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M.Sc. in ENGINEERING PHYSICS

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SCIENCES

APPLICATION OF VARIATIONAL METHOD AND  
SUPERSYMMETRIC TECHNIQUE TO THE FOKKER-  
PLANCK EQUATION

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YUNUS BAŞAK  
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**Application of Variational Method and Supersymmetric  
Technique to the Fokker-Planck Equation**

**MSc Thesis**  
**in**  
**Engineering Physics**  
**University of Gaziantep**

**Supervisor**  
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**by**  
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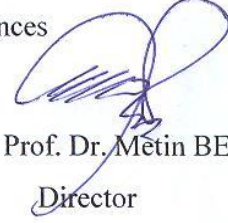
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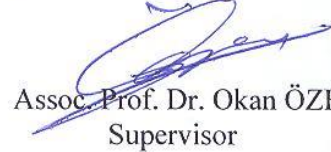
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## ABSTRACT

### APPLICATION OF VARIATIONAL METHOD AND SUPERSYMMETRIC TECHNIQUES FOR THE FOKKER-PLANCK PROBABILITY

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The time dependent probability density for the one-dimensional Fokker-Planck equation is determined by the variational method within the context of the Supersymmetric Quantum Mechanics. Using an *ansatz* function for the superpotential, one can obtain the trial wavefunctions of the variational method and then the construction of the hierarchy of the effective Hamiltonians allows us to obtain the variationaleigenfunctions and energies of the excited states to the evaluation of the probability. The symmetric bistable potentials, whose energy eigenvalues are calculated for some potential parameters, are studied. The numerical results obtained in this study are in very good agreement with the eigenvalues obtained by numerical integration in previous studies. The error percent is also presented in all calculations.

**Keywords:** ansatz, superpotential, variational method.

## ÖZET

# FOKKER-PLANCK OLASILIK HESABI İÇİN VARYASYONEL METOD VE SÜPERSİMETRİK TEKNİKLERİ

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Tek boyutlu Fokker-Planck denklemi için zamana bağlı olasılık yoğunluğu varyasyon yöntemi ile Süpersimetrik Kuantum Mekanikini kullanarak belirlenir. Superpotansiyel için yaklaşım fonksiyonunu kullanarak, varyasyon yönteminin deneme dalga fonksiyonları elde edilebilir ve daha sonra etkin Hamilton hiyerarşisinin yapısı bize, zamana bağlı olasılığın hesaplanmasındaki değişken özfonksiyonların ve uyarılmış durumların enerjilerini bulmanıza olanak sağlar. Bazı potansiyel parametreler için hesaplanmış enerji özfonksiyonları olan, simetrik bistabil potansiyelleri incelenmiştir. Bu çalışmada elde edilen sayısal sonuçlar daha önceki çalışmalarda sayısal integralleme ile elde edilen özdeğerler ile çok iyi bir uyum içindedir. Yüzdeler hata ayrıca her hesapta sunulmuştur.

**Anahtar kelimeler:** yaklaşım, süperpotansiyel, varyasyon metodu.

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## LIST OF SYMBOLS

$\psi$	Wavefunction of the system
$\epsilon$	Energy of the Hamiltonian
$\hbar$	Planck constant
$\hat{H}$	Hamiltonian operator
$V$	Potentialfunctionof the system
$A^{\pm}$	Ladder operator
$W$	Superpotential function

## CHAPTER 1

### GENERAL INTRODUCTION

Particle in a box, simple harmonic oscillator, hydrogen atom and such kind of quantum systems of which Hamiltonians are well known and can be solved exactly are good examples in undergraduate courses to understand the behavior of particles in a potential well [1]. On the other hand, there are some potential functions, in quantum physics, whose solution can not be solved exactly; no analytical energy eigenvalues and eigenfunctions are obtained explicitly. Therefore, there are many methods to solve these kinds of potential problems to find the eigenvalues and eigenfunctions of the Schrödinger equation. One of the basic approximation methods that are suitable for solving such problems is the Variational Method, which is also called the Rayleigh-Ritz method [2]. In other words, the variational method is one way of finding approximations to the lowest energy eigenstate or ground state, and some excited states. This allows calculating the approximate wavefunctions of systems such as molecular orbitals [3].

This method consists of choosing a “trial wavefunction” depending on one or more parameters and finding the values of these parameters for which the expectation value of the energy is the lowest possible. The wavefunction obtained by fixing the parameters to such values is then an approximation to the ground state wavefunction, and the expectation value of the energy in the state is an upper bound to the ground state energy. In general; for a Hamiltonian operator  $\hat{H}$  that describes the studied system and any normalizable function  $\psi$  with arguments approximate for the unknown wavefunction of the system, we define the energy function as

$$\epsilon[\psi] = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (1.1)$$

The variational principle states that;

-  $\epsilon \geq E_0$  where  $E_0$  is the lowest energy eigenstate(ground state) of the Hamiltonian.

-  $\epsilon = E_0$  if and only if  $\psi$  is exactly equal to the wavefunction of the ground state of the studied system.

Choosing a “trial wavefunction” in variational method can be done by suggesting an ansatz wavefunction which can be obtained from the SUSYQM.

## **CHAPTER 2**

### **SUPERSYMMETRIC QUANTUM MECHANICS and FOKKER-PLANCK EQUATION**

A unified description of all basic interactions of nature, i.e. strong, electroweak, and gravitational interactions has been studied for a long period by the scientists. There are many ambitious attempts made in the last years, and now it is considerably believed that supersymmetry (SUSY) is a necessary element in any unifying approach [4]. Basically, the SUSY gets relation between bosonic and fermionic degrees of freedom and it includes a graded Lie algebra that has combination of commutation and anti-commutation relations.

The idea in SUSY has given new comprehensions in the studies of statistical physics, mathematical physics, nuclear physics and condensed matter physics [5]. In particular, supersymmetric quantum mechanics (SUSYQM) originally has been introduced by Nicolai in 1976 [6], re-discovered by Witten [7] in 1981, and has been attracted much attention in the last decades [8].

The Fokker–Planck equation was first introduced by Fokker and Planck (for instance, see [9]) to describe the Brownian motion of a particle: When a small particle of mass  $m$  is immersed in a fluid, the equation of motion for the distribution function is defined by a time-dependent linear second-order partial differential equation. Recently, the Fokker–Planck equation has taken much attention in a number of different fields in natural science such as chemical physics, quantum optics, solid-state physics, circuit theory and theoretical biology [See Ref. 10 and references there in].

## 2.1 Supersymmetric Quantum Mechanics

It is well known that the time-independent Schrödinger equation describing a particle of mass  $m$  moving in a one-dimensional potential  $V(x)$  is given by [1]

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (2.1)$$

Now, we ask that if this equation can be factorized? According to the basic quantum mechanics, the Schrödinger equation can be factorized if one suggests the appropriate quantum mechanical "operators" [6]. Then, Eq. (2.1) can be factorized. Let's focus on Eq. (2.1) and its ground state wave function

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_0(x)}{dx^2} + V^-(x)\psi_0^-(x) = E_0^-\psi_0^-(x) \quad (2.2)$$

We use the 'superscripts' because our purpose is to obtain a "partner" of that equation, and these two systems should be distinguished from each other shortly. We start with the ground state wave function, which has a great importance in the procedure and the reason will be clearly seen in next steps. If we assume that  $H^-$  is the Hamiltonian operator for this system, then we can write

$$H^- = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V^-(x). \quad (2.3)$$

Since  $H^-$  is operator and  $E_0^-$  is its eigenvalue, then it can be convenient to re-write the equation as following:

$$\left(H^- - E_0^-\right)\psi_0^-(x) = 0 \quad (2.4)$$

Where  $E_0^-$  is the ground-state energy eigenvalue and  $\psi_0^-(x)$  is the *normalizable* ground-state eigenfunction of the operator  $H^-$  [11]. Thus, we obtain an equation in



terms of Hamilton operator for the system. Therefore, one can now factorize the operator on the left-hand side of the wave function as:

$$H^- - E_0^- = A^- A^+ \quad (2.5)$$

and it is guessed that these operators can be given in the following forms [12]

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

$$A^+ = +\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W(x), \quad (2.6)$$

