THE UNIVERSITY OF HULL

PERTURBATION AND NON-PERTURBATION NUMERICAL CALCULATIONS TO COMPUTE ENERGY EIGENVALUES FOR THE SCHRÖDINGER EQUATION WITH VARIOUS TYPES OF POTENTIAL

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ABSTRACT

The present work is concerned with methods of finding the energy eigenvalues of the one-particle Schrödinger equation for various model potentials in one, two, three and N-dimensional space. One major theme of this thesis is the study of divergent Rayleigh-Schrödinger perturbation series which are encountered in non-relativistic quantum mechanics and on the behaviour of the series coefficients E(n) in the energy expansion $E(\lambda)=E(0)+\sum E(n)\lambda^{n}$. Several perturbative techniques are used. Hypervirial and Hellmann-Feynman theorems with renormalised constants are used to obtain perturbation series for large numbers of potentials. Padé approximant methods are applied to various problems and also an inner product method with a renormalised constant is used to calculate energy eigenvalues with very high accuracy. The non-perturbative methods which are used to calculate energy eigenvalues include finite difference and power series methods. Expectation values are determined by an approach based on eigenvalue calculations, without the explicit use of wave functions. The first chapter provides a glance back into history and a preview of the problems and ideas to be investigated. Chapter two deals with one dimensional problems, including the calculation of the energy eigenvalues for quasi-bound states for some types of perturbation (λx^{2n+1}). Chapter three is concerned with two, three and N-dimensional problems. Chapter four deals with non-polynomial potentials in one and three dimensions. The final chapter is devoted to a variety of eigenvalue problems. Most of the energy eigenvalues are computed by more than one method with double precision accuracy, and the agreement between the results serves to illustrate the accuracy of the methods.

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CHAPTER ONE

Introduction

1.1 Introductory remarks

The aim of this work is to use numerical techniques to compute the energy eigenvalues for one-particle Schrödinger equations in one, two, three and (N=1,2,3,4,.....1000) dimensions, for a large number of potentials with different forms, as we shall see later. We face convergence difficulties in dealing with perturbation methods. However, there are an extensive range of techniques in the mathematical literature to deal with divergence problem e.g renormalised series, Padé approximants and the Aitken procedure. We wish to point out that we overcome the convergence problem, to ensure that our results are correct. by using the renormalised constant (K) which is given in the review of Killingbeck [12,1980;14,1982]. The renormalization constant (K) plays an important role in the convergence aspects of the calculations which are investigated in this work. Also, Padé approximants and the Aitken procedure have been used to calculate the energy eigenvalues for some problems. The results are compared with those produced by different methods which can be used to calculate energies for the same perturbed potentials.

1.2 Summary of selected previous and present work for chapter two

Bender and Wu [1,1969] have calculated 75 terms of the ground state energy perturbation series for the 2N=4 case of the anharmonic oscillator defined by the Hamiltonian

$$H=P^2+\mu x^2+\lambda x^{2N} \quad (2N=4,6,8,10,10...18,20 \ ; \ \mu=0,1) \qquad (1.1)$$

However, Simon [2,1970] has studied the analytic properties of the energy series for (2N=4) and its Padé approximants. Biswas, et. al. [3,1973] have calculated the ground state and the excited state energies for power (2N=4,6,8) by using a non-perturbative method (Hill determinants). Banerjee [4,1978] calculated energy levels for the (2N=4,6,8) cases, for high state number ($0 \leq n \leq 1000$). Also J.E. Drummond [5,1981] used 25 terms of the perturbation series to calculate the first five energy levels. G.Schiffrer and D. Stanzial [7,1985] treat the Schrödinger equation to calculate energy eigenvalues using a gradient method, for perturbation power index (2N=6,8,10,12); they give results with high accuracy (more than 20-digits). Killingbeck [8,9,10,11,12,13,14,15,16] presented a number of works using many perturbative and non-perturbative numerical methods which give results of very high accuracy. In chapter two, the hypervirial theorem and Hellmann-Feynman theorem are used to obtain energy eigenvalues and expectation values for the harmonic oscillator with λx^{2N} perturbing potential. We have also used non-perturbative methods, the finite difference method and the power series method, to calculate the energy eigenvalues for perturbations with high N values (2N=4,6,8,10....18,20). Some typical results are listed in tables (2.1,2.2,2.3,2.4).

Also the problem of quasi-bound states is considered for the Hamiltonians given below:

$$H=P^2+x^2+\lambda x^3 \qquad (1.2)$$

$$H=P^2+x^2+\lambda x^5 \tag{1.3}$$

$$H=P^2+x^2-\lambda x^4 \tag{1.4}$$

J.E. Drummond [5,1981;6,1982] used 11 to 20 terms of the perturbation series to calculate the first six energy levels for (1.2) and (1.4). The energy eigenvalues have been calculated here by renormalised series for (1.2) and (1.4), and Padé approximants for (1.3). Our results are in good agreement with those given in ref [5,1981]; our results are reported in tables (2.5,2.6,2.7).

R.Balsa, et. al [17,1983] used a non-perturbative method which involves matrices to calculate the energy eigenvalues for a double well Potential. R.M. Quick and H.G.Miller [18,1984] also computed the energy eigenvalues for a double well potential by a matrix method . In our case we investigate their double well potential with the Hamiltonian

$$H=P^2-Z^2x^2+x^{2N} \quad (2N=4,6,8,10,12..26,28,30....) \tag{1.5}$$

but for a wider range of the potential parameters and state numbers. The renormalised series work well in computing the eigenvalues even for high values of $(Z^2\ ,2N)$ and state number n. We also use power series and finite difference methods, and show how the accuracy in the calculated energy depends on the choice of the strip width h in the finite-difference method. It is shown how to get a projected energy eigenvalue by means of an extrapolation process in the quantity h^2. Many of our results are not reported previously in the literature, so we made many checks. The results are shown in tables (2.8 to 2.13).

1.3 Summary of selected previous and present work for chapter three

Perturbation problems in two and three dimensions have been studied less often than one-dimensional problems. Hioe, et. al [19,1978] have studied the two dimensional problem:

$$H=-\frac{1}{2}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]+\mu\left[x^2+y^2\right]+\lambda\left[a_{11}x^4+2a_{12}x^2y^2+a_{22}y^4\right] \qquad (1.6)$$

They have calculated the energy eigenvalues by using matrix diagonalistation for different values of the perturbation parameters ($a_{11}, a_{22}, a_{12}, \lambda$), and different values of state numbers ($n_1=n_2=0,1,2,3$). Nasit and Metin [20,1985] applied a characteristic function approach, and used Padė approximant methods to compute energy eigenvalues for different values of the potential parameters, comparing their results with those in ref [19,1978], J.Killingbeck and M.N.Jones [21,1986] used an inner product method to calculate the accurate energies for six states $E_{0,0}, E_{1,1}, E_{0,2}, E_{2,0}, E_{1,3}, E_{3,1}$ and three different values of (a_{11}, a_{22}, a_{12}). The convergence of the perturbation series depends upon the choice of the value of a renormalised constant K. In the present work inner product, renormalised series and power series methods are applied to calculate the energy eigenvalues of a two dimension perturbed oscillator for various values of (a_{12}, a_{22}, a_{21}), ($0.05 \le \lambda \le 5000$) and state numbers ($n_1, n_2=0,1,2,3$).

For three and N dimensional problems Killingbeck [22,1985] used a Hill determinant method to calculate the energy eigenvalues for a perturbed oscillator for high values of angular momentum ℓ. The Hamiltonian used was

$$H(r)=-\nabla^{2}+\mu r^{2}+\ell(\ell+1)r^{-2}+\lambda r^{2M} \qquad (2M=4,6,8) \qquad (1.7)$$

Killingbeck also calculated the energy eigenvalues for s-states (ℓ=0) in (N=1,2,3,24,5,...320) dimensions using the Hamiltonian

$$H_{N}(r)=-D^{2}+\mu r^{2}+\frac{1}{4}\left[[N+2\ell-3][N+2\ell-1]\right]r^{-2}+\lambda r^{4} \qquad (1.8)$$

The energy eigenvalues for (1.7) and (1.8) have been computed by us for power series and renormalised series methods. The energy eigenvalues for (1.7) and (1.8) obtained by these methods are in good agreement with each other, and with available results reported in the literature.

1.4 Summary of selected previous and present work for chapter four

Mitra [23,1978] calculated the ground states and first two excited states (2N=2) for the perturbed Hamiltonian:

$$H=P^{2}+x^{2}+\frac{\lambda x^{2N}}{(1+gx^{2})} \qquad (2N=2,4,6,8,10..18,20) \qquad (1.9)$$

He used the Ritz variational method in combination with the Givens-Householder algorithm for numerical computations. Galicia and Killingbeck [24,1979] give a simple numerical finite difference method to calculate the energy eigenvalues for the three lowest even parity states. Kaushal [25,1979] has obtained the asymptotic expansions for the eigenenergies and eigenfunctions of the wave function for the potential given by (1.9) by expanding the factor $1/(1+gx^{2})$ as a power series in gx^{2}. Bessis and Bessis [26,1980] have studied the same problem by taking advantage of a two parameter (λ and g) scale transformation, and Hautot [27,1981] has used a Hill determinant method for the potential. Lai and Lin [28,1982] have applied the Hellmann-Feynman theorem and hypervirial theorem to obtain the perturbation series for the energy eigenvalues; they have employed the Padé approximant method to sum the energy series. Their results, however, require the asymptotic expansion of the factor $1/(1+gx^2)$ as a power series in gx^2, which is valid for low values of $g\leq2$ only. On the other hand, V.Fack and Vanden Berghe [29,1985] used a finite difference method in combination with matrix diagonalisation for numerical computation, and transformed the Schrödinger equation into an algebraic eigenvalue problem involving special forms of matrix. They calculated the energy eigenvalues for various values of g and λ and strip width h and compared their results with those of [28,1982]. This problem has received great attention from us, and we used perturbative and non-perturbative methods to attack the problem. We determined the energy eigenvalues for various values of the state number (n), and over a wide range of values of λ,g and power index (2N=2,4,6,..18,20).

G.Auberson [30,1982], G.Auberson and Boissiere [31,1983] studied numerically and analytically the energy levels of a one dimensional oscillator:

$$H=\frac{1}{2}P^2+\frac{1}{2}x^2\pm\frac{gx^{2N}}{(1+g\alpha x^2)} \qquad (2N=4,6) \qquad (1.10)$$

They used various methods to calculate the ground state energy eigenvalues for different values of g and α, for the case 2N=4. We calculate in the present work energies for the ground state and many excited states, for different values of g and α and for (2N=4,6), using the renormalised series and finite difference methods. The results are compared in tables (4.7 to 4.14) On the other hand, it is interesting to point out that the one dimensional problems (1.9) and (1.10) can be extended to the three dimensional form

$$H=-\frac{d^2}{dr^2}+r^2+\ell(\ell+1)r^{-2}+\frac{\lambda r^2}{(1+gr^2)} \qquad (1.11)$$

$$H=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{1}{2}r^2+\frac{\ell}{2}(\ell+1)r^{-2}\pm\frac{gr^4}{(1+g\alpha r^2)} \qquad (1.12)$$

The numerical results obtained for (1.11) and (1.12) by perturbative method agree with those obtained by a nonperturbative method and the results are listed in tables (4.15,4.20). Our methods for the non-polynomial potential allow us to study the numerical behaviour of the energy levels for (2N=2,4,6...18,20), and many λ,g and state number values, at the same time comparing the results with those for the ordinary anharmonic oscillator g=0, which has been studied in chapter two.

1.5 Summary of selected previous and present work for chapter five

Praddaude [32,1972] calculated the 14 lowest-energy levels of hydrogen atoms in a magnetic field, using the Hamiltonian

$$H= \frac{1}{2}P^2-r^{-1}+ \frac{1}{2}\gamma\ell_z + \frac{1}{8}\gamma^2\left[x^2+y^2\right] \qquad (1.13)$$

assuming an appropriate expansion of the wave function in terms of Laguerre polynomials and solving the Schrödinger equation in cylindrical coordinates using a matrix variational method. The results of Praddaude are in good agreement with those of our calculation (described later) shown in table (5.2). The calculations of Gallas [34,1984] involve variational estimates of eigenvalues for first 13 states. Killingbeck [33,34] investigated the problem of the hydrogen quadratic Zeeman effect using several techniques (power series, renormalised series and finite difference methods) to calculate the energy eigenvalues and the expectation values $\langle r^N\rangle$ N=1,2,3 for different states. Killingbeck [36,1987] treated the hydrogen atom in a magnetic field by using simple basis functions, such that the Schrödinger eigenvalue equation is transformed into a recurrence relation, which gives accurate energy levels when solved by a new shooting-relaxation technique. In the present work we use renormalised series to calculate energy eigenvalues for 30 states in magnetic field strengths ($0.005\le\gamma\le0.01$), and energies and expectation values $\langle r^N\rangle$ in magnetic field strength $\gamma=0.1$ for 14 states. The renormalised series gives very good accuracy even for high excited states. The results are listed in tables (1.5 to 5.5).

In section (5.2) we investigated the problem of the Yukawa potential:

$$H= -\frac{1}{2}\nabla^2+\frac{\ell}{2}(\ell+1)r^{-2}+Zr^{-1}e^{-\lambda r} \qquad (1.14)$$

M.Grant and C.S.Lai [37,1979] have applied the hypervirial relations with the Hellmann-Feynman theorem to study screened Coulomb potentials. They calculated (K,L,M) shell binding energies for different values of Z ($2\leq Z\leq 50$), using power series in λ up to order λ^{20}, Lai [38,1984] studied the problem of the Yukawa potential by using the hypervirial-Padé scheme for various eigenstates for Z=1, and found that the [6,6] and [6,7] Padé approximants to the energy series can account for various energy eigenvalues to a very high accuracy. Edward. R. Vrscay [39,1986] developed a simple power series method to calculate to high order the Rayleigh-Schrödinger perturbation expansions for energy levels of a Yukawa-type screened coulomb potential. He produced results to very high accuracy (20-digits) for 1s,2s and 2p states. In the present work we attacked this problem by using renormalised series, and performed our calculation for many eigenstates. The renormalised series yields energy eigenvalues with excellent accuracy (more than 15-digits), the results being listed in tables (5.6,5.7,5.8).

Bessis, et. al [40,1982] have computed the bound state energies of the Gaussian potential.

$$H= -\frac{d^2}{dr^2}+\ell(\ell+1)r^{-2}-Ae^{-\lambda r^2} \qquad (1.15)$$

using a perturbational and variational treatment on a conveniently chosen basis of transformed Jacobi functions.

They have calculated the energy eigenvalues for different values of the quantum numbers (ℓ,n). C.S.Lai [41,1983] calculated the bound state energies of the same potential for various eigenstates (ℓ,n=0 to 7) by using the Hypervirial-Padé scheme. Also Chatterjee [42,1985] has applied the method of 1/N expansion to obtain the bound state energy levels of a Gaussian potential. The method of 1/N expansion yields energy values which are in good agreement with those results which are available in the literature. In this work, we used the hypervirial method to calculate the energy eigenvalues for various bound states. We extended our calculation to high excited states ($0\le\ell\le12$) and ($0\le n\le7$), and our method achieved 20-digit accuracy. Such a high degree of precision has not been obtained before by any other method. The results are shown in tables (5.9).

Killingbeck [43,1977] attacked the problem of the perturbed hydrogen atom with Hamiltonian

$$H= - \frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{2}\ell(\ell+1)r^{-2} - r^{-1} + \lambda r \qquad (1.16)$$

by using non-perturbative methods (finite difference methods) to calculate the energy eigenvalues. In a subsequent paper Killingbeck and Galicia [44,1980] used hypervirial relations together with the Hellmann-Feynman theorem to get the energy coefficients of the energy perturbation series. Lai and Lin [45,1981] calculated the energy eigenvalues of various eigenstates, by applying the hypervirial-Padé framework. Austin and Killingbeck [46,1982] calculated the energy eigenvalues with very high accuracy by using renormalised series. We calculated the energy eigenvalues for this problem by using power series, finite difference and renormalised series methods. The results produced by these methods are in good agreement with each other. The results are listed in table (5.10). The ground state of the s-wave Hamiltonian for a hydrogen atom with a polynomial perturbation

$$H=\frac{1}{2}P^{2}-r^{-1}+2\lambda r+2\lambda^{2}r^{2} \qquad (1.17)$$

has been studied by Killingbeck [47,1978;48,1980]. He pointed out that the system possesses an exact solution for the ground state energy and wavefunction for $\lambda > 0$ given by

$$E= -\frac{1}{2}+3\lambda \qquad (1.18)$$

$$\Psi(r)= e^{-(r+\lambda r^{2})} \qquad (1.19)$$

while for $\lambda<0$ the potential has bound states but their energy differs from (1.18). R.P.Saxena and V.S.Varma [49,1982 ;50,1982] studied the same system and gave the exact solutions

$$E_{n}= -\frac{1}{2}+\left(2n+3\right)|\lambda| \qquad (1.20)$$

which hold only for special values of the parameter λ. Cohen and Herman [51,1982] listed results for $(-0.2\le\lambda\le-20480)$ by using a variational modification of Rayleigh-Schrödinger perturbation theory. We used renormalised series and finite difference methods to calculate the eigenvalues for the Hamiltonian given by (1.17). Our results are in good agreement with those in the references mentionedabove; the results are reported in tables (5.11,5.12).

The exponential cosine screened coulomb [ECSC] potential with Hamiltonian

$$H= \frac{1}{2}P^{2}+ \frac{1}{2}\ell(\ell+1)r^{-2}- r^{-1}e^{-\lambda r}\, \mathrm{Cos}(\lambda r) \qquad (1.21)$$

has been treated by several approximate methods. Aparna and Pirtam [52,1980] applied the generalized virial theorem and Hellmann-Feynman theorem to calculate perturbatively the bound state energy levels without using a perturbed wavefunction. C.S. Lai [53,1982] has calculated the energy eigenvalues of (1.21) for various eigenstates within the framework of the hypervirial-Padé scheme. We used renormalised series to calculate the energy eigenvalues for various states and different values of screening parameter. Our method yields 15-digits accuracy, and the results are given in table (5.13). C.S.Lai and W.Lin [54,1980] have applied the Padé approximant technique to perturbation series obtained through the use of hypervirial and Hellmann-Feynman theorems. They computed the energies of 2p,3p,4p,4d and 4f states.

R.Dutt and U.Mukherji [55,1982] proposed a new approximation scheme to obtain analytic expressions for the bound-state energies and eigenfunctions for any arbitrary bound (ℓ,n)-state of the Hulthen potential.

$$H=\frac{1}{2}P^{2}+ \frac{\ell}{2}(\ell+1)r^{-2}-\lambda\left[\frac{e^{-\lambda r}}{1-e^{-\lambda r}}\right] \qquad (1.22)$$

They compared their results with those given in ref

[22,1982]. We used the renormalised series to calculate the energy eigenvalues for (1.22) for various values of λ and for high excited states (2p to 8h). The renormalised series give high accuracy (15-digits).

Finally, we calculated the energy eigenvalues for potentials in (one and three dimension):

$$H= P^2+ x^2 - 2\left[\frac{e^{-2\lambda x^2}}{1+ e^{-2\lambda x^2}}\right] \tag{1.23}$$

$$H= P^2+ r^2+ \ell(\ell+1)r^{-2} - 2\left[\frac{e^{-2\lambda r^2}}{1+ e^{-2\lambda r^2}}\right] \tag{1.24}$$

We used Padé approximant and the hypervirial method to compute the energy eigenvalues for different values of λ and excited states (n=0 to 5). The results are reported in tables (5.15,5.16).

CHAPTER TWO

ONE-DIMENSIONAL MODEL PROBLEMS

2.1 Numerical calculation for $H=P^2+\mu x^2+\lambda x^{2N}$ (2N=4,6,8,10..18,20)

2.1.1 Introduction

The investigation of eigenvalues has long been a fruitful and active field of research, and a variety of techniques have been employed to calculate energy eigenvalues. In many kinds of eigenvalue problem one wishes to improve the accuracy of results obtained by previous methods, so we have tried to obtain eigenvalues of high accuracy. For purpose of clarity, this chapter is divided into four sections. Section one is concerned with the eigenvalue problem defined by the Hamiltonian (2.1), section two is concerned with the eigenvalue problems defined by (2.42,2.43,2.44), section three is concerned with the double well potential defined by (2.63) and section four is concerned with the expectation value calculation. In section one we would like to discuss the eigenvalue problem of the general anharmonic oscillator, described in the one-dimensional case by the Hamiltonian:

$$H=P^2+\mu x^2+\lambda x^{2N} \qquad (2N=4,6,8,\ldots 18,20) \qquad (2.1)$$

The one-dimensional anharmonic oscillator has been studied intensively in the past by various authors using several powerful methods. The most studied system of this kind is the quartic anharmonic oscillator (2N=4). Bender and Wu [1,1969] have calculated 75 terms of the ground state energy series. Simon [2,1970] has studied the analytic properties of the series and its Padé approximants. Biswas et. al [3,1973] have calculated energies of the ground state and the first seven excited states for 2N=4 as well as energies of the ground state and first excited state for N=3,4, for λ values between $(0.1\leq\lambda\leq100)$, using Hill determinants. Banerjee [4,1978] calculated energy levels for 2N=4,6,8 for $(10^{-5}\leq\lambda\leq4\mathrm{x}10^{4})$. Drummond [5,1981] used 25 terms of the perturbation series to calculate the first five energy levels. G.Schiffrer and D.Stanzial [7,1985] have reported excellent numerical results of energy calculations for the ground state and first excited state for 2N=6,8,10,12 and $(10^{-6}\leq\lambda\leq10^{6})$ by using a gradient method. Killingbeck [8,9,10,11,12,13,14,15,16] presented several works using many perturbative and non-perturbative numerical methods which give results of high accuracy. We extended our calculated results to higher values of the index N $(\lambda x^{2N}$, 2N=14,16,18,20). In spite of the high value of 2N, our methods (non-perturbation methods) are still capable of handling this perturbation. We use three methods to calculate energy eigenvalues for the λx^{2N} perturbation.

2.1.2 Renormalised series to calculate energy eigenvalues for 2N=4,6,8

In order to find the eigenvalues E of the Schrödinger equation:

$$\left[-\frac{d^2}{dx^2}+\mu x^2+\lambda x^{2N}\right]\Psi(x)=E\Psi(x) \qquad \mu{:}1 \quad (2N=4,6,8) \qquad (2.2)$$

we shall use the hypervirial relations in calculating the perturbation energy series. These relations are given by Killingbeck [12,1982] as follows, for a potential $\Sigma\, V_n x^n$;

$$2E\left(N+1\right)\langle x^{N}\rangle=\sum V_{n}\left(2N+2+n\right)\langle x^{N+n}\rangle - \frac{N}{2}\left(N^{2}-1\right)\langle x^{N-2}\rangle \qquad (2.3)$$

This formula has an obvious use; if the energy E and a sufficient number of the $\langle x^N\rangle$ are known (analytically or numerically) then it allows computation of other $\langle x^N\rangle$ values. This formula also has the interesting property that it yields the Rayleigh-Schrödinger series for the eigenvalues and $\langle x^N\rangle$ values (as we will show later) without using any perturbed wave function. We should comment here that an application of the present method to a large variety of more complicated potentials will be studied in the forthcoming chapters. It is note worthy that although this approach is very attractive for the one dimensional problem, its application to a system of many dimensions has not yet been accomplished. We can write the potential appearing in equation (2.2) as:

$$V(x)=\mu x^{2}+\underline{\lambda}^{I}(x^{2N}-Kx^{2}) \qquad (2N=4,6,8) \qquad (2.4)$$

where

$$\mu=1+\underline{\lambda}^{I}K \quad , \quad \underline{\lambda}=\lambda^{\frac{1}{I}} \qquad (I=1,2,3,4) \qquad (2.5)$$

If we insert the series expansions given by:

$$E=\sum_{J} E(J)\lambda^{J} \qquad (2.6)$$

and

$$\langle x^{M}\rangle=\sum_{N} A(M,N)\lambda^{N} \qquad (2.7)$$

into (2.3) and take into account the potentials coefficients

$$V_{2}=(\mu-\underline{\lambda}^{I}K) \qquad (2.8)$$

$$V_{2n+2}=\underline{\lambda}^{I} \qquad (n=1,2,3) \qquad (2.9)$$

we obtain the recurrence relation

$$\left(2N+2\right)\sum_{0}^{M} E(J)A(N,M-J)=\left(2N+4\right)\left[\mu A(N+2,M)-KA(N+2,M-1)\right]$$
$$+\left[2N+2n+4\right]A(N+2n+2,M-I)$$
$$-\frac{N}{2}\left[N^{2}-1\right]A(N-2,M) \qquad (n=1,2,3) \qquad (2.10)$$

We use the series expansions in equation (2.6) and (2.7) to obtain the relation between the energy series (E) and the coefficient series A(N,M) as given below.

$$E=E(0)+E(1)\lambda+E(2)\lambda^{2}+E(3)\lambda^{3}+\ldots\ldots \qquad (2.11)$$

$$\langle x^{2}\rangle=A(2,0)+A(2,1)\lambda+A(2,2)\lambda^{2}+\ldots \qquad (2.12)$$

$$\langle x^{2n+2}\rangle=A(2n+2,0)+A(2n+2,1)\lambda+A(2n+2,2)\lambda^{2}+\ldots \quad (n=1,2,3) \quad (2.13)$$

Applying the Hellmann-Feynman theorem in the form

$$\frac{\partial E}{\partial\lambda}=\langle\frac{\partial V}{\partial\lambda}\rangle \qquad (2.14)$$

We obtain a recurrence relation of the form

$$\left(M+1\right)E(M+1)=IA(2n+2,M+1-I)-KA(2,M) \qquad (n=1,2,3) \qquad (2.15)$$

The Hellmann-Feynman theorem and Hypervirial theorem provide relationships between the energy E and the expectation values $\langle x^{N}\rangle$. It is clear now that from relations (2.10) and (2.15), we obtain the full set of A and E coefficients starting from the unperturbed energy.

$$E(0)=\left(2n+1\right)\sqrt{\mu} \qquad (n=0,1,2,\ldots) \qquad (2.16)$$

and the initial condition A(0,0)=1. The convergence properties of the resulting perturbation series are controlled by varying K.

The renormalised series work very well for the quartic perturbation (2N=4,I=1). The interesting point about this approach for (2N=6,8) calculations is that the accuracy varies with the power (I). We use this modified (variable I) technique to perform more accurate calculations. These calculations by the renormalised series technique become progressively more difficult as N increases; thus one must keep in mind that we can partly overcome this difficulty by introducing $\underline{\lambda}^{I}$. The primary motivation of this idea is to improve the accuracy of our eigenvalues results, using a very simple extension of the original renormalised series technique. It is important to point out that the effect of varying K , the renormalised constant, is to allow us to obtain results of high accuracy. The best K values in this calculation have been obtained by numerical search, so our calculation reveals the importance of finding the best values of the renormalised constant. The convergence rate decreases remarkably when λ and 2N increase. Problems with computer overflow were avoided by using the definition $A(N,M) \longrightarrow 2^{N} A(N,M)$. The renormalised technique has been used by Killingbeck for many eigenvalues problems, and has provided an excellent way to overcome divergence problems as well as to obtain eigenvalues with very high accuracy.

2.1.3 Finite-difference eigenvalue calculations

The finite-difference approach is a nonperturbative method capable of arbitrarily high accuracy. This method has been described by Killingbeck in reference [12,1982]. We will only mention the essential feature here; the reader interested in details should consult that reference. The finite-difference method for calculating energy eigenvalues of the Schrödinger equation

$$\left[\frac{d^2}{dx^2} - V(x)+E\right]\Psi(x)=0 \qquad (2.17)$$

with the potential

$$V(x)=\mu x^2+\lambda x^{2N} \qquad (2N=4,6,8...,20) \qquad (2.18)$$

produces results with high accuracy for a wide range of λ ($10^{-1}\le\lambda\le 5\times10^4$). For large λ values it seems that the present method works quite well, whereas various other methods have some problems. Although the results displayed are restricted to even-parity states, the method can be used for odd-parity states. To treat equation (2.13) or any similar problem, we define the finite-difference quantity

$$\delta^2\Psi(x)=\Psi(x+h)+\Psi(x-h)-2\Psi(x) \qquad (2.19)$$

where h is the strip width for the numerical integration. It is well known that (2.19) can be expressed as series expansion of even powers, by using the Taylor expansion

$$\delta^2\Psi(x)=h^2D^2\Psi(x)+ \frac{1}{12}h^4D^4\Psi(x)+----- \qquad (2.20)$$

Then we can combine (2.17) and (2.20) to give

$$h^{-2}\delta^2\Psi(x)=D^2\Psi(x)+ \frac{1}{12}h^2D^4\Psi(x) \qquad (2.21)$$

$$=\Big[V(x)-E\Big]\Psi(x)+V_P \qquad (2.22)$$

where the perturbation V_P has a leading term of order h^2. The most simple procedure is to ignore V_P as the first approximation; then the equation (2.22) reduces to the form

$$\delta^2\Psi(x)=h^2\Big[V(x)-E\Big]\Psi(x) \qquad (2.23)$$

We use two quantities R(x) and F(x) which are defined as follows

$$\Psi(x+h)=\Psi(x)R(x) \qquad (2.24)$$

$$\Psi(x+h)=\Psi(x)\Big[1+h^2F(x)\Big] \qquad (2.25)$$

If we insert equations (2.24) and (2.25) in equation (2.23) the following equations are obtained

$$R(x)+\frac{1}{R(x-h)}=2+h^2\Big[V(x)-E\Big] \qquad (2.26)$$

$$F(x)-\frac{F(x-h)}{R(x-h)}=V(x)-E \qquad (2.27)$$

For even states we have

$$\Psi(-h)=\Psi(h) \qquad (2.28)$$

which leads to the starting conditions

$$R(0)=\frac{1}{R(-h)} \qquad (2.29)$$

$$F(0)=\frac{1}{2}\Big[V(0)-E\Big] \qquad (2.30)$$

To apply equation (2.26) or (2.27), we need some initial value for R(x) or F(x) and can then calculate successive R(x) or F(x) values along the x-axis, with some test energy E. The wave function $\Psi(x)$ is calculated using equation (2.26) or equation (2.27) for two trial energies E_1 and E_2. We suppose that $E_2 > E_1$, so that (Ψ_2) has its nodes earlier than (Ψ_1). Then the calculation of the projected energy is given as

$$E_P=E_1+\frac{E_2-E_1}{(1-\Psi_2/\Psi_1)} \tag{2.31}$$

E_P is actually a function of x; it is the interpolated energy which would have given $\Psi(x)=0$. As x increases, however, E_P settles down to a limiting value, provided that E_2-E_1 is not too large. This limiting energy corresponds to the boundary condition $\Psi(\infty)=0$. The true energy is related to the calculated energies for varying strip widths by a formula of type

$$E(h)=E_0+h^2E_2+h^4E_4+\text{-------} \tag{2.32}$$

$$E(2h)=E_0+4h^2E_2+16h^4E_4+\text{----} \tag{2.33}$$

$$E(4h)=E_0+16h^2E_2+256h^4E_4+\text{-----} \tag{2.34}$$

From equations (2.32,2.33,2.34), we can obtain the equation

$$E_0=\frac{1}{45}\left[64E(h)-20E(2h)+E(4h)\right] \tag{2.35}$$

Here E(h) is the energy calculated using strip width h and E_0 is the exact energy (for $h\longrightarrow 0$). Now we turn back to equation (2.22) and ask what the first-order energy shift would be if a perturbing term $h^2D^4/12$ were added to a Hamiltonian. This shift would be the expectation value.

$$E_1=\frac{1}{12}h^2\int_{-\infty}^{+\infty}\Psi(x)D^4\Psi(x)dx \tag{2.36}$$

The integral can easily be evaluated by parts to yield

$$E_1=\frac{1}{12}h^2\langle(E-V)^2\rangle \tag{2.37}$$

This shift E_1 could be produced by using the extra term

$$V_P = \frac{1}{12}h^2\left[V(x)-E\right]^2 \qquad (2.38)$$

to simulate the more complicated term $h^2D^4/12$

2.1.4 power series eigenvalue calculations

The power series approach has been used by Killingbeck for calculations on many types of eigenvalues problem. He has developed and modified this approach to give very high accuracy for eigenvalues, comparable to that of the finite difference method. The success of this approach allows us to calculate eigenvalues for high value of λ ($0.1 \le \lambda \le 50000$) and ($2N=4,6..18,20$). We used the non-perturbative power series method as another approach to calculate the energy eigenvalues for the Schrödinger equation given by (2.17), which we earlier treated by perturbation theory. We take the wavefunction in the form

$$\Psi(x)=\exp\left(-\beta x^2\right)\sum_0^\infty A(N)x^N \qquad (2.39)$$

If we insert equation (2.39) in equation (2.17) we obtain the following equation:

$$\left(N+1\right)\left(N+2\right)T(N+2)=\left[4\beta N+2\beta-E\right]T(N)x^2$$

$$+\left[\mu-4\beta^2\right]T(N-2)x^4+\lambda T(N-2M)x^{2M+2} \quad (2M=4,6,..18,20) \qquad (2.40)$$

In the above equations we use the notation

$$\sum_0^\infty T(N)=\sum_0^\infty A(N)x^N \qquad (2.41)$$

We can take the initial condition T(0)=1 for even states or T(1)=0 for odd states, with all lower T(N) zero. We can give a clear physical picture for this method; we want the bound state wavefunction $\Psi(x,E)$ to become zero as x approach infinity (or sometimes for some finite x). We can describe the calculational method as follows: we pick out some value for x and take two trial energies $E_1$and $E_2=E_1+H$; we take sufficient terms of the series (2.41) to get converged values for $\Psi(x,E_1)$ and $\Psi(x,E_2)$. Then by linear interpolation we estimate the E value E_0 which would have made $\Psi(x,E)$ zero. We then repeat using $E_1= E_0$, $E_2= E_0+H$ with a small value of H. H is typically $\simeq 10^{-3}$. After a few repetitions we should get a close estimate of an eigenvalue, appropriate to the boundary condition $\Psi(x)=0$. The interpolated value depends on wavefunction ratio $\psi(E+H)/\Psi(E)$. The number of terms of the series needed can be reduced by a factor of up to twenty by using this ratio directly instead of waiting for separate convergence of the $\Psi(E+H)$ and $\Psi(E)$ series. In this approach we have the convergence factor $\exp(-\beta x^2)$. The choice of the β parameter helps to achieve or improve convergence. We consider the success of this approach as being related to its physical interpretation. We emphasize that the method gives us the freedom to work with any value of 2N and λ.

2.1.5 Results and discussion

The energy eigenvalues of the generalized anharmonic oscillator defined by the Hamiltonian (2.1) have been calculated for various values of λ, using three different methods; the renormalised series, finite difference and power series methods. Our results as obtained by these methods are compared with each other, the agreement between them being very good. In table (2.1) we list the energy eigenvalue for $(2N=4)$ arising from the renormalised series and power series methods. It is clear from the listed results that the power series method is able to produce more accurate results than those from the renormalised series at high values of λ. Table (2.2) gives the values of the energies of the anharmonic oscillator $(2N=6,8,..20)$, calculated by power series and finite difference methods for $(0.1 \leq \lambda \leq 50000)$ and $(\mu=1,0)$. We have computed ten eigenvalues in this range. From our results we observed the order of levels $E^4 < E^6 < E^8, \ldots . E^{18} < E^{20}$ for small values of $(\lambda=0.1,1..,5)$, but for large values of $(\lambda=10,50,5000)$, we observed the order reversed. The physical reason behind this is that the eigenvalues are non-analytic at each crossing points, as discussed by Simon [2,1970] and C.M.Bender [1,1969] and this has been proved by them. It seems from our eigenvalue results for $E^{2N}(\lambda)$ that the crossing occurs approximately at the same value $(\lambda \approx 5)$ for various levels. As can be seen from these calculations, the accuracy of our results is around 16 significant digits. The energies quoted in table (2.2) agree to the number of digits given with those obtained by other calculations. We wish to stress that the finite difference method and power series method work very well for any value of the index $(2N=4,6,..,20)$. These methods have obvious advantages over the renormalised series method, which can only handle the values $(2N=4,6,8)$. The results for this approach are shown in table (2.3) and it is clear that the accuracy is decreased as 2N increases, although it is still very good in comparison with the results of Biswas et.al [3,1973]. In order to illustrate the effect of the use of the $\underline{\lambda}^I$ technique on the convergence rate we have calculated many eigenvalues for various $\underline{\lambda}^I$ (I=1,2,3,4),and the results have been listed in table (2.4). It is clear from our calculations that the accuracy is poor for 2N=6 at I=1 but at I=2,3,4, it is clearly better and we obtain 6 digits accuracy. For 2N=8 we find better accuracy at I=4, although we obtain only 4 digits. The confidence in the accuracy of the computed eigenvalues is derived from the following checks;

1. The agreement between the two computed eigenvalues by the two techniques which have been used is excellent, as is clear from our results which list in tables (2.1,2.2,2.3).
2. Two separate computations for (2N=4,6,..20) by using power series and finite difference methods with an increasing and decreasing (x,β), yielded eigenvalues agreeing to 16 significant figures.
3. The agreement between some of our results and the results which have been given by G.Schiffner and Stanzial [7,1985], and Banerjee [4,1978] for (2N=6,8,10,12), to about 16th figures.

In conclusion, we remark that the present results are to our knowledge the best available so far in the literature; for 2N>12 we have not found numerical results in the literature. The method is able to deal with perturbations that other methods cannot handle due to numerical difficulties, for example the cases (2N=14,16,18,20). In the limit $2N \longrightarrow \infty$ the potential becomes a square well potential and our methods should allow this limit to be studied.

Table (2.1). Energy eigenvalues of $H=P^2+x^2+\lambda x^4$, First line renormalised series calculation, Second line; power series calculation, with digits before the last digit omitted.

