

SUPER SYMMETRIC QUANTUM MECHANICS APPLICATIONS ON SOME
DIATOMIC POTENTIALS

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SOME DIATOMIC POTENTIALS**

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I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

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ABSTRACT

SUPER SYMMETRIC QUANTUM MECHANICS APPLICATIONS ON SOME DIATOMIC POTENTIALS

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One dimensional molecular potentials are studied by solving the Schrödinger Equation for some well known potentials, such as the deformed Morse, Eckart and the Hua potentials. Parametric generalization of Hamiltonian Hierarchy is introduced. Nikiforov-Uvarov method and SUSYQM with Hamiltonian Hierarchy method is used in the calculations to get energy eigenvalues and the corresponding wave functions exactly.

Keywords: Nikiforov-Uvarov Method, Supersymmetric Quantum Mechanics, Morse Potential, Eckart Potential, Hua Potential.

ÖZ

BAZI ÇİFT ATOMLU POTANSİYELLER ÜZERİNE SÜPER SİMETRİK QUANTUM MEKANİĞİ UYGULAMALARI

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Tek boyutlu moleküler potansiyeller deforme Morse, Eckart, Hua gibi bilinen bazı potansiyeller için Schrödinger denklemini çözülerek çalışıldı. Hamilton Hiyerarşi'nin parametrik genellemesi gösterildi. Enerji özdeğerleri ve ilgili dalga fonksiyonlarının tam çözümlerinin hesaplamalarında Nikiforov-Uvarov metodu ve süper simetrik kuantum mekaniği Hamilton Hiyerarşi ile beraber kullanıldı.

Anahtar Kelimeler: Nikiforov-Uvarov Metodu, Süper Simetrik Kuantum Mekaniği, Morse Potansiyeli, Eckart Potansiyeli, Hua Potansiyeli.

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CHAPTER I

INTRODUCTION

For the last twenty years, the need for the solution of the Schrodinger equation (SE) occurred in many fields of physics and chemistry [1–7]. Unfortunately it is not generally possible to obtain analytical solutions of the SE because of the potential term except some potentials such as harmonic oscillator potential [8], Kratzer potential [9], etc. The most well known method for solving such an equation is to expand the solution in a power series and then find the expansion coefficients with help of the recursion relationships. In mathematical physics many other analytical techniques have been developed some of which are group theory [10], supersymmetry [11-19], point canonical transformation [20], shifted 1/N expansion [21], asymptotic iteration method [22], quantization rules [23, 24], wave function ansatz method [25, 26], variational, Nikiforov-Uvarov method [27-29], hypervirial perturbation [30], perturbative formalism [31], path integral approach [32] and polynomial solution [33], etc.

Nikiforov-Uvarov method (NUM) and Supersymmetry (SUSY) are the methods which are studied and used to solve some potentials in this thesis. Since a few decades, there has been a significant increase in the number of studies in which Nikiforov-Uvarov (NU) method is used for solving quantum mechanical problems. This method is improved to solve certain kind of second-order linear differential equations. The NU method is one of the easiest, most systematic and direct methods which are used to solve SE for some potentials [28].

On the other side, supersymmetry is a symmetry which is used to understand all particle interactions in nature by the relations between fermions and bosons [13]. SUSY connects every fermion and boson with each other one by one in particle physics. In this context, supersymmetric quantum mechanics (SUSYQM) was introduced as a method for testing the breaking of supersymmetry [14-15]. As the SUSY work progressed, it was understood that this method offers much more than a simple model testing of field theory methods. As a simple statement, for a given potential V_- a partner potential V_+ is created with a new Hamiltonian H_2 by using SUSY. These potentials have identical energy eigenvalue spectrum except for the ground state. This method uses factorization of Hamiltonian. When this method is applied together with the Hamilton Hierarchy [15] method and shape invariance [13, 16-19] concept, it becomes a very powerful tool to find the energy spectrum and wave functions of some Hamiltonians.

In this thesis, the parametric generalization of NU method [29, 34-35] is applied to the solution of the SE by using SUSY quantum mechanics. Firstly, ground state wave function is obtained. Then superpotential and partner potentials are calculated. We found energy eigenvalues with the help of shape invariance. Eigenfunctions and related energy eigenvalues are calculated for the some potentials exactly. These potentials are Morse, [36] Eckart [37], and Hua [38] potentials.

The organization of the thesis is as follows: In Chapter II, firstly the NU method is explained. Then, parametric generalization of this method is presented. In Chapter III, respectively SUSYQM, Hamiltonian Hierarchy Method, Shape Invariance reviewed and parametric generalization of Hamiltonian Hierarchy [35] is described with shape invariance condition. In Chapter IV, dynamics of diatomic molecules explained and some of one dimensional molecular potentials are introduced. In Chapter V, we present the solutions of the SE for some potentials. In the last chapter, conclusions are given.

CHAPTER II

THE NIKIFOROV-UVAROV METHOD

2.1 General

A very systematic method to solve the non-relativistic SE analytically for some kind of potentials is to use the Nikiforov-Uvarov method. In this method, one dimensional SE is transformed to a hypergeometric-type equation with coordinate transformation $x = x(s)$. Then NU method is used to find exact solutions of the SE in terms of special orthogonal functions [21].

The equation which NU method is based on is [28];

$$\frac{d^2\Psi(s)}{ds^2} + \frac{\tilde{\tau}(s)}{\sigma(s)} \frac{d\Psi(s)}{ds} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)} \Psi(s) = 0 \quad (2.1)$$

Where σ and $\tilde{\sigma}$ are at most second degree polynomials, and $\tilde{\tau}$ is a first-degree polynomial. $\Psi(s)$ is a hypergeometric-type function. The transformation $\Psi(s) = \phi(s)y(s)$ with an appropriate function $\phi(s)$ can be used to transform the Equation (2.1) into more easily solvable form,

$$y''(s) + \left(2 \frac{\phi'(s)}{\phi(s)} + \frac{\tilde{\tau}(s)}{\sigma(s)}\right) y'(s) + \left(\frac{\phi''(s)}{\phi(s)} + \frac{\phi'(s)}{\phi(s)} \frac{\tilde{\tau}(s)}{\sigma(s)} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\right) y(s) = 0 \quad (2.2)$$

Now let us define first degree polynomial $\tau(s)$ with the following equation by using coefficient of the second term of the equation (2.2).

$$2 \frac{\phi'(s)}{\phi(s)} + \frac{\tilde{\tau}(s)}{\sigma(s)} = \frac{\tau(s)}{\sigma(s)}, \quad (2.3)$$

and define $\pi(s)$ as follows,

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \quad (2.4)$$

Solving the equation (2.4) for $\pi(s)$ with the help of equation (2.3), one can get

$$\pi(s) = \frac{1}{2} [\tau(s) - \tilde{\tau}(s)], \quad (2.5)$$

Since the polynomials $\tau(s)$ and $\tilde{\tau}(s)$ are first degree, $\pi(s)$ must be a first degree polynomial. The coefficient of $y(s)$ in Eq.(2.2), can be rewritten as follows by using derivation identity and Eq.(2.4);

$$\frac{\phi''(s)}{\phi(s)} = \left(\frac{\phi'(s)}{\phi(s)} \right)' + \left(\frac{\phi'(s)}{\phi(s)} \right)^2 = \left(\frac{\pi(s)}{\sigma(s)} \right)' + \left(\frac{\pi(s)}{\sigma(s)} \right)^2. \quad (2.6)$$

By using the equality Eq. (2.4), we can deal with the third coefficient in Eq. (2.2) more easily;

$$\frac{\phi''(s)}{\phi(s)} + \frac{\phi'(s)}{\phi(s)} \frac{\tilde{\tau}(s)}{\sigma(s)} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)} = \frac{\Lambda(s)}{\sigma^2(s)} \quad (2.7)$$

$$\left(\frac{\pi(s)}{\sigma(s)} \right)' + \left(\frac{\pi(s)}{\sigma(s)} \right)^2 + \frac{\pi(s)}{\sigma(s)} \frac{\tilde{\tau}(s)}{\sigma(s)} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)} = \frac{\Lambda(s)}{\sigma^2(s)}$$

$$\frac{\pi'(s)\sigma(s) - \sigma'(s)\pi(s)}{\sigma^2(s)} + \frac{\pi^2(s)}{\sigma^2(s)} + \frac{\pi(s)\tilde{\tau}(s)}{\sigma^2(s)} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)} = \frac{\Lambda(s)}{\sigma^2(s)}$$

\Rightarrow

$$\Lambda(s) = \tilde{\sigma}(s) + \pi^2(s) + \pi(s)[\tilde{\tau}(s) - \sigma'(s)] + \pi'(s)\sigma(s) \quad (2.8)$$

If we substitute Eq.(2.3) and Eq.(2.7) into Eq.(2.2), we will get the following equation,

$$y''(s) + \frac{\tau(s)}{\sigma(s)}y'(s) + \frac{\Lambda(s)}{\sigma^2(s)}y(s) = 0 \quad (2.9)$$

If $\Lambda(s) = \lambda\sigma(s)$ with constant λ Eq.(2.9) takes the following form,

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0, \quad (2.10)$$

Defining k as follows;

$$k = \lambda - \pi'(s) \quad (2.11)$$

we can write the Eq.(2.8) in a quadratic equation form for $\pi(s)$,

$$\pi^2(s) + \pi(s)[\tilde{\tau}(s) - \sigma'(s)] + \tilde{\sigma}(s) - k\sigma(s) = 0, \quad (2.12)$$

We can solve this quadratic equation by using well known discriminant formula;

$$\pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)} \quad (2.13)$$

Since $\pi(s)$, $\sigma'(s)$ and $\tilde{\tau}(s)$ are first degree polynomials, the term with square root must be a polynomial of degree one. So the expression in the square root sign must be exact square of a first degree polynomial. As a result of this information we can write a discriminant equation for constant k . Since the expression in the square root sign is an exact square, its discriminant must be equal to zero.

As we know the polynomials $\sigma(s)$, $\tilde{\sigma}(s)$ and $\tilde{\tau}(s)$ by definition with the help of Eq. (2.1), we can calculate the only unknown “k” using discriminant formula. As soon as we determine k, polynomials $\pi(s)$, $\tau(s)$ and λ are calculated from Eq.(2.5), Eq.(2.11) and Eq.(2.13).

$$\lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s), \quad (n = 0,1,2, \dots) \quad (2.14)$$

We can also write from equation (2.11) as follows;

$$\lambda = k + \pi'(s) \quad (2.15)$$

Energy eigenvalues can be obtained by equating λ and λ_n through the equations (2.14) and (2.15). Polynomial hypergeometric-type functions $y_n(s)$ are solved by the Rodrigues relation;

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)] \quad (2.16)$$

With normalization constant B_n and weight function $\rho(s)$ which is calculated through the condition;

$$(\sigma(s)\rho(s))' = \tau(s)\rho(s) \quad (2.17)$$

Using Eq. (2.4) $\phi(s)$ is determined and general solution set becomes

$$\Psi(s) = \phi(s) \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)] \quad (2.18)$$

2.2 Parametric Generalization Of The Nikiforov-Uvarov Method

Now let us introduce the parametric generalization of the NUM [29, 34-35]. The general form of the SE can be written as follows with a suitable coordinate transformation for any potential;

$$\left[\frac{d^2}{ds^2} + \frac{\alpha_1 - \alpha_2 s}{s(1 - \alpha_3 s)} \frac{d}{ds} + \frac{-\xi_1 s^2 + \xi_2 s - \xi_3}{[s(1 - \alpha_3 s)]^2} \right] \Psi = 0 \quad (2.19)$$

Since the Eq. (2.19) must be equal to Eq. (2.1);

$$\tilde{\tau}(s) = \alpha_1 - \alpha_2 s \quad (2.20)$$

$$\sigma(s) = s(1 - \alpha_3 s) \quad (2.21)$$

$$\tilde{\sigma}(s) = -\xi_1 s^2 + \xi_2 s - \xi_3 \quad (2.22)$$

Rewriting Eq. (2.13) to calculate $\pi(s)$;

$$\pi(s) = \alpha_4 + \alpha_5 s \pm \sqrt{(\alpha_6 - k\alpha_3)s^2 + (\alpha_7 + k)s + \alpha_8} \quad (2.23)$$

Where

$$\alpha_4 = \frac{1 - \alpha_1}{2} \quad (2.24)$$

$$\alpha_5 = \frac{(\alpha_2 - 2\alpha_3)}{2} \quad (2.25)$$

$$\alpha_6 = \alpha_5^2 + \xi_1 \quad (2.26)$$

$$\alpha_7 = 2\alpha_4\alpha_5 - \xi_2 \quad (2.27)$$

$$\alpha_8 = \alpha_4^2 + \xi_3 \quad (2.28)$$

We know that the expression in the square root sign in Eq. (2.23) must be square of a first degree polynomial from the previous section. So the discriminant of the the expression in the square root sign must be zero;

$$k^2 + 2(\alpha_7 + 2\alpha_3\alpha_8)k + \alpha_7^2 - 4\alpha_8\alpha_6 = 0 \quad (2.29)$$

So we can solve for k;

$$k_{\mp} = -(\alpha_7 + 2\alpha_3\alpha_8) \mp 2\sqrt{\alpha_8\alpha_6} \quad (2.30)$$