Where  $W(x)$  is some function, called *superpotential function* in SUSYQM, whose exact form will be determined soon. As it is seen in the process, these operations do not change anything in the physics. It is also clear that the wave functions of the system are not affected and the potential of the system is just re-scaled by the constant term  $E_0^-$  in Eq.(2.4). One can ask to examine what exactly  $A^-$  and  $A^+$  operators 'do' on any function  $f(x)$ , for example. To see the effect, we just apply these operators on the function as it is done in quantum mechanics:

$$\begin{aligned} (A^- A^+)f(x) &= \left[ -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W(x) \right] \left[ \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W(x) \right] f(x) \\ &= \left[ -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W(x) \right] \left[ \frac{\hbar}{\sqrt{2m}} \frac{df(x)}{dx} + W(x)f(x) \right] \\ &= -\frac{\hbar^2}{2m} \frac{d^2 f(x)}{dx^2} - \left[ \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} W(x)f(x) \right] + W(x) \frac{\hbar}{\sqrt{2m}} \frac{df(x)}{dx} + W^2(x)f(x) \quad (2.7) \\ &= \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \frac{\hbar}{\sqrt{2m}} W'(x) + W^2(x) \right] f(x) \end{aligned}$$

For this result, it is required

$$W^2(x) - \frac{\hbar}{\sqrt{2m}} W'(x) = V^-(x) - E_0^- . \quad (2.8)$$

At that point it is clearly seen that if one can find a function  $W(x)$  satisfying this equation, then the Hamiltonian in Eq. (2.5) will have been successfully factorized. Now, the question is how one can determine the function  $W(x)$ ? We can suppose that it were the case  $A^+$  has annihilated the ground state wave function  $\psi_0^-$ , that means  $A^+\psi_0^-(x) = 0$ . Then  $A^-\left(A^+\psi_0^-(x)\right)$  would automatically be zero, and Eq.(2.4) would be satisfied. At his point, it is clearly seen as a reason why we have started by the ground-state wave function  $\psi_0^-(x)$ . Then we can look for a function  $W(x)$  which forces this condition to be satisfied. If we explicitly write the condition in terms of Eq.(2.8), then we get

$$A^+\psi_0^-(x) = \frac{\hbar}{\sqrt{2m}} \frac{d\psi_0^-(x)}{dx} + W(x)\psi_0^-(x) = 0 \quad (2.9)$$

and this equation leads us to find out that

$$W(x) = -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} \ln \psi_0^-(x) \quad (2.10)$$

It is obvious that one can also obtain  $\psi_0^-(x)$  from this equation if  $W(x)$  is known:

$$\psi_0^-(x) = N \exp \left[ -\frac{\sqrt{2m}}{\hbar} \int^x W(y) dy \right] \quad (2.11)$$

Where  $N$  is the normalization constant. Eq.(2.10) says that we can find  $W(x)$  explicitly if we know the ground state wave function. To do this, we are to solve the Schrödinger equation completely. We find that we need to know the solutions already. On the other hand, the Eq.(2.11) says something quite different: It says that if one somehow can find  $W(x)$  independently of any knowledge of  $\psi_0^-$ , then one can obtain the ground state wave function of the system by using Eq. (2.11). In essence,

we have transformed the Schrödinger equation into a completely different equation, but equivalent one. In more general terms, we have found a first-order, nonlinear differential equation equivalent to our original second-order linear differential equation. Such first-order nonlinear equivalents are classified under the general name of *Riccati equations*.

In order to obtain a partner potential and to factorize the Schrödinger equation, the only thing we do is to reverse the order of the factors  $A^\pm$  and get something interesting. Reversing the order of factors leads to a new Hamiltonian such as [12, 13]

$$A^+ A^- = H^+ - E_0^- \quad (2.12)$$

Where  $H^+ = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V^+(x)$  and it is found that

$$\begin{aligned} (A^+ A^-) f(x) &= \left[ \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W(x) \right] \left[ -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + W(x) \right] f(x) \\ &= \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{\hbar^2}{\sqrt{2m}} W'(x) + W^2(x) \right] f(x), \end{aligned} \quad (2.13)$$

for this result, it is required that the potential of this new Hamiltonian  $H^+$  must satisfy

$$W^2(x) + \frac{\hbar}{\sqrt{2m}} W'(x) = V^+(x) - E_0^- \quad (2.14)$$

From that equation, it is seen that there is a relation between partner potentials and it can be found as following: If we rewrite that equation with a little difference,

$$V^+(x) = W^2(x) + \frac{\hbar}{\sqrt{2m}} W'(x) + \frac{\hbar}{\sqrt{2m}} W'(x) - \frac{\hbar}{\sqrt{2m}} W'(x) + E_0^- \quad (2.15)$$

and using another fact,

$$V^-(x) = W^2(x) - \frac{\hbar}{\sqrt{2m}} W'(x) + E_0^-, \quad (2.16)$$

one obtains

$$V^+(x) = V^-(x) + 2 \frac{\hbar}{\sqrt{2m}} W'(x), \quad (2.17)$$

When the superpotential term is replaced in terms of wave function, we get finally,

$$V^+(x) = V^-(x) - \frac{\hbar^2}{m} \frac{d^2}{dx^2} \ln \psi_0^- \quad (2.18)$$

We can easily find interesting connections between these two systems described by  $H^-$  and  $H^+$ . First, consider an eigenfunction of  $H^-$  satisfying

$$H^- \psi_n^- = E_n^- \psi_n^-, \quad (2.19)$$

where  $E_n^-$  is the  $n^{\text{th}}$  energy of  $H^-$ . In terms of  $A^\pm$ , we get

$$(A^- A^+ + E_0^-) \psi_n^- = E_0^- \psi_n^- \quad (2.20)$$

Applying  $A^+$  to the left of both equations, we obtain

$$A^+ A^- A^+ \psi_n^- + E_0^- A^+ \psi_n^- = E_n^- A^+ \psi_n^-, \quad (2.21)$$

then we can group terms

$$(A^+ A^- + E_0^-) (A^+ \psi_n^-) = E_n^- (A^+ \psi_n^-) \quad (2.22)$$

which we notice Eq. (2.12) to get

$$H^+(A^+\psi_n^-) = E_n^-(A^+\psi_n^-) \quad (2.23)$$

This is a quite interesting result and it says that  $A^+\psi_n^-$  is a solution to the Schrödinger equation for  $H^+$ , with energy  $E_n^-$ . It is obvious that we can go the other way around. Starting with an eigenfunction  $\psi_m^+$  of  $H^+$  with energy  $E_m^+$  leads us to obtain

$$(A^+A^- + E_0^-)\psi_m^+ = E_m^+\psi_m^+ \quad (2.24)$$

Applying  $A^-$  to the left of both sides and grouping terms appropriately we get

$$(A^-A^+ + E_0^+)\psi_m^+ = E_m^+(A^-\psi_m^+) \quad (2.25)$$

or shortly

$$H^-(A^-\psi_m^+) = E_m^+(A^-\psi_m^+) \quad (2.26)$$

so  $A^-\psi_m^+$  is an eigenfunction of  $H^-$ , with an energy  $E_m^+$ .

In summary,  $A^+$  applied to any eigenfunction of  $H^-$  gives an eigenfunction of  $H^+$ , with the same energy eigenvalue;  $A^-$  applied to any eigenfunction of  $H^+$  gives an eigenfunction of  $H^-$ , again with the same eigenvalue. This guarantees that the two systems in fact have identical energy spectra, almost. Notice that  $A^+$  kills the ground state wave function  $\psi_0^-$  of  $H^-$ , by construction, so  $H^+$  has no corresponding eigenstate at the same energy. The lowest state of  $H^+$  must then correspond to the first 'excited' state of  $H^-$ , or  $E_0^+ = E_1^-$ . In general,

$$E_{n+1}^- = E_n^+ \quad (2.27)$$

As we have shown above if the ground-state eigenvalue of a potential can be shifted to zero and the ground-state eigenfunction can be normalized, then the system is called “*unbroken supersymmetry*”. This is why we obtain Eq. (2.27). Therefore, one can conclude that partner potentials have identically the same bound spectra, except the ground state of  $V^-(x)$  which does not appear in the spectrum of  $V^+(x)$ . This procedure is sometimes useful if one of the partner potentials is quite complex for to be solved than the other one.

