are Rosen-Morse and Manning-Rosen potential functions. Yet, Mustafa [13] has suggested a new deformed Schiöberg-type potential for diatomic molecules,

$$U(r) = \sigma (\delta + \tanh_q \alpha r)^2, \quad (1.5)$$

Where $\sigma > 0$, δ , q , and the screening parameter $\alpha > 0$ are real adjustable parameters to be determined. Additionally, the q -deformation of the standard hyperbolic function is characterized through

$$\begin{aligned} \tanh_q \alpha r &= \frac{\sinh_q \alpha r}{\cosh_q \alpha r}; \quad \sinh_q \alpha r = \frac{e^{\alpha r} - qe^{-\alpha r}}{2}; \\ \cosh_q \alpha r &= \frac{e^{\alpha r} + qe^{-\alpha r}}{2}. \end{aligned} \quad (1.6)$$

The main goal of this thesis is to study the deformed Schiöberg-type potential (1.5) by using the radial spherically symmetric Schrödinger equation to investigate the central attractive/repulsive core $l(l+1)/2\mu r^2$ to get the rotational-vibration energy levels. To achieve this goal we present the necessary information in the subsequent chapters. In Chapter two, Varshni's conditions for the deformed Schiöberg-type potential (1.5) are highlighted. In Chapter three, there is a brief review of the basic formulae of the supersymmetric quantum mechanics. A four-parameter exponential-type potential is used and the exact energy spectra is obtained. Moreover, we also convert expression (2.7) into a proper form to be able to use the supersymmetric quantization recipe of [2] and find the rotational-vibration energy levels. In addition, Chapter four, discusses the obtained results using three-diatom molecules $H_2(x^1\Sigma_g^+)$, $HF(x^1\Sigma_g^+)$ and $N_2(x^1\Sigma_g^+)$. They compare

great with those from a generalized pseudospectral numerical method (GPS). Finally, Chapter five concludes the thesis through discussing the findings.

Chapter 2

DIATOMIC MOLECULAR POTENTIAL

An experimental diatomic molecular potential energy function, $U(r)$, necessary and desirably has to satisfy the Varshni's conditions [21, 15]

$$\left. \frac{dU(r)}{dr} \right|_{r=r_e} = 0, \quad (2.1)$$

$$U(\infty) - U(r_e) = D_e, \quad (2.2)$$

$$\left. \frac{d^2U(r)}{dr^2} \right|_{r=r_e} = K_e = (2\pi c)^2 \mu \omega_e^2, \quad (2.3)$$

where D_e is the dissociation energy, r_e is the equilibrium bond length, c is the speed of light, $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass, and ω_e is the equilibrium harmonic oscillator vibrational frequency.

From Eq. (1.5) and (1.6), we can convert our potential into an exponential form to obtain,

$$U(r) = \sigma \left(\delta + \frac{e^{\alpha r} - q}{e^{\alpha r} + q} \right)^2. \quad (2.4)$$

We use the first and second Varshni's conditions (2.1) and (2.2), on our (2.4), we obtain,

$$\left. \frac{dU(r)}{dr} \right|_{r=r_e} = 0 \Rightarrow \delta = - \left(\frac{e^{\gamma r_e} - q}{e^{\gamma r_e} + q} \right)^2, \gamma = 2\alpha \quad (2.5)$$

And

$$U(\infty) - U(r_e) = D_e \Rightarrow \sigma = \frac{D_e}{4q^2} (e^{\gamma r_e} + q)^2. \quad (2.6)$$

Equations (2.5) and (2.6) into (2.4), yield

$$U(r) = D_e \left[1 - \frac{e^{\gamma r_e + q}}{e^{\gamma r} + q} \right]^2. \quad (2.7)$$

Now, if we apply the third Varshni's conditions (2.3), we get

$$\begin{aligned} \frac{d^2 U(r)}{dr^2} \Big|_{r=r_e} &= K_e, \\ F &= \frac{\gamma e^{\gamma r_e}}{e^{\gamma r_e} + q} \Rightarrow q = -\left(1 - \frac{\gamma}{F}\right) e^{\gamma r_e}, \\ F &= \sqrt{\frac{K_e}{2D_e}}. \end{aligned} \quad (2.8)$$