Where

$$\alpha_9 = \alpha_3\alpha_7 + \alpha_3^2\alpha_8 + \alpha_6 \quad (2.31)$$

For k -;

$$\pi(s) = \alpha_4 + \alpha_5s - [(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8})s - \sqrt{\alpha_8}] \quad (2.32)$$

$$\pi'(s) = \alpha_5 - (\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \quad (2.33)$$

Using Eq. (2.5) with Eq. (2.32) we get;

$$\tau(s) = \alpha_1 + 2\alpha_4 - (\alpha_2 - 2\alpha_5)s - 2[(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8})s - \sqrt{\alpha_8}] \quad (2.34)$$

$$\tau'(s) = -(\alpha_2 - 2\alpha_5) - 2[(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8})] \quad (2.35)$$

Remembering the Eq. (2.21);

$$\sigma'(s) = -2\alpha_3 s + 1 \quad (2.36)$$

$$\sigma''(s) = -2\alpha_3 \quad (2.37)$$

Now we will insert the Eqs. (2.35 and 2.37) into Eq. (2.14) and insert the Eq. (2.30) of k - and (2.33) into Eq. (2.15) and equate λ_n and λ ;

$$\begin{aligned} & \alpha_2 n - 2\alpha_5 n + 2(\sqrt{\alpha_9} + \alpha_3 \sqrt{\alpha_8})n + n(n-1)\alpha_3 \\ & = -\alpha_7 - 2\alpha_3 \alpha_8 - 2\sqrt{\alpha_8 \alpha_9} + \alpha_5 - \sqrt{\alpha_9} - \alpha_3 \sqrt{\alpha_8} \\ \Rightarrow & \\ & \alpha_2 n - (2n+1)\alpha_5 + (2n+1)(\sqrt{\alpha_9} + \alpha_3 \sqrt{\alpha_8}) + n(n-1)\alpha_3 + \alpha_7 \\ & + 2\alpha_3 \alpha_8 + 2\sqrt{\alpha_8 \alpha_9} = 0 \end{aligned} \quad (2.38)$$

Remembering Eq. (2.17);

$$\begin{aligned} & (\sigma(s)\rho(s))' = \tau(s)\rho(s) \\ & \sigma'(s)\rho(s) + \sigma(s)\rho'(s) = \tau(s)\rho(s) \\ & \sigma'(s) + \frac{\sigma(s)\rho'(s)}{\rho(s)} = \tau(s) \\ \Rightarrow & \\ & \frac{\rho'(s)}{\rho(s)} = \frac{\tau(s) - \sigma'(s)}{\sigma(s)}, \quad (2.39) \\ & \frac{d(\ln \rho(s))}{ds} = \frac{\tau(s) - \sigma'(s)}{\sigma(s)} \end{aligned}$$

Eqs. (2.21, 2.34 and 2.36) are inserted to get;

$$\begin{aligned} & d(\ln \rho(s)) \\ &= \frac{\alpha_1 + 2\alpha_4 - (\alpha_2 - 2\alpha_5)s - 2[(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8})s - \sqrt{\alpha_8}] + 2\alpha_3s - 1}{s(1 - \alpha_3s)} ds \end{aligned}$$

Using Eq. (2.25);

$$d(\ln \rho(s)) = \frac{\alpha_1 + 2\alpha_4 - 2[(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8})s - \sqrt{\alpha_8}] - 1}{s(1 - \alpha_3s)} ds$$

$$d(\ln \rho(s)) = \frac{-\alpha_{11}s + 2\alpha_3s + \alpha_{10} - 1}{s(1 - \alpha_3s)} ds$$

Where

$$\alpha_{10} = \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8} \quad (2.40)$$

$$\alpha_{11} = \alpha_2 - 2\alpha_5 + 2(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \quad (2.41)$$

Solving for $\rho(s)$;

$$\rho(s) = s^{(\alpha_{10}-1)}(1 - \alpha_3s)^{\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1} \quad (2.42)$$

Now the solution of the Eq. (2.16) by using Eq. (2.42) becomes,

$$y_n(s) = P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}(1 - 2\alpha_3s) \quad (2.43)$$

where $P_n^{(\alpha,\beta)}$ are Jacobi polynomials. When we put Eq. (2.32) into Eq. (2.4) we solve,

$$\phi(s) = s^{\alpha_{12}}(1 - \alpha_3s)^{-\alpha_{12}-\frac{\alpha_{13}}{\alpha_3}} \quad (2.44)$$

With,

$$\alpha_{12} = \alpha_4 + \sqrt{\alpha_8} \quad (2.45)$$

$$\alpha_{13} = \alpha_5 - (\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \quad (2.46)$$

And,

$$\Psi(s) = \phi(s)y(s)$$

$$\Psi(s) = s^{\alpha_{12}}(1 - \alpha_3 s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_3}} P_n^{\left(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1\right)} (1 - 2\alpha_3 s) \quad (2.47)$$

Now we will examine the case where $\alpha_3 = 0$. Firstly let's consider second factor in the right hand side of Eq. (2.47);

$$\begin{aligned} C &= \lim_{\alpha_3 \rightarrow 0} \left[(1 - \alpha_3 s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_3}} \right] \\ \ln C &= \lim_{\alpha_3 \rightarrow 0} \ln \left[(1 - \alpha_3 s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_3}} \right] \\ &= - \lim_{\alpha_3 \rightarrow 0} \frac{(\alpha_{12}\alpha_3 + \alpha_{13}) \ln[1 - \alpha_3 s]}{\alpha_3} \end{aligned}$$

Applying L'Hopital Rule;

$$\begin{aligned} \ln C &= - \lim_{\alpha_3 \rightarrow 0} [\alpha_{12} \ln(1 - \alpha_3 s) - (\alpha_{12}\alpha_3 + \alpha_{13})s] \\ &= \alpha_{13}s \end{aligned}$$

So;

$$C = \lim_{\alpha_3 \rightarrow 0} \left[(1 - \alpha_3 s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_3}} \right] = e^{\alpha_{13} s} \quad (2.48)$$

Now we will examine the third factor on the right hand side of Eq. (2.47). If we write definition of Jacobi Polynomials by the Rodriguez formula;

$$P_n^{(a,b)}(x) = \left[\frac{(-1)^n}{2^n n! (1-x)^a (1+x)^b} \right] \cdot \frac{d^n}{dx^n} [(1-x)^{n+a} (1+x)^{n+b}] \quad (2.49)$$

then;

$$P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1)}(1 - 2\alpha_3 s) = \left[\frac{(-1)^n}{2^n n! (2\alpha_3 s)^{\alpha_{10}-1} (2 - 2\alpha_3 s)^{\frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1}} \right] \cdot \frac{d^n}{d(1 - 2\alpha_3 s)^n} \left[(2\alpha_3 s)^{n+\alpha_{10}-1} (2 - 2\alpha_3 s)^{n+\frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1} \right] \quad (2.50)$$

Using Leibniz formula [39];

$$\frac{d^n}{dx^n} [A(x)B(x)] = \sum_{k=0}^n \frac{n!}{k! (n-k)!} \left(\frac{d^{n-k} A}{dx^{n-k}} \right) \left(\frac{d^k B}{dx^k} \right) \quad (2.51)$$

and using

$$\frac{d^n}{d(1 - 2\alpha_3 s)^n} = \frac{(-1)^n}{2^n \alpha_3^n} \frac{d^n}{ds^n} \quad (2.52)$$

in Eq. (2.50) lead us;

$$P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1)}(1 - 2\alpha_3 s) = \left[\frac{(-1)^n}{2^n n! (2\alpha_3 s)^{\alpha_{10}-1} (2 - 2\alpha_3 s)^{\frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1}} \right] \cdot \frac{(-1)^n}{(2\alpha_3)^n} \sum_{k=0}^n \left[\left(\frac{n!}{k! (n-k)!} \frac{(n + \alpha_{10} - 1)!}{(k + \alpha_{10} - 1)!} (2\alpha_3)^{n-k} (2\alpha_3 s)^{k+\alpha_{10}-1} \right) \cdot \frac{\left(n + \frac{\alpha_{11}}{\alpha_3} - \alpha_{10} - 1 \right)!}{\left(n + \frac{\alpha_{11}}{\alpha_3} - \alpha_{10} - 1 - k \right)!} (-2\alpha_3)^k (2 - 2\alpha_3 s)^{n+\frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1-k} \right]$$

⇒

$$\begin{aligned}
& P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}(1-2\alpha_3s) = \\
& \frac{1}{2^{2n+\frac{\alpha_{11}}{\alpha_3}-2} \alpha_3^{n+\alpha_{10}-1} s^{\alpha_{10}-1} (1-\alpha_3s)^{\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1}} \\
& \sum_{k=0}^n \frac{(-1)^k (n+\alpha_{10}-1)! \left(n+\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1\right)!}{k!(n-k)!(k+\alpha_{10}-1)! \left(n+\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1-k\right)!} \\
& 2^{2n+\frac{\alpha_{11}}{\alpha_3}-2} \alpha_3^{n+k+\alpha_{10}-1} s^{k+\alpha_{10}-1} (1-\alpha_3s)^{n+\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1-k}
\end{aligned}$$

⇒

$$\begin{aligned}
& P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}(1-2\alpha_3s) = \\
& \sum_{k=0}^n \frac{(-1)^k (n+\alpha_{10}-1)! \left(n+\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1\right)!}{k!(n-k)!(k+\alpha_{10}-1)! \left(n+\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1-k\right)!} \alpha_3^k s^k (1-\alpha_3s)^{n-k} \quad (2.53)
\end{aligned}$$

If we use

$$\begin{aligned}
& \frac{\left(n+\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1\right)!}{\left(n+\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1-k\right)!} = \frac{\left(\frac{\alpha_{11}+\alpha_3(n-\alpha_{10}-1)}{\alpha_3}\right)!}{\left(\frac{\alpha_{11}+\alpha_3(n-\alpha_{10}-1-k)}{\alpha_3}\right)!} = \\
& \frac{[\alpha_{11}+\alpha_3(n-\alpha_{10}-1)][\alpha_{11}+\alpha_3(n-\alpha_{10}-2)] \dots [\alpha_{11}+\alpha_3(n-\alpha_{10}-k)]}{\alpha_3^k}
\end{aligned}$$

in Eq (2.53) then;

$$\begin{aligned}
& P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}(1-2\alpha_3s) = \\
& \sum_{k=0}^n \frac{(-1)^k (n+\alpha_{10}-1)!}{k!(n-k)!(k+\alpha_{10}-1)!} s^k (1-\alpha_3s)^{n-k} \\
& [\alpha_{11}+\alpha_3(n-\alpha_{10}-1)] \dots [\alpha_{11}+\alpha_3(n-\alpha_{10}-k)] \quad (2.54)
\end{aligned}$$

If $\alpha_3 = 0$ in a problem, Eq (2.54) becomes;

$$P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}(1-2\alpha_3 s) = \sum_{k=0}^n \frac{(-1)^k}{k! (n-k)!} \frac{(n+\alpha_{10}-1)!}{(k+\alpha_{10}-1)!} s^k \alpha_{11}^k \quad (2.55)$$

This is in the form of associated Laguerre polynomials [39]:

$$L_n^a(x) = \sum_{k=0}^n (-1)^k \frac{(n+a)! x^k}{(n-k)! (k+a)! k!} \quad (2.56)$$

So for $\alpha_3 = 0$;

$$P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}(1-2\alpha_3 s) = L_n^{(\alpha_{10}-1)}(\alpha_{11} s) \quad (2.57)$$

Finally we can write the complete wave function for $\alpha_3 = 0$ using Eqs.(2.48 and 2.57);

$$\Psi(s) = s^{\alpha_{12}} e^{\alpha_{13} s} L_n^{(\alpha_{10}-1)}(\alpha_{11} s) \quad (2.58)$$

CHAPTER III

SUSYQM

3.1 General

Supersymmetry is a symmetry which is used to understand all particle interactions in nature by the relations between fermions and bosons. These particles are called superpartners of each other. If SUSY really exists in nature, then every superpartners should have equal mass and quantum numbers except spin numbers. Since SUSY foresees that every elementary particle has a superpartner, the scope of the standard model raises the double in the framework of a unified theory explaining the fundamental interactions in nature [13].

As the SUSY work progressed, it was understood that this method offers much more than a simple model testing of field theory methods. Super-symmetric quantum mechanics has helped a better understanding of the non-relativistic quantum mechanics. It explains why only certain potentials have analytical solutions and furthermore discovered potentials with analytical solutions. It also uses the factorization method, and when used in conjunction with the shape invariant condition, has led to the identification of a potential class which can be solved analytically [19].