On the other hand, if the partner potentials have ground-state energy eigenvalues greater than zero, then the system is called “*broken supersymmetry*”, and the energy eigenvalues satisfy the condition:

$$E_n^- = E_n^+ \quad (2.28)$$

As we have shown above one can obtain the eigenvalue and the eigenfunction among the partner potentials if the initial potential is in the exactly solvable form, such as Simple Harmonic Oscillator, Coulomb, Morse and Pösch-Teller potential [12]. One can easily obtain the partner potentials for them by following the procedure given above. At this point a question is asked that what the general relation among these potentials is and why they can be solved? In the paper by Gendenshtein [14], it is shown that these potentials have a property of “shape invariance” that is of importance point in the SUSYQM to obtain eigenvalues of the partner potentials. In the procedure we have given above if the potentials  $V^-(x)$  and  $V^+(x)$  can be written in a more general case than Eq.(2.18) as

$$V^+(x; a_0) = V^-(x; a_1) + R(a_1) \quad (2.29)$$

where  $a_0$  is a set of parameters and  $a_1$  is a function of  $a_0$  and the last term  $R(a_1)$  is a independent function of  $x$ , then the potentials  $V^-(x)$  and  $V^+(x)$  are called “shape invariant” potentials: They are similar in shape and differ only in the parameters appearing in their function forms. Following the hierarch process given above one can write the Hamiltonians in the form of the following structure

$$H^k = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V^-(x; a_k) + \sum_{i=1}^k R(a_i) \quad (2.30)$$

where  $a_k = f^k(a_0)$ , the function  $f$  applied  $k$  times. If we take the next member of the hierarchy and compare its spectrum with the previous one, we obtain

$$\begin{aligned} H^{k+1} &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V^-(x; a_{k+1}) + \sum_{i=1}^{k+1} R(a_i) \\ &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V^+(x; a_k) + \sum_{i=1}^k R(a_i) \end{aligned} \quad (2.31)$$

From Eqs. (2.30) and (2.31), we obtain that the Hamiltonians have identical bound-state spectra except for the lowest level of the member  $H^k$  whose energy is given by

$$E_0^k = \sum_{i=1}^k R(a_i) \quad (2.32)$$

This can be written from Eq.(31) and it is known that  $E_0^- = 0$ . The complete energy spectrum of  $H^-$  is found as

$$E_n^- = \sum_{i=1}^n R(a_i), \quad E_0^- = 0 \quad (2.33)$$

In several branches of physics, chemistry and biology the Fokker-Planck equation has many applications in the processes involving diffusion of neutrons, transfer of electrons, transfer of protons and protein folding [15].

## 2.2 The Fokker-Planck Equation

The general form of the Fokker-Planck equation (See *Appendix A* for a detailed derivation of the Fokker-Planck equation) is defined as [9, 16]

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ \frac{\partial}{\partial x} + D U'(x) \right] P(x,t) \quad (2.34)$$

In the steady-state case the probability function can be defined as  $P(x,t) = e^{-Et} \psi(x)$  and then one can write

$$\left[ \frac{d^2}{dx^2} + D U'(x) \frac{d}{dx} + D U''(x) \right] \psi(x) = -E \psi(x) \quad (2.35)$$

The transformation  $\psi(x) = e^{-DU(x)/2} \phi(x)$  makes possible to write Eq.(2.35) in the form of Schrödinger equation:

$$-\phi''(x) + \left( \frac{D^2}{4} U'(x)^2 - \frac{D}{2} U''(x) \right) \phi(x) = E \phi(x) \quad (2.36)$$

where one can define the Schrödinger potential by  $V_S(x) = \frac{D^2}{4} U'(x)^2 - \frac{D}{2} U''(x)$  and then one gets

$$-\phi''(x) + V_S(x) \phi(x) = E \phi(x) \quad (2.37)$$

where  $\hbar^2 = 2m = 1$ . Comparing Eq.(38) with Eq.(2.6), one finds a relation between the superpotential and the fluctuation functions as

$$W(x) = \frac{1}{2} D U'(x) \quad (2.38)$$

where the operators  $A^+$  and  $A^-$  are as given in Eq.(2.6).



## CHAPTER 3

### THE VARIATIONAL METHOD and SUPERSYMMETRIC TECHNIQUE

#### 3.1 The Variational Method

It is well known that there are some quantum systems of which Hamiltonians are well known, but they can not be solved exactly or by a perturbative treatment. That means there is no closely related Hamiltonian that can be solved exactly or approximately by perturbation theory because the first order is not sufficiently accurate, for example. One of the basic approximation methods that is suitable for solving such problems is the *variational method*, which is also called the Rayleigh–Ritz method [2]. The variational method is useful for determining upper bound values for the eigenenergies of a system of which Hamiltonian is known where as its eigenvalues and eigenstates are not known. Therefore, it is particularly useful for determining the ground state. However, it becomes quite cumbersome to determine the energy levels of the excited states.

In the context of the variational method, one does not attempt to solve the eigenvalue problem

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \quad (3.1)$$

but rather one uses a variational scheme to find the approximate eigenenergies and eigenfunctions from the variational equation

$$\delta E(\Psi) = 0 \quad (3.2)$$

where  $E(\Psi)$  is the expectation value of the energy in the state  $|\Psi\rangle$ :

$$E(\Psi) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (3.3)$$

If  $\Psi$  depends on a parameter, let us say  $\alpha$ , then  $E(\Psi)$  will also depend on  $\alpha$ . The variational ansatz Eq.(3.3) enables us to vary  $\alpha$  so as to minimize  $E(\Psi)$ . The minimum value of  $E(\Psi)$  provides an upper limit approximation for the true energy of the system. The variational method is particularly useful for determining the ground state energy and its eigenstate without explicitly solving the Schrödinger equation. Note that for any (arbitrary) trial function  $|\Psi_0\rangle$  we choose, the energy  $E$  as given by Eq.(3.3) is always larger than the exact energy  $E_0$ :

$$E(\Psi) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0 \quad (3.4)$$

the equality condition occurs only when  $|\Psi\rangle$  is proportional to the true ground state  $|\Psi_0\rangle$ . To prove this, we simply expand the trial function in terms of the exact eigenstates of  $\hat{H}$ :

$$|\Psi\rangle = \sum_n \alpha_n |\phi_n\rangle \quad (3.4)$$

With

$$\hat{H} |\phi_n\rangle = E_n |\phi_n\rangle \quad (3.5)$$

and since  $E_0 < E_n$ ,  $E_n$  for nondegenerate one-dimensional bound systems, we have

$$E(\Psi) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\sum_n |\alpha_n|^2 E_n}{\sum_n |\alpha_n|^2} \geq \frac{E_0 \sum_n |\alpha_n|^2}{\sum_n |\alpha_n|^2} = E_0 \quad (3.6)$$

which proves Eq.(3.4).

### 3.2 Supersymmetric Quantum Mechanics Formalism and the Variational Method

The hierarchy of Hamiltonians provides an efficient way to obtain the solution for excited states of the Schrödinger equation [17]. This general construction was originally conceived for exactly analytical solvable potentials. In what follows we give the main idea and fix the notation in this study.

The method of supersymmetric quantum mechanics starts from an original Hamiltonian  $H_0$  :

$$H_0 = -\frac{d^2}{dx^2} + V_0(x) \quad (3.7)$$

Next step is to factorize this Hamiltonian in terms of the "bosonic" operators  $a_1^\mp$ , defined in terms of a function  $w_1(x)$  known as the superpotential,

$$a_1^\mp = \mp \frac{d}{dx} + w_1(x) \quad (3.8)$$

And

$$H_0 = H_{1,-} = a_1^+ a_1^- + E_0^{(1)} = -\frac{d^2}{dx^2} + w_1^2(x) - w_1'(x) + E_0^{(1)} \quad (3.9)$$

where  $E_0^{(1)}$  is the ground state eigenvalue. Thus the superpotential  $w_1(x)$  satisfies the Riccati equation:

$$w_1^2(x) - w_1'(x) = V_0(x) - E_0^{(1)} \quad (3.10)$$

The supersymmetric partner of  $H_{1,-}$  is constructed by changing the order of operators  $a_1^\mp$  :

$$H_{1,-} = a_1^- a_1^+ + E_0^{(1)} = -\frac{d^2}{dx^2} + w_1^2(x) + w_1'(x) + E_0^{(1)} \quad (3.11)$$

where the potential associated to this Hamiltonian is:

$$V_{1,+}(x) = w_1^2(x) + w_1'(x) + E_0^{(1)} \quad (3.12)$$

The Hamiltonian  $H_{1,+}$  can be identified with another Hamiltonian. If this new Hamiltonian can be factorized by new operators  $a_2^\mp = \mp \frac{d}{dx} + w_2(x)$  then we obtain,

$$H_{1,+} = a_1^+ a_1^- + E_0^{(2)} = -\frac{d^2}{dx^2} + w_2^2(x) + w_2'(x) + E_0^{(2)} \quad (3.13)$$

where the superpotential  $w_2(x)$  must satisfy the Riccati equation similar to Eq. (3.10). This equation is obtained through the imposition that  $H_{1,+}$  be equal to  $H_{2,-}$ , then,

$$V_{1,+}(x) = w_2^2(x) + w_2'(x) + E_0^{(2)} \quad (3.14)$$

With  $V_{1,+}(x)$  indicated in Eq.(3.12). The difference between Eq.(3.12) and Eq.(3.14) is only an additive constant that is related to the energy eigenvalue.

