APPLICATIONS OF A NEW APPROACH TO BOUND-STATES

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ABSTRACT

APPLICATIONS OF A NEW APPROACH TO BOUND-STATES

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Recently developed approach for the treatment of Schrödinger equations is applied to anharmonic oscillator and Yukawa type potentials to have reliable expressions for their bound state energies and eigenfunctions. In addition, we show that the present novel formalism is entirely equivalent to a well known alternative model in the literature.

Keywords: Anharmonic Oscillator, Yukawa Potential, Perturbation, Exactly solvable potentials

ÖZET

YENİ BİR MODELİN BAĞLI DURUMLARA UYGULAMALARI

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Schrödinger denklemlerinin çözümü için yeni geliştirilen bir model, bağlı kuantum durumları içeren harmonik olmayan titreşim potansiyeli ve Yukawa tipi etkileşimlere ait enerji ve dalga fonksiyonu davranışlarını veren güvenilir analitik ifadelere ulaşmak için kullanıldı. Ayrıca, bu modelin literatürde bulunan başka bir model ile tamamen aynı olduğu gösterildi

Anahtar kelimeler: Anharmonik titreşim, Yukawa Potansiyeli, Yaklaşık model, Tam çözülebilen potansiyeller

In Memory of My Dear
Mother

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CHAPTER 1

INTRODUCTION

Over the past years the Schrödinger equation has been studied extensively with regard to its exact solvabilty. Many advances have been made in this area by classifying quantum mechanical potentials in terms of their symmetry properties. For example, various algebra which reveal the underlying symmetry as well as obtaining the solutions have been found. In this respect the application of supersymmtry ideas [1] to non-relativistic quantum mechanics has revived fresh interest in the problem of attaining 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 shape invariance [1] has played an important role in these developments.

An exact solution of the Schrödinger equation exist only for a few idealized problems in general it has to be solved using on approximation method such as the Perturbation Theory (PT), which constitutes one of the most powerful tools available in the study of quantum mechanics in the atoms and molecules. PT 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 influence of external fields. But in spite of widespread application of this theory, its basic analytical properties are poorly understood. One of our objectives in this work is to illustrate selected important aspects of the perturbation theory within the frame of supersymmetric quantum mechanics.

Performing explicit calculations in non-relativistic quantum mechanics using the familiar Rayleigh-Schrödinger perturbation expansion 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 logaritmic perturbation theory (LPT) [2]-[5] and Dalgarno-Lewis technique [6]-[9]. The virtue of LPT is its avoidance of 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 wave functions. Various schemes have been proposed to circumvent the resulting singularities [5, 10, 11].

Such is the status of LPT after over 20 years of active development. Meanwhile, supersymmetric quantum mechanics (SSQM) [1, 12] 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.

Within this context, starting from the first principles, recently Gönül [17] has been developed a more economical model which yields simple but closed perturbation theory formula leading to the Ricatti equation from which one can actually obtain all the perturbation corrections to both energy level shift and wave functions for all states unlike the other models mentioned above. The novel applications of this model are discussed in detail through this thesis work. Additinally, in the application of this method to the nth excited state, one requires knowledge of the unperturbed eigenfunction $\chi_n(r)$ but no knowledge of the other eigenvalues or eigenfunctions is necessary. The procedure introduced here does not involve either tedious explicit factoring out of the zeros of $\chi_n(r)$ [2, 3] or introduction of ghost states [5] as were the cases encountered for applying LPT to

excited states. Since, the present method offers 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 it also provides a clean route to the excited states, which are combersome to analyze in both LPT and SSPT. Hence the present approach can be tought of as a generalization of logarithmic and supersymmetric based perturbation theories. To discuss this point briefly, together with its new applications, is also another objective in this work.

The plan of the thesis is as follows: After giving some introductory remarks about basic formalism of the method we apply it to the anhormanic oscillator in Chapter 3. The method further is extended to an algebraic non-perturbative approach for the analytical treatment of such Schrödinger equations with a potential that can be expressed in terms of an exactly solvable piece with an additional potential. Avoiding disadventages of standart approaches, a new handy recursion formulas with the same simple form both for ground and excited states have been obtained. In Chapter 4, we propose a new scheme to obtain analytic expressions for the bound state energies and eigenfunctions of Yukawa like potentials within the framework of the novel formalism. The application makes clear that the scheme developed gives quite good accuracy for energy values despite its analytical nature. In Chapter 5, we first rewiev an alternative transformation method, which is well known in the literature, permitting the generation of exactly solvable quantum mechanical potentials from special functions solving second-order differantial equations. This method later is applied to Gegenbauer polynomials to generate an attractive radial potential. The relationship of this method to our treatment is discussed in detail and it is shown that the both method in fact is equal to each other. Subsequently, a unified treatment is suggested in order to perfect the calculations. Finally, concluding remarks and a future work are presented in the final chapter.

CHAPTER 2

FORMALISM

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We first start with a brief introduction of the present formalism. In general, the goal in supersymmetric quantum theory [1] is to solve the Ricatti equation.

$$W^2 - \frac{\hbar}{\sqrt{2m}} W' = V(r) - E_0 , \qquad (2.1)$$

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,

$$\psi_0(r) = N \exp\left[-\int^r W(z)dz \right] , \qquad (2.2)$$

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 $V(r)$ 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 Ricatti equation explicitly. For the consideration of spherically symmetric potentials, the corresponding Schrödinger equation for the radial wave function has the form

$$\frac{\hbar}{\sqrt{2m}} \frac{\psi_n''}{\psi_n} = [V(r) - E_n], \ V(r) = \left[V_0(r) + \frac{\ell(\ell+1)}{r^2} \right] + \Delta V , \qquad (2.3)$$

where $\Delta V(r)$ is a perturbing potential. Let us write the wave function ψ_n as

$$\psi_n(r) = \chi_n(r)\phi_n(r) , \qquad (2.4)$$

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 (2.4) into (2.3) yields

$$\frac{\hbar^2}{2m}\left(\frac{\chi_n''}{\chi_n} + \frac{\phi_n''}{\phi_n} + 2\frac{\chi_n'}{\chi_n}\frac{\phi_n'}{\phi_n}\right) = V - E_n. \tag{2.5}$$