λ	E_0	N	K	E_1	N	K
0.1	1.06528550954371768888 8	47	20	3.30687201315291350070 1	42	20
1.0	1.3923516415302 2918557	39	8	4.64881270421207 775364	42	9
10.	2.44917407211 183869183	40	4	8.59900345480 077726028	47	5
100	4.999417545 51375878293	37	170	17.8301927159 952522387	36	200
λ	E_2	N	K	E_3	N	K
0.1	5.74795926883356633045 7	42	18	8.35267782578575471l6 22	42	20
1.0	8.655049957759 93096881	5	10	13.15680389805 49875079	42	12
10.	16.635921492 2413757783	50	6	25.806276215 5055640450	28	4
100	34.873984262 1994777546	36	200	54.385291571 1603103269	34	200
λ	E_4	N	K	E_5	N	K
0.1	11.09859562263304301l 1	38	20	13.969926197742799300 0	44	25
1.0	18.057557436303 3252895	49	14	23.29744145122 23189085	49	16
10.	35.885171222 2253873712	58	9	46.729080900 0817113006	59	10
100	75.8770040286 669724181	37	220	99.0328373 315407491228	22	200
λ	E_6	N	K	E_7	N	K
0.1	16.9547946861441513336 6	41	25	20.0438636041884612232 4	42	25
1.0	28.83533845950 04248840	12	18	34.64084832111 11332543	54	20
10.	58.241298739 9753240285	57	18	70.3510519392 234653309	57	10
100	123.64069762667 7816767	38	250	149.545657443 328822117	31	280

Table (2.2). Eigenvalues of the anharmonic oscillator $H=P^2+\mu x^2+\lambda x^{2N}$, First line, power series method; Second line, finite difference method, with digits before last digit omitted.

λ	(2N=6), μ=1	β , X h	(2N=6), μ=0	β , X h
0.1	1.1090870784655584 4	10, 12 0.004	0.6437697289493398 8	10, 12 0.004
1	1.4356246190033392 2	10, 12 0.004	1.1448024537970553 3	10, 12 0.004
5	1.9124538322228856 6	10, 12 0.004	1.7118789540244485 5	10, 12 0.004
10	2.2057232695956632 2	10, 12 0.004	2.0357786321493334 4	15, 12 0.004
50	3.1590212010596554 4	10, 12 0.004	3.0441990964207110 0	15, 12 0.004
100	3.7169747292086620 0	10, 12 .004	3.6201832249483663 3	10, 6 0.002
500	5.4783790904627791 1	10, 6 0.002	5.4134365732240443 2	10, 6 0.002
1000	6.4923501323296772 1	12, 6 0.0015	6.4376972894939880 0	15, 3 0.001
10000	11.478798042264554 4	15, 3 0.001	11.448024537970553 3	15, 3 0.001
50000	17.139375868861889 9	15, 3 0.001	17.118789540244485 5	15, 3 0.0009
λ	(2N=8), μ=1	β , X h	(2N=8) μ=0	β , X h
0.1	1.1689704532459866 6	8 , 6 0.0025	0.7734402038139666 6	8 , 6 0.0025
1	1.4910198956622055 5	10, 6 0.002	1.2258201138004922 2	10, 6 0.002
5	1.8874871430320622 2	15, 6 0.002	1.6913003706263011 1	10, 6 0.002
10	2.1145446219421299 9	10, 6 0.002	1.9427939535443088 8	10, 6 0.002
50	2.8060650893162866 6	15, 6 0.002	2.6805304438125833 3	15, 6 0.002
100	3.1886543464922688 8	15, 6 0.002	3.0791209113269866 6	20, 6 0.002
500	4.3280123802505633 3	24, 6 0.002	4.2483544525833299 9	20, 6 0.002
1000	4.9494874400327433 3	20, 6 0.002	4.8800777711268000 0	20, 6 0.0015
10000	7.7782722143110999 9	25 , 6 0.0015	7.7344020381396688 8	30, 6 0.0015
50000	10.703197380124888 8	40, 6 0.0015	10.671383905687377 7	40, 6 0.0015

Table (2.2 continued)

λ	(2N=10), μ=1	β , X h	(2N=10), μ=0	β , X h
0.1	1.2338889706082700	20, 6 0.002	0.8848919122181699	20, 6 0.002
1	1.5462635125723466	20, 6 0.002	1.2988437006785211	20, 6 0.002
5	1.8905049648525822	20, 6 0.002	1.6984465848826800	20, 6 0.002
10	2.0783027869748266	20, 6 0.002	1.9064418326114722	20, 6 0.002
50	2.6253425166656877	20, 6 0.002	2.4929786533860033	20,6 0.002
100	2.9164422693587099	20, 6 0.002	2.7982739256711955	20, 6 0.002
500	3.7498604727534744	30, 6 0.002	3.6591922416374288	30, 6 0.002
1000	4.1881592340936666	30, 6 0.002	4.1073044187061133	30, 6 0.002
10000	6.0838949772928366	50, 6 0.001	6.0286984176777233	50, 6 0.001
50000	7.9257314465184500	90, 6 0.001	7.8834907028792066	90, 6 0.001
λ	(2N=12), μ=1	β , X h	(2N=12), μ=0	β , X h
0.1	1.2978255995072699	40, 6 0.002	0.9814796022472956	40, 6 0.002
1	1.5979904992759977	45, 6 0.002	1.3637614851417577	45, 6 0.002
5	1.9045814160856600	40, 5 0.002	1.7162923979766400	40, 5 0.002
10	2.0660950169768722	45, 5 0.002	1.8949404390040900	45, 5 0.002
50	2.5216143481371088	50, 5 0.002	2.3847805540154100	50, 5 0.002
100	2.7571798005984766	50, 5 0.002	2.6330112021016399	50, 5 0.002
500	3.4126221224391366	50, 5 0.002	3.3136418348730877	50, 5 0.002
1000	3.7482945891043944	50,5 0.002	3.6585572019542265	50, 5 0.002
10000	5.1482723474050433	70, 5 0.001	5.0835487480217900	70, 5 0.001
50000	6.4491144728362066	95, 5 0.001	6.3976407649219955	95, 5 0.001

Table (2.2 continued)

λ	(2N=14), μ=1	β , X h	(2N=14), μ=0	β , X h
0.1	1.3582600972089699	40 ,5 0.002	1.0659287883947544	40 ,5 0.002
1	1.6454273016675300	45 ,5 0.001	1.4214388844842899	45 ,5 0.001
5	1.9230940610807200	42 ,6 0.001	1.7381987859337599	42 ,6 0.001
10	2.0655848669930211	46 ,5 0.001	1.8955192169701277	46 ,5 0.001
50	2.4577453915696922	45 ,5 0.001	2.3179253344029377	45 ,5 0.001
100	2.6561527487818666	45 ,5 0.001	2.5277155009071066	45 ,5 0.001
500	3.1963538820403522	50 ,4 0.001	3.0910031115806566	50 ,4 0.001
1000	3.4674643575128088	50 ,4 0.001	3.3707627948710788	50 ,4 0.001
10000	4.5676648963859733	70 ,4 0.001	4.4949844296993288	70 ,4 0.001
50000	5.5561602511674799	98 ,4 0.001	5.4966671896901244	98 ,4 0.001
λ	(2N=16), μ=1	β , X h	(2N=16), μ=0	β ,X h
0.1	1.4143629933806299	60 ,5 0.001	1.1403916274128788	60 ,5 0.001
1	1.6886443554088022	70 ,3 0.001	1.4728724243708811	70 ,3 0.001
5	1.9431341163633477	70 ,4 0.001	1.7612802494210466	70 ,4 0.001
10	2.0711020698254600	50 ,5 0.001	1.9022878863058711	50 ,5 0.001
50	2.4166226483466044	70 ,5 0.001	2.2747809161370833	70 ,5 0.001
100	2.5884346961194200	70 ,5 0.001	2.4568992823202199	70 ,4 0.001
500	3.0483044971762800	60 ,3 0.001	2.9379925302191011	60 ,3 0.001
1000	3.2754398843852388	70 ,3 0.001	3.1732074450559888	70 ,3 0.001
10000	4.1776919144105900	90 ,3 0.001	4.0983550126847977	90 ,3 0.001
50000	4.9672812669047833	110,3 0.001	4.9008669179482422	110,3 0.001

Table (2.2 continued)

λ	$(2N=18)$, $\mu=1$	β , X h	$(2N=18)$, $\mu=0$	β , X h
0.1	1.4660511079402923	80, 2 0.001	1.2065611903664033	80 , 2 0.001
1	1.7279826652359922	80, 2 0.001	1.5189705434368855	80 , 2 0.001
5	1.9633395750481711	85, 2 0.001	1.7842115743136677	85 ,2 0.001
10	2.0797847627251544	85, 2 0.001	1.9122706168994900	85 , 2 0.001
50	2.3894070878440833	75, 2 0.001	2.2461892909207533	75 , 2 0.001
100	2.5412271627975411	65, 2 0.001	2.4074060738420777	65 , 2 0.001
500	2.9420194583712355	90, 2 0.001	2.8277847780400577	90 , 2 0.001
1000	3.1374276159495011	100, 2 0.001	3.0307446828674156	100, 2 0.001
10000	3.9004171024695822	120, 2 0.001	3.8154814979218444	120, 2 0.001
50000	4.5541240762311366	140, 2 0.001	4.4817368444608488	140 ,2 0.001
λ	$(2N=20)$, $\mu=1$	β , X h	$(2N=20)$, $\mu=0$	β , X h
0.1	1.5135519832599833	90, 2 0.001	1.2657764286507211	95, 2 0.001
1	1.7638480600908033	92, 2 0.001	1.5605083429246655	92, 2 0.001
5	1.9830578706002199	90, 2 0.001	1.8063787787365600	92, 2 0.001
10	2.0900925950219877	90, 2 0.001	1.9238676224468155	92, 2 0.001
50	2.3711391716639499	90, 2 0.001	2.2269881875627099	95, 3 0.001
100	2.5073631404681633	67, 2 0.001	2.3718339254517166	95, 3 0.001
500	2.8629144984356944	110, 2 0.001	2.7455351258126822	110, 2 0.001
1000	3.0344164846907233	120, 2 0.001	2.9241077214912244	120,2 0.001
10000	3.6946539612752966	140, 2 0.0009	3.6049766702178255	140, 2 0.001
50000	4.2505260515873011	160, 2 0.0009	4.1729692663592733	160, 2 0.0009

Table (2.3). Energy eigenvalues of $H=P^2+x^2+\lambda^I x^{2N}$, First line; power series calculation, Second line; renormalised series, with digits before the last digit omitted.

λ	(2N=4) I=1	N	K	(2N=6) I=4	N	K	(2N=8) I=4	N	K
0.1	1.06528550954371 1	47	20	1.10908707846558 7	128	50	1.16897045324598 9	70	80
0.2	1.11829265436704 4	47	20	1.17388934512543 3	100	50	1.24102790505586 0	68	80
0.3	1.16404715735384 4	51	18	1.22368713082245 1	89	50	1.29235601011702 3	62	80
0.4	1.20481032737249 9	48	14	1.26509938921472 3	81	50	1.33326839519428 2	59	80
0.5	1.24185405965149 4	43	13	1.30098697190627 6	75	50	1.36772100954772 7	58	80
0.6	1.27598356634255 5	47	12	1.33289594337339 5	78	50	1.39770876202691 7	57	80
0.7	1.30774865112003 0	43	10	1.36177259515288 2	66	50	1.42439586248017 3	53	80
0.8	1.33754520814817 1	44	10	1.38824494503033 5	67	50	1.44852785641937 5	61	90
0.9	1.36566982578443 4	43	9	1.41275436082138 4	78	60	1.47061414630140 0	46	80
1.0	1.39235164153029 2	39	8	1.43562461900339 4	76	60	1.49101989566220 1	54	80
2.0	1.60754130246854 8	42	7	1.60993195202308 1	81	70	1.64137035713246 1	43	80
3.0	1.76958884428039 0	42	6	1.73285711751614 5	71	75	1.74320451094779 3	41	80
4.0	1.90313694545900 5	43	6	1.83043734375010 3	71	80	1.82217987008594 2	39	80
5.0	2.01834064936531 6	40	5	1.91245383222285 5	64	80	1.88748714303206 7	35	80
6.0	2.12053292939427 9	43	5	1.98378052759545 8	66	80	1.94357976099209 3	45	100
7.0	2.21291421117415 7	46	5	2.04723907601261 3	70	90	1.99298567568301 2	43	100
8.0	2.29757782825207 2	34	4	2.10462590821951 2	75	100	2.03729023148001 7	44	100
9.0	2.37597854978311 7	40	4	2.15716300414840 6	113	150	2.07755877362301 7	53	120
10.	2.44917407211838 1	40	4	2.20572326959563 2	70	100	2.11454462194212 4	52	120
20.	3.00994481555778 5	49	4	2.56464464550004 4	94	150	2.38184367142942 1	45	120
30.	3.41016853263682 6	38	80	2.80938113102966 8	82	150	2.55894138891585 8	51	140
40.	3.73139160205310 0	39	100	3.00031532076312 1	83	160	2.69468105951785 4	53	150
50.	4.00399276827762 2	40	120	3.15902120105965 2	76	160	2.80606508931628 6	55	150
60.	4.24308144642364 6	29	120	3.29595194934978 5	84	180	2.90119763491835 1	56	160
70.	4.45740819230319 2	30	125	3.41704571758164 4	70	160	2.98462697679431 4	49	150
80.	4.65255184730633 7	34	150	3.52603057224061 3	65	160	3.05918117713722 9	49	150
90.	4.83231440623305 6	34	160	3.62541489540524 1	67	160	3.12674784921351 6	50	160
100	4.99941754513758 5	37	170	3.71697472920862 7	80	180	3.18865434649226 8	46	150

Table (2.4). Energy of ground state levels, by using renormalised series method at $\lambda=1$, The number in the bracket correspond to exact value.

I	2N=6	N	K	2N=8	N	K
1	1.4355	72	80	1.5	24	120
2	1.435624	81	70	1.49	51	150
3	1.435624	54	40	1.490	55	100
4	1.435624	76	60	1.491	54	80
	(1.4356246)			(1.49102)		

2.2 Numerical calculation for Quasi-bound states.

2.2.1 Introduction

This section is concerned with potentials of the types:

$$V(x)=x^2+\lambda x^3 \tag{2.42}$$

$$V(x)=x^2+\lambda x^5 \tag{2.43}$$

$$V(x)=x^2-\lambda x^4 \tag{2.44}$$

and the hypervirial recurrence relations have been used to calculate perturbed energy eigenvalues. There are many studies of potentials of the form

$$V(x)=\mu x^2+\lambda x^{2N} \qquad (2N=4,6,..10,12) \tag{2.45}$$

whereas for potentials of the form

$$V(x)=x^2+\lambda x^{2N+1} \qquad (2N=2,4) \tag{2.46}$$

there are few reported results. The energy levels of an anharmonic oscillator with a perturbation of type λx^3have been calculated by Drummond [5,1981;6,1982]. The potential functions given by (2.42,2.43,2.44) describe a system which has no true bound states. For large x, $\Psi(x)$ does not tend to zero and is not admissible as a normalizable wavefunction, so that the particle is not permanently confined to the neighbourhood of the centre of force. However, in spite of there being no true bound states, we can still compute an average real energy for small values of λ.

2.2.2 Renormalised series method to calculate energy eigenvalues for λx^{2N+1}. (2N=2,4) perturbation

In order to find the eigenvalues E of the Schrödinger equation:

$$\left[-\frac{d^2}{dx^2}+x^2+\lambda x^{2N+1}\right]\Psi(x)=E\Psi(x) \qquad (2N=2,4) \tag{2.47}$$

We shall use the hypervirial relations (2.3) in calculating the perturbation energy series. Drummond's approach is based on a method due to Bender and Wu [1,1969]. It uses recurrence relations to calculate the perturbed energy and wave function. We should point out that Drummond used extrapolated values based on the first few terms of the energy series, but in our approach we calculate many terms of the series. Also in our approach we tried out Aitken's transformation in order to increase the accuracy, but unfortunately it did not seem to help to improve the accuracy of our results for this problem. In order to improve the convergence properties of the perturbation series we used a rearrangement of terms in the potential (renormalised perturbation series).

To illustrate this technique we can rewrite the potential (2.46) as follows

$$V(x)=\mu x^2+\lambda\left(x^{2N+1}-Kx^2\right) \tag{2.48}$$

where

$$\mu=1+\lambda K \tag{2.49}$$

The new perturbation series is still divergent but its divergence begins for high values of λ, so that for low values of λ we findagood energy value. Inserting the series expansions given by equations (2.6) and (2.7) into (2.3) and taking into account the potentials coefficients

$$V_2=\left(\mu-\lambda K\right) \tag{2.50}$$

$$V_{2N+1}=\lambda; \qquad (N=1,2) \qquad (2.51)$$

we obtain the recurrence relations

$$\left(2N+2\right)\sum_{0}^{M} E(J)A(N,M-J)=\left(2N+4\right)\left[\mu A(N+2,M)-KA(N+2,M-1)\right]$$

$$+\left[2N+2n+3\right]A(N+2n+1,M-1)-\frac{N}{2}\left[N^{2}-1\right]A(N-2,M) \quad (n=1,2) \qquad (2.52)$$

Applying the Hellmann-Feynman theorem as given by equation (2.14), we obtain a recurrence relation in the form

$$\left(M+1\right)E(M+1)=A(2n+1,M)-KA(2,M) \quad (n=1,2) \qquad (2.53)$$

It is clear now that from equations (2.52) and (2.53) we obtain the full set of A and E coefficients starting from the unperturbed energy

$$E(0)=\left(2n+1\right)\sqrt{\mu} \qquad (2.54)$$

2.2.3 Energy levels for negative quartic oscillator

It is interesting to note that the renormalised series method can even be extended to the case of a negative but small value of λ. Strictly speaking, no bound states are present in this case. We can write the potential appearing in equation (2.44) as

$$V(x)=\mu x^{2}-\lambda\left(x^{4}+kx^{2}\right) \qquad (2.55)$$

If we use the series given by equations (2.6) and (2.7) and the potential coefficients which are given by equation (2.56) as

$$V_{2}=\left(\mu-\lambda K\right), \quad V_{4}=-\lambda \qquad (2.57)$$

in the hypervirial relation (2.3) we obtain the recurrence relation

$$\left(2N+2\right)\sum_{0}^{M} E(J)A(N,M-J)=\left(2N+4\right)\left[\mu A(N+2,M)-KA(N+2,M-1)\right]$$

$$-\left(2N+6\right)A(N+4,M-1)-\frac{N}{2}\left[N^{2}-1\right]A(N-2,M) \qquad (2.58)$$

If we use the same approach as used to obtain equation (2.53) we get the energy equation

$$\left(M+1\right)E(M+1)=-KA(4,M)-KA(2,M) \qquad (2.59)$$

The above recurrence relation together with relation (2.58) and (2.59) are sufficient to determine the coefficients E and A of the perturbation series, starting with initial conditions for E(0) and A(0,0) as quoted previously. We calculated the eigenvalues of the $(-\lambda x^{4})$ oscillator for ground and excited states for different values of λ as shown in table (2.7). It is worth noticing here that varying the renormalised constant K improves the convergence our results. The numerical eigenvalues of $(x^{2}-\lambda x^{4})$ are in reasonable agreement with the previous results which have been obtain by J.E.Drummond [5,1981], who used 25 coefficients of the energy series to calculate the eigenvalues of energy. Our calculations were done on an ICL system using double precision arithmetic.

2.2.4 Results and discussion

The ground state as well as excited energy levels of the generalized anharmonic oscillator defined by the Hamiltonians:

$$H_{M}=-\frac{d^{2}}{dx^{2}}+x^{2}+\lambda x^{2N+1} \qquad (2N=2,4) \qquad (2.60)$$

$$H=-\frac{d^2}{dx^2}+x^2-\lambda x^4 \tag{2.61}$$

have been calculated for various λ values, using the renormalised series method. Our results for $(\lambda x^3, -\lambda x^4)$ perturbations have been compared with previous results of J.E.Drummond [5,4] in order to have an idea about the accuracy of our approach. In table (2.5) we present the energy eigenvalues for a $(-\lambda x^4)$ perturbation for the first five excited states, for different values of λ lying between $(0.01 \leq \lambda \leq 0.12)$. Our results lead to the following observation:

1. Our perturbation energies series for λx^3 converge very well for small values of λ $(\lambda < 0.12)$, where our approach has obtained 20 significant figures. The precision of the energies seems good even for excited states, but J.E.Drummonds' approach achieves only 12 figures; our results can thus considered as more accurate.

2. The renormalised series approach for $(\lambda > 0.12)$ deteriorates in convergence. This approach has a limited range of application, and seems not to work for this range of λ, presumably because the quasi-bound states are not well defined for such large λ.

3. The most important difference between the J.E.Drummond approach and our approach is that the former computed only 20 coefficients while we have computed any number of coefficients until we obtain the best converged energy.

4. The Padé approximant technique has been used to calculate the energy eigenvalue of the potential given by equation

(2.43) for low values of λ, because the energy series is more speedily divergent than that for the potential (2.42). Our results in table (2.6) exhibit this behaviour. This technique is reviewed in more detail in chapter 4. In the absence of other reported results (to the best of our Knowledge), we have calculated each eigenvalue for two values of [M,N] in order to estimate the accuracy of our results.

Table (2.5). Energy eigenvalues of $H=P^2+x^2+\lambda x^3$, First line; Renormalised series calculation, Second line; Drummond calculation, with digits before the last digit omitted.

λ	E_0	N	K	E_1	N	K
0.01	0.99993123182623556912 6	12	2	2.9995560300711536057 1	13	2
0.02	0.99972470875265969188 3	16	2	2.9982214713809320871 1	17	2
0.03	0.99937977159498842338 5	21	2	2.9959883032176996116 8	22	2
0.04	0.99889530980223136279 2	24	2	2.9928429058397717080 40	26	2
0.05	0.99826974304395106074 4	29	2	2.9887656636459711189 6	34	2
0.06	0.99750099428744908392 8	34	2	2.9837303688393113876 40	38	2
0.07	0.99658645309226050407 3	40	2	2.9777033776119970087 7	48	2
0.08	0.99552292727908772567 80	47	2	2.970642444800281916 9	51	2
0.09	0.99430658035499637812 0	57	2	2.96249512297422822 30	58	2
0.10	0.99293285097631609853 1	75	2	2.9531965472043759 3	74	2
0.12	0.98969072098313 1	83	2	2.930803974978 2	80	2
0.15	0.98347687 9	93	2	2.88557423 2	92	2
0.20	0.96863 3	77	8	2.7564 5	48	6

λ	E_2	N	K	E_3	N	K
0.01	4.9988053317405753541 4	14	2	6.9976788050043899205 0	15	2
0.02	4.9952102465829434515 9	19	2	6.9906856587857592698 8	21	2
0.03	4.9891810363434278186 5	24	2	6.9789301813199445386 4	26	2
0.04	4.9806599152895584412 30	31	2	6.6922558458118062523 9	33	2
0.05	4.9695624320799928932 1	37	2	6.9404302370588397541 1	41	2
0.06	4.9557734480182652681 0	44	2	6.9131293458398142655 9	50	2
0.07	4.9391411788801258984 9	56	2	6.87991308220897580 3	64	2
0.08	4.9194684602435089298 3	68	2	6.84018686405584 4	68	2
0.09	4.8964998050337740 1	71	2	6.7931394446125 4	72	2
0.10	4.8699017069532 7	75	2	6.73763664172 6	76	2
0.12	4.80388361 4	74	2	6.593703 0	81	2
0.15	4.658 8	51	2	6.208 8	54	2

Table (2.5 continued)

λ	E_4	N	K	E_8	N	K
0.01	8.99617611734871565665	15	2	10.99429693555736764517	15	2
0.02	8.98464228756966487357	24	4	10.97707466707551724688	22	2
0.03	8.96520741602457701663	33	4	10.94798386960034161600	30	2
0.04	8.93753702986342064069	42	4	0.90640644540485123244	36	2
0.05	8.90112615749962459515	52	4	10.85139294284377858229	50	2
0.06	8.85525386659719176	62	4	10.78155328405708795221	60	2
0.07	8.798908380381521777	63	2	10.694865910061050	63	2
0.08	8.730660498669968	68	2	10.588327513785	68	2
0.09	8.648436836177	71	2	10.4572471037	70	2
0.10	8.5490729433	74	2	10.2935778	74	2
0.12	8.27233	72	2	9.766	62	2

Table (2.6). Energy eigenvalues of $H=P^2+x^2+\lambda x^6$ the result produced by Padé approximants E [M,N]

λ	E_0	E [M,N]	E_1	E [M,N]
0.005	0.99982353	[7,7]	2.99771	[7,7]
	0.99982353	[9,9]	2.99771	[8,8]
0.01	0.99927923	[8,8]	2.9904	[7,7]
	0.99927923	[9,9]	2.9907	[8,8]
0.02	0.99679	[7,7]	2.906	[8,8]
	7	[8,8]	2.996	[8,9]
λ	E_2	E [M,N]	E_3	E [M,N]
0.005	4.98719	[7,7]	6.95381	[7,7]
	4.98719	[8,8]	6.95387	[8,8]
0.01	4.94	[7,7]	6.6	[7,7]
	4.94	[8,8]	6.7	[8,8]

Table (2.7). Energy eigenvalues of $H=P^2+x^2-\lambda x^4$, First line Renormalised series calculation, Second line; Drummond calculation, with digits before the bracket omitted.

λ	E_0	N	K	E_1	K	N
0.01	0.99236322064691319978 (6)	24	4	2.96140190352361172 89 (5)	30	4
0.05	0.95823 (3336)	18	10	2.771 (126)	21	20
λ	E_2	N	K	E_3	N	K
0.01	4.89830203662898068 39 (6)	35	4	6.8014327584883497 (5)	31	2
0.05	4.316 (5)	34	50	5.54 (4)	21	50

2.3 Energy levels of double-well anharmonic oscillator

2.3.1 Introduction

The aim of this section is to investigate numerically the eigenvalues of double-well potentials with form given as below:

$$V(x)=-\ Z^2x^2+\ x^{2N} \qquad (2N=4,6,8,\ldots\ldots28,\ 30) \qquad (2.62)$$

The most studied system of this kind is the quartic double-well potential (2N=4). The calculation of eigenvalues for the Schrödinger equation with double-well potential has received great attention from us. We extended our calculations to higher powers (2N=4,6,8.....28,30), since our methods free our hands to compute the eigenvalues for such higher values of 2N. The treatment of the double-well potential (2N=4) has attracted many authors. For instance, R.Balsa et. al [17,1983] have computed the energy eigenvalues for 2N=4,($0\le Z^2\le 100$) and $0\le n\le 21$; their results produce 12 digits accuracy. R.M.Quick and H.G.Miller [18,1984] have computed for 2N=4, $Z^2=50$ and ($0\le n\le 79$); they used a non-perturbative method involving matrix diagonalization to calculate some energy levels. Our approaches will use a perturbative method as well as a non-perturbative method. Our main object is to demonstrate that both approaches work and are able to produce excellent accuracy in spite of high values of Z^2, 2N and state number n. It is important to point out that some of our results for this problem are not available in the literature, so the values which are listed in our tables have been checked at least by two methods. The agreement in our calculated results by both methods gives us faith that the accuracy yielded by our methods is high. The depth of the double well is controlled by a parameter Z^2 (in equation 2.64 below). In some cases, particularly for $Z^2 \geq 1$ or $Z^2 \leq 10^6$, one approach works better than the other. The perturbation approach works excellently for large values of Z^2 because as Z^2 increases the depth of the two wells become deeper and for deep wells the perturbation series converge quickly.

2.3.2 Renormalised series for Double well potential

To calculate energy eigenvalues for the double well potential, we consider the Schrödinger equation

$$\left[\frac{d^2}{dx^2}+E-V(x)\right]\Psi(x)=0 \qquad (2.63)$$

where

$$V(x)=-Z^2x^2+x^{2N} \quad (2N=4,6,\ldots 26,28,30) \qquad (2.64)$$

The SDWP energy levels are found by simply setting $\mu x^2 \longrightarrow -Z^2x^2$ in the equation (2.1), and shifting the energy so that the zero of the energy is at the bottom of the well, with $Z^2>0$. The minima of V(x) are located at

$$x=x_0 \qquad (2.65)$$

where

$$x_0=\left[\frac{Z^2}{N}\right]^{\left[\frac{1}{2N-2}\right]} \qquad (2.66)$$

In this case we expand V(x) about its minimum at x_0 in order to estimate the eigenvalues E around x_0. The Taylor expansion for the potential V(x) about x_0 is

$$V(x)=V(x_0)+V'(x_0)x+\frac{1}{2}V''(x_0)x^2+\frac{1}{6}V'''(x_0)x^3 \;.......$$

$$+\sum_{n=4}^{2N} V^n(x_0)\frac{x^n}{n!} \qquad (2N=4,6,8,...26,28,30) \qquad (2.67)$$

If we follow the same procedure as used to obtain relations (2.10) and (2.15), we obtain hypervirial recurrence relations corresponding to the double well potential case as follows:

$$\left(2N+2\right)\sum_{0}^{M} E(J)B(N,M-J)=-\frac{N}{2}\left[N^2-1\right]A(N-2,M)$$

$$-\left(2N+4\right)\left[\mu A(N+2,M)+KA(N+2,M-1)\right]$$

$$\sum_{n=3}^{2N}\frac{d^nV(x)}{dx^n}\bigg|_{x=x_0}\frac{1}{n!}\left(2N+2+n\right)A(N+n,M-1) \qquad (2.68)$$

$$\left(M+1\right)E(M+1)=\sum_{n=3}^{2N}\frac{d^nV(x)}{dx^n}\bigg|_{x=x_0}\frac{1}{n!}A(n,M)-KA(2,M) \qquad (2.69)$$

The unperturbed energy corresponding to the double well potential can be expressed as

$$E=-V(x_0)+\left(2n+1\right)\sqrt{\mu} \qquad (n=0,1,2,...) \qquad (2.70)$$

and we obtain a hypervirial perturbation formalism for the problem. We also used a non-perturbative power series method to calculate the energy levels of the double well potential, as noted in the introduction and in the beginning of this section. If we use the wavefunction (2.39) in equation (2.63) and follow the same route that led us to recurrence relation (2.40), we get the following recurrence relation:

$$\left(N+2\right)\left(N+1\right)T(N+2)=\left[4\beta N+2\beta-E\right]T(N)x^{2}-\left[Z^{2}+4\beta^{2}\right]T(N-2)x^{4}$$

$$+\lambda T(N-4M)x^{2M+4} \qquad (M=1,2,3,4) \qquad (2.71)$$

which gives the terms in the power series for the wavefunction. The use of the recurrence relation (2.71) it similar to that of the recurrence relation (2.40). We also used the finite difference method to compute the energy eigenvalues, to give another check on the eigenvalues for this potential.

2.3.3 Results and discussion

Three methods have been used for calculating the eigenvalues ofthe double well potential:

$$V(x)=-Z^{2}x^{2}+x^{2N} \qquad (2N=4,6,8,10,...30) \qquad (2.72)$$

Each method has its own limited range of applicability in which it gives excellent numerical eigenvalues. The computations were carried out to double-precision accuracy (20 decimal places) on a VME system with a Fortran (77) program. We list some of our results in tables (2.8,2.9,2.10,2.11). We present the eigenvalues for different values of Z^2, 2N and state number (n). The results shown in table (2.9) are yielded by power series and finite difference methods for (2N=4), ($1\le Z^2\le 100$) and state number (n= 0,10). The two methods achieve the same accuracy (18-figure), and the accuracy of our results is in good agreement with the accuracy results produced by other methods. The results in table (2.9) are computed by renormalised series and power series methods for 2N=4, ($100\le Z^2\le 200$) and ($0\le n\le 100$). The agreement between the two methods is in general good to about 16-figures but at low Z^2values (Z^2=100) and high state number (80≤n≤100), the renormalised series faces difficulties in producing the eigenvalues, while the power series method is able to give very high accuracy. In table (2.10) we list ground state results for (2N=6,8,10,12), and for 2N=6,8; $10 \le Z^2 \le 200$, and for (2N=10,12); ($50 \le Z^2 \le 5000$). The agreement between results is very good (20-digits). In the present work, we consider not only 2N=4, but extend the work to high powers (2N=6,8, 10...28,30). We list in table (2.11) the results for ($200 \le Z^2 \le 10^6$), (2N=4,8,10,12,...16,18) and ($0 \le n \le 10^6$). It is clear from our results that the renormalised series method achieves very high accuracy (20 digits). We show in table (2.12) the results for (2N=4,6,8...30); $Z^2=10^6$and n=0,5,10. Our results for the double well potential have the following consequences:

First the three methods all yielded excellent accuracy for high values of Z^2, 2N=4,6,8,..28,30 and state number n. The renormalised series produce 20-digits while the power series and finite different method yield around 18-digits.

Secondly the renormalised series work and converge very well (even with zero renormalised constant k=0) for high values of Z^2, but for low values of Z^2 the accuracy depends on the choice of the constant K. On the other hand, there was seen in some perturbation series calculations the phenomenon of bogus convergence of the perturbation series. We can overcome this situation by running the same series for different values of the renormalisation constant K, or by using another method to compute the eigenvalues.

Thirdly, as 2N increases the order of the series (M) must be increased to get converged eigenvalues. For instance at (2N=6, $Z^2=10^6$, n=100) the order of series M=9 suffices but for 2N=16 with the same parameters as for 2N=6 the order M=221 is needed. Therefore, the computation requires more time to obtain a converged eigenvalue. The numerical investigations of the double well potential shows the applicability of the renormalised series method is limited to small values of Z^2; this behaviour is clear from our results in table (2.9). In conclusion, we remark that a large part of our results (as noted in beginning of this section) are not available so far in the literature for any value of 2N and λ.

Table (2.8). Energy eigenvalues for $H=P^2-Z^2x^2+\lambda x^4$, first line by using Power series method, Second line by using Finite difference method.

Z^2	E_0	K	E_{10}	K
1	0.65765300518071512 33	8	117.49809600941412 55	5
2	0.13778584818822250 88	8	112.29611182022330 44	5
4	-1.71035045013263901 22	8	101.59911496522932 33	5
5	-3.41014276123982947 55	9	96.10173784272303 333	6
10	-20.6335767029477991 55	9	67.13680076168951 622	6
15	-50.8413872843819543 66	9	36.10324015499149 555	8
50	-615.020090902757816 55	8	-422.068788468890653 3	8
100	-2485.86788034207529 44	9	-2206.39793308583867 7	10

Table (2.9). Energy eigenvalues for $H=P^2-Z^2x^2+x^4$, first line by using Renormalised series, Second line by using Finite difference method.

n	Z^2=100	N	K	Z^2=200	N	K
0	-2485.867880342075294 4	15	4	-9980.005002815982695 5	12	10
10	-2206.397933085838670 0	37	10	-9581.667513417091650 1	23	10
20	-1933.346914656864991 1	55	10	-9186.399286294146024 9	30	10
30	-1667.186570446339405 8	90	10	-8794.269970126812022 37	35	10
40	-1408.490911220260490 5	112	15	-8405.353470599673696 7	43	10
50	-1157.977638546861798 5	164	20	-8019.728387026959805 8	53	10
60	-916.577031362996460 9 5	214	40	-7637.478513238368133 2	63	10
70	-685.55684328917519 2	277	50	-7258.693415282352855 3	76	10
80	-466.7787859914 5598	280	50	-6883.469101614010341 5	100	10
90	-263.34133 396322586	277	80	-6511.908805493704025 3	120	10
100	-81.96 8568086503131	266	90	-6144.123904678133375 8	50	10

Table (2.10) Ground-Eigenvalues of $H=P^2-Z^2x^2+x^{2N}$, first line; Power series method, second line; Finite difference method.

Z^2	2N=6	2N=8
10	-6.49926775322720373855 5	-3.89894214172766175299 9
20	-25.87334193313496322211 1	-15.62781591739413309777 7
30	-52.60592938534157782444 4	-31.42542756409901051999 9
40	-84.99472361799993657555 5	-49.86570114185737813333 3
50	-122.18207663325821604 4	-70.38126435978874599222 2
60	-163.61339155967104506 6	-92.63788167422606936777 7
70	-208.89144940573581971 1	-116.40920258886600541 1
80	-257.71347607128204661 1	-141.53001914553649406 6
90	-309.83870807596104881 1	-167.87356568705615233 3
100	-365.06971153870182453 3	-195.33899037173939921 1
200	-1060.49730659884007477 7	-518.38616407723543045 5

Table (2.10 continued)

z^2	2N=10	2N=12
50	-52.3654734889334252755	-43.1928699096025457977
100	-141.9424457741485644444	-116.330519988214583400
150	-247.150721715750570499	-200.783170018454183033
200	-363.264785592818111988	-292.821735185777180499
300	-619.770695822513347033	-493.279211261750019744
400	-901.202646602101485177	-710.129513834382311133
500	-1202.37352106781657844	-939.676279331803543055
1000	-2919.63630063364190188	-2219.48972081813268355
5000	-22294.0527656254710155	-15771.0182538124130333

Table (2.11). Energy eigenvalues for $H=P^2-Z^2x^2+x^{2M}$, by using renormalised series method.