This process can be repeated “ $n$ ” times since successive Hamiltonians can be factorized and a family or hierarchy of Hamiltonians can be constructed as:

$$H_{n,-} = a_n^+ a_n^- + E_0^{(n)} \quad (3.15)$$

Where

$$a_n^\mp = \mp \frac{d}{dx} + w_n(x) \quad (3.16)$$

And

$$w_n^2(x) - w_n'(x) = V_{n,-}(x) - E_0^{(n)} \quad (3.17)$$

The lowest state eigenfunction is obtained by applying the operator  $a_1^-$ , given by Eq. (3.16), in the ground state wave function,

$$a_1^- \Psi_0^{(1)}(x) = 0 \quad (3.18)$$

This results in

$$\Psi_0^{(1)}(x) \propto e^{-\int w_1(x) dx} \quad (3.19)$$

The first excited state  $\Psi_1^{(1)}(x)$  can be obtained through the operator  $a_1^+$  applied to  $\Psi_0^{(1)}(x)$ . This relation can be extended to all the members of the hierarchy; it is possible to get a general form for the eigenfunctions of the excited states by the application of the bosonic operators successively. These are simple relations connecting the eigenfunctions and eigenvalues of the members of the hierarchy:

$$\Psi_n^{(1)}(x) = a_1^+ a_2^+ a_3^+ \cdots a_n^+ \Psi_0^{(n+1)}(x) \text{ and } \Psi_0^{(n)}(x) = N e^{-\int w_n(x) dx} \quad (3.20)$$

And

$$E_n^{(1)} = E_0^{(n+1)} \quad (3.21)$$

The superscript and subscript notations represent the member of the hierarchy of Hamiltonians and the energy level of each member, respectively. See Ref. [18] for detail.

The exactly analytical solvable potentials can be studied by the general construction presented above. However, the relation between the variational method and the formalism of supersymmetric quantum mechanics can provide an appropriate and successful way to determine trial eigenfunctions in order to find out the energy eigenvalues variationally for the non-exactly solvable potentials [19]. The approach to obtain these trial functions is based on an *ansatz* for the superpotential generally used in supersymmetric quantum mechanic formalism. If an approximate function that depends on free parameters is used to obtain an effective potential, then one obtains Eq.(3.14). Using Eq. (3.20) one finally gets the eigenfunction which depends on a set of free parameters, denoted by  $\alpha$ , that is used in the variational method to minimize the energy expectation value, given by the following expression:

$$E(\alpha) = \frac{\langle \Psi(x, \alpha) | \hat{H} | \Psi(x, \alpha) \rangle}{\langle \Psi(x, \alpha) | \Psi(x, \alpha) \rangle} \quad (3.22)$$

It is also possible to apply an extension of the procedure described above for excited states. Since one factorizes the effective Hamiltonian, it is possible to build a supersymmetric partner as indicated in Eq. (3.13). Then one can search for an effective Hamiltonian in order to obtain a trial eigenfunction and through this procedure the first excited state can be found. The procedure can be followed to obtain a set of effective Hamiltonians, one for each state of the original Hamiltonian. Therefore, it is a constructive approach to obtain trial functions for excited states for a given Hamiltonian. The eigenfunctions and eigenvalues obtained variationally by this method can be used in the calculation of the transition probability for the Fokker-Planck equation.

## CHAPTER 4

### APPLICATIONS

As a first application we consider the even-power potential [20]

$$V_0(x) = Ax^6 + Bx^4 + Cx^2 + D \quad (4.1)$$

The partner potential is found as

$$V_{1,-}(x) = w_1^2(x) - w_1'(x) + E_0^{(1)} = Ax^6 + Bx^4 + Cx^2 + D \quad (4.2)$$

which is satisfied by the following superpotential

$$w_1(x) = a_1x + b_1x^3 \quad (4.3)$$

We note here that there is an exact solution for the ground state when the potential and superpotential parameters are defines as  $A=1, B=-2, C=-1, D=1$  and  $a_1=-1, b_1=1$ , respectively. Using Eq. (3.15), one gets

$$\Psi_0^{(1)}(x) = e^{-\frac{x^2}{2}a_1 - \frac{x^4}{4}b_1} \quad (4.4)$$

Following the procedure given above one can construct the partner Hamiltonian.

Thus, we get

$$H_{1,+} = -\frac{d^2}{dx^2} + w_1^2(x) + w_1'(x) + E_0^{(1)} \quad (4.5)$$

in which the partner potential is determined as

$$V_{1,+}(x) = w_1^2(x) + w_1'(x) + E_0^{(1)} = a_1^2x^2 + 2a_1b_1x^4 + b_1^2x^6 + 3b_1x^2 + a_1 + E_0^{(1)} \quad (4.6)$$

If the parameters  $a_1=-1, b_1=1$  are given, then we find

$$V_{1,+}(x) = x^6 - 2x^4 + 4x^2 - 1 \quad (4.7)$$

Following the factorization procedure in SQM, one obtains the second partner Hamiltonian as

$$H_{2,-} = -\frac{d^2}{dx^2} + w_2^2(x) - w_2'(x) + E_0^{(2)} = -\frac{d^2}{dx^2} + V_{2,-}(x) \quad (4.8)$$

in which the superpotential  $w_2(x)$  satisfies

$$w_1^2(x) + w_1'(x) + E_0^{(1)} = w_2^2(x) - w_2'(x) + E_0^{(2)} \quad (4.9)$$

Now there is not an exact solution for the Riccati equation for  $w_2(x)$  and then one can make the following ansatz for the superpotential since  $V_{1,+}(x)$  and  $V_{1,-}(x)$  are in the same functional form. Therefore, one can set

$$w_1(x) = a_2x + b_2x^3 \quad (4.10)$$

And

$$\Psi_0^{(2)}(x) = e^{-\frac{x^2}{2}a_2 - \frac{x^4}{4}b_2} \quad (4.11)$$

where the constants  $a_2$  and  $b_2$  are now parameters that minimize the energy of  $E_0^{(2)}$  by the variationa method:

$$E_0^{(2)} = E_1^{(1)} = \frac{\int \Psi_0^{(2)} H_{1,+} \Psi_0^{(2)} dx}{\int \Psi_0^{(2)} \Psi_0^{(2)} dx} \quad (4.12)$$

The excited states can be determined by the same procedure if one suggests the ansatz superpotential in the form of

$$w_n(x) = a_nx + b_nx^3 \quad (4.13)$$

and then the ground state wavefunctions of each partner can be determined by

$$\Psi_0^{(n)}(x) = Ne^{-\int w_n(x')dx'} = e^{-\frac{x^2}{2}a_n - \frac{x^4}{4}b_n} \quad (4.14)$$



In Table 1, we give the values of  $a_n$  and  $b_n$  minimized parameters, the energy eigenvalues obtained from the variational method, the numerical results of the potential function in Eq.(3.13) for the certain parameters. We also present the percent Error in the last column. It is observed that the variational results are in a good agreement for the low values of energy with the ones obtained by numerical calculation. For higher states the more approximations are needed. In Figure 1, we present the first four states normalized wave functions for the minimized parameters of  $a_n$  and  $b_n$  values given in Table 1.

