

**Comprehensive Treatments for Schrödinger Equations Involving
Constant and Non-constant Masses**

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by
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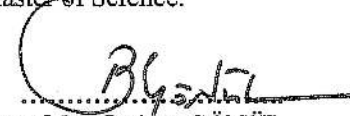
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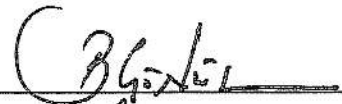
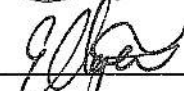

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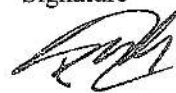
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ABSTRACT

COMPREHENSIVE TREATMENTS FOR SCHRÖDINGER EQUATIONS INVOLVING CONSTANT AND NON-CONSTANT MASSES

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The concept of the elegant work introduced by Lévai in Ref. [21] is extended for the solutions of the Schrödinger equation with more realistic other potentials used in different disciplines of physics within the constant mass consideration. The connection between the present model and the other alternative algebraic technique [32] in the literature is discussed in detail. Extending the point canonical transformation approach introduced in this thesis in a manner distinct from the previous ones, we also propose a unified approach of generating potentials of all classes having non-constant masses.

Keywords: Schrödinger equation, PCT method, exactly-solvable potentials, non-solvable potentials, position-dependent mass.

ÖZ

SABİT VE DEĞİŞKEN KÜTLE İÇEREN SCHRÖDINGER DENKLEMLERİ İÇİN KAPSAMLI ÇÖZÜMLER

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Sabit kütle içeren Schrödinger dalga denkleminin analitik çözümleri için Levai [21] tarafından önerilen titiz çalışmanın kapsamı, fiziğin farklı disiplinlerinde kullanılan daha gerçekçi potansiyellere de uygulanabilmesi için genişletilmiştir. Geliştirilen bu model ile literatürde bulunan [32] ve analitik çözüm içerebilen diğer model arasındaki ilişki detaylı olarak incelenmiştir. Bu tez çalışmasında ayrıca, sabit kütle içeren sistemler için ileri sürülen ve kapsamı noktasal kanonik dönüşüm içeren benzer çalışmalardan farklı olarak genişletilen yaklaşım yardımı ile sabit olmayan kütle içeren sistemlerde dahil olmak üzere tüm etkileşim potansiyellerini, çözümleri ile birlikte, türetebilen diğer bir model teklif edilmiştir.

Anahtar Kelimeler: Sch denklemi, PCT modeli, tam-çözülebilir potansiyeller, tam çözilemeyen potansiyeller, sabit olmayan (hareket ile değişen) kütle.

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TABLE OF CONTENTS

ABSTRACT.....	v
ÖZ	vi
ACKNOWLEDGEMENT	vii
TABLE OF CONTENTS	viii
LIST OF TABLES	ix
CHAPTER 1: INTRODUCTION	1
CHAPTER 2: THEORETICAL BACKGROUND.....	5
2.1. Previous Consideration	5
2.2. The Previous Model	7
2.3. Application.....	10
2.3.1. Calculations for $n=0$ and $n=1$ states	11
2.3.2. Calculations for $n \geq 2$ states	14
2.3.3. Large-order calculations.....	18
2.4. Concluding Remarks	19
CHAPTER 3: AN EXTENDED FORMALISM FOR THE SCHRÖDINGER EQUATION WITH CONSTANT MASS	21
3.1. Formalism	22
3.2. Application.....	26
3.2.1. Quartic oscillator.....	26
3.2.2. Sextic oscillator.....	30
3.3. Concluding Remarks	34
CHAPTER 4: AN ALTERNATIVE APPROACH TO SCHRÖDINGER EQUATION WITH A SPATIALLY VARYING MASS.....	36
4.1. Formalism	37
4.2. Application.....	41
4.3. Concluding Remarks	43
CHAPTER 5: CONCLUDING REMARKS.....	45
REFERENCES.....	47

LIST OF TABLES

Table 2.1 Lowest eigenvalue of the anharmonic oscillator.....	12
Table 2.2 First excited state energies of the anharmonic oscillator	14
Table 2.3 Second excited state energies of the anharmonic oscillator.....	15
Table 2.4 Third excited state energies of the anharmonic oscillator.....	17
Table 2.5 Lowest eigenvalues calculated for $g = 1$ at large orders	18
Table 2.6 Lowest eigenvalues calculated for $g = 10$ at large orders	19
Table 3.1 Comparison of the first four eigenvalues of the potential $\mu x^2 + \eta x^6$ obtained by the present method with the exact values ([Ref. 40] for $\mu = 1$, and Ref. [54] for $\mu = 0$)	33
Table 3.2 Comparison of the present calculation results for the first four eigenvalues of the potential $\mu x^2 + \sigma x^4 + \eta x^6$, where $\mu = 30$, $\sigma = 20\sqrt{30}$ and $\eta = 100$, with those obtained with the two different algebraic models	34

CHAPTER 1

INTRODUCTION

One of the challenging problems in non-relativistic quantum mechanics is to find solutions to the Schrödinger equation for potentials that are used in different fields of physics. However, an exact solution of the Schrödinger equation exists only for a few idealized problems. Normally it has to be solved using an approximation method such as the usual perturbation theory which constitutes one of the most powerful tools available in the study of quantum mechanics in the atoms and molecules. Perturbation theory is applied to those cases in which the real system can be described by a small change in an exactly solvable idealized system. In this form we can describe a great number of problems encountered especially in atomic physics, in which the nucleus provides the strong central potential for the electrons; further interactions of less strength are described by the perturbation. Examples of these additional interactions are: the magnetic interaction (spin-orbit coupling), the electrostatic repulsion of electrons and the influence of external fields. But in spite of widespread application of this theory, its basic analytical properties are poorly understood and the corresponding framework is not easily applicable. In addition, performing explicit calculations in non-relativistic quantum mechanics using the familiar Rayleigh-Schrödinger perturbation expansion mentioned above is rendered difficult by the presence of summations over all intermediate unperturbed eigenstates. Alternative perturbation procedures have been proposed to avoid this difficulty, notably the logarithmic perturbation theory (LPT) [1-4] and the Dalgarno-Lewis technique [5-8]. The virtue of LPT is its avoidance of the cumbersome summation over states for second and higher-order corrections in Rayleigh-Schrödinger perturbation theory. Unfortunately, it has problems of its own in calculating corrections to excited states, owing to presence of nodes in the wavefunctions. Various schemes have been proposed to circumvent the resulting

singularities [4, 9, 10]. In spite of the progress given above, over the years the Schrödinger equation has been studied extensively regarding its exact solvability. Many advances have been made in this area by classifying quantum mechanical potentials according to their symmetry properties. For instance, various algebras which reveal the underlying symmetry as well as facilitating and obtaining the solutions have been found. In this respect, the application of supersymmetry ideas to non-relativistic quantum mechanics has revived fresh interest in the problem of obtaining algebraic solutions of exactly solvable non-relativistic potentials and provided a deeper understanding of analytically solvable Hamiltonians, as well as a set of powerful approximate schemes for dealing with problems admitting no exact solutions. The concept of supersymmetry and its application to quantum mechanics [11,12], together with the shape invariance, have played a fundamental role in these developments. Supersymmetric quantum mechanics (SSQM) has developed immensely since the first models were introduced [13,14]. Several approximation methods using SSQM formalism have been developed, including the supersymmetric perturbation theory (SSPT) of Cooper and Roy [15]. Recently, Lee [16] has shown that SSPT and LPT are entirely equivalent and fortuitously, each turns out to resolve difficulties encountered in the other. Namely, LPT formulas for energy corrections obviate tedious procedures in the SSQM method, while the use of SSQM partner potentials with virtually identical bound state spectra solves difficulties with excited states encountered in LPT. Although the iterative procedure in SSPT may not actually reduce the calculational workload, it does cast the calculations into a physically-motivated, visualizable framework. Along this line, recently a more economical scheme has been introduced, which yields simple but closed perturbation theory formulae [17] leading to the Riccati equation from which one can actually obtain all the perturbation corrections to both energy level shifts and wavefunctions for all states, unlike the other models mentioned above. In the application of this method to the n th excited state, one requires knowledge of the unperturbed eigenfunction but no knowledge of the other eigenvalues or eigenfunctions is necessary. The procedure underlined does not involve either tedious explicit factoring out of the zeros of unperturbed eigenfunction [1,2] or introduction of ghost states [4] as were the cases encountered for applying LPT to excited states. The model discussed in Ref. [17] offers the explicit expressions for the energy corrections, which are absent in the original SSPT while the treatment of Lee [16] for

such calculations has mathematical complexity, and provides a clean route to the excited states, which are cumbersome to analyze in both LPT and SSPT. Thus, the results obtained in [17] can be thought of as a generalization of logarithmic and supersymmetric based perturbation theories.

Nevertheless, no single approximation method available in the literature is ideal for every problem. SSPT and LPT based theories [1-17] avoid the Rayleigh-Schrödinger summation, but it can in general lead to nasty integrals and more effort in particular for excited states. The method is valuable when the integrals can be done exactly or by a reliable numerical procedure. Otherwise, the Rayleigh-Schrödinger summation, even when it does not give an exact answer, starts not to look so bad after all. This was the motivation behind the work introduced in this thesis. One needs at this stage an algebraic model for the analysis of quantum mechanical problems of sub-atomic world, providing a quick route to the calculation of all corrections within the frame of an easily applicable perturbation theory to considerably simplify one's calculational workload including any interaction (corresponding to any potential) in micro-world.

Considering all these, and keeping the main aim of the thesis work in mind, we remind another simple method of investigating the solution of the Schrödinger equation, which is related to the work of Bhattacharjie and Sudarsan [18] that has been known for a long time. These authors applied their method to the hypergeometric, confluent hypergeometric and Bessel equations. Later it turned out that it can be related to algebraic techniques of solving differential equations [19]. Another systematic application of this method (to the hypergeometric functions) has been carried out by Natanzon [20] independently. Further, Lévai [21] in his pioneering work discussed a significant question, through the consideration of the link between the works in [18-20], if there are any other special functions which are solutions of the Schrödinger equation with shape invariant potentials deducing a condition which has to be satisfied by any special function leading to the orthogonal polynomials and exactly solvable shape invariant potentials discussed above. Besides the results obtained, the combination of SSQM with traditional approaches to solvable potentials proved to be fruitful. For instance, Refs. [22-31] involve some significant applications of the original idea discussed in [21], clarifying the physics behind a variety of interactions in sub-atomic world.

However, to our knowledge, this formalism up to now has been used only to study for exactly solvable systems. Therefore, bearing in mind that realistic physical problems can practically never be solved exactly, it needs a meticulous modification to also solve more realistic other systems as the ones of interest in this thesis. This is the main motivation behind the present work suggesting a more comprehensive and generalized model using the spirit of the investigation in [21], which escaped notice in other publications.