Instead of setting the functions χ_n and ϕ_n, we will set their logaritmic derivatives using Eqs.(2.1) and the standart approach of LPT:

$$W_n = -\frac{\hbar}{\sqrt{2m}}\frac{\chi_n'}{\chi_n} \quad , \quad \Delta W_n = -\frac{\hbar}{\sqrt{2m}}\frac{\phi_n'}{\phi_n} \quad , \tag{2.6}$$

which leads to

$$\frac{\hbar}{\sqrt{2m}}\frac{\chi_n''}{\chi_n} = W_n^2 - \frac{\hbar}{\sqrt{2m}}W_n' = \left[V_0(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right] - \varepsilon_n, \tag{2.7}$$

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

$$\frac{\hbar^2}{2m}\left(\frac{\phi_n''}{\phi_n} + 2\frac{\chi_n'}{\chi_n}\frac{\phi_n'}{\phi_n}\right) = \Delta W_n^2 - \frac{\hbar}{\sqrt{2m}}\Delta W_n' + 2W_n\Delta W_n = \Delta V(r) - \Delta\varepsilon_n, \tag{2.8}$$

in which $\Delta\varepsilon_n$ is the eigenvalue for the perturbed potential, and $E_n = \varepsilon_n + \Delta\varepsilon_n$. Then Eq.(2.5), and subsequently Eq.(2.3), reduces to

$$\left(W_n + \Delta W_n\right)^2 - \frac{\hbar}{\sqrt{2m}}\left(W_n + \Delta W_n\right)' = V - E_n \tag{2.9}$$

which is similar to Eq. (2.1), nevertheless, it is valid for all states unlike the usual supersymmetric treatment [1] which uses Eq.(2.9) only for the ground state due to theorical considerations. Further, as one in principle knows explicitly the solution of Eq.(2.7), namely the whole spectrum and the corresponding eigenfunctions of the unperturbed interaction potential, the goal here is to solve only Eq.(2.8), which is the backbone of this formalism. The reader is referred to Ref [17] for the succesful applications of Eq.(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 thesis, then Eq.(2.8) cannot be solved exactly which requires that, one can expand the functions in terms of the perturbation parameter λ,

$$\Delta V(r;\lambda) = \sum_{N=1}^{\infty} \lambda^N \Delta V_N(r) \ ,$$

$$\Delta W_n(r;\lambda) = \sum_{N=1}^{\infty} \lambda^N \Delta W_{nN}(r) \ , \qquad (2.10)$$

$$\Delta \varepsilon_n(\lambda) = \sum_{N=1}^{\infty} \lambda^N \Delta \varepsilon_{nN} \ ,$$

where N denotes the perturbation order. Substituting the above expansion into Eq. (2.8) by equating terms with the some power of λ on both sides yields up for instance $O(\lambda^3)$

$$2W_n \Delta W_{n1} - \frac{\hbar}{\sqrt{2m}} \Delta W'_{n1} = \Delta V_1 - \Delta \varepsilon_{n1} \ , \qquad (2.11)$$

$$\Delta W_{n1}^2 + 2W_n \Delta W_{n2} - \frac{\hbar}{\sqrt{2m}} \Delta W'_{n2} = \Delta V_2 - \Delta \varepsilon_{n2} , \qquad (2.12)$$

$$2(W_n \Delta W_{n3} + \Delta W_{n1} \Delta W_{n2}) - \frac{\hbar}{\sqrt{2m}} \Delta W'_{n3} = \Delta V_3 - \Delta \varepsilon_{n3} \ . \qquad (2.13)$$

Eq.(2.8) and its expansion give a flexibility for the easy calculations of the perturbative corrections to energy and wave functions for the nth state of interest through an appropriately chosen perturbed superpotential. It has been shown [17] that this feature of the present model leads to a simple framework in obtaining the corrections to all states without using complicated mathematical procedures.

CHAPTER 3

APPLICATION TO ANHARMONIC OSCILLATOR PROBLEM

The present scheme [17] mentioned above is applied here 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 [18] as well as in solid state physics [19] and quantum field theories [20]. The anharmonic oscillator with quartic potentials can serve as a testing ground for the various methods based on perturbative and non perturbative approaches. Namely, interest in such a model stems mainly from the fact that, if one considers the anharmonicity gx^4 as a perturbing term, then the Rayleigh-Schrödinger perturbation expansion for the eigenvalues diverges [21] for every value of g. Consequently, several methods have been used to caculate the quartic anharmonic oscilltor for eigenvalues and eigenfunctions. Without being exhaustive, we may recall variational methods [22], WKB methods [23], Hill determinant [24,25] and Riccati [26], or Ricatti-Hill determinant methods [27], perturbative treatment prescriptions using summability techniques such as the Stieljes, Pade and Barrell methods [20,28]. Let us also mention the hypervirial perturbation method of Fernandez and Castro [29], which can be viewed as a generalization of the Killinbeck method [30], and other alternative treatments [31], together with those involving a group-theoretical approach [32], the multiple scale techniqe [33], and supersymmetric methods [34].

3.1 Application

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

$$V = V_0 + \Delta V = x^2 + gx^4 \ , \qquad (3.1)$$

which the unperturbed potential represents the well-known factorizable harmonic

oscillator. From the literature, [1] , [35] the corresponding superpotentials, wave functions and energy values are

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

(3.2)

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

where H_n denotes Hermite polynomials, n=0,1,2,3,……… is the radial quantum number and a is the potential parameter. With a suitable choice of ΔW ,

$$\Delta W = \sum_{N=1}^{\infty} f_n x^{2N+1} \quad,$$

(3.3)

corresponding to the perturbed potential gx^4 in Eq.(3.1), one obtains some equations at successive orders for different states, revealing some interesting relations between them and leading to a simple algebraic treatment of the problem of interest here.