Firstly, factorisation process should be illustrated. Consider the one dimensional quantum mechanical Hamiltonian for the ground state wavefunction $\Psi_0(x)$;

$$H_1 \Psi_0(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x) \right] \Psi_0(x) \quad (3.1)$$

Instead of solving a particular potential, we will develop an approach that enables us to solve varying potentials and thus also general Hamiltonians. In this approach we define the ground state wave function as nodeless, and we will assume that it takes a value of zero in both infinities in order to be normalized. In addition, we will make the ground state energy equal to zero. This does not affect the energy spectrum except for a constant shift. Thus, SE for the ground-state is

$$V_1(x) = \frac{\hbar^2 \Psi_0''(x)}{2m \Psi_0(x)} \quad (3.2)$$

Thus, if we know the ground-state wave function, we can calculate the $V_1(x)$ except the constant term. To apply the super-symmetric quantum mechanics we need to factorise Hamiltonian.

$$H_1 = A^\dagger A \quad (3.3)$$

Where the operators A and A^\dagger are defined as follows;

$$A = W(x) + \frac{\hbar}{\sqrt{2m}} \frac{d}{dx}, \quad A^\dagger = W(x) - \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} \quad (3.4)$$

$W(x)$ term is called super potential. Using equations (3.3) and (3.4) we can write the $V_1(x)$ potential as follows;

$$V_1(x) - W^2(x) + \frac{\hbar}{\sqrt{2m}} W'(x) = 0 \quad (3.5)$$

Equation (3.5) is called the Riccati equation [40]. Equation (3.2) is still valid, and provides additional information about the potential $V_1(x)$. If $A\Psi_0(x)$ value is zero, then it is clear that $A^\dagger A\Psi_0(x) = H_1\Psi_0(x)$ is to be zero. In this case, $W(x)$ values can be written in terms of the known ground state function. This also means that A operator is an annihilation operator. We find a general solution of the ground-state wave function in terms of $W(x)$ with the help of A operator. Since it destroys the ground-state wave function, we arrive at the following solution.

$$A\Psi_0(x) = \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} \Psi_0(x) + W(x)\Psi_0(x) = 0 \quad (3.6)$$

$$\Rightarrow W(x) = -\frac{\hbar}{\sqrt{2m}} \left(\frac{\Psi_0'}{\Psi_0} \right) = -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} \ln[\Psi_0(x)] \quad (3.7)$$

$$\Rightarrow \Psi_0(x) = N \exp \left[-\frac{\sqrt{2m}}{\hbar} \int^x W(k) dk \right] \quad (3.8)$$

So it is seen that if we know the super potential, we can turn the second-order differential equation to first order differential equation. Hereby SUSY provides a great advantage over the standard quantum mechanics. Now we need to define a new Hamilton (H_2) by reversing the order of factorization to create the SUSY theory. H_1 and H_2 are partner Hamiltonians of each other. Now we will repeat the calculations to get V_2 as we did to get V_1 .

$$H_2 = AA^\dagger = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_2(x) \right] \quad (3.9)$$

and this yields

$$V_2(x) = W^2(x) + \frac{\hbar}{\sqrt{2m}} W'(x) \quad (3.10)$$

The potentials $V_1(x)$ and $V_2(x)$ are called supersymmetric partner potentials. We will see that the partner Hamiltonians H_1 and H_2 , their energy eigenvalues and wave functions are related through SUSY.

Let $\Psi_n^{(1)}$ and $\Psi_n^{(2)}$ be the eigenfunctions and $E_n^{(1)}$ and $E_n^{(2)}$ the energy eigenvalues of Hamiltonians H_1 and H_2 where “n” is the the number of nodes starting from 0. Now we will see that bound states of potentials $V_1(x)$ and $V_2(x)$ completely the same except for the ground state energy $E_0^{(1)} = 0$.

$$\begin{aligned} H_1 \Psi_n^{(1)}(x) &= A^\dagger A \Psi_n^{(1)}(x) \\ &= E_n^{(1)} \Psi_n^{(1)}(x) \end{aligned} \quad (3.11)$$

Using this,

$$\begin{aligned} H_2 [A \Psi_n^{(1)}(x)] &= (A A^\dagger) [A \Psi_n^{(1)}(x)] \\ &= A [A^\dagger A \Psi_n^{(1)}(x)] \\ &= A [H_1 \Psi_n^{(1)}(x)] \end{aligned}$$

\Rightarrow

$$H_2 [A \Psi_n^{(1)}(x)] = E_n^{(1)} A \Psi_n^{(1)}(x) \quad (3.12)$$

Here we are convinced that if $\Psi_n^{(1)}(x)$ is eigenfunction of H_1 then $A \Psi_n^{(1)}$ is an eigenfunction of H_2 with the same eigenvalue $E_n^{(1)}$. Now let us repeat the same calculations by switching H_1 and H_2 ,

$$\begin{aligned} H_2 \Psi_m^{(2)}(x) &= A A^\dagger \Psi_m^{(2)}(x) \\ &= E_m^{(2)} \Psi_m^{(2)}(x) \end{aligned} \quad (3.13)$$

Using this,

$$\begin{aligned}
H_1[A^\dagger\Psi_m^{(2)}(x)] &= (A^\dagger A)[A^\dagger\Psi_m^{(2)}(x)] \\
&= A^\dagger[AA^\dagger\Psi_m^{(2)}(x)] \\
&= A^\dagger[H_2\Psi_m^{(2)}(x)]
\end{aligned}$$

⇒

$$= E_m^{(2)} A^\dagger\Psi_m^{(2)}(x) \quad (3.14)$$

So similarly we see that if $\Psi_m^{(2)}(x)$ is an eigenfunction of H_2 then $A^\dagger\Psi_m^{(2)}(x)$ is an eigenfunction of H_1 with the same eigenvalue $E_m^{(2)}$. With the help of last calculations it is inevitable that

$$E_m^{(2)} = E_n^{(1)} \quad (3.15)$$

If we assume that the eigenfunctions of H_1 is normalised then we can calculate the normalized eigenfunctions $\Psi_m^{(2)}(x)$ of H_2 as follows;

$$\begin{aligned}
1 &= \int Z\Psi_m^{*(2)}Z\Psi_m^{(2)} \quad (3.16) \\
&= Z^2 \int \Psi_n^{(1)}A^\dagger A\Psi_n^{(1)} \\
&= Z^2 \int \Psi_n^{(1)} H_1\Psi_n^{(1)} \\
&= Z^2 E_n^{(1)}
\end{aligned}$$

⇒

$$Z = [E_n^{(1)}]^{-\frac{1}{2}} \quad (3.17)$$

In Eq. (3.18) “Z” is not the normalization constant. Normalization constant “N” is embedded in the right hand side of the Eq. (3.18). Now we can write normalized eigenfunctions of H_2 ;

$$\Psi_m^{(2)} = [E_n^{(1)}]^{-\frac{1}{2}} A\Psi_n^{(1)} \quad (3.18)$$

We also can calculate $\Psi_n^{(1)}$ starting from $\Psi_m^{(2)}$;

$$\begin{aligned} A^\dagger \Psi_m^{(2)} &= [E_n^{(1)}]^{-\frac{1}{2}} A^\dagger A \Psi_n^{(1)} \\ &= [E_n^{(1)}]^{-\frac{1}{2}} H_1 \Psi_n^{(1)} \\ &= [E_n^{(1)}]^{-\frac{1}{2}} E_n^{(1)} \Psi_n^{(1)} \end{aligned} \quad (3.19)$$

\Rightarrow

$$\Psi_n^{(1)} = [E_m^{(2)}]^{-\frac{1}{2}} A^\dagger \Psi_m^{(2)} \quad (3.20)$$

Since $A\Psi_0(x) = 0$ by definition H_2 does not have any eigenfunction with zero energy ground state. Now we can define $m = n - 1$ through equations (3.11)-(3.17) and so we can conclude the relations between eigenstates and eigen values of H_1 and H_2 as follows;

$$\Psi_n^{(2)} = [E_{n+1}^{(1)}]^{-\frac{1}{2}} A \Psi_{n+1}^{(1)} \quad (3.21)$$

$$\Psi_{n+1}^{(1)} = [E_n^{(2)}]^{-\frac{1}{2}} A^\dagger \Psi_n^{(2)} \quad (3.22)$$

$$E_n^{(2)} = E_{n+1}^{(1)} \quad (3.23)$$

for $n = 0, 1, 2, \dots$ and $E_n^{(1)} = 0$. If the eigenfunctions $\Psi_{n+1}^{(1)}$ normalizable, then the eigenfunctions $\Psi_n^{(2)}$ are also normalizable. In addition, the operator A turns eigenfunctions of H_1 to eigenfunctions of H_2 and the operator A^\dagger turns eigenfunctions of H_2 to eigenfunctions of H_1 with the same energy eigenvalues. Furthermore A annihilates and A^\dagger creates a node in the related eigenfunctions. As a result, we can say that if we know the all eigenfunctions and eigenvalues of H_1 we can determine the solution of H_2 and if we know the all eigenfunctions and eigenvalues of H_2 we can determine the solution of H_1 by using A and A^\dagger operators.

3.2 Hierarchy of Hamiltonians

In the previous section, we observed that the energy of the ground state must be zero in order to factorise the Hamiltonian. This is accomplished by shifting the ground state energy up to a constant. With the aid of the factorisation of Hamiltonian we have constructed a partner Hamiltonian with the same energy spectrum except for the ground state. The number of bound states of the second Hamiltonian should be one less than the number of bound states of the second Hamiltonian. If we apply the same idea to H_2 as we did to H_1 , we can achieve a new Hamiltonian H_3 that is partner to H_2 . It will also be partner Hamiltonian of H_1 . To do so, we should equate ground state energy of H_2 to zero by shifting. After that, we can create the partner Hamiltonian H_3 by using the principles developed in the previous section. We can find a set Hamiltonians by applying this process again and again. Each new Hamiltonian will have one missing bound state from the previous one. This iteration can be applied as many times as the number of bound states of H_1 . Therefore, we can obtain all of the energy eigenvalues and eigenfunctions of a set of partner Hamiltonians if we have a Hamiltonian H_1 with an analytically solvable potential. Similarly, we know all of the ground states of set of partner Hamiltonians, we can create solutions to actual problem. This is a very powerful tool when it is used together with shape invariance described in the next section.

Let $\Psi_0^{(1)}$ and $E_0^{(1)}$ be the ground state eigenfunction and ground state energy of H_1 respectively. Then from Eq. (3.3),

$$H_1(x)\Psi_n^1(x) = [A_1^\dagger A_1 + E_0^{(1)}]\Psi_n^1(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x) \right] \Psi_n^1(x) \quad (3.24)$$

where a zero energy ground state of the H_1 is obtained by shifting. Then following Eq. (3.5), $V_1(x)$ is rewritten as

$$V_1(x) = W_1^2(x) - \frac{\hbar}{\sqrt{2m}} W_1'(x) + E_0^{(1)} \quad (3.25)$$

where

$$A_1 = \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W_1(x), A_1^\dagger = -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W_1(x), \quad (3.26)$$

$$W_1(x) = \frac{\hbar}{\sqrt{2m}} \frac{\Psi_0^{(1)'}(x)}{\Psi_0^{(1)}(x)} = -\frac{\hbar}{\sqrt{2m}} \frac{d \ln \Psi_0^{(1)}}{dx} \quad (3.27)$$

following from Eqs. (3.4) and (3.7). Since we have to consider many super partners, it is very important to use indices carefully. As we continue,

$$H_2(x) \Psi_n^2(x) = [A_1 A_1^\dagger + E_0^{(1)}] \Psi_n^2(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_2(x) \right] \Psi_n^2(x) \quad (3.28)$$

with

$$\begin{aligned} V_2(x) &= W_1^2(x) + \frac{\hbar}{\sqrt{2m}} W_1'(x) + E_0^{(1)} = V_1(x) + 2 \frac{\hbar}{\sqrt{2m}} W_1' \\ &= V_1(x) - 2 \frac{\hbar}{\sqrt{2m}} \frac{d^2}{dx^2} \ln \Psi_0^{(1)} \end{aligned} \quad (3.29)$$

gives

$$\begin{aligned} E_n^{(2)} &= E_{n+1}^{(1)} \\ \Psi_n^{(2)} &= (E_{n+1}^{(1)} - E_0^{(1)})^{-\frac{1}{2}} A_1 \Psi_{n+1}^{(1)} \end{aligned} \quad (3.30)$$

What we do here is actually the same as what we did in the previous section. Based on the fact that $E_0^{(2)}$, the ground state energy of H_2 , is equal to $E_1^{(1)}$ Hamiltonian H_3 can be constructed. But firstly H_2 should be written as follows;

$$\begin{aligned}
H_2 \Psi_n^2(x) &= [A_1 A_1^\dagger + E_0^{(1)}] \Psi_n^2(x) = [A_2^\dagger A_2 + E_0^{(2)}] \Psi_n^2(x) \\
&= [A_2^\dagger A_2 + E_1^{(1)}] \Psi_n^2(x)
\end{aligned} \tag{3.31}$$

with

$$A_2 = \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W_2(x), \quad A_2^\dagger = -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W_2(x), \tag{3.32}$$

$$W_2(x) = -\frac{\hbar}{\sqrt{2m}} \frac{d \ln \Psi_0^{(2)}}{dx}. \tag{3.33}$$

Then H_3 is obtained by the same method we did to obtain H_2 but this time we will use A_2 instead of A_1 .

$$H_3 \Psi_n^3(x) = [A_2 A_2^\dagger + E_1^{(1)}] \Psi_n^3(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_3(x) \right] \Psi_n^3(x), \tag{3.34}$$

Then the related potential becomes;

$$\begin{aligned}
V_3(x) &= W_2^2(x) + \frac{\hbar}{\sqrt{2m}} W_2'(x) + E_1^{(1)} = V_2(x) + 2 \frac{\hbar}{\sqrt{2m}} W_2' \\
&= V_2(x) - 2 \frac{\hbar}{\sqrt{2m}} \frac{d^2}{dx^2} \ln \Psi_0^{(2)}
\end{aligned} \tag{3.35}$$