The deformation parameter q is defined as

$$q = -\varepsilon e^{\gamma r_e}; \quad \varepsilon = \left(1 - \frac{\gamma}{F}\right), \quad (2.9)$$

Where, q takes positive or negative values depending on whether the optimization parameter ε is negative or positive, respectively. Obviously, q represents a deformation function that depends on the spectroscopic parameters F , γ , and r_e . That is $q = q(F, \gamma, r_e)$. One should notice that for the Morse potential the deformation parameter $q \rightarrow 0$ (i.e. $\varepsilon \rightarrow 0$), for the Deng-Fan potential and improved for the Manning-Rosen potential $q = -1$ (i.e., $\varepsilon = e^{-\gamma r_e}$), and for the Tietz-Hua potential $q = -\varepsilon e^{\gamma r_e}; \varepsilon = c_h$,

Chapter 3

SUPERSYMMETRIC QUANTUM MECHANICAL TREATMENT

In this chapter, we give a brief review for the supersymmetric shape invariance. The Schrödinger equation for a particle of mass m in one – dimensional potential is,

$$\left[-\beta \frac{d^2}{dr^2} + V(r) \right] \psi(r) = E \psi(r) , \quad (3.1)$$

Where $\psi(r)$ is the wavefunction, $\beta = \left(\frac{\hbar^2}{2m}\right)$, $V(r)$ is the potential and E is the energy. The ground – state wavefunction $\Psi_0(r)$ can be written as,

$$\psi_0(r) = A \exp\left(-\frac{1}{\sqrt{\beta}} \int W(r) dr\right), \quad (3.2)$$

where A is a normalized constant and $W(r)$ is called superpotential in supersymmetric quantum mechanics. Substituting (3.2) into (3.1), we obtain ,

$$W^2(r) - \sqrt{\beta} \frac{dW(r)}{dr} = V(r) - E_0, \quad (3.3)$$

Where E_0 is the ground – state energy. Equation (3.3) is a nonlinear Riccati equation. In terms of the superpotential $W(r)$, the supersymmetric partner potentials $V^+(r)$ and $V^-(r)$ are given by,

$$V^+(r) = W^2(r) + \sqrt{\beta} \frac{dW(r)}{dr}, \quad (3.4)$$

$$V^-(r) = W^2(r) - \sqrt{\beta} \frac{dW(r)}{dr}. \quad (3.5)$$

And the operator A and A^+ are defined by

$$A^+ = -\sqrt{\beta} \frac{d}{dr} + W(r), \quad (3.6)$$

$$A = \sqrt{\beta} \frac{d}{dr} + W(r). \quad (3.7)$$

Incorporating (3.3) and (3.5), the potential $V(r)$ and $V^-(r)$ have the following relation,

$$V(r) = V^-(r, a_0) + E_0, \quad (3.8)$$

If $V^+(r)$ and $V^-(r)$ have similar shapes, they are said to be shape – invariant. And they satisfy the following relation,

$$V^+(r, a_0) = V^-(r, a_1) + R(a_1), \quad (3.9)$$

Where a_0 is a set of parameter, a_1 is a function of a_0 , and the reminder $R(a_1)$ is independent of r . The Hamiltonians corresponding to the potentials $V^+(r)$ and $V^-(r)$ are given by,

$$H^+ = -\beta \frac{d^2}{dr^2} + V^+(r), \quad (3.10)$$

$$H^- = -\beta \frac{d^2}{dr^2} + V^-(r). \quad (3.11)$$

The supersymmetric partner potential $V^+(r)$ and $V^-(r)$ have the same energy spectra except for the fact that $V^+(r)$ has one bound state less than $V^-(r)$,

$$E_n^{(+)} = E_{n+1}^{(-)} \quad (n = 0, 1, 2, \dots),$$

The ground – state energy of $V^+(r)$ is zero. For the partner potential $V^-(r)$, the energy spectrum is given in the fashion [5],

$$E_0^{(-)} = 0, \quad E_n^{(-)} = \sum_{k=1}^n R(a_k), \quad (k = 1, 2, 3, \dots). \quad (3.12)$$