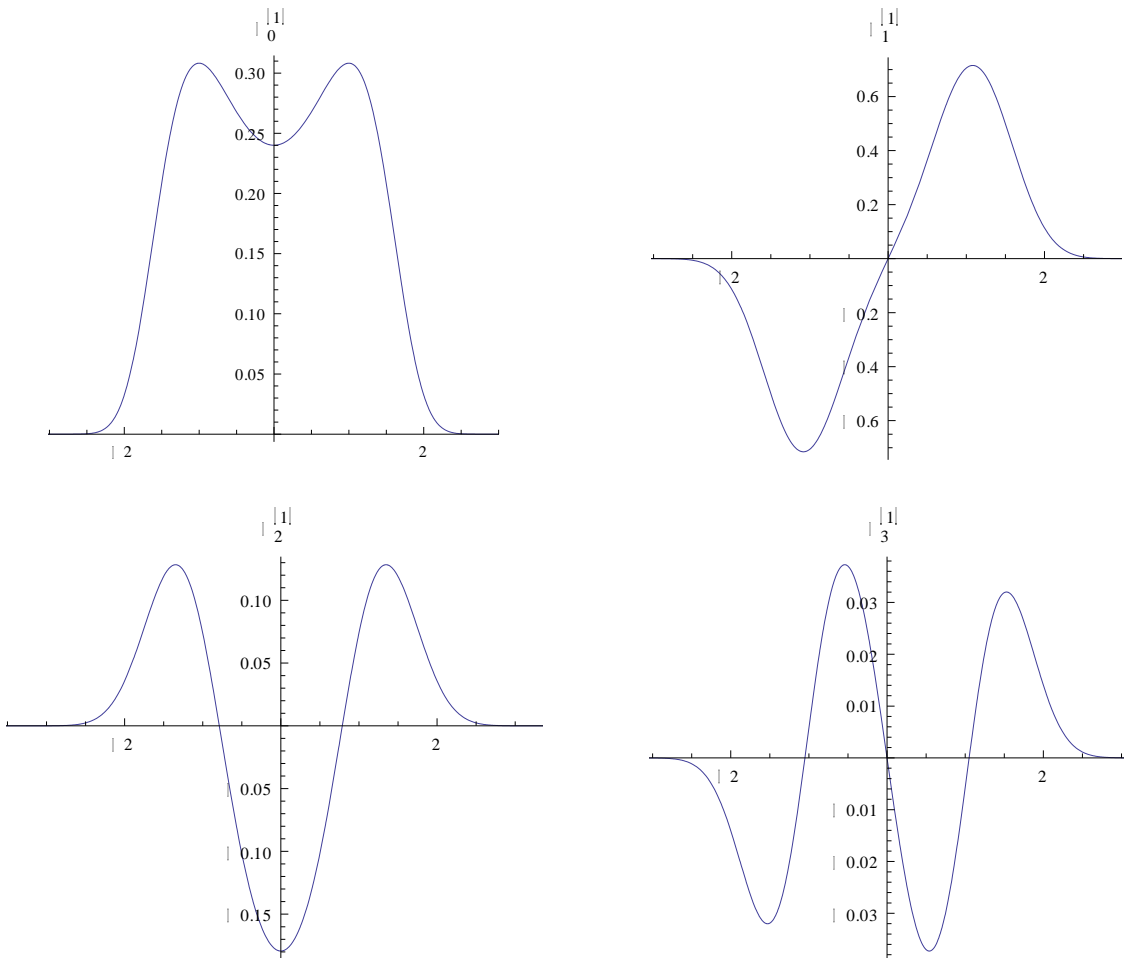
**Table 1:** The minimized values of  $a_n$  and  $b_n$ , the energy eigenvalues by the variational method ( $E_n^V$ ) with supersymmetric formalism, the numerical results ( $E_n^N$ ) and the percent errors for the potential in Eq.(64) with potential parameters  $A=1, B=-2, C=-1, D=1$ .

$a_n$	$b_n$	$E_n^V$	$E_n^N$	Error (%)
$a_1 = -1$	$b_1 = 1$	$E_0^V = 0$	$E_0^N = 0$	0
$a_2 = 1.6895$	$b_2 = 0.2850$	$E_1^V = 0.4238$	$E_1^N = 0.4229$	0.21
$a_3 = 2.0990$	$b_3 = 0.2440$	$E_2^V = 2.3192$	$E_2^N = 2.3149$	0.18
$a_4 = 2.4040$	$b_4 = 0.2194$	$E_3^V = 4.5713$	$E_3^N = 4.5038$	1.49
$a_5 = 2.6525$	$b_5 = 0.2025$	$E_4^V = 7.0998$	$E_4^N = 7.1755$	1.55

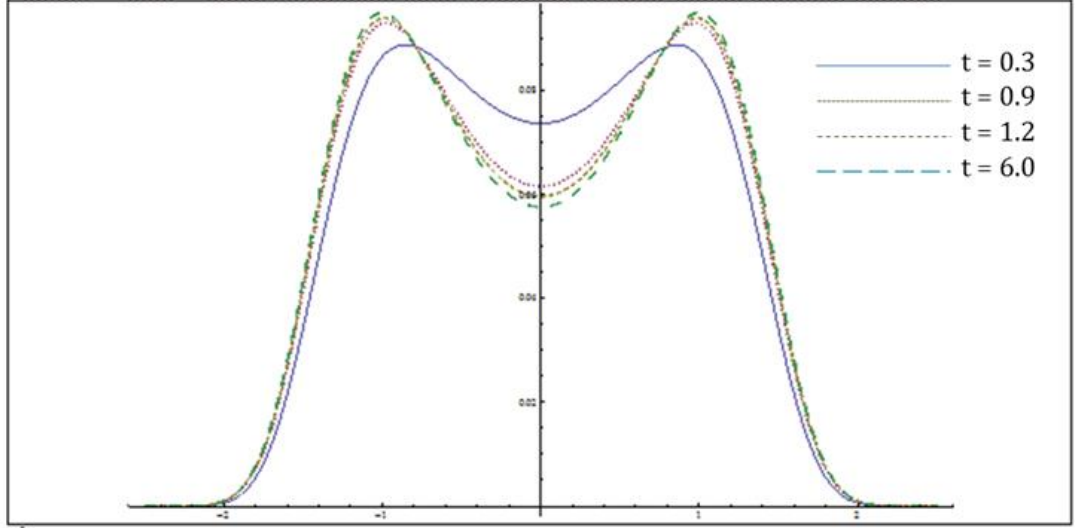
One can now calculate the transition probability

$$P(x,t|0,0) = e^{(-x^2/2 - x^4/4)} \sum_{n=0}^4 \Psi_n^{(1)}(x) \Psi_n^{(1)}(0) \times e^{-\lambda_n t} \quad (4.15)$$

where it is set  $\lambda_n = E_n^{(1)}$  for the truncation of the series for the transition probability function. We show the transition probability  $P(x,t|0,0)$  for four different time values,  $t$ , in Figure 2.



**Figure 1:** The first four states normalized wave functions for  $\Psi_n^{(1)}$  where  $n=0,1,2,3$ .



**Figure 2:** The transition probability functions for four different values of time,  $t$ .

As a second application, we consider the quartic potential [21]

$$V_0(x) = -\beta x^2 + x^4 \quad (4.16)$$

Following the procedure given above, one can obtain the partner potential functions, the wave functions and the eigenvalues of the quartic potential in Eq.(78) by determining the values of the minimized parameters of  $a_n$  and  $b_n$ . We give our results in Table 2a, 2b, 2c and 2d for the first 4 states of the quartic potential for different  $\beta$  values. We also compare our results with numerical results and present the percent error in the calculations.

As a third application, we consider the following sextic potential which has a great importance in class of quasi-exactly solvable potentials [22-24]:

$$V_0(x) = x^6 - 3x^2 \quad (4.17)$$

Following the same procedure, one can determine the partner Hamiltonians and the energy eigenvalues of the potential in Eq. (4.17). We present our results in Table 3.

**Table 2a:** The minimized values of  $a$  and  $b$ , the ground state energy eigenvalues by the variational method ( $E_0^V$ ) with supersymmetric formalism, the numerical results ( $E_0^N$ ) and the percent errors for the potential in Eq.(4.16) for different  $\beta$  values.

$\beta$	$a$	$b$	$E_0^V$	$E_0^N$	Error (%)
0.1	1.060	0.300	1.023911	1.023810	0.01
0.2	1.020	0.305	0.986647	0.986540	0.01
0.4	0.945	0.315	0.909823	0.909680	0.02
0.6	0.875	0.320	0.829672	0.829488	0.02
0.8	0.800	0.330	0.745853	0.745613	0.03
1.0	0.720	0.340	0.657974	0.657656	0.05

**Table 2b:** The minimized values of  $a$  and  $b$ , the first excited state energy eigenvalues by the variational method ( $E_1^V$ ) with supersymmetric formalism, the numerical results ( $E_1^N$ ) and the percent errors for the potential in Eq.(4.16) for different  $\beta$  values.