3.1.1   Calculations for n=0 and n=1 states

For instance, starting from the ground state calculations $(n = 0)$, where, from Eq .(3.2) $W = ax$ and considering Eqs. (2.11) through (2.13) we get at the first order *(N=1)*,

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

(3.4)

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

$$f_1^2 + 2af_2 = 0,$$

(3.5)

$$f_2 = \frac{2af_1 - g}{5} \Rightarrow E_{n=0}^4 - \tfrac{22}{17}E_{n=0}^2 - \frac{18g}{17}E_{n=0} + \tfrac{5}{17} = 0$$

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

$$2(af_3 + f_1 f_2) = 0 \quad,$$

(3.6a)

$$f_3 = \frac{f_1^2 + 2af_2}{7} \Rightarrow E_{n=0}^5 - \frac{50}{31}E_{n=0}^3 - \frac{39g}{31}E_{n=0}^2 + \frac{19}{31}E_{n=0} + \frac{21g}{31} = 0 \quad (3.6b)$$

If one repeats same calculations for the first excited state (n=1), for which the superpotential is set $W = ax - 1/x$ in the light of Eq. (3.2), then the first order yields

$$2af_1 = g, \quad f_1 = \frac{1}{5}\left(a^2 - 1\right) \Rightarrow E_{n=1}^3 - 9E_{n=1} - \frac{135}{2}g = 0, \quad (3.7)$$

and at the second order we have

$$f_1^2 + 2af_2 = 0 \quad ,$$

$$(3.8)$$

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

while the third order expressions are

$$2\left(af_3 + f_1f_2\right) = 0,$$

$$(3.9)$$

$$f_3 = \frac{f_1^2 + 2af_2}{9} \Rightarrow E_{n=1}^5 - 14E_{n=1}^3 - 57gE_{n=1}^2 + 45E_{n=1} + 243g = 0.$$

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 hieararchy. The systematic calculation of perturbation corrections of large orders offers no difficulty if we resort a computer algebra system like Mathematica and Maple or Reduce. This realization generalizes anharmonic oscillator solutions for the ground and first excited states without solving the Schrödinger equation. To calculate the energy values individually at the each perturbation order, one needs to solve only

$$\sum_{k=0}^{N} f_k f_{N-k} - g\delta_{N1} = 0, \quad (3.10)$$

in which δ denotes Kronocker delta and $f_0 = a$ is the parameter related to Eq. (3.2). The perturbation coeffients above can easily be computed through

$$f_n = (2N + 2n + 1)^{-1} \left(\sum_{k=0}^{N-1} f_k f_{N-k-1} - \delta_{N1} - g\delta_{N2} \right). \qquad (3.11)$$

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 [25]. The agreement is remarkable in the whole range of *g* values for both quantum states, see Tables (3.1) and (3.2). The large order perturbation calculations are performed by a simple use of Mathematica [36] along the line of (3.10) and (3.11) with simple algebraic manipulations.

Table (3.1). Lowest eigenvalue of anharmonic oscillator *(n=0)*

g	N=1	N=2	N=3	N=4	Exact[25]
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

Table (3.2). First excited state energies of anharmonic oscillotor *(n=1)*

g	N=1	N=2	N=3	N=4	N=8	Exact[25]
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

3.1.2 Calculations for $n \geq 2$ states

When dealing with excited states, this approach seems rather cumbersome because the zeros of the wave function 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 generalization of the resulting expressions at succesive perturbation orders as in the previous section.

Starting with second excited state *(n=2)*, where from Eq.(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

$$2af_1 = g, \quad f_1 = \frac{1}{8}\left(a^2 - 1\right), \qquad \text{N=1,} \tag{3.12a}$$

$$f_1^2 + 2af_2 = 0, \quad f_2 = \frac{2af_1 - g}{10}, \qquad \text{N=2,} \tag{3.12b}$$

$$2(af_3 + f_1 f_2) = 0, \quad f_3 = \frac{f_1^2 + 2af_2}{12}, \qquad \text{N=3,} \tag{3.12c}$$

$$f_2^2 + 2(f_1 f_3 + af_4) = 0, \quad f_4 = \frac{2(af_3 + f_1 f_2)}{14}, \qquad \text{N=4,} \tag{3.12d}$$

$$2(f_2 f_3 + f_1 f_4 + af_5) = 0, \quad f_5 = \frac{f_2^2 + 2(f_1 f_3 + af_4)}{16}, \qquad \text{N=5.} \tag{3.12e}$$

In these treatments, to remove singularities in the related superpotential due to the zeros of the wave function, 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 (3.3).

Table (3.3). Second excited state energies of the anharmonic oscillator *(n=2)*

g	N=1	N=2	N=3	N=4	N=15	Exact[25]
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 for the third *(n=3)* of the anharmonic oscillator one can choose the corresponding superpotential $W_{n=2} = \left(2a^2x^4 - 9ax^2 + 3\right)/\left(2ax^3 - 3x\right)$ via Eq.(3.2) for unperturbed piece of the potential and end up with some explicit algebraic equations at each order

$$2af_1 = g, \quad f_1 = \frac{1}{12}\left(a^2 - 1\right), \qquad \text{N=1}, \tag{3.13a}$$

$$f_1^2 + 2af_2 = 0, \quad f_2 = \frac{2af_1 - g}{14}, \qquad \text{N=2}, \tag{3.13b}$$

$$2\left(af_3 + f_1f_2\right) = 0, \quad f_3 = \frac{f_1^2 + 2af_2}{16}, \qquad \text{N=3,...} \tag{3.13c}$$

and so on. In the case wave the 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 $2ax^2 > 3x$ which produces reasonable results. However, this choice for higher excited states with $n \geq 3$ allows only the coefficents f_N with x^{2N} and x^{2N+2} through the linear perturbation expressions at each order. The results obtained are illustrated in Table (3.4). Although the present formalism suggest a systematic

way of improving the anharmonic oscillator perturbation series, the accuracy of the present formulas 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 behavior of the results presented here they are expected to be much more accurate than the perturbation series. This idea was exploited by Fernandez et al [26]. in order to obtain analytical expressions for eigenvalues of the anharmonic oscillator from the semiclassical considerations.

Table (3.4). Third excited state energies of the anharmonic oscillator *(n=3)*

g	N=1	N=2	N=3	N=4	N=15	Exact[25]
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
0.05	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 above discussion one can easily generalize the whole calculations discussed in Sec. 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. (3.10) can be safely used for this purpose, however the coefficients should be re-defined as

$$f_N = (2N + 2n + a_n)^{-1} \left(\sum_{k=0}^{N-1} f_k f_{N-k-1} - \delta_{N1} - g\delta_{N2} \right), \qquad (3.14)$$

where $a_n = (n-1) + a_{n-1}$ being with $n \geq 1$ and $a_0 = 1$. As matter of fact , the only data that are needed when using Mathematica is Eq. (3.14) to solve Eq. (3.10) yielding energy values through the perturbation orders for any quantum state.

3.1.3 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. Our numerical results almost confirm this assumption. We have calculated low-lying energy levels of the anharmonic oscillator for several values, finding almost the same behaviour in all cases. Tables (3.5) and (3.6) 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 is obtained from the N value corresponding to the smallest oscillation amplitude. Such an accuracy cannot be obtained from the other perturbation series.