In other words, using the basic ingredient of the elegant work introduced by Lévai in Ref. [21] we have developed in the present thesis work a simple alternative approach to perturbation theory in one-dimensional non-relativistic quantum mechanics for the solutions of the Schrödinger equation with more realistic other potentials used in different disciplines of physics. The formulae for the energy shifts and wave functions do not involve tedious calculations which appear in the available perturbation theories discussed above. The present model applicable in the same form to both the ground state and excited bound states involving all classes of potentials including exactly-/quasi-exactly solvable and non-solvable potentials, unlike earlier algebraic techniques for the analytical or perturbative treatment of Schrödinger equation. The power and elegance of the present unified model, which is in a sense complete, are illustrated via specifically chosen examples. We now have clear and explicit ways to get corrections to all energy levels and state wave functions for a given perturbed potential.

In Chapter 2, we give a theoretical background based on the previous work in Ref [32] which is interestingly in connection with the one we developed in this thesis. Chapter 3 discusses the framework of the present formalism together with distinct examples in order to convince the reader regarding the reliability and flexibility of the model introduced, where we also discuss a significant result behind the calculations and clarifies the inter-relation between the present formalism and the one used in the related literature [32] that was performed within the frame of an extended SSQM theory. The applications of the new model for position-dependent masses is discussed in Chapter 4. Some concluding remarks and summary of the work, together with the outlook, are drawn in the last chapter.

CHAPTER 2

THEORETICAL BACKGROUND

An algebraic non-perturbative approach has been recently proposed [32] for the analytical treatment of Schrödinger equations with a potential that can be expressed in terms of an exactly solvable piece with an additional potential involving constant masses. Avoiding disadvantages of standard approaches, new handy recursion formulae with the same simple form both for ground and excited states have been obtained in there. As an illustration the procedure, well adapted to the use of computer algebra, has been successfully applied to quartic anharmonic oscillators by means of very simple algebraic manipulations. The trend of the exact values of the energies has been rather well reproduced for a large range of values of the coupling constant ($g = 0.001 - 10000$).

As the novel algebraic model presented in Chapter 3, being as an alternative to the one presented in [32], reproduces similar numerical results to those of [32] we will first focus in this chapter to the previous model introduced by [32] due to the interesting inter-relation between the two different methods mentioned for solving Schrödinger equation. The link between the models will also be discussed in detail through the next chapter.

2.1 Previous Consideration

The main task in application of the quantum mechanics is to solve Schrödinger equations with different potentials. Unfortunately, realistic physical problems can practically never be solved exactly. Then one has to resort to some approximations. Most widely used among them is the perturbation theory. However, the explicit calculation with the Rayleigh-Schrödinger perturbation theory, described in most

quantum mechanics textbooks, runs into the difficulty of the summation over all intermediate unperturbed eigenstates. To avoid this difficulty, alternative perturbation procedures have been proposed. Unfortunately, as discussed in Chapter 1, they have other problems in calculating corrections to excited states, owing to presence of nodes in the wavefunctions. Various schemes have been proposed to circumvent the resulting singularities, which however cause to clumsy and cumbersome procedures.

Considering such drawbacks of the available treatments and gaining confidence from their success of the recent works, Gönül and his co-workers [32], have presented an alternative approach to perturbation theory in one-dimensional non-relativistic quantum mechanics, which yields simple but closed perturbation theory formulae leading to the Riccati equation from which one can actually obtain all the perturbation corrections to both energy level shifts and wavefunctions for all state. These quantities can be calculated to any given accuracy since the generation of successive corrections in the perturbative expansions introduced only requires the solution of simple algebraic solutions. The model applicable in the same form to both the ground state and excited bound states without involving tedious calculations which appear in the available perturbation theories. In particular they noted that the procedure introduced in [32] does not involve either tedious explicit factoring out of the zeros of [1,2] or introduction of ghost states [4] as were the cases encountered for applying LPT to excited states. In the application of the present method to the n th excited state, one requires only knowledge of the unperturbed state eigenfunction but no knowledge of the other eigenvalues or eigenfunctions is necessary.

As an illustration, their scheme in [32] has been applied to quartic anharmonic oscillator since there has been a great deal of interest in the analytical and numerical investigation of the one-dimensional anharmonic oscillator. They are of interest because of their importance in molecular vibrations [33] as well as in solid state physics [34] and quantum field theories [35]. Since anharmonic oscillators model intrinsic anharmonic effects of the real world, they continue to play a crucially important role in contemporary physics. On the other hand, the anharmonic oscillators with quartic potentials can serve as a testing ground for the various methods based on perturbative and non-perturbative approaches. In other words, interest in such a model stems mainly from the fact that, if one considers the

anharmonicity gx^4 as a perturbing operator, then the Rayleigh-Schrödinger perturbation expansion for the eigenvalues diverges [36] for every value of g . Consequently, several methods have been used to calculate the quartic anharmonic oscillator eigenvalues and eigenfunctions. Without being exhaustive, we may recall variational methods [37], WKB methods [38], Hill determinant [39-40], Riccati [41] or Riccati-Hill determinant methods [42], perturbative treatment prescriptions using summability techniques such as the Stieljes, Pade and Borrell methods [35-43]. We should also mention the hypervirial perturbation method of Fernandez and Castro [44], which can be viewed as a generalization of the Killingbeck method [45], and other alternative treatments [46], together with those involving a group-theoretical approach [47], the multiple scale technique [48], and supersymmetric methods [49]. After all, it appears challenging to test the new formalism in [32] avoiding the failure of the other perturbation series for the treatment of the quartic anharmonic oscillator.

The layout of this section is as follows. In the next sub-section we summarize the main ideas of the approach in Ref. [32] to understand deeply the physics behind the formalism, which leads to the clear understanding of the inter-connection between the model presented here and our novel method introduced in the next chapter. The application of the present model to quartic anharmonic oscillators leading to simple recursion relations for the calculations at each successive perturbation order and the results obtained are shown in sub-section 2.3. This section ends with a brief summary and concluding remarks given by the Section 2.4.

2.2 The previous model

We first start with a brief introduction of the present formalism. Throughout the work the unit system $\hbar = 2m = 1$ is chosen. In general, the goal in the supersymmetric quantum theory [50] is to solve the Riccati equation,

$$W^2(r) - W'(r) = V(r) - E_0 \quad (2.2.1)$$

where $V(r)$ is the potential of interest and E_0 is the corresponding ground state

energy. If we find $W(r)$, the so called superpotential, we have of course found the ground state wave function via,

$$\psi_0(r) = N \exp \left[- \int^r W(z) dz \right], \quad (2.2.2)$$

where N is the normalization constant. If $V(r)$ is a shape invariant potential, we can in fact obtain the entire spectrum of bound state energies and wave functions via ladder operators.

Keeping in mind this point, now suppose that we are interested in a potential for which we do not know $W(r)$ exactly. More specifically, we assume that $V(r)$ differs by a small amount from a potential $V_0(r)$ plus angular momentum barrier if any, for which one solves the Riccati equation explicitly. For the consideration of spherically symmetric potentials, the corresponding Schrödinger equation for the radial wave function has the form

$$\frac{\psi_n''(r)}{\psi_n(r)} = [V(r) - E_n], \quad V(r) = \left[V_0(r) + \frac{\ell(\ell+1)}{r^2} \right] + \Delta V(r), \quad (2.2.3)$$

where ΔV is a perturbing potential. Let us write the wave function ψ_n as

$$\psi_n(r) = \chi_n(r) \phi_n(r), \quad (2.2.4)$$

in which χ_n is the known normalized eigenfunction of the unperturbed Schrödinger equation whereas ϕ_n is a moderating function corresponding to the perturbing potential. Substituting Eq. (2.2.4) into Eq. (2.2.3) yields

$$\left(\frac{\chi_n''}{\chi_n} + \frac{\phi_n''}{\phi_n} + 2 \frac{\chi_n'}{\chi_n} \frac{\phi_n'}{\phi_n} \right) = V - E_n. \quad (2.2.5)$$

Instead of setting the functions χ_n and ϕ_n , we will set their logarithmic derivatives using the spirit of Eqs. (2.2.1-2.2.2)

$$W_n = - \frac{\chi_n'}{\chi_n}, \quad \Delta W_n = - \frac{\phi_n'}{\phi_n} \quad (2.2.6)$$

which leads to

$$\frac{\chi_n''}{\chi_n} = W_n'^2 - W_n' = \left[V_0(r) + \frac{\ell(\ell+1)}{r^2} \right] - \varepsilon_n, \quad (2.2.7)$$

where ε_n is the eigenvalue of the exactly solvable unperturbed potential, and

$$\left(\frac{\phi_n''}{\phi_n} + 2 \frac{\chi_n' \phi_n'}{\chi_n \phi_n} \right) = \Delta W_n'^2 - \Delta W_n' + 2W_n \Delta W_n' = \Delta V(r) - \Delta \varepsilon_n, \quad (2.2.8)$$

in which $\Delta \varepsilon_n$ is the eigenvalue for the perturbed potential, and $E_n = \varepsilon_n + \Delta \varepsilon_n$.

Then, Eq. (2.2.5), and subsequently Eq. (2.2.3), reduces to

$$(W_n + \Delta W_n)^2 - (W_n + \Delta W_n)' = V - E_n, \quad (2.2.9)$$

which is similar to Eq. (2.2.1), nevertheless it is valid for all states unlike usual supersymmetric treatments [50] which use (2.2.9) only for the ground state due to theoretical considerations. Further, as one in principle knows explicitly the solution of Eq. (2.2.7), namely the whole spectrum and corresponding eigenfunctions of the unperturbed interaction potential, the goal here is to solve only Eq. (2.2.8), which is the backbone of this formalism. The reader is referred to [17] for the successful applications of Eq. (2.2.8) involving different problems in quantum theory through exactly solvable potentials.