2M	Z^2	n	Energy eigenvalues	K	N
4	200	0	-9980.0050028159826954	4	13
		109	-5816.4449312862250544	50	113
		129	-5100.0590318897258274	50	144
	1000	0	-249955.27964050032130	80	10
		100	-241041.50309696648561	80	24
		200	-232188.90692320119850	80	31
	1000000	0	-249999998585.78643863	30	1
		200	-249999432900.48208944	30	3
		500	-249998584372.97556629	30	3
		1000	-249997170161.66469846	30	3
		10000	-249971714614.57498827	30	5
		50000	-249858584730.45059914	30	7
		100000	-249717185879.62466239	30	9
		1000000	-247174577498.01323762	30	9
6	500	0	-4258.6688774276245144	30	15
		5	-3819.2954146189564726	61	300
		10	-3393.3180268582713776	98	300
	1000	0	-12108.420121823300736	18	20
		10	-10863.823057843175515	76	20
		15	-10255.624888140762639	75	300
	1000000	0	-384898179.46143444907	7	10
		100	-384498237.78001669689	9	10
		500	-382899626.49112269457	14	10
		1000	-380903964.87520528163	18	10
		10000	-345481878.91352133277	71	10
8	500	0	-1820.5389205617856685	155	5000
		5	-1308.16607088513062	333	5000
	1000	0	-4647.4912270594430333	54	2000
		10	-3201.2486360212548444	262	5000
	1000000	0	-47244589.906007874090	6	500
		100	-46755627.489189453771	22	500
		500	-44818331.790043854243	53	500
		1000	-42438588.627165190403	159	500

Table (2.11 continued)

2M	Z^2	n	Energy eigenvalues	N	K
10	500	0	-1202.37352106781	326	20000
	1000	0	-2919.6363006336419018	146	10000
	1000000	0	-16915111.894318432037	7	5000
		100	-16353718.777944851718	45	10000
		200	-15800800.650501761684	163	30000
		400	-14720236.325035974160	138	6000000
		500	-14192510.169525537853	227	10000000
		1000	-11677743.500966862589	276	5000000
12	1000	0	-2219.4897208181	316	50000
	5000	0	-15771.018263812413102	72	30000
	1000000	0	-9226557.5252702159236	11	5000
		50	-8913272.8692413813494	60	50000
		100	-8605713.0285369980016	81	1000000
		200	-8007487.6090856718034	144	6000000
		400	-6876576.6381132161111	273	8000000
		500	-6342697.57289155199	336	11000000
14	5000	0	-12569.894878042290449	154	100000
	1000000	0	-6193850.9596831714354	12	100000
		100	-5524739.6392872711763	153	9000000
		200	-4900537.3935722085611	327	5000000
16	5000	0	-10712.019695833569	308	280000
	1000000	0	-4675097.7776189004440	14	100000
		100	-3967520.7561902368199	221	12000000
		200	-3333753.123067	326	24000000
18	5000	0	-9512.740331150	326	500000
	1000000	0	-3794108.1595137526644	17	400000
		50	-3410435.5868953036452	151	9000000
		100	-3056514.452061896070	333	20000000

Table (2.12). Energy eigenvalue E_n of $H=P^2-10^6x^2+x^{2M}$

2M	E_0	N	K
4	-249999998585.78643863	1	30
6	-382901623.60062969913	3	10
8	-47244589.906007874090	6	500
10	-16915111.894318432037	7	5000
12	-9226557.5252702159236	11	5000
14	-6193850.9596831714354	12	100000
16	-4675097.7776189004440	14	100000
18	-3794108.1595137526644	17	400000
20	-3231448.2137844684225	52	200000
22	-2844228.9042498099145	38	300000
24	-2564211.6965375207819	48	400000
26	-2353439.4381257253101	77	400000
28	-2189691.1294772728892	127	400000
30	-2057317.5404059334392	69	400000
2M	E_5	N	K
4	-249999984443.65090490	2	900
6	-384878179.63464054929	6	6000
8	-47220097.786578726274	9	10000
10	-16886840.389585966567	11	50000
12	-9194969.4946575680202	17	30000
14	-6159281.7823838970287	21	200000
16	-4637807.1533750004834	26	800000
18	-3754306.3381539108434	29	800000
20	-3203487.4823806587166	303	5000000
22	-2811292.2855402582908	130	1200000
24	-2528588.1864523074806	54	5000000
26	-2315303.1307335050271	67	9000000
28	-2149192.4833116563563	69	1000000
30	-1995935.6018646606083	62	1200000
2M	E_{10}	N	K
4	-249999970301.51552117	3	900
6	-384858180.09652682594	6	2000
8	-47195610.297303128682	11	4000
10	-16858590.159141109283	15	5000
12	-9163439.3251966807468	21	50000
14	-6124832.0681987239915	30	60000
16	-4600725.5125355944917	43	60000
18	-3714832.3451350217949	65	80000
22	-2811292.2855402582908	130	1200000
24	-2492902.3316859334126	84	1200000
26	-2315303.1307335050270	67	1200000
28	-2108695.3955166933663	118	20000000

Table (2.13). Eigenvalues of double well potential, $H=P^2-Z^2x^2+x^4$, the empty spaces mean that the corresponding eigenvalues cannot be reached by the renormisled series method.

Z^2	E_0	N	K	E_{10}	N	K
50	-615.02009090275781659	25	4	-422.06878846889065343	91	16
60	-889.06227300486193004	25	10	-675.74835854298220857	67	10
70	-1213.1821651898549119	20	4	-981.43650963590381001	62	20
80	-1587.3634172895388897	20	10	-1338.6355945195635901	47	10
90	-2011.5947240357247713	17	4	-1747.0286463771624767	44	12
100	-2485.8678803420752944	16	4	-2206.3979330858386704	41	16
110	-3010.1767065098313495	16	4	-2716.5857716451493226	38	12
120	-3584.5164100613252041	16	10	-3277.4733922495277308	43	40
130	-4208.8831850873868429	15	4	-3888.9685692722225034	34	10
140	-4883.2739492013529658	15	4	-4550.9979232479539362	31	10
150	-5607.6861643754981177	14	4	-5263.5018928297392613	33	30
160	-6382.1177111017456297	14	4	-6026.4313199897000921	28	10
170	-7206.5667976672927759	14	4	-6839.7450548666047199	32	30
180	-8081.0318932598986501	13	4	-7703.4082296071414350	36	32
190	-9005.5116776698542078	12	4	-8617.3909851971302838	26	12
200	-9980.0050028159826956	13	4	-9581.6675134170916509	30	40

Z^2	E_{19}	N	K	E_{29}	N	K
50	-261.1128009969884	140	16	-101.3177	138	20
60	-493.72832020120837456	123	16	-304.82574418310	140	20
70	-781.10461613643258906	108	30	-568.9768629413375	140	32
80	-1121.8227459175537037	79	20	-889.58953481053710986	124	25
90	-1515.0768823846056310	67	20	-1264.7817258812299097	99	30
100	-1960.3504161623486054	61	20	-1693.4771234525348979	89	40
110	-2457.2860580368153526	51	12	-2174.9809381305608263	71	20
120	-3005.6233730498282292	46	12	-2708.8095772576156449	67	24
130	-3605.1650135444209181	38	12	-3294.6084917739769907	56	14
140	-4255.7568905364548164	41	10	-3932.1076040214296442	52	16
150	-4957.2757839946847806	39	12	-4621.0950319044286029	49	12
160	-5709.6212164992748582	36	10	-5361.4006061377582123	46	16
170	-6512.7099110272935837	35	12	-6152.8850175885580946	44	16
180	-7366.4718875908759766	34	10	-6995.4323880555912290	41	12
190	-8270.8476389026458667	34	16	-7888.9450191385672056	40	16
200	-9225.7860392421012573	31	10	-8833.3395796932385018	39	20

Z^2	E_{39}	N	K	E_{49}	N	K
50	23.65	56	40			
60	-134.3864	138	30			
70	-369.92345375	140	32	-187.6350	140	40
80	-667.680142016913	140	30	-457.882527	140	50
90	-1023.086737184011599	140	32	-791.05252170448	140	40
100	-1434.0054906171744749	117	30	-1182.636349770178584	137	30
110	-1899.1888163171216232	98	30	-1630.405663585995842	121	32
120	-2417.8201990908239908	84	24	-2133.0234640467371385	107	30
130	-2989.3253702521091727	70	16	-2689.5989401543841285	89	20
140	-3613.2797649313515071	70	30	-3299.4974196083640116	79	20
150	-4289.3577097095471324	61	16	-3962.2449651344950678	76	24
160	-5017.3021810218428557	57	20	-4677.4750803558315765	68	20
170	-5796.9056833124374165	53	16	-5444.8965679782860865	63	20
180	-6627.9975726007569325	51	16	-6264.2729886536170344	61	32
190	-7510.4353268231872679	48	16	-7135.4089225448923636	57	24
200	-8444.0983426739195579	48	24	-8058.1404367453636516	55	2

Table (2.13 continued)

Z^2	E_{59}	N	K	E_{69}	N	K
50						
60						
70	-31.3	170	50			
80	-263.121	140	40	-89.47	140	56
90	-570.1662364	140	50	-362.7145	140	56
100	-940.2743771491	140	36	-708.1452123	140	40
110	-1369.239504119219	139	40	-1116.457064712	133	50
120	-1854.8549208896795879	136	40	-1583.8398505019	95	36
130	-2395.7557500210651164	116	40	-2108.17737919477166	139	46
140	-2991.0138268741596687	103	40	-2688.1181443495960919	128	50
150	-3639.9584608428570838	86	24	-3322.7244062434622529	109	40
160	-4342.0833137029717077	80	30	-4011.3083110492964484	96	36
170	-5096.9933963064054984	73	24	-4753.3446350647740583	85	30
180	-5904.3726007046359721	68	32	-5548.4199298315017611	80	32
190	-6763.9626916746914429	67	30	-6396.2008403338927144	73	30
200	-7675.5491116678069292	62	24	-7296.4133277748366471	71	32
Z^2	E_{79}	N	K	E_{89}	N	K
50						
60						
70						
80						
90	-172.84	140	60	-11.2	140	64
100	-488.032402	138	42	-282.855	140	50
110	-873.05870389	155	40	-640.4631818	159	40
120	-1320.627466309276	159	30	-1066.0461733	135	56
130	-1827.3171424886562101	169	40	-1553.7247034176151	171	40
140	-2391.1444265362416835	145	40	-2100.484060462868652	161	40
150	-3010.7987700769314178	95	40	-2704.4741529950278715	147	40
160	-3685.3521178273382944	126	36	-3364.4414582393011809	133	50
170	-4414.1135420543346174	109	60	-4079.4806988304248378	122	60
180	-5196.5494174466278255	91	32	-4848.9080726802675185	111	60
190	-6032.2358317382823444	85	40	-5672.1894960584758516	94	40
200	-6920.8284161009304491	80	40	-6548.8968485308347987	88	40
Z^2	E_{99}	N	K	E_{109}	N	K
50						
60						
70						
80						
90						
100	-98.5	140	60			
110	-420.7599	151	40	-217.65	170	64
120	-821.199853	136	60	-587.6543	170	60
130	-1288.0840886	136	70	-1031.2760630	170	66
140	-1816.603509440355	162	40	-1540.07063786699	167	40
150	-2404.0890583259665518	168	50	-2110.0407404457227	166	50
160	-3048.8329917475477910	152	50	-2738.8202482064881885	171	50
170	-3749.6471827168237798	136	50	-3424.8385989487090213	149	50
180	-4505.6574830881116335	125	64	-4166.9762973144787464	138	60
190	-5316.1943569464700038	110	50	-4964.3952316470177006	121	50
200	-6180.7291424458160399	103	60	-5816.4449312862256552	112	60

Table (2.13 continued)

Z^2	E_{119}	N	K	E_{129}	N	K
150	-1822.8035987948	162	50	-1542.2956578997	167	50
160	-2434.7429901443612	162	50	-2137.00019932509	163	50
170	-3105.3102938846409295	170	60	-2791.3542283902294	160	50
180	-3833.0633305013937080	153	50	-3504.1415060634419202	172	50
190	-4616.9511808588504792	136	58	-4274.0379119004966888	148	50
200	-5456.1742418345963221	124	60	-5100.0590318897258282	132	50

2.4 Expectation value calculations $\langle x^{2N}\rangle$

2.4 .1 Introduction

Our aim in this section to find expectation values $\langle x^{2N}\rangle$ for the potential

$$V(x) = x^2 + \lambda x^4 \tag{2.73}$$

However to find an expectation value such as $\langle x^{2N}\rangle$ for a bound state, we need to have the eigenfunction $\Psi(x)$ for all x if we wish to apply the definition

$$\langle x^{2N}\rangle = \int \Psi^2(x)\ x^{2N} dx \tag{2.74}$$

To find $\Psi(x)$ for arbitrary x and for any state number (n=0,1,2..9,10), is not easy. However Killingbeck [12,1979] has applied a very simple perturbative numerical algorithm for the calculation of an expectation value, based on the formula

$$\langle x^{2N}\rangle = \mathrm{Lt}_{\varepsilon\longrightarrow 0} \frac{1}{2\varepsilon}\left[E(H + \varepsilon x^{2N}) - E(H - \varepsilon x^{2N})\right] \tag{2.75}$$

This algorithm demonstrate that expectation values can be determined by an approach based on eigenvalue calculations, without the explicit use of wavefunctions. The way in which we can calculate is as follows; we do two calculations, to get two E values, with $\mp\varepsilon x^{2N}$ included in the potential

$$E_+ = x^2 + \lambda x^4 + \varepsilon x^{2N} \tag{2.76}$$

$$E_- = x^2 + \lambda x^4 - \varepsilon x^{2N} \tag{2.77}$$

where ε is a very small number. The value of $\langle x^{2N}\rangle$ is then given by

$$\langle x^{2N}\rangle = \frac{1}{2\varepsilon}\left[E_{+} - E_{-}\right] \tag{2.78}$$

The Hellmann-Feynman and the virial theorem also provide relationships between the energy and the expectations values $\langle x^2\rangle$, $\langle x^4\rangle$ which take the form

$$2E\left[N+1\right]\langle x^{N}\rangle = \left[2N+4\right]\langle x^{N+2}\rangle + \left[2N+6\right]\lambda\langle x^{N+4}\rangle - \frac{N}{2}\left[N^2-1\right]\langle x^{N-2}\rangle \tag{2.79}$$

We used the Hellmann-Feynman theorem to calculate the expectation values along with the energies for potential (2.73), and can calculate the coefficients in the series

$$\langle x^{2n}\rangle = A(2n,0)+A(2n,1)\lambda+A(2n,2)\lambda^2+A(2n,3)\lambda^3+\ldots \quad (n=1,2) \tag{2.80}$$

$$E=E(0)+E(1)\lambda\ +E(2)\lambda^2+E(3)\lambda^3+E(4)\lambda^4\ldots\ldots\ldots \tag{2.81}$$

2.4.2 Results and discussion

The energy eigenvalues and expectation values $\langle x^{2N}\rangle$ (2N=2,4) of the potential $V(x)=x^2+\lambda x^4$ have been calculated for state number $0\le n\le 10$ and for various values of (λ=0.1,1,10,100) using three different methods; the renormalised series method, the finite difference method and the power series method. The energy and expectation values as obtained by these methods are compared with each other, the agreement between them being very good. To use power series or finite difference methods to calculate the expectation values $\langle\Psi|x^{2N}|\Psi\rangle$ (2N=2,4) of the x^{2N}, we simply calculate the energy twice, once for Hamiltonian $H+\varepsilon x^{2N}$ and once for

$H-\epsilon x^{2N}$. According to the first order energy formula the difference between them equals $2\epsilon\langle\Psi|x^{2N}|\Psi\rangle$ if ϵ is sufficiently small. It is important to point out the effect of the parameter value ϵ in obtaining high accuracy of $\langle x^{2N}\rangle$. The best values of ϵ in this calculations have been obtained by numerical search. An ϵ value $\epsilon=10^{-8}$ gave 15 digits accuracy, but larger values such as $\epsilon>10^{-8}$ produced less accuracy. Our results were checked by noting that the independently calculated values of E, $\langle x^2\rangle$ and $\langle x^4\rangle$ obeyed the virial theorem

$$E=2\langle x^2\rangle+3\lambda\langle x^4\rangle \qquad (2.83)$$

In tables (2.15) and (2.16) we list the energy E_-, E_+ and the expectation values for $\langle x^{2N}\rangle$ (2N=2,4) for state number $0\leq n\leq 10$ and for (λ=0.1,1,10,100), with the value $\epsilon=10^{-3}$. This value seems good for high values of λ and gives 10 digits accuracy, but the accuracy decrease with small values of λ. The results presented in tables (2.15,2.16) are computed by power series and renormalised series methods. The agreement between them is very good. In table (2.17) we present the energy eigenvalues and the expectation values by using renormalisd series and power series, with the smaller value $\epsilon=10^{-8}$. The two methods achieve the same accuracy. We wish to mention that to produce results by using renormalised series with a high accuracy, we worked hard to achieve that, e.g by changing the value of the overflow parameter (2^N, N=1,2,3..) and also by increasing the dimension of B(N,M) together with varying the renormalised constant. We checked some of our results which are given in tables (2.16,2.17,2.18) by using the finite difference method, which gives the same accuracy as that achieved by the power series. Our results also agree with those available results reported in the literature.

Table (2.14) Calculations for energy and expectation values for potential $V(x)=x^2+\lambda x^4$, First line; renormalised series calculation, Second line; power series calculations, with digits before the last digit omitted; by applying approach

$$\langle x^N\rangle = Lt_{\varepsilon \longrightarrow 0} \frac{E(H+\varepsilon x^N)-E(H-\varepsilon x^N)}{2\varepsilon}\text{, where } \varepsilon=10^{-3}$$

n	λ	E_+	E_-	$\langle x^2\rangle$
0	0.1	1.0657312508 8	1.0648396060 0	0.4458223854 4
	1	1.3926574323 3	1.3920458050 0	0.3058136507 7
	10	2.4493355238 8	2.4490126139 9	0.0161454961 1
	100	4.9994948571 1	4.9993402324 4	0.0773123734 4
1	0.1	3.3081357074 4	3.3056079231 1	1.2638921729 9
	1	4.6496139110 0	4.6480114098 8	0.8012505993 3
	10	8.5994107868 8	8.5985961196 6	0.4073374364 4
	100	17.830385818 8	17.829999612 2	0.1931030445 5
2	0.1	5.7499260520 0	5.7459919765 5	1.9670377164 4
	1	8.6562053559 9	8.6538944749 9	1.1554405209 9
	10	16.636489980 0	16.635352994 4	0.5684930636 6
	100	34.874251496 6	34.873717026 6	0.2672348645 5
3	0.1	8.3552785070 0	8.3500765658 8	2.6009706620 0
	1	13.158271378 8	13.155336331 1	1.4675232168 8
	10	25.806989984 4	25.805562436 6	0.7137739458 8
	100	54.385626271 1	54.384956870 0	0.3347008638 8
4	0.1	11.101781814 4	11.095408804 4	3.1865048938 8
	1	18.059308332 2	18.055806453 3	1.7509395029 9
	10	35.886016698 8	35.884325736 6	0.8454807074 4
	100	75.877399853 3	75.876608202 2	0.3958257267 7

Table (2.14 continued)

5	0.1	13.9736613655	13.9661903688	3.73549869988
	1	23.2994554744	23.2954273399	2.01406774622
	10	46.7300486422	46.7281131499	0.96774664688
	100	99.0332898900	99.0323847399	0.45257507266
6	0.1	16.9590498655	16.9505388177	4.25552383533
	1	28.8376001199	28.8330767111	2.26170395977
	10	58.2423815288	58.2402159411	1.08279342022
	100	123.641203600	123.640191655	0.50597467888
7	0.1	20.0486150333	20.0391114633	4.75178505555
	1	34.6433452333	34.6383513199	2.49695708222
	10	70.3522440066	70.3498598622	1.19207230944
	100	149.546214144	149.545100744	0.55669760000
8	0.1	23.2347798677	23.2243237633	5.22805198944
	1	40.6931080222	40.6876640522	2.72198485177
	10	83.0051636233	83.0025704422	1.29659012144
	100	176.629261166	176.628050744	0.60521082288
9	0.1	26.5112415455	26.4998672177	5.68716399899
	1	46.9679478222	46.9620710988	2.93836210944
	10	96.1576600588	96.1548658955	1.39708150522
	100	204.795426366	204.794122655	0.65185526722
10	0.1	29.8726561833	29.8603935300	6.13132616899
	1	53.4522493777	53.4459548122	3.14728269011
	10	109.774064966	109.771076755	1.49410316655
	100	233.966922766	233.965528988	0.69889213422

Table (2.15) Calculations for energy and expectation values for potential $V(x)=x^2+\lambda x^4$, First line; Renormalised series calculation, Second line; Power series calculations, with digits before the last digit omitted; by applying approach

$$\langle x^N\rangle=\mathop{Lt}_{\varepsilon\longrightarrow 0}\frac{E(H+\varepsilon x^N)-E(H-\varepsilon x^N)}{2\varepsilon}\text{ , where }\varepsilon=10^{-3}$$

n	λ	E_+	E_-	$\langle x^4\rangle$
0	0.1	1.0658637339 9	1.0647061263 3	0.5788037991 1
	1	1.3926118200 0	1.3920913371 1	0.2602414736 6
	10	2.4498826072 2	2.4484650975 5	0.0708754831 1
	100	5.0010319464 4	4.9978020840 0	0.1614931223 3
1	0.1	3.3094655735 5	3.3042716379 9	2.5969677958 8
	1	4.6498278726 6	4.6477969980 0	1.0154372948 8
	10	8.6015974093 3	8.5964078561 1	0.2594776632 2
	100	17.836005462 2	17.824376135 5	0.0581466326 6
2	0.1	5.7539959659 9	5.7419033499 9	6.0463079955 5
	1	8.6571640856 6	8.6529346391	2.1147232607 7
	10	16.641086144 4	16.630753518 8	0.5166312684 4
	100	34.885426983 3	34.862533969 9	0.1144650693 3
3	0.1	8.3631613706 6	8.3421563357 7	10.502517462 2
	1	13.160210159 9	13.153395653 3	3.4072529821 1
	10	25.814399827 7	25.798147339 9	0.8126244202 2
	100	54.403190940 0	54.367380340 0	0.1790529989 9
4	0.1	11.114316655 5	11.082812529 9	15.752062771 1
	1	18.062407887 7	18.052704100 0	4.8518935404 4
	10	35.896565586 6	35.873769442 2	1.1398071955 5
	100	75.902024185 5	75.851967274 4	0.2502845544 4

Table (2.15 continued)

5	0.1	13.9915440477	13.9482175155	21.6632659300
	1	23.3038626177	23.2910164111	6.42310297833
	10	46.7440072277	46.7141448300	1.49311985299
	100	99.0655356977	99.0001172277	0.32709235064
6	0.1	16.9828789022	16.9265867733	28.1460645255
	1	28.8434399679	28.8272320111	8.10397812266
	10	58.2599845344	58.2226007200	1.86919073100
	100	123.681560311	123.599807800	0.40876256933
7	0.1	20.0789181300	20.0086488611	35.1346342311
	1	34.6507275977	34.6309629711	9.88231296488
	10	70.3737001577	70.3283888777	2.26556398399
	100	149.595118444	149.496163588	0.49477429844
8	0.1	23.2720307344	23.1868735855	42.5785740833
	1	40.7021312555	40.6786336411	11.7488073599
	10	83.0306618122	82.9770546788	2.68035670877
	100	176.687109288	176.570163777	0.58472755511
9	0.1	26.5558712455	26.4549953744	50.4379354000
	1	46.9787013444	46.9513091499	13.6960973322
	10	96.1873734666	96.1251320555	3.11207056000
	100	204.862582344	204.726921600	0.67830367144
10	0.1	29.9250611733	29.8077007800	58.6801966988
	1	53.4648154111	53.4333790488	15.7181815077
	10	109.808153955	109.736964366	3.55947946055
	100	234.043724277	233.888675944	0.77524163422

Table (2.16) Calculations for energy and expectation values for potential $V(x)=x^2+\lambda x^4$, first line by using power series, second line by using renormalised series method with $\varepsilon=10^{-8}$.

n	λ	E_n	$\langle x^2\rangle$	$\langle x^4\rangle$
0	0.1	1.0652855095437176 6	0.44582235824066 6	0.57880264354132 2
	1	1.3923516415302918 8	0.30581365071758 8	0.26024144669837 7
	10	2.4491740721183869 7	0.16145496089184 4	0.07087547167782 2
	100	4.9994175451375878 8	0.07731237343730 0	0.01614930932750 0
1	0.1	3.3068720131529135 5	1.26389211766864 4	2.59695925938542 2
	1	4.6488127042120775 5	0.80125059554115 5	1.01543717104325 5
	10	8.5990034548077726 6	0.40733743637874 4	0.2947761940167 7
	100	17.830192715952522 2	0.19310304450722 2	0.05814662208979 9
2	0.1	5.7479592688335633 3	1.96703766221280 0	6.04627981469316 6
	1	8.6550499577593096 6	1.15544051919958 8	2.11472297312004 4
	10	16.635921492413757 5	0.56849306360089 9	0.51663117884040 0
	100	34.873984261994777 7	0.26723486462936 6	0.11446504844245 5
3	0.1	8.3526778257857547 7	2.60097061177047 7	10.5024553408159 9
	1	13.156803898049875 5	1.46752321539066 6	3.40725248908951 1
	10	25.806276215055640 39	0.71377394584474 4	0.81262427744553 3
	100	54.385291571603103 3	0.33470086388409 9	0.17905296614611 1
4	0.1	11.098595622633043 3	3.18650484762779 9	15.7519530912581 1
	1	18.057557436303252 2	1.75093950176114 4	4.85189281092698 8
	10	35.885171222253873 3	0.84548070739381 1	1.13980699358220 0
	100	75.877004028669724 4	0.39582572678423 3	0.25028450858367 7
5	0.1	13.969926197742799 9	3.73549865728394 4	21.6630962772497 7
	1	23.297441451223189 9	2.01406774527822 2	6.42310198688891 1
	10	46.729080900817113 2	0.96774664678119 9	1.49311958690849 9
	100	99.032837315407491 1	0.45257507264502 2	0.32709229056705 5

Table (2.16 continued)

6	0.1	16.9547946861441511	4.25552379593961 1	28.14582364754977
	1	28.8353384595042488	2.26170395885470 0	8.103976847264944
	10	58.2412987397532400	1.082793420257411	1.869190396641288
	100	123.640697626678166	0.505974678819200	0.408762494230133
7	0.1	20.0438636041884611	4.751785018897811	35.134311887976 11
	1	34.6408483211113322	2.496957081437433	9.882311386078822
	10	70.3510519392346533	1.192072309472300	2.265563577343000
	100	149.545657443288222	0.556697600065233	0.494774207477199
8	0.1	23.2295521799392899	5.228051955206888	42.57816089841833
	1	40.6903860821064444	2.721984850986511	11.74880546004444
	10	83.0038670375852900	1.296590121385933	2.680356226493788
	100	176.628655957714355	0.605210842289588	0.584727447577111
9	0.1	26.5055547525366177	5.687163966763822	50.43742273002999
	1	46.9650095056755277	2.938362108797033	13.69609509602711
	10	96.1562629811977599	1.397081505257622	3.112069999022755
	100	204.795477451294477	0.651855267254744	0.678303546594788
10	0.1	29.8665252346712788	6.131326138564711	58.67957652513955
	1	53.4491021396652644	3.147282689543199	15.71817892019299
	10	109.772570843329744	1.494103166531900	3.559478817708977
	100	233.966922587623599	0.698892134263044	0.775241491497944

CHAPTER THREE

TWO, THREE AND (N=4,5,6..) DIMENSIONAL PROBLEMS

3.1 Introduction

The aim of this chapter is to investigate numerically the potentials in two, three and N dimensions which are given as below

$$V(x,y)=\frac{1}{2}\left[x^{2}+y^{2}\right]+\lambda\left[a_{11}x^{4}+2a_{12}x^{2}y^{2}+a_{22}y^{4}\right] \qquad (3.1)$$

$$V(r)=\mu r^{2}+\ell(\ell+1)r^{-2}+\lambda r^{2M} \qquad (2M=4,6,8) \qquad (3.2)$$

$$V_{N}(r)=\mu r^{2}+\frac{1}{4}\left[[N+2\ell-3][N+2\ell-1]\right]r^{-2}+\lambda r^{4} \qquad (3.3)$$

We used three methods, the inner product method, the renormalised series method, and the power series method to calculate the eigenvalues for the potentials given above. In two dimensions we computed the eigenvalues for different values of the potential parameters (a_{11},a_{22},a_{12}) and for many eigenstates ($E_{n1,n2}$ n_1,n_2=0,1,2,3), over a wide range of λ values. In three dimensions we computed the eigenvalues for high values of the state number n, for various values of the angular momentum ℓ, perturbation parameter λ, and for different power indices (2M=4,6,8). We also calculated the s-state energy eigenvalues for spherically symmetric states in N dimensions. This chapter is divided into two sections as follows. Section one is concerned with the two- dimensional oscillator, and contains all the necessary equations and recurrence relations to calculate the energy eigenvalues for different eigenstates. Section two is concerned with three and N (N=1,2,3,4,5,6----1000) dimensional oscillators and with relations which can be used to compute the energy eigenstates. The abundance of studies of the one-dimensional anharmonic oscillator eigenvalue problem is not matched in the case of multidimensional problems; there are few reported results. We may divide the main methods used in this work to compute eigenvalues into two groups. Our perturbative methods (of inner product and hypervirial type) use a renormalisation parameter K, which is helpful in improving convergence. We also use a non-perturbative method, the power series method. These methods have been used effectively to calculate the energy eigenvalues even for high state numbers and large values of the perturbation parameters.

3.2 TWO DIMENSIONAL PROBLEM

3.2.1 Review of the two dimension oscillator problem

A review and investigation of the two-dimensional perturbed oscillator is the main objective of this section. Many techniques have been used to obtain the energy eigenvalues for this two-dimensional problem. The work of Hioe, et. al [19,1978] involved matrix diagonalisation. They were able to calculate energy eigenvalues for different values of λ and for various quantum numbers. To obtain high accuracy by their methods involves dealing with large matrices. Ari and Demiralp [20,1985] computed the eigenvalues of a two-dimensional oscillator by using perturbation theory and Padé approximants. J Killingbeck and M.N.Jones [21,1986] used the inner product method to calculate accurate energies for six states, $E_{0,0}$,$E_{1,1}$,$E_{0,2}$,$E_{2,0}$, $E_{1,3}$,and $E_{3,1}$, for different values of (a_{11},a_{22},a_{12}).

In this section we present some extended numerical calculations using the inner product technique for a greater range of values of the perturbation constant $0.05 \le \lambda \le 5000$, and for different values of the potential parameters (a_{11}, a_{22}, a_{12}). The inner product method to calculate eigenvalues has been investigated by Killingbeck, et. al [11,1985] to compute energy eigenvalues for one-dimensional problems. We also used renormalised series and power series methods, for the special case $a_{12}=1$, to calculate the energy eigenvalues for the perturbed oscillator potential in two dimensions:

$$V(x,y)=\frac{1}{2}\left[x^2+y^2\right]+\lambda\left[a_{11}x^4+2a_{12}x^2y^2+a_{22}y^4\right] \qquad (3.4)$$

The potential is non-separable, and the energy perturbation series is expected to be divergent, so we start by introducing a renormalisation parameter, and write the potential in the form

$$V(x,y)=\mu^2\left[x^2+y^2\right]+\lambda\left[V(x,y)-\beta(x^2+y^2)\right] \qquad (3.5)$$

where

$$\mu^2=1+\lambda\beta \qquad (3.6)$$

The use of parameter β is helpful in improving convergence in this techniques and β plays the same role as the renormalisation constant K used for the one-dimensional oscillator. The Schrödinger equation for the potential (3.5) can be written

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right]\Psi(x,y)=E\Psi(x,y) \qquad (3.7)$$

The energy eigenvalues of the unperturbed oscillator is given by

$$E=\left[n_1+n_2+1\right]\mu \qquad n_1,n_2= 0,1,2,3\ldots\ldots \qquad (3.8)$$

In each state the energy eigenvalues depend on a pair of quantum numbers (n_1,n_2).

3.2.2 The recurrence relation for the Inner product

To find the recurrence relations which allow us to calculate the eigenvalues we use the function:

$$\Phi(x,y)=\left(x^{P_1}y^{P_2}\right)\exp\left[-\frac{\mu}{2}\left(x^2+y^2\right)\right] \qquad (3.9)$$

where the p_1 and p_2 are parity indices, with values 0 for even parity and 1 for odd parity. The inner products

$$A(N,M)=\langle\Phi|x^{2M}y^{2N}|\Psi\rangle \qquad (3.10)$$

play a key role in this technique. The next step is to work out the quantity

$$EA(M,N)=\langle\Psi|H\ x^{2M}y^{2N}|\Phi\rangle \qquad (3.11)$$

and then to substitute the perturbation expansions

$$A(M,N)=\sum_K A(M,N,K)\lambda^K \qquad (3.12)$$

$$E=\sum_K E(K)\lambda^K \qquad (3.13)$$

into the A(M,N) recurrence relation. The result is the new recurrence relation

$$\sum_{1}^{k} E(I)A(M,K,K-I)=a_{11}A(M+2,N,K-1)+a_{22}A(M,N+2,K-1)$$

$$+a_{12}A(M+1,N+1,K-1)-\beta A(M+1,N,K-1)$$

$$+4\mu\left[M+N-S_1-S_2\right]A(M,N,K)-2M\left[2M+2P_1-1\right]A(M-1,N,K)$$

$$-2N\left[2N+2P_2-1\right]A(M,N-1,K) \qquad (3.14)$$

In writing the relation (3.14) we have moved one term E(0)A(M,N,K) from the sum over I to the right of the equation, and have expressed the unperturbed energy in the form

$$E(0)=\mu\left[2+2P_1+2P_2+4S_1+4S_2\right] \qquad (3.15)$$

The parity indices for x and y are P_1 and P_2 (0 or 1). The x and y state numbers S_1 and S_2 (0,1,2), specify which particular state is being treated. When $P_1=P_2$, we can further specify an x-y interchange symmetry index P_3 (0 or 1) such that

$$A(N,M,K)=\left(-\right)^{P_3} A(M,N,K) \qquad (3.16)$$

The initial condition imposed on the A(N,M,K) if $P_1=P_2$ is

$$A(S_1,S_2,0)=\left(-\right)^{P_3} A(S_2,S_1,0)=1 \qquad (3.17)$$

and the recurrence relation (3.14) is then used as follows. If the energy sum up to $E(Q)\lambda^Q$ is required, then the indices have the ranges set out below if $P_1=P_2$, with the convention $S_1\leq S_2$ on the state labels):

$$K=0,1,2,........Q,$$

(fixed K) $N=0,1,2,\ldots\ldots\ldots,S_2+2Q-2K$,

(fixed K, N) $M=0,1,\ldots\ldots,N-P_3$.

The indices are scanned in the order given above and the relation (3.17) is used to work out A(M,N,K) in term of lower order elements which are already known. Then we can get A(N,M,K) from the symmetry relation (3.17). E(K) is found from the equation for the special case $M=S_1$, $N=S_2$

3.2.3 The recurrence relation for the renormalised series approach

The renormalised series method was seen to work very well in previous chapters and produced highly accurate results for the problems investigated in chapter one. As we indicated in section (3.1) the renormalised series can be used to compute the energy eigenvalues for equation (3.7) in some cases. When the relationship $a_{12}=a_{11}=a_{22}=1$ holds, the equation (3.7) has a circular symmetry. The energy levels are then most appropriately characterized by the quantum numbers (n_r,m) rather than (n_1, n_2). Letting $x=r\cos\theta$, $y=r\sin\theta$, such that $r^2=x^2+y^2$, the radial part of the eigenvalue equation (3.7) is

$$\left[\frac{1}{2}\left(-\frac{d^2}{dr^2}-r^{-1}\frac{d}{dr}+\frac{m^2}{r^2}+r^2\right)+\lambda r^4\right]\Psi(r)=E\Psi(r) \qquad (3.18)$$

If we set

$$\Psi(r)=\left[\ r\ \right]^{-\frac{1}{2}}\Phi(r) \qquad (3.19)$$

we get

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{1}{2}V_m\right]\Phi(r)=E\Phi(r) \qquad (3.20)$$

$$V_m=\left[m^2-\frac{1}{4}\right]r^{-2}+r^2+2\lambda r^4 \qquad (3.21)$$

$$=\left[m^2-\frac{1}{4}\right]r^{-2}+\left(\mu-\lambda K\right)r^2+2\lambda r^4,\ \mu=1+\lambda K$$

If we apply the Hypervirial and Hellmann-Feynman theorems to the potential given by (3.21), we get the following recurrence relation after some algebra

$$\left(2N+2\right)\sum_{0}^{M} E(I)B(N,M-I)=N\left[\left(m^2-\frac{1}{4}\right)-\frac{1}{4}\left(N^2-1\right)\right]B(N-2,M)$$

$$+\left(N+2\right)\left[\mu A(N+2,M)-KB(N+2,M-1)\right]+\left(2N+6\right)B(N,M-1) \qquad (3.22)$$

$$\left(M+1\right)E(M+1)=B(4,M)-KA(2,M) \qquad (3.23)$$

From the recurrence relations (3.22) and (3.23), we can find the energy coefficients with the help of the E(0) value and the condition B(0,0)=1. The unperturbed energy is

$$E(0)=\left[2n_r+|m|+1\right]\sqrt{\mu} \qquad (3.24)$$

$$\mu=1+\lambda K$$

$$2n_r+|m|=n$$

$$n_r=0,1,2,3,.......$$

$$m = 0,\mp1,\mp2,.......$$

where n_r and m are the orbital quantum number and the magnetic quantum number. The expression $(2n_r+|m|+1)$ show that a degeneracy exists between energy levels to the degree that all allowable combinations of n_r and m consistent with the same values of the m and n_r yield the same energy levels. For example $E_{1,1}$ and $E_{0,2}$ have the same quantum numbers (n_r=0,m=2) and have the same perturbed energy eigenvalues.

3.2.4 The Power series method

We used the power series method to compute the energy eigenvalues in two-dimensions for the case ($a_{12}=a_{11}= a_{22}=1$). We start from the Schrödinger equation (3.21). The regular solution to equation (3.21) will behave as r^{ℓ} near the origin, so we postulate $\Phi(r)$ to be of the form:

$$\Phi(r)=\text{Exp}\left(-\tfrac{1}{2}\beta r^2\right)\sum_{0}^{\infty} A(N)r^{N+\ell} \tag{3.25}$$

and use the notation

$$\sum T(N)=\sum A(N)r^{N} \tag{3.26}$$

Inserting these relations (3.25) and (3.26) into equation (3.20) yields the recurrence relation

$$\begin{aligned}\left(N+2\right)\left[N+2\ell+3\right]T(N+2)&=\left[\left(2N+2\ell+3\right)\beta-E\right]r^2T(N)\\ &+\left[\mu-\beta^2\right]r^4T(N-2)+\lambda r^6T(N-4)\end{aligned} \tag{3.27}$$

where

$$\ell=|m|-\frac{1}{2}$$

The calculation starts at N=0, with T(0)=1, and with all lower coefficient zero.