So, by using the expression for $V_2(x)$ which was obtained earlier,

$$\begin{aligned}
V_3(x) &= V_1(x) - 2 \frac{\hbar}{\sqrt{2m}} \frac{d^2}{dx^2} \ln \Psi_0^{(1)} - 2 \frac{\hbar}{\sqrt{2m}} \frac{d^2}{dx^2} \ln \Psi_0^{(2)} \\
&= V_1(x) - 2 \frac{\hbar}{\sqrt{2m}} \frac{d^2}{dx^2} \ln(\Psi_0^{(1)} \Psi_0^{(2)})
\end{aligned} \tag{3.36}$$

Again, now some relations can be written for H_3 ;

$$E_n^3 = E_{n+1}^{(2)} = E_{n+2}^{(1)} \quad (3.37)$$

$$\begin{aligned} \Psi_n^{(3)} &= (E_{n+1}^{(2)} - E_0^{(2)})^{-\frac{1}{2}} A_2 \Psi_{n+1}^{(2)} \\ &= (E_{n+2}^{(1)} - E_1^{(1)})^{-\frac{1}{2}} (E_{n+2}^{(1)} - E_0^{(1)})^{-\frac{1}{2}} A_2 A_1 \Psi_{n+2}^{(1)} \end{aligned} \quad (3.38)$$

where Eq. (3.30) was used for $\Psi_{n+1}^{(2)}$. This means that the solutions of H_3 completely can be written in terms of the solutions of H_1 . It is also possible for all partner Hamiltonians in this hierarchy. So it can be seen that H_1 , which has $k \geq 1$ bound states having eigenfunctions $\Psi_n^{(1)}$ and energy eigenvalues $E_n^{(1)}$ with $0 \leq n \leq k$, lets us to always construct a hierarchy of $k - 1$ Hamiltonians. Those Hamiltonians' eigenvalues are related with their order in the hierarchy. In other words, the l^{th} Hamiltonian has identical energy spectrum with the first Hamiltonian H_1 , except the $(0, \dots, l-1)$ states. Hence, knowing that H_1 has k bound states, we can always write (for $l = 2, 3, \dots, k$)

$$H_l \Psi_n^l(x) = [A_l A_l^\dagger + E_{l-1}^{(1)}] \Psi_n^l(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_l(x) \right] \Psi_n^l(x), \quad (3.39)$$

with

$$A_l = \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W_l(x), \quad A_l^\dagger = -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W_l(x), \quad (3.40)$$

$$W_l(x) = -\frac{\hbar}{\sqrt{2m}} \frac{d \ln \Psi_0^{(1)}}{dx} \quad (3.41)$$

And thereby the previously derived relations;

$$E_n^3 = E_{n+1}^{(2)} = E_{n+2}^{(1)} \quad (3.42)$$

$$\Psi_n^{(1)} = (E_{n+1}^{(1)} - E_{l-2}^{(1)})^{-\frac{1}{2}} \dots (E_{n+1}^{(1)} - E_0^{(1)})^{-\frac{1}{2}} A_{l-1} \dots A_1 \Psi_{n+1}^{(1)} \quad (3.43)$$

$$V_l(x) = V_1(x) - 2 \frac{d^2}{dx^2} \ln(\Psi_0^{(1)} \dots \Psi_0^{(l-1)}). \quad (3.44)$$

Thus, we can find all the energy eigenvalues and eigenfunctions of Hamiltonians in this hierarchy. In this way, we can get the solutions of all Hamiltonians immediately if we know the solutions of a Hamiltonian which is related to them all super symmetrically. Lastly, to get the exact energy eigenvalues the constant value by which ground state energy of H_1 was shifted should be added back.

3.3 Shape Invariance

We can not say that there are too many potentials which can be analytically solvable in quantum mechanics. The condition that decides which potentials are analytically solvable was not known until the shape invariant condition discovered. Many of the exactly solvable potentials are shape invariant and some of them [19] are Morse, Eckart, Coulomb and Pöschl-Teller [41-43] potentials. Now we will explain what a shape invariant potential (SIP) means and show how we can employ shape invariant condition together with Hamilton Hierarchy to solve SE for some potentials.

Let us start with considering potentials V_1 and V_2 which are partner potentials by SUSY. If V_1 and V_2 have similar shapes but their parameters are different then they are said to be shape invariant. This is expressed mathematically as follows;

$$V_2(x; a_1) = V_1(x; a_2) + R(a_1) \quad (3.45)$$

Here a_1 and a_2 are two groups of parameters where $a_2 = f(a_1)$ which means a_2 is a function of a_1 . The terms which are independent of x are expressed as $R(a_1)$. If the SUSY is not broken the eigenfunctions and energy eigenvalues of any SIP can be determined easily by using equation (3.21) and the Hamiltonian hierarchy illustrated in the previous chapter.

Let us consider two partner Hamiltonians connected through unbroken SUSY. Then from section 2.1 we know that

$$E_0^{(1)}(a_0) = 0 \quad (3.46)$$

$$\Psi_0^{(1)}(x; a_0) = N. \exp\left(-\frac{\sqrt{2m}}{\hbar} \int^x W_1(k; a_0) dk\right) \quad (3.47)$$

By using the hierarchy of Hamiltonians and Eq. (3.45), we can write Hamiltonian H_1 and H_2 ;

$$H_1 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_1) \quad (3.48)$$

and

$$\begin{aligned} H_2 &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_2(x; a_1) \\ &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_2) + R(a_1) \end{aligned} \quad (3.49)$$

where Eq. (3.45) was used. Now we will repeat the same procedure for H_2 . First of all we must make H_2 proper for the factorisation. So H_2 has to be shifted by the amount of $R(a_1)$ in order to create a zero energy ground state. Then shape invariance condition is implemented to construct H_3 ;

$$\begin{aligned}
H_3 &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_2(x; a_2) \\
&= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_3) + R(a_2)
\end{aligned} \tag{3.50}$$

By the help of Eq. (3.45) and $a_3 = f(a_2) = f(f(a_1))$. Remembering that we have shifted H_2 by $R(a_1)$ to get this result, we have to shift H_3 back by $R(a_1)$, leading to following results,

$$\begin{aligned}
H_1 &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_1) \\
H_2 &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_2) + R(a_1) \\
H_3 &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_3) + R(a_2) + R(a_1)
\end{aligned} \tag{3.51}$$

The rule that is governing the shape invariant Hamiltonians can be realised easily by a careful observation. Now we can generalise this rule for any partner Hamiltonian in this ranking;

$$H_k = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_k) + \sum_{i=1}^{k-1} R(a_i) \tag{3.52}$$

Thus we can use the obtained Hamiltonians to determine all energy eigenvalues of H_1 or in other words of all partner Hamiltonians. Let us apply the SE to H_2

$$\begin{aligned}
H_2 \Psi_0^{(1)}(x; a_2) &= \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_2) \right] \Psi_0^{(1)}(x; a_2) + R(a_1) \Psi_0^{(1)}(x; a_2) \\
&= R(a_1) \Psi_0^{(1)}(x; a_2)
\end{aligned} \tag{3.53}$$

By using

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_2) \right] \Psi_0^{(1)}(x; a_2) = H_1 \Psi_0^{(1)}(x; a_2) = 0 \quad (3.54)$$

since SUSY is unbroken, $E_0^{(1)}$ is zero. Thus Eq. (3.53) yields;

$$E_0^{(2)} = R(a_1) \quad (3.55)$$

So we can see that one can simply write the ground state energy $E_0^{(2)}$ of H_2 by just calculating the remainder $R(a_1)$. As we know it is also the first excited state of H_1 . This method enable us find out the ground energy of potentials by just comparing the shapes of the partner potentials. We can generalise the expression to find the ground energy of k^{th} Hamiltonian H_k ;

$$\begin{aligned} H_k \Psi_0^{(1)}(x; a_k) &= \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_1(x; a_k) \right] \Psi_0^{(1)}(x; a_k) + \sum_{i=1}^{k-1} R(a_i) \Psi_0^{(1)}(x; a_k) \\ &= \sum_{i=1}^{k-1} R(a_i) \Psi_0^{(1)}(x; a_k) \end{aligned} \quad (3.56)$$

$$\rightarrow E_0^{(k)} = \sum_{i=1}^{k-1} R(a_i) \quad (3.57)$$

Eq. (3.57) allows us to determine the first energy eigenvalue of the k^{th} Hamiltonian H_k . Since the ground state energy of the H_k is equal to $(k - 1)$ 'th energy eigenvalue of the H_1 , we can determine the whole energy eigenvalue spectrum of H_1 and of all partner Hamiltonians except first $k - 1$ energy levels. General formula is written as;

$$E_k^{(1)} = \sum_{i=1}^k R(a_i), \quad E_0^{(1)} = 0 \quad (3.58)$$

So we can say that it is possible to determine the eigenstates $\Psi_n^{(1)}(x; a_1)$ of shape invariant potentials from the ground state wave function $\Psi_0^{(1)}(x; a_1)$. $\Psi_0^{(1)}(x; a_1)$ can be found through Eq. (3.8) with help of super potential. Operators A and A^\dagger are used to do this since these operators convert the wave functions of any super symmetric Hamiltonian to a wave function of its partner Hamiltonian with the same energy level. We can write the ground state wave function of H_s as $\Psi_0^{(1)}(x; a_s)$ by using Eq. (3.56). Now with help of the equation (3.22) we can reach s 'th eigenfunction of H_1 , $\Psi_s^{(1)}(x; a_1)$, by using operators $[A^\dagger(x; a_{s-1}), A^\dagger(x; a_{s-2}) \dots A^\dagger(x; a_1)]$ one by one on $\Psi_0^{(1)}(x; a_s)$;

$$\Psi_n^{(1)}(x; a_1) \propto A^\dagger(x; a_1) A^\dagger(x; a_2) \dots A^\dagger(x; a_n) \Psi_0^{(1)}(x; a_{n+1}) \quad (3.59)$$

but it is not normalised. Hence, the energy eigenvalues and energy eigenfunctions of any shape invariant potential can be determined by knowing the super potential, the remainder and $f(a_1)$. The main importance of shape invariant condition comes from the fact that many of the potentials which we come across through atomic investigations have shape invariance condition.

More useful explicit expressions can be defined for the wave functions with normalised relation as follows,

$$\Psi_n^{(1)}(x; a_1) = \left(E_{n-1}^{(1)}\right)^{\left(-\frac{1}{2}\right)} A^\dagger(x; a_1) \Psi_{n-1}^{(1)}(x; a_2) \quad (3.60)$$

3.4 Parametric Generalization Of The Hamiltonian Hierarchy Method

In this section, very newly generated Parametric Generalization of the Hamiltonian Hierarchy Method [35] will be explained. Ground state wave function for an arbitrary potential can be determined by using Eq. (2.44);

$$\Psi_0(s) = s^{\alpha_{12}}(1 - \alpha_3 s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_3}} \quad (3.61)$$

In additon we can define the super potential $W(r)$ by rewriting Eq. (3.27);

$$W(r) = \frac{d}{dr} \ln \Psi_0(r) \quad (3.62)$$

To make calculations easier let us define;

$$a = \alpha_{12}\alpha_3 + \alpha_{13} \quad (3.63)$$

So we get;

$$\begin{aligned} W(r) &= \frac{ds}{dr} \frac{d}{ds} \ln \left[s^{\alpha_{12}}(1 - \alpha_3 s)^{-\frac{a}{\alpha_3}} \right] \\ &= \frac{1}{s} \frac{ds}{dr} \left[\alpha_{12} - a \frac{s}{\alpha_3 s - 1} \right] \end{aligned} \quad (3.64)$$

If we factorise

$$\frac{s}{\alpha_3 s - 1} = \left[1 + \frac{1}{\alpha_3 s - 1} \right] \frac{1}{\alpha_3}$$

Then,

$$W(r) = \frac{1}{s} \frac{ds}{dr} \left[\alpha_{12} - a \left(1 + \frac{1}{\alpha_3 s - 1} \right) \frac{1}{\alpha_3} \right]$$

$$W(r) = \frac{1}{s} \frac{ds}{dr} \left(\frac{\alpha_3 \alpha_{12} - a}{\alpha_3} - \frac{a}{\alpha_3 (\alpha_3 s - 1)} \right) \quad (3.65)$$