We can now use the four – parameters exponential – type potential,

$$V(r) = P_1 + \frac{P_2}{e^{2\alpha r} + q} + \frac{P_3}{(e^{2\alpha r} + q)^2}, \quad (3.13)$$

Putting the superpotential as,

$$W(r) = -\sqrt{\beta} \left(Q_1 + \frac{Q_2}{e^{2\alpha r} + q} \right). \quad (3.14)$$

We may use (3.13) and (3.14) into (3.3), we get

$$\begin{aligned} Q_1^2 &= \frac{1}{\beta} (P_1 - E_0), \\ 2Q_1Q_2 - 2\alpha Q_2 &= \frac{1}{\beta} P_2, \\ Q_2^2 + 2\alpha q Q_2 &= \frac{1}{\beta} P_3. \end{aligned} \quad (3.15)$$

Also, solving (3.15) we can produced,

$$Q_1 = \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right], \quad (3.16)$$

Using (3.16) and (3.14) in to (3.4) and (3.5), the supersymmetric potentials $V^+(r)$ and $V^-(r)$ can be find as,

$$\begin{aligned} V^+(r) &= W^2(r) + \sqrt{\beta} \frac{dW(r)}{dr} = \beta \left\{ \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right]^2 + \frac{(qP_2 + P_3)}{q\beta(e^{2\alpha r} + q)} - \right. \\ &\quad \left. \frac{Q_2^2}{q(e^{2\alpha r} + q)} + \frac{Q_2^2}{(e^{2\alpha r} + q)^2} + \frac{2\alpha Q_2}{(e^{2\alpha r} + q)} - \frac{2\alpha q Q_2}{(e^{2\alpha r} + q)^2} \right\}, \end{aligned} \quad (3.17)$$

$$V^-(r) = W^2(r) - \sqrt{\beta} \frac{dW(r)}{dr} = \beta \left\{ \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right]^2 + \frac{(qP_2 + P_3)}{q\beta(e^{2\alpha r} + q)} - \frac{Q_2^2}{q(e^{2\alpha r} + q)} + \frac{Q_2^2}{(e^{2\alpha r} + q)^2} - \frac{2\alpha Q_2}{(e^{2\alpha r} + q)} + \frac{2\alpha q Q_2}{(e^{2\alpha r} + q)^2} \right\}. \quad (3.18)$$

Putting $a_0 = Q_2$ and $a_1 = (Q_2 - 2\alpha q)$, the partner $V^+(r, a_0)$ and $V^-(r, a_1)$ satisfy following relationship,

$$\begin{aligned} R(a_1) &= V^+(r, a_0) - V^-(r, a_1) \\ &= \beta \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right]^2 - \beta \left[\frac{(qp_2 + P_3)}{2q\beta(Q_2 - 2\alpha q)} - \frac{(Q_2 - 2\alpha q)}{2q} \right]^2. \end{aligned} \quad (3.19)$$

Using Eq. (2.12), the energy levels for the partner potential $V^-(r)$ are given by

$$E_0^{(-)} = 0, \quad (3.20)$$

$$\begin{aligned} E_n^{(-)} &= \sum_{k=1}^n R(a_k) = R(a_1) + R(a_2) + \dots + R(a_n) \\ &= \beta \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right]^2 - \beta \left[\frac{(qp_2 + P_3)}{2q\beta(Q_2 - 2\alpha q)} - \frac{(Q_2 - 2\alpha q)}{2q} \right]^2 + \beta \left[\frac{(qP_2 + P_3)}{2q\beta(Q_2 - 2\alpha q)} - \frac{(Q_2 - 2\alpha q)}{2q} \right]^2 \\ &\quad - \beta \left[\frac{(qp_2 + P_3)}{2q\beta(Q_2 - 4\alpha q)} - \frac{(Q_2 - 4\alpha q)}{2q} \right]^2 + \dots + \\ &\quad \beta \left[\frac{(qp_2 + P_3)}{2q\beta(Q_2 - (n-1)2\alpha q)} - \frac{(Q_2 - (n-1)2\alpha q)}{2q} \right]^2 - \beta \left[\frac{(qp_2 + P_3)}{2q\beta(Q_2 - n2\alpha q)} - \frac{(Q_2 - n2\alpha q)}{2q} \right]^2 \\ &= \beta \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right]^2 - \beta \left[\frac{(qp_2 + P_3)}{2q\beta(Q_2 - n2\alpha q)} - \frac{(Q_2 - n2\alpha q)}{2q} \right]^2. \end{aligned} \quad (3.21)$$