Table (3.5). 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 (3.6). Lowest eigenvalue 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

$$E_{n=0}^{exact} = 2.449174$$

3.2 Conclusion

We have shown [47] that the eigenvalues of quantum mechanical systems can be approximately obtained from the present formalism which is non-perturbative, self-consistent and sistematically improvable. Although we have limited ourselves to one illustrative example, the range of application of the method is rather large and and appears to be straightforward. The perturbation procedure here 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 vales of g for different quantum numbers does not imply special difficulty since the perturbed contributions merely follow from the solution of a linear system of equations of small order. Within this contex, we may for example recall that Hill determinants of orders as high as 100×100 are required [24] for large values of $g(g \approx 50)$ and that, when applying summation procedures, the calculations become more and more cumbersome as increases, because of the strong divergence of the coefficients in the Rayleigh-Schrödinger expansions. Furthermore, the remove of the singularities in the unperturbed wave function via the superpotential introduced in the present formalism does not cause tedious calculations which are difficult when dealing with excited states in LPT. Finally, although in this thesis we have focused only the calculations of eigenvalues for the quartic anharmonic oscillator, one can also find analytical solutions easily for the corresponding total wave function, through the use of Eqs. (2.4), (2.6), (3.2), (3.3).

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 competitive with other methods developed to deal with perturbation treatments. As a matter of fact , 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.

where the first piece is the zeroth order and shape invariant exactly solvable piece corresponding to the unperturbed potential with $V_0 = -A/r$ while ΔV is the perturbation term $\Delta V = A\alpha - (A\alpha^2/2)r + (A\alpha^3/6)r^2 - (A\alpha^4/24)r^3 + \ldots\ldots$ through the expansion of the exponential terms. Our careful calculations have clarified that the main contributions come from the first three terms. Hence, the present calculations are performed up to the second-order involving only these additional potential terms, which surprisingly provide highly accurate results.

4.1.1 Ground state calculations *(n=0)*

In the light of Eq. (2.7), the zeroth-order calculations leading to exact solutions can be carried out readily with the choice of a suitable $W_{n=0}$ yielding the Coulomb potential,

$$W_{n=0}(r) = -\frac{\hbar}{\sqrt{2m}}\frac{\ell+1}{r} + \sqrt{\frac{m}{2}}\frac{A}{(\ell+1)\hbar} \quad , \quad \varepsilon_n = -\frac{mA^2}{2\hbar^2(n+\ell+1)^2} \quad , \quad n=0,1,2,\ldots$$

$$(4.3)$$

$$\chi_n(r) = \left[\frac{2mA}{(n+\ell+1)\hbar^2}\right]^{\ell+1}\left(\frac{1}{n+\ell+1}\right)\frac{r^{\ell+1}}{\sqrt{\frac{\hbar}{mAn!}(n+2\ell+1)!}}\exp\left[-\frac{mA}{(n+\ell+1)\hbar^2}r\right]L_n^{2\ell+1}\left[\frac{2mA}{(n+\ell+1)\hbar^2}\right]$$

in which $L_n^\ell(r) = \sum_{m=0}^{n}\frac{\Gamma(n+\ell+1)(-r)^m}{(m+\ell+1)(n-m)!m!}$ is an associate Laguerre polynomial.

These analytical solutions are already exist in literature, providing a superiority to the present calculations. For the calculation of corrections to the zeroth-order energy and wavefunctions, one needs to consider the expressions leading to first- and second-order perturbation given by Eqs.(2.11) and (2.12). Multiplication of each term by χ_n^2 in these equations, and keeping in mind the relation

$$W_n = -\frac{\hbar}{\sqrt{2m}}\frac{\chi_n'}{\chi_n}$$ in Eq (2.6) , one can obtain general expressions for corrections in the first- order

$$\Delta\varepsilon_{n1} = \int\limits_{-\infty}^{\infty} \chi_n^2(r)\left(-\frac{A\alpha^2}{2}r\right)dr$$

(4.4)

$$\Delta W_{n1}(r) = \frac{\sqrt{2m}}{\hbar}\frac{1}{\chi_n^2(r)}\int\limits^{r}\chi_n^2(z)\left(\Delta\varepsilon_{n1}+\frac{A\alpha^2}{2}z\right)dz$$

and the second-order calculations are

$$\Delta\varepsilon_{n2} = \int\limits_{-\infty}^{\infty}\chi_n^2(r)\left[\frac{A\alpha^3}{6}r^2 - \Delta W_{n1}^2(r)\right]dr \;,$$

(4.5)

$$\Delta W_{n2}(r) = \frac{\sqrt{2m}}{\hbar}\frac{1}{\chi_n^2(r)}\int\limits^{r}\chi_n^2(z)\left[\Delta\varepsilon_{n2}+\Delta W_{n1}^2(z)-\frac{A\alpha^3}{6}z^2\right]dz \;,$$

for any state of interest. According to these formulas, we can calculate ΔW_{n1} and ΔW_{n2} when we know what the energy correction $\Delta\varepsilon_{n1}$ and $\Delta\varepsilon_{n2}$ are, from which the whole of the perturbed wevefunction can be calculated in a closed form by Eq. (2.6). It is also noted that the lower limit of the integration for energy caculations should be changed from $-\infty$ to 0 to accomodate the fact r that is always positive. Thus, the ground state calculations within the frame of Eqs. (4.4) and (4.5) give

$$\Delta\varepsilon_{01} = -\frac{\hbar^2(\ell+1)(2\ell+3)}{4m}\alpha^2 \;,$$

(4.6a)

$$\Delta\varepsilon_{02} = \frac{\hbar^4(\ell+1)^2(\ell+2)(2\ell+3)}{12Am^2}\alpha^3 - \frac{\hbar^6(\ell+1)^4(\ell+2)(2\ell+3)}{16A^2m^3}\alpha^4 \;,$$

$$\Delta W_{01}(r) = -\frac{(\ell+1)\hbar\alpha^2}{2\sqrt{2m}}r \;,$$

(4.6b)

$$\Delta W_{02}(r) = \frac{\left\{(\ell+1)\hbar\alpha^3 r\left[mAr+(\ell+1)(\ell+2)\hbar^2\left[3\alpha\hbar^2(\ell+1)^2-4mA\right]\right]\right\}}{24\sqrt{2m}(mA)^2}$$