3.2.5 Results and discussion

In this section we investigate and discuss the results of the numerical calculations for the two-dimensional systems. It is clear from our listed results in tables (3.1-3.4) that the accuracy can be expected to decrease rapidly as λ increases. Let us now turn to the renormalisation constant (K) which is the heart of this calculation for perturbative methods. We can see from the results that the accuracy depends on the value of the renormalised constant (K). One continues to change the renormalised constant until energy eigenvalues of the best required accuracy are obtained. The values of energy in table (3.1) are for the case $a_{12}=a_{11}=a_{22}=1$; we show some energies for states $(n_1,n_2=0,1,2,3)$ and for $0.05\leq\lambda\leq5000$. The three approaches work very well for two-dimensional oscillator, and the results obtained by these methods are in good agreement with each other. We observe that the three approaches yield a high number of accurate digits (14) for the eigenvalues at low values of λ. For higher values of the perturbation constant λ the power series method gives more digits than the inner product method with renormalised series.

One main difference between the two perturbative techniques lies in the values of the renormalised constant. For the hypervirial approach the values of (K) increases as the perturbation constant increase, while for the inner product method the values of (K) decrease as the perturbation constant increases. Also the hypervirial method can only work for the case of a symmetric potential $a_{11}=a_{22}=a_{12}=1$ in which the potential reduces to a one dimensional potential. The inner product method deals with more general parameter values, but still requires $a_{11}=a_{22}$, since the equations used exploit this symmetry to reduce computation. To get the energy eigenvalues of Killingbeck and Jones [21,1980] it is necessary to multiple our values by 2, since they used $-\nabla^2$ in their Hamiltonian. All numerical calculations were done on the ICL (VME) system using double precision arithmetic. A good rate of convergence was achieved for all techniques and was relatively insensitive to the choice of the state number. Summarising our results we can say the following:

1. We succeeded in finding the energy eigenvalues for states $E_{0,0}$, $E_{1,0}$, $E_{0,1}$, $E_{1,1}$, $E_{0,2}$, $E_{2,0}$, $E_{1,3}$,$E_{3,1}$, with excellent accuracy in two-dimension even for high values of λ ($0.05 \le \lambda \le 5000$) and for different values of the potential parameters ($a_{12}=1,-1,0$); ($a_{11}=a_{22}=1,0$). The set of tables (3.1,3.2,3.3,3.4) cover a wide range values of (λ).

2. We have found that the three methods work very well to determine the energy eigenvalues, and give high accuracy. Our results are in good agreement with other reported results given by Killingbeck [21,1986], Hioe, et. al [22,1978], Ari and Demiralp [20,1985].

3. We avoid the phenomenon of bogus convergence by computing the energy eigenvalues for different values of the renormalisation constant K. We believe that some of our results may be improved in accuracy with a better choice of K.

4.We calculated the energy eigenvalues for (68) states for the symmetric potential $V(r)=(m^2-\frac{1}{4})r^{-2}+2r^4$ by using the power series method for high quantum numbers $(0\leq m\leq 400)$ and $(1\leq n\leq 600)$. This approach produces (20) digits and the results are presented in table (3.4). We wish to note that the results yielded by the inner product were improved by using Aitken extrapolation; it seem that extrapolation improves the convergence of the perturbation series and gives extra digits.

Table (3.1) Energy eigenstates $E_{n1,n2}$ for $a_{11}=a_{22}=1$ upper line; power series method, second line; inner product, lower line renormalised series method, the numbers in the bracket corresponding to $(n_r, |m|)$.

λ	$E_{00}, a_{12}=1,(0,0)$	N	K	$E_{11}, a_{12}=1,(0,2)$	N	K
0.05	1.0842986056346 1.0842986056346 6	22 27	15 20	3.4541660556159 3.4541660556159 9	19 26	14 20
0.1	1.1501881250606 1.1501881250606 6	31 55	14 25	3.7723225907160 3.7723225907160 0	24 35	13 20
0.3	1.3396594184964 1.3396594184964 6	36 79	10 25	4.6179820140228 4.6179820140228 8	36 74	12 15
0.5	1.4760250459814 1.4760250459814 8	35 152	8 40	5.1953136477518 5.1953136477518 8	40 62	10 17
0.7	1.5866048866704 1.5866048866704 7	45 169	8 40	5.6530457466566 5.6530457466566 5	39 74	9 25
1	1.7241840692602 1.7241840692602 2	50 177	8 30	6.2138150782789 6.2138150782789 9	39 71	8 30
2	2.0603939148148 2.0603939148148 8	49 89	6 60	7.5587968359841 7.5587968359841 8	44 55	7 40
3	2.3057043582553 2.305704358255 2	44 90	5 80	8.5262241756526 8.5262241756526 5	44 54	6 50
4	2.5046993203828 2.504699320382 0	50 93	5 100	9.3055741968355 9.3055741968355 3	48 52	5.5 60
5	2.6746764097032 2.674676409703 9	44 91	4 120	9.9684501870056 9.968450187005 0	42 61	5 80
10	3.3012105709687 3.30121057096 0	35 66	3 140	12.396815561409 12.396815561409 0	46 50	4 100
50	5.5117989643904 5.51179896 64	31 37	2 220	20.884372171987 20.884372171 2	30 66	2 500
100	6.9118993381066 6.9118993 3	21 167	1.2 2000	26.236239882895 26.23623988 8	27 82	1.8 1000
500	11.756694591564 11.756694 5	22 154	0.75 6000	44.716717016874 44.71671702 0	20 70	0.8 3000
1000	14.797339112653 14.797338 9	16 135	0.5 8000	56.303967659458 56.303967 76	15 75	0.6 5000
5000	25.274022474051 25.2740 2	15 51	0.4 10000	96.210280600953 96.21028 80	15 38	0.4 8000

Table (3.1 continued)

λ	$E_{02}, a_{12}=1,(1,0)$	N	K	$E_{20}, a_{12}=1,(0,2)$	N	K
0.05	3.5198537922332			3.4541660556159		
	3.5198537922332	29	20	3.4541660556159	19	14
	2	29	20	9	21	16
0.1	3.8766416198911			3.7723225907160		
	3.8766416198911	38	17	3.7723225907160	24	13
	1	39	18	0	32	18
0.3	4.8105255385415			4.6179820140228		
	4.810525538541	37	12	4.6179820140228	36	12
	1	68	13	8	76	16
0.5	5.4412177884099			5.1953136477518		
	5.441217788409	37	9	5.1953136477518	40	10
	8	56	15	8	58	16
0.7	5.9388856534267			5.6530457466566		
	5.93888565342	35	8	5.6530457466566	39	9
	2	52	18	6	67	24
1	6.5465683556350			6.2138150782789		
	6.54656835563	39	7.5	6.2138150782789	39	8
	3	50	20	8	56	25
2	7.9981590720375			7.5587968359841		
	7.9981590720	37	6	7.5587968359841	44	7
	01	47	30	4	42	30
3	9.0389864961385			8.5262241756526		
	9.0389864961	36	5	8.5262241756526	44	6
	1	42	35	5	36	35
4	9.8761746038637			9.3055741968355		
	9.8761746038	35	4.5	9.3055741968355	46	5
	8	39	40	3	33	40
5	10.587567685461			9.9684501870056		
	10.587567685	29	4	9.9684501870056	43	5
	53	47	60	0	45	60
10	13.190071603429			12.396815561409		
	13.190071603	33	3.5	12.39681556140	42	4
	33	60	120	0	52	110
50	22.266904679055			20.884372171987		
	22.2669047	32	2.5	20.884372171	30	2
	678	31	200	19	33	220
100	27.984562615242			26.236239882895		
	27.9845626	27	1.5	26.23623988	27	1.8
	614	35	350	829	35	350
500	47.718724902029			44.716717016874		
	47.718724	22	0.9	44.71671702	20	0.8
	490	33	1000	16	29	1000
1000	60.089282034393			56.303967659458		
	60.08928	18	0.6	56.303967	15	0.6
	821	34	2000	766	29	1800
5000	102.68887287128			96.210280600953		
	102.6888	11	0.3	96.21028	15	0.4
	873	28	5000	806	24	4500

Table (3.1 Continued)

λ	$E_{13}, a_{12}=1, (0,4)$	N	K	$E_{31}, a_{12}=1, (1,2)$	N	K
0.05	6.0422359263878 6.0422359263878 8	25	20	6.2076280889676 6.2076280889676 6	27 25	20 20
0.1	6.7213125523637 6.7213125523637 7	29 31	18 20	6.9707691664077 6.9707691664077 7	30 37	16 20
0.3	8.4545696693009 8.4545696693009 9	43 78	16 18	8.8854630915511 8.885463091551 11	32 93	12 18
0.5	9.6087617479444 9.6087617479444 4	46 66	14 20	10.146914853768 10.14691485376 68	31 82	10 24
0.7	10.514815636683 10.514815636683 3	47 56	13 22	11.132938889040 11.13293888904 40	32 58	9 22
1	11.617519077229 11.617519077229 9	48 49	12 25	12.329546221690 12.32954622169 90	31 59	8 26
2	14.241725289107 14.241725289107 7	41 37	8 30	15.167593664968 15.1675936649 96	29 41	6 30
3	16.118242454196 16.118242454196 6	43 34	7 35	17.191851764040 17.1918517640 03	30 47	5.5 40
4	17.625712314489 17.625712314489 9	37 37	5.5 45	18.816020919322 18.8160209193 32	31 52	5 60
5	18.905701125845 18.905701125845 5	37 44	5 60	20.194071485057 20.194071485 506	29 59	4.5 80
10	23.583299477205 23.583299477205 5	37 36	4 80	25.224641863887 25.224641863 388	31 48	4 100
50	39.871524826155 39.8715248261 15	30 37	2.2 250	42.713491135003 42.713491135 50	31 44	2.2 300
100	50.124243611725 50.124243611 172	25 33	1.6 350	53.713552989007 53.71355298 890	24 37	1.6 380
500	85.498889140468 85.4988891 1404	19 29	0.9 1000	91.653169053892 91.653169 9054	19 31	0.9 1050
1000	107.67035206511 107.670352 206	18 30	0.8 2000	115.42830289918 115.42830 0289	17 33	0.8 2000
5000	184.01504122412 184.0150 0412	15 32	0.5 7000	197.28870356871 197.288 8703	10 32	0.4 7000

Table (3.1 Continued)

λ	$E_{01}, a_{12}=1, (0,1)$	N	K	$E_{10}, a_{12}=1, (0,1)$	N	K
0.05	2.2388001803841 2.2388001803841 1	23 26	14 20	2.2388001803841 2.2388001803841 1	23 26	14 20
0.1	2.4143403273687 2.4143403273687 7	31 39	14 18	2.4143403273687 2.4143403273687 7	31 39	14 18
0.3	2.8959049500709 2.8959049500709 9	43 68	13 22	2.8959049500709 2.8959049500709 9	43 68	13 22
0.5	3.2314529999319 3.2314529999319 1	40 102	10 25	3.2314529999319 3.2314529999319 1	40 102	10 25
0.7	3.4997488466601 3.4997488466601 0	38 96	8 32	3.4997488466601 3.4997488466601 0	38 96	8 32
1	3.8303238562966 3.8303238562966 6	44 107	8 45	3.8303238562966 3.8303238562966 6	44 107	8 45
2	4.6286453903987 4.6286453903987 9	42 84	6 55	4.6286453903987 4.6286453903987 9	42 84	6 55
3	5.2058549925116 5.2058549925116 1	45 72	5.5 65	5.2058549925116 5.2058549925116 1	45 72	5.5 65
4	5.6720139476076 5.6720139476076 6	46 62	5 70	5.6720139476076 5.6720139476076 6	46 62	5 70
5	6.0691123694494 6.0691123694494 4	44 58	4.5 78	6.0691123694494 6.0691123694494 4	44 58	4.5 78
10	7.5270433782113 7.52704337821 2	44 52	3.8 110	7.5270433782113 7.52704337821 2	44 52	3.8 110
50	12.639925716725 12.639925716 67	30 33	2 220	12.639925716725 12.639925716 67	30 33	2 220
100	15.868971472615 15.86897147 726	27 31	1.5 300	15.868971472615 15.86897147 726	27 31	1.5 300
500	27.027427897759 27.027427 7897	21 30	0.8 860	27.027427897759 27.027427 7897	21 30	0.8 860
1000	34.026189981976 34.026190 01	18 39	0.65 2600	34.026189981976 34.026190 01	18 39	0.65 2600
5000	58.133690484124 58.13369 904	14 27	0.3 4500	58.133690484124 58.13369 904	14 27	0.3 4500

Table (3.2). Energy eigenstates $E_{n1,n2}$ for $a_{11}=a_{22}=0$, by using inner product method, the letters in the brackets corresponding to even or odd parity.

λ	E_{00}, a_{12}=1,(e)	N	K	E_{11}, a_{12}=1,(e)	N	K
0.1	2.0241383214157	28	8	6.2082907985657	26	8
0.2	2.0467957188325	38	6	6.3912911417583	32	6
0.3	2.0682421306988	43	5	6.5564773059808	37	5
0.4	2.0886676590731	35	3	6.7081422885770	41	4
0.5	2.1082137796985	45	3.5	6.8490530489122	38	3.5
0.6	2.1269899290285	48	3.2	6.981128077230	38	3.5
0.7	2.145083242883	50	3.2	7.105767237544	43	3.5
0.8	2.16256468586	47	3	7.224031480660	44	3.4
0.9	2.1794931149	45	3	7.33674892366	44	3.3
1.0	2.1959180852	44	2.8	7.44458136157	44	3.2
2.0	2.3395662	43	2.5	8.339449323	50	3
3.0	2.458377	41	2.2	9.03485424	49	2.5
4.0	2.561626	50	2	9.61758777	50	2.3
5.0	2.653910	48	1.8	10.1256931	46	2.2
6.0	2.73792	38	1.6	10.5798578	46	2
7.0	2.81540	39	1.5	10.0992791	42	2
8.0	2.88755	44	1.5	11.372950	45	2
9.0	2.95526	46	1.5	11.726290	48	2
10.0	3.01918	50	1.5	12.057188	45	1.8
15.0	3.2968	45	1.4	13.469681	49	1.5
20.0	3.5270	48	1.4	14.616918	50	1.4
λ	E_{02}, a_{12}=1,(e)	N	K	E_{20}, a_{12}=1,(o)	N	K
0.1	6.1592857507523	37	10	6.0716400174184	36	10
0.2	6.2953249520699	45	7	6.1377408133565	47	7
0.3	6.4155065471639	48	5	6.1995318631918	46	4.5
0.4	6.5239694436917	48	4	6.2578183515335	49	4
0.5	6.62332398024	45	3.5	6.313168654731	47	3.6
0.6	6.7153450867	46	3.5	6.36600479493	50	3.5
0.7	6.8013050520	49	3.5	6.4166518870	48	3.4
0.8	6.882152491	50	3.4	6.465367562	48	3.4
0.9	6.95861670	47	3.4	6.512360604	48	3.2
1.0	7.03127234	47	3.2	6.557803327	51	3.2
2.0	7.620032	47	2.5	6.950634	45	2.5
3.0	8.06620	48	2.4	7.27168	49	2.4
4.0	8.4360	45	2.2	7.54917	50	2.2
5.0	8.7568	49	2	7.7964	49	2
λ	E_{13}, a_{12}=1,(o)	N	K	E_{31}, a_{12}=1,(e)	N	K
0.1	10.343899981402	30	10	10.588281727226	31	10
0.2	10.642274833394	40	8	11.062705074846	40	8
0.3	10.909687297357	45	6	11.468592204749	44	6
0.4	11.154084419444	46	5	11.827386430149	48	5
0.5	11.380431070714	48	4.5	12.15131154316	50	4.5
0.6	11.592096589142	51	4.2	12.4481243454	44	4
0.7	11.79150094595	48	3.8	12.7231097106	47	3.8
0.8	11.9804560656	45	3.5	12.980056955	46	3.6
0.9	12.1603626387	45	3.4	13.221790115	47	3.5
1.0	12.3323312711	50	3.4	13.45047872	43	3.4
2.0	13.7564464	46	3	15.2786864	51	3
3.0	14.861855	45	2.6	16.64511	39	3
4.0	15.788322	49	2.5	17.76911	47	2.5
5.0	16.59651	43	2.2	18.73871	48	2.2

Table (3.2 Continued)

λ	$E_{01}, a_{12}=1$, (e)	N	K	$E_{10}, a_{12}=1$, (e)	N	K
0.1	4.0708639128944	39	12	4.0708639128944	39	12
0.2	4.1350822342067	47	8	4.1350822342067	47	8
0.3	4.1942935736199	46	5	4.1942935736199	46	5
0.4	4.2495313630102	51	4	4.2495313630102	51	4
0.5	4.301504505315	45	3.6	4.301504505315	45	3.6
0.6	4.35072736225	49	3.4	4.35072736225	49	3.4
0.7	4.3975886228	47	3.4	4.3975886228	47	3.4
0.8	4.4423912545	50	3.2	4.4423912545	50	3.2
0.9	4.485377268	46	3	4.485377268	46	3
1.0	4.526743874	49	3	4.526743874	49	3
2.0	4.8777096	48	2.4	4.8777096	48	2.4
3.0	5.157977	48	2.2	5.157977	48	2.2
4.0	5.39680	49	2	5.39680	49	2
5.0	5.60757	45	1.8	5.60757	45	1.8

Table (3.3). Energy eigenstates $E_{n1,n2}$ for $a_{11}=a_{22}=1$, by using; inner product method.

λ	E_{00} ,a_{12}=-1	N	K	E_{11} ,a_{21} =-1	N	K
0.05	1.04433382953 6575	44	10	3.12890917576 6778	46	12
0.1	1.0812823429327	44	9.5	3.232683781270	49	10
0.3	1.194693708	50	7	3.542778	48	9
0.5	1.2808133	42	6	3.774578	52	6.5
0.7	1.3525907	49	5.5	3.96682	46	6
1	1.443775	46	5	4.2105	39	5
2	1.67296	47	4.5	4.8231	48	4.5
3	1.84417	46	3.5	5.281	48	3.8
4	1.98480	48	3.2	5.659	48	3.5
5	2.1058	49	3	5.985	44	3
10	2.5577	46	2.5	7.207	46	2.5
50	4.185	31	1.4	11.6	28	1.5
100	5.22	30	1.3	14.5	22	1
500	8.85	22	0.65			
1000	11.12	21	0.4			
5000	18.9	16	0.2			
λ	E_{02} ,a_{12} =-1	N	K	E_{20} ,a_{12}=-1	N	K
0.05	3.261984721845845	46	12	3.354071144288548	40	12
0.1	3.44107624580	46	10	3.6120157403298	42	11
0.3	3.9052148	34	8	4.3174414428	47	9
0.5	4.21799	33	7	4.80879388	32	8
0.7	4.4660	24	6.5	5.2018647	27	7
1	4.7711	33	6	5.6864749	30	6
2	5.512	34	5	6.858039	30	5
3	6.055	32	4	7.706011	39	4
4	6.498	35	4	8.391257	43	3.5
5	6.878	34	3.5	8.975224	29	3.5
10	8.29	34	3.2	11.12060	27	3
50	13.4	20	2	18.65251	30	2
λ	E_{13} ,a_{12}=-1	N	K	E_{31} ,a_{12}=-1	N	K
0.05	5.577042209722313	46	14	5.313459809272	38	12
0.1	5.990228032831	47	12	5.51652835	38	10
0.3	7.113043	33	14	6.04410	31	9.5
0.5	7.894161	33	10	6.40938	28	7
0.7	8.519471	43	7	6.705	17	6
1	9.291179	39	5.5	7.075	21	5.5
2	11.16038	41	5	7.996	31	5
3	12.5159	30	5	8.686	30	4.6
4	13.6127	28	4.5	9.25	28	4.4
5	14.5481	29	4	9.74	30	4
10	17.9891	28	3	11.6	17	3
50	30.097	24	2	18.4	25	2

Table (3.4) Values of E for $V_m = (m^2 - \frac{1}{4})r^{-2} + 2r^4$, $n = 2n_r + m + 1$.

n	m	$E_{n,m}$	n	m	$E_{n,m}$
1	0	1.4771497535779945721	2	1	3.3981501760276967464
3	0	6.0033860833082771514	3	2	5.6243393493913396531
4	1	8.7004538139555255613	4	3	8.0906677703608193746
5	0	11.802433595134781574	5	2	11.534749463408076728
6	1	14.977808372321000000	6	3	14.508675257695970504
7	0	18.458818704077168861	7	2	18.245419047079048918
8	1	21.999601034420900742	8	3	21.611340607414397172
9	0	25.791792378517220594	9	2	25.611488488280248047
10	1	29.634879556288082362	10	3	29.299902799490796558
11	0	33.694279876607792998	11	2	33.536632154175749853
12	1	37.798347753896714409	12	3	37.501528172629380043
13	0	42.093807710826166293	13	2	41.952815503257419596
5	4	10.758265165443797408	6	5	13.600878059158590077
7	4	17.616153535989094860	7	6	16.599393814776394337
8	5	20.849518216129607466	8	7	19.739173054344587276
9	4	25.076185950170202224	9	6	24.201285335452976530
10	5	28.638196688780136641	10	7	27.664612666846010149
11	4	33.066977461811458538	11	6	32.294610862541875823
1	5	36.913007746802281817	12	7	36.042296443612372112
13	4	41.531946454275438213	13	6	40.837258834021116975
9	8	23.008582870458735348	10	9	26.398118422669436590
11	8	31.233371375757594792	11	10	29.899842302768836228
12	9	34.902099507843364602	12	11	33.507008578384495977
13	8	39.878053076615649884	13	10	38.665924463870911206
15	12	46.461859815974355445	13	12	37.213800511625613223
25	10	98.374602981775359967	50	25	244.70647279713012760
80	61	436.55737473447115869	80	79	411.92626609958683169
100	51	615.72015957476693747	100	81	581.45987058782485898
150	101	1028.2632957809553818	150	121	999.19230724062377362
300	201	2592.7329574173396208	300	221	2557.7535843371696925
401	300	3756.7756669860561374	401	350	3647.3034038845666264
501	350	5108.0404929172998556	601	400	6553.4105446949506296

3.3 THREE AND N DIMENSIONAL PROBLEMS

3.3.1 Introduction

J.Killingbeck [22,1985] has used the Hill determinant method to calculate the energy eigenvalues for a three-dimensional oscillator and also investigated all spherically symmetric states in any dimension (N=1,2,3 ....320). He computed the energy eigenvalues and expectation values such as $\langle r^2\rangle$ for potentials $\ell^{-1}r^4$ and $N^{-1}r^4$ and gave results of high accuracy. We extended our numerical calculations for higher powers of the perturbation index (2N=4,6,8), and for a wide range of values of angular momentum, perturbation parameter, and state number. We used two methods to produce our results for this problem, the renormalised series method and the power series method. The radial part of the three-dimensional Schrödinger equation can be written conventionally in the form

$$\left[-\frac{d^2}{dr^2}+\mu r^2+\ell(\ell+1)r^{-2}+\lambda r^{2N}\right]\Psi(r)=E\Psi(r) \qquad (3.28)$$

where (ℓ) is the angular momentum, and the energies of unperturbed levels are

$$E(0)=\left[2n+3\right]\sqrt{\mu} \qquad (3.29)$$

where n is the principal quantum number, which can be expressed as

$$n=\left(2n_r+\ell\right) \qquad (3.30)$$

Here n_r is called the radial quantum number. The energy values include zero-point energy 3 corresponding to the three degrees of freedom. n is seen to be even or odd according as

(ℓ) is even or odd. The main difference between one and three dimensional perturbations lies in the presence of the angular momentum. We have presented two methods to compute energy eigenvalues. The first approach uses a hypervirial scheme based on the formulation of recurrence relations, and the second approach uses a power series, based on relations derived by using wavefunctions.

3.3.2 Renormalised series to calculate energy eigenvalues for $H=P^2+\mu r^2+\ell(\ell+1)r^{-2}+\lambda r^{2N}$ $(2N=4,6,8)$

We used renormalised series to calculate the energy eigenvalues for the potential

$$V(r)=\mu r^2+\ell(\ell+1)r^{-2}+\lambda r^{2N} \quad (2N=4,6,8)$$

Using recurrence relations derived from the hypervirial and Hellmann-Feynman theorems which have been used by Killingbeck, with the potential terms

$$V_{-2}=\ell(\ell+1) \tag{3.31}$$

$$V_2=(\mu-\lambda K) \tag{3.32}$$

$$V_4=\lambda \tag{3.33}$$

we obtain the following recurrence relations after some algebra

$$\begin{aligned}\left(2N+2\right)\sum_{0}^{M} E(J)A(N,M-J)=N\left[2\ell(\ell+1)-\frac{1}{2}\left(N^2-1\right)\right]A(N-2,M)\\ +\left(2N+4\right)\left[\mu A(N+2,M)-KA(N+2,M-1)\right]\\ +\left[2N+2n+2\right]A(N+2n,M-1)\end{aligned} \tag{3.34}$$

$$\left(M+1\right)E(M+1)=A(2n,M)-KA(2,M) \qquad (2n=4,6,8) \tag{3.35}$$

The recurrence relations (3.34) and (3.35) suffice to compute the coefficients of energy E(M) and A(N,M) and this procedure allows us to calculate the expectation values of powers (r^N) without the explicit use of eigenfunctions. The input for our calculations are the renormalised constant K, the angular momentum ℓ and the state number n. The values of $\mu=1+\lambda K$, $E(0)=(4n+2\ell+3)\sqrt{\mu}$, are worked out by the program. The renormalised series approach seems to give results of excellent accuracy, whereas at K=0 the perturbation series diverge and do not give satisfactory numerical results.

3.3.3 The power series approach

We used the power series method to compute the energy eigenvalues for the three-dimensional perturbed oscillator , and this method works very well, producing results of high accuracy, even for large perturbation parameters. When an angular spherical harmonic factor Y_ℓ^m has been factored out of the wavefunction for a three-dimensional problem, the Schrödinger equation can be expressed as

$$\left[-D^2 - 2r^{-1}D + \ell(\ell+1)r^{-2} + r^2 + V(r)\right]\Psi(r)=E\Psi(r) \qquad (3.36)$$

We take the radial potential V(r) to have the form

$$V(r)=\lambda r^{2m} \qquad 2m=4,6 \qquad (3.37)$$

The regular solution to equation (3.37) will behave as r^ℓ near the origin. The eigenfunction $\Psi(r)$ is then given by the general form

$$\Psi(r)=\mathrm{Exp}\left[-\tfrac{1}{2}\beta r^2\right] \sum_0^\infty A(N)r^{N+\ell} \qquad (3.38)$$

We use the notation

$$T(N)=A(N)r^{N} \qquad (3.39)$$

Inserting the relations (3.38) and (3.39) into equation (3.36) yields the recurrence relation

$$\left(N+2\right)\left[N+2\ell+3\right]T(N+2)=\left[\left(2N+2\ell+3\right)\beta-E\right]r^{2}T(n)$$

$$+\left[\mu-\beta^{2}\right]r^{4}T(N-2)+\lambda T(N-2M)r^{2M+2} \quad (2M=4,6,8) \qquad (3.40)$$

The calculation starts at N=0, with T(0)=1, and all lower coefficient zero.

3.3.4 N dimensional calculations.

J.Killingbeck has applied the Hill determinant to N-dimensional anharmonic oscillators. He calculated energy eigenvalues and expectation values of type $\langle r^{N}\rangle$. Killingbeck [22,1985] has expressed the Schrödinger equation in N dimensions as:

$$D^{2}\Psi(r)-\left(N-1\right)r^{-1}D\Psi(r)+V(r)\Psi(r)=E\Psi(r) \qquad (3.41)$$

where $V(r)=\left[\mu-\lambda K\right]r^{2}+\lambda r^{4}, \quad \mu=1+\lambda K$

We used the renormalised series approach to calculate the energy eigenvalues. If we apply the hypervirial and Hellmann-Feynman theorem to the potential given by equation (3.3) we get the following recurrence relations.

$$\left(2I+2\right)\sum_{0}^{M} E(J)A(I,M-J)=\frac{I}{2}\left[\left(N+2\ell-3\right)\left(2N+2\ell-1\right)-\left(I^{2}-1\right)\right]A(I-2,M)$$

$$\left(2I+4\right)\left[\mu A(I+2,M)-KA(I+2,M-1)\right]$$

$$+\left(2I+6\right)A(I+4,M-1) \tag{3.42}$$

$$\left(M+1\right)E(M+1)=A(4,M)-KA(2,M) \tag{3.43}$$

Here N is number of dimensions. The recurrence relations (3.34) and (3.35) for three dimensions reduce to the recurrence relations (3.42) and (3.43), if we insert $\ell=(N+2\ell-3)/2$. We also used the power series method to calculate energy eigenvalues for the N-dimensional problem. If we insert $\ell=(N+2\ell-3)/2$ in relation (3.27) we obtain the relation corresponding to N dimensions.

3.3.5 Results and discussion

We have used the techniques described in this section, the renormalised series and power series methods, to compute the energy eigenvalues. Our results are given in tables (3.5,3.6,3.7, 3.8,3.9). Our energy eigenvalues cover a large range of values of angular momentum, perturbation constant λ and state number n. We have performed various numerical checks on the obtained energy eigenvalues. For example we did some calculations at zero value of angular momentum and at ($\ell=-1$). At these values the problem reduces to a one dimensional problem. Also the power series approach has been used as another approach to compute the energy eigenvalue, and the agreement between the results is very good. We list some results in table (3.5) for different values of angular momentum, and state number. We note particularly that in the case of high values of angular momentum the renormalised series approach works well. We notice from table (3.5) that for ($\lambda=100$, $\ell=100$, $n=20$) the accuracy of this approach achieves 12 significant figures. To our knowledge such a high degree of precision for the potentials considered is unprecedented. We also wish to draw attention to the fact that the renormalised series approach applies equally well to any value of (λ,ℓ,n). Our calculations in three dimensions may be regarded as a guide to future numerical calculations. As far we know, we are the first to investigate numerically the energy eigenvalues for a wide range of potential parameters in three dimensions. A sample of energy eigenvalues for potentials in three dimensions computed by using renormalised series and power series methods are displayed in table (3.6) for different values of angular momentum, and state number n. These methods lead to very accurate results. We also calculated the energy eigenvalues for higher power of the perturbation index $(2N=6,8)$. The renormalised series method was used to compute the energy eigenvalues for $(2N=6)$, $n,\ell=0,1,2,3,4$ and $\lambda=0.1$. This method achieved 6-digits accuracy; the renormalised series method has limited capability to deal with high powers $\langle r^{2N}\rangle$ $(2N=8)$ and we can only manage to calculate a few energy eigenvalues with a low accuracy. In this respect we face the same situation as for the one-dimensional oscillator in dealing with high powers of perturbation. However the power series method works excellently and gives results with 16 digits accuracy. We also computed the energy eigenvalues for s-states in $(N=1,2,3,..1000)$ dimensions for potentials $V(r)=Nr^4,N^{-1}r^4$. The renormalised series work very well for calculating the energy eigenvalues even for higher values of

N. The energy eigenvalues are compared with corresponding ones obtain by the power series method and listed in table (3.8). The agreement of our results with those of Killingbeck is good.

Table (3.5). Eigenvalues of $H=P^2+r^2+\ell(\ell+1)r^{-2}+\lambda r^4$, by using renormalised series method, the two numbers in the bracket correspond to Quantum number (n) and Angular momentum (ℓ) respectively.

λ	(0,100)	N	K	(1,100)	N	K
10	1941.43718812085389	43	20	2003.62055851455466	49	25
20	2442.33603327688921	42	15	2520.65181680286960	42	15
30	2794.05812020431	41	15	2883.69331314046	38	15
40	3074.1949418234	37	14	3172.8425759472	34	14
50	3310.826669040	34	14	3417.08551270	33	15
60	3517.710003191	33	13	3630.62225010	33	15
70	3702.734756023	34	12	3821.59680389	31	12
80	3870.896104981	29	12	3995.16524219	28	10
90	4025.580334828	28	10	4154.82289345	29	10
100	4169.201422351	31	10	4303.06145372	29	10
λ	(2,100)	N	K	(3,100)	N	K
10	2066.09518504967081	44	20	2128.85970059119358	43	20
20	2599.334455047768	42	18	2678.3822347300208	42	16
30	2973.74840103652	38	15	3064.2214269365	33	15
40	3271.95233392781	36	13	3371.5220644981	34	15
50	3523.8421427834	33	12	3631.0942437592	34	13
60	3744.063457751	33	12	3858.031166943	33	12
70	3941.015689849	31	12	4060.988826166	34	15
80	4120.016551825	30	10	4245.447329285	29	10
90	4284.670926787	29	10	4415.12162272	33	10
100	4437.54859426	27	10	4572.65993200	29	10
λ	(4,100)	N	K	(5,100)	N	K
10	2191.91271486181399	43	20	2255.252817482268746	45	20
20	2757.793412902427	40	20	2837.56622080886168	37	15
30	3155.110399690855	37	14	3246.413298382831	36	14
40	3471.54957861064	38	14	3572.0326543166	34	14
50	3738.8394593109	33	13	3847.0753975792	34	13
60	3972.5228750505	34	12	4087.536041603	31	12
70	4181.513579299	31	12	4302.587275857	34	12
80	4371.454822058	29	10	4498.036235874	28	10
90	4546.172119287	31	10	4677.819510998	29	10
100	4708.392503294	27	9	4844.74329941	29	10
λ	(6,100)	N	K	(7,100)	N	K
10	2318.87858078395864	44	20	2382.788562408605161	43	20
20	2917.698867453038	44	20	2998.189542897865	45	20
30	3338.12807642583	38	15	3430.252665351057	37	14
40	3672.96904128309	36	14	3774.3564649682	31	14
50	3955.7996360364	32	13	4065.0097259891	34	13
60	4203.0680934731	35	14	4319.1164296606	33	12
70	4424.2072079790	31	12	4546.3706384184	30	12
80	4625.1887404104	31	10	4752.9094745678	30	10
90	4810.060854865	31	10	4942.8931758487	31	10
100	4981.709272753	28	10	5119.287342452	30	10

Table (3.5 continued)

λ	(8,100)	N	K	(9,100)	N	K
10	2446.98130770891136	44	20	2511.45535196346692	41	20
20	3079.0364213129957	46	20	3160.237663787287	41	20
30	3522.7849783066610	40	15	3615.722913287366	43	20
40	3876.19263047968	36	14	3978.47522813514	38	14
50	4174.7031967392	33	13	4284.87755942354	32	12
60	4435.6784257188	33	12	4552.7514378387	32	12
70	4669.0748051960	31	12	4792.3169259014	31	12
80	4881.1955513491	29	10	5010.0440623569	29	10
90	5076.313471937	27	10	5210.318718830	29	10
100	5257.474399705	29	10	5396.267312586	27	10
λ	(10,100)	N	K	(20,100)	N	K
10	2576.20922241841174	45	22	3238.81196569573192	45	25
20	3241.7914209219405	46	20	4076.30718561972	44	25
30	3709.0643561112464	39	15	4664.202776599	33	20
40	4081.20192674615	35	14	5132.378895292	34	16
50	4395.53031055566	33	14	5527.813775535	30	15
60	4670.3328066151	31	12	5873.516071757	30	14
70	4916.094201661	30	12	6182.679475874	30	14
80	5139.452081943	34	10	6463.656086087	29	13
90	5344.905874255	28	10	6722.107336324	24	12
100	5535.662930529	28	10	6962.06877997	27	12
λ	(0,50)	N	K	(1,50)	N	K
5	629.16532829185147	53	22	668.647665496408	47	20
10	789.730556441783	57	20	839.426750777384	54	20
15	902.64397422707	50	18	959.509601105681	49	15
20	992.6387313402	42	15	1055.2136538311	44	15
25	1068.689129338	40	15	1136.086207736	42	15
30	1135.197711392	41	14	1206.810431464	39	13
35	1194.691648051	31	10	1270.074407705	40	13
40	1248.771929449	25	8	1327.580987666	35	10
45	1298.524395323	35	10	1380.485055975	35	10
50	1344.723395085	25	8	1429.610177565	30	8
λ	(2,50)	N	K	(3,50)	N	K
5	708.4935268594213	40	16	748.69932767330315	43	18
10	889.580679098124	41	15	940.1878757319985	43	15
15	1016.89907154239	51	15	1074.807297275903	45	15
20	1118.36505886080	45	15	1182.08736077491	45	15
25	1204.1042251075	44	15	1272.737174868	41	15
30	1279.082953494	41	15	1352.008902418	42	15
35	1346.151723198	37	12	1422.916889612	38	12
40	1407.116186019	25	8	1487.370519579	25	8
45	1463.200908251	27	8	1546.664671100	28	8
50	1515.279124223	28	8	1601.722697508	28	8

Table (3.5 continued)