However, if the whole potential has no analytical solution as the case considered in this section, which means ΔW and subsequently Eq. (2.2.8) cannot be exactly solvable, then one can expand the functions in terms of the perturbation parameter λ ,

$$\Delta V(r; \lambda) = \sum_{N=1}^{\infty} \lambda^N \Delta V_N(r), \Delta W_n(r; \lambda) = \sum_{N=1}^{\infty} \lambda^N \Delta W_{nN}(r), \Delta \varepsilon_n(\lambda) = \sum_{N=1}^{\infty} \lambda^N \varepsilon_{nN} \quad (2.2.10)$$

where N denotes the perturbation order. Substitution of the above expansion into Eq. (2.2.8) by equating terms with the same power of λ on both sides yields up to for instance $O(\lambda^3)$

$$2W_n\Delta W_{n1} - \Delta W'_{n1} = \Delta V_1 - \Delta\mathcal{E}_{n1} \quad , \quad (2.2.11)$$

$$\Delta W_{n1}^2 + 2W_n\Delta W_{n2} - \Delta W'_{n2} = \Delta V_2 - \Delta\mathcal{E}_{n2} \quad , \quad (2.2.12)$$

$$2(W_n\Delta W_{n3} + \Delta W_{n1}\Delta W_{n2}) - \Delta W'_{n3} = \Delta V_3 - \Delta\mathcal{E}_{n3} \quad , \quad (2.2.13)$$

Eq. (2.2.8) and its expansion give a flexibility for the easy calculations of the perturbative corrections to energy and wave functions for the n th state of interest through an appropriately chosen perturbed superpotential. It has been shown [17, 32] that this feature of the present model leads to a simple framework in obtaining the corrections to all states without using complicated mathematical procedures.

2.3 Application

For clarity, in this paper we restrict ourselves to the Schrödinger equation in one dimension ($\ell = 0$) and consider the anharmonic potential as

$$V = V_0 + \Delta V = x^2 + gx^4 \quad , \quad (2.3.1)$$

in which the unperturbed potential represents the well known factorizable harmonic oscillator. From the literature [11,50], the corresponding superpotentials, wave functions and energy values are

$$w_n = -\sqrt{a} \left[\sqrt{a}x - \frac{H_{n+1}(\sqrt{a}x)}{H_n(\sqrt{a}x)} \right] \quad ,$$

$$\chi_n = H_n(\sqrt{a}x) \exp(-ax^2/2) \quad , \quad \varepsilon_n = 2a \left(n + \frac{1}{2} \right) \quad (2.3.2)$$

where H_n denotes the Hermite polynomials, $n = 0, 1, 2, \dots$ is the radial quantum number and a is the potential parameter. With a suitable choice of ΔW ,

$$\Delta W = \sum_{N=1}^{\infty} f_N x^{2N+1} \quad , \quad (2.3.3)$$

corresponding to the perturbed potential gx^4 in Eq. (2.3.1), one obtains some equations at successive orders for different states, which reveal some interesting relations between them leading to a simple algebraic treatment of the problem of interest here.

2.3.1 Calculations for $n=0$ and $n=1$ states

For instance, starting from the ground state calculations ($n=0$), where, from Eq. (2.3.2), $W=ax$ and considering Eqs. (2.2.11) through (2.2.13) we get at the first order ($N=1$),

$$2af_1 = g \quad , \quad f_1 = \frac{1}{3}(a^2 - 1) \Rightarrow E_{n=0}^3 - E_{n=0} - \frac{3}{2}g = 0 \quad . \quad (2.3.4)$$

Similarly, at the second order ($N=2$) of the perturbation we have

$$f_1^2 + 2af_2 = 0 \quad , \quad f_2 = \frac{2af_1 - g}{5} \Rightarrow E_{n=0}^4 - \frac{22}{17}E_{n=0}^2 - \frac{18g}{17}E_{n=0} + \frac{5}{17} = 0 \quad , \quad (2.3.5)$$

and the third order ($N=3$) calculations give

$$2(af_3 + f_1f_2) = 0, \quad f_3 = \frac{f_1^2 + 2af_2}{7} \Rightarrow$$

$$E_{n=0}^5 - \frac{50}{31}E_{n=0}^3 - \frac{39g}{31}E_{n=0}^2 + \frac{19}{31}E_{n=0} + \frac{21g}{31} = 0 \quad (2.3.6)$$

The results for the ground state energy values at successive orders within the frame of the above expressions are given below. The agreement between our calculation and the corresponding exact values is remarkably reasonable.

Table 2.1 Lowest eigenvalue of the anharmonic oscillator

g	N=1	N=2	N=3	N=4	Exact [40]
0.001	1.00075	1.00075	1.00075	1.00075	1.000748
0.01	1.00742	1.00737	1.00737	1.00737	1.007373
0.05	1.03558	1.03467	1.03474	1.03473	1.034729
0.1	1.06792	1.06500	1.06533	1.06528	1.065286
0.5	1.26255	1.23689	1.24347	1.24118	1.2418541
1.0	1.43113	1.38082	1.39672	1.39017	1.392352
10	2.60124	2.38404	2.47867	2.42910	2.449174
100	5.37603	4.82115	5.08211	4.93770	4.999417
1000	11.4763	10.2346	10.8285	10.4960	10.639789
10000	24.6756	21.9784	23.2731	22.5463	22.861608

If one repeats the same calculations for the first excited state ($n = 1$), for which the superpotential is set $W = ax - \frac{1}{x}$ in the light of Eq. (2.3.2), then the first order yields

$$2af_1 = g \quad , \quad f_1 = \frac{1}{5}(a^2 - 1) \Rightarrow E_{n=1}^3 - 9E_{n=1} - \frac{135}{2}g = 0 \quad , \quad (2.3.7)$$

and at the second order we have

$$f_1^2 + 2af_2 = 0 \quad , \quad f_2 = \frac{2af_1 - g}{7} \Rightarrow E_{n=1}^4 - \frac{34}{3}E_{n=1}^2 - 50gE_{n=1} + 21 = 0 \quad , \quad (2.3.8)$$

while the third order expressions are

$$2(af_3 + f_1f_2) = 0 \quad , \quad f_3 = \frac{f_1^2 + 2af_2}{9} \Rightarrow$$

$$E_{n=1}^5 - 14E_{n=1}^3 - 57gE_{n=1}^2 + 45E_{n=0} + 243g = 0 \quad (2.3.9)$$

In our calculations, the upper bounds which are the largest real and positive roots in these equations are chosen as the energy of the anharmonic oscillator in the related quantum state.

The repeat of such calculations for large successive orders reproduces similar relations in a manner of hierarchy. The systematic calculation of perturbation corrections of large orders offer no difficulty if we resort a computer algebra system like Mathematica, Maple or Reduce. This realization leads us to generalize anharmonic oscillator solutions for the ground and first excited states without solving the Schrödinger equation. To calculate the energy values individually at each perturbation order, one needs to solve only

$$\sum_{k=0}^N f_k f_{N-k} - g \delta_{N1} = 0 , \quad (2.3.10)$$

in which δ is the Kronecker delta and $f_0 = a$ is the parameter related to Eq. (2.3.2).

The perturbation coefficients above can easily be computed through

$$f_N = (2N + 2n + 1)^{-1} \left(\sum_{k=0}^{N-1} f_k f_{N-k-1} - \delta_{N1} - g \delta_{N2} \right) . \quad (2.3.11)$$

The calculations are carried out for different range of g values and the results obtained for the ground and first excited state energies are compared to the one computed numerically. The agreement is remarkable in the whole range of g values for the first excited state ($n=1$), see Table 2.2. The large order perturbation calculations are performed by a simple use of Mathematica [51] along the line of Eq. (2.3.10) and Eq. (2.3.11) with simple algebraic manipulations.

Table 2.2 First excited state energies of the anharmonic oscillator

g	N=1	N=2	N=3	N=4	N=8	Exact [40]
0.001	3.00374	3.00374	3.00374	3.00374	3.00374	3.003739
0.01	3.03682	3.03652	3.03653	3.03653	3.03653	3.036525
0.05	3.17236	3.16683	3.16727	3.16722	3.16723	3.167225
0.1	3.32148	3.30511	3.30718	3.30681	3.30687	3.306872
0.5	4.14123	4.03032	4.05869	4.04924	4.05171	4.051932
1.0	4.80180	4.60453	4.66448	4.64159	4.64784	4.648813
10	9.11388	8.39998	8.68054	8.55128	8.58582	8.599004
100	19.0576	17.3193	18.0446	17.6965	17.7864	17.83019
1000	40.7899	36.9427	38.5693	37.7818	37.9829	38.08683
10000	87.7547	79.4176	82.9526	81.2378	81.6747	81.90331

2.3.2 Calculations for $n \geq 2$ states

When dealing with excited states this approach seems rather cumbersome because the zeros of the wavefunction have to be taken into account explicitly. However, with some simple but physically acceptable algebraic manipulations, we can obtain simple analytical expressions for higher excited states easily from a straightforward generalisation of the resulting expressions at successive perturbation orders as in the previous section.

Starting with the second excited state ($n=2$), where from Eq. (2.3.2) the superpotential is $W_{n=2} = ax(2ax^2 - 5)/(2ax^2 - 1)$, energies up to for example the fifth order ($N=5$) can be obtained through

$$2af_1 = g \quad , \quad f_1 = \frac{1}{8}(a^2 - 1) \quad , \quad N=1 \quad ,$$

$$f_1^2 + 2af_2 = 0 \quad , \quad f_2 = \frac{2af_1 - g}{10} \quad , \quad N = 2 \quad ,$$

$$2(af_3 + f_1f_2) = 0 \quad , \quad f_3 = \frac{f_1^2 + 2af_2}{12} \quad , \quad N = 3 \quad ,$$

$$f_2^2 + 2(f_1f_3 + af_4) = 0 \quad , \quad f_4 = \frac{2(af_3 + f_1f_2)}{14} \quad , \quad N = 4 \quad ,$$

$$2(f_2f_3 + f_1f_4 + af_5) = 0 \quad , \quad f_5 = \frac{f_2^2 + 2(f_1f_3 + af_4)}{16} \quad , \quad N = 5 \quad . \quad (2.3.12)$$

In these treatments, to remove the singularities in the related super potential due to the zeros of the wavefunction, we accept that $2ax^2 > 1$ leading to physically acceptable results. This simple assumption reproduces good accuracy in the calculations when compared to tedious calculations of LPT for higher excited states. The results obtained are shown in Table 2.3

Table 2.3 Second excited state energies of the anharmonic oscillator

g	N=1	N=2	N=3	N=4	N=15	Exact [40]
0.001	5.00997	5.00996	5.00996	5.00996	5.00996	5.009711
0.01	5.09715	5.09606	5.09609	5.09609	5.09609	5.093939
0.05	5.44017	5.42257	5.42423	5.42401	5.42404	5.417261
0.1	5.79852	5.75129	5.75799	5.75670	5.75694	5.747959
0.5	7.60690	7.35517	7.41992	7.39911	7.40489	7.396900
1.0	8.98161	8.56694	8.68960	8.64563	8.65908	8.655049
10	17.5870	16.2662	16.7452	16.5461	16.6188	16.63592
100	37.0665	33.9532	35.1363	34.6287	34.8238	34.87398
1000	79.4750	72.6342	75.2605	74.1261	74.5674	74.68140
10000	171.046	156.245	161.940	160.830	160.437	160.6859

Finally, within the same framework one can readily get similar expressions for other excited states. For instance, in order to deal with the third excited state ($n = 3$) of the

anharmonic oscillator one can choose the corresponding super potential $W_{n=3} = (2a^2x^4 - 9ax^2 + 3)/(2ax^3 - 3x)$ via Eq. (2.3.2) for the unperturbed piece of the potential and end up with some explicit algebraic equations at each order,

$$2af_1 = g \quad , \quad f_1 = \frac{1}{12}(a^2 - 1) \quad , \quad N = 1 \quad ,$$

$$f_1^2 + 2af_2 = 0 \quad , \quad f_2 = \frac{2af_1 - g}{14} \quad , \quad N = 2 \quad ,$$

$$2(af_3 + f_1f_2) = 0 \quad , \quad f_3 = \frac{f_1^2 + 2af_2}{16} \quad , \quad N = 3 \quad , \quad (2.3.13)$$

...and so on. In this case the wave function and consequently the superpotential have three zeros at $x = \pm\sqrt{3/2a}$. As argued above, to circumvent the resulting singularities the present calculations here make a similar assumption that is $2ax^3 > 3x$ which produces reasonable results. This choice however for higher excited states with $n \geq 3$ allows only the coefficients f_N with x^{2N} and x^{2N+2} through the linear perturbation expressions at each order. The results obtained are illustrated in Table 2.3. Although the present formalism suggest a systematic way of improving the anharmonic oscillator perturbation series, the accuracy of the present formulae as expected gets decrease with the increase of the quantum number since the perturbation becomes more important.