The analytical expressions for the lowest energy and radial wavefunction of a Yukawa-type potential are then given by

$$E_{n=0} \approx \varepsilon_{n=0} + A\alpha + \Delta\varepsilon_{01} + \Delta\varepsilon_{02} ,$$

$$\psi_{n=0}(r) \approx \chi_n(r)\phi_n(r) , \qquad (4.7)$$

$$\phi_{n=0}(r) \approx \exp\left(-\frac{\sqrt{2m}}{\hbar} \int^r (\Delta W_{01} + \Delta W_{02})dz \right).$$

These explicit expressions support the similar works in [16, 40, 41]. Table (4.1) shows numerical values of the perturbed energies for a few values of n and α. The result obtained are compared with those of [16, 40, 41], together with the results of Rogers and his co-workers [38] who solved the Schrödinger equation numerically. Our results are in remarkably good agrement. Table (4.2) and (4.3) illustrate another comparison of our calculations with those of [41] who carried out their calculations in a different unit. These two different comparison make clear the sensitivity of present calculations although the procedures in [16 ,40, 41] to reproduce the corrections anallytically seem similar to ours. In particular, Table (4.2) clarifies that the present method is very useful one for large potential parameters (A), for which numerical solution of the Schrödinger equation is extremely difficult. Because, for a large strength the Yukawa potential is very deep and the wave function becomes very sharply peaked near the origin. This causes a great deal of difficulty in the numerical solution of the Schrödinger equation, which is reflected in the instability of the wavefunction thus obtained, although the energy eigenvalue is fairly stable and accurate.

4.1.2. Excited state caculations ($n \geq 1$)

The procedures leads to a handy recursion relations in the case of ground states, but becomes extremely cumbersome in the description of radial excitations when nodes of wavefunctions are taken into account , in particular during the higher order calculations. Although several attempts have been made to by pass this difficulty and improve calculations in dealing with excited states, e.g [16] within

the frame of supersymmetric quantum mechanics and, the related references therein regarding the Logarithmic Perturbation Theory, they have not resulted in simple algorithm. Therefore, as an another objective of this work, here an explicit treatment is introduced in within the frame of the present formalism and described a straightforword procedure for obtaining the perturbation corrections through handy recursion formula, having the same form both for ground and excited states.

Using our expertise due to our earlier calculations, the function W_n related to excited states can be calculated explicitly for the computation of perturbations expressed by (4.4) and (4.5). So, the first-order corrections in the first excited state (n=1) are

$$\Delta\varepsilon_{11} = -\frac{\hbar^2(\ell+4)(2\ell+3)}{4m}\alpha^2,$$

$$(4.8)$$

$$\Delta W_{11} = -\frac{(\ell+2)\hbar\alpha^2 r\left[A^2m^2r^2 - (\ell+1)(2\ell+5)\hbar^2 mAr + (\ell+1)^2(\ell+2)(\ell+4)\hbar^4\right]}{2\sqrt{2m}\left[Amr - (\ell+1)(\ell+2)\hbar^2\right]^2}.$$

However, higher-order calculations have singularity problems during the integrations because of the nodes appearing in ΔW_{11}. To remove this problem, we focus on a hidden relation in the above equation and with some confidence suggest that

$$\left[Amr - (\ell+1)(\ell+2)\hbar^2\right]^2 \approx \left[A^2m^2r^2 - (\ell+1)(2\ell+5)\hbar^2 mAr + (\ell+1)^2(\ell+2)(\ell+4)\hbar^4\right]$$

$$(4.9)$$

which transforms eq.(4.8) into

$$\Delta W_{11}(r) \approx \frac{(\ell+2)\hbar\alpha^2}{2\sqrt{2m}}r. \qquad (4.10)$$

Use of the approximate ΔW_{11} in Eq.(4.10) gives the energy correction in the second-order as

$$\Delta\varepsilon_{12} = \frac{\hbar^4(\ell+2)^2(\ell+7)(2\ell+3)}{12Am^2}\alpha^3 - \frac{\hbar^6(\ell+2)^2(\ell+7)(2\ell+3)}{16A^2m^3}\alpha^4. \qquad (4.11)$$

Therefore, the appoximate energy value of the Yukawa potential corresponding to the first excited state is

$$E_{n=1} \approx \varepsilon_{n=1} + A\alpha^2 + \Delta\varepsilon_{11} + \Delta\varepsilon_{12}. \qquad (4.12)$$

The related radial wavefunction can be expressed in an analytical form in the light of Eqs. (4.4), (4.5) and (4.7), if required.

One can easily check the similarities as in (4.9), between the terms of any $W_n = -\dfrac{\hbar}{\sqrt{2m}}\dfrac{\chi'_n}{\chi_n}$ of interest to by pass the nodal difficulty as in the first excited state. Our careful and exhausted investigations have revealed that the ratio between these similar terms in W_n for any state is approximately 1, which means, that the approximation used here would not affect considerably the sensitivity of the calculations. Furthermore, these investigations put forword interesting hiearachy between ΔW_{n1} terms of different quantum states in the first order, circumventing the nodal difficulties elegantly,

$$\Delta W_{n1} \approx \frac{(n+\ell+1)\hbar\alpha^2}{2\sqrt{2m}}r \qquad (4.13)$$

which, for example, for second excited state (n=2) leads to,

$$\Delta\varepsilon_{21} = -\frac{\hbar^2\left(2\ell^2+17\ell+27\right)}{4m}\alpha^2 ,$$

$$(4.14)$$

$$\Delta\varepsilon_{22} = \frac{\hbar^4(\ell+2)(\ell+3)^2(2\ell+23)}{12Am^2}\alpha^3 - \frac{\hbar^6(\ell+2)(\ell+3)^4(2\ell+23)}{16A^2m^3}\alpha^4 .$$

Calculations for higher excited states can be carried out in the same manner without employing tedious integrals, results of which are fairly in good agreement with the accurate numerical integration results, see tables (4.1) and (4.3), when compared to the other theoretical works. Finally, though the comparison of these results with those of [38] for large $n-$ and $\ell-$ values yields excellent results, we do not illusrate these tables here for clarity, which may be reproduced easily within the scheme described in this chapter.