λ	(4,50)	N	K	(5,50)	N	K
5	789.2614098875849	45	20	830.176065294112	61	30
10	991.243777094699	45	18	1042.7437514735	52	25
15	1133.22907540585	37	14	1192.1591227496	47	15
20	1246.37484615	23	10	1311.221711797	47	20
25	1341.97891168	23	10	1411.823192504	41	15
30	1425.58175488	24	10	1499.794882915	39	15
35	1500.36304520	25	9	1578.48321763	38	14
40	1568.33681893	24	10	1650.00779840	33	12
45	1630.86889192	25	8	1715.80599679	23	8
50	1688.93318179	23	8	1776.90273540	34	8
λ	(0,1)	N	K	(0,2)	N	K
0.2	6.1650668551133289	47	20	8.964493907927813081	45	18
0.4	6.9017850347770	52	20	10.15048703243291	49	18
0.6	7.47664934944	52	18	11.063537072093	49	16
0.8	7.95920408956	75	25	11.82449582386	54	20
1.0	8.3803425300	47	16	12.48555605099	60	20
1.2	8.7569760328	38	12	13.07483391163	64	20
1.4	9.0995351570	33	10	13.60948572185	70	20
1.6	9.4149786743	35	10	14.1008680499	42	14
1.8	9.7082163463	37	10	14.5569453429	37	10
2.0	9.9828610540	38	10	14.9835501066	35	10
4.0	12.107915541	46	10	18.271035707	39	10
8.0	14.87549356	40	8	22.530961046	52	10
16.	18.43724415	42	6	27.9952905	45	10
20.	19.78325190	42	6	30.0571990	47	8
λ	(0,3)	N	K	(0,4)	N	K
0.2	11.915467413289146178	44	18	15.00199301040248031	46	20
0.4	13.6112847202701596	42	15	17.25899374373014841	43	15
0.6	14.90402836035570	46	15	18.96654863720368	42	15
0.8	15.97590852220218	47	15	20.37686233369806	43	15
1.0	16.9040367035113	50	15	21.59503757424409	45	12
1.2	17.7294839852236	44	12	22.67657939480145	37	10
1.4	18.4771234244251	47	12	23.65491350281611	42	10
1.6	19.1633297680839	42	10	24.55195567083628	42	10
1.8	19.7995386098443	44	10	25.38296350143428	43	10
2.0	20.3940964325156	43	10	26.15904542728026	45	10
4.0	24.963006350820	43	8	32.110495991136	49	10
8.0	30.86283763085	51	8	39.775885005345	49	8
16.	38.413674887	50	8	49.57009862581	52	7
20.	41.259988282	43	6	53.2592845086	44	6

Table (3.5 continued)

λ	(0,5)	N	K	(0,6)	N	K
0.2	18.2117554620041711175	44	20	21.53492733399226632	41	20
0.4	21.074809613665338	48	20	25.044062605126524	34	15
0.6	23.227833563434205	43	15	27.669907540554367	50	20
0.8	25.0006114600427	43	15	29.82660338720456	40	14
1.0	26.5289175581239	48	15	31.682981512789	57	20
1.2	27.8839784388655	32	10	33.327135080818	40	12
1.4	29.1084996939278	35	10	34.811696239964	31	10
1.6	30.2303929416295	39	10	36.170976971602	37	10
1.8	31.2690430441013	38	10	37.428760968811	34	10
2.0	32.2385361700628	39	10	38.602304177711	35	10
4.0	39.6611949276483	43	8	47.575599405435	47	10
8.0	49.202495044920	44	7	59.091780144589	47	8
16.	61.37800743234	52	8	73.77239137440	48	7
20.	65.96150003067	48	6	79.2963766707	42	6
λ	(0,7)	N	K	(0,8)	N	K
0.2	24.963450521912494731	42	20	28.49057521034573453	36	20
0.4	29.1549318155875613	39	16	33.397651540446745	43	20
0.6	32.2783906427811582	44	15	37.0414061017115	46	20
0.8	34.838464422125062	44	15	40.0228778000281	48	20
1.0	37.03919765481263	44	15	42.582832667399	50	20
1.2	38.9865846699327	44	15	44.846447027866	53	20
1.4	40.7437685851541	49	15	46.887819701773	54	20
1.6	42.3518274368493	49	15	48.755129513699	60	20
1.8	43.8391893432362	36	10	50.481673892473	35	20
2.0	45.2264537604095	37	10	52.09155494175	56	20
4.0	55.8226359351935	46	10	64.37712292803	29	8
8.0	69.40381848329	51	10	80.1063093642	36	8
16.	86.7023288396	50	8	100.126668507	43	8
20.	93.2089020399	39	6	107.654314292	37	6
λ	(0,9)	N	K	(0,10)	N	K
0.2	32.11054936137011260	34	20	35.818401307982826	29	20
0.4	37.7639928600849362	42	18	42.24690950911906	26	16
0.6	41.949239731676567	40	16	46.99324638908133	33	15
0.8	45.368357482504512	42	15	50.86562617229216	37	15
1.0	48.30158155212828	43	15	54.18498461045444	42	15
1.2	50.89347528567889	43	14	57.11642024607385	44	15
1.4	53.22976729225708	44	13	59.75766162354566	46	15
1.6	55.36604659360524	44	13	62.17199622658863	44	12
1.8	57.34068787512017	42	12	64.40306979793429	44	12
2.0	59.18144308568	27	10	66.4824213570910	31	10
4.0	73.21815644059	36	10	82.32806025866	37	10
8.0	91.17248633208	37	8	102.5797423723	41	10
16.	114.0113421757	43	8	128.327598116	37	8
20.	122.596778339	34	6	138.004302608	31	6

Table (3.5 continued)

λ	(1,15)	N	K	(1,20)	N	K
1	101.91678684638399	46	20	138.04987367414238	42	20
2	125.977653245378	47	18	171.0495927508109	49	20
3	143.078976236345	51	16	184.4641817161947	51	18
4	156.777542032226	49	15	2132046935105180	50	16
5	168.388641932864	53	15	229.081655174241	51	16
6	178.563920818335	54	15	242.990634729459	51	15
7	187.679825186614	49	12	255.448445574032	50	15
8	195.975921885432	52	12	266.783777322107	46	12
9	203.615252035510	45	10	277.220148770836	40	13
10	210.714402318751	47	10	286.917354016062	41	10
15	240.540526129253	49	8	327.648559692898	38	8
20	264.335696314341	35	6	360.134624942840	41	8
25	284.455637107849	38	6	387.598465804466	34	6
30	302.05819459135	32	5	411.623282456859	37	6
35	317.80881320795	35	5	433.118658419101	38	6
40	332.12942621539	35	5	452.66118035179	31	5
50	357.5440225623	35	5	487.34049691812	35	5
60	379.7715900750	28	4	517.668757889	28	5
λ	(2,15)	N	K	(2,20)	N	K
1	118.49387948531204	44	20	155.955430901458956	42	20
2	146.73582098958453	42	15	193.4934419287675	47	20
3	166.7826427958949	46	15	220.1029137473840	49	18
4	182.8307170484548	48	14	241.391033626497	43	15
5	196.428210007448	50	15	259.421457342401	47	15
6	208.341202350853	54	15	275.214058838910	49	15
7	219.011899042153	46	12	289.357061837706	52	15
8	228.721556342141	49	12	302.224378194105	44	12
9	237.661505931336	47	10	314.070259030449	34	10
10	245.968518111394	44	10	325.076388374757	40	10
15	280.862566787661	41	8	371.299029187458	36	8
20	308.694922294554	46	8	408.159192262949	40	8
25	332.225439810830	37	6	439.317996377129	43	8
30	352.810024996765	38	6	466.573354333842	35	6
35	371.227740718914	39	6	490.958004699244	37	6
40	387.97246577136	32	5	513.12651103713	36	6
50	417.6874430307	35	5	552.46420523621	32	5
60	443.674664860	24	4	586.86499343	25	5

Table (3.5 continued)

λ	(3,15)	N	K	(3,20)	N	K
1	135.506365072906843	46	20	174.2308690641695408	43	20
2	168.042762436886417	44	15	216.40313276183877	44	18
3	191.1145148505109	46	15	246.274629469015	41	15
4	209.5753083927461	47	15	270.164043587794	45	15
5	225.212564414063	48	15	290.393152213244	43	15
6	238.909917637434	52	15	308.108906344687	50	15
7	251.177117469138	55	15	323.972441213952	50	15
8	262.338239325261	45	12	338.403877711859	42	13
9	272.613670838482	39	12	351.688816803555	37	10
10	282.160911304826	41	10	364.031304426724	39	10
15	322.258605749117	37	8	415.860427127846	34	8
20	354.236193561922	37	7	457.186283141929	39	8
25	381.268529981204	35	6	492.117402922014	36	7
30	404.914899741898	36	6	522.67091961202	30	6
35	426.07103309008	34	6	550.00531075326	30	6
40	445.30468386464	36	6	574.85475214411	34	6
50	479.43500361690	35	5	618.9482929265	31	6
60	509.28237048	24	5	657.5068097759	30	5
λ	(1,1)	N	K	(1,2)	N	K
0.2	12.352276634042668	44	20	15.5580293095556 5183	45	20
0.4	14.2409592995497	51	20	18.04816857012701	47	18
0.6	15.667863465357	52	20	19.9169611039371	42	15
0.8	16.845347929914	49	15	21.4539830953581	40	12
1.0	17.86179690040	43	13	22.778076043111	32	10
1.2	18.76383244512	42	12	23.951458625944	36	10
1.4	19.57950453935	46	12	25.011382598346	40	10
1.6	20.32719024211	39	10	25.982168939479	40	10
1.8	21.01967538972	33	8	26.880694482287	44	10
2.0	21.66626381870	34	8	27.71921445856	31	8
4.0	26.62156995574	44	8	34.13482677528	40	8
6.0	30.15915998432	41	6	38.70730053761	47	8
8.0	32.99875808622	44	6	42.37471213006	45	6
10.	35.40867481235	46	6	45.4857021249	41	6
15.	40.29871749436	46	5	51.795254392	42	6
20.	44.20927997315	41	4	56.838828346	43	5
λ	(1,3)	N	K	(1,4)	N	K
0.2	18.87003947992126263	45	20	22.28294403978606562	44	20
0.4	21.9981807456203860	45	15	26.0836404495626789	43	16
0.6	24.3339207559629	42	15	28.9100446342l316	41	15
0.8	26.2501809502373	37	12	31.2241929317796	35	12
1.0	27.898417760082	40	12	33.2121946629290	38	12
1.2	29.357484748402	39	12	34.9705201655879	41	12
1.4	30.674423256764	42	12	36.5565565699307	40	11
1.6	31.879866636593	39	10	38.0075983405180	40	10
1.8	32.995030498365	41	10	39.3494344260591	41	10
2.0	34.03529693500	38	10	40.600739898195	35	9
4.0	41.98456068903	48	10	50.15309753946	38	8
6.0	47.6429427220	40	8	56.94569842738	43	8
8.0	52.1786232972	46	8	62.38795258059	48	8
10.	56.0247638183	51	8	67.00150973042	41	6
15	63.8224421451	45	6	76.35228536354	45	6
20	70.0535245305	31	4	83.8224793766	45	6

Table (3.5 continued)

λ	(1,5)	N	K	(5,1)	N	K
0.2	25.79159711822616016	43	20	43.02003446494085997	45	20
0.4	30.297277422588188	45	20	51.4659307154537972	43	20
0.6	33.636606912870932	43	15	57.62645844234190	44	20
0.8	36.366150892962	34	12	62.62245894913870	44	18
1.0	38.708583610736	39	12	66.88902102510251	45	16
1.2	40.77891330265	24	10	70.64723195457507	41	14
1.4	42.64539463739	28	10	74.02691099153794	41	13
1.6	44.35231032458	32	10	77.11163959617097	42	13
1.8	45.93024267891	38	10	79.95880357528195	44	13
2.0	47.40131557735	38	10	82.6097245106638	44	14
4.0	58.62201030259	35	8	102.749763632043	47	12
6.0	66.59423360866	36	8	117.001698046682	42	10
8.0	72.97906736539	47	8	128.394195246495	41	8
10.	78.39037455221	36	6	138.038515046643	38	7
15.	89.35533477808	43	6	157.55784505046	42	7
20	98.1131645379	45	6	173.1318447503	35	6
λ	(5,2)	N	K	(5,3)	N	K
0.2	47.25181616055158948	42	25	51.53412329767382839	42	25
0.4	56.63568444847436669	46	20	61.8697224207838047	42	20
0.6	63.469078865339469	46	18	69.3854985004110643	44	18
0.8	69.00636570305774	42	18	75.471606729801238	46	16
1.0	73.73290256864148	43	16	80.664464371131188	40	15
2.0	91.13639236712172	44	14	99.7736803801925	45	14
4.0	113.4162108558533	40	10	124.222111815616	44	12
6.0	129.1763735904936	42	9	141.510711453496	42	10
8.0	141.7722610934256	41	8	155.326072409934	46	10
10.	152.4341697808606	45	8	167.019149524716	41	8
λ	(5,4)	N	K	(5,5)	N	K
0.2	55.86736976530330601	40	25	60.2516271560787083	36	25
0.4	67.1690029351599099	45	22	72.5339030253549529	42	22
0.6	75.377057085102206	45	20	81.44434455280887	40	20
0.8	82.019819752492763	44	18	88.65176007466746	39	18
1.0	87.685591263303033	43	16	94.79717504992373	41	16
2.0	108.52433697323802	44	14	117.3897269823141	41	14
4.0	135.1712477730185	45	12	146.2655429525857	45	12
6.0	154.0091928350215	45	10	166.6741183030235	42	10
8.0	169.0606575535068	48	10	182.978610173453	45	10
10.	181.798393314306	42	8	196.776376883182	37	8

Table (3.6). Eigenvalues of $H=P^2+r^2+\ell(\ell+1)r^{-2}+\lambda r^4$, First line results yielded by renormalised series method; Second line results yielded by power series method.

λ	n	ℓ	Energy	N	K
0.1	1	1	11.04088651003545688	59	30
0.1	10	10	113.6627169353884688	60	70
0.1	20	20	265.0314509035827655	48	100
0.1	50	50	848.0851187798380322	48	120
0.1	100	100	2084.7736303306986 33	41	180
0.1	500	500	17360.10724228866676	77	1000
0.1	1000	1000	43534.72083673737367	74	2000
10	5	5	196.7763768831827633	49	8
10	10	10	464.2267382273237377	55	13
20	10	10	583.4026361152836500	43	8
50	20	20	1926.551230985222025	35	10
100	20	100	6962.068779976634781	29	12

Table (3.7). Eigenvalues of $H=P^2+ r^2+\ell(\ell+1)r^{-2}+\lambda r^{2N}$, at $\lambda=0.1$. First line results yielded by power series, second line results yielded by renormalised series method, the numbers in the brackets correspond to (K,N). The empty spaces mean that the corresponding eigenvalues cannot be reached by the renormalised series approach.

n	ℓ	2N=6, I=1	2N=8, I=4
0	0	3.596036921220455 3.596036 (250,76)	3.939721361041987 3.939 (100,72)
0	1	6.439143322321712 6.43914 (260,70)	7.288474617608067 7.288 (159,129)
1	0	10.237873721423873 10.23787 (240,70)	12.281167732276058 12.28 (180,140)
0	2	9.617462285290456 9.61746 (250,63)	11.185812492801674 11.185 (260,215)
1	1	14.117061485224455 14.11706 (250,67)	17.424614887050766 17.42 (300,221)
2	0	18.801758333358159 18.80175 (300,58)	23.997088021463533 23.9 (350,212)
0	3	13.107473752755803 13.10747 (280,71)	15.598154928645939 15.59 (310,177)
1	2	18.253525389313848 18.25352 (260,68)	23.016781600186331
2	1	23.513885011366269 23.51388 (350,69)	30.623751038636159
3	0	28.928957081664627 28.92895 (350,68	38.519256956770986
0	4	16.888004695310679 16.88800 (270,67)	20.495332597266005
1	3	22.631658348338379 22.63166 (290,67)	29.028799590779936
2	2	28.434856717360885 28.43485 (330,70)	37.626800216924090
3	1	34.353199367450016 34.35319 (370,71)	46.442399043138764
4	0	40.408244096093465 40.40824 (370,72)	55.522079758670015

Table (3.8) Lowest s state energy in N dimensions for potentials ($V=N^{-1}r^4$, $V=Nr^4$), first line renormalised series, second line power series method.

N	$V=N^{-1}r^4$	M	K	$V=Nr^4$	M	K
1	1.06036209043 4841828	81	19	1.06036209043 4841828	81	19
2	1.861092068378 799400	73	20	2.9542995071 71559891	33	6.6
3	2.63454613405888 8318	74	22	5.48007679453 397092	36	6.4
4	3.39815017602771 76967	68	23	8.5628018749625 5274	49	6.5
5	4.15704336756073 346	71	25	12.1552685452677 735	56	7
10	7.92675754804411159 160	62	30	36.79274932175737 79	53	6
20	15.437713304665885 55	45	38	113.746044162737577 7	73	180
40	30.443495308478298 8	42	60	356.069281180762855 5	63	300
80	60.4464655899995 529	32	100	1122.270558855603 5 5	42	500
160	120.447970891098 850	28	180	3549.8729468101802 2	41	1000
320	240.448728618409 908	29	340	11249.221561775356 6	37	2400
400	300.4488805712 23209	26	440	16310.874686175430 0	37	3200
500	375.449002231 137532	23	550	23651.805053666849 9	47	5200
750	562.94916458 8031373	22	850	46470.429656755093 3	42	8000
1000	750.44924581 1284135	21	1100	75044.924581284135 5	39	10800

Table (3.9). Eigenvalues of $H=P^2+r^2+\frac{1}{4}(N+2\ell-3)(N+2\ell-1)r^{-2}+\lambda r^4$, in N dimensions , First line results yielded by power series method, Second line, results yielded by renormalised series method.

λ	n	ℓ	N	Energy	M	K
1	2	2	5	39.8899296600671224092	106	30
5	5	5	5	169.2326726468838667337	137	150
10	5	10	10	331.9680291461382137077	105	200
20	10	10	10	666.5816106404612830500	143	550
50	20	20	20	2269.6613514391479641 1	70	700
25	25	25	25	2426.10280527400274699	95	700
50	50	50	50	7688.08368787150832299	48	700
10	5	5	100	1119.80727601711931000	119	400
10	10	10	500	7636.07317026975480755	61	450
20	10	10	500	96136.43839288103391000	61	700
100	10	10	10	1136.75150052352652494	56	600
200	20	20	20	3599.78110799882231626	54	1500
10	20	20	750	13804.30141279078241611	54	600
20	10	10	750	15620.88525433949566888	46	700

CHAPTER FOUR

4. NON-POLYNOMIAL POTENTIALS IN ONE AND THREE DIMENSIONS

4.1 Introduction.

This chapter has been devoted to the computation of the eigenvalues in one and three-dimensional cases by using perturbative and nonperturbative methods for the following perturbed Hamiltonians

$$H= -\frac{d^2}{dx^2}+x^2+\frac{\lambda x^{2N}}{(1+gx^2)} \qquad (2N=2,4,6\ldots 18,20) \tag{4.1}$$

$$H= -\frac{1}{2}\frac{d^2}{dx^2}+\frac{x^2}{2}+\frac{gx^{2N}}{(1+g\alpha x^2)} \qquad (2N=4,6) \tag{4.2}$$

$$H= -\frac{1}{2}\frac{d^2}{dx^2}+\frac{x^2}{2}-\frac{gx^{2N}}{(1+g\alpha x^2)} \qquad (2N=4,6) \tag{4.3}$$

$$H= -\frac{d^2}{dr^2}+\ell(\ell+1)r^{-2}+\frac{\lambda r^2}{(1+gr^2)} \tag{4.4}$$

$$H= -\frac{1}{2}\frac{d^2}{dr^2}+\frac{\ell}{2}(\ell+1)r^{-2}+\frac{r^2}{2}+\frac{gr^4}{(1+g\alpha r^2)} \tag{4.5}$$

$$H= -\frac{1}{2}\frac{d^2}{dr^2}+\frac{\ell}{2}(\ell+1)r^{-2}+\frac{r^2}{2}-\frac{gr^4}{(1+g\alpha r^2)} \tag{4.6}$$

We drop quantities such as $\hbar$,m and e from the Hamiltonians in the equations above, in order to present the equations which have been used in simple forms. However, it is obvious that for certain limiting parameter values (e.g $\lambda\longrightarrow 0$, $g\longrightarrow 0$ or $g\longrightarrow\infty$) the differential equations corresponding to (4.1,4.2, 4.3,4.4,4.5,4.6) behave like the differential equations of the harmonic oscillator.

There are a variety of techniques which have been employed to calculate and to investigate these eigenvalue problems. Most of the calculations has been devoted to the Hamiltonian given by (4.1) for (2N=2). However as far as we know the other potentials have not been so much studied, except the potentials given by (4.2,4.3) for (2N=4), as we will see in later sections. We have been unable to find a reference in the literature dealing with the other types of potentials. We have used four methods to treat the eigenvalue problem for even and odd parity for different values of λ and g:

1. The Renormalised series method.
2. The Power series method.
3. The Finite difference method.
4. The Padé approximant method.

Also we tested some of our results by running the code which was used by V.Fack and Vanden Berghe [29,1985]. The agreement between our results using a finite difference method and the results using their code depends on the number of terms which are taken into account in the expansion of the kinetic energy operator:

$$h^2D^2 = \delta^2 - \frac{\delta^4}{12} + \frac{\delta^6}{90} \qquad (4.7)$$

The basic idea of the Fack and Vanden Berghe [29,1985] method is to use a finite difference method with matrix diagonalisation; this approach is more complicated than our finite difference method. Some of our reported results have not been previously available in the literature, so we used more than one method in order to check the accuracy of our results. In the present calculation we have been able to consider the effect of the extension of the range of values of the index (2N=2,4,6,8,...20) on our eigenvalue calculations. It should be useful to have such calculations to get an idea of the numerical limits of applicability of our methods for investigation of these types of potentials, and to prepare the way for further study of these potentials in the future. The perturbation series only converges for some appropriate ranges of λ and g. Precautions must be taken not to exceed critical values of λ and g. Some of our methods depend on the ranges which are used for λ and g if they are to give eigenvalue results of high accuracy.

4.2 Introductory remarks concerning potential $\lambda x^{2N}/(1+gx^2)$

The purpose of this section is to investigate the Schrödinger equation.

$$\left[\frac{d^2}{dx^2}-V(x)+E\right]\Psi(x)=0 \tag{4.8}$$

with the potential

$$V(x)=x^2+\frac{\lambda x^{2N}}{(1+gx^2)} \qquad (2N=2,4,6,8,10...18,20) \tag{4.9}$$

This potential with 2N=2 , has recently been studied by many authors using different techniques. Mitra [23,1978] calculated the ground state and first two excited states using the Ritz variational method in combination with a Givens-Householder matrix eigenvalue algorithm. Galicia and Killingbeck [24,1979] used the finite difference method to compute the energy eigenvalues for the three lowest even parity states. Kaushal [25,1970] has obtained the asymptotic expansions for the eigenenergies and eigenfunctions for the potential by expanding the factor $1/(1+gx^2)$ as a power series in gx^2. Bessis and Bessis [26,1980] have studied the same problem by taking advantage of a two parameter (λ and g) scale transformation. Hautot [27,1981] has used a Hill determinant method to calculate the energy eigenvalues. Lai and Lin [28,1982] have applied the Hellmann-Feynman and hypervirial theorem and used Padé approximants to calculate the energy eigenvalues from the perturbation series. Fack and Vanden Berghe [29,1985] used the finite difference method in combination with matrix diagonalisation for a numerical computation. The interest in this type of potential arises in several areas and these have been summarized by Mitra [23,1978] and Kaushal [25,1970]. In particular, this type of potential occurs when considering models in laser theory. In this calculation we have presented four numerical methods for the determination of energy eigenvalues. However, for large value of g some difficulties are encountered for some of these methods, so we restricted our calculation to a rather small range of $0.1\leq g\leq 0.5$ and a large range of $(20\leq\lambda\leq 1000)$. In spite of these restrictions on the values of λ and g, the agreement between the power series, hypervirial, and finite difference methods is excellent. The results can be considered as an improvement over previous results. Our results, which have twenty significant figure, are more accurate than previous results, which do not exceed ten significant figures. The finite difference method is a powerful method which covers a large range of $0.1\leq\lambda\leq1000$ and $0.1\leq g\leq1000$ and we can use this method to show up the drawbacks of other methods mentioned previously. While the finite difference method appears to be recommendable for a large range of λ and g, the power series and hypervirial methods should be reserved for a small range of (g) and large range of (λ). We also used the [6,6] Padé approximants to the energy series, which was obtained from the Hellmann-Feynman theorem and the hypervirial theorem.

4.3 Hypervirial relations for the potential $x^2+\lambda x^2/(1+gx^2)$

The Schrödinger equation for this potential can be written as

$$\left[\frac{d^2}{dx^2}-V(x)+E\right]\Psi(x)=0 \tag{4.10}$$

where the potential V(x) is given by

$$V(x)=x^2+\frac{\lambda x^2}{(1+gx^2)} \tag{4.11}$$

The perturbation calculation for the potential $[\lambda x^2/(1+gx^2)]$ is made by expanding the factor $1/(1+gx^2)$ as a power series in gx^2 which is valid for $gx^2\leq 1$. As x varies from $(-\infty\leq x\leq+\infty)$, the function $f(x)=1/(1+gx^2)$ runs from (0 to 0) through 1 at $x=0$, f(x) being always non-negative. In this section, we apply the hypervirial relation Killingbeck [12,1982] and the Hellmann -Feynman theorem to the Schrödinger equation, starting from the basic hypervirial relation and the Hellmann-Feynman theorem which have been given in a previous chapter (2.3) and (2.14). The potential in equation (4.11) can be expressed as

$$V(x)=\left(1+\lambda\right)x^{2}+\sum_{n=1}^{\infty} g^{n}\ V_{n}x^{2(n+1)} \qquad (4.12)$$

where

$$V_{n}=\lambda\left(-1\right)^{n} \qquad (4.13)$$

The coefficient given by (4.13) alternate in sign; the coefficient take (+ sign) for even n values, and (- sign) for odd n values. We have expanded the potential as given by equation (4.12) to the limit at which any term beyond that limit makes no difference to our eigenvalues. For our calculations this limit was reached for n=20. The series in equation (4.12) is valid only for $gx^{2}\leq 1$. For large g and small λ, it is found that our hypervirial method underestimates the eigenenergies. The unperturbed value of E(0) is given by

$$E(0)=\left(2n+1\right)\sqrt{(1+\lambda)} \qquad (4.14)$$

Now we use the energy E and the expectation values $\langle x^{N}\rangle$ which are given by (2.6) and (2.7) and the potential which is given by (4.12) in the Hypervirial relation and the Hellmann-Feynman relation. Using the same approach that led us to the recurrence relations (2.10) and (2.15), we find the relations

$$\left(2N+2\right)\sum_{0}^{M} E(I)B(N,M-I)=-\frac{N}{2}\left[N^{2}-1\right]B(N-2,M)$$

$$+\left(1+\lambda\right)\left(2N+4\right)B(N+2,M)+\sum_{n=1}^{\infty} V_{n}\left[2N+2\left(n+2\right)\right]B(N+2(n+1)),M-n) \qquad (4.15)$$

$$\left(M+1\right)E(M+1)=\sum_{n=0}^{\infty}\left(n+1\right)V_{n}B(N+2(n+1)),M-n) \qquad (4.16)$$

The energy coefficients E(M) can be determined from the relations (4.15) and (4.16) with the aid of E(0) and the condition B(0,0)=1. At K=0 the perturbation series converges and gives satisfactory numerical results for high values of λ ($20\le\lambda\le1000$) together with low values of g ($0.1\le g\le0.5$).

4.4 Power series method calculation of the energy eigenvalues

The power series method is a non-perturbative approach which has been used to calculate eigenvalues for many problems, Killingbeck has applied this approach to perform many eigenvalue calculations and our confidence in the accuracy of this method in numerical calculations of the energies for various problems has been indicated in previous chapters. From our results this approach can be seen to provide excellent accuracy, but for the type of potential of equation (4.11) there is some restriction on the values of λ and g. At large values of g the perturbing potential is concentrated in a small bump near the origin. The energy levels of the Schrödinger equation (4.10) with the potential ($x^2+ \lambda x^2/(1+gx^2)$) can be calculated by applying the power series approach. The wavefunction in equation (4.10) is defined as

$$\Psi(x)=\exp\left(-\beta x^{2}\right)\sum_{0}^{\infty} A(N)x^{N} \qquad (4.17)$$

Substituting the wavefunction as given by equation (4.17) into equation (4.10) reduces (4.10) to the following equation

$$\left(N+1\right)\left(N+2\right)T(N+2)=\left[2\beta N-gN\left(N-1\right)+2\beta\left(N+1\right)-E\right]x^{2}T(N)$$

$$+\left[2\beta g\left(2N-3\right)-4\beta^{2}+1+\lambda-Eg\right]x^{4}T(N-2)$$

$$+\left(g-4\beta g\right)x^{6}T(N-4) \qquad (4.18)$$

where

$$\sum_{0}^{\infty} T(N)=\sum_{0}^{\infty} A(N)x^{N} \qquad (4.19)$$

and β is an arbitrary parameter on which the eigenvalues cannot depend. In the previous chapter we have mentioned this parameter β as being used to improve the rate of convergence of the resulting computations. The initial conditions for the recurrence relation (4.18) are $T(0)=1$ (to get an even eigenstate) or $T(1)=0$ (to get odd states) with all other coefficients zero for $N<0$. The calculated eigenvalues vary with x_0 , if we require $\psi(x_0) = 0$. In the power series approach the results are accurate only when certain relation between λ and g hold. These relations can be given as

$$\frac{g}{\lambda}\ll 1 \qquad (4.20)$$

and

$$gx^{2}\leq 1 \qquad (4.21)$$

The conditions (4.20) and (4.21) limit the range of values of $0.1\leq g\leq 0.5$ and $20\leq\lambda\leq 1000$. Within these limits, the energy eigenvalues for this potential as given by the power series approach are very accurate.

4.5 Finite-difference eigenvalue calculations

Recent times have seen the development of non-perturbative methods of computing energy eigenvalues. Such methods are necessary since the perturbative methods provide insufficient information about accuracy, and give convergence difficulties. Recently Killingbeck has applied finite difference methods to various eigenvalue calculations and published many papers dealing with this type of method. He also described modified approaches of high order for finding Schrödinger equation eigenvalues, which can be expressed as

$$h^2\delta^2\psi(x)=4\left[\mathrm{Sinh}(\tfrac{1}{2}hD)\right]^2\Psi(x) \quad D^2>0$$

$$=4\left[\mathrm{Sin}(\tfrac{1}{2}hD)\right]^2\Psi(x) \quad D^2<0$$

In the present eigenvalues calculations, we used the above relations instead of using the relations (2.21) and (2.22). The error of the method used here should be smaller when a smaller h (step length) is used. The energy eigenvalues calculated by finite-difference methods in this section are subject to further modifications if high-term expansions are used. It will be our aim in this section to compute energy eigenvalues of the Schrödinger equation

$$\left[\frac{d^2}{dx^2}-V(x)+E\right]\Psi(x)=0 \qquad (4.22)$$

with the potential

$$V(x)=x^2+\frac{\lambda x^{2N}}{(1+gx^2)} \qquad (2N=2,4,6,..18,20) \qquad (4.23)$$

where E denotes the energy eigenvalue. The wavefunction $\Psi(x)$ can be restricted to the region $[0,+\infty]$. Furthermore we shall suppose that the wavefunctions are restricted to obey the Dirichlet boundary condition $\Psi(x)=0$ at some x value ($x=R$). An acceptable R value will be guessed numerically. The interval $[0,R]$ is subdivided into equal parts of length h, with $x=kh$ ($k=0,1,2,..\ n$; $nh=R$). The ground state and the first three even energy levels were computed by our approach for a large range of (λ) and (g). In this section the finite difference method for calculating eigenvalues of the Schrödinger equation (4.22) will be discussed by introducing a finite difference representation of $D^2\Psi(x)$. Chapter two explained the simple mathematics which forms the basis of our method. It is worth noting here that the finite difference method which is under discussion in the present section is different from that of the V.Fack and Vanden Berghe but it shares with it the use of finite difference expressions. Those previous workers used a finite difference method in combination with a matrix diagonalisation for numerical computations and transformed the Schrödinger equation into an algebraic eigenvalue problem, with a special form of matrix. A Finite difference representation for $D\Psi^{2}(x)$ is introduced such that the Schrödinger equation is transformed into an algebraic eigenvalue problem. Our method gives results with high accuracy for a wide range of $0.1\le g\le 1000$ and $0.1\le\lambda\le 1000$ for ($2N=2,4,6..18,20$). For large g values it seems that the present method works quite well, whereas the other methods have some problems. Although the displayed results are restricted to even-parity states, the method can be used for odd-parity states. We believe that the extrapolation procedure (for $h \longrightarrow 0$) is very accurate if the h values are chosen in the safe region.

4.6 The Padé approximant calculation of energy eigenvalues

We will now define the Padé approximant, and the Padé table. Definition: Let the [L,M] Padé approximant to the series A(x) be denoted by:

$$[L,M] = \frac{P_L(x)}{Q_M(x)}$$

where $P_L(x)$ is a Polynomial of degree at most L and $Q_M(x)$ a polynomial of degree at most M. We require that the formal power series for P/Q agrees with the A(x) series up to the (L+M)th power. The following theorem is due to Frobenius.G. and Padé, (Theorem of Uniqueness). The [L,M] Padé approximant to any formal power series A(x), when it exists, is Unique. (For the proof see ref [56,1975]. This theorem holds whether the defining equations are non singular or not. If they are non singular, then they can be solved directly to obtain:

$$[L,M] = \frac{\begin{vmatrix} a_{L-M+1} & a_{L-M+1} & \cdots & a_{L+1} \\ \vdots & \vdots & \ddots & \vdots \\ a_L & a_{L+1} & \cdots & a_{L+M} \\ \sum\limits_{J=M}^{L} a_{J-M}\lambda^{J} & \sum\limits_{J=M-1}^{L} a_{J-M+1}\lambda^{J} & \cdots & \sum\limits_{J=0}^{L} a_J \lambda^{J} \end{vmatrix}}{\begin{vmatrix} a_{L-M+1} & a_{L-M+2} & \cdots & a_{L+1} \\ \vdots & \vdots & \ddots & \vdots \\ a_L & a_{L+1} & \cdots & a_{L+M} \\ \lambda^{M} & \lambda^{M-1} & \cdots & 1 \end{vmatrix}}$$

where we define $a_n \equiv 0$ if $n<0$; $q_j \equiv 0$ if $j > M$ and, if the lower index on a sum exceeds the upper, the sum is replaced by zero. It is customary to arrange the Padé approximants in a table as follows:

[0,0]	[0,1]	[0,2]	[0,3]
[1,0]	[1,1]	[1,2]	[1,3]
[2,0]	[2,1]	[2,2]	[2,3]
[3,0]	[3,1]	[3,2]	[3,3]

The set [N,0] [N,1] [N,2] with N fixed is a row of the table; likewise the set [N,M] with M fixed is a 'column' while the set [N,N] is the diagonal sequence; we call a set [N,N+j] with j fixed, a paradiagonal. The top row is composed of the partial sums of the Taylor series. The Padé approximants are a particular type of rational fraction approximation to the value of a function, Padé approximation is a useful technique when the convergence of the series is unacceptably slow or even nonexistent. The Padé approximant is in the form of one polynomial divided by another polynomial. Padé approximants provide us with a practical method of calculating results from energy series E(n), since their use frequently accelerates convergence.The E [M,N] Padé approximants to the energy series is given by

$$E\ [N,M]=\frac{a_0+a_1\lambda\ +\ a_2\lambda^2+a_3\lambda^3\ .....a_n\lambda^N}{b_0+b_1\lambda\ +\ b_2\lambda^2+b_3\lambda^3\ ....b_M\lambda^M} \tag{4.24}$$

$$\equiv E(0)+E(1)\lambda+E(2)\lambda^2+\ \text{------}E(N+M)\lambda^{M+N}+\ \text{---} \tag{4.25}$$

with b_0 defined to be unity. The coefficients (a_i i=1,-----N) and (b_i i=0,-----M)in the numerator and denominator are calculated from the knowledge of E(1),E(2),-------,E(M+N), which can be computed from the hypervirial relations. The energy series for the interaction $\lambda x^2/(1+gx^2)$ appears to be convergent for $g>5$ and for large value of λ. Thus we can still calculate the energy E_n for $g>5$ to very high accuracy. Our calculated energy values E_n used the [6,6] Padė approximants to the energy series for the ground and the first three excited states.

4.7 Hypervirial relations for the potential given by $\left[\frac{1}{2}x^2-gx^{2N}/(1+g\alpha x^2)\right]$ (2N=4,6)

In this section, we want to investigate the Schrödinger equation

$$\left[\frac{1}{2}\frac{d^2}{dx^2}+E-V(x)\right]\Psi(x)=0 \qquad (4.26)$$

with a potential of the type

$$V^{\mp}=\frac{x^2}{2}\mp\frac{gx^{2N}}{(1+g\alpha x^2)}, \qquad (2N=4,6) \qquad (4.27)$$

The potential described by equation (4.27) for (2N=4) has recently been studied by G.Auberson [30,1982], who has shown that the perturbation expansion of eigenvalues E in terms of g at fixed α, is Borel summable. For the validity of this results, it is essential that the potential $V(x;g)$ be positive for all physical values of g and α, where the physical range of the parameters (g and α) is given as; for the potential $V^{+}(x;g)$, $g\geq 0$, $\alpha>0$, and for $V^{-}(x;g)$, $g\geq 0$, $\alpha>2$, (in order that $V^{-}(x,g)\longrightarrow\infty$, as $x^2\longrightarrow\infty$).