Nevertheless, owing to the nearly correct large g behaviour of the results presented here they are expected to be much more accurate than the perturbation series. This idea exploited by Fernandez et al [41] in order to obtain analytical expressions for the eigenvalues of the anharmonic oscillator from the semiclassical considerations.

Table 2.4 Third excited state energies of the anharmonic oscillator

g	N=1	N=2	N=3	N=4	N=15	Exact [40]
0.001	7.02091	7.02087	7.02087	7.02087	7.02087	7.018652
0.01	7.20124	7.19823	7.19833	7.19832	7.19832	7.178573
0.05	7.87793	7.83590	7.84053	7.83985	7.83995	7.770271
0.1	8.54838	8.44564	8.46179	8.45849	8.45913	8.352677
0.5	11.7019	11.2511	11.3683	11.3315	11.3415	11.11515
1.0	14.0000	13.2973	13.5021	13.4319	13.4524	13.15680
10	28.0000	25.9479	26.6524	26.3804	26.4698	25.80627
100	59.3169	54.5806	56.2681	55.5997	55.4001	54.38529
1000	127.327	116.968	120.689	119.207	119.712	116.60319
10000	274.100	251.711	259.767	256.555	257.651	250.95073

In the light of the above discussions one can easily generalize the whole calculations discussed in Section 3 in a compact form to determine the solutions of quartic anharmonic oscillator in a closed algebraic form, which should be valid for the all states. Eq. (2.3.10) can be safely used for this purpose, however the coefficients should be re-defined as

$$f_N = (2N + 2n + \alpha_n)^{-1} \left(\sum_{k=0}^{N-1} f_k f_{N-k-1} - \delta_{N1} - g \delta_{N2} \right), \quad (2.3.14)$$

where $\alpha_n = (n-1) + \alpha_{n-1}$ being with $n \geq 1$ and $\alpha_0 = 1$. As a matter of fact, the only data that is needed when using Mathematica is Eq. (2.3.14) to solve Eq. (2.3.10) yielding energy values through the perturbation orders for any quantum state.

2.3.3 Large-order calculations

A question now arises about the convergence of the method just described. Since it seems closely related to perturbation theory, one expects it to be asymptotic divergent. The numerical results shown here almost confirm this assumption. We have calculated low-lying energy levels of the anharmonic oscillator for several g values, finding almost the same behavior in all cases. Tables 2.5 and 2.6 represent the oscillations of our results, though they remain quite close to the true eigenvalue, about its actual value as the perturbation order (N) increases, which are carried out for $g=1$ and $g=10$ respectively for the lowest state. Although divergent the present method is still useful because it certainly improves the perturbation series. The most accurate results are obtained from the N value corresponding to the smallest oscillation amplitude. Such an accuracy cannot be obtained from the other perturbation series.

Table 2.5 Lowest eigenvalues calculated for $g=1$ at large orders

N	$E_{n=0}$	N	$E_{n=0}$
5	1.39357	15	1.39269
6	1.39155	16	1.39196
7	1.39291	17	1.39272
8	1.39191	18	1.39221
9	1.39271	19	1.39273
10	1.39202	20	1.39231
11	1.39265	21	1.39273
12	1.39201	22	1.39235
13	1.39266	23	1.39272
14	1.39186	24	1.39238
$E_{n=0}^{exact} = 1.392352$			

Table 2.6 Lowest eigenvalues calculated for $g = 10$ at large orders

N	$E_{n=0}$	N	$E_{n=0}$
5	2.46214	15	2.45815
6	2.43752	16	2.44941
7	2.45804	17	2.45808
8	2.43856	18	2.45067
9	2.45720	19	2.45800
10	2.43125	20	2.45176
11	2.45752	21	2.45798
12	2.44277	22	2.45276
13	2.45799	23	2.45798
14	2.44735	24	2.45358
$E_{n=0}^{exact} = 2.449174$			

2.4 Concluding Remarks

We have discussed that the eigenvalues of quantum mechanical systems can be approximately obtained from the present formalism of Ref. [32] which is non-perturbative, self-consistent and systematically improvable. Although we have limited ourselves to one illustrative example, the range of application of the method is rather large and appears to be straightforward. The perturbation procedure is well adapted to the use of software systems such as Mathematica and allows the computation to be carried out up to high orders of the perturbation. For any given state, simple algebraic manipulations provide, at the same time, analytical expressions of the perturbed eigenvalues and eigenfunctions, without having to compute any matrix elements or to perform any integration.

The increase in the value of g for different quantum numbers do not imply special difficulty, unlike the other perturbation theories available in the literature. Furthermore, the remove of the singularities in the unperturbed wavefunction via the superpotential introduced in the present formalism does not cause tedious calculations which are great pain when dealing with excited states in the other theoretical treatments.

As a concluding remark, due to its simplicity and accuracy in particular for small g -values at low-lying states we believe this method to be competitive with other methods developed to deal with perturbation treatments. As a matter of fact that, the degree of precision of the results can be drastically improved by raising the perturbative order in the expansion, a step which does not bear any technical difficulty. It would be interesting to extend the present scheme to other non-exactly solvable potentials.

In the next chapters, we will introduce alternative schemes to solve all classes of potentials, involving solvable and non-solvable potentials, with constant and also position- dependent masses. We will further discuss the relation between the model presented here and the one that will be introduced in the following chapter.

CHAPTER 3

AN EXTENDED FORMALISM FOR THE SCHRÖDINGER EQUATION WITH A CONSTANT MASS

A simple method of investigating the solution of the Schrödinger equation, which is related to the work of Bhattacharjie and Sudarsan [18] has been known for a long time. These authors applied their method to the hypergeometric, confluent hypergeometric and Bessel equations. Later it turned out that it can be related to algebraic techniques of solving differential equations [19]. Another systematic application of this method (to the hypergeometric functions) has been carried out by Natanzon [20] independently. In the following years, there has been also renewed interest in simple quantum mechanical systems as a result of the introduction of two important concepts: supersymmetric quantum mechanics (SUSYQM) and shape invariance. For a comprehensive review on this topic, the reader is referred to [11] and the related references therein. In the light of this progress and the previous works mentioned, a significant question has then arisen regarding if there are any other special functions which are solutions of the Schrödinger equation with shape invariant potentials. This question has been answered in detail by Lévai [21] through the consideration of the link between the works in [18-20] and the formalism of SUSYQM, deducing a condition which has to be satisfied by any special function leading to the orthogonal polynomials and exactly solvable shape invariant potentials. Besides the results obtained, the combination of SUSYQM with traditional approaches to solvable potentials proved to be fruitful. For instance, Refs. [22-31] involves some applications of the original idea discussed in [21].

However, to our knowledge, this formalism up to now has been used only to study exactly solvable systems. Therefore, it needs a meticulous modification to also solve more realistic other systems as the ones of interest in this article. Within this context the main motivation behind the present work, bearing in mind that realistic

physical problems can practically never be solved exactly, is to suggest a more comprehensive and generalized model [57] using the spirit of the investigation in [21], which escaped notice in other publications. As an illustration, the present novel scheme is applied first to quartic anharmonic oscillator since there has been a great deal of interest in anharmonic oscillators due to their phenomenological as well as methodological use in physics.

These potentials also has the characteristics of being a rather simple model where many non-trivial features essential to understanding quite complicated system may be implemented. Their exact solutions however for arbitrary couplings are hard to find. This has culminated into the development of many fascinating techniques based on perturbative and non-perturbative approaches, which was well discussed in the previous chapter. Thus, it appears challenging to test our formalism in avoiding the failure of other perturbation series for the treatment of the quartic anharmonic oscillator. For completeness, the model proposed will also be applied to the well-known sextic oscillator problem, which provides an alternative perspective in justifying the capability of widespread applicability of the present scheme.

In Section 3.1 we present the formalism of our method, and in Section 3.2 we apply it to distinct cases including different potentials in order to convince the reader regarding the reliability and flexibility of the model introduced. Section 3.2 also discusses a significant result behind the calculations and clarifies the inter-relation between the present formalism and the one used in [32] that was performed within the frame of an extended SUSYQM theory. Finally, concluding remarks are given in Section 3.3.

3.1 Formalism

It is well known that the general framework of non-relativistic quantum mechanics is by now well understood and its predictions have been carefully proved against observations. Physics is permanently developing in a tight interplay with mathematics. It is of importance to know therefore whether some familiar problems are of particular case of a more general scheme or to search if a map between the

radial equations of two different scenarios exist. It is hence worthwhile to devote ourselves to the clarification of this point through the rest of this article.

Considering the Schrödinger equation ($\hbar = 2m = 1$)

$$\frac{d^2\Psi}{dx^2} + (E - V(x))\Psi = 0 \quad (3.1.1)$$

we suggest, for a generalized formalism, that

$$\Psi(x) = f(x)F(g(x))h(x) \quad , \quad (3.1.2)$$

where $f(x)F(g)$ yields an algebraic closed solution for exactly solvable potentials [21-31] with $F(g)$ being a special function which satisfies a second-order differential equation

$$\frac{d^2F}{dg^2} + Q(g)\frac{dF}{dg} + R(g)F(g) = 0 \quad , \quad (3.1.3)$$

while $h(x)$ is the moderating function in connection with a perturbing piece of the full potential corresponding to Eq. (3.1.2). The form of $Q(g)$ and $R(g)$ is already well defined for any special function $F(g)$ when dealing with analytically solvable potentials. However, in case of the consideration of a realistic non-exactly solvable problem one should derive reliable expressions, in an explicit form, for plausible definitions of the related $Q(g)$ and $R(g)$. This is the significant point in the framework of the new formalism to reach physically meaningful solutions.