Table (4.1). Energy eigenvalues of the Yukawa potential in units of $\hbar = m = 1$. For comparison, we set $A = \sqrt{2}$ and $\alpha = gA$

State	g	Present calculations	Ref[38] (exact)	Ref.[40]	Ref.[16]
1s	0.002	-0.99601	-0.9960	-0.99601	-0.9960
	0.005	-0.99004	-0.9900	-0.99004	-
	0.01	-0.98015	-0.9801	-0.98015	-0.9801
	0.02	-0.96059	-0.9606	-0.96059	-0.9606
	0.025	-0.95092	-0.9509	-0.95092	-
	0.05	-0.90363	-0.9036	-0.90363	-0.9036
2s	0.002	-0.24602	-0.2460	-0.24602	-0.2460
	0.005	-0.24015	-0.2401	-0.24015	-
	0.01	-0.23059	-0.2306	-0.23058	-0.2306
	0.02	-0.21230	-0.21230	-0.21229	-0.2124
	0.025	-0.20355	-0.2036	-0.20352	-
	0.05	-0.16351	-0.1635	-0.16325	-0.1650
2p	0.002	-0.24602	-0.2460	-0.24602	-0.2460
	0.005	-0.24012	-0.2401	-0.24012	-
	0.01	-0.23049	-0.2305	-0.23049	-0.2305
	0.02	-0.21192	-0.2119	-0.21193	-0.2120
	0.025	-0.20299	-0.2030	-0.20299	-
	0.05	-0.16144	-0.1615	-0.16155	-0.1625
3p	0.002	-0.10716	-0.1072	-0.10716	-0.1072
	0.005	-0.10142	-0.1014	-0.10142	-
	0.01	-0.09231	-0.09232	-0.09236	-0.09236
	0.02	-0.07570	-0.07570	-0.07563	-0.07611
	0.025	-0.06814	-0.06816	-0.06799	-
	0.05	-0.03739	-0.03712	-0.03486	-0.04236
3d	0.002	-0.10715	-0.1072	-0.10715	-0.1072
	0.005	-0.1014	-0.1014	-0.10137	-
	0.01	-0.09212	-0.09212	-0.09212	-0.09216
	0.02	-0.07502	-0.07503	-0.07504	-0.07531
	0.025	-0.06713	-0.06715	-0.06718	-
	0.05	-0.3388	-0.034383	-0.03477	-0.03736

Table (4.2). The same as in Table (3.1) , but $\hbar = 2m = 1$, $\alpha = fm^{-1}$ and $n = 0$

A	ℓ	Present calculations	Ref.[41] (Numerical)	Ref.[41](Analytical)
4	0	-3.2563	-3.2565	-3.2199
8	0	-14.4581	-14.4571	-14.4199
	1	-2.5830	-2.5836	-2.4332
16	0	-60.8590	-60.8590	-60.8193
	1	-12.9908	-12.9910	-12.8375
24	0	-139.2590	-139.2594	-139.2201
	1	-31.3937	-31.3938	-31.2385
	2	-11.5951	-11.5959	-11.2456

Table (4.3). The same as in Table (3.2), but $n \succ 0$

A	ℓ	n	Present Calculations	Ref.[41](Numerical)	Ref.[41](Analytical)
16	0	1	-13.0271	-13.0273	-13.0326
	0	2	-4.3937	-4.3720	-4.4057
	1	1	-4.3612	-4.3480	-4.3886
24	0	1	-31.4311	-31.4313	-31.4356
	0	2	-11.6992	-11.6998	-11.7093
	0	3	-5.0448	-5.0442	-5.0590
	0	4	-2.2194	-2.2033	-2.2237
	1	1	-11.6645	-11.6653	-11.6839
	1	2	-5.0133	-5.0135	-5.0541
	1	3	-2.1908	-2.1770	-2.2414
	2	1	-4.9504	-4.9516	-5.0085
	2	2	-2.1337	-2.1241	-2.2428

4.2 Concluding Remarks

In conclusion, a new useful technique for solving the bound state problem for Yukawa-type potentials within the frame of Riccati equation have been obtained and the comparison of calculation results with the accurate numerical values has been proven the success of the formalism. Avoiding the disadvantages of the standard non-relativistic perturbation theories, the present formula have the same simple form both for ground and excited states and provide, in principle, the calculation of the perturbation corrections up to an arbitrary order in analytical or numerical form.

Additionally, the application of the present technique to Yukawa potential is really of great interest leading to analytic expressions for both energy values and wavefunctions. Of particular importance is the apperance of ground state energy in a simple form. Comparing various energy levels with different works in the literature we feel that our analytic treatment quite reliable and further analytic calculation with this non-perturbative scheme would be useful. In particular, our method becomes more reliable as the potential strength increases while the numerical solution of the Schrödinger equation gets unstable and unreliable in calculating especially the wavefunction. Thus, the present method nicely complements the existing numerical methods.

Finally, it is noted that the present results can be extended easily to $N-$dimension with the consideration of the work in [42] by the replacement of the angular momentum term ℓ with $\Lambda = (M-3)/2$ where $M = N + 2\ell$.

CHAPTER 5

EQUIVALENCE OF TWO ALTERNATIVE APPROACHES

5.1 Introduction of the other model

It has been recently shown that the supersymmetric perturbation techniques [43] and other approaches [9, 10, 11] based logarithmic perturbation theory [2, 3, 4, 5] are involved within the more general framework of the novel formalism [17] discussed in this thesis , considering only non-exactly solvable potentials. Within this context, in this Chapter we go further and show that the present model also is entirely equivalent to the other significant approach [44] in the literature for exactly solvable Schrödinger equations. Before clarifying this point, the other model and its one application is briefly reviewed.

In their exposure to quantum mechanics in undergraduate courses in physics and chemistry, most students obtain a grounding in the solutions to exactly solvable model systems such as the hydrogen atom and the harmonic oscillator. While these are certainly essential for a student to know about, the manner of presentation often gets the sense that there are relatively few exactly solvable quantum mechanical systems, as well as the view that the mathematics involved in finding exact solutions is beyond their capabilities. Simple techniques permitting students to generate for themselves exactly solvable quantum mechanical potentials should hence be of general interest. Below, we outline one such method and apply it to generate a somewhat novel, exactly solvable quantum mechanical radial potential. The method essentially involves developing secondary differential equations from the differential equations solved by special functions by use of the chain rule, and finding their solutions. These solutions then determine the form of the solvable potential, as well as the allowed energy eigenvalues and the variables appearing in the wavefunctions.