As we remember from section 3.1 the partner potentials are written as follows;

$$V_{\mp} = W^2 \mp \frac{dW}{dr} \quad (3.66)$$

We need to calculate

$$\begin{aligned} \frac{dW(r)}{dr} &= \frac{d^2 s}{dr^2} \frac{1}{s} \left[\frac{\alpha_3 \alpha_{12} - a}{\alpha_3} - \frac{a}{\alpha_3 (\alpha_3 s - 1)} \right] \\ &+ \left(\frac{ds}{dr} \right)^2 \left[-\frac{1}{s^2} \left(\frac{\alpha_3 \alpha_{12} - a}{\alpha_3} - \frac{a}{\alpha_3 (\alpha_3 s - 1)} \right) \right. \\ &\left. + \frac{1}{s} \left(-\frac{a}{\alpha_3} \frac{-\alpha_3}{(\alpha_3 s - 1)^2} \right) \right] \end{aligned} \quad (3.67)$$

$$A = \frac{1}{s^2} \left(\frac{ds}{dr} \right)^2 \quad (3.68)$$

$$B = \frac{1}{s} \frac{d^2 s}{dr^2} \quad (3.69)$$

Then Eq. (3.68) and (3.69) are inserted into Eq. (3.67),

$$\begin{aligned} \frac{dW(r)}{dr} &= B \left[\frac{\alpha_3 \alpha_{12} - a}{\alpha_3} - \frac{a}{\alpha_3 (\alpha_3 s - 1)} \right] \\ &+ A \left[-\left(\frac{\alpha_3 \alpha_{12} - a}{\alpha_3} - \frac{a}{\alpha_3 (\alpha_3 s - 1)} \right) + \left(a \frac{s}{(\alpha_3 s - 1)^2} \right) \right] \\ &= B \frac{\alpha_3 \alpha_{12} - a}{\alpha_3} - B \frac{a}{\alpha_3 (\alpha_3 s - 1)} - A \frac{\alpha_3 \alpha_{12} - a}{\alpha_3} + A \frac{a}{\alpha_3 (\alpha_3 s - 1)} \\ &+ A \frac{a}{\alpha_3 (\alpha_3 s - 1)} \left(1 + \frac{1}{(\alpha_3 s - 1)} \right) \end{aligned}$$

$$= (B - A) \frac{\alpha_3 \alpha_{12} - a}{\alpha_3} + \left[-\frac{a}{\alpha_3} (B - A) + A \frac{a}{\alpha_3} \right] \frac{1}{(\alpha_3 s - 1)} + \frac{a}{\alpha_3} \frac{A}{(\alpha_3 s - 1)^2} \quad (3.70)$$

Now we can put Eq. (3.70) into Eq. (3.66);

$$\begin{aligned} V_{\mp} &= A \left[\frac{\alpha_3 \alpha_{12} - a}{\alpha_3} - \frac{a}{\alpha_3 (\alpha_3 s - 1)} \right]^2 \mp (B - A) \frac{\alpha_3 \alpha_{12} - a}{\alpha_3} \\ &\quad \mp \left[-\frac{a}{\alpha_3} (B - A) + A \frac{a}{\alpha_3} \right] \frac{1}{(\alpha_3 s - 1)} \mp \frac{a}{\alpha_3} \frac{A}{(\alpha_3 s - 1)^2} \\ &= A \left(\frac{\alpha_3 \alpha_{12} - a}{\alpha_3} \right)^2 - A \frac{2a}{\alpha_3^2} \frac{\alpha_3 \alpha_{12} - a}{\alpha_3 s - 1} + A \frac{a^2}{\alpha_3^2 (\alpha_3 s - 1)^2} \\ &\quad \mp (B - A) \frac{\alpha_3 \alpha_{12} - a}{\alpha_3} \mp \left[-\frac{a}{\alpha_3} (B - A) + A \frac{a}{\alpha_3} \right] \frac{1}{\alpha_3 s - 1} \\ &\quad \mp \frac{a}{\alpha_3} \frac{A}{(\alpha_3 s - 1)^2} \\ &= \frac{\alpha_3 \alpha_{12} - a}{\alpha_3} \left[\frac{\alpha_3 \alpha_{12} - a}{\alpha_3} A \mp (B - A) \right] \\ &\quad + \left[\mp \frac{a}{\alpha_3} (A - B) \mp \frac{a}{\alpha_3} A - \frac{2a(\alpha_3 \alpha_{12} - a)}{\alpha_3^2} A \right] \frac{1}{\alpha_3 s - 1} \\ &\quad + \frac{a^2 \mp a \alpha_3}{\alpha_3^2 (\alpha_3 s - 1)^2} A \end{aligned} \quad (3.71)$$

If we put Eq. 3.(64) into Eq. (3.71);

$$\begin{aligned} V_{\mp} &= \left(\frac{-\alpha_{13}}{\alpha_3} \right) \left[\frac{-\alpha_{13}}{\alpha_3} A \mp (B - A) \right] + \frac{a}{\alpha_3} \left[\mp (A - B) \mp A + \frac{2}{\alpha_3} \alpha_{13} A \right] \frac{1}{\alpha_3 s - 1} \\ &\quad + \frac{a(a \mp \alpha_3)}{\alpha_3^2 (\alpha_3 s - 1)^2} A \end{aligned}$$

$$\begin{aligned}
&= \frac{\alpha_{13}^2}{\alpha_3^2} A \mp \frac{\alpha_{13}}{\alpha_3} (A - B) + \left[\frac{2\alpha_{13} \mp \alpha_3}{\alpha_3} A \mp (A - B) \right] \frac{a}{\alpha_3} \frac{1}{\alpha_3 s - 1} \\
&\quad + \frac{a(a \mp \alpha_3)}{\alpha_3^2} \frac{1}{(\alpha_3 s - 1)^2} A
\end{aligned} \tag{3.72}$$

For the shape invariance to be valid $A=B=\text{constant}$, then;

$$V_+ = \frac{\alpha_{13}^2}{\alpha_3^2} A + \left[\frac{2\alpha_{13} + \alpha_3}{\alpha_3} \right] A \frac{a}{\alpha_3} \frac{1}{\alpha_3 s - 1} + \frac{a(a + \alpha_3)}{\alpha_3^2} \frac{1}{(\alpha_3 s - 1)^2} A \tag{3.73}$$

$$V_- = \frac{\alpha_{13}^2}{\alpha_3^2} A + \left[\frac{2\alpha_{13} - \alpha_3}{\alpha_3} \right] A \frac{a}{\alpha_3} \frac{1}{\alpha_3 s - 1} + \frac{a(a - \alpha_3)}{\alpha_3^2} \frac{1}{(\alpha_3 s - 1)^2} A \tag{3.74}$$

$$V_+ = \left[\alpha_{13}^2 + \frac{(2\alpha_{13} + \alpha_3)a}{\alpha_3 s - 1} + \frac{a(a + \alpha_3)}{(\alpha_3 s - 1)^2} \right] \frac{A}{\alpha_3^2} \tag{3.75}$$

$$V_- = \left[\alpha_{13}^2 + \frac{(2\alpha_{13} - \alpha_3)a}{\alpha_3 s - 1} + \frac{a(a - \alpha_3)}{(\alpha_3 s - 1)^2} \right] \frac{A}{\alpha_3^2} \tag{3.76}$$

Since

$$\begin{aligned}
(2\alpha_{13} \mp \alpha_3)a &= 2\alpha_{13}^2 + 2\alpha_{13}\alpha_3\alpha_{12} \mp \alpha_3 a \\
&= \alpha_{13}^2 - \alpha_{12}^2\alpha_3^2 + \alpha_{13}^2 + \alpha_{12}^2\alpha_3^2 + 2\alpha_{13}\alpha_3\alpha_{12} \mp \alpha_3 a \\
&= \alpha_{13}^2 - \alpha_{12}^2\alpha_3^2 + a^2 \mp \alpha_3 a \\
&= \alpha_{13}^2 - \alpha_{12}^2\alpha_3^2 + a(a \mp \alpha_3)
\end{aligned}$$

Then we rewrite Eq. (3.75) and (3.76);

$$V_+ = \left[(a - \alpha_{12}\alpha_3)^2 + \frac{\alpha_{13}^2 - \alpha_{12}^2\alpha_3^2 + a(a + \alpha_3)}{\alpha_3 s - 1} + \frac{a(a + \alpha_3)}{(\alpha_3 s - 1)^2} \right] \frac{A}{\alpha_3^2} \tag{3.77}$$

$$V_- = \left[(a - \alpha_{12}\alpha_3)^2 + \frac{\alpha_{13}^2 - \alpha_{12}^2\alpha_3^2 + a(a - \alpha_3)}{\alpha_3 s - 1} + \frac{a(a - \alpha_3)}{(\alpha_3 s - 1)^2} \right] \frac{A}{\alpha_3^2} \tag{3.78}$$

Since

$$\begin{aligned}
(a - \alpha_{12}\alpha_3)^2 &= \left(\frac{a - 2\alpha_{12}\alpha_3}{2} + \frac{a}{2}\right)^2 \\
&= \left(\frac{-\alpha_{12}\alpha_3 + \alpha_{13}}{2} + \frac{a}{2}\right)^2 \\
&= \left[\frac{(-\alpha_{12}\alpha_3 + \alpha_{13})a}{2a} + \frac{a}{2}\right]^2 \\
&= \left[\frac{-\alpha_{12}^2\alpha_3^2 + \alpha_{13}^2}{2a} + \frac{a}{2}\right]^2
\end{aligned}$$

So finally;

$$\begin{aligned}
V_+ &= \left[\left(\frac{-\alpha_{12}^2\alpha_3^2 + \alpha_{13}^2}{2a} + \frac{a}{2} \right)^2 + \frac{\alpha_{13}^2 - \alpha_{12}^2\alpha_3^2 + a(a + \alpha_3)}{\alpha_3 s - 1} \right. \\
&\quad \left. + \frac{a(a + \alpha_3)}{(\alpha_3 s - 1)^2} \right] \frac{A}{\alpha_3^2}
\end{aligned} \tag{3.79}$$

$$\begin{aligned}
V_- &= \left[\left(\frac{-\alpha_{12}^2\alpha_3^2 + \alpha_{13}^2}{2a} + \frac{a}{2} \right)^2 + \frac{\alpha_{13}^2 - \alpha_{12}^2\alpha_3^2 + a(a - \alpha_3)}{\alpha_3 s - 1} \right. \\
&\quad \left. + \frac{a(a - \alpha_3)}{(\alpha_3 s - 1)^2} \right] \frac{A}{\alpha_3^2}
\end{aligned} \tag{3.80}$$

With the help of Eq. (3.45) we can write

$$R(a_1) = V_+(a_0) - V_-(a_1) \tag{3.81}$$

$$a_1 = a_0 + \alpha_3 \tag{3.82}$$

$$a_0 = \xi \tag{3.83}$$

so

$$R(a_1) = V_+(a_0) - V_-(a_0 + \alpha_3) \tag{3.84}$$

$$R(a_1) = \left[\left(\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2\xi} + \frac{\xi}{2} \right)^2 - \left(\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2(\xi + \alpha_3)} + \frac{(\xi + \alpha_3)}{2} \right)^2 \right] \frac{A}{\alpha_3^2} \quad (3.85)$$

We can generalise the above expressions as follows;

$$a_n = \xi + n\alpha_3 \quad (3.86)$$

$$R(a_n) = V_+(a_{n-1}) - V_-(a_n) \quad (3.87)$$

$$R(a_n) = \left[\left(\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2\{\xi + (n-1)\alpha_3\}} + \frac{\xi + (n-1)\alpha_3}{2} \right)^2 - \left(\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2(\xi + n\alpha_3)} + \frac{\xi + n\alpha_3}{2} \right)^2 \right] \frac{A}{\alpha_3^2} \quad (3.88)$$

And remembering the Eq. (3.58);

$$E_n^- = \sum_{i=0}^n R(a_i), \quad E_0^- = 0 \quad (3.89)$$

At last,

$$E_n^- = \left[\left(\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2\xi} + \frac{\xi}{2} \right)^2 - \left(\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2(\xi + n\alpha_3)} + \frac{(\xi + n\alpha_3)}{2} \right)^2 \right] \frac{A}{\alpha_3^2} \quad (3.90)$$

$$E_n = E_n^- + E_0 \quad (3.91)$$

CHAPTER IV

DIATOMIC MOLECULES

4.1 Structure of Diatomic Molecules

Now the structure of diatomic molecules will be examined. Molecules are made up from atoms that are using valence electrons commonly. Basically there is no significant difference between the definition of the states and transitions of the molecules and atoms since both of them are studied with the same principles of quantum mechanics. However, molecules have extra types of motion that atoms do not have. Experimental results show that the internal energy of the molecule consists of three different components whose energy scales are largely different from each other [44]. In order to understand the spectrum characteristics of these molecules, the wave functions must be found by solving Schrödinger equation. But these solutions are very difficult even for the simplest molecule. Therefore, describing a molecule by quantum mechanical principles can only be achieved with some approximations. The overall motion of the molecule can be divided into several components.

Like many quantum mechanical system the Hamiltonian for any molecule is composed of kinetic (T) and potential (V) energies. The overall internal kinetic energy of the molecule is the sum of kinetic energies of the electrons (T_e) and kinetic energies of the nuclei (T_n). On the other hand, the potential energy has three components which are due to electric attraction force between electrons and nuclei (V_{en}), repulsion forces between electrons (V_{ee}) and between nuclei (V_{nn}). In addition, if the distance between atoms is very long, then potential energy is equal to the sum of the individual energies of both atoms.

As the atoms get closer to each other, an attraction force rises. On the other side, if the separation distance goes to zero, a high repulsive force occurs. For stable molecules these forces are in equilibrium.