$\beta$	$a$	$b$	$E_1^V$	$E_1^N$	Error (%)
0.1	1.63	0.23	3.714926	3.70897	0.16
0.2	1.6	0.23	3.626268	3.61704	0.26
0.4	1.56	0.23	3.428299	3.42950	0.04
0.6	1.52	0.24	3.245721	3.23679	0.28
0.8	1.49	0.24	3.044770	3.03859	0.20
1.0	1.45	0.24	2.842032	2.83456	0.26

**Table 2c:** The minimized values of  $a$  and  $b$ , the second excited state energy eigenvalues by the variational method ( $E_2^V$ ) with supersymmetric formalism, the numerical results ( $E_2^N$ ) and the percent errors for the potential in Eq.(4.16) for different  $\beta$  values.

$\beta$	$a$	$b$	$E_2^V$	$E_2^N$	Error (%)
0.1	1.98	0.20	7.32667	7.33079	0.06
0.2	1.95	0.20	7.18273	7.20491	0.31
0.4	1.92	0.20	6.91123	6.95033	0.56
0.6	1.90	0.21	6.66891	6.69197	0.34
0.8	1.88	0.20	6.413241	6.42982	0.26
1.0	1.84	0.21	6.137756	6.16393	0.42

**Table 2d:** The minimized values of  $a$  and  $b$ , the third excited state energy eigenvalues by the variational method ( $E_3^V$ ) with supersymmetric formalism, the numerical results ( $E_3^N$ ) and the percent errors for the potential in Eq.(4.16) for different  $\beta$  values.

$\beta$	$a$	$b$	$E_3^V$	$E_3^N$	Error (%)
0.1	2.25	0.18	11.55487	11.48857	0.58
0.2	2.22	0.18	11.35422	11.33136	0.20
0.4	2.19	0.18	11.02608	11.01406	0.11
0.6	2.19	0.19	10.75837	10.69288	0.61
0.8	2.16	0.18	10.45268	10.36778	0.82
1.0	2.14	0.18	10.11452	10.03872	0.76

**Table 3:** The minimized values of  $a$  and  $b$ , the first few excited state energy eigenvalues by the variational method ( $E_n^V$ ) with supersymmetric formalism, the numerical results ( $E_n^N$ ) and the percent errors for the potential in Eq.(4.17) for different  $\beta$  values (Note that  $E_0^{V,N} = 0$ ).

n	$a_n$	$b_n$	$E_n^V$	$E_n^N$	Error (%)
1	1.9	0.5	1.93596	1.9354	0.03
2	2.5	0.4	6.344699	6.2985	0.73
3	2.9	0.4	11.75929	11.6809	0.58
4	3.3	0.3	17.92811	18.0426	0.63
5	3.6	0.2	24.78196	25.2546	1.87

As a last, the Morse potential is considered. For the diatomic system, the three dimensional Morse oscillator [25] can be written as

$$V_M = D(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}) \quad (4.18)$$

where  $D$  is the dissociation energy,  $r_e$  is the equilibrium internuclear distance and  $a$  is the range parameter. One can write the Schrödinger equation in terms of a new variable  $y$  as

$$\left( -\frac{d^2}{dy^2} + \frac{l(l+1)}{y^2} + \lambda^2(e^{-2(y-y_e)} - 2e^{-(y-y_e)}) \right) \Psi(y) = \epsilon \Psi(y) \quad (4.19)$$

where  $y = ar$  and the constants are set like

$$y_e = ar, \quad \lambda^2 = \frac{2mD}{a^2\hbar^2}, \quad E = \epsilon \frac{\hbar^2 a^2}{2m} \quad (4.20)$$

and the parameter  $m$  is the reduced mass of the molecule.

The Schrödinger equation can be exactly solvable and therefore one can construct the hierarchy of Hamiltonians as shown above. In this case, the Schrödinger equation can be reduced to the form

$$\left( -\frac{d^2}{dy^2} + \frac{l(l+1)}{y^2} + \lambda^2(e^{-2(y-y_e)} - 2e^{-(y-y_e)}) \right) \Psi(y) = \epsilon \Psi(y) \quad (4.21)$$

Using the behaviour of the wavefunction at  $y = 0$  and  $y$  goes to infinity, one can write the eigenfunction obtained from Eq.(4.21) as

$$\Psi(y) \propto e^{-\lambda e^{-(y-y_e)}} y^{(l+1)} e^{-Cy} \quad (4.22)$$

where one can suggest the variational parameter “ $C$ ” in the equation. Using the ansatz wave function in Eq. (4.22) one can also obtain the superpotential  $w_1(y)$  as

$$w_1(y) = -\frac{d}{dy} \ln[\Psi(y)] = -\lambda e^{-(y-y_e)} - \frac{(l+1)}{y} + C \quad (4.23)$$

Using expression in Eq. (4.22) as a trial wavefunction in the variational method we can change the parameter  $C$  by the variational parameter  $\mu$ :

$$\Psi_\mu = \Psi(y, C = \mu) \propto e^{-\lambda e^{-(y-y_e)}} y^{(l+1)} e^{-\mu y} \quad (4.24)$$

Following the process given in Eq. (3.22) the energy eigenvalues can then obtained by minimisation of the energy expectation value with respect to  $\mu$ . Therefore, the equation we have to consider to minimize is given as

$$E_\mu = \frac{\int_0^\infty \Psi_\mu(y) \left[ -\frac{d^2}{dy^2} + \frac{l(l+1)}{y^2} + \lambda^2(e^{-2(y-y_e)} - 2e^{-(y-y_e)}) \right] \Psi_\mu(y) dy}{\int_0^\infty \Psi_\mu(y)^2 dy} \quad (4.25)$$

Using this expression one can calculate the ground state energy expectation value of various molecules such as  $H_2$ ,  $HCl$ ,  $CO$  and  $LiH$  for known values of their respective potentials parameters  $D$ ,  $a$ ,  $r_e$ , and  $m$  of the molecules in Table 4[26]

**Table 4:** Potential parameters  $D$ ,  $a$ ,  $r_e$ , and  $m$  for different molecules [26].

Molecule	$D$ (eV)	$r_e$ (Å)	$m$ (amu)	$a$ (Å <sup>-1</sup> )	$\lambda$
H <sub>2</sub>	4.7446	0.7416	0.50391	1.9426	17.4129
LiH	2.5152672118	1.5956	0.8801221	1.1280	28.8558
HCl	4.619030905	1.2746	0.9801045	1.8677	24.9221
CO	10.845073641	1.1283	6.8606719	2.2994	82.0662

The results are given for different values of  $l$  for the molecules under investigation as shown in Tables 5-8.

**Table 5:** Comparison of bound states energy eigenvalues (in eV) for the H<sub>2</sub> molecule for different values of the angular momentum quantum number.

$l$	$\mu$	Present Results	[27]	[28]	[29]	[30]	[31]	[32]	[33]
0	17.595	4.475936	4.4762	4.47601	4.47601	4.47601	4.4760	4.4760084	4.4760131
5	20.349	4.256705	4.2592	4.25880	4.25901	4.25880	4.2590	4.2590038	4.2590180
10	21.953	3.719804	3.7251	3.72193	3.72473	3.72193	3.7247	3.7247181	3.7247471
15	22.538	2.959578	2.9669	2.95158	2.96635	–	–	2.9663319	2.9663814
20	22.289	2.075983	–	2.02864	2.08401	–	–	2.0839937	2.0840636

**Table 6:** Comparison of bound states energy eigenvalues (in eV) for the HCl molecule for different values of the angular momentum quantum numbers.