5.1.1 Generation of solvable potentials from special functions

In the following, we shall adapt the notation and approach used by Levai [44]. Many of the special functions $F(g)$ of mathematic, including orthogonal polynomials, represent solutions to differential equations of the form

$$\frac{d^2 F(g)}{dg^2} + Q(g)\frac{dF(g)}{dg} + R(g)F(g) = 0 \tag{5.1}$$

where the functions $Q(g)$ and $R(g)$ are defined for a particular function. The form of this differential equation can be compared to that of a single variable Schrödinger equation

$$\frac{d^2\psi}{dx^2} + (E - V(x))\psi(x) = 0 \tag{5.2}$$

where atomic units have been adopted such that $h=2m=1$. Wiriting wavefunction solutions to (5.2) in the form $\psi(x) = f(x)F(g(x))$, applying the chain rule and equating like terms between the resulting expression and (5.1) results in the equalities

$$\frac{g''}{(g)^2} + \frac{2f'}{g'f} = Q(g(x)) \tag{5.3}$$

and

$$\frac{f''}{f(g')^2} + \frac{E - V(x)}{(g')^2} = R(g(x)). \tag{5.4}$$

This permits representation of the term $E - V(x)$ in several ways, when both (5.3) and (5.4) are considered simultaneously:

$$E - V(x) = (g')^2 R(g(x)) - f''/f$$

$$= (g')^2 R(g(x)) - (f'/f)^2 - (f'/f)' \tag{5.5}$$

$$= (g')^2 \left[R(g) - \frac{1}{2}\frac{dQ}{dg} - \frac{1}{4}Q^2(g(x)) \right] + \frac{g''}{2g'} - \frac{3}{4}\left[\frac{g''}{g'}\right]$$

$$= (g')^2 \left[R(g) - \frac{1}{2}\frac{dQ}{dg} - \frac{1}{4}Q^2(g(x)) \right] + \left[\frac{g''}{2g'}\right] - \left[\frac{g''}{2g'}\right]^2.$$

Now, whenever g' can be found such that one of the terms on the right becomes a real constant repesenting the energy and the remaining terms become independent of any quantum number, a solvable quantum mechanical potential results. Specifically, whenever 'secondary' differential equations of the forms

$$(g')^2 R(g) = C$$

$$(g')^2 \left[\frac{dQ}{dg} \right] = C \qquad (5.6)$$

$$(g')^2 (Q(g))^2 = C \text{ , etc}$$

can be solved (where C is a real constant) solvable potentials $V(x)$ are possible. Often, since special functions solving equations of the form (5.1) are defined by integral indices which become quantum numbers, some algebraic manipulation is usually reguired in order to remove any dependence of a specific potential $V(x)$ on the index. Such manipulation determines the sipecific mathematical form of the energy eigenvalues. The Jacobi, Laguerre, and Hermite polynomials represent examples where several different types of exactly solvable potentials have been derived using this approach, including many of the better known model potentials [44].

5.1.2 Application of the method: an attractive radial potential

Solutions to the differential equation

$$\frac{d^2 F(g)}{dg^2} + \left[\frac{(n+\alpha)^2}{1-g^2} + \frac{2+4\alpha-4\alpha^2+g^2}{4\left(1-g^2\right)} \right] F(g) = 0 \qquad (5.7)$$

are given in terms of the Gegenbauer polynomials $C_n^\alpha(g(r))$ by

$F(g(r)) = \left(1-g^2\right)^{\left(\alpha+\frac{1}{2}\right)/2} C_n^\alpha(g(r))$ [46]. Multiplying the numerator and denominator of the first non-derivative term in (5.7) by $4\left(1-g^2\right)$ and defining $R(g)$ as in (5.1) gives

$$R(g) = \left[\frac{4(n+\alpha)^2 + 2 + 4\alpha - 4\alpha^2}{4\left(1-g^2\right)^2} + \frac{\left(1-4(n+\alpha)^2 g^2\right)}{4\left(1-g^2\right)^2} \right]. \tag{5.8}$$

Derivation of solvable potential requires that one of the terms in (5.8) becomes a real constant representing the energy E when multiplied by $(g')^2$. This gives two secondary differantial equations:

$$(g')^2 / \left(1 - g^2\right)^2 = C,$$

$$(g')^2 g^2 / \left(1 - g^2\right)^2 = C \quad (C{=}\text{constant}). \tag{5.9}$$

Solutions to the first differantial equations give a type of potential previously derived for Jacobi polynomials by Levai [44], as the Gegenbauer polynomials can be represented by Jacobi polynomials. We choose the other one leading a solution $g(r) = (1 - \exp(2ar))^{1/2}$ and results in a somewhat novel radial potential.

To complete derivation of this solvable potential, it is also necessary to remove any dependence of the potential $V(x)$ on the polynomial index n, which becomes the quantum number. For the choice of $g(r)$ above, this means that any dependence on n be removed from the first term of the right in (5.8). This accomplished by requiring that

$$4(n + \alpha)^2 + 2 + 4\alpha - 4\alpha^2 = A, \tag{5.10}$$

where A is a real constant. Expansion this polynomial results in the expression

$$\alpha = \frac{A - 2 - 4n^2}{8n + 4} \tag{5.11}$$

and ultimately the energy E for this solvable potential is given by

$$E = \left(a^2/4\right)\left(1 - 4(n + \alpha)^2\right) \tag{5.12}$$

$$= \left(a^2/4\right)\left[1 - 4\left[\frac{n^2 + n + (A-2)/4}{2n+1}\right]^2\right].$$

The corresponding potential energy $V(r)$ and unnormalized wavefunctions $\psi(g(r))$ are then given by

$$V(r) = \left[\frac{g''}{2g'}\right]^2 - \left[\frac{g''}{2g'}\right] - \frac{a^2 A}{4g^2}$$

$$= \left(a^2/4\right)\left[\frac{g^4 + (6-A)g^2 - 3}{g^4}\right] \tag{5.13}$$

$$= \left(a^2/4\right)\left[\frac{\exp(-4ar) + (A-8)\exp(-2ar) + (4-A)}{(1-\exp(-2ar))^2}\right]$$

and

$$\psi(g(r)) \propto (g')^{-1/2}\left(1 - g^2\right)^{(\alpha+1/2)/2} C_n^\alpha(g) \tag{5.14}$$

$$= (1 - \exp(-2\alpha r)) - 1/4\exp(-(\alpha-1/2)ar) \times C_n^\alpha\left((1 - \exp(-2\alpha r))^{1/2}\right).$$

The boundary conditions $\psi(r = 0) = 0$ and $\psi(r = \infty) = 0$ for a radial potential are met by requiring that $\alpha > \frac{1}{2}$.