Electrons and nuclei in the molecular system is exposed to similar forces. However, the mass of the electron is thousands of times smaller than the mass of the nucleus. As a result, electrons are accelerated faster than the nuclei and move much faster. Therefore, the movement of electrons and nuclei can be considered largely independently of each other. So, when the motions of electrons are defined quantum mechanically, position of the nuclei can be assumed constant. This approximation is called Born-Oppenheimer approximation [45]. Based on this fact, the time scales of motion of electrons and nuclei can be assumed separable. Because of the separability of time scales of nuclear and electronic we can assume a separable wave function form:

$$\Psi(\vec{r}, \vec{R}) = \Psi_{\text{El},n}(\vec{r}, \vec{R})\Psi_{\text{N}}(\vec{R}) \quad (4.1)$$

In Eq. (4.1) wave function $\Psi_{\text{El},n}(\vec{r}, \vec{R})$ is named as electronic wave function. The subscript “n” is the electronic quantum number which specifies the electronic state. Furthermore, each electronic wave function has electronic variables \vec{r} and nuclear variable \vec{R} . By using the fixed nuclei assumption mentioned above $\Psi_{\text{El},n}(\vec{r}, \vec{R})$ wave functions can be calculated by solving SE for electrons. The electronic energy eigenvalues are parametrically dependent on the nuclear positions. So, for each value of \vec{R} an eigenvalue spectrum $E_{\text{El},n}(\vec{R})$ and eigenfunctions $\Psi_{\text{El},n}(\vec{r}, \vec{R})$ are found by solving SE. These wave equations are the same wave equations of valence electrons.

In Eq. (4.1) wave function $\Psi_{\text{N}}(\vec{R})$ is named as nuclear wave function and solved in nuclear variables \vec{R} . Eigenvalue solutions of the nuclear wave function give the rotational and vibrational energy levels. Since the rotational and translational

variables of the Hamiltonian in the SE for the nuclear wave function are independent, the wave equation is solved by separation of variables.

Firstly, the wave equation which we obtain for the motions of nuclei has two components. These are translational motion of center of mass of nuclei and motions of nuclei relative to each other. Translational motion of the center of mass of nuclei, actually, is the translational motion of the molecule. Since this motion is not related with molecular structure, it is ignored.

The other wave equation, which is about the motions of nuclei relative to each other, is solved by separating it into two wave functions with the help of separation of variables. Unfortunately, another approximation method is needed here: The potential energy due to the nuclei and electronic states is represented by approximate functions, e.g. Morse Potential [36]. The solution of the wave function with angular variables gives the eigenstates and eigenvalues of the rotational motion of the nuclei. On the other side, the solution of the wave function with radial variable gives the vibrational eigenstates and eigenvalues of the nuclei. To sum up, there are four motions of a molecule which are motion of electrons, vibration of nuclei, rotation of nuclei and translational motion of molecule. So, if we ignore the translational motion of the molecule, the internal complete wave function of the diatomic molecules becomes;

$$\Psi = \Psi_{el}(r, R) \Psi_{vib}(R) \Psi_{rot}(\theta, \phi) \quad (4.2)$$

And energy eigenvalues are;

$$E = E_{El} + E_{vib} + E_{rot} \quad (4.3)$$

This means the internal excitations in diatomic molecules are rotational, vibrational, and electronic.

The energy levels with the largest energy scale corresponds to the electronic states. Energy level of an electronic state also has different energy groups due to different vibrational states of the nuclei. Vibrational energy levels are also divided into different energy levels with narrower gaps because of the rotational states. The difference between the rotational energy levels grows proportionally with increasing energy.

$$E_{\text{el}} \gg E_{\text{vib}} \gg E_{\text{rot}} \quad (4.4)$$

Absorption and emission of radiation of molecules are directly connected to changes of their electronic, rotational and vibrational energies. When a molecule makes a transition between electronic states, the related radiation energy is so high that it appears in ultraviolet or visible region. Diatomic molecules can have many different electronic states. The energy eigenvalues of these states are determined by measuring the changes during electronic transitions. While the spectra for vibrational transitions of molecules is in the infrared region, the spectra for rotational transitions is in the microwave region [44].

4.2 Molecular Potentials

Since the intermolecular forces are encountered in many fields of physics, biology and chemistry (the properties of crystals, phonon spectra, stability of compounds like DNA and RNA, in the formation of chemical complexes etc.[46]), it is an important research field. Instead of direct measurement of intermolecular forces experimentally, researchers determine them by measuring some other characteristics depending on these forces.

To solve an intermolecular interaction problem, firstly necessary data gathered by experiments. Then some potential models fitting to these data are used.

Model potential is chosen according to the studied problem. One variable function fitting to potential describes the interaction between two molecules. The potential $V(R)$ is called the intermolecular potential and it is a function of the distance (R) between the centers of molecules. Depending on the distance between the atoms, interatomic potential is classified in three types.

I. In short distance range atoms repulse each other and atomic interaction is dominated by exchanging of electrons.

II. In medium distance range there is a balance between repulsive and attractive forces.

III. In long distance range exchanging of electrons are ineffective and atomic interaction is dominated by attractive force.

Only a theory based on quantum mechanics can be consistent in understanding of intermolecular forces. Since the electrons and nuclei have motions in quantum scale, one must solve SE to find the solution to the interacting atoms. Analytical solution to the studied problem can be found solving SE for an appropriate potential. There are many model potentials which are used in molecular and condensed matter physics (e.g. Morse, Eckart and Pöschl-Teller potentials)[46].

CHAPTER V

CALCULATIONS

5.1 Solution Of The Generalized Morse Potential

The Morse potential is one of the most well known potentials is used to describe the potential energy in diatomic molecules. Van der Waals complexes between molecules or vibrational motion of covalent diatomic molecules can be defined by The Morse potential [44 and 47]. Generalized Morse Potential [36] is defined as

$$V(r) = V_1 e^{-2\alpha r} - V_2 e^{-\alpha r} \quad (5.1)$$

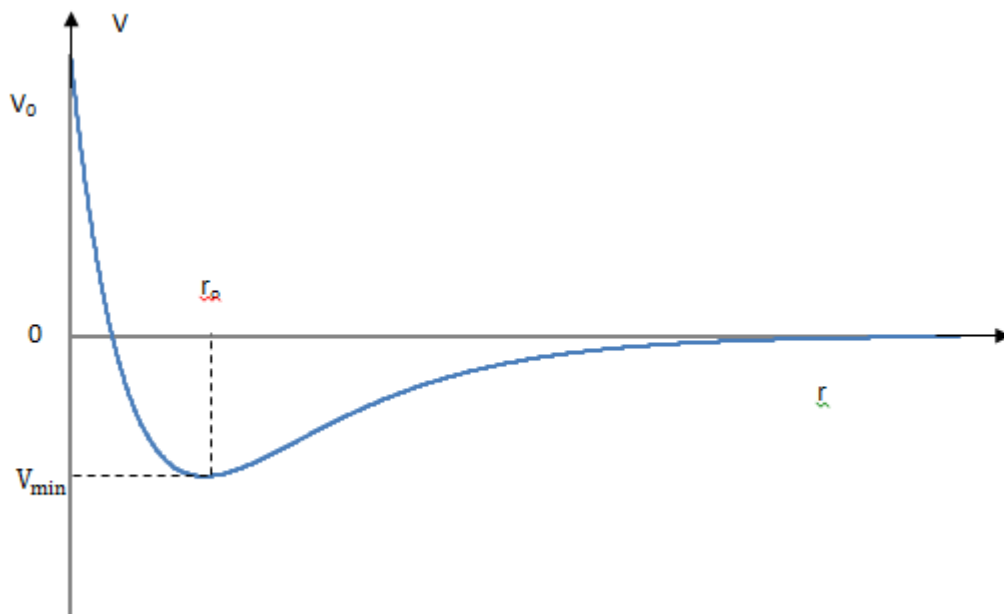


Figure 1: Morse Potential

If we define a new parameter $s = \sqrt{V_1}e^{-\alpha r}$ and let $2m = \hbar = 1$, SE transforms to

$$\frac{d^2\Psi}{ds^2} + \frac{1}{s} \frac{d\Psi}{ds} - \frac{1}{s^2} \left(\frac{s^2}{\alpha^2} - \frac{1}{\alpha^2} \frac{V_2}{\sqrt{V_1}} s + 4\varepsilon^2 \right) \Psi = 0 \quad (5.2)$$

where

$$4\varepsilon^2 = -\frac{E}{4\alpha^2} \quad (5.3)$$

Meanwhile;

$$\frac{ds}{dr} = -\alpha s, \quad \frac{d^2s}{dr^2} = \alpha^2 s \quad (5.4)$$

$$\Rightarrow A = \frac{1}{s^2} \left(\frac{ds}{dr} \right)^2 = B = \frac{1}{s} \frac{d^2s}{dr^2} = \alpha^2 \quad (5.5)$$

making the shape variance condition satisfied. Using eqs. (2.19), (2.24-2.28), (2.30), (2.37 and 2.38), (2.40 and 2.42);

$$\begin{aligned} \alpha_1 &= 1, & \alpha_2 &= 0, & \alpha_3 &= 0, & \alpha_4 &= 0 \\ \alpha_5 &= 0, & \alpha_6 &= \xi_1, & \alpha_7 &= -\xi_2, & \alpha_8 &= \xi_3 \\ \alpha_9 &= \xi_1, & \alpha_{10} &= 1 + 2\sqrt{\xi_3}, & \alpha_{11} &= 2\sqrt{\xi_1}, \\ \alpha_{12} &= \sqrt{\xi_3}, & \alpha_{13} &= -\sqrt{\xi_1}, \end{aligned} \quad (5.6)$$

and

$$\xi_1 = \frac{1}{\alpha^2}, \quad \xi_2 = \frac{1}{\alpha^2} \frac{V_2}{\sqrt{V_1}}, \quad \xi_3 = 4\varepsilon^2 \quad (5.7)$$

Using Eq. (2.38);

$$-\alpha_5 + \sqrt{\alpha_9} + \alpha_7 + 2\sqrt{\alpha_8\alpha_9} = 0 \quad (5.8)$$

From the Eqs. (5.6) and (5.7);

$$\sqrt{\xi_1} - \xi_2 + 2\sqrt{\xi_3 \xi_1} = 0 \quad (5.9)$$

$$\sqrt{\frac{1}{\alpha^2} - \frac{1}{\alpha^2} \frac{V_2}{\sqrt{V_1}}} + 2\sqrt{4\varepsilon_0^2 \frac{1}{\alpha^2}} = 0 \quad (5.10)$$

$$\Rightarrow \varepsilon_0 = -\frac{1}{4} \left[1 - \frac{1}{\alpha} \frac{V_2}{\sqrt{V_1}} \right] \quad (5.11)$$

From the Eq. (5.3) and (5.11) we can find ground state energy eigenvalue;

$$E_0 = -\frac{1}{4} \alpha^2 \left[1 - \frac{1}{\alpha} \frac{V_2}{\sqrt{V_1}} \right]^2 \quad (5.12)$$

Furthermore we can use the Eq. (3.90) for calculating the all shifted energy eigenvalues;

$$\begin{aligned} E_n^- &= \left[\left(\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2\xi} + \frac{\xi}{2} \right)^2 - \left(\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2(\xi + n\alpha_3)} + \frac{(\xi + n\alpha_3)}{2} \right)^2 \right] \frac{A}{\alpha_3^2} \\ &= \left[\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2\xi} + \frac{\xi}{2} + \frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2(\xi + n\alpha_3)} + \frac{(\xi + n\alpha_3)}{2} \right] \\ &\quad \left[\frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2\xi} + \frac{\xi}{2} - \frac{-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2}{2(\xi + n\alpha_3)} - \frac{(\xi + n\alpha_3)}{2} \right] \frac{A}{\alpha_3^2} \\ &= \left[\frac{(-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2)(2\xi + n\alpha_3)}{2\xi(\xi + n\alpha_3)} + \xi + \frac{n\alpha_3}{2} \right] \left[\frac{(-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2)(n\alpha_3)}{2\xi(\xi + n\alpha_3)} - \frac{n\alpha_3}{2} \right] \frac{A}{\alpha_3^2} \\ &= \left[\frac{(-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2)(2\xi + n\alpha_3)}{2\xi(\xi + n\alpha_3)} + \xi + \frac{n\alpha_3}{2} \right] \left[\frac{(-\alpha_{12}^2 \alpha_3^2 + \alpha_{13}^2)}{2\xi(\xi + n\alpha_3)} - \frac{1}{2} \right] \frac{n}{\alpha_3} A \quad (5.13) \end{aligned}$$

using Eq. (3.63) we can simplify the second term in the above expression as follows;

$$\begin{aligned}
\frac{(-\alpha_{12}^2\alpha_3^2 + \alpha_{13}^2)}{2\xi(\xi + n\alpha_3)} - \frac{1}{2} &= \frac{-\alpha_{12}^2\alpha_3^2 + \alpha_{13}^2 - \xi^2 - \xi n\alpha_3}{2\xi(\xi + n\alpha_3)} \\
&= \frac{-2\alpha_{12}^2\alpha_3^2 - 2\alpha_{12}\alpha_{13}\alpha_3 - \xi n\alpha_3}{2\xi(\xi + n\alpha_3)} \\
&= \frac{-2\alpha_{12}\alpha_{13}\xi - \xi n\alpha_3}{2\xi(\xi + n\alpha_3)} \\
&= \frac{-2\alpha_{12}\alpha_3 - n\alpha_3}{2(\xi + n\alpha_3)}
\end{aligned}$$