Also G.Auberson and T.Boissiere [31,1983] calculated ground state energy levels for a large range of values of α and g, by using a Padė method, Borel-Padė method, an improved Borel-Padė method and Borel-mapping method). The potential

$V^{\mp}_{2N}(x,g)$ can be written in this form

$$V^{\mp}_{4}(x;g)=\left[\frac{1}{2} \mp \frac{1}{\alpha}\right]x^{2}\pm \frac{x^{2}}{\alpha(1+g\alpha x^{2})} \tag{4.28}$$

$$V^{\mp}_{6}(x;g)=\left[\frac{1}{2} \mp \frac{1}{\alpha}x^{2}\right]x^{2}\pm \frac{x^{2}}{g\alpha^{2}} \mp \frac{x^{2}}{g\alpha^{2}(1+g\alpha x^{2})} \tag{4.29}$$

We want to study the limit of this potential

$$V^{\mp}(x;g)\Big|_{\alpha=0} =\frac{1}{2}x^{2}\mp gx^{2M} \qquad (2N=4,6) \tag{4.30}$$

The potential given by equation (4.30) is a pure anharmonic oscillator The singularity of $V^{\mp}(x;g)$ at $x^{2}= -1/\alpha g$ is responsible for a singularity of $E_{\mp}(g)$ and for the divergence of the potential series expansion. We investigate three methods to compute the energy eigenvalues, the hypervirial method, the Padé approximants method and the finite difference method. The first two methods are excellent for computing the energy for a small range of values of α and g, but the finite difference approach is applied to a wide range of values of α and g. In this section, we apply the hypervirial theorem and the Hellmann-Feynman theorem to calculate the eigenvalues of the Schrödinger equation for this potential. The potential $V^{\mp}(x)$ can be expanded as

$$V^{\mp}(x)=\frac{1}{2}\left[\mu-\lambda k\right]x^{2} \mp \frac{1}{\alpha}\sum_{n=0}^{\infty} V_{n}\lambda^{n+1}x^{2(n+2)} \tag{4.31}$$

where the potential coefficient V_{n} is

$$V_{n}=\left(-1\right)^{n} \tag{4.32}$$

and

$$\lambda=g\alpha \tag{4.33}$$

The unperturbed energy eigenvalue E(0) is given by

$$E(0)=\left(n+\frac{1}{2}\right)\sqrt{\mu} \quad ; \quad \mu=1+\lambda K \tag{4.34}$$

If we insert the energy (E) series and the expectation value $\langle x^N \rangle$ series in the hypervirial relation, the following relation is obtained

$$\left(2N+2\right)\sum_{0}^{M} E(I)B(N,M-I)=-\frac{N}{4}\left[N^2-1\right]B(N-2,M)$$

$$+\left(N+2\right)\left[\mu B(N+2,M)-KB(N+2,M-1)\right]$$

$$\mp\frac{1}{\alpha}\sum_{n=0}^{\infty}V_n\left[2N+2\left(n+3\right)\right]B(N+2(n+2),M-n-1) \tag{4.35}$$

If we apply the Hellmann-Feynman theorem

$$\frac{\partial E}{\partial \lambda}=\left\langle\frac{\partial V}{\partial \lambda}\right\rangle \tag{4.36}$$

the following relation is obtained

$$\left(M+1\right)E(M+1)=-\frac{K}{2}B(2,M)\mp\frac{1}{\alpha}\sum_{n=0}^{\infty}V_n\left(n+1\right)B(2(n+2),M-n) \tag{4.37}$$

We can calculate the energy eigenvalues from equations (4.35) and (4.37) by using the unperturbed energy E(0) and the initial coefficient value B(0,0)=1. We also used the same technique with g as the perturbation parameter. The agreement between the results from the two approaches is excellent, particularly for low value of α, but at high values of α the agreement between the two eigenvalues decreases, and this is very clear from our results in table (4.10). The potential

$V^{\mp}(x)$ in equation (4.27) can be expanded in the form

$$V^{\mp}(x)=\frac{1}{2}\left[\mu-\lambda k\right]x^{2}\mp\sum_{n=0}^{\infty}V_{n}\ g^{n+1}x^{2(n+2)} \qquad (4.38)$$

where

$$V_{n}=\left(-\alpha\right)^{n},\ \mu=1+\lambda k \qquad (4.39)$$

The coefficients given by equation (4.39) alternate in sign, taking positive and negative values for even and odd powers respectively. If we follow the same procedure used to get the relations (4.35) and relation (4.37), we get the following relations

$$\left(2N+2\right)\sum_{0}^{M}E(I)B(N,M-I)=-\frac{N}{4}\left[N^{2}-1\right]B(N-2,M)$$

$$+\left(N+2\right)\left[\mu B(N+2,M)-KB(N+2,M-1)\right]$$

$$\mp\sum_{n=0}^{\infty}V_{n}\left[2N+2\left(n+3\right)\right]B(N+2(n+2),M-n-1) \qquad (4.40)$$

$$\left(M+1\right)E(M+1)=-\frac{K}{2}B(2,M)\mp\sum_{n=0}^{\infty}V_{n}\ \left(n+1\right)B(2(n+2),M-n) \qquad (4.41)$$

The above equation (4.40) and (4.41), together with initial conditions $E(0)=\ \frac{1}{2}\ [2n+1]\sqrt{\mu}$ $(n=0,1,2)$ and $B(0,0)=1$ are sufficient to compute the coefficients $E(M)$ of the perturbation series for the energy. The method outlined above can also be used for the potential which is given by equation (4.29). For high-index $(2N=4,6)$ perturbation calculation by the hypervirial method, the method seems to work only for small value of g. The recurrence relations corresponding to the case (2N=6) are

$$\left(2N+2\right)\sum_{0}^{M} E(I)B(N,M-I)=-\frac{N}{4}\left[N^{2}-1\right]B(N-2,M)$$

$$+\left(N+2\right)\left[\mu B(N+2,M)-KB(n+2,M-1)\right]$$

$$\mp\frac{1}{\alpha}\sum_{n=0}^{\infty} V_{n}\left[N+2\left(n+4\right)\right]B(N+2(n+3),M-n-1) \qquad (4.42)$$

$$\left(M+1\right)E(M+1)=-\frac{K}{2}B(2,M) \mp \frac{1}{\alpha}\sum_{n=0}^{\infty} V_{n}\left(n+1\right)B(2(n+3),M-n) \qquad (4.43)$$

We used the recurrence relations (4.42) and(4.43) but with $\lambda=g\alpha$ as the perturbation parameter.

4.8 Three dimensional calculation for the potential $\lambda r^{2}/(1+gr^{2})$

It is interesting to note that this model can be extended to the three dimensional case, and we used more than one method to calculate the eigenvalues. The numerical results obtained by the perturbative method agree with those obtained by the non-perturbative (power series) method. As is expected, the eigenvalue accuracy decreases steadily with increasing λ and fixed g in accord with our previous experience In one dimensional problems for this type of potential, for large g, the perturbing potential is almost entirely concentrated near r=0. In this section, we want to investigate the three-dimensional Schrödinger equation, which can be written conventionally in the form

$$\left[\frac{d^{2}}{dx^{2}} + E-V(r)\right]\Psi(r)=0 \qquad (4.44)$$

where

$$V(r)=r^2+\ell(\ell+1)r^{-2}+\frac{\lambda r^2}{(1+gr^2)} \qquad (4.45)$$

We shall not distinguish between the one and three-dimensional interpretation of the perturbed Hamiltonian, and assume that we have either (ℓ=-1,0 and $-\infty<r<+\infty$) or (ℓ=0,1, and $0<r<+\infty$) The potential in equation (4.45) can be expressed as

$$V(r)=r^2+\ell(\ell+1)r^{-2}+\sum_{n=0}^{\infty}V_n\; g^n\; r^{2(n+1)} \qquad (4.46)$$

where

$$V_n=\lambda\left(-1\right)^n \qquad (4.47)$$

If we insert the energy and expectation value series in the hypervirial relation, and use the Hellmann-Feynman theorem, we get the following relations

$$\left(2N+2\right)\sum_{0}^{M} E(I)B(N,M-I)=N\left[\ell(\ell+1)-\frac{1}{2}\left(N^2-1\right)\right]B(N-2,M)$$

$$+\left(\lambda+1\right)\left(2N+4\right)B(N+2,M)$$

$$+\sum_{n=0}^{\infty}V_n\left[2N+2\left(n+2\right)\right]B(N+2(n+1),M-n-1) \qquad (4.48)$$

$$\left(M+1\right)E(M+1)=\sum_{n=0}^{\infty}V_n\;\left(n+1\right)B(2(n+1),M-n) \qquad (4.49)$$

The energy of the nth unperturbed state can be written as follows

$$E(0)=\left(4n+2\ell+3\right) \qquad (4.50)$$

The above equations (4.48,4.49,4.50) with coefficient

$B(0,0)=1$ allow us to compute the energies for different value of angular momentum ($\ell=5,10,20$). We used the power series method as another approach to compute the energy eigenvalues, to check our results. The first step in applying this approach is to write the Schrödinger equation in the form

$$\left[\frac{d^2}{dr^2} + E - r^2 - \frac{\lambda r^2}{(1+gr^2)} - \ell(\ell+1)r^{-2}\right]\Psi(r)=0 \qquad (4.51)$$

The wavefunction in equation (4.51) can be expressed as

$$\Psi(r)=\exp\left(-\beta r^2\right)\sum_0^\infty A(N)r^{\ell+N+1} \qquad (4.52)$$

We substitute equation (4.52) in equation (4.51). The result of this substitution is

$$\left[\left(N+2\right)\left(N+2\ell+3\right)\right]T(N+2)=$$

$$+\left[g\left\{\ell\left(\ell+1\right)-\left(N+\ell\right)\left(N+\ell+1\right)\right\}+4\beta N+4\beta\ell+6\beta-E\right]r^2T(N)$$

$$+\left[g\left(4\beta\left(N-2\right)+4B\ell+6\beta-E\right)+1-4\beta^2+\lambda\right]r^4T(N-2)$$

$$+g\left[1-4\beta^2\right]r^6T(N-4) \qquad (4.53)$$

where

$$\sum_0^\infty T(N)=\sum_0^\infty A(N)\ r^{\ell+N+1} \qquad (4.54)$$

The energy eigenvalues calculated by the power series approach are valid only for $gr^2\leq 1$, using the Dirichlet condition $\psi(r)=0$. We used the Padé approximant method as another approach to calculate the energy eigenvalues corresponding to a range of values g and λ for which it is impossible to calculate results by hypervirial and power series methods. We calculated the energy eigenvalues using the [6,6] approximant for ground and first excited states; the energy levels were calculated for different values of angular momentum.

4.9 Three dimensional calculation for the potential $1/2r^2 \mp gr^4/(1+g\alpha r^2)$

The Schrödinger equation (4.27) for three dimensions takes the form

$$\left[\frac{d^2}{dr^2} + E - V(r)\right]\Psi(r)=0 \tag{4.55}$$

where the potential in equation (4.55) is given as

$$V^{\mp}(r)=\frac{r^2}{2} + \frac{\ell}{2}(\ell+1)r^{-2} \mp \frac{gr^4}{(1+g\alpha r^2)} \tag{4.56}$$

The potential (4.56) can be expressed as

$$V^{\mp}(r)=\frac{r^2}{2} + \frac{\ell}{2}(\ell+1)r^{-2} \mp \frac{1}{\alpha}\sum_{n=0}^{\infty} V_n \lambda^{n+1} r^{2(n+2)} \tag{4.57}$$

where the potential coefficients V_n are

$$V_n=\left(-\right)^n ; \quad \lambda=\alpha g \tag{4.58}$$

The series in equation (4.57) is valid only for $g\alpha r^2 \leq 1$. By substituting the energy and expectation value series, as given by equations (2.6,2.7), in the hypervirial relation (2.3), the following relation is obtained

$$\left(2N+2\right)\sum_{0}^{M} E(I)B(N,M-I)=N\left[\ell(\ell+1) - \frac{1}{4}\left(N^2-1\right)\right]B(N-2,M)$$

$$+\left(N+2\right)B(N+2,M)\mp\frac{1}{\alpha}\sum_{n=0}^{\infty}V_n\left[2N+2\left(n+3\right)\right]B(N+2(n+2)),M-n-1) \tag{4.59}$$

If we apply the Hellmann-Feynman theorem, we obtain the following relation

$$\left(M+1\right)E(M+1)= \mp\frac{1}{\alpha}\sum_{n=0}^{\infty}V_n\left(n+1\right)B(2(n+2),M-n) \qquad (4.60)$$

Using the unperturbed value of energy $E(0)=\frac{1}{2}[4n+2\ell+3]$, with the initial condition $B(0,0)=1$, the equations (4.59) and (4.60) are sufficient to calculate the energy series. Also we use the same approach with g as perturbation parameter, so that the potential takes the form

$$V(r)=\frac{r^2}{2}+\frac{\ell}{2}(\ell+1)r^{-2}\mp\sum_{n=0}^{\infty}V_n g^{n+1}r^{2(n+2)} \qquad (4.61)$$

Using the same technique which gave relations (4.59,4.60), we can get the relation

$$\left(2N+2\right)\sum_{0}^{M}E(I)B(N,M-I)=N\left[\ell(\ell+1)-\frac{1}{4}\left(N^2-1\right)\right]B(N-2,M)$$

$$+\left(N+2\right)B(n+2,M)\mp\sum_{n=0}^{\infty}V_n\left[2N+2\left(n+3\right)\right]B(N+2(n+2),M-n-1) \qquad (4.62)$$

where

$$V_n=\left(-\alpha\right)^n \qquad (6.63)$$

and also the relation

$$\left(M+1\right)E(M+1)=\mp\sum_{n=0}^{\infty}V_n\left(n+1\right)B(2(n+2),M-n) \qquad (4.64)$$

4.10 Results and discussion

Our aim in this section is to investigate and to discuss the results for the energy eigenvalues of the Hamiltonians given by equations (4.1-4.6), in one and three dimensions.

Our aim also is to push the numerical analysis as far as possible, and in this respect we go further than other people in our analysis. We study here the three dimensional problem and high indices 2N of the perturbation. In addition we have succeeded in finding the energy eigenvalues with excellent accuracy. This problem received great attention from us , and we have attacked it by many methods, as we mentioned in a previous section. In summary, we have analysed numerically four different methods to determine the energy eigenvalues for these problems for different values of state number n and a wide range of values of (λ&g) and indices (2N=2,4,..18,20). The finite difference method has been used for calculations outside the limits applicable to the other three methods (hypervirial, Padé approximant and power series), particularly in respect to the values of parameters (g&λ) and of the index of the perturbation (2N=2,4,6,... 18,20). It is note worthy that the methods which have been applied to compute our results are applicable within a limited range of (2N,λ,g), except for the finite difference method, which seems to present fewer difficulties. We have used the hypervirial method to calculate results for various model problems, such as those given by (4.1,4.2,4.3,4.4,4.5,4.6), for different values of (2N,λ,g,n). The present work is intended to point out one feature which has not been noted in previous problems. The hypervirial method can produce a good accuracy even without use of the renormalisation parameter K, which usually plays an important role in obtaining convergent perturbation series, as we have seen in previous chapters. We have performed a series of computations for the problems of this chapter, which revealed the following fact. As the index (2N) increases the sums of the perturbation series converge very well for small values of λ, and as λ increases the convergence begin to decrease. If we review briefly our listed results in tables (4.3,4.7,4.10,4.12 ,4.13), we can get a clear picture of this behaviour. We can say that the accuracy of our listed results is very good in comparison with other results which are available in the literature. Also the results which are produced by the hypervirial method are in good agreement with our results which have been calculated by the power series and finite difference methods. This agreement provides a check on the accuracy of our results. We have computed the first four energy eigenvalues for index (2N=2), with parameter values $50\le\lambda\le1000$, $0.1\le g\le0.50$, by using three methods (hypervirial, power series and finite difference). The accuracy of our results in general is more than 16 significant digits, as shown in tables (4.1,4.2). The power series method seems to work very well and the convergence of this method will be controlled by the parameter β. We also listed in table (4.4) the four first energy eigenvalues for (2N=2) and for values $0.2\le g\le50$ and $500\le\lambda\le10^6$, obtained by using Padé approximants [6,6] and the hypervirial method. The agreement between the two methods is very good. Also we have calculated the first five energy levels by using the hypervirial method for (2N=4), with case $V^-(x)$ for $10^{-3}\le g\le0.02$; $1\le\alpha\le50$. In addition we used Padé approximants for ($0.1\le g\le2$; $2\le\alpha\le50$). We have observed a strong similarity between the behaviour of the hypervirial method in one and three dimensional calculations for changing index of perturbation (2N) and value of (g&λ). The series converge very quickly for large λ and small g with (2N=2), but with (2N=4,6) the situation is not similar;the series converges for small values of λ and larger values of g. Further more it clearly appeared from our listed results in tables (4.12,4.14), that the perturbation calculations (Hypervirial calculations) can yield very high accuracy for large values of α, if we take αg as perturbation parameter in stead of g. For small values of α,it does not make any different to the accuracy whether we take αg or g as perturbation parameter. Also we have not observed any fundamental difference in behaviour between the $V^-$and V^+cases as we vary the perturbation parameters (α,g) and index (2N=4,6). We have calculated the first five energy eigenvalues in three dimensions for different sets of λ,g, index (2N=2,4,6) and angular momentum. It is note worthy that the Padé approximant method [M,N] has been applied to this problem for one and three dimension and is able to handle this problem over a wide range of $0.1\le g\le 50$; $0.1\le\lambda\le 10^6$, and index power (2N=2,4,6). Some of the present calculations of eigenvalues have been repeated with two different values of N and M in order to check the accuracy, since there is an absence of reported results in the literature. The agreement between the two eigenvalues is very good. We wish to draw attention to the fact that the present Padé approximant approach works very well even for higher values of (g,λ), whereas the Padé approximant method of Lai and Lin [28,1982] is restricted to low values of g ($g \le 2$). Our results allow us to study the numerical behaviour of this potential for varying index (2N), perturbation parameter (g&λ), and for a number of excited states. For the ordinary anharmonic oscillator ($g=0$) of chapter one, we have seen that as the index 2N varies the order of the ground state levels obeys

$$E^4 < E^6 < E^8 \ldots\ldots E^{16} < E^{20}$$

for small values of ($\lambda=0.1,1,5$), while for large values of ($\lambda=50,100$), the order is reversed. For the present type of perturbation the picture is more complicated because there are two parameters (g&λ). Many energy levels have been calculated, and we mentioned previously that the behaviour of the eigenvalues is nonanalytic at each crossing point. We have seen from our results that some energy eigenvalues for ($g=\lambda$) decrease or increase with increasing index ($2N=2,4,..20$). For example at ($g=\lambda=0.1$) the energy eigenvalues increase as 2N increases, as is clear from our listed results in table (4.4,4.5). The ordering of the eigenvalues can be expressed as below:

$$E^2(n) < E^4(n) < E^6(n) \; < E^{2N-2}(n) \; < E^{2N}(n) \quad (2N=2,4,..20)$$

Here n is the state number and its values in the present calculations are $n=0,2,4,6$. With another set of values of the perturbation parameters ($g=\lambda=10$) the order of levels can be given as:

$$E^2(0,4) > E^4(0,4), \; E^2(2,6) < E^4(2,6)$$

For index values greater than (2N=6) the energy eigenvalues increase as 2N increases as follows:

$$E^{4}(n) < E^{6}(n)<E^{8}(n).......<E^{16}(n)<E^{18}(n)<E^{20}(n)$$

With other sets of values of ($g=\lambda=100,1000$) the energy levels have the same behaviour; the energy levels increase as 2N increases except the ground levels

$$E^{2}(0)>E^{4}(0)>E^{6}(0)<E^{8}(0)<E^{10}(0),..<E^{18}(0)<E^{20}(0)$$

For states n=2,4,6 the order of levels is :

$$E^{2}(n)<E^{6}(n)<E^{8}(n)< E^{10}(n)...E^{18}(n)<E^{20}(n)$$

We computed the energy levels with different values of $g\&\lambda$; for the values ($g=100,\lambda=0.1$), the order of levels is:

$$E^{2}(0)>E^{4}(0); \quad E^{2}(2,4,6)<E^{4}(2,4,6);$$

$$E^{4}(n)<E^{6}(n)<E^{8}(n)......<E^{18}(n)<E^{20}(n)$$

for n=0,2,4,6. With the values g=1 and $\lambda=100$ the order of levels is given by

$$E^{2}(n)>E^{4}(n)>E^{6}(n)>E^{8}(n)....E^{18}(n)>E^{20}(n) \qquad (n=0,2,4)$$

while for n=6 the order of levels is;

$$E^{2}(6)<E^{2N-2}(6) <E^{2N} (6) \qquad (2N=6,8...20)$$

The computation was carried out to double-precision accuracy by using the ICL and VME system with Fortran (77) programs. In order to give a clear picture of our results for this chapter, in tables (I,II,III,VI), we present the ranges of values of the parameters ($g\&\lambda$), and of the state number n and angular momentum, together with the table numbers in which the relevant results were reported for the various methods.

PARAMETER RANGES

Table (I). $H= p^2 + x^2 + \lambda x^{2N}/(1+gx^2)$

2N	methods	λ	g	n	table
2	Power series Finite difference	$20-10^3$	0.1-0.5	2	4.1
2	Hypervirial Power series	$50-10^3$	0.1-0.5	4	4.2
2	Hypervirial Padé approximants	$50-10^6$	2-50	4	4.3
2	Padé approximants	$0.1-9\times10^3$	0.10-10	4	4.4
2-20	Finite difference	$0.1-10^3$	$0.1-10^3$	4	4.5-6

Table (II). $H=P^2+x^2+(\ell(\ell+1)r^{-2}+\lambda r^2/(1+gr^2)$

2N	method	λ	g	n	ℓ	table
2	Hypervirial Power series	$200-10^4$	0.1-0.5	4	5,10,20	4.14
2	Padé approximants	$0.1-10^3$	0.1-5	4	1,2,3	4.15

Table (III) $H = \frac{P^2}{2} + \frac{x^2}{2} \mp gx^{2N}/(1+g\alpha x^2)$ $2N = 4,6$

2N	method	g	α	$V_\mp$	n	table
4	Hypervirial	0.001-0.02	0.5-100	+	5	4.7
4	Padé approximants	0.01-10	0.1-50	+	4	4.8
4	Hypervirial	0.001-0.02	1-100	-	5	4.9-10
4	Padé approximants	0.1-2	2-50	-	4	4.11
6	Hypervirial	0.0001-0.0005	4-100	+	5	4.12
6	Hypervirial	0.0001-0.0006	3-100	-	5	4.13

Table (IV) $H=\frac{P^2}{2} + \frac{r^2}{2} + \frac{\ell}{2}(\ell+1)r^{-2} \mp gr^4/(1+g\alpha r^2)$

2N	method	$V_\mp$	gx1000	α	n	ℓ	table
4	Hypervirial	+	1-5	0.25-10	5	1,2,5,10	4.16
4	Padé approximants	+	10-200	2-50	1	1,2,3,4	4.17
4	Hypervirial	-	1-5	1-10	5	1,2,5,10	4.18-19
4	Padé approximants	-	10-400	1-100	4	1,2,3,4,5	4.20

Table (4.1). Eigenvalues of $H=p^2+x^2+\lambda x^2/(1+gx^2)$, for ground state and the first even state, First line; power series method, Second line; finite difference method; the numbers in the bracket correspond to $(g)\&(\lambda)$.

(0.1,500)	β, X h	(0.1,1000)	β, X h
22.30842993445491522	40, 3 0.0015	31.56383647646583973	50, 3 0.0015
110.94588224555598079	40, 3 0.0015	157.22156717304200021	50, 3 0.0015
(0.2,500)		(0.2,1000)	
22.23432842711840034	40, 2 0.001	31.48944190129190676	50, 2 0.001
109.98417163813053222	40, 2 0.001	156.25554681794073000	50, 2 0.001
(0.3,500)		(0.3,1000)	
22.16071878572099145	40, 1.6 0.0008	31.41539729424046122	50, 1.6 0.0008
109.02997679666895111	40, 1.6 0.0008	155.29483961720882566	50, 1.6 0.0008
(0.4,500)		(0.4,1000)	
22.08759516321136999	40, 1.5 0.00075	31.34169968327075266	50, 1.5 0.00075
108.08326113127335104	40, 1.5 0.00075	154.33942649652595555	50, 1.5 0.00075
(0.5,500)		(0.5,1000)	
22.014951838478025741	40, 1.4 0.0007	31.26834614237787211	50, 1.4 0.0007
107.14398920298777877571	40, 1.4 0.0007	153.38928880219417888	50, 1.4 0.0007
(0.1,200)		(0.1,50)	
14.10321682800423266	40, 3 0.0015	7.068696472300124013	20, 3 0.0015
69.923125553469652355	40, 3 0.0015	34.76382969377249211	20, 3 0.0015
(0.1,100)		(0.1,20)	
9.976180087723021055	40, 3 0.0015	4.51242099189001387260	20, 3 0.0015
49.29269050462686088	40, 3 0.0015	22.0055699335623527558818	20, 3 0.0015
(0.2,200)		(0.2,100)	
14.02977038265679199	40, 2 0.001	9.903588530458731472640	30, 2 0.001
68.97103698954511300	40, 2 0.001	48.35321196661020415865631	30, 2 0.001

Table (4.2). Eigenvalues of $H=P^2+x^2+\lambda x^2/(1+gx^2)$, for the first four energy levels, First line; power series method, Second line; Hypervirial method; the numbers in the bracket correspond to g & λ.

(0.1,500)	β , X N	(0.1,1000)	β , X N
22.308429934454915232 2	40, 3 8	31.563836476465839774 8	50, 3 7
66.776095400961728774 5	40, 3 9	94.542015961555579220 3	50, 3 8
110.945882245555598088 8	40, 3 8	157.221567173042002 94 3	50, 3 8
154.818812750317864 07 6	40, 3 8	219.603208380955897 11 1	50, 3 7
(0.1,50)		(0.1,100)	
7.0686964723001240 22 3	20, 3 12	9.9761800877230210 51 4	40, 3 10
21.0607382647098919 3 3	20, 3 12	29.7811911107765744 7 8	40, 3 10
34.7638296937724921 8 7	20, 3 13	49.2926905046268608 1 1	40, 3 11
48.1814981927716147 3 38	40, 3 13	68.5130622345111346 4 3	40, 3 11
(0.2,500)		(0.2,1000)	
22.2343284271184003 8 9	40, 2 9	31.4894419012919067 86 7	50, 2 9
66.4056045778459592 7 9	40, 2 10	94.1700499432476337 20 4	50, 2 9
109.984171638130532 4 4	40, 2 9	156.255546817940730 24 3	50, 2 9
152.974149420465918 7 7	40, 2 11	217.748820745966303 93 2	50, 2 10
(0.3,500)		(0.3,1000)	
22.1607187857209915 0 0	40,1.6 11	31.4153972942404612 1 1	50,1.6 9
66.0375911385046321 1 2	40,1.6 11	93.7998417643379529 0 1	50,1.6 10
109.029976796668951 5 494	40,1.6 11	155.294839617208825 9 9	50,1.6 11
151.147213935882350 7 2535	40,1.6 12	215.906923255882685 8 7	50,1.6 10
(0.4,1000)		(0.5,1000)	
31.3416996832707526 3 3	50,1.5 11	31.268346142377872 2	50,1.4 10
93.4313793247623147 0 1	50,1.5 12	93.064650716496147 7	50,1.4 11
154.339426496525955 0 0	50,1.5 11	153.389288802194 17 7	50,1.4 10
214.077514335810180 9 9	50,1.5 11	212.260592887339 55 2	50,1.4 12

Table (4.3). Eigenvalues of $H=p^2+x^2+\lambda x^2/(1+gx^2)$, for the first four energy levels, First line; Padé approximants E[6,6], Second line; Hypervirial method, the numbers in the bracket correspond to g & λ.

(2,500)	(2,1000)	(3,1000)
20.9793853161 5	30.2074696503 6	29.5385893988 9
60.1392564150 6	87.7642116155 6	84.4284577789 5
93.9269144470 1	139.7586931046 3	131.3026334252 3
122.8043486438 4	186.5053066071 6	170.8958329278 8
(2,10000)	(5,10000)	(10,10000)
98.5272494340 3	96.3899452770 7	93.0223623058 3
292.6266296841 8	281.9453701041 0	265.1442062295 2
480.8619132637 2	453.3505908064 0	410.6813658326 1
663.3260941431 4	611.2130190804 9	532.2133179828 3
(5,100000)	(10,100000)	(15,100000)
312.5232226960 9	308.9023429341 9	305.3632607161 0
930.1579978317 3	912.0575568601 8	894.3726387992 3
1533.0601272580 2	1486.2835519312 1	1440.7950550314 5
2121.4121264812 4	2032.3283407535 0	1946.3522929991 9
(15,1000000)	(25,1000000)	(50,1000000)
988.8753661364 1	981.5942714810 4	963.8461236953 2
2944.3773870170 0	2907.9774809773 8	2819.2850260431 2
4855.6398420920 0	4761.4749945992 9	4533.2030348177 0
6723.1814910755 1	6543.5504361985 3	6111.6710565087 1

Table (4.4). Eigenvalues of $H=p^2+x^2+\lambda x^2/(1+gx^2)$ for the first five energy levels, calculated from the Padé approximants E [6,6]; the numbers in the bracket correspond to (g) & (λ).

(0.1,0.1)	(2,0.1)	(2,50)
1.0431737131	1.0172815965	5.8318898330
3.1200818644	3.0329572730	15.4975387596
5.1810947875	5.0345519112	21.3878955934
7.2310099806	7.0377588528	25.0164059096
(2,100)	(5,500)	(10,500)
8.7582786322	19.1685333012	16.7327514335
23.7433260421	51.1818569177	39.5754394019
34.2577412431	72.1400383450	48.1038613194
41.4928240348	85.1765680378	52.4391828133
(0.5,0.5)	(0.5,5)	(0.5,50)
1.1515634020	2.1921184695	6.7827895303
3.3638015565	6.1210592341	19.6850376488
5.4632114193	9.3207606655	31.2380422733
7.5278886000	12.0923480220	41.5492530493
(1,1)	(1,100)	(1,200)
1.2323535261	9.3594180264	13.4687482263
3.5073979060	26.7059656288	38.9825190308
5.5898335474	41.4410897462	61.7775336881
7.6490689893	53.8390929601	82.0052851252
(3,500)	(3,750)	(3,1500)
20.3403609835	25.3260708824	36.6165571250
56.9614598560	71.8385859542	105.6057200506
85.9949684543	110.4934667581	166.3941150102
108.5270735407	142.1540209781	219.5685782022
(4,2000)	(4,4000)	(4,8000)
41.9205051279	60.3888919111	86.5454114322
120.1518287267	175.4447994176	253.8340971246
187.6111222784	279.3640214949	409.7309965677
245.2134888879	372.7726752273	554.6676122546
(5,3000)	(5,6000)	(5,9000)
51.2701342846	73.8883731803	91.2655428397
146.8062318991	214.5189371947	266.5867728404
228.9052478261	341.2492805607	427.8041652813
298.7357244491	454.8791439607	575.5603962093

Table (4.5) Eigenvalues of $H=p^2+x^2+\lambda x^{2N}/(1+gx^2)$, for the first four even energy levels calculated from finite difference method:the numbers in the bracket correspond to g & λ.

2N	(0.1,0.1)	(10,10)	(100,100)
2	1.043173713044	1.580022327391	1.838335833448
	5.181094785884	5.832767532465	5.928328571544
	9.272816970035	13.905251334974	9.949160962809
	13.339390726973	17.918865935944	13.959285222368
4	1.055297707257	1.359774662157	1.406065452883
	5.574522322948	6.990545314996	7.061901755091
	10.456102206292	12.641626177581	12.718510053100
	15.527085931694	18.295827777899	18.375244956667
6	1.094134891239	1.366850746128	1.389372026300
	6.400322742109	8.546584784823	8.643580194793
	13.438095185462	17.890113503822	18.040135250589
	21.798915062902	28.617080307170	28.812809980223
8	1.151514504374	1.417528105627	1.433638679938
	7.383294498903	9.849002405294	9.954237354521
	16.941331851282	22.688954068384	22.887204444789
	29.198386385942	38.726642405555	39.018341106677
10	1.215878634348	1.476109774767	1.489420177825
	8.343517967069	10.877002260298	10.981472033116
	20.170797539421	26.495085595570	26.717641645910
	36.026256433816	47.001366822781	47.352859541727
12	1.280182859803	1.533170988252	1.544873619363
	9.197921053984	11.707675148976	11.808190624164
	22.993264654376	29.505481413627	29.737527537625
	42.007180092887	53.656055492948	54.040415693047
14	1.341354528636	1.586121222133	1.596737866007
	9.955132586841	12.397847402773	12.493517331184
	25.438823035348	31.935163276650	32.168244360628
	47.192045758317	59.063768230162	59.463513300016
16	1.398313628112	1.634469145224	1.644275007573
	10.626048883982	12.984420658732	13.075207911050
	27.565806963300	33.940982509003	34.170496409418
	51.694783070945	63.528796292616	63.932980434225
18	1.450867110050	1.678410054248	1.687570756347
	11.223051083941	13.491825483811	13.577996382110
	29.429398500059	35.631030232473	35.854600782728
	55.628346093512	67.275793958806	67.677675952840
20	1.499195895316	1.718348479054	1.726973707590
	11.757261716042	13.936891803671	14.018803426232
	31.075486317130	37.080020447702	37.296532262040
	59.089626726601	70.467858967117	70.863367896662

Table (4.6) Eigenvalues of $H=P^2+x^2+\lambda x^{2N}/(1+gx^2)$, for the first four even energy levels calculated from finite difference method; numbers in the bracket correspond to g & λ.

2N	(1000,1000)	(100,1.0)	(0.1,100)
2	1.945115962246	9.359418026324	1.000841102403
	5.973871294466	41.441099751484	5.000927544679
	9.980844496690	64.187440995096	9.000948590765
	13.984309011922	79.911771037615	13.000958871383
4	1.413277479827	4.551943690436	1.000491464345
	7.070098533826	30.032354991385	5.002490100021
	12.726944524023	61.606494425908	9.004489389761
	18.383794662647	95.540315090111	13.006488787180
6	1.392046738681	3.379530522796	1.000743784230
	8.653895433124	25.553317440935	5.009687062013
	18.055807419917	58.942539708101	9.030504963328
	28.833077682717	99.359790269248	13.063099296382
8	1.435423858640	2.916439495691	1.001841471859
	9.965376749087	23.352777555213	5.044707772528
	22.907873768005	57.343691294529	9.218311541801
	39.048539250890	101.091557364302	13.592656194818
10	1.490858685346	2.687699701924	1.005840947517
	10.992504406862	22.122616368764	5.190668793727
	26.740857548661	56.331803557092	10.044315726459
	47.389313237020	102.113154388781	15.834302784052
12	1.546123212747	2.559566787748	1.017304112745
	11.818784253499	21.379015891983	5.538312461608
	29.761753514174	55.671617557702	11.654214351369
	54.080343451799	102.815736737674	19.634358792624
14	1.597864518960	2.481972823456	1.039468918489
	12.503583878929	20.906733711552	56.045814670986
	32.192539969290	55.236609028179	13.633559470727
	59.505092854508	103.350952041603	23.979716235410
16	1.645311460919	2.432559266677	1.071175971148
	13.084748387255	20.597368905582	6.626819240530
	34.194483210206	54.952691225111	15.685083305035
	63.975063699382	103.789938694360	28.347149684929
18	1.688536455215	2.400063940870	1.109227794604
	13.587042575353	20.391273776539	7.224690702921
	35.877971924946	54.773396474927	17.677889685561
	67.719551758007	104.170086964780	32.526472722653
20	1.727881280722	2.378295762785	1.150657947532
	14.027395631206	20.253376994017	7.810470001495
	37.319168240829	54.668139736770	19.561158228393
	70.904604121144	104.512350040639	36.441449502621

Table (4.7). Eigenvalues of $H^{\pm}= 1/2P^2+1/2x^2 \pm gx^4/(1+g\alpha x^2)$, for the ground-state energy levels calculated from finite difference method.

α	g	E_0^+	Ref 31	E_0^-	Ref 31
50	0.01	0.503676241304	0.50367624	0.496256025610	0.4962560
	0.10	0.507955018588	0.5079549	0.491869010232	0.491869
	0.20	0.508718597784	0.508718	0.491025383716	0.491093
	0.50	0.509333177139	0.509332	0.490470329585	0.49047
	1	0.509588747931	0.50958	0.490212618236	0.49021
	2	0.509734009232	0.50973	0.490066458426	0.49007
	5	0.509830390245	0.50982	0.489969665448	0.48997
	10	0.509864996405	0.50986	0.489934960900	0.48994
	15	0.509876957373	0.50987	0.489922974358	0.48993
	20	0.509883043737	0.50988	0.489916877069	0.48992
	1000	0.509901554538	0.50990195	0.489898345433	0.48989795

Table (4.8). Eigenvalues of $H=1/2P^2+1/2x^2+gx^4/(1+g\alpha x^2)$, for the first five energy levels calculated from Hypervirial method; the numbers in the bracket correspond to (g) & (α).

(0.001,0.5)	N	K	(0.001,5)	N	K
0.50074647074764394145	9	0	0.50073828777355865815	13	0
1.50372318292878927 20	10	0	1.5036665319444506778	14	0
2.50965154156177726 91	11	0	2.50945179884940872165	16	0
3.51850014293877716 48	12	0	3.5180038831642341607	20	0
4.53023834076249261 13	13	0	4.5292372284608061748	20	0
(0.001,10)	N	K	(0.001,20)	N	K
0.50072947976709422277	19	0	0.50071269224348549426	37	0
1.5036060772489412314	21	0	1.503492319497928984	36	0
2.5092408909632772410	24	0	2.508850115404986976	44	0
3.5174860974896648367	28	0	3.5165431520351894	42	0
4.5282057666965039694	31	0	4.526360808570728	43	0
(0.001,50)	N	K	(0.001,100)	N	K
0.5006678376	15	10	0.5006073	15	10
1.503197920	14	10	1.502818	13	10
2.50787393	12	10	2.50668	11	10
3.5142766	10	10	3.511	7	10
4.522095	11	10	4.517	7	10
(0.005,1)	N	K	(0.005,5)	N	K
0.50364328312043147469	32	0	0.5034819805166	15	10
1.5179671613901822218	32	0	1.51689308272	16	10
2.54594982503971	24	0	2.5423246614	30	10
3.5868079952874	29	0	3.578207916	28	10
4.6398468050	22	0	4.6075	12	10
(0.005,10)	N	K	(0.005,15)	N	K
0.5033046682	13	10	0.50314886	14	10
1.51574764	19	10	1.514770	10	10
2.538594	9	10	2.53355	6	10
3.56969	7	10	3.5629	7	10
4.6075	12	10	4.595	5	10
(0.005,20)	N	K	(0.01,0.1)	N	K
0.503010	11	10	0.50723945969	13	0
1.51392	10	10	1.5355368515	17	0
2.5329	8	10	2.59046858	17	0
3.557	5	10	3.670194	15	0
4.58	4	10	4.77361	13	0
(0.01,0.5)	N	K	(0.01,1)	N	K
0.50717349508	17	0	0.507093239851	21	10
1.535099404	18	0	1.534570408	13	10
2.5889936	19	0	2.58722278	15	10
3.66669	18	0	3.662515	12	10
4.766	6	0	4.7583	11	10
(0.01,2)	N	K	(0.01,3)	N	K
0.50693958345	14	10	0.506794314	9	10
1.533567343	10	10	1.53263064	16	10
2.5839027	11	10	2.580846	13	10
3.65478	8	10	3.64777	11	10
4.7437	8	10	4.730	5	10
0.02,1.5)	N	K	(0.02,2)	N	K
0.5132395	8	10	0.5129848	7	10
1.56288	8	10	1.56130	8	10
2.654	6	10	2.649	4	10
3.77	5	10	3.76	3	10

Table (4.9). Eigenvalues of $H=1/2P^2+1/2x^2+gx^4/(1+g\alpha x^2)$, for the first five energy levels calculated from the Padé approximants E [N,N]; the numbers in the bracket correspond to (g) & (α).