Solving (3.15) yields

$$E_0 = P_1 - \beta \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right]^2, \quad (3.22)$$

$$Q_2 = -\alpha q \pm \sqrt{\alpha^2 q^2 + \frac{P_3}{\beta}}. \quad (3.23)$$

Incorporating (3.8), (3.21) and (3.22), we can get the energy spectra for the four – parameters exponential – type potential,

$$\begin{aligned}
E_n &= E_n^{(-)} + E_0 = \beta \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right]^2 - \beta \left[\frac{(qp_2 + P_3)}{2q\beta(Q_2 - n2\alpha q)} - \frac{(Q_2 - n2\alpha q)}{2q} \right]^2 \\
&\quad + P_1 - \beta \left[\frac{(qP_2 + P_3)}{2q\beta Q_2} - \frac{Q_2}{2q} \right]^2 \\
&= P_1 - \beta \left[\frac{(qp_2 + P_3)}{2q\beta(Q_2 - n2\alpha q)} - \frac{(Q_2 - n2\alpha q)}{2q} \right]^2, \\
n &= 0, 1, 2, \dots
\end{aligned} \tag{3.24}$$

In put (3.23) into (3.24), the above energy spectrum can be express,

$$\begin{aligned}
E_n &= P_1 - \frac{\beta}{4} \left[\frac{\frac{1}{q^2\beta} (qp_2 + p_3)}{(-\alpha - 2n\alpha \pm \sqrt{\alpha^2 + \frac{p_3}{q^2\beta}})} - (-\alpha - 2n\alpha \pm \sqrt{\alpha^2 + \frac{p_3}{q^2\beta}}) \right]^2, \\
n &= 1, 2, 3, \dots
\end{aligned} \tag{3.25}$$

3.1 Application To The Deformed Schiöbeg-Type Potential

We use the radial spherically symmetric Schrödinger equation to deal with the central attractive/repulsive core $l(l+1)/2\mu r^2$.

$$-\frac{\hbar^2 d^2 u_{n,l}(r)}{2\mu dr^2} + \left[\frac{l(l+1)\hbar^2}{2\mu r^2} + U(r) \right] u_{n,l}(r) = E_{n,l} u_{n,l}(r). \tag{3.26}$$

Substituting expression (2.7) into (3.26), we get

$$-\frac{\hbar^2 d^2 u_{n,l}(r)}{2\mu dr^2} + \left[D_e \left[1 - \frac{e^{\gamma r e + q}}{e^{\gamma r + q}} \right]^2 + \frac{l(l+1)\hbar^2}{2\mu r^2} \right] u_{n,l}(r) = E_{n,l} u_{n,l}(r), \tag{3.27}$$

Where $E_{n,l}$ denotes the energy spectrum of the diatomic molecular, n and l are the vibrational and rotational quantum numbers, respectively. Eq. (3.27) is explained just for the case $l \neq 0$.

We change our potential (2.7) into an appropriate structure to have the capacity to apply the supersymmetric quantization (3.13) method by Jia et al [2],

$$U(r) = P_1 + \frac{P_2}{e^{\gamma r} + q} + \frac{P_3}{(e^{\gamma r} + q)^2}, \quad (3.28)$$

Where

$$\begin{aligned} P_1 &= D_e, \\ P_2 &= -2D_e(e^{\gamma r_e} + q), \\ P_3 &= D_e(e^{\gamma r_e} + q)^2. \end{aligned} \quad (3.29)$$