Then

$$\begin{aligned}
E_n^- &= \left[\frac{(-\alpha_{12}^2\alpha_3^2 + \alpha_{13}^2)(2\xi + n\alpha_3)}{2\xi(\xi + n\alpha_3)} + \xi + \frac{n\alpha_3}{2} \right] \left[-\frac{2\alpha_{12}\alpha_3 + n\alpha_3}{2(\xi + n\alpha_3)} \right] \frac{n}{\alpha_3} A \\
&= \left[\frac{(-\alpha_{12}^2\alpha_3^2 + \alpha_{13}^2)(2\xi + n\alpha_3)}{2\xi(\xi + n\alpha_3)} + \xi + \frac{n\alpha_3}{2} \right] \left[-\frac{2\alpha_{12} + n}{2(\xi + n\alpha_3)} \right] nA
\end{aligned} \tag{5.14}$$

Using $\alpha_3 = 0 \Rightarrow \xi = \alpha_{13}$ we reach a simple general expression for the shifted energy eigenvalues;

$$\begin{aligned}
E_n^- &= \left[\frac{\alpha_{13}^2(2\alpha_{13})}{2\alpha_{13}^2} + \alpha_{13} \right] \left[-\frac{2\alpha_{12} + n}{2\alpha_{13}} \right] nA \\
&= -(2\alpha_{12} + n)nA
\end{aligned} \tag{5.15}$$

From the eqs. (5.5), (5.6) and (5.7);

$$E_n^- = -(4\varepsilon_0 + n)n\alpha^2 \tag{5.16}$$

Now we can write the energy eigenvalues by back shifting with help of Eq. (3.91);

$$\begin{aligned}
E_n &= -(4\varepsilon_0 + n)n\alpha^2 - 4\alpha^2\varepsilon_0^2 \\
E_n &= -\frac{1}{4}[4\varepsilon_0 + 2n]^2\alpha^2
\end{aligned} \tag{5.17}$$

Finally by inserting Eq. (5.11) into Eq. (5.17);

$$E_n = -\frac{1}{4} \left[1 - \frac{1}{\alpha} \frac{V_2}{\sqrt{V_1}} + 2n \right]^2 \alpha^2 \quad (5.18)$$

And the wave function is;

$$\Psi_n = B_n s^{2\epsilon} e^{-\frac{s}{\alpha}} L_n^{4\epsilon} \left(\frac{2s}{\alpha} \right) \quad (5.19)$$

Table 1: The energy eigenvalues of the Morse potential in atomic units ($2m = \mu = 1$). For H_2 ; $2V_1 = V_2 = 9,4892$, $\alpha = 0,1440558$. For $NaCl$; $2V_1 = V_2 = 5,030574$ and $\alpha = 0,11998912$.

n	H_2		LiH	
	Our work	Nasser [48]	Our work	Nasser [48]
0	-4,436	-4,4360	-2,32859	-2,3286
1	-3,84994	-3,8499	-1,97679	-1,9768
2	-3,30538	-3,3054	-1,65378	-1,6538
3	-2,80233	-2,8023	-1,35956	-1,3596
4	-2,34078	-2,3408	-1,09415	-1,0941
5	-1,92073	-1,9207	-0,85752	-0,8575
6	-1,54219	-1,5422	-0,64969	-0,6497
7	-1,20515	-1,2051	-0,47066	-0,4707
8	-0,90961	-0,9096	-0,32042	-0,3204
9	-0,65558	-0,6556	-0,19898	-0,1990
10	-0,44306	-0,4431	-0,10633	-0,1063

5.2 Solution Of The Eckart Potential

The Eckart potential [37] is an exponential-type potential and one of the most widely used potentials in physics[13] and chemistry [7]. The conventional Eckart potential is;

$$V_{A,B}(r) = \gamma(\gamma - 1)\operatorname{cosech}^2(r) - 2\beta\coth(r), \quad 0 < r < \infty \quad (5.20)$$

where $\gamma, \beta > 0$

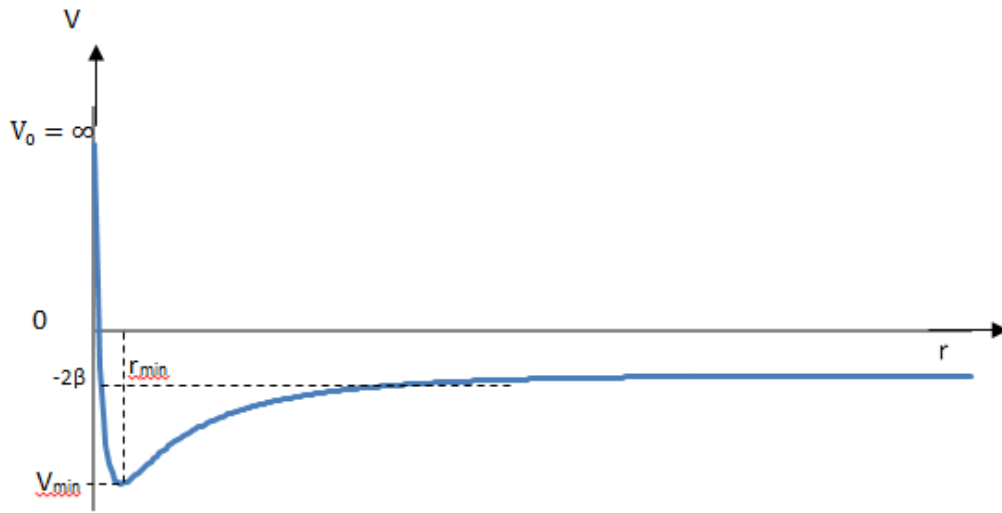


Figure 2: Eckart Potential

Rewriting the equation;

$$V_{\gamma,\beta}(r) = \gamma(\gamma - 1) \frac{4e^{-2r}}{(1 - e^{-2r})^2} - 2\beta \frac{1 + e^{-2r}}{1 - e^{-2r}} \quad (5.21)$$

If we define a new parameter $s = e^{-2r}$ and let $2m = \hbar = 1$, SE transforms to;

$$\frac{d^2\Psi}{ds^2} + \frac{1}{s} \frac{d\Psi}{ds} + \frac{1}{4s^2} \left(-\frac{\gamma(\gamma-1)4s}{(1-s)^2} + 2\beta \frac{(1+s)}{(1-s)} + E \right) \Psi = 0 \quad (5.22)$$

Meanwhile,

$$\frac{ds}{dr} = -2s, \quad \frac{d^2s}{dr^2} = 4s \quad (5.23)$$

$$\Rightarrow \frac{1}{s^2} \left(\frac{ds}{dr} \right)^2 = \frac{1}{s} \frac{d^2s}{dr^2} = 4 \quad (5.24)$$

making the shape variance condition satisfied. Using eqs. (2.19), (2.24-2.28), (2.30), (2.37 and 2.38), (2.40 and 2.42),

$$\begin{aligned} \alpha_1 &= 1, & \alpha_2 &= 1, & \alpha_3 &= 1, & \alpha_4 &= 0 \\ \alpha_5 &= -\frac{1}{2}, & \alpha_6 &= \frac{1}{4} + \xi_1, & \alpha_7 &= -\xi_2, & \alpha_8 &= \xi_3 \\ \alpha_9 &= \xi_1 - \xi_2 + \xi_3 + \frac{1}{4}, & \alpha_{10} &= 1 + 2\sqrt{\xi_3}, \\ \alpha_{11} &= 2 + 2 \left(\sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} + \sqrt{\xi_3} \right), \\ \alpha_{12} &= \sqrt{\xi_3}, & \alpha_{13} &= -\frac{1}{2} - \sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} - \sqrt{\xi_3}, \end{aligned} \quad (5.25)$$

and

$$\xi_1 = \frac{2\beta - E}{4}, \quad \xi_2 = -\frac{+2E + 4\gamma(\gamma-1)}{4}, \quad \xi_3 = -\frac{E + 2\beta}{4} = \varepsilon^2 \quad (5.26)$$

Using Eq. (2.38) for n=0;

$$-\alpha_5 + \sqrt{\alpha_9} + \alpha_3 \sqrt{\alpha_8} + \alpha_7 + 2\alpha_3 \alpha_8 + 2\sqrt{\alpha_8 \alpha_9} = 0 \quad (5.27)$$

Rewriting the Eq. (5.27);

$$\frac{1}{2} + \sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} + \sqrt{\xi_3} - \xi_2 + 2\xi_3 + 2\sqrt{(\xi_1 - \xi_2 + \xi_3 + 1/4)\xi_3} = 0 \quad (5.28)$$

\Rightarrow

$$\left(\sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} + \sqrt{\xi_3} + 1\right) \left(\sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} + \sqrt{\xi_3}\right) - \xi_1 + \frac{1}{4} = 0 \quad (5.29)$$

$$\xi_1 - \xi_2 + \xi_3 + 1/4 = \left(\frac{2\gamma - 1}{2}\right)^2 \quad (5.30)$$

So we rewrite Eq. (5.29);

$$\left(\gamma - \frac{1}{2} + \varepsilon_0 + 1\right) \left(\gamma - \frac{1}{2} + \varepsilon_0\right) - \frac{2\beta - E_0 + 1}{4} = 0 \quad (5.31)$$

solving Eq. (5.31) for ε_0 by inserting ε_0^2 from Eq. (5.26);

$$\varepsilon_0 = \frac{\beta - \gamma^2}{2\gamma} \quad (5.32)$$

\Rightarrow

$$E_0 = -\frac{\beta^2}{\gamma^2} - \gamma^2 \quad (5.33)$$

Furthermore we can use the Eq. (3.90) for calculating the all shifted energy eigenvalues;

$$E_n^- = 4 \left[\left(\frac{(\alpha_{13} + \alpha_{12})(\alpha_{13} - \alpha_{12})}{2(\alpha_{13} + \alpha_{12})} + \frac{\alpha_{13} + \alpha_{12}}{2} \right)^2 - \left(\frac{(\alpha_{13} + \alpha_{12})(\alpha_{13} - \alpha_{12})}{2(\alpha_{13} + \alpha_{12} - n)} + \frac{\alpha_{13} + \alpha_{12} - n}{2} \right)^2 \right] \quad (5.34)$$

Using

$$\alpha_{12} = \varepsilon_0 = \frac{\beta - \gamma^2}{2\gamma}, \quad \alpha_{13} = -\frac{\beta + \gamma^2}{2\gamma} \quad (5.35)$$

Inserting eq. (5.34)

$$E_n^- = \left[\frac{\beta^2}{\gamma^2} + \gamma^2 - \frac{\beta^2}{(\gamma + n)^2} - (\gamma + n)^2 \right] \quad (5.36)$$

And

$$E_n = E_n^- + E_0 = \left[-\frac{\beta^2}{(\gamma + n)^2} - (\gamma + n)^2 \right] \quad (5.37)$$

$$\Psi_n = B_n s^{\frac{\sqrt{-E-2\beta}}{2}} (1-s)^{\gamma} P_n^{(\sqrt{-E-2\beta}, 2\gamma-1)} (1-2s) \quad (5.38)$$

Table 2: Comparison of the calculated energy eigenvalues of the Eckart potential with Taskin [52] in atomic units ($2m = \mu = 1$), $\gamma = 1,8$ and $\beta = 100$.

n	Our work	Taskin [49]
0	-3089,66	-3089,66
1	-1283,35	-1283,35
2	-706,961	-706,961
3	-457,068	-457,068
4	-330,905	-330,905
5	-262,503	-262,503
6	-225,206	-225,206
7	-206,572	-206,572
8	-200,163	-200,163

5.3 Solution Of The Hua Wei Potential

Wei Hua anharmonic oscillator is used for diatomic molecules to describe their bond-stretching vibrations [50]. It is widely used in molecular physics and chemistry [51]. Hua Potential is defined as [38];

$$V(r) = V \left(\frac{1 - e^{-br}}{1 - ce^{-br}} \right)^2 \quad (5.39)$$

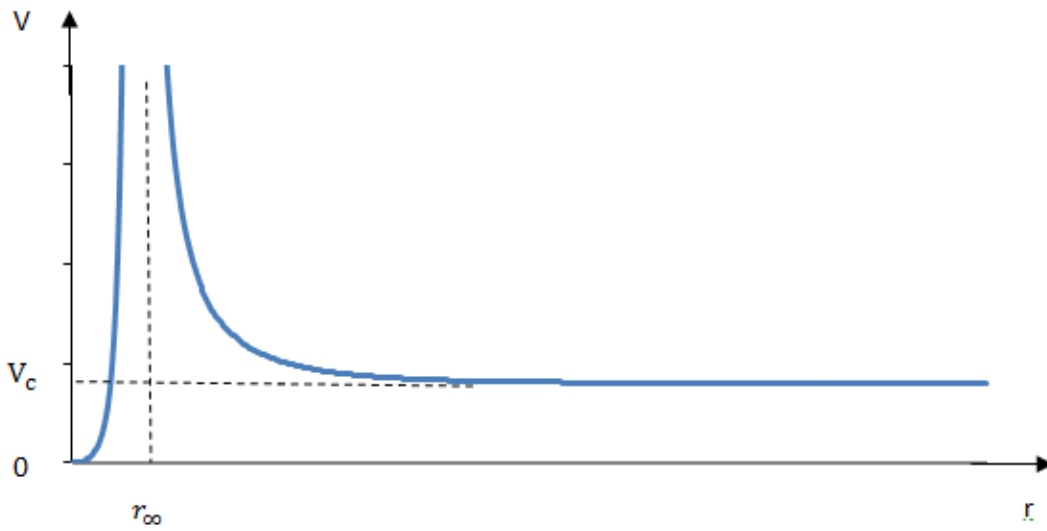


Figure 3: Hua Potential

If we define a new parameter $s = ce^{-br}$ and let $2m = \hbar = 1$, SE transforms to