Substituting Eq. (3.1.2) into Eq. (3.1.1) leads to

$$\begin{aligned} & \frac{d^2F}{dg^2} + \frac{dF}{dg} \left(\frac{g''}{(g')^2} + \frac{2f'}{fg'} + \frac{2h'}{hg'} \right) + \\ & F(g) \left(\frac{f''}{f(g')^2} + \frac{2f'h'}{fh(g')^2} + \frac{h''}{h(g')^2} + \frac{E - V(x)}{(g')^2} \right) = 0 \end{aligned} \quad (3.1.4)$$

From the comparison of Eqs. (3.1.3) and (3.1.4) it follows that

$$Q(g(x)) = \frac{g''}{(g')^2} + \frac{2f'}{fg'} + \frac{2h'}{hg'} \quad (3.1.5)$$

and

$$R(g(x)) = \frac{f''}{f(g')^2} + \frac{2f'h'}{fh(g')^2} + \frac{h''}{h(g')^2} + \frac{E-V(x)}{(g')^2} \quad (3.1.6)$$

Obviously, Eqs. (3.1.4-3.1.6) reduce to Eqs. (3.4-3.6) in Ref. [21] for the consideration of exact solvability, in which case $h(x)$ in the equations above goes to a constant value. Gaining confidence from this observation we proceed with

$$\begin{aligned} V(x) &= V_{ES}(x) + \Delta V(x) \\ E &= E_{ES} + \Delta E \end{aligned} \quad (3.1.7)$$

in accordance with our choice in Eq. (3.1.2), which means that potentials considered in this article are admitted as the sum of an exactly solvable potential with a perturbation or a moderating piece. Hence, the aim in this perspective is to reveal the corrections to energy (ΔE) and wavefunction $h(x)$ for a given $\Delta V(x)$, as the main piece of the solutions leading to exact solvability can easily be found from the literature.

The use of Eq. (3.1.7) within Eq. (3.1.6) produces coupled equations in the form of

$$E_{ES} - V_{ES}(x) = R_{ES}(g(x))(g')^2 - f''/f \quad , \quad (3.1.8)$$

and

$$\Delta E - \Delta V(x) = \Delta R(g(x))(g')^2 - 2f'h'/(fh) - h''/h \quad (3.1.9)$$

where $R_{ES}(g) + \Delta R(g)$ should certainly reproduces Eq. (3.1.6). Similarly, Eq. (3.1.5) can be decomposed as

$$Q_{ES}(g(x)) = g''/(g')^2 + 2f'/fg' \quad , \quad \Delta Q(g(x)) = 2h'/hg' \Rightarrow Q = Q_{ES} + \Delta Q \quad (3.1.10)$$

To be more practical it is reminded that $f''/f = (f'/f)^2 + (f'/f)'$ and the same is valid for h''/h in the equations above, which transform Eqs. (3.1.8) and (3.1.9) into more applicable forms

$$E_{ES} - V_{ES}(x) = \frac{g'''}{2g'} - \frac{3}{4} \left(\frac{g''}{g'} \right)^2 + (g')^2 \left[R_{ES}(g(x)) - \frac{1}{2} \frac{dQ_{ES}}{dg} - \frac{1}{4} Q_{ES}^2(g(x)) \right] \quad , \quad (3.1.11)$$

and

$$\Delta E - \Delta V(x) = -\left(\frac{g''}{2} + \frac{f'g'}{f}\right)\Delta Q(g(x)) + (g')^2\left[\Delta R(g(x)) - \frac{1}{2}\frac{d(\Delta Q)}{dg} - \frac{1}{4}\Delta Q^2(g(x))\right] \quad (3.1.12)$$

The result of this brief investigation opens a gate to the reader for the visualization of the explicit form of the correction (ΔE) to the energy. Unfortunately, there seems a problem naturally arised in calculating the correction term owing to the presence of two unknown: $\Delta Q(g)$ and $\Delta R(g)$ on the right hand side of Eq. (3.1.12). To circumvent the resulting drawback and proceed safely we need to go back Eq. (3.1.4) and substitute the definitions given by Eq. (3.1.7) in it, which leads us to handle

$$\Delta E - \Delta V(x) = -\frac{2h'}{h}\left(\frac{f'}{f} + \frac{F'(g(x))g'}{F(g(x))}\right) - \frac{h''}{h} \quad (3.1.13)$$

that is another form of Eq. (3.1.9). Thus, equating Eq. (3.1.9) and Eq. (3.1.13) and remembering the form of $\Delta Q(g)$ in Eq. (3.1.10) we arrive at

$$\Delta R(g) = -\Delta Q(g) \frac{F'(g)}{F(g)} \quad (3.1.14)$$

which is vital to overcome the problem encountered in Eq. (3.1.12). As $F(g)$ is well defined for a given exactly solvable potential, evidently one needs here to find only an appropriate expression for $\Delta Q(g)$ to be employed in Eq. (3.1.12) that reveals clearly the full solution. However, singular functions appearing in Eqs. (3.1.13-3.1.14), and subsequently in Eq. (3.1.12), are systematically generated when dealing with excited state wavefunctions of any given potential due to the zeros of $F(g)$ function. The effects of this consideration on the calculations are discussed in Section 3.2.

Before closing this section, we should remark that once choosing carefully $Q_{ES}(g)$ and $R_{ES}(g)$ for the analytically solvable part ($V_{ES}(x)$) of the full potential under

investigation we can easily set a proper internal function $g(x)$ and considering Eq. (3.1.5)

$$f(x) \approx (g')^{-1/2} \exp \left[\frac{1}{2} \int_{ES}^{g(x)} Q_{ES}(g) dg \right] , \quad (3.1.15)$$

as discussed in Ref. [21], which are used in Eq. (3.1.12) to find corrections to the solutions of the exactly solvable piece.

The application of the model to specifically chosen different potentials is discussed in the following section.

3.2 Application

Special care has to be taken in the application of the model as the results obtained are crucial in the interpretation of the system behavior in terms of the Hamiltonian described in this work. To reveal especially the flexibility of the scheme used particular cases are discussed below.

3.2.1 Quartic oscillator

In the light of experiences gained from successful modeling based on anharmonic oscillators, an obvious step in the direction of improvement is to define modifications more accurately brought by anharmonic terms leading to more precise descriptions of the systems considered.

Keeping this point in mind, and also to clarify the relationship between the procedure proposed in this article and the one [32] that was presented in Chapter 2, together with the comparison of the results obtained, we restrict ourselves to the Schrödinger equation in one dimension ($\ell = 0$) and consider the anharmonic potential as

$$V(x) = x^2 + \beta x^4 , \quad (3.2.1)$$

in which the first piece $V_{ES}(x) = x^2$ represents the well-known exactly solvable harmonic oscillator potential. From the differential equation of the Hermite polynomials [52] one can see that

$$F(g) = \exp(-g^2/2)H_n(g) \quad , \quad R_{ES}(g) = 2n+1-g^2 \quad ,$$

$$Q_{ES}(g) = 0 \quad , \quad g(x) = a^{1/2}x \quad (3.2.2)$$

where $a(=w/2)$ is the parameter related to E_{ES} . Clearly, from Eqs. (3.1.11) and (3.1.15), the main contributions through to the closed analytical solutions of the harmonic oscillator are

$$E_{ES} = 2a(n + \frac{1}{2}) \quad , \quad n = 0, 1, 2, \dots \quad , \quad \Psi_{ES} = f(x)F(g) = \exp(-\frac{g^2}{2})H_n(g) \quad (3.2.3)$$

in which Ψ_{ES} is the unnormalized wavefunction for the exactly solvable piece of the unharmonic oscillator.

As the whole potential in Eq. (3.2.1) has no analytical solution, one may expand the related functions in terms of the perturbation such that $\Delta V(r) = \sum_{N=1}^{\infty} \Delta V_N(r)$ and

$\Delta \mathcal{E}_n = \sum_{N=1}^{\infty} \mathcal{E}_{nN}$ where N denotes the perturbation order. In connection with this idea

we choose, after some exhaustive analyses, the form of ΔQ as

$$\Delta Q(g) = -\frac{2}{g} \sum_{N=1}^{\infty} j_N x^{2N+1} \quad (3.2.4)$$

and substitute all the above expansions into Eq. (3.1.12) by equating terms with the same power of the perturbation order on both sides, which yield the modifying terms in the frame of coupled equations at successive orders for different states. It is stressed that as $g(x)$, $f(x)$, $F(g)$ and finally $\Delta R(g)$, from Eqs. (3.1.14) and (3.2.4), are known one can compute readily the corrections to the whole solution using Eq. (3.1.12) at each perturbation order for a quantum state of interest. Before discussing the calculation technique of the corrections to the energy, it is reminded that the modifying function in Eq. (3.1.2) is formed consistently as

$$h(x) = \exp\left(\frac{1}{2} \int \Delta Q dg\right) \quad (3.2.5)$$

as a consequence of the choice in Eq. (3.2.4) and the eventual use of it in Eq. (3.1.10).

The systematic calculation of energy corrections in different orders involving large N – values offers no difficulty if we resort a computer algebra system like Mathematica. The repeat of our calculations for large successive orders reproduces similar relations in a manner of equation hierarchy. This realization leads us to generalize anharmonic oscillator solutions obtained within the frame of Eq. (3.1.12), without solving the Schrödinger equation. To calculate the energy values individually at each order we need to solve

$$\sum_{k=0}^N j_k j_{N-k} - \beta \delta_{N1} = 0 \quad (3.2.6)$$

in which δ is the Kronecker delta and $j_0 = a = w/2$. The perturbation coefficients above can be computed through

$$j_N = (2N + 2n + \alpha_n)^{-1} \left(\sum_{k=0}^{N-1} j_k j_{N-k-1} - \delta_{N1} - \beta \delta_{N2} \right) \quad (3.2.7)$$

where $\alpha_n = (n-1) + \alpha_{n-1}$ for the excited states ($n \geq 1$) and $\alpha_0 = 1$ in the case of ground ($n = 0$) and first excited state ($n = 1$) calculations. As a matter of fact, the only data that are needed when using Mathematica is Eq. (3.2.7) to solve Eq. (3.2.6) producing energy values through the perturbation orders for any quantum state.