The parameter α, besides meeting the requirement that $\alpha > \frac{1}{2}$, has complitated dependence on the parameter A and the quantum number n. These conditions imply that there are no eigenstates for the potential $V(g(r))$ unless $A > 4$ and that relatively few eigenstates are allowed for even large values of the parameter A.

5.1.3 Superpotentials and supersymmetric quantum mechanics

The method described above has an immediate application in the emerging area of supersymmetric quantum mechanics. An accesable introduction to the general theory is given by Dutt et al [45]. Brifly, in supersymmetric quantum mechanics two one-dimensional Hamiltonian partners $H\_$ and H_+ can written as

$$H_\pm = -\frac{d^2}{dx^2} + V_\pm(x) \tag{5.15}$$

where $V_-(x)$ and $V_+(x)$ are expressed in terms of a superpotential $W(x)$ such that

$$V_\pm(x) = W^2(x) \pm W'(x). \tag{5.16}$$

The energy eigenvalues of H_- and H_+ are identical, except for the ground state, where $E_{n=0}^- = 0$ and eigenfunctions of each Hamiltonian are connected through operators related to the factorization of the Hamiltonians.

Comparison of (5.16) with the expressions in (5.5) shows an immediate connection. With the defination

$$W(x) = -\left(\ln(f(x))\right)' \tag{5.17}$$

the term $E - V(x)$ can be expessed as

$$E - V(x) = (g')^2 R(g) - (W(x))^2 + (W(x))' \tag{5.18}$$

and whenever $R(g) = 0, E = 0$ for a potential $V_-(x)$ defined by the superpotential $W(x)$. The function $f(x)$ can be determined from (5.3) by

$$f(x) = (g')^{-1/2}\left[\exp\left(\frac{1}{2}\int^g Q(z)dz\right)\right] \tag{5.19}$$

or from the ground state eigenfunction when $F(g(x))_{n=0}$ is a constant. Since the form of $R(g)$ in (5.1) is such that $R(g) = 0$ when the polynomial index $n = 0$ for many orthogonal polynomials, this observation permitted the facile generation of the superpotentials associated with the solvable potentials described earlier by Levai in 1989 [44].

Superpotentials defined by

$$W(g(x)) = \left[\frac{-g''}{2g'}\right] \tag{5.20}$$

are also possibilty whenever g' can be found such that

$$(g')^2\left[R(g) - \frac{1}{2}\frac{dQ}{dg} - \frac{1}{4}Q^2(g(x))\right] = 0 \qquad (5.21)$$

when the polynomial index $n = 0$.

5.1.4 Conclusion

A simple method [44] for generating exactly solvable, single variable Schrödinger equation based on the special functions solving second-order linear ordinary differantial equations has been reviewed. Application of this method in the case of a differantial equation related to the Gegenbauer polynomials results in generation of an exactly solvable radial potential, and the quantum mechanical supersymmetric superpotential for this solvable potential can also be easily derived. The relative mathematical case with which this method can be applied, as well as its relationship to the developing area of supersymmtric quantum mechanics, should make it of use to both teachers and students of introductory and intermediate quantum mechanics.

Now, the equivalence of both models, the one introduced in this Chapter and other used through the thesis work, is discussed in detail below for analytically solvable potentials.

5.2. Equivalence of two models

The substitution of $\Psi(x) = f(x)F[g(x)]$ in the one-dimensional time-independent Schrödinger equation

$$-\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x) \quad , \qquad (5.22)$$

leads to the second-order differential equation

$$\frac{f''}{f} + \frac{F''g'^2}{F} + \frac{g''F'}{F} + 2\frac{F'g'f'}{Ff} = V - E . \qquad (5.23)$$

Splitting the equation in two parts as have done earlier in our calculations one gets

$$W^2(x) - W'(x) = V_0(x) - \varepsilon \quad , \quad W = -\frac{f'}{f} , \qquad (5.24)$$

and

$$\Delta W^2(x) - \Delta W'(x) + 2W(x)\Delta W(x) = \Delta V(x) - \Delta E \quad , \quad \Delta W = -\frac{F'g'}{F} \quad , (5.25)$$

where $E = \varepsilon + \Delta E$ and $V = V_0 + \Delta V$. Eqs. (5.23) and (5.24) are the concrete proof of the equivalence between the two alternative models.

Afterall, it can be clearly seen that Eq. (5.24) is the one required for obtaining an explicit expression for W term corresponding to exactly solvable systems in one-dimension. However, to proceed further, the functions f and g should be solved as F, Q and R are known in principle. Now, equating like terms between the resulting expression in (5.22) and (5.1) gives

$$Q[g(x)] = \frac{1}{g'}\left(\frac{g''}{g'} + \frac{2f'}{f}\right) \quad , \quad R[g(x)] = \frac{1}{g'^2}\left[\frac{f''}{f} + (E - V)\right] \quad , \qquad (5.26)$$

where, from the definition of Q,

$$f(x) \approx (g')^{-1/2} \exp\left[\frac{1}{2}\int^{g(x)} Q(g)dg\right] . \qquad (5.27)$$

Consideration of Eqs. (5.23) through (5.26) suggests a novel prescription

$$\Delta V(x) - \Delta E = -g'^2 R(g) \quad , \qquad (5.28)$$

which, for R functions, provides a reliable expression for $g(x)$. Though the both model of interest seem different, in fact they are entirely equivalent as clarified within the frame of the present unified formalism to solve underlined problems in physics.

CHAPTER 6

GENERAL CONCLUSION

Within the powerful framework of a novel approach introduced recently [17], we have solved successfully significant problems of physics. This investigation confirms once more the reliability and usefulness of the model for both exactly and non-exactly solvable Schrödinger equations.

The search of anharmonic oscillator potential in the light of a perturbative treatment of the technique has shown flexibility of the formalism by the comparison of the results obatined at different orders with those of a numerical integration work. In addition, large order calculations have made clear rapid convergence of the calculations. The algebraic closed expressions obtained for the energy values and wave functions at ground and higher excited states are found in well agreement with the others in the literature.

Application of the approach to Yukawa type potentials justifies the sensitivity of the calculations through the method for approximately solvable Schrödinger equations. The comparison of our calculation results with those of other techniques put forwards the superiority of the formalism within its elegant algebraic framework.

Finally, we have proven that the prescription used through the present thesis work is entirely equivalent to the other well known approach in the literature for exactly solvable Schrödinger equations. The two methods have been unified to perfect the calculations removing deficiency of each other.

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