$$\frac{d^2\Psi}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{d\Psi}{ds} + \left[\frac{(Ec^2 - V)s^2 + 2(Vc - Ec^2)s + c^2(E - V)}{b^2c^2s^2(1-s^2)} \right] \Psi = 0 \quad (5.40)$$

meanwhile

$$\frac{ds}{dr} = -bs, \quad \frac{d^2s}{dr^2} = b^2s \quad (5.41)$$

$$\Rightarrow \frac{1}{s^2} \left(\frac{ds}{dr} \right)^2 = \frac{1}{s} \frac{d^2s}{dr^2} = b^2 \quad (5.42)$$

making the shape variance condition satisfied. Using eqs. (2.19), (2.24-2.28), (2.30), (2.37 and 2.38), (2.40 and 2.42),

$$\begin{aligned} \alpha_1 &= 1, & \alpha_2 &= 1, & \alpha_3 &= 1, & \alpha_4 &= 0 \\ \alpha_5 &= -\frac{1}{2}, & \alpha_6 &= \frac{1}{4} + \xi_1, & \alpha_7 &= -\xi_2, & \alpha_8 &= \xi_3 \\ \alpha_9 &= \xi_1 - \xi_2 + \xi_3 + \frac{1}{4}, & \alpha_{10} &= 1 + 2\sqrt{\xi_3}, \\ \alpha_{11} &= 2 + \left(2\sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} + \sqrt{\xi_3} \right), \\ \alpha_{12} &= \sqrt{\xi_3}, & \alpha_{13} &= -\frac{1}{2} - \sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} - \sqrt{\xi_3}, \end{aligned} \quad (5.43)$$

and

$$\xi_1 = \frac{V - Ec^2}{b^2c^2}, \quad \xi_2 = \frac{2(Vc - Ec^2)}{b^2c^2}, \quad \xi_3 = \frac{V - E}{b^2} = \varepsilon^2 \quad (5.44)$$

Using Eq. (2.38) for n=0;

$$-\alpha_5 + \sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8} + \alpha_7 + 2\alpha_3\alpha_8 + 2\sqrt{\alpha_8\alpha_9} = 0 \quad (5.45)$$

From the Eq. (5.45);

$$\left(\sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} + \varepsilon_0 + 1 \right) \left(\sqrt{\xi_1 - \xi_2 + \xi_3 + 1/4} + \varepsilon_0 \right) - \xi_1 + \frac{1}{4} = 0 \quad (5.46)$$

$$\xi_1 - \xi_2 + \xi_3 + 1/4 = \frac{V(c-1)^2}{b^2c^2} + \frac{1}{4} = \beta^2 \quad (5.47)$$

Solving Eq. (5.46) for ε_0 by inserting ε_0^2 from Eq. (5.44);

$$\varepsilon_0 = \frac{V(1 - c^2)}{b^2 c^2 (2\beta + 1)} - \frac{2\beta + 1}{4} \quad (5.48)$$

\Rightarrow

$$E_0 = V - b^2 \varepsilon_0^2 \quad (5.49)$$

Furthermore we can use the Eq. (3.90) for calculating the all shifted energy eigenvalues with using Eqs. (5.47) and (5.48);

$$E_n^- = -b^2 \left(\frac{(n - 2\beta - 1)(n - 2\beta - 1 - 2\varepsilon_0)(n + 2\varepsilon_0)}{(2n - 2\beta - 1)^2} \right) n \quad (5.50)$$

And

$$E_n = V - b^2 \left[\varepsilon_0^2 + \left(\frac{(n - 2\beta - 1)(n - 2\beta - 1 - 2\varepsilon_0)(n + 2\varepsilon_0)}{(2n - 2\beta - 1)^2} \right) n \right] \quad (5.51)$$

This eigenvalue equation is consistent with the formula which is given for Hua Potential in Hassanabadi [51].

$$\Psi_n = B_n s^{\frac{\sqrt{V-E}}{b}} (1-s)^{\frac{2\beta+1}{2}} P_n \left(\frac{2\sqrt{V-E}}{b}, 2\beta \right) (1-2s) \quad (5.52)$$

CHAPTER VI

CONCLUSION

We explained Nikiforov-Uvarov Method which is one of the most systematic and direct methods being used for solving potentials in molecular physics. We briefly described newly developed parametric generalization of the Nikiforov-Uvarov method. Then Supersymmetric Quantum Mechanics was studied in detail. Hamilton Hierarchy Method and Shape Invariance concepts and how these methods are implemented together were explained. It was pointed out that how SUSYQM is a very powerful method for solving some potentials when it is used together with Hierarchy of Hamiltonians and Shape Invariance. Furthermore it was specified that many of the well known exactly solvable potentials have shape invariance property. In addition, very newly generated parametric generalization of the Hamilton Hierarchy Method was introduced in detail. Since all these mathematical tools have been developed and studied to find out the correct mathematical descriptions of characteristics of diatomic molecules, we explained dynamics and spectral properties of diatomic molecules in Chapter IV. Molecular potentials and motions of diatomic molecules with the consequences of these dynamics on the spectroscopy of diatomic molecules were examined in the frame of quantum mechanical principles.

Finally in chapter V, we implemented all these mathematical tools to solve three of the very famous diatomic potentials, Morse, Eckart and Hua Wei. Firstly we used parametric generalization of Nikiforov-Uvarov method to define the parameters of related Schrödinger Equation of each potential. Secondly, we calculated the ground state energy eigenvalue of the Hamiltonians. Thirdly, shifted energy eigenvalue spectrum of the Hamiltonians are calculated by using parametric generalization of the Hamilton Hierarchy Method.

Then ground state energy added onto these shifted energy eigenvalues and true energy eigenvalue spectrum was obtained. Wave functions were written with applying energy eigenvalues with Nikiforov-Uvarov method.

The numerical values of the energy eigenvalues for H_2 and LiH diatomic molecules were computed and presented for the Morse potential. These eigenvalues were compared with the findings of the Nasser [48]. Since our calculations are made using atomic units ($m = \mu = 1$), the energy eigenvalues presented in Nasser [48] were recalculated in atomic units by using the formulas given in Nasser [48] for the energy eigenvalues. It is seen that these adjusted eigenvalues are very consistent with our results. For angular quantum number $l = 0$, Morse potential has exact solution. But for $l \neq 0$, some approximations must be made to find analytical solutions. SE is solved for $l = 0$ in this thesis. The numerical values of the energy eigenvalues for the conventional Eckart Potential are also determined by choosing some arbitrary parameters. These calculated eigenvalues were compared with the results presented in Taskin [49]. The calculations in Taskin [49] were adjusted according to the our chosen parameters and were also consistent with our results. The eigenvalue solution of the Hua Potential was also obtained. This equation is also consistent with the expression which is given in Hassanabadi [51] with different form. Furthermore, it is observed that values of the calculated energy eigenvalues of the bound states of these potentials starts to decrease beyond certain “n” number. This means that these proposed potentials are only working for values of $n < k$.

So it is seen that applying parametric generalization of Hamilton Hierarchy Method with parametric generalization of Nikiforov-Uvarov Method to the potentials which have required shape invariance conditions (especially exponential type potentials) lets simple and direct solutions.

REFERENCES

- [1] H. Hassanabadi, B. H. Yazarloo and L. L. Lu. *Chin. Phys. Lett.* 29, 020303, (2012).
- [2] X. Y. Gu and S. H. Dong. *J. Math. Chem.* 49, 2053, (2011).
- [3] B. H. Yazarloo, H. Hassanabadi and S. Zarrinkamar. *Eur. Phys. J. Plus* 127, 51, (2012).
- [4] S. H. Dong. *Int. J. Theor. Phys.* 41, 1991, (2002).
- [5] S. H. Dong. *Int. J. Theor. Phys.* 39, 1529, (2000).
- [6] Weiss J. J. *J. Chem. Phys.* 41 1120, (1964).
- [7] Cimas A, Aschi M, Barrientos C, Ray`on V M, Sardo J A and Largo. *A Chem. Phys. Lett.* 374, 594, (2003).
- [8] L D Landau and E M Lifshitz. *Quantum Mechanics-Non-Relativistic Theory* (Oxford, Pergamon 1977).
- [9] Kratzer, A. *Z. Phys.* 3, 289, (1920).
- [10] S. H. Dong. *Phys. Scr.* 65, 289, (2002).
- [11] G F Wei and S H Dong. *Canadian J. Phys.* 89, 1225, (2011).
- [12] D. A. Morales. *Chem. Phys. Lett.* 394, 68, (2004).
- [13] F. Cooper, A. Khare. U. Sukhatme. *Phys. Rep.* 251, 267, (1995).
- [14] F. Cooper and B. Freedman. *Ann. Phys.* 146, 262, (1983).
- [15] C. Sukumar. *J. Phys.* 18, 297, (1985).
- [16] G. Lévai. *Lect. Notes in Phys.* 427, 427, (1993).
- [17] A. B. Balantekin. *Physical Review A.* 57, 4188, (1998).
- [18] D. T. Barclay, R. Dutt, A. Gangopadhyaya, A. Khare, and U. Sukhatme. *Physical Review A.* 48, 2786, (1993).

- [19] F. Cooper, A. Khare, U. Sukhatme. *Supersymmetry in Quantum Mechanics*, (World Scientific, Singapore, 2001).
- [20] R. De, R. Dutt, and U. Sukhatme. *J. Phys. A Mat. Gen.* 25, L843, (1992).
- [21] M. Bag, M. M. Panja, and R. Dutt. *Phys. Rev. A* 46, 6059, (1992).
- [22] H. Ciftci, R. L. Hall, and N. Saad. *J. Phys. A Math. Gen.* 36, 11807, (2003).
- [23] X Y Gu and S H Dong *J. Math. Chem.* 49, 2053, (2011).
- [24] W. C. Qiang and S. H. Dong. *Phys. Lett. A* 363, 169, (2007).
- [25] H Hassanabadi, B H Yazarloo, S Zarrinkamar and H. Rahimov. *Commun. Theor. Phys.* 57, 339, (2012).
- [26] S. H. Dong. *Int. J. Theor. Phys.* 39, 1119, (2000).
- [27] A D Antia, A N Ikot, I O Akpan and O A Awoga. *Indian J. Phys.* 87 155, (2013).
- [28] A. F. Nikiforov and V. B. Uvarov. *Special Functions of Mathematical Physics*, (Birkhauser, Basel, 1988).
- [29] C. Tezcan and R. Sever. *Int. J. Theor. Phys.* 48, 337, (2008).
- [30] J. B. Killingbeck, A. Grosjean, and G. Jolicard. *J. Chem. Phys.* 116, 447, (2002).
- [31] B. Gonul, K. Koksal, and E. Bakir. *Phys. Scr.* 73, 279, (2006).
- [32] I. H. Duru and H. Kleinert. *Fortschr. Phys.* 30, 401, (1982).
- [33] S. M. Ikhdaire and R. Sever. *J. Mol. Struct.: THEOCHEM* 806, 155, (2007).
- [34] A. Arda, R. Sever, C. Tezcan. *Chinese J. Phys.* 48 1, 27, (2008).
- [35] C. Tezcan and Ramazan Sever. *Journal of Mathematical Physics* 55, 032014, (2104).
- [36] P. M. Morse. *Phys. Rev.* 34, 57, (1929).
- [37] Eckart C. *Phys. Rev.* 35 1303, (1930).
- [38] W. Hua *Phys. Rev. A*, 42, 2524, (1990).

- [39] S. S. Baym. *Mathematical Methods in Science and Engineering*, (Wiley, New Jersey, 2006).
- [40] W.T. R. Riccati. *Differential Equations, Math. in Sci. and Eng.*, (Academic Press, N.Y. 1972).
- [41] Dutt R., Khare, A., Varshni, Y.P. *J. Phys. A Math. Gen.* 28, L107, (2004).
- [42] Jia C.S., Li Y. *Phys. Lett. A* 305, 231, (2002).
- [43] Pöschl G., Teller E. *Z. Phys.* 83, 143, (1933).
- [44] G. Herzberg. *Molecular Spectra and Molecular Structure I. Spectra of Diatomic molecules*, (Van Nostrand–Reinhold, New York, 1950).
- [45] M. Born, R. Oppenheimer. *Ann. Phys.* 84, 457, (1927).
- [46] G. Kaplan. *Intermolecular Interactions, Physical Picture, Computational Methods and Model Potentials*. (John Wiley and Sons, 2006).
- [47] S. Cho, H. Sun,. *Korean Chem. Soc.* 25 1397, (2004).
- [48] I. Nasser, M. S. Abdelmonem, H. Bahlouli and A. D. Alhaidari. *J. Phys. B* 40, 4245, (2007)
- [49] F. Taşkin, G. Koçak. *Chin. Phys. B*, 19 9, 090314 (2010).
- [50] Mikulski D., Molski M., Konarski J., and Eder K. *J. Math. Chem* 52, 162, (2014).
- [51] H. Hassanabadi, B. H. Yazarloo, A. N. Ikot, N. Salehi and S. Zarrinkamr. *Indian J. Phys.* doi:10.1007/s12648-013-0317-1, (2013)