Incorporating (3.28) and (3.29) into (3.26) we write the effective potential as,

$$U_{eff}(r) = \frac{l(l+1)\hbar^2}{2\mu r^2} + U(r) = \tilde{p}_1 + \frac{\tilde{p}_2}{e^{\gamma r} + q} + \frac{\tilde{p}_3}{(e^{\gamma r} + q)^2}, \quad (3.30)$$

$$\tilde{p}_1 = P_1 + \lambda C_0,$$

$$\tilde{p}_2 = P_2 + \lambda C_1,$$

$$\tilde{p}_3 = P_3 + \lambda C_3,$$

$$\lambda = \frac{l(l+1)\hbar^2}{2\mu r_e^2}. \quad (3.31)$$

In the present proposition, we suggest Badawi et al [1] factorization formula,

$$\frac{r_e^2}{r^2} = C_0 + \frac{C_1}{e^{ar} + q} + \frac{C_2}{(e^{ar} + q)^2}. \quad (3.32)$$

The estimations of the C_i 's are gotten utilizing the factorization formula of Badawi et al [1] in the accompanying way. Let $y = \gamma (r - r_e)$ then with $\gamma r = y + b$ and $b = \gamma r_e$ one suggests that,

$$\frac{r_e^2}{r^2} = \frac{1}{\left(\frac{y}{b}+1\right)^2},$$

$$\frac{r_e^2}{r^2} = C_0 + \frac{C_1}{e^{y+b+q}} + \frac{C_2}{(e^{y+b+q})^2}. \quad (3.33)$$

When $r \rightarrow r_e$, $y=0$. We take the Taylore's expansion to both sides in (3.33), we get three linear equations. The solutions are,

$$C_0 = 1 - \left(\frac{1-\varepsilon}{b}\right)^2 \left[\frac{4b}{1-\varepsilon} - (3+b)\right], \quad (3.34)$$

$$C_1 = 2e^b (1-\varepsilon) \left[3\left(\frac{1-\varepsilon}{b}\right) - (3+b)\left(\frac{1-\varepsilon}{b}\right)^2\right], \quad (3.35)$$

$$C_2 = \frac{e^{2b}}{b^2} (1-\varepsilon)^4 \left[(3+b) - \frac{2b}{1-\varepsilon}\right]. \quad (3.36)$$

In such potential parametric situation, the supersymmetric quantum recipe used by Jia et al [2] is most probably utilized. This is also followed consequently for our schrödenger equation and the effective potential in both (2.7) and (3.30), respectively. More specifically, one should set their P_1 , P_2 , and P_3 are our current \tilde{p}_1 , \tilde{p}_2 , and \tilde{p}_3 , respectively. Hereby, we only cast the necessary formulae where our superpotential would read [13],

$$\tilde{W}(r) = -\sqrt{\beta} \left(\tilde{Q}_1 + \frac{\tilde{Q}_2}{e^{2\alpha r} + q}\right), \quad (3.37)$$

and the ground-state like wave function is given by

$$\Psi(r) = A \exp\left(-\frac{1}{\sqrt{\beta}} \int \tilde{W}(r) dr\right). \quad (3.38)$$

Substituted (3.30), (3.37) and (3.38) into (3.26), we get

$$\tilde{Q}_1 = \left[\frac{(q\tilde{p}_2 + \tilde{p}_3)}{2q\beta\tilde{Q}_2} - \frac{\tilde{Q}_2}{2q}\right], \quad (3.39)$$

$$E_0 = \tilde{p}_1 - \beta \left[\frac{(q\tilde{p}_2 + \tilde{p}_3)}{2q\beta\tilde{Q}_2} - \frac{\tilde{Q}_2}{2q} \right]^2, \quad (3.40)$$

$$\tilde{Q}_2 = -\alpha q \pm \sqrt{\alpha^2 q^2 + \frac{\tilde{p}_3}{\beta}}. \quad (3.41)$$

The corresponding rotational-vibrational energy levels are,

$$E_{n,l} = \tilde{p}_1 - \frac{\hbar^2 \gamma^2}{2\mu} \left[\frac{\frac{2\mu}{\hbar^2 q^2 \gamma^2} (\tilde{p}_3 + q\tilde{p}_2)}{\left(-1 - 2n \pm \sqrt{1 + \frac{8\mu \tilde{p}_3}{\hbar^2 q^2 \gamma^2}} \right)} - \frac{\left(-1 - 2n \pm \sqrt{1 + \frac{8\mu \tilde{p}_3}{\hbar^2 q^2 \gamma^2}} \right)}{4} \right]^2, \quad (3.42)$$

Where the positive and negative signs (\pm) are corresponding to the cases $q > 0$ and $q < 0$.