(0.01,10)	N	N	(0.01,20)	N	N	(0.01,50)	N	N
0.5059575080	7	7	0.5051139884	8	8	0.5036757394	6	6
1.5274463072	7	7	1.5225668046	7	7	1.5150007532	6	6
2.5646974761	6	6	2.5506500867	6	6	2.5310182764	6	6
3.6124950756	6	6	3.5841841943	6	6	3.5482670605	6	6
(0.1,0.1)	N	N	(0.1,2)	N	N	(0.1,5)	N	N
0.5582333913	5	5	0.5453998375	7	7	0.5341718973	7	7
1.7642326395	4	4	1.6945334318	6	6	1.6378922422	7	7
3.1228901590	4	4	2.9279904156	6	6	2.7837371250	6	6
4.5947999549	4	4	4.2037147105	6	6	3.9412533225	6	6
(0.1,10)	N	N	(0.1,20)	N	N	(0.1,50)	N	N
0.5245297214	7	7	0.5159205999	8	8	0.5078744867	8	8
1.5932661578	7	7	1.5568866871	7	7	1.5263350805	7	7
2.6809753605	6	6	1.6048590962	7	7	2.5463132887	7	7
3.7701773930	6	6	3.6517785538	6	6	3.5655210362	6	6
(0.2,10)	N	N	(0.2,20)	N	N	(0.2,50)	N	N
0.5315549492	8	7	0.5186447380	8	8	0.5085465285	8	8
1.6107937612	7	7	1.5632400714	7	7	1.5276758156	7	7
2.7077561342	7	6	2.6123469423	7	7	2.5477261709	7	7
3.8008563585	7	6	3.6595690660	6	6	3.5669336660	6	6
(0.5,1)	N	N	(0.5,10)	N	N	(0.5,20)	N	N
0.6367842514	8	8	0.5403867827	8	9	0.5209789505	8	8
2.0506190597	6	7	1.6357182641	7	8	1.5775333602	7	8
3.5707739173	5	5	2.7306590810	7	8	2.6175082283	7	7
5.1611009800	5	5	3.8330786791	6	7	3.6806084300	6	7
(1,10)	N	N	(1,20)	N	N	(1,50)	N	N
0.5404218004	7	7	0.5219457808	8	8	0.5092104985	8	8
1.6323985776	7	7	1.5698405566	7	7	1.5288868018	7	7
2.7288343227	6	6	2.6193625994	7	7	1.5489359130	7	7
3.8214696406	6	6	3.6665464775	7	7	3.5681200249	7	7
(2,10)	N	N	(2,20)	N	N	(2,50)	N	N
0.5421754838	7	7	0.5224763153	8	8	0.5093037479	8	8
1.6359113182	7	7	1.5707971290	7	7	1.5290482467	7	7
2.7324352014	6	6	2.6203175163	7	7	2.5490925352	7	7
3.8250366890	6	6	3.6674723743	6	6	3.5682720688	6	6
(5,50)	N	N	(10,10)	N	N	(10,50)	N	N
0.5093609603	8	8	0.5437277814	7	7	0.5093802478	8	8
1.6422446166	7	8	2.0510177453	7	8	1.7753765226	7	8
2.6091210151	7	8	3.0025250343	7	8	2.6726023094	7	8
3.6899213557	7	8	4.3120162909	7	6	3.8210832897	7	8

Table (4.10). Eigenvalues of $H=1/2P^2+1/2x^2-gx^4/(1+g\alpha x^2)$, for the first five Energy levels calculated from Hypervirial method; the numbers in the bracket correspond to (g) & (α).

(0.001,1)	N	K	(0.001,10)	N	K
0.49924924509082103087	8	0	0.499265588785765898283	16	0
1.4962424317659615658	8	0	1.49635689769681264690	14	0
2.4902196292455903232	9	0	2.4906259959688469599	14	0
3.4811699825024634359	10	0	3.4821857773654487833	21	0
4.4690824528709260691	11	0	4.4711439430890412558	21	0
(0.001,20)	N	K	(0.001,50)	N	K
0.49928283815577382018	30	10	0.4993284415	15	10
1.4964743488656095074	33	10	1.4967767403	16	10
2.491033392031268146	32	10	2.492043943	16	10
3.483179154792483	16	10	3.48554266	12	10
4.47310733766121	17	10	4.4775843	14	10
(0.001,100)	N	K	(0.005,1)	N	K
0.4993900	14	10	0.49623061843859388133	14	0
1.497164	14	10	1.4810535774523086622	16	0
2.49326	12	10	2.4504506307929553916	19	0
3.4882	8	10	3.4041090393018610892	22	0
4.482	6	10	4.3416858782640029960	26	0
(0.005,5)	N	K	(0.005,10)	N	K
0.496410220946958321	17	0	0.4966047151	17	10
1.4823111693092516	17	0	1.483617596	16	10
2.454927624666918	16	0	2.459345776	17	10
3.41532551991532	16	0	3.425767168	16	10
4.36448638412074	17	0	4.38443866	14	10
(0.01,2)	N	K	(0.01,2.5)	N	K
0.49261048842431841116	15	0	0.49270083568284728418	18	0
1.4630542754167881338	15	0	1.4636958224910252902	18	0
2.4041742821521898813	16	0	2.4064888346975272	15	0
3.3164352655255853622	17	0	3.322306851416587	15	0
4.200308983473177091	17	0	4.212382312008046	16	0
(0.01,3)	N	K	(0.01,4)	N	K
0.49278813286769149	17	0	0.49295433222635	15	0
1.4643087072318182	17	0	1.4654574556056	16	0
2.408667765195180	17	0	2.412672075247	16	0
3.3277381346791	14	0	3.33749365618	14	0
4.223332041512	14	0	4.2425196812	17	0
(0.01,8)	N	K	(0.01,10)	N	K
0.49352818	16	10	0.49377219	18	10
1.4692593	16	10	1.470806	16	10
2.4252650	16	10	2.43013	12	10
3.36650	12	10	3.3771	9	10
4.29644	12	10	4.3152	8	10
(0.02,1)	N	K	(0.02,2)	N	K
0.48465430456	28	10	0.4854342883	19	10
1.42129904	25	10	1.42718578	19	10
2.288670	22	10	2.3116477	18	10
3.0757	24	10	3.14073	16	10
3.759	19	10	3.91642	16	10
(0.02,4)	N	K	(0.02,5)	N	K
0.4867027	16	0	0.4872327	17	10
1.436017	15	10	1.439495	16	10
2.342453	17	10	2.35372	15	10
3.21546	15	10	3.24065	16	10
4.06237	16	10	4.1076	12	10

Table (4.11). Eigenvalues of $H=1/2P^2+1/2x^2-gx^4/(1+g\alpha x^2)$, for the first five energy levels calculated from Hypervirial method; the numbers in the bracket corresponds to (g) & (α) First line corrspond to (gα) as perturbation constant; Second line to (g) as perturbation constant.

(0.001,10)	N	K	(0.001,20)	N	K
0.4992656878576565696263	16	0	0.4992828381557738201 8	30	10
3	14	0	7	10	10
1.496356976968126469 0	14	0	1.4964743488656095074	33	10
0	14	0	6	13	10
2.4906259959688469599	14	0	2.4910333920312 68146	32	10
9	14	0	2	14	10
3.4821857773654487833	21	0	3.483178154792483	16	10
3	20	0	4	16	10
4.4711439430890412558	21	0	4.473107337 66121	17	10
8	21	0	2	17	10
(0.001,50)	N	K	(0.005,1)	N	K
0.4993284415	15	10	0.4962306184385938813 3	14	0
2	12	10	3	14	0
1.4967767403	16	10	1.4810535774523086622	16	0
7	12	10	2	16	0
2.492043943	16	10	2.4504506307929553916	19	0
0	13	10	6	19	0
3.48554266	12	10	3.4041090393018610892	22	0
5	15	10	2	22	0
4.4775843	14	10	4.3416858782640029960	26	0
7	14	10	0	26	0
(0.005,5)	N	K	(0.01,2)	N	K
0.4964102209469583 21	17	0	0.4926104884243184111 6	15	0
1	17	0	6	15	0
1.4823111693092516	17	0	1.4630542754167881338	15	0
6	17	0	8	15	0
2.454927624666918	16	0	2.4041742821521898813	16	0
8	16	0	3	16	0
3.415325519915 32	16	0	3.3164352655255853622	17	0
2	16	0	2	17	0
4.364486384120 74	17	0	4.2003089834731770 91	17	0
4	17	0	1	17	0
(0.01,5)	N	K	(0.02,2)	N	K
0.493110419714	16	0	0.4854342883	19	10
4	16	0	26	17	10
1.4665158856	14	0	1.42718578	19	10
6	14	0	82	16	10
2.416275286	13	0	2.3116477	18	10
6	13	0	63	17	10
3.346040309	17	0	3.14073	16	10
9	17	0	354	16	10
4.258866543	17	0	3.91642	16	10
3	17	0	15	16	10

Table (4.12). Eigenvalues of $H=1/2P^2+1/2x^2-gx^4/(1+g\alpha x^2)$ for the first four energy levels calculated from the Padé approximants E[N,N]; the numbers in the bracket correspond to (g) & (α).

(0.1,2)	N	N	(0.1,2.5)	N	N	(0.1,3)	N	N
0.4345832964	8	8	0.4412762084	8	8	0.4462758528	9	9
1.1744233671	8	8	1.2252581949	8	8	1.2575765719	9	9
1.6831031070	8	8	1.8617228194	8	8	1.9566367048	9	9
2.0151554685	8	8	2.4251600025	8	8	2.6097159514	9	9
(0.1,5)	N	N	(0.1,10)	N	N	(0.1,15)	N	N
0.4587898978	9	9	0.4727319810	8	8	0.4782532747	8	8
1.3280416331	9	9	1.3953728384	8	8	1.4236849697	8	8
2.1411909221	8	8	2.2968398450	8	8	2.3567717433	8	8
2.9408181736	9	9	3.1971246268	7	7	3.1788622622	8	8
(0.2,2)	N	N	(0.2,2.5)	N	N	(0.2,3)	N	N
0.3836567073	7	7	0.4037167692	8	8	0.4159779485	8	8
0.9281407509	7	7	1.0788453405	8	8	1.1481938772	8	8
1.1455258520	7	7	1.6037923857	8	8	1.7744403191	8	8
1.2206580711	7	7	2.0974228055	8	8	2.3839422086	8	8
(0.2,5)	N	N	(0.2,10)	N	N	(0.2,15)	N	N
0.4417394844	8	8	0.4652409492	8	8	0.4748397321	8	8
1.2748491752	8	8	1.7354519173	8	8	1.4129171006	8	8
2.0625474492	8	8	2.2712345226	8	8	2.3439153813	8	8
2.8484836356	8	8	3.1686818077	8	8	3.2763114084	8	8
(0.5,2)	N	N	(0.5,2.5)	N	N	(0.5,3)	N	N
0.2810581365	8	8	0.3440407085	7	7	0.3718192169	9	9
0.4951438653	7	7	0.8971718533	7	7	1.0212534971	9	9
0.5557256829	9	9	1.3359424602	7	7	1.6040289426	9	9
1.1283491890	7	7	1.7971751960	7	7	2.1947562151	9	9
(0.5,5)	N	N	(0.5,10)	N	N	(0.5,15)	N	N
0.4206661507	9	9	0.4575899416	7	7	0.4707208408	8	8
1.2210327895	8	8	1.3582779746	7	7	1.4043002434	8	8
1.9960067456	8	8	2.2520265292	8	8	2.3348082096	7	7
2.7744683184	8	8	3.1479537392	7	7	3.2665125789	7	7
(1,3)	N	N	(1,5)	N	N	(1,15)	N	N
0.3431570119	10	10	0.4086902923	8	8	0.4688843439	8	8
0.9562204783	10	10	1.1954308829	8	8	1.4008787418	8	8
1.5317717035	10	10	1.9688573248	8	8	2.3314809029	8	8
2.1186156264	10	10	2.7466352484	8	8	3.2629190879	8	8
(1,50)	N	N	(2,5)	N	N	(2,50)	N	N
0.4905390334	8	8	0.4002714352	9	9	0.4904410593	8	8
1.4704215488	7	7	1.1802036273	9	9	1.4702554737	7	7
2.4500288406	7	7	1.9540673614	8	8	2.4498709063	7	7
3.4301396212	7	7	2.7258489369	8	8	3.3299775368	7	7

Table (4.13). Eigenvalues of $H = 1/2P^2 + 1/2x^2 - gx^6/(1+g\alpha x^2)$, For the first five energy levels calculated from Hypervirial method;the numbers in the bracket correspond to (g)&(α),First line corrspond to (gα) as perturbation constant;Second line to (g) as perturbation constant.

(0.0001,5)	N	(0.0001,10)	N	(0.0001,20)	N
0.49981227962688195559 9	12 12	0.49981260877599879487 7	11 12	0.49981326263023232111 094	10 13
1.4986830203391436274 4	16 16	1.4986860018377311175 5	13 13	1.4986919153374103074 087	11 9
2.4952790842668085520 0	18 18	2.4952928059703008330 0	17 17	2.4953199695038252729 36	16 11
3.48803751212950265 5	17 17	3.4880813288034949205 2	23 17	3.4881678723838316991 29	19 13
4.475318709124738 8	17 17	4.4754289637285439 4	19 16	4.4756491365545428671 0	24 16
(0.0001,100)	N	(0.0002,10)	N	(0.0002,20)	N
0.4998182907837595591 1	22 22	0.4996254294479404345 4	22 19	0.4996280355457631462 4	25 8
1.4987369875120074141 1	23 23	1.49736884834399597 9	21 19	1.49739253775022120 2	25 7
2.4955247809883051070 0	25 25	2.49054411589624 2	23 16	2.4906539011114878 55	26 18
3.4888122166482404402 2	28 28	3.475934128335 3	23 17	3.47628883899059 6	24 18
4.4772578321247956935 5	29 29	4.450008702 2	16 16	4.45092601795 9	23 18
(0.0003,3)	N	(0.0003,5)	N	(0.0004,10)	N
0.49943426656917 7	15 15	0.4994354710480190 0	23 19	0.499251670691 1	16 16
1.49600980232 2	12 12	1.496020892537 8	21 18	1.4947240220 0	14 14
2.485568969 9	12 12	2.485621375 5	16 16	2.48090744 4	11 11
3.4629279 9	10 10	3.4631022 2	10 10	3.450829 9	9 9
4.421949 9	10 10	4.422419 9	13 13	4.3958 8	5 5
(0.005,2)	N	(0.0005,5)	N	(0.0006,8)	N
0.4990516248 8	10 10	0.4990567271 1	9 9	0.498869022 2	6 6
1.49327002 2	10 10	1.49331788 8	9 9	1.4919725 5	7 7
2.475398 8	9 9	2.475632 2	7 7	2.47060 0	5 5
3.4356 6	4 4	3.43646 6	7 7	3.4226 6	8 8
4.359 9	8 8	4.362 2	5 5	4.329 9	7 7

Table (4.14). Eigenvalues of $H=1/2P^2+1/2x^2+gx^6/(1+g\alpha x^2)$, for the first five energy levels calculated from Hypervirial method; the numbers in the bracket corresponds to (g) & (α), First line corrspond to (gα) as perturbation constant; Second line to (g) as perturbation constant.

(0.0001,10)	N	(0.0001,100)	N
0.50018631161181683179	14	0.50018073361783520246	26
1.50128946562205326667	16	1.50125013470858294 34	30
2.50461645179303576 88	20	2.50439675301365722	33
3.51155118318366 73	21	3.510878803521578	34
4.523443927058427	20	4.521823800663	32
(0.0002,4)	N	(0.0002,20)	N
0.50037182660944569	17	0.50036779117745 3172	27
1.502587266898668	21	1.50255163333155	20
2.5091581159278	18	2.509000000754	21
3.5228005302	12	3.522318551	12
		4.5448345	9
(0.0003,5)	N	(0.0004,4)	N
0.50055485771084	18	0.50073753505	9
1.50384885187	11	1.50510337	8
2.51356329	7	2.5179195	8
3.5335744	9	3.544150	9
4.56725	6	4.5879	5
(0.0004,6)	N	(0.0005,5)	N
0.50073555629	9	0.5009166570	9
1.50508602	9	1.5063232	6
2.5178438	9	2.522108	7
3.54392	5	3.5541	5
4.5874	6	4.607	4

Table (4.15). Eigenvalues of $H=P^2+r^2+\lambda r^2/(1+gr^2)$, for the first four energy levels, First line; power series method, Second line; Hypervirial method; the numbers in the bracket correspond to (g) & (λ) and [ℓ].

(0.1,500) [5]	β , r N	(0.1,1000) [10]	β , r N
286.13076490527473583 9	50, 3 9	406.44313182902570483 9	50, 3 9
371.22042907411788362 1	50, 3 9	528.53607611601199889 7	50, 3 9
455.14748332068983119 25	50, 3 11	649.45475697358916874 9	50, 3 8
537.82033223623150988 94	50, 3 11	769.20503286345577039 6	50, 3 8
(0.1,500) [20]		(0.1,1000) [20]	
914.36631099435518106 29	50, 3 15	1312.2516748089389117 6 9	50, 3 13
990.80662152100375692 713	50, 3 15	1425.5860016386655690 0	50, 3 12
1066.1483033938278229 32	50, 3 14	1537.7804590395244318 6	50, 3 13
1140.4001942815468116 21	50, 3 15	1648.8711228851733896 6	50, 3 13
(0.1,200) [5]		(0.1,200) [10]	
179.48311321895504768 74	50, 3 10	311.86088089276042370 8	50, 3 14
231.79347770320596206 4	50, 3 12	361.30878862459200039 7	50, 3 14
282.96632629393405987 97	50, 3 12	409.65356499765353914 24	50, 3 15
333.01539438085999032 35	50, 3 12	456.90932312687538308 6	50, 3 16
(0.5,10000) [5]		(0.5,10000) [10]	
1275.7839677457011592 2	50,1.4 9	2228.5184345249449665 4	50,1.4 11
1653.5754640897516671 1	50,1.4 9	2591.7305830130772647 7	50,1.4 11
2025.5619017911742377 7	50,1.4 9	2949.2545750114440892 1	50,1.4 11
2391.7900375221419928 8	50,1.4 10	3301.1380480892597575 7	50,1.4 11
(0.4,10000) [5]		(0.4,10000) [10]	
1280.6255224944247831 1	50,1.4 9	2242.7941758856259097 7	50,1.4 10
1662.8193920643831413 3	50,1.4 9	2613.2566724792696371 2	50,1.4 10
2040.3377379823186474 4	50,1.4 10	2979.1179119985850306 6	50,1.4 11
2413.2102671628264615 4	50,1.4 11	3340.4080590976735523 3	50,1.4 11
(0.2,1000) [5]		(0.2,1000) [10]	
401.60803348855637720 2	50, 2 10	699.10562257451248607 10	50, 2 13
519.30844710805602854 2	50, 2 10	811.02606253526313711 08	50, 2 13
634.71038117717253462 2	50, 2 12	920.70801035417738037 40	50, 2 13
747.83782016102183348 7	50, 2 12	1028.1760134993310156 7	50, 2 14

Table (4.16). Eigenvalues of $H=P^2+r^2+\lambda r^2/(1+gr^2)$, for the first five energy levels, calculated from the Padé approximants E [6,6]; the numbers in the bracket correspond to (g), (λ) and [ℓ].

(0.1,0.1)[1]	(0.1,0.1)[2]	(0.1,0.1)[3]
5.1863730031	7.2439618411	9.2943591118
9.2765419870	11.3179977480	13.3557272953
13.3421984324	15.3738528950	17.4034522612
17.3927308919	19.4179144888	21.4419338622
(0.1,5)[1]	(0.1,5)[2]	(0.1,5)[3]
11.5587455831	15.9170986413	20.1306138402
19.7987423849	23.7658049064	27.6128545825
27.3160524161	30.9539439974	34.4954980980
34.2309589246	37.5974669447	40.8891097666
(0.5,0.5)[1]	(0.5,0.5)[2]	(0.5,0.5)[3]
5.4998837608	7.5917869769	9.6568791274
9.5919229690	11.6466627410	13.6910540038
13.6438990724	15.6885686213	17.7222565012
17.6875754104	19.7163820232	21.7440321550
(0.5,50)[1]	(0.5,50)[2]	(0.5,50)[3]
31.6592687604	42.7250391678	52.8947367975
51.0837491364	59.8601905694	67.9020149596
66.3789651981	73.3071780289	79.6769793648
78.4172864626	83.9412018964	89.0795821529
(1,50)[1]	(1,50)[2]	(1,50)[3]
28.0789946886	36.4030821775	43.2227912191
40.8728593723	46.1845533815	50.7798984456
49.1901626340	53.0463643460	56.7135011768
55.2382048224	58.1092055687	60.8014575383
(1,100)[1]	(1,100)[2]	(1,100)[3]
42.2375607416	55.9778041155	67.9608076904
64.8194034146	74.4373894408	82.7693357495
80.3937290506	87.1066457238	93.0193049200
91.2485998040	96.1350495173	100.5576277803
(2,500)[1]	(2,500)[2]	(2,500)[3]
95.5803706134	127.3216094886	155.3869965188
148.6098717171	171.3920797463	191.2127639316
185.8851576987	201.7065198328	215.3169441763
211.2839677147	222.0671507250	231.3670836370
(5,1000)[1]	(5,1000)[2]	(5,1000)[3]
119.3154421104	151.7988052722	175.8756903428
165.2034322656	181.6192066874	193.2683695238
187.3168908208	195.5744071826	202.4102794043
198.5135699380	204.1633890606	211.2001773100

Table (4.17) Eigenvalues of $H=1/2P^2+1/2r^2+gr^4/(1+g\alpha r^2)$, for the first five energy levels calculated from Hypervirial methods. The numbers in the bracket correspond to (g) & (α) and $<\ell>$.

(0.001,2)<1>	N	(0.001,10)<1>	N
2.5086092925084448022	13	2.5083202242185217689	24
4.5289412362445608226	16	4.5273411523390132269	30
6.5603505790868401431	18	6.5557621744605236698	37
8.6024681561332499412	21	8.59268950843783	34
10.654947388501173618	22	10.637352650852	32
(0.001,2)<5>	N	(0.001,10)<5>	N
6.5472403360866197125	17	6.5443876107859155020	37
8.5896062539413339822	21	8.58194431159574531	37
10.642323666264598321	22	10.6271771957659	36
12.705067193300432272	25	12.67942473622	35
14.7775300888412425	24	14.73810754	28
(0.001,2)<10>	N	(0.001,10)<10>	N
11.636752190015929766	21	11.6243639035517	32
13.705031891469307294	25	13.6812912058	30
15.7828596702109861	24	15.744273	20
17.869955315101557	26	17.812843	26
19.966053454454	21	19.88658	31
(0.002,5)<2>	N	(0.002,5)<5>	N
3.529381979370159554	33	6.58768081339508	33
5.576571189484475	36	8.66123416650	37
7.641023223462	34	10.749453164	35
9.721019279	32	12.851005	33
11.8150998	31	14.9647	22
(0.003,2)<2>	N	(0.004,2)<2>	N
3.544594052253502709	31	3.55840576203442	32
5.61704994895376	30	5.6518583832	27
7.71699916310	29	7.7792316	25
9.84221323	29	9.9371	15
11.990773	28	12.12	8
(0.005,1)<1>	N	(0.005,0.5)<1>	N
2.541366559899216	30	2.5417914913193910	25
4.63554346741	30	4.637819301005	26
6.775981	15	6.782318632	23
8.95840	21	8.971570	21
11.179	18	11.2024	16
(0.005,0.25)<1>	N	(0.005,0.25)<2>	N
2.542007801743604	20	3.57486773054679	22
4.638987472277	22	5.69751271419	24
6.785597954	22	7.86797093	20
8.978434	16	10.08311	15
11.214	7	12.3402	21

Table (4.18). Eigenvalues of $H=1/2P^2+1/2r^2+gr^4/(1+g\alpha r^2)$, for the ground state energy level calculated from Padé approximants E[N,M]; numbers in the bracket correspond to (g) & (α) and <ℓ>.

(0.01,10)<1>	N	M	(0.01,20)<2>	N	M	(0.01,25)<1>	N	M	(0.01,25)<2>	N	M
2.559403684	7	7	3.576614	7	6	2.542745	7	7	3.56875	7	6
2.559403698	7	6	3.576613	6	6	2.542745	7	6	3.56875	6	6
(0.01,50)<1>	N	M	(0.01,50)<2>	N	M	(0.01,50)<3>	N	M	(0.01,50)<4>	N	M
2.529452	7	7	3.54566	7	6	4.5629	6	6	5.5808	6	6
2.529459	7	6	3.54565	6	6	4.5629	6	5	5.5808	6	5
(0.03,2)<1>	N	M	(0.03,4)<2>	N	M	(0.03,6)<2>	N	M	(0.03,8)<2>	N	M
2.6852918	7	6	3.764767	7	6	3.72925	7	6	3.7022	7	6
2.6852914	6	6	3.764762	6	6	3.72924	6	6	3.7022	6	6
(0.04,2)<1>	N	M	(0.04,4)<2>	N	M	(0.04,6)<3>	N	M	(0.04,8)<4>	N	M
2.72763	7	6	3.81229	7	6	4.8754	7	6	5.91962	6	6
2.72763	6	6	3.81227	6	6	4.8754	6	6	5.91999	6	5
(0.05,5)<1>	N	M	(0.05,10)<2>	N	M	(0.05,20)<1>	N	M	(0.05,20)<2>	N	M
2.69907	7	6	3.7189	7	6	2.5896	7	7	3.6347	7	6
2.69903	6	6	3.7187	6	6	2.5899	7	6	3.6343	6	6
(0.06,,2<2>	N	M	(0.06,4)<2>	N	M	(0.06,6)<2>	N	M	(0.06,8)<2>	N	M
3.9891	6	6	3.8830	6	6	3.8143	6	6	3.766	6	6
3.9893	6	5	3.8833	6	5	3.8148	6	5	3.767	6	5
(0.08,4)<4>	N	M	(0.08,4)<2>	N	M	(0.08,6)<2>	N	M	(0.08,8)<2>	N	M
2.7747	7	6	3.934	6	6	3.848	6	6	3.791	6	6
2.7744	6	6	3.935	6	5	3.849	6	5	3.792	6	5
(0.1,2)<1>	N	M	(0.1,2)<2>	N	M	(0.1,4)<1>	N	M	(0.1,4)<2>	N	M
2.899	7	6	4.142	6	6	2.8027	7	6	3.973	7	6
2.899	6	6	4.143	6	5	2.8022	6	6	3.973	6	6
(0.15,2)<2>	N	M	(0.15,3)<2>	N	M	(0.15,4)<2>	N	M	(0.15,5)<2>	N	M
4.27	6	6	4.137	7	6	4.04	6	6	3.97	6	6
4.27	6	5	4.134	6	6	4.04	6	5	3.97	6	5
(0.2,2)<1>	N	M	(0.2,4)<1>	N	M	(0.2,6)<1>	N	M	(0.2,8)<1>	N	M
3.05	7	6	2.88	6	6	2.79	6	6	2.74	6	6
3.05	6	6	2.89	6	5	2.80	6	6	2.75	6	5

Table (4.19). Eigenvalues of $H=1/2P^2+1/2r^2-gr^4/(1+g\alpha r^2)$, for the first five energy levels calculated from Hypervirial method. The numbers in the bracket correspond to (g) & (α) and <ℓ>.

(0.001,2)<1>	N	(0.001,10)<1>	N
2.49126310973569004 75	7	2.4915654185981646077	14
4.4703209098626626 4601	7	4.4720384032432318316	17
6.4374599847414786137	7	6.4425130642421144292	18
8.3927166630793602145	7	8.4037518404895297	18
10.336127390802639802	8	10.356446671250888	17
(0.001,2)<5>	**N**	**(0.001,10)<5>**	**N**
6.4513231377501644703	7	6.4544310511385735820	17
8.4065375048857602018	6	8.41512488949682234	17
10.349905840171106936	7	10.3673114224817555	17
12.281464708012676318	8	12.31161616038458	17
14.201250789780285442	8	14.248607780243	16
(0.001,2)<10>	**N**	**(0.001,10)<10>**	**N**
11.356466025517407830	8	11.37060280542148	15
13.282012436129986100	8	13.30988181125121	17
15.195804217767798362	8	15.242196695642	16
17.097878228073353224	9	17.16803472738	16
18.988271440081638932	9	19.08780204	16
(0.003,5)<2>	**N**	**(0.004,5)<2>**	**N**
3.4551947842483942627	17	3.441285158679119 6	16
5.38241530522555255	17	5.34756301634048	17
7.282281166135826	17	7.220562915774	17
9.157402007571	16	9.0644256779	16
11.01012535683	16	10.88273141	16
(0.005,0.5)<1>	**N**	**(0.005,0.5)<2>**	**N**
2.4550159896717549118	24	3.4183365040822728954	28
4.3435674261949896	25	5.272789543280191	26
6.161611838663	28	7.053618142957	27
7.9022786583	26	8.752887897	26
9.55618173	25	10.359380	20
(0.005,1)<1>	**N**	**(0.005,1)<2>**	**N**
2.4555182642734604 39	19	3.4195468600070907884	22
4.3468793496272357119	27	5.2785363111551442055	30
6.172341788422471186	31	7.07001052754106 15	28
7.9283885503556	26	8.7900057898161	30
9.61054340321	28	10.43344590542	30
(0.005,0.25)<1>	**N**	**(0.005,0.25)<2>**	**N**
2.4547417623982326966	25	3.417713820390711	21
4.34184523090877	23	4.34184523090877	23
6.1559135127	20	7.044817879	23
7.88803158	21	8.73231	13
9.525380	21	10.3164	13

Table (4.20) Eigenvalues of $H=1/2P^2+1/2r^2-gr^4/(1+g\alpha r^2)$, for the first five energy levels calculated from Hypervirial method. The numbers in the bracket correspond to (g) & (α).

(0.001,2)<1>	N	(0.001,10)<1>	N
2.49126310973569004785	7 7	2.49186654185981646077 7	14 14
4.47032080962662646011	7 7	4.47203840324323183166	17 17
6.43745998474147861377	7 7	6.44251306424211442922	18 18
8.39271666307936021455	7 7	8.4037518404895287 7	18 18
10.33612739080263980222	8 8	10.356446671250888 8	17 17
(0.001,2)<10>	N	(0.001,10)<10>	N
11.35646602551740783000	8 8	11.37060280542148 8	15 15
13.28201243612998610000	8 8	13.30988181125121 1	17 17
15.19580421776779836222	8 8	15.242198669564 2 2	16 16
17.09787822807335322444	9 9	17.16803472738 8	16 16
18.98827144008163893222	9 9	19.08780204 4	16 16
(0.003,5)<2>	N	(0.004,5)<2>	N
3.45519478424839426277	17 17	3.4412851586791196 6	16 16
5.382415305222555525555	17 17	5.34756301634048 8	17 17
7.282281166135826 6	17 17	7.220562915774 4	17 17
9.157402007571 1	16 16	9.0644256779 9	16 16
11.01012535683 3	16 16	10.88273141 1	16 16
(0.005,1)<1>	N	(0.005,1)<2>	N
2.45555182642734604399	19 19	3.41954686000709078844	22 22
4.34687934962723571199	27 27	5.27853631115514420555	30 30
6.17234178842247118666	31 31	7.0700105275410615 5	28 28
7.9283885503556 6	26 26	8.7900057998161 1	30 30
9.61054340321 1	28 28	10.43344590542 2	30 30

CHAPTER FIVE

SOME DIFFERENT PROBLEMS

5.1 Introduction

Chapter five is devoted to investigating numerically various eigenvalue problems in one and three dimensions, using perturbative and nonperturbative methods for the following perturbative Hamiltonians:

1. $H=\frac{1}{2}P^2- r^{-1}+ \frac{1}{2}\gamma\ell_z + \frac{\gamma^2}{8}\left[x^2+y^2\right]$

2. $H=\frac{1}{2}P^2+ \frac{1}{2}\ell(\ell+1)r^{-2}- Zr^{-1}e^{-\lambda r}$

3. $H=P^2+ \ell(\ell+1)r^{-2}-Ae^{-\lambda r^2}$

4. $H=\frac{1}{2}P^2+ \frac{1}{2}\ell(\ell+1)r^{-2}- r^{-1}+\lambda r$

5. $H=\frac{1}{2}P^2- r^{-1}+ 2\lambda r + 2\lambda^2 r^2$

6. $H=\frac{1}{2}P^2+ \frac{1}{2}\ell(\ell+1)r^{-2}-r^{-1}e^{-\lambda r}\mathrm{Cos}(\lambda r)$

7. $H=\frac{1}{2}P^2+ \frac{1}{2}\ell(\ell+1)r^{-2}- \lambda e^{-\lambda r}\left[1-e^{-\lambda r}\right]^{-1}$

8. $H=P^2+x^2-2e^{-2\lambda x^2}\left[1+e^{-2\lambda x^2}\right]^{-1}$

9. $H=P^2+r^2+\ell(\ell+1)r^{-2}-2e^{-2\lambda r^2}\left[1+e^{-2\lambda r^2}\right]^{-1}$

The energy eigenvalues as computed by more than one method agree with each other and with those reported in the literature. Beside the methods described in the various sections of chapter five, we should note that all the traditional methods of accelerating convergence of a series can be used in perturbation theory (e.g renormalised series and Padé approximants).