The calculations are carried out for different range of β – values and the results obtained for different states at various orders are compared to those of the work in [32] given in the previous chapter. The agreement is remarkable in the whole range of β – values. All the numerical results produced by completely different mathematical procedures of the two alternative approaches, the present one and the other in [32], are exactly the same, which for clarity are not repeated here. This interesting coincidental outcome is of course due to the natural inheritance of the same calculation scheme, Eq. (3.2.6.) and (3.2.7), in both model. As the same results

tabulated in [32] through the Tables 2.1 and 2.6, which are illustrated in Chapter 2, are appeared naturally in the present work with the same precision, and also the accuracy, convergency and the success of the identical model are well discussed in [32] when compared to other techniques available in the related literature, we intend in this section to focus our attention only to this interesting inter-connection between the seemingly alternative but in fact identical prescriptions for the treatments of bound states in non-relativistic domain of the subatomic world.

The most significant piece in [32] is Eq. (2.2.8) discussed in Chapter 2 to find energy corrections through the model used,

$$\Delta E - \Delta V(x) = -\left[\Delta W_n^2(x) + 2W(x)\Delta W(x)\right] + \Delta W'(x) \quad (3.2.8)$$

where $W(x)$ and $\Delta W(x)$ are the superpotentials, concerning with the exactly solvable part $V_{ES}(x)$ and the perturbing piece $\Delta V(x)$ respectively, as appeared correspondingly in Eq. (3.2.1) above. From the extended definitions of superpotential terms in Ref. [32] by employing the spirit of the standard treatment of SUSYQM, we make clear that

$$W_n(x) = -\frac{d}{dx} \ln \Psi_n^{ES} = -\left(\frac{f'}{f} + \frac{F_n' g'}{F_n}\right), \quad \Delta W(x) = -\frac{h'}{h} \quad (3.2.9)$$

Certainly, the substitution of Eq. (3.2.9) into Eq. (3.2.8) yields Eq. (3.1.13) which can easily be transformed to Eqs. (3.1.9) and subsequently (3.1.12) as discussed in the previous section, clarifying the reason behind obtaining the identical results. Further, from the definitions of ΔW in Eq. (3.2.9) and ΔQ in Eq. (3.1.10) and also Eq. (3.2.5) one can find an explicit relationship such that $\Delta Q = -2\Delta W/g'$ which makes another link between the theoretical considerations of the models being analysed in this section.

Afterall, this brief but concrete analysis sheds a light on a remarkable coincidence regarding the identical treatment of the two alternative scenarios underlined. This investigation also completes the idea of Lévai [21] in which he has related his simple analytic scheme with the treatment procedure in the standard SUSYQM, as the present discussion has made clear the close relation between the

generalized work introduced in this article and the method proposed in [32] within the extended framework of SUSYQM, in a similar but extended manner used by [21].

3.2.2 Sextic oscillator

To improve the precision of the description of bistable systems one has to add a sextic term to the quadratic anharmonic oscillator equation discussed above. Though this section deals with the applications involving general form of sextic oscillators, we need first to remind briefly a peculiar behaviour of such potentials in case it is quasi-exactly solvable, which would be useful in understanding the mathematical procedure behind the present calculations leading to the energy values in case the sextic oscillator potential of interest is non-solvable.

The quasi-exactly solvable form of sextic oscillator potentials with a centrifugal barrier is defined [53]

$$V(x) = \frac{(2s-1/2)(2s-3/2)}{x^2} + \left[a^2 - 4b \left(s + \frac{1}{2} + M \right) \right] x^2 + 2abx^4 + b^2x^6 \quad (3.2.10)$$

where $x \in [0, \infty)$ and M is a non-negative integer. For any value of M , leading to certain combinations of potential parameters, only $M+1$ solutions for the related Schrödinger equation can be obtained in an algebraic fashion. The simplest solutions are obtained for $M=0$ and $M=1$.

Starting with $M=0$ case and considering Eq. (3.1.7),

$$V_{ES}(x) = a^2x^2 + \frac{(2s-1/2)(2s-3/2)}{x^2} \quad , \quad \Delta V(x) = -4b \left(s + \frac{1}{2} \right) x^2 + 2abx^4 + b^2x^6 \quad (3.2.11)$$

where the exactly solvable piece, in general, requires

$$F(g) = L_n^{2(s-\frac{1}{4})}(g) \quad , \quad Q_{ES}(g) = (2s-g)/g \quad , \quad R_{ES}(g) = n/g \quad , \quad (3.2.12)$$

in which $g = ax^2$ that yields $f \sim x^{2(s-1/4)} \exp(-ax^2/2)$. Hence the corresponding ground state algebraic solutions for $V_{ES}(r)$ are

$$E_{ES}^{n=0} = 4as \quad , \quad \Psi_{ES}^{n=0}(x) \sim x^{2(s-1/4)} \exp(-ax^2/2). \quad (3.2.13)$$

To obtain the modifying terms to the solutions in Eq. (3.2.13), due to the additional term (ΔV) in Eq. (3.2.11), we set ΔQ as

$$\Delta Q(g) = -\frac{b}{a^2} g = -\frac{b}{a} x^2 \quad , \quad (3.2.14)$$

and the substitution of which into Eq. (3.1.12) reveals that

$$E_{n=0}^{M=0} = 4as \quad , \quad \Psi_{n=0}^{M=0}(x) = f(x)h(x) \sim x^{2(s-1/4)} \exp\left(-\frac{b}{4}x^4 - \frac{a}{2}x^2\right) \quad (3.2.15)$$

Obviously, the solutions reduce to the analytically solvable harmonic oscillator for the choice of $b=0$, which clarifies that the contributions to $E_{ES}^{n=0}$ due to the two pieces of ΔV in Eq. (3.2.11), having opposite signs, cancel each other.

However, the situation for the case of $M=1$ is different. Because, the generalized Laquerre polynomial now is not constant, which appears as

$F(g) = L_{n=1}^{2(s-\frac{1}{4})}(g) = 2s - ax^2$. Moreover, the change in the potential parameter of the harmonic oscillator like term forces us to re-consider the structure of $g = ax^2$ which now should be $\lambda(a,b,s)x^2$ due to the presence of anharmonic terms in the potential.

This behaviour thus requires the replacement of $L_{n=1}^{2(s-\frac{1}{4})} = 2s - ax^2$ with an appropriate

another orthogonal polynomial $P_{n=1}^{2(s-\frac{1}{4})}(g) = 2s - \lambda x^2$. With this new consideration the full wavefunction for the first excited state becomes

$$\Psi_{n=1}^{M=1}(x) \sim \left(1 - \frac{\lambda(a,b,s)}{2s} x^2\right) x^{2(s-1/4)} \exp\left(-\frac{b}{4}x^4 - \frac{a}{2}x^2\right) \quad (3.2.16)$$

which guides us to use the exact treatment, $\frac{\Psi''}{\Psi} = V - E$, unlike the ground state case, that produces the related energy value as

$$E_{n=1}^{M=1} = 4(as + \lambda) \quad , \quad \lambda_{\mp}(a, b, s) = \frac{1}{2}(a \mp \sqrt{a^2 + 8bs}) \quad (3.2.17)$$

As stated in Ref. [53], $\lambda_{\mp}$ choice has to be made for $n=0$ and $n=1$ state calculations, respectively. Note that $b=0$ case causes $\lambda_{\pm} \rightarrow a$, subsequently $P_{n=1}^{2(s-\frac{1}{4})} \rightarrow L_{n=1}^{2(s-\frac{1}{4})}$ which reproduces the known solutions of the usual harmonic oscillator problem.

It has to be finally remarked that the solutions for $M=0$ and $M=1$ belong to different sextic potentials if $s \left(= \frac{\ell}{2} + \frac{3}{4} \right)$ is the same, as the coefficient of the quadratic term is different then. This shifting in the parameters defines the corresponding energy value for different considerations which are certainly related to the same subsequent perturbation order solutions in distinct quantum states if one deals with non-solvable sextic oscillator problems discussed below.

To complete the discussion in this section, we consider now a general form of the sextic potential in one dimension

$$V(x) = \mu x^2 + \sigma x^4 + \eta x^6 \quad , \quad (3.2.18)$$

and solve the corresponding Schrödinger equation approximately within the frame of the present scheme. In this case, Eqs. (3.2.6) and (3.2.7) become

$$\sum_{k=0}^N j_k j_{N-k} - \sigma \delta_{N1} - \eta \delta_{N2} = 0$$

$$j_N = (2N + 2n + \alpha_n)^{-1} \left(\sum_{k=0}^{N-1} j_k j_{N-k-1} - \mu \delta_{N1} - \sigma \delta_{N2} - \eta \delta_{N3} \right) \quad (3.2.19)$$

for the systematic calculations of the energy corrections concerning with the quadratic and sextic pieces in Eq. (3.2.18) , where α_n discussed in the previous section. For clarity, as the details of the similar calculation procedure for the quadratic potential were well discussed in Ref. [32] through Hermite polynomials, we illustrate only our application results in Tables 3.1 and 3.2

Table 3.1 Comparison of the first four eigenvalues of the potential $\mu x^2 + \eta x^6$ obtained by the present method with the exact values ([Ref. 40] for $\mu = 1$, and Ref. [54] for $\mu = 0$)

μ	σ	η	$N = 4$	$N = 8$	$N = 12$	<i>Exact</i>
1	0	0.1	1.104 923	1.109 628	1.109 070	1.109 087
			3.576 125	3.598 684	3.595 729	3.596 037
			6.609 983	6.662 450	6.655 648	6.644 392
			10.391 040	10.483 375	10.472 339	10.237 874
		1.0	1.418 059	1.442 229	1.435 465	1.435 625
			4.971 886	5.051 659	5.034 736	5.033 396
			9.831 164	9.974 381	9.958 135	9.966 622
			16.219 169	16.435 265	16.391 053	15.989 441
		10.0	2.174 017	2.221 521	2.205 998	2.205 723
			8.002 447	8.156 497	8.110 650	8.114 843
			16.353 667	16.624 921	16.587 359	16.641 218
			27.537 122	27.940 075	27.843 302	27.155 086
		100.0	3.665 363	3.745 295	3.718 101	3.716 975
			13.751 708	14.023 562	13.966 820	13.946 207
			28.440 597	28.925 950	28.863 060	28.977 294
			48.230 105	48.952 973	48.770 486	47.564 985
		1000.0	6.404 635	6.542 058	6.487 758	6.492 350
			24.184 202	24.664 085	24.557 556	24.525 316
			50.214 147	51.077 401	50.968 447	51.182 480
			85.350 546	86.638 619	86.308 303	84.175 584
0	0	1	1.129 584	1.153 559	1.143 340	1.144 802
			4.278 386	4.363 353	4.340 883	4.338 599
			8.899 753	9.053 228	9.034 111	9.073 085
			15.143 475	15.372 717	15.313 502	14.935 169

Table 3.2 Comparison of the present calculation results for the first four eigenvalues of the potential $\mu x^2 + \sigma x^4 + \eta x^6$, where $\mu=30$, $\sigma=20\sqrt{30}$ and $\eta=100$, with those obtained with the two different algebraic models

Average SWKB [Ref. 55]	Modified Hill Determinant Method [Ref. 56]	Present Calculations
7.3786	7.3569	7.3569
24.6861	24.6462	24.6462
46.3690	46.3355	46.3585
71.3823	71.3534	73.0669

The agreement is remarkable in the whole range of the potential parameters in the low-lying states. Similar accuracy is observed for the higher quantum levels. Nevertheless, when dealing with excited states the present approach becomes rather cumbersome because the zeros of the wavefunction have to be taken into account explicitly. As expected, due to the consequence of the radial nodes in - more specifically - $F(g)$ and subsequently $\Delta R(g)$ in Eqs. (3.1.14) and (3.1.12), the present formulae gives small accuracy for large quantum numbers since the perturbation becomes more more important.