$l$	$\mu$	Present Results	[28]	[30]	[31]	[33]	[34]	[34]
0	24.838	4.43555	4.43556	4.4356	4.4355	4.4355522	4.43556	4.43556
5	26.826	4.39667	4.39681	4.3968	4.3968	4.3968066	4.39681	4.39682
10	28.648	4.29363	4.28408	4.2841	4.2940	4.2940628	4.28407	4.28409
15	30.290	4.12803	4.12889	-	-	4.1288846	4.12889	4.12893
20	31.740	3.90241	3.90375	-	-	3.9037744	3.90374	3.90385

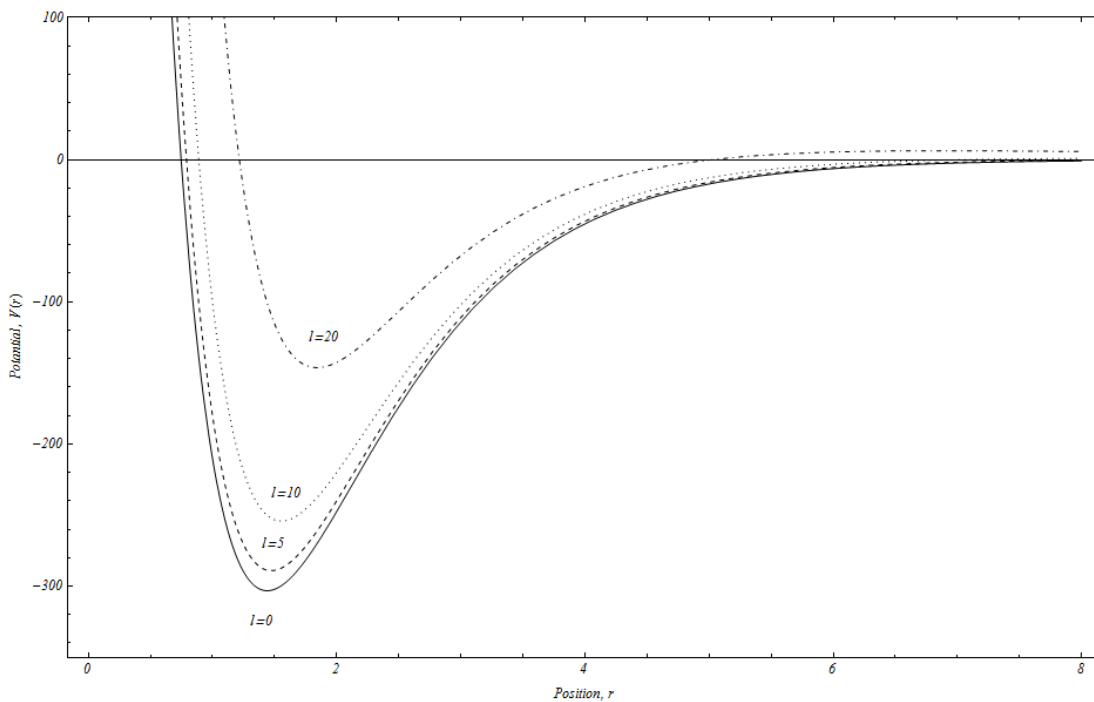


**Table 7:** Comparison of bound states energy eigenvalues (in eV) for the CO molecule for different values of the angular momentum quantum numbers.

$l$	$\mu$	Present Results	[28]	[30]	[31]	[33]	[34]	[34]	[35]
0	83.378	11.0916	11.0915	11.0915	11.092	11.0915353	11.0915	11.0915	11.091
5	85.279	11.0844	11.0844	11.0845	11.084	11.0843875	11.0844	11.0844	11.084
10	87.146	11.0653	11.0653	11.0653	11.065	11.0653334	11.0653	11.0653	11.065
15	88.915	11.0344	11.0344	-	-	11.0343911	11.0344	11.0344	-
20	90.768	10.9916	10.9916	-	-	10.9915902	10.9916	10.9916	-

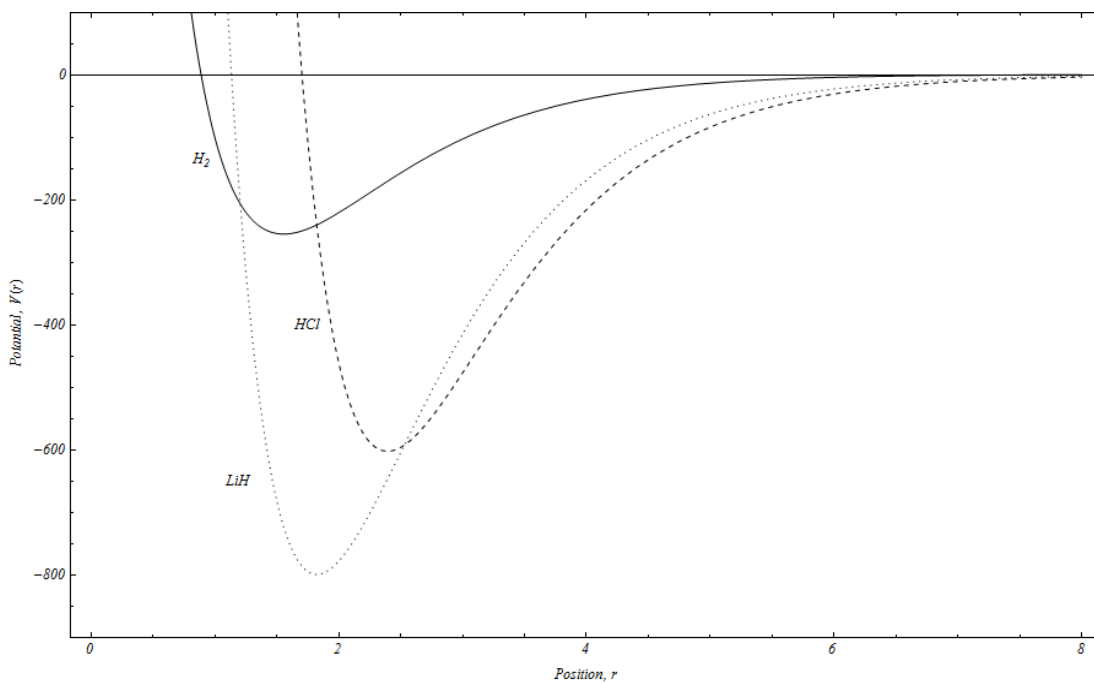
**Table 8:** Comparison of bound states energy eigenvalues (in eV) for the LiH molecule for different values of the angular momentum quantum numbers.

$l$	$\mu$	Present Results	[28]	[30]	[31]	[33]	[34]	[34]	[35]
0	28.906	2.42885	2.42886	2.4289	2.4280	2.4288627	2.42886	2.42886	2.4287
5	31.469	2.40118	2.40133	2.4013	2.4000	2.4013352	2.40133	2.40133	2.4012
10	33.688	2.32842	2.32883	2.3288	2.3261	2.3288530	2.32883	2.32885	2.3287
15	35.539	2.21306	2.21377	-	-	2.2138464	2.21377	2.21385	-
20	37.012	2.05885	2.05977	-	-	2.0600073	2.05977	2.06001	-



**Figure 3:** The Morse potential for  $H_2$  molecule for different  $l$  values

The Figure 3 shows graph of the Morse potential for four different values of the orbital angular momentum quantum number,  $l$ . The graph says that the behaviour of the Morse potential is typical of the substantial variance of  $V(r)$  for  $l \neq 0$  and  $l = 0$ . The different molecules for the same  $l$  (where  $l = 10$ ), The Morse potential seems as in Figure 4. The relation between the potential energy and distance separating two bonded atoms as HCL, is the great importance such that chemical processes.



**Figure 4:** The Morse potential for different molecules for  $l = 10$

## CHAPTER 5

### CONCLUSION

In this work we have studied a method to determine the time dependent probability density for the one-dimensional Fokker-Planck equation. The treatment is based on an analysis of the Schrödinger equation through the variational method associated to the formalism of the supersymmetric quantum mechanics. We have used an ansatz superpotential which allows us to obtain the trial wavefunction of the variational method. Using SUSYQM, the hierarchy of the effective Hamiltonians can be constructed. The superpotentials give us the variational eigenfunctions and the effective potentials. The adjustable parameters allow one to calculate the minimum eigenenergy of the partner potential for the full spectra. The symmetric bistable potentials are studied to illustrate the approach whose results are in good agreement with the numerical calculations [36].

As a result, our study shows that the variational supersymmetric approach can be useful and effective for a group of polynomial potentials.