Chapter 4

RESULTS AND DISCUSSION

Table 1 shows Amlan K. Roy's [17] spectroscopic parameters for three diatomic molecules $H_2(x^1\Sigma_g^+)$, $HF(x^1\Sigma_g^+)$ and $N_2(x^1\Sigma_g^+)$. Now, we utilize the results shown in (3.42) and calculate the ro-vibrational energy levels provided, in Table 2, for $H_2(x^1\Sigma_g^+)$, $HF(x^1\Sigma_g^+)$ and $N_2(x^1\Sigma_g^+)$ molecules, and the vibrational energies for the $N_2(x^1\Sigma_g^+)$ molecule (given in table 3). For each of the aforementioned diatomic molecules, we have tested the sign of q and accordingly used the proper sign of the square root in (3.42). In addition, in Table 2, we have compared the results we obtained with those of Amlan K. Roy [17], who employs a generalized pseudospectral (GPS) numerical method. It can be seen from the Roy's study that his results are compared excellently with those of the Nikiforov-Uvarov formalism of Hamzavi [7]. Furthermore, in the conversion of the (eV)-units, which are used by Roy, into cm^{-1} units, we have used the relation [13],

$$E_{n,l}(cm^{-1}) = D_e(cm^{-1}) + \frac{Roy's(eV)}{1.23984188 \times 10^{-4}(eV cm^{-1})}.$$

It is apparent that the results we achieved from (3.42) are in good agreement with those from the GPS numerical method. However, when we want to explore any relationship between the accuracy of our results shown in Table 2 and the potential parameters given in Table 1, we can see a general trend that the heavier the reduced mass the more exact our results are contrasted with the GPS ones. This is mostly

connected to the semi-classical limit nature of the Taylor's expansion near the equilibrium inter-nuclear distance, $r \rightarrow r_e$, used in the factorization recipe (3.32) of Badawi et al. [1]. It is also apparent that the larger the reduced mass, in the central core term $l(l + 1) / 2\mu r^2$, the less the effect of the rotational quantum number l .

Moreover, the authors of [8, 19] have used the common diatomic molecular potential (2.7) as an equivalent form for their deformed modified Rosen-Morse (DMRM) potential. As a result, the introduction of table 3 cannot be avoided in the process. In this table we compare our results with those given by Lino da Silva et al. [10] (who have used the RKR method to construct the potential curve of the $N_2(x^1\Sigma_g^+)$) along with the results reported by Sun et al. [19] and those of Morse potential. It can be seen from the comparison between our results and those of Lino da Silva et al [10] that the accuracy is still high. However, if our results are compared with those of Sun et al. [19], we can see small discrepancies.

Table 4.1: The values of the molecular parameters are taken from Roy [17].

Molecule	\mathcal{E}	$\mu / 10^{-23}(\text{g})$	$\gamma (\text{\AA}^{-1})$	$r_0(\text{\AA})$	$F(\text{\AA}^{-1})$	$D_e(\text{cm}^{-1})$
$H_2(x^1\Sigma_g^+)$	0.170066	0.084	1.61890	0.741	1.9506	38318
$HF(x^1\Sigma_g^+)$	0.127772	0.160	1.94207	0.917	2.2266	49382
$N_2(x^1\Sigma_g^+)$	-0.032325	1.171	2.78585	1.097	2.6986	79885

Table 4.2: Rotational-vibrational energy $E_{n,l}$ in cm^{-1} for $n = 0, 3, 5$ for different l values using