3.3 Concluding Remarks

An attempt has been made [57] to generalize the work in [21] and shown that the mathematically rigorous new scheme unifies different theories for the solution of Schrödinger equation with analytically/approximately solvable conventional and energy-dependent potentials. The presented algorithm is also found to be equivalent to the alternative model reported previously [32]. This remarkable coincidence has revealed the bridge between the algebraic approach in the scenario introduced in this work and the one carried out within the frame of an extended SUSYQM theory [32], completing the discussion of Lévai [21] regarding the connection between the simple

prescription used in his work and the procedure within the usual SUSYQM theory. Although the literature covered similar problems, to our knowledge an investigation such as the one presented here was missing.

Beyond its intrinsic importance as a new solution for a fundamental equation in physics, we expect that the present simple method would find a widespread application in the study of different quantum mechanical systems with constant and position-dependent masses. In particular, the present discussion would be useful in perturbational treatments of the exact spectra of a few particle systems, and thus provide a further insight on discussion of the fractional nature of such systems.

The application of the present scenario, introduced in this chapter for the systems with a constant mass, to the systems with spatially varying masses, will be discussed in the next chapter.

CHAPTER 4

AN ALTERNATIVE APPROACH TO SCHRÖDINGER EQUATIONS WITH A SPATIALLY VARYING MASS

Tracking down solvable quantum potentials has always aroused interest. Apart from being useful in understanding of many physical phenomena, investigations of such potentials also provide a good starting point for undertaking perturbative calculations of more complex systems. Within this context, we have recently suggested [57] a novel algebraic framework for the unified treatment of Schrödinger equations, with a constant mass, involving solvable and non-solvable potentials, which was also well discussed in the previous chapter.

For the completeness, and also considering the importance of quantum mechanical systems with position dependent masses in describing the physics of many microstructures of current interest [58], the model [57] discussed in the previous chapter is to be extended in this chapter for also analysing the systems having non-constant masses.

Unfortunately, up to now, the related previous works have dealt with only either exact or quasi-exact solutions of the Schrödinger equation in a position-dependent effective mass back-ground. In the other words, to the best of our knowledge, there has been no ongoing discussion in the literature regarding approximate solutions of non-solvable potentials for the case of non-constant masses. Therefore, at present, there seems no room for a precise test of the application results of the prescription introduced in Section 4.1. However, we believe that the present algebraic scenario would find a widespread application in the near future due to the current interest in microstructures, Ref [58], which eventually would require physically acceptable approximate descriptions of such systems that should be investigated within the frame of more complex and non-exactly solvable potentials. In addition, the recent

progress [59,60] in analysing experimental data within the frame of algebraic models to investigate nuclear structure gives us a signal for the possibility of using a prescription such as the one presented in this chapter.

4.1 Formalism

As is well known the general Hermitian position-dependent effective mass Hamiltonian, initially proposed by von Roos [61] in terms of ambiguity parameters α , β , γ such that $\alpha + \beta + \gamma = -1$, gives rise to the time independent Schrödinger equation

$$H\psi(x) = \left[-\frac{d}{dx} \frac{1}{M(x)} \frac{d}{dx} + V_{\text{eff}}(x) \right] \psi(x) = E\psi(x) \quad , \quad (4.1.1)$$

where the effective potential

$$V_{\text{eff}}(x) = V(x) + \frac{1}{2}(\beta + 1) \frac{M''}{M^2} - [\alpha(\alpha + \beta + 1) + \beta + 1] \frac{M'^2}{M^3} \quad (4.1.2)$$

depends on the mass term. Here the prime denotes derivative with respect to x , $M(x)$ is the dimensionless form of the mass function $m(x) = m_0 M(x)$ and we have set $\hbar = 2m_0 = 1$.

Considering the suggestion in Ref. [57], which is shown by Eq. (3.1.2) in the previous chapter,

$$\psi(x) = [f(x)F(g(x))] h(x) \quad , \quad (4.1.3)$$

where $f(x)F(g)$ yields an algebraic closed solution for exactly and quasi-exactly solvable potentials with $F(g)$ being a special function satisfying Schrödinger-like equations

$$\frac{d^2 F}{dg^2} + Q(g) \frac{dF}{dg} + R(g)F(g) = 0 \quad , \quad (4.1.4)$$

while $h(x)$ is the moderating function in connection with a perturbing piece of the full potential corresponding to, in our present consideration, Eq. (4.1.2). The form of $Q(g)$ and $R(g)$ is already well defined for any special function $F(g)$ when dealing with analytically solvable potentials. However, in case of the consideration of a realistic non-exactly solvable system one should suggest reliable expressions, in an explicit form, for plausible definitions of the related $Q(g)$ and $R(g)$ functions. This is the significant point in the framework of the new formalism to reach physically meaningful solutions.

On inserting Eq. (4.1.3) in Eq. (4.1.1) and comparing the result with Eq. (4.1.4), we arrive at

$$Q(g(x)) = \frac{g''}{(g')^2} + \frac{2f'}{fg'} - \frac{M'}{Mg'} + \frac{2h'}{hg'} \quad (4.1.5)$$

and

$$R(g(x)) = \frac{f''}{f(g')^2} + \frac{2f'h'}{fh(g')^2} + \frac{h''}{h(g')^2} - \frac{M'}{M} \frac{f'}{f(g')^2} - \frac{M'}{M} \frac{h'}{h(g')^2} + M \frac{[E - V_{eff}(x)]}{(g')^2} \quad (4.1.6)$$

where

$$f(x) \propto \left(\frac{M}{g'}\right)^{1/2} \exp\left[\frac{1}{2} \int^g Q(y) dy\right]. \quad (4.1.7)$$

Obviously, Eqs. (4.1.5 - 4.1.7) reduce to their standard forms (see, e.g., Ref. [21]) for the consideration of exact solvability of Schrödinger equations with a constant mass in which case $M(x)$ and $h(x)$ in the equations above appear as a constant. Gaining confidence from this observation we proceed with

$$V_{eff}(x) = V_{ES}(x) + \Delta V(x) \quad , \quad E = E_{ES} + \Delta E \quad (4.1.8)$$

in accordance with our choice in Eq. (4.1.2), which means that potentials considered in this chapter are admitted as the sum of an exactly (or quasi-exactly) solvable potential with a perturbation or a moderating piece. Hence, the aim in this

perspective is to reveal the corrections to energy (ΔE) and wavefunction, $h(x)$, for a given $\Delta V(x)$ as the main piece of the solutions leading to exact solvability can easily be found from the literature.

The use of Eqs. (4.1.5) and (4.1.8) within the frame of Eq. (4.1.6) leads to the coupled equations in the form of

$$E_{ES} - V_{ES}(x) = \frac{g'''}{2Mg'} - \frac{3}{4M} \left(\frac{g''}{g'} \right)^2 + \frac{(g')^2}{M} \left[R_{ES}(g) - \frac{1}{2} \frac{dQ_{ES}(g)}{dg} - \frac{1}{4} Q_{ES}^2(g) \right] - \frac{M''}{2M^2} + \frac{3M'^2}{4M^3} \quad (4.1.9)$$

and

$$\Delta E - \Delta V(x) = -\frac{1}{2M} \left(g'' + \frac{2f'g'}{f} - \frac{M'g'}{M} \right) \Delta Q(g) + \frac{g'^2}{M} \left[\Delta R(g) - \frac{1}{2} \frac{d(\Delta Q)}{dg} - \frac{1}{4} \Delta Q^2(g) \right] \quad (4.1.10)$$

in which, from Eq. (4.1.5), $\Delta Q(g) = \frac{2h'}{hg'}$ leading to

$$h(x) = \exp \left(\frac{1}{2} \int \Delta Q(g) dg \right), \quad (4.1.11)$$

and

$$\Delta R(g) = \frac{2f'h'}{f h(g')^2} + \frac{h''}{h(g')^2} - \frac{M'}{M} \frac{h'}{h(g')^2} + M \frac{[\Delta E - \Delta V(x)]}{(g')^2}.$$

It is clear that $Q_{ES}(g)$, together with $R_{ES}(g)$, related to algebraically solvable potentials, can be obtained from Eqs. (4.1.5) and (4.1.6) such that $Q(g) = Q_{ES}(g) + \Delta Q(g)$ and $R(g) = R_{ES}(g) + \Delta R(g)$. Again, in case of exact solvability Eqs. (4.1.10) and (4.1.11) disappear naturally by reducing the scheme to Eq. (4.1.9), which justifies the reliability of the present work, see, e.g., Refs. [28,30,31]. This realization puts forward the significance of Eq. (4.1.10) for approximately solvable more complex quantum potentials, which is the main point in this section.

The result of this brief investigation opens a gate to the reader for the visualization of the explicit form of the correction (ΔE) to the energy. Unfortunately, there seems a problem arised in calculating the correction term owing to the presence of two unknown: ΔQ and $\Delta R(g)$ on the right hand side of Eq. (4.1.10). To circumvent the resulting drawback and proceed safely, one needs to use the interesting expression yielding inter-connection between ΔQ and $\Delta R(g)$ functions, as was discussed earlier,

$$\Delta R(g) = -\Delta Q(g) \frac{F'(g)}{F(g)} \quad , \quad (4.1.12)$$

that is obtained, after some exhaustive analyses, by considering the another form of Eq. (4.1.10)

$$\Delta E - \Delta V(x) = -\frac{1}{M} \left[\frac{h''}{h} + \frac{2h'}{h} \left(\frac{f'}{f} + \frac{g'F'(g)}{F(g)} - \frac{M'}{2M} \right) \right] . \quad (4.1.13)$$

As $F(g)$ is well defined for solvable potentials, we obviously need here to find only an appropriate expression for ΔQ to be employed eventually in Eq. (4.1.10), or in Eq. (4.1.13) with the use of Eq. (4.1.11), that reveals the full solution.