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## APPENDIX

### APPENDIX A

#### Derivation of the Fokker-Planck Equation

Let  $\{X(t): t \geq 0\}$  be a one-dimensional stochastic process with  $t_1 > t_2 > t_3$  [37]. We use  $P(X_1, t_1; X_2, t_2)$  to denote the joint probability distribution, i.e., the probability that  $X(t_1) = X_1$  and  $X(t_2) = X_2$ , and  $P(X_1, t_1 | X_2, t_2)$  to denote the conditional (or transition) probability distribution, i.e., the probability that  $X(t_1) = X_1$  given that  $X(t_2) = X_2$ , defined as  $P(X_1, t_1; X_2, t_2) = P(X_1, t_1 | X_2, t_2)P(X_2, t_2)$ . We will assume  $X(t)$  is a Markov process, namely,

$$P(x_1, t_1 | X_2, t_2; X_3, t_3) = P(X_1, t_1 | X_2, t_2). \quad (\text{A.1})$$

For any continuous state Markov process, the following Chapman-Kolmogorov equation is satisfied [38, 9]:

$$P(x_1, t_1 | X_3, t_3) = \int P(x_1, t_1 | X_2, t_2) P(x_2, t_2 | X_3, t_3) dX_2. \quad (\text{A.2})$$

In the following, We also assume  $X(t)$  is time homogenous:

$$P(X_1, t_1 + s; X_2, t_2 + s) = P(X_1, t_1, X_2, t_2), \quad (\text{A.3})$$

So that  $X$  is invariant with respect to a shift in time. For simplicity of notation, we use  $P(X_1, t_1 - t_2 | X_2) \equiv P(X_1, t_1 | X_2, t_2)$ .

We will now outline the derivation of the Fokker-Planck equation, a partial differential equation for the time evolution of the transition probability density function. This closely follows the derivation in Ref. [39]. Consider

$$\int_{-\infty}^{\infty} h(Y) \frac{\partial P(Y, t | X)}{\partial t} dY, \quad (\text{A.4})$$

where  $h(Y)$  is any smooth function with compact support. Writing

$$\frac{\partial P(Y, t | X)}{\partial t} = \lim_{\Delta t \rightarrow 0} \frac{P(Y, t + \Delta t | X) - P(Y, t | X)}{\Delta t}, \quad (\text{A.5})$$

and interchanging the limit with the integral, it follows that

$$\int_{-\infty}^{\infty} h(Y) \frac{\partial P(Y, t | X)}{\partial t} dY = \lim_{\Delta t \rightarrow 0} \int_{-\infty}^{\infty} h(Y) \left[ \frac{P(Y, t + \Delta t | X) - P(Y, t | X)}{\Delta t} \right] dY \quad (\text{A.6})$$

Applying the Chapman-Kolmogorov identity (Eq. A.2), the right hand side of Eq. A.6 can be written as

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[ \int_{-\infty}^{\infty} h(Y) \int_{-\infty}^{\infty} P(Y, \Delta t | Z) P(Z, t | X) dZ dY - \int_{-\infty}^{\infty} h(Y) P(Y, t | X) dY \right], \quad (\text{A.7})$$

Interchanging the limits of integration in the first term of Eq. 7, letting  $Y \rightarrow Z$  in the second term, and using the identity  $\int_{-\infty}^{\infty} P(Y, \Delta t | Z) dY = 1$ , we have

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[ \int_{-\infty}^{\infty} P(Z, t | X) \int_{-\infty}^{\infty} P(Y, \Delta t | Z) (h(Y) - h(Z)) dY dZ \right] \quad (\text{A.8})$$

Taylor expanding  $h(Y)$  about  $Z$  gives

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[ \int_{-\infty}^{\infty} P(Z, t | X) \int_{-\infty}^{\infty} P(Y, \Delta t | Z) \sum_{n=1}^{\infty} h^{(n)}(Z) \frac{(Y - Z)^n}{n!} dY dZ \right]. \quad (\text{A.9})$$

Defining the jump moments as



$$D^{(n)}(Z) = \frac{1}{n!} \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{-\infty}^{\infty} (Y - Z)^n P(Y, \Delta t | Z) dY \quad (\text{A.10})$$

It follows that

$$\int_{-\infty}^{\infty} h(Y) \frac{\partial P(Y, t | X)}{\partial t} dY = \int_{-\infty}^{\infty} P(Z, t | X) \sum_{n=1}^{\infty} D^{(n)}(Z) h^{(n)}(Z) dZ. \quad (\text{A.11})$$

Integrating each term on the right side of Eq. (A.11) by parts  $n$  times and using the assumptions on  $h$ , after moving terms to the left hand side, it follows that

$$\int_{-\infty}^{\infty} h(Z) \left( \frac{\partial P(Z, t | X)}{\partial t} - \sum_{n=1}^{\infty} \left( -\frac{\partial}{\partial Z} \right)^n \left[ D^{(n)}(Z) P(Z, t | X) \right] \right) dZ = 0. \quad (\text{A.12})$$

Now, because  $h$  is an arbitrary function, it is necessary that

$$\left( \frac{\partial P(Z, t | X)}{\partial t} \right) = \sum_{n=1}^{\infty} \left( -\frac{\partial}{\partial Z} \right)^n \left[ D^{(n)}(Z) P(Z, t | X) \right]. \quad (\text{A.13})$$

We define the probability distribution function  $P(X; t)$  of  $X(t)$  as the solution of Eq. (A.13) with initial condition given by a  $\delta$ -distribution at  $X_0$  at  $t = 0$ . In this case,  $P(X, t) \equiv P(X, t | X_0, 0)$  and we may write Eq. 13 as

$$\left( \frac{\partial P(Z, t | X)}{\partial t} \right) = \sum_{n=1}^{\infty} \left( -\frac{\partial}{\partial Z} \right)^n \left[ D^{(n)}(X) P(X, t) \right], \quad (\text{A.14})$$

with

$$D^{(n)}(X_0) = \frac{1}{n!} \lim_{\Delta t \rightarrow 0} \left\langle \left[ X(t + \Delta t) - X(t) \right]^n \right\rangle \Big|_{t=0}, \quad (\text{A.15})$$

which is commonly called the Kramers-Moyal expansion. Now, if we assume  $D^{(n)}(X) = 0$  for  $n > 0$ , then we have the Fokker-Planck equation:

$$\frac{\partial P(X,t)}{\partial t} = -\frac{\partial}{\partial X}[V(X)P(X,t)] + \frac{\partial^2}{\partial X^2}[D(X)P(X,t)], \quad (\text{A.16})$$

where,  $V(X) \equiv D^{(1)}(X)$  is the drift coefficient and  $D(X) \equiv D^{(2)}(X) > 0$  is the diffusion coefficient, which can be written as

$$V(X_0) = \left. \frac{\partial \langle X(t; X_0) \rangle}{\partial t} \right|_{t=0}, \quad D(X_0) = \left. \frac{1}{2} \frac{\partial \sigma^2(t; X_0)}{\partial t} \right|_{t=0}, \quad (\text{A.17})$$

where angular brackets denote ensemble averaging,  $\sigma^2$  denotes the variance of  $X$ , and  $X(t; X_0)$  denotes a realization with  $X(0) = X_0$ . Any stochastic process  $X(t)$  whose probability distribution function satisfies the Fokker-Planck equation is known mathematically as a diffusion process [38].

## APPENDIX B

The Mathematica program used for the calculation of the energy eigenvalues presented in Table 2a.

```
Timing[WorkingPrecision→10;

Do[i=k;
  gamma=i/10.;
  Vp0=-gamma*x2+x4;
  En0=0.;
  Do[
Print["gamma= ",gamma," iken ",j-1,". enerji seviyesi hesabı
baslar!"];
Clear[energy];
energy=50.;
  Do[
  Do[
wi=a*x+b*x3;
Ψ0i=Exp[-\[Integral]wi@x];
  term1=-D[Ψ0i,x,x];
  term2=Vpj-1*Ψ0i;
hamilton=term1+term2;
  term3=Ψ0i*hamilton;
  term4=Ψ0i*Ψ0i;
  term5=NIntegrate[term3,{x,-10,10}];
  term6=NIntegrate[term4,{x,-10,10}];
ratio=N[term5/term6,7]//N;
If[ratio<energy,{energy=ratio,A=a,B=b},rr=10],{b,1./10,2./1,1./100},
{a,1./10,3./1,1/100}];Vpj=(A*x+B*x3)2+D[A*x+B*x3,x];
Enj=energy+Enj-1;
Print[NumberForm[{"gamma=",gamma," ise",j-1,". enerji seviyesi
E= ",Enj//N," ve bu şartı saglayan","a=",A//N,
"b=",B//N,"degerleri bulunur"},7]],{j,1,4}},{k,1,10}]]
```