		$H_2(x^1\Sigma_g^+)$		$HF(x^1\Sigma_g^+)$		$N_2(x^1\Sigma_g^+)$	
n	l	GPS[10]	Eq.(3.42)	GPS[10]	Eq.(3.42)	GPS[10]	Eq.(3.42)
0	0	2171.682	2171.620	2047.271	2047.583	1174.939	1174.927
0	1	2289.372	2289.389	2088.368	2088.372	1178.870	1178.881
0	2	2523.794	2523.868	2169.893	2169.899	1186.778	1186.787
0	3		2872.971		2292.067		1198.653
0	4		3333.648		2454.724		1214.465
0	5		3901.964		2657.674		1234.235
0	10		8173.751		4266.494	1392.325	1392.337
0	15	14184.546	14257.357	6824.964	6825.640	1649.086	1649.101
0	20	21121.346	21406.208	10257.291	10259.283	2004.287	2004.306
3	0	13641.123	13641.153	13298.714	13298.702	8047.875	8074.931
3	1	13738.725	13740.002	13334.713	13334.767	8051.716	8051.773
3	2	13932.924	13936.843	13406.667	13406.849	8059.397	8059.454
3	3		14229.985		13514.858		8070.982
3	4		14616.957		13658.654		8086.343
3	5		15094.572		13838.054		8105.549
3	10		18692.978		15259.572	8259.034	8259.147
3	15		23845.985		17518.420	8508.407	8508.590
3	20		29951.318		20544.347	8853.370	8853.656
5	0	19916.186	19915.781	19858.084	19860.675	12460.465	12460.549
5	1	20000.398	20003.348	19893.600	19893.731	12464.229	12464.315
5	2	20168.806	20177.740	19959.350	19959.799	12471.756	12471.845
5	3		20437.497		20058.790		12483.147
5	4		20780.480		20190.575		12498.207
5	5		21203.936		20354.979		12517.037
5	10		24399.295		21657.201	12667.396	12667.620
5	15		28992.422		23724.734	12911.768	12912.163
5	20		34465.726		26490.807	13249.805	13250.446

Table 4.3: $E_{n,l}$ for $l = 0$ (i.e., vibrational energy) compared with RKR [10], DMRM [19] and Morse [19]

n	l	RKR[10]	Eq.(3.42)	DMRM[19]	Morse[19]
0	0	1184.4539	1174.9270	1174.9971	1174.9477
1	0	3526.3576	3499.7431	3499.8409	3498.7289
2	0	5833.4516	5790.7602	5790.8755	5787.6913
3	0	8107.0460	8047.9317	8048.0809	8041.8351
4	0	10348.312	10271.210	10271.387	10261.160
5	0	12558.287	12460.549	12460.725	12445.666
6	0	14737.876	14615.901	14616.138	14595.353
7	0	16887.859	16737.218	16737.473	16710.222
8	0	19008.895	18824.453	18824.747	18790.272
9	0	21101.519	20877.559	20877.869	20835.503

Chapter 5

CONCLUSION

The main goal of this thesis is to study the deformed Schiöberg- type potential by using the radial spherically symmetric Schrödinger equation to investigate the central attractive/repulsive core $l(l+1)/2\mu r^2$ (3.26) to obtain the rotational-vibration energy levels. To obtain this aim, we started by using the Morse potential (1.1) with the Manning-Rosen potential (1.2), the Deng-Fan potential (1.3) and the Schiöberg-type potential (1.4) to show their relationship. In addition, each of them was used to investigate the diatomic molecules. Some previous studies have found that the Manning-Rosen potential (1.2), the Deng-Fan potential (1.3) and the Schiöberg-type potential (1.4) are more accurate than the Morse potential (1.1) to explore the ro-vibrational levels for diatomic molecules and the Manning-Rosen potential (1.2), the Deng-Fan potential (1.3) and the Schiöberg-type potential (1.4) are equivalent empirical potential functions for diatomic molecules.

In this part of the thesis, We have used the Varshni's [21,15] conditions for deformed Schiöberg-type potential (2.4) to obtain common diatomic molecular potential (2.7) . Also, We have used the radial spherically symmetric Schrödinger equation (3.26), the supersymmetric quantization method (3.28) by Jia et al [2], Badawi et al [1] factorization recipe (3.32) and ground-state like wave function (3.38) to obtain a closed form solution for the rotatinal-vibrational energy levels (3.42).

In the last part of this thesis, we discussed our results using three-diatomic molecules $H_2(x^1\Sigma_g^+)$, $HF(x^1\Sigma_g^+)$ and $N_2(x^1\Sigma_g^+)$. The results of our analysis turned out to have great comparison with those from a generalized pseudospectral numerical method (in table 2), Lino da Silva et al. [10] and Sun et al. [19] (in table 3).

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