It is however reminded that if the whole potential such as in Eq. (4.1.2) has no analytical solution, one should expand the related functions in terms of the perturbation such that $\Delta V(x) = \sum_{N=1}^{\infty} \Delta V_N(x)$ and $\Delta E_n = \sum_{N=1}^{\infty} \Delta E_{nN}$ where N denotes the perturbation order and $n(= 0, 1, 2, \dots)$ is the radial quantum number relating to bound-state energy levels. In connection with this idea, the form of ΔQ should be chosen carefully depending on N – values and the substitution of reasonable ΔQ values into either Eq. (4.1.10) or Eq. (4.1.13), and consequently equating terms with the same power of the perturbation order on both sides, yields the modifying terms in the frame of coupled equations at successive orders for different states. The procedure has been well discussed in Ref. [57], and also in Chapter 3, for approximately solvable unharmonic potentials involving constant masses.

4.2 Application

This section gives a clue for exploring new potentials within the unique frame of the formalism introduced. For clarity, we start with a simple example from the work of Bagchi and his co-workers [28] where the form of the mass is chosen as $M = \lambda g'$ with λ being a constant, which simplifies Eq. (4.1.9) as

$$E_{ES} - V_{ES}(x) = \frac{g'}{\lambda} \left[R_{ES}(g) - \frac{1}{2} \frac{dQ_{ES}(g)}{dg} - \frac{1}{4} Q_{ES}^2(g) \right], \quad (4.2.1)$$

that is responsible for the piece of the interaction having closed analytical solutions. Another appropriate choice for the $F(g)$ within the list of the orthogonal

polynomials used frequently in physics, $F(g) = \exp\left(-\frac{g}{2}\right) g^{\left(\frac{\alpha+1}{2}\right)} L_n^\alpha(g)$, implies that

$$R(g) = \frac{2n + \alpha + 1}{2g} + \frac{1 - \alpha^2}{4g^2} - \frac{1}{4}, \quad Q(g) = 0. \quad (4.2.2)$$

The use of Eq. (4.2.2) in Eq. (4.2.1) requires that $g'/\lambda g = \beta^2$ which must be restricted to positive values in order to get a constant term on the right-hand side of Eq. (4.2.1). Setting $\lambda = -1/\beta$, we arrive at $g(x) = e^{-\beta x}$ and, from the definition of the mass form, $M(x) = e^{-\beta x}$. Therefore, the related solutions appear as

$$E_{ES} = \beta^2 \left(n + \frac{\alpha + 1}{2} \right), \quad \psi_{ES} = f(x) F(g) \propto \exp\left(-\frac{g}{2}\right) g^{\left(\frac{\alpha+1}{2}\right)} L_n^\alpha(g), \quad (4.2.3)$$

for the constructed solvable potential

$$V_{ES}(x) = \frac{\beta^2}{4} \left[(\alpha^2 - 1) e^{\beta x} + e^{-\beta x} \right]. \quad (4.2.4)$$

At this stage, we focus on Eq. (4.1.10) to observe how additional potential terms can be generated. This observation would clarify how the present model copes with the perturbed piece of the potential, as well as the understanding of the procedure for the

generation of new non-solvable potentials. With the use of $M = \lambda g'$ in Eq. (4.1.10),

$$\text{we obtain } \Delta E - \Delta V(x) = \frac{g'}{\lambda} \left[\Delta R(g) - \frac{1}{2} \frac{d(\Delta Q)}{dg} - \frac{1}{4} \Delta Q^2(g) \right], \quad (4.2.5)$$

which is similar to Eq. (4.2.1). Bearing the structure of Eq. (4.2.1) in mind, in particular n -dependence of $R(g)$ term, we transform the above equation, with the remind of Eq. (4.1.12),

$$\Delta E - \Delta V(x) = -\frac{g'}{\lambda} \left[\frac{F'}{F} \Delta Q + \frac{1}{2} \frac{d(\Delta Q)}{dg} + \frac{1}{4} \Delta Q^2 \right], \quad (4.2.6)$$

into the more applicable form. As the study of Eq. (4.2.1) has already defined $F(g)$, $g(x)$ and λ , one needs here to deal with only $\Delta Q(g)$ term which is the central part of the whole discussion. Obviously different choice of this term, depending of course on the perturbation order (N) discussed in the previous section, would lead to distinct functions generating new additional potentials including the corresponding energy

terms in each order. For instance, a possible choice of $\Delta Q(g) = -\frac{b}{g'} \sum_{i=1}^N G(i, x)$, where

b is a constant and G is a general form of the physically reasonable functions, would help us to define energy term from the first term in the bracket while generating modifications to the main part of the potential in Eq. (4.2.4). It is clear that there is no strict definition for the generating function $G(i, x)$ which should be determined by considering the structure of the realistic system of interest. It is however stressed that the modifications in each order for successive quantum levels should be individually considered. This requires a meticulous search for the corrections brought by Eq. (4.2.6), in which expressions giving the structure of $F(g)$ for each state ($n = 0, 1, 2, \dots$) ought to be used properly.

Finally, to clarify the flexibility of the approach used, it should be noticed that additional exactly and quasi-exactly solvable quantum potentials in a spatially varying mass context may also be generated. As an illustration, we choose again $M = \lambda g'$ option and employ it in Eq. (4.1.10). This consideration leads to

$$\Delta E - \Delta V(x) = -\frac{\Delta Q(g)}{\lambda} \frac{[\psi_{ES}(x)]'}{\psi_{ES}(x)} - \frac{g'}{2\lambda} \frac{d[\Delta Q(g)]}{dg} - \frac{g'}{4\lambda} [\Delta Q(g)]^2, \quad (4.2.7)$$

where, from Eq. (4.1.3), $\psi_{ES}(x) = f(x)F(g)$ is the exact (or quasi-exact) solution for a solvable potential undertaken. To proceed we choose a specific example assuming that the sum of the second and third terms on the right hand side of the above equation is zero. This feasible assumption requires that $\Delta Q = 2/g$ which transforms Eq. (4.2.7) to

$$\Delta E - \Delta V(x) = -\frac{2}{\lambda g} \frac{[\psi_{ES}(x)]'}{\psi_{ES}(x)}. \quad (4.2.8)$$

As, in general, ψ_{ES} and $g(x)$ are readily obtained from Eq. (4.1.9), or they can be extracted from the literature, Eq. (4.2.8) together with Eq. (4.1.8) may generate new solvable potentials. In addition, the modification to the wavefunction ($h(x)$) due to the additional potential ($\Delta V(x)$) can easily be obtained through Eq. (4.1.11). More specifically, the substitution of ψ_{ES} in Eq. (4.2.3) into Eq. (4.2.8) generates a modification in a closed form to the solvable potential in Eq. (4.2.4), the summation of these terms ($V_{ES} + \Delta V$) is a new potential having algebraic solutions involving either the whole or some part of the spectra.

Overall, the method described here has an ability of generating all classes of potentials depending of course on the choice of the mass function and the use of different orthogonal polynomials ($F(g)$) within the frame of Eqs, (4.1.9), (4.1.10) and (4.1.12), providing closed analytical or approximate solutions to the corresponding Schrödinger equation.

4.3 Concluding Remarks

The literature covers many applications regarding the description of collective nuclear properties in terms of the corresponding collective variables within the framework of Bohr Hamiltonian involving exactly solvable potentials. However, the

recent analysis [59] has introduced special solutions for the Morse potential which is known to be exactly soluble only for $\ell = 0$, unlike the previous applications. For the approximate treatment of quantum states having non-zero angular momenta, the well-known Pekeris approximation has been used. This unusual consideration, however, has suppressed the overestimation of the energy spacings within the beta-band due to right branch of the Morse potential that imitates the sloped wall, which has removed a main drawback of the earlier considerations. Furthermore, the Bohr Hamiltonian and its extensions, for a recent review see Ref. [59] and the references therein, have provided for several decades a sound framework for understanding the collective behavior of atomic nuclei. It has been customary to consider in the Bohr Hamiltonian the mass to be constant, as in [59]. However, evidence has been accumulating that this approximation might be inadequate [60] in which significant effects of using a mass depending upon nuclear deformation on the calculations of spectra and analytical expression of the wavefunction describing the collective motion of deformed nuclei was discussed in detail. Within this context, the present algebraic model [63] seems promising as the scheme has a power of yielding the required expressions in an explicit form for the Morse-like potentials mentioned above and also the corrections due to the corresponding angular momentum barrier involving deformation-/position-dependent mass systems. Along this line the works are in progress.

CHAPTER 5

CONCLUDING REMARKS

An attempt has been made to generalize the work in [21] and shown that the mathematically rigorous new scheme [57] unifies different theories for the solution of Schrödinger equation with analytically/approximately solvable all conventional potentials. In addition, the procedure used here for approximately solvable potentials is illustrated as to be well adapted to the use of software systems such as Mathematica and allows the computation to be carried out up to high orders of the perturbation. Further, the presented algorithm is also found to be equivalent to the alternative model reported previously [32]. This remarkable coincidence has revealed the bridge between the algebraic approach introduced in this work [57] and the one carried out within the frame of an extended SUSYQM theory [32], completing the discussion of Lévai [21] regarding the connection between the simple prescription used in his work and the procedure within the usual SUSYQM theory. Although the literature covered similar problems, to our knowledge an investigation such as the one presented here was missing.

Beyond its intrinsic importance as a new solution for a fundamental equation in physics, we expect that the present simple method [57] would find a widespread application in the study of different quantum mechanical systems with constant and position-dependent masses. In particular, the present discussion would be useful in perturbational treatments of the exact spectra of a few particle systems, and thus provide a further insight on discussion of the fractional nature of such systems. Finally, the remaining question here is to know if the scenario put forward in the present work is applicable to non-central potentials and also, after some necessary modifications, to the related problems in the relativistic region. Along this line the works are in progress.

Final chapter in this thesis has been devoted to the extension of the formalism introduced in Chapter 3, where the model is applied to the systems involving position dependent masses. The novel scheme developed originally [57] for the solutions of Schrödinger equations with constant masses, has been successfully applied [63] to other systems involving spatially varying masses. We also showed that the present algebraic model is capable for the generation of potentials in all classes. We intend to use this flexible technique [63] to answer some unsolved questions in nuclear physics dealing with the structure of atomic nuclei with deformation- (like position-) dependent potentials [59,60].

Moreover, recently, a modified factorization technique [62] of a quantum system characterized by spatially varying mass-Hamiltonians has been presented and shown that excited state wavefunctions of a given singular Hamiltonian can be used to construct non-singular isospectral partner potentials. This work would be helpful to remove the singularity problem naturally arised in the present formalism due to zeros of $F(g)$ function, which should be necessary for the case of considering higher quantum states.

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