5.2 Quadratic Zeeman effect

5.2.1 Introduction

The problem of the quadratic Zeeman effect for the hydrogen atom has attracted much attention because of its applications in astrophysics and solid state physics. The problem of the Zeeman effect has been studied by many authors using a number of approximate methods. The literature provides an exhaustive range of numerical results for different range of field strength H.Praddaude [32,1972] calculated the 14 lowest-energy levels, assuming an appropriate expansion of the wave function in terms of Laguerre polynomials, Gallas [34,1984] gave variational estimates of the energies for the first 13 states. Also an investigation of this problem was given by Killingbeck [33,1981; 35,1985; 36,1985] using several techniques (power series, renormalised series and finite difference methods). The hamiltonian for a hydrogen atom in the presence of a constant magnetic field is

$$H=\frac{1}{2}m_e\left[\underline{P}+\frac{e}{c}\underline{A}\right]^2-\frac{e^2}{r} \tag{5.1}$$

where $(\underline{A}=\frac{1}{2}\underline{B}\times\underline{r})$ is the vector potential. Assuming the magnetic field B to be along the Z direction ($\underline{B}=0,0,B$), and choosing atomic units such that $\hbar=e=m_e=1$, the magnitude of the vector potential is

$$A=\frac{1}{2}\left|\underline{B}x\underline{r}\right|=\frac{1}{2}BrSin\theta \qquad (5.2)$$

so that

$$\underline{A}.\underline{P}=B\left(xPy-yPx\right)=B\ell z \qquad (5.3)$$

$$\underline{P}=iPx+jPy+kPz \qquad (5.4)$$

$$\underline{A}=\frac{1}{2}B\left[-iy+jx\right] \qquad (5.5)$$

Here r makes angle θ with the Z axis. ℓz is the operator for the Z component of the orbital angular momentum. Using equations (5.2,5.3,5.4), then the equation (5.1) takes the form

$$H=\frac{1}{2}P^{2}-r^{-1}+\frac{1}{2}\gamma\ell z+\frac{1}{8}\gamma^{2}r^{2}Sin^{2}\theta \qquad (5.6)$$

with $\gamma=\frac{eB}{m_e c}$, in S.I.units. B represents the magnetic field strength and e, m_e the electronic charge and mass respectively. In the units used the parameter γ is equal to the cyclotron frequency. It measures the magnetic field strength in units of $2.35x10^{9}$ G; equivalently $2.35x10^{5}$ T corresponds to the value $\gamma=1$. By using the spherical coordinates

$$x=rSin\theta Cos\phi \qquad (5.7)$$

$$y=rSin\theta Sin\phi \qquad (5.8)$$

$$z=rCos\theta \qquad (5.9)$$

Then

$$x^{2}+y^{2}=r^{2}Sin^{2}\theta \qquad (5.10)$$

Therefore the hamiltonian can be written as

$$H=-\frac{1}{2}D^2-r^{-1}+\frac{1}{2}\gamma\ell_z+\frac{1}{8}\gamma^2\left[x^2+y^2\right] \qquad (5.11)$$

In these units the ground state energy is -1/2 at $\gamma=0$, and $\gamma=0.1$ corresponds to a magnetic field of ($2.35\mathrm{x}10^4$T). The term in equation (5.6) $\frac{1}{8}\gamma^2r^2\mathrm{Sin}^2\theta$ has the expectation value

$$\frac{1}{8}\gamma^2\langle n\ell m|r^2\mathrm{Sin}^2\theta|n\ell m\rangle=\frac{1}{8}\gamma^2\langle\ell n|r^2|\ell n\rangle\langle\ell m|\mathrm{Sin}^2\theta|\ell m\rangle \qquad (5.12)$$

Where

$$|n\ell m\rangle=R_{n\ell}Y_\ell^m(\theta,\phi) \qquad (5.13)$$

In order to evaluate the quantity (5.12) it is convenient to write down the recurrence relations

$$\left(2\ell+1\right)\mathrm{Cos}\theta P_\ell^m=\left(\ell+m\right)P_{\ell-1}^m+\left(\ell-m+1\right)P_{\ell+1}^m \qquad (5.14)$$

$$\mathrm{Cos}\theta P_\ell^m=\left[\frac{(\ell+m)}{(2\ell+1)}\right]P_{\ell-1}^m+\left[\frac{(\ell-m+1)}{(2\ell+1)}\right]P_{\ell+1}^m \qquad (5.15)$$

$$Y_\ell^m(\theta,\phi)=\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}\,(-)^m e^{im\phi}\,P_\ell^m\,\mathrm{Cos}\theta \qquad (5.16)$$

From equations (5.15,5.16), it is easy to obtain the relation

$$\mathrm{Cos}\theta Y_\ell^m(\theta,\phi)=$$

$$\left[\sqrt{\frac{(\ell+m)(\ell-m)}{(2\ell+1)(2\ell-1)}}\right]Y_{\ell-1}^m(\theta,\phi)+\left[\sqrt{\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}}\right]Y_{\ell+1}^m(\theta,\phi) \qquad (5.17)$$

$$\langle\ell m|\mathrm{Sin}^2\theta|\ell m\rangle=1-\langle\ell m|\mathrm{Cos}^2\theta|\ell m\rangle \qquad (5.18)$$

$$=1-\int Y_\ell^{*m}(\theta,\phi)\mathrm{Cos}^2\theta\,Y_\ell^m(\theta,\phi)\,d\Omega \qquad (5.19)$$

$$=1-\left[\frac{(\ell+m)(\ell-m)}{(2\ell-1)(2\ell+1)}+\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}\right] \quad (5.20)$$

$$=\frac{1}{4}\left[\frac{\ell(\ell+1)+m^2-1}{(2\ell+3)(2\ell-1)}\right] \quad (5.21)$$

Also the $\frac{1}{2}\gamma\ell_z$ term contribution is given by

$$\langle n\ell m|\frac{1}{2}\gamma\ell_z|n\ell m\rangle=\frac{\gamma}{2}\langle e^{-im\phi}|\frac{\partial}{i\partial\phi}|e^{im\phi}\rangle=\frac{1}{2}\gamma m \quad (5.22)$$

Therefore to lowest order equation (5.6) can be replaced by a spherically symmetric Hamiltonian

$$H=\frac{1}{2}P^2-r^{-1}+\frac{\gamma}{2}m+\frac{1}{4}\left[\frac{\ell(\ell+1)+m^2-1}{(2\ell+3)(2\ell-1)}\right]\gamma^2r^2 \quad (5.23)$$

This use of a lowest order effective Hamiltonian is described in detail below. The quantum states of energy E_0 for a particle in a spherically symmetric field are characterised by wave function of the form

$$\Psi_{n\ell m}=R_{n\ell}(r)Y_\ell^m(\theta,\phi) \quad (5.24)$$

The direction of the Z-axis is arbitrary and can be chosen along the direction of the magnetic field B. The operator ℓ_z commutes with the Hamiltonian H for all values of the magnetic field and m is thus a good quantum number, i.e the Hamiltonian describes a system invariant to rotation about the Z-axis. The operators H and ℓ_z must have simultaneous eigenfunctions. The functions Y_ℓ^m contain the angle ϕ only in the factor $e^{im\phi}$, and the commutation relation $[H,\ell_z]=0$, expresses the fact that the Z-component of ℓ is a constant of the motion for any spherically symmetric potential. The hamiltonian contains a linear and a quadratic term in the magnetic field strength. The ground state (S-state) of the hydrogen atom has zero angular momentum, which means that the magnetic quantum number must be m=0. For such a state the linear term vanishes; therefore the full Hamiltonian (5.11) reduces to the form

$$H=-\frac{1}{2}D^{2}-r^{-1}+\frac{1}{8}\gamma^{2}\left[y^{2}+x^{2}\right] \tag{5.25}$$

The perturbing potential due to the magnetic field is not of a single tensor type but is a sum of tensor operator of rank 0 (with $\ell=0$) and of rank 2 (with $\ell=2$). which may be referred to as the s and d parts of the perturbation. By using tensor operators of definite ℓ we can express the perturbation as an $\ell=0$ term plus an $\ell=2$ term as follows

$$\frac{1}{8}\gamma^{2}\left[x^{2}+y^{2}\right]=A_{1}\gamma^{2}r^{2}+V_{2} \tag{5.26}$$

where

$$A_{1}=\frac{1}{12} \tag{5.27}$$

and

$$V_{2}=\frac{1}{24}\gamma^{2}\left[r^{2}-3z^{2}\right] \tag{5.28}$$

Therefore the equation (5.25) takes the form

$$H=-\frac{1}{2}D^{2}-r^{-1}+\frac{1}{12}\gamma^{2}r^{2}+\frac{1}{24}\left[r^{2}-3z^{2}\right] \tag{5.29}$$

where the s part is given by $\frac{1}{12}\gamma^{2}r^{2}$ and the d part by

$$\frac{1}{24}\gamma^{2}\left[3z^{2}-r^{2}\right]$$

The Hamiltonian for the different states can be written as follows, with

$$H_0 = -\frac{1}{2}D^2 - r^{-1}$$

$$1s \quad , \quad H=H_0+\frac{1}{12}\gamma^2r^2+\frac{1}{24}\gamma^2\left(r^2-3z^2\right) \tag{5.30}$$

$$2p_0 \quad , \quad H=H_0+\frac{1}{20}\gamma^2r^2+\frac{1}{40}\gamma^2\left(3r^2-5z^2\right) \tag{5.31}$$

$$2p_{-1}, \quad H=H_0+\frac{1}{10}\gamma^2r^2+\frac{1}{2}\gamma m+\frac{1}{40}\gamma^2\left(r^2-5z^2\right) \tag{5.32}$$

$$3d_{-1}, \quad H=H_0+\frac{1}{14}\gamma^2r^2+\frac{1}{2}\gamma m+\frac{1}{56}\gamma^2\left(3r^2-7z^2\right) \tag{5.33}$$

$$3d_{-2}, \quad H=H_0+\frac{3}{28}\gamma^2r^2+\frac{1}{2}\gamma m+\frac{1}{56}\gamma^2\left(r^2-7z^2\right) \tag{5.34}$$

Each V_2 term has zero expectation value for the states concerned

$[1s,\ 2s,\ 2p_0\ ,\ 2p_{-1}\ ,\ 2p_{+1}\ ,\ 3d_{-1}\ ,\ 3d_{-2}]$ i.e

$$E_1=\langle\Phi_0|V_2|\Phi_0\rangle=0 \tag{5.35}$$

The spherically symmetric Hamiltonian $H-V_2$ can be treated accurately by various methods. To obtain the full perturbed energy (E) it will then be necessary to include the second order and third order energy shift which is produced by adding the V_2 part of the potential function. As we pointed out above, the addition of the V_2 potential term to the Hamiltonian does not alter the energy eigenvalue in first order. We can estimate the second-order energy shift caused by the residual perturbation V_2. E_2 and E_3 can actually be closely estimated starting from the Hylleraas functional, which takes the following form

$$F(\psi)=2\langle\psi|V|\phi_0\rangle-\langle\psi|(H_0-E_0)|\psi\rangle \qquad (5.36)$$

where ψ is a trial function estimate for the first order perturbed wavefunction. By using the renormalised series method, it is easy to find E_0, $\langle r\rangle$ and to get higher $\langle r^n\rangle$. To find the E_2 produced by V_2 we start from the eigenfunction of the perturbed radial problem as the unperturbed function. Calling this function ϕ_0 and taking the trial function ψ in the form $\psi=f\phi_0$, with f some function of the coordinates, the second term in (5.36) then takes the following form after using the relation

$$H_0\phi_0=E_0\phi_0 \qquad (5.37)$$

$$\langle\phi_0|f(H_0-E_0)f|\phi_0\rangle=\langle\phi_0|f[H_0,f]|\phi_0\rangle \qquad (5.38)$$

If the Hamiltonian $H_0=-\alpha D^2+U$, with U any function of position, then relation (5.38) after tedious algebra and use of the identity

$$\nabla^2(fg)=f\nabla^2g+g\nabla^2f+2\mathrm{grad}(f).\mathrm{grad}(g) \qquad (5.39)$$

takes the form

$$\langle\phi_0|f[H_0,f]|\phi_0\rangle=\alpha\langle\phi_0|\mathrm{grad}(f).\mathrm{grad}(f)|\phi_0\rangle \qquad (5.40)$$

Then the Hylleraas functional takes the form (with $f=kV_2$)

$$f(\psi)=2k\langle\phi_0|V_2^2|\phi_0\rangle-\alpha k^2\langle\phi_0|\mathrm{grad}\ V_2.\mathrm{grad}\ V_2|\phi_0\rangle \qquad (5.41)$$

The whole set of terms involve only expectation values over ϕ_0, and standard angular integrals over (θ). The radial expectation values can be obtained from the renormalised series approach. In order to work out the angular terms in the functional we can use the relation

$$\langle F(\mu)\rangle=\frac{\langle\langle \mu^2 F(\mu)\rangle\rangle}{\langle\langle \mu^2\rangle\rangle} \qquad (5.42)$$

$$\langle\langle \mu^n\rangle\rangle=(n+1)^{-1} \qquad (5.43)$$

where

$$\mu=\mathrm{Cos}\theta \qquad (5.44)$$

We also have

$$\mathrm{grad}V_2.\mathrm{grad}V_2=\left(\frac{\partial V_2}{\partial x}\right)^2+\left(\frac{\partial V_2}{\partial y}\right)^2+\left(\frac{\partial V_2}{\partial z}\right)^2 \qquad (5.45)$$

E_3 can be estimated from the formula

$$E_3=\langle\psi_1|V_2|\psi_1\rangle \qquad (5.46)$$

$$=k^2\langle\phi_0|V_2^3|\phi_0\rangle \qquad (5.47)$$

To calculate E_2, we need the minimum of a function of form

$$F(k)=2Ak-Bk^2 \qquad (5.48)$$

The minimum is A^2B^{-1}. Taking A and B from the above results we can estimate the total second-order E_2 effect due to V_2. We performed the calculation at $\gamma=0.1$ for the states in the table below. We found the expectation values $\langle r^n\rangle$ $(n=2,4,6)$ by using the renormalised series approach. For example the total second-order effect for $2P_{-1}$ is given as

$$-0.1632653\left[\frac{\gamma^2}{40}\right]^2\frac{\langle r^4\rangle^2}{\langle r^2\rangle}=-27.302\times10^{-5} \qquad (\text{at } \gamma=0.1)$$

and also the total third-order effect for the same state $2P_{-1}$ is given as

$$\left[\frac{\gamma^2}{40}\right]^3\left[2k^2(-\frac{32}{31})\langle r^6\rangle\right]=-4.78852\times10^{-5} \quad (\text{at } \gamma=0.1)$$

where the value of k it can be determined from the second-order calculation and equals $k=AB^{-1}$. The perturbation coefficient in the above calculation is $(\gamma^2/40)$, which is actually (λ) (see (5.32)). The $(H-V_2)$ energy eigenvalue for state $2p_{-1}$is -0.1505220 as found by the renormalisd series approach, which also gives expectation values $\langle r^2\rangle=21.1594$, $\langle r^4\rangle=752.424$,$\langle r^6\rangle=38967.179$. The second and third order shifts due to V_2 are estimated to be (-0.000302, -0.0000478852) respectively. The second-order correction to the energy is six times the third-order correction, E_2 and E_3 together give a corrected energy (-0.1508429). This energy is in good agreement with Praddaude; using a large scale matrix calculation he obtained (-0.150845). The second and third order corrections thus bring our results closer to the results of Praddaude and indicate that it is sufficient to take the second and third order corrections to obtain a good energy. The unperturbed $2p_{-1}$energy is -1/8, so the V_1 part of the perturbation has given an energy shift (-0.025522), while V_2 has given a second order shift (-0.00027302) and a third order shift (-0.0000478852). The calculation described above can be carried out for various other states, as shown in table (5.2), which gives the required expressions for each state.

state	$2k\langle\phi_0\|V_2^2\|\phi_0\rangle$	$\alpha k^2\langle\phi_0\|[\frac{\partial V_2}{\partial r}]^2\|\phi_0\rangle$	$k^2\langle\phi_0\|V_2^3\|\phi_0\rangle$
s	$2k\,\frac{4}{5}\langle r^4\rangle$	$\frac{1}{2}\,k^2 8\,\langle r^2\rangle$	$2k^2[-\frac{16}{35}]\langle r^6\rangle$
$2p_0$	$2k\,\frac{12}{7}\langle r^4\rangle$	$\frac{1}{2}\,k^2 24\langle r^2\rangle$	$2k^2[\frac{16}{21}]\langle r^6\rangle$
$2P_{-1}$	$2k\,\frac{8}{7}\langle r^4\rangle$	$\frac{1}{2}\,k^2 16\langle r^2\rangle$	$2k^2[-\frac{32}{21}]\langle r^6\rangle$
$3d_{-1}$	$2k\,\frac{8}{3}\langle r^4\rangle$	$\frac{1}{2}\,k^2 48\langle r^2\rangle$	$2k^2[-\frac{32}{33}]\langle r^6\rangle$
$3d_{-2}$	$2k\,\frac{4}{3}\langle r^4\rangle$	$\frac{1}{2}\,k^2 24\langle r^2\rangle$	$2k^2[-\frac{38}{33}]\langle r^6\rangle$

We also used the more complicated wavefunctions, $\psi_1=kV_2(1+\alpha r)\phi_0$ as a trial function and followed the same method above to calculate E_2. We obtained the following relation corresponding to this trial wavefunctions for the 1s state

$$E_2 = \frac{A_1}{A_2}$$

where

$$A_1= -0.64\left[\frac{\gamma^2}{24}\right]^2\left[\langle r^4\rangle+\alpha\langle r^5\rangle\right]^2$$

$$A_2=4\left[\langle r^2+2\alpha\langle r^3\rangle+\alpha^2\langle r^4\rangle\right]+o.4\left[4\alpha\langle r^3\rangle+5\alpha^2\langle r^4\rangle\right]$$

The above approach does not improve the correction since it gave a best correction at $\alpha=0$.

5.2.2 The renormalised series method to compute the initial energy eigenvalues

To find the energy of a state in the spherically symmetric potential

$$V(r)=-r^{-1}+A(\ell,m)\gamma^2r^2 \qquad (5.49)$$

We write the radial Schrödinger equation in this form

$$-\frac{1}{2}D^2\Psi(r)-\left[r^{-1}-\frac{1}{2}\ell(\ell(+1)r^{-2}-\lambda r^2\right]\Psi(r)=E\Psi(r) \qquad (5.50)$$

Using the renormalised series approach we rewrite the potential given in equation (5.50) as

$$V(r)=-\left(\mu+k\lambda\right)r^{-1}+\frac{1}{2}\ell(\ell+1)r^{-2}+\lambda r^2 \qquad (5.51)$$

where

$$A(\ell,m)=\frac{1}{4}\left[\frac{\ell(\ell+1)+m^2-1}{(2\ell+3)(2\ell-1)}\right], \quad \mu=1-\lambda k \qquad (5.52)$$

and

$$\lambda=A(\ell,m)\gamma^2 \qquad (5.53)$$

For the potential given by equation (5.51) the hypervirial relation (2.3) gives the following relation between the various expectation values for states of angular momentum ℓ takes the form

$$\begin{aligned}2\left(N+1\right)\sum_{0}^{M}E(I)A(N,M-I)=N\left[\ell(\ell+1)-\frac{1}{4}\left(N^2-1\right)\right]A(N-2,M)\\ -\left(2N+1\right)\left[\mu A(N-1,M)+kA(N-1,M-1)\right]\\ +\left(2N+4\right)A(N+2,M-1) \qquad (5.54)\end{aligned}$$

By using the Hellmann-Feynman theorem we obtain the recurrence relation

$$\left(M+1\right)E(M+1)=A(2,M)-kA(-1,M) \tag{5.55}$$

We can determine the energy coefficients E(M+1) and the series coefficients A(N,M), by using equations (5.54,5.55), with the aid of the unperturbed energy $E(0)=-\mu^2/2n^2-\frac{1}{2}\gamma m$, and the initial coefficient A(0,0) =1. We also tried another renormalised series approach to compute the energy eigenvalues. The renormalised potential corresponding to this approach takes the form

$$V(r)=-\mu_p r^{-1}+\frac{1}{2}\ell(\ell+1)r^{-2}+\underline{\lambda}\left[r^2-Kr^{-1}\right] \tag{5.56}$$

$$\underline{\lambda}=\lambda^2 \tag{5.57}$$

$$\mu_p=1+\underline{\lambda}k \tag{5.58}$$

i.e the perturbation involves λ^2 rather than λ. The purpose of using this modified renormalised technique was to seek an improvement in the accuracy of the results. This approach seemed helpful for higher excited states at low values of magnetic field. The recurrence relations corresponding to the modified renormalised series approach are

$$\begin{aligned}\left(2N+2\right)\sum_{0}^{M} E(I)A(N,M-I)=N&\left[\ell(\ell+1)-\frac{1}{4}\left(N^2-1\right)\right]A(N-2,M)\\ &-\left(2N+1\right)\left[\mu_p A(N-1,M)+kA(N-1,M-1)\right]\\ &+\left(2N+4\right)A(N+2,M-2)\end{aligned} \tag{5.59}$$

$$\left(M+1\right)E(M+1)=2A(2,M-1)-KA(-1,M) \tag{5.60}$$

The difference between the two approaches can be seen from equations (5.54,5.55.5.59,5.60), in the third term and first term of the right hand sides of the equations. The same technique was used for anharmonic oscillators in chapter 2 and helped to compute energy eigenvalues for $(\lambda x^6, \lambda x^8)$ perturbations which were an improvement over those given by the usual approach.

5.2.3 Results and discussion

We have calculated energy levels for all thirty states which have principal quantum number $n=1,2,3,4$, for magnetic field strengths in the range $0.005 \le \gamma \le 0.01$. Also we calculated thirteen states with $(n=1,2,3)$ at $\gamma = 0.1$. We computed the results using the renormalised series approach. Our results are converged to (14-figures) at field values corresponding to $\gamma=0.005$ and $\gamma=0.01$. This accuracy decreases for higher states. While the ordinary renormalised series $(\lambda^I, I=1)$ does not work at $\gamma=0.01$ and $n=4$, the other approach $(\lambda^I, I=2)$ works satisfactorily. Our results at $\gamma=0.005$ are in good agreement with the results of Gallas[34,1984], which are converged only to four significant figures. Two considerations govern our calculation at low magnetic fields; first, to show that the two perturbation approaches work very well and, second, to compute the energy eigenvalues for higher states.In table (5.3), it is clear that the renormalised series method for $H-V_2$ gives a very good upper bound to the total energies, while using the second and third order corrections to the energy bring our results very close to the results obtained by Praddaude; this is clear from table (5.2). Killingbeck [14,1981] estimated second-order corrections, so our work is an extension of this work. Table 5.1 shows the expectation value for $\langle r^n \rangle$, table 5.2 shows the energy and the second and third order corrections to the energy. Table (5.4) shows that the agreement between the results of the two perturbation approaches are very satisfactory at (γ=0.1) for states with n=1,2. The number of coefficients required to get a converged energy eigenvalue from the renormalised series is less with the λ^2 approach; this is clear from our results as shown in the tables (5.4,5.5). We believe our results demonstrate that the renormalised series method work excellently for low range values of magnetic field (where the series converge quickly) but does not work for high values of magnetic field. The energy eigenvalue associated with the 2p(+1) state can easily be calculate from the results for the 2P(-1) state. The term $\frac{1}{2}\gamma m$ gives the linear Zeeman term in equation (5.30-5.31); for the 2p(-1) state we have m=-1 and for the 2p(+1) state we have m=1, therefore they differ in energy by amount (γ),which means that to get the energy eigenvalue for the 2p(+1) state it will only be necessary to add this amount to the resulting energy for the 2p(-1) state. In a similar way we can compute the energy eigenvalues for the other states; therefore states with m>0 cannot treated separately, since $E(\ell,m)-E(\ell,-m)$ has the fixed value $m\gamma$.

Table (5.1) some $\langle r^{n} \rangle$ values at $\gamma=0.1$.

state	$\langle r^{1} \rangle$	$\langle r^{2} \rangle$	$\langle r^{3} \rangle$	$\langle r^{4} \rangle$	$\langle r^{5} \rangle$	$\langle r^{6} \rangle$
1s	1.48919	2.94887	7.27689	21.47604	73.674802	287.71007
2s	5.18465	30.9783	203.25814	1446.64	11090.159	91024.32
2p(0)	4.51631	24.0078	146.0403	995.987	7498.307	61562.655
2p(+1)	4.25626	21.1594	119.538	752.424	5198.383	38967.179
2p(−1)	4.25626	21.1594	119.538	752.424	5198.383	38967.179
3d(−1)	6.96121	53.4333	446.2065	4011.81	38516.423	392244.29
3d(−2)	6.49885	46.4433	360.24112	3002.45	26675.328	251009.29

Table (5.2) Energies with second and third correction to the energy at $\gamma=0.1$; the figure between the bracket is the power of (10) multiplying the number.

state	E	E_2	E_3	$E+E_2+E_3$
1s	−0.4975216	−4.3446 (−6)	−4.03701(−8)	−0.4975259
2S	−0.0956530	−18.7655(−4)	−5.25135(−4)	−0.0980546
2P(0)	−0.1117526	−63. (−5)	5.14842(−5)	−0.1123312
2p(+1)	−0.0505220	−27.302 (−5)	−4.78852(−5)	−0.0508429
2p(−1)	−0.1505220	−27.302 (−5)	−4.78852(−5)	−0.1508429
3d(−1)	−0.0543089	−2.84589(−3)	−3.0146 (−4)	−0.0574562
3d(−2)	−0.0865749	−9.16956(−4)	−3.57562(−4)	−0.0878494

Table (5.3). comparison of our energy eigenvalues, which are calculated by using renormalised series approach with those of Jason (1984) and Praddaude (1972) at (γ=0.1).

State	JASON	Praddaude	E (λ^I, I=1)	N	K
1s	-0.497512	-0.497525	-0.49752165289784317	12	-80
2s	-0.0958	-0.098085	-0.0956530	7	-800
2p(0)	-0.11135	-0.11241	-0.11175251	13	-900
2p(-1)	-0.1495	-0.150845	-0.1505220	19	-800
2p(+1)	-0.0495	-0.050845	-0.0505220	17	-710
3s	0.031235	-0.02493	0.0374	14	-1500
3p(-1)	-0.01609	-0.03118	-0.0147	18	-1700
3p(+1)	-0.0839	-0.068815	-0.0859	8	-1450
3d(0)	-0.008635	-0.01216	-0.0108	11	-1700
3d(-1)	-0.05165	-0.05781	-0.0543	11	-1400
3d(+1)	0.04832	0.042185	0.0457	4	-1000
3d(-2)	0.0828	-0.087835	0.0864	19	-1400
3d(+2)	0.11715	0.11216	0.1135	19	-1400

Table (5.4). comparison between the calculations of the two approaches of the renormalised series for 1s, 2s, 2p(0), 2p(+1), 2p(-1) at γ=0.1

State	E (λ^I, I=2)	N	-K	E (λ^I, I=1)	N	-K
1s	-0.49752165289784317225	46	8	-0.49752165289784317	12	80
2s	-0.0956530	49	40	-0.0956530	7	800
2p(0)	-0.11175251	42	40	-0.11175251	13	900
2p(-1)	-0.150523	47	40	-0.1505220	19	800
2p(+1)	-0.050523	42	35	-0.0505220	17	710

Table (5.5) comparison of the energy eigenvalues, upper lines, renormalised series calculations from equation (5.60) lower line, renormalised series calculations from equation (5.55). The empty spaces mean that the corresponding eigenvalues cannot be reached through that approach.

state	γ=0.005	N	K	γ=0.01	N	K
1s	-0.49999375013996 6	6 2	-8 -10	-0.49997500223880 0	10 3	-12 -40
2s	-0.12491256398736 6	9 4	-8 -10	-0.12465101534992 2	14 6	-12 -40
2p(-1)	-0.12742506579170 0	9 5	-8 -10	-0.12970104287480 0	15 7	-12 -40
2p(0)	-0.12496251647389 9	9 3	-8 -10	-0.12485026234232 2	11 5	-12 -40
2p(+1)	-0.12242506579170 0	9 5	-8 -10	-0.11970104287480 0	15 6	-12 -40
3s	-0.05512714835713 3	16 7	-10 -15	-0.053873226274 2	29 14	-40 -50
3p(-1)	-0.05760909221494 4	19 7	-10 -15	-0.058808167016 6	29 8	-95 -60
3p(0)	-0.05533145157546 6	17 7	-10 -15	-0.0546693455128 8	24 12	-95 -60
3p(+1)	-0.05260909221494 4	19 7	-10 -15	-0.048808167016 6	29 8	-95 -60
3d(-2)	-0.06022071043309 9	18 8	-10 -15	-0.064245045208 5	28 13	-95 -60
3d(-1)	-0.05783174597558 8	15 7	-10 -15	-0.0596736605849 8	26 10	-95 -60
3d(0)	-0.05536888470656 6	14 6	-10 -15	-0.05481826517181 8	28 13	-95 -60
3d(+1)	-0.05283174597558 8	15 7	-10 -15	-0.0496736605849 8	26 10	-95 -60
3d(+2)	-0.05022071043309 9	18 8	-10 -15	-0.044245045208 5	28 13	-95 -60
4s	-0.029942181 8	24 9	-12 -20	-0.0263782	28	-120
4p(-1)	-0.03230520 0	16 8	-12 -20	-0.030935	29	-120
4p(0)	-0.03501460768 8	19 10	-12 -20	-0.02845022	25	-120
4p(+1)	-0.02730520 0	16 8	-12 -20	-0.020935	29	-120
4d(-2)	-0.034951942 4	23 9	-12 -20	-0.036491	25	-220
4d(-1)	-0.03287397814 4	23 12	-12 -20	-0.0329654	26	-120
4d(0)	-0.03051687437 7	21 11	-12 -20	-0.0284775	20	-120
4d(+1)	-0.02787397814 4	23 12	-12 -20	-0.0229654	26	-120
4d(+2)	-0.024951942 4	23 9	-12 -20	-0.016491	25	-220

Table (5.5 continued)

4f(-3)	-0.0377856722	21 13	-12 -20	-0.042693	26	-280
4f(-2)	-0.03552061888	19 10	-12 -20	-0.038518	20	-280
4f(-1)	-0.033163422800	19 10	-12 -20	-0.0340302	21	-280
4f(0)	-0.0307113445933	23 11	-12 -20	-0.0292040	20	-280
4f(+1)	-0.028163422800	19 10	-12 -20	-0.0240302	21	-280
4f(+2)	-0.02552061888	19 10	-12 -20	-0.018518	20	-280
4f(+3)	-0.0227856722	21 13	-12 -20	-0.012693	26	-280

5.3 Hydrogen atom with a Yukawa potential

The general screened Coulomb potential for hydrogen like atoms may be written in the form

$$V(r)=-Zr^{-1}\sum_{n=0}^{\infty} V_n(\lambda r)^n \qquad (5.61)$$

where Z is the nuclear charge and λ represents the screening constant. Screened Coulomb potentials have received a great deal of attention , not only in the field of nuclear physics but also in other fields such as atomic, solid state and plasma physics. The problem of the Yukawa potential has been studied by many authors, employing different approaches. C.S.Lai [38,1984] obtained, using Padé approximants [6,6] and [6,7], the energy eigenvalues for different values of λ and for various eigenstates. Edward R. Vrscay [39,1985] developed a power series method to calculate to large order the Rayleigh-Schrödinger perturbation expansions for energy levels of a hydrogen atom with a Yukawa type screened Coulomb potential, treating the 1s,2s and 2p levels. We employ the Hellmann-Feynman theorem and the hypervirial theorem to calculate the energy eigenvalues of various energy eigenvalues to high accuracy. In our work we wish to show that the renormalised series method can be used to calculate the bound-state energies of a screened Coulomb potential to very high accuracy. The present section treats the Yukawa potential. This study was motivated by the work of Lai [38,1984], who observed that [N-1,N] and [N,N] Padé approximants to the energy series provide accurate estimates of eigenvalues. The method which he used raises the question of whether or not the renormalised series method can gives accurate estimates of the eigenvalues. The two approaches (his and ours) which have been employed to study the potential use the Hellmann-Feynman and hypervirial theorems but our approach uses no Padé approximants. The renormalised series method for this problem is complicated by the presence of the renormalising constant K. A proper treatment would necessarily involve the choice of an ideal value for the renormalising constant K. The Hamiltonian for the Yukawa potential can be written as

$$H= -\frac{1}{2}D^2+\frac{1}{2}\ell(\ell+1)r^{-2}-Zr^{-1}e^{-\lambda r} \qquad (5.62)$$

$$= -\frac{1}{2}D^2+\frac{1}{2}\ell(\ell+1)r^{-2}-Z\left(\mu+\lambda K\right)r^{-1}-Zr^{-1}\sum_{n=1}^{\infty}V_n(\lambda r)^n$$

where

$$\mu=1-\lambda K$$

where ℓ is the orbital angular momentum quantum number. Here we are using atomic units, ħ=e=m=1. By employing the Hellmann-Feynman theorem and the hypervirial theorem as in previous sections the following two relations are obtained

$$\left(2N+2\right)\sum_{0}^{M}E(J)A(N,M-J)=N\left[\ell(\ell+1)-\frac{1}{4}\left(N^2-1\right)\right]B(N-2,M)$$

$$-\left(2N+1\right)\left[\mu B(N-1,M)+KB(N-1,M-1)\right]$$

$$-\sum_{n=0}^{\infty}V_n\left(2N+n+2\right)B(N+n,M-n-1) \qquad (5.63)$$

$$\left(M+1\right)E(M+1)=-KB(-1,M)-\sum_{n=0}^{\infty}V_n\left(n+1\right)B(n,M-n) \qquad (5.64)$$

The coefficients V_n in (5.63) and (5.61) can be written as

$$V_n=\frac{(-1)^{n+1}}{(n+1)!} \qquad (5.65)$$

for the case of the Yukawa potential. The coefficients V_n in general alternate in sign and decrease with increasing n. Where the energy of the unperturbed nth state $E(0)=-\mu^2/2n^2$ is known, the equations (5.63,5.64) suffice to calculate the full set of E and B coefficients, with the aid of equation (5.65) and the starting term B(0,0) which is obtained from the condition of normalization $\langle r^0\rangle=\langle 1\rangle=1$. Our numerical results, presented in table (5.6), reveal that at low values of λ for states (1s,2s,2p) we have excellent agreement with the values of Edward R.Vrscay [39,1985]. Our approach provides extremely accurate eigenvalues at low λ. These values are accurate to all the digits shown and agree to over (19) digits with those of Vrscay. The power of this renormalised series techniques at low values of λ has thus been demonstrated. However, at larger values of λ, the accuracy decreases as expected from our previous renormalised series calculations, although the accuracy is better than that of Lai [38,1984].

Table (5.6). The energy eigenvalues of $H=\frac{1}{2}P^2+\frac{1}{2}\ell(\ell+1)r^{-2}-r^{-1}e^{-\lambda r}$ by using renormalisd series.

λ	State	Energy	N	K
0.1	1S	-0.40705803061340315676	32	-2
0.2	1S	-0.32680851136919338490	61	-2.5
0.25	1S	-0.290919587521274335	75	-2.5
0.3	1S	-0.25763858630305	77	-3
0.4	1S	-0.19837608334	69	-2.5
0.5	1S	-0.1481170	63	-2.65
0.6	1S	-0.106134	67	-3
0.7	1S	-0.07181	59	-3
0.8	1S	-0.0445	53	-3
0.9	1S	-0.024	49	-2
0.01	2S	-0.11529328516799425622	14	-2
0.02	2S	-0.10614832024469550325	22	-2
0.03	2S	-0.097531786134660862775	34	-2
0.04	2S	-0.089414634185159188418	40	-3.5
0.05	2S	-0.081771195795253124176	58	-3.5
0.06	2S	-0.074578534412709709700	53	-5
0.07	2S	-0.067815959981462181221	65	-6
0.08	2S	-0.061464656212300385	68	-6.2
0.09	2S	-0.0555073885532907	67	-5.8
0.10	2S	-0.049928271331918	70	-6
0.20	2S	-0.0121075	72	-6
0.25	2S	-0.00337	82	-7
0.01	2P	-0.11524522409056418590	15	-4
0.02	2P	-0.10596339817993990476	22	-4
0.03	2P	-0.097131366795691310675	29	-4
0.04	2P	-0.088729373582879526291	35	-4
0.050	2P	-0.080740387037784609716	51	-4
0.060	2P	-0.073149619385860625029	57	-5
0.070	2P	-0.0659441769961565733	59	-5
0.080	2P	-0.05911280478703123	68	-6
0.090	2P	-0.05264570133158	62	-6
0.100	2P	-0.046534390486	57	-6
0.025	3S	-0.03432950991154377	35	-10
0.025	3P	-0.03407891042893813	35	-8
0.025	3d	-0.03357312208666600	34	-8
0.050	3S	-0.019352554814	37	-8
0.050	3P	-0.01855775188	46	-10
0.050	3d	-0.0169155705	41	-10
0.080	3S	-0.0077758	56	-14
0.080	3P	-0.0063299	62	-13
0.080	3d	-0.00324	44	-15
0.025	4S	-0.01250323831800	39	-12
0.025	4P	-0.0122943204363	39	-12
0.025	4d	-0.0118704489361	38	-12
0.025	4f	-0.011218210790	35	-10
0.050	4S	-0.0030915	42	-15
0.050	4P	-0.0025978	44	-15
0.050	4d	-0.001580	48	-15
0.060	4S	-0.001235	47	-14
0.060	4P	-0.00072	36	-13

5.4 The K-and L-shell binding energies of atom:

In the preceding section we have calculated the bound-state energy eigenvalues for a Yukawa potential with Z=1. In this section we will extend our discussion of the Yukawa potential of the form

$$V(r)=-Zr^{-1}\exp(-\lambda r) \qquad (5.66)$$

to the case Z>1, where the screening parameter λ is given by

$$\lambda=\lambda_0\left[Z\right]^{\frac{1}{3}} \qquad (5.67)$$

corresponding to the Z dependence of the reciprocal of the Thomas-Fermi radius of the atom. Grant and Lai [37,1979] have recently evaluated the energy levels for atoms with $(4\le Z\le 84)$ using Padé approximants [6,6] and [6,7], for K-and L-shell electrons with $(\lambda_0=0.98)$. The potential given by equation (5.66) can be expanded as

$$V(r)=-Zr^{-1}\sum_{n=0}^{\infty}V_n\left[\lambda_0 Z^{\frac{1}{3}}\right]^n \qquad (5.68)$$

$$=-Z\left(\mu+\lambda K\right)r^{-1}-Zr^{-1}\sum_{n=1}^{\infty}V_n\left[\lambda_0 Z^{\frac{1}{3}}\right]^n,\mu=1-\lambda K$$

By employing the Hellmann-Feynman theorem and the hypervirial theorem, the following two relations are obtained

$$\left(2N+2\right)\sum_{0}^{M}E(J)B(N,M-J)=N\left[\ell(\ell+1)-\frac{1}{4}\left(N^2-1\right)\right]B(N-2,M)$$

$$-Z\left(2N+1\right)\left[\mu B(N-1,M)+KB(N-1,M-1)\right]$$

$$-Z\sum_{n=0}^{\infty}V_n\left(2N+n+2\right)B(N+n,M-n-1) \tag{5.69}$$

$$\left(M+1\right)E(M+1)=-ZKB(-1,M)-Z\sum_{n=0}^{\infty}V_n\left(n+1\right)B(n,M-n) \tag{5.70}$$

where the energy of the unperturbed nth state is

$$E(0)=-\frac{Z^2\mu^2}{2n^2} \tag{5.71}$$

Here we use atomic units $\hbar=e=m_e=1$, so that distances are measured in units of the Bohr radius a_0 and energies in units of 2Ry=27.212ev. The coefficients V_n can be written for $\lambda=\lambda_0 Z^{\frac{1}{3}}$ as

$$V_n=\frac{(-)^{n+1}}{(n+1)!} \tag{5.72}$$

and for $\lambda=\lambda_0$ as

$$V_n=\left[-Z^{\frac{1}{3}}\right]^{n+1}[(n+1)!]^{-1} \tag{5.73}$$

The two coefficients (5.72,5.73) in general alternate in sign and the coefficients (5.72) decrease with increasing n, but the coefficients (5.73) decrease less quickly than the coefficients (5.72). For the case Z>1, in table (5.7) we list the energy of states (1s,2s,2p,3s) for different values of λ_0 and different values of Z ($2\le Z\le 65$). Our results are summarized in table (5.8), ranging from ($4\le Z\le 84$) at intervals of 5, in order to cover the range of low to high atomic number. For a given shell the results improve with increasing Z, but the accuracy of the results decreases as we go to higher shells. The renormalised series approach as introduced by Killingbeck is a very elegant and powerful approach to compute the energies eigenvalues with high accuracy. The approach achieved an accuracy of fifteen significant figures for higher values of atomic number Z; to our knowledge such a high degree of accuracy for the eigenvalues of the Yukawa potential has never been obtained by any other method. As a next comment we wish to draw attention to the fact that the renormalised series work equally well for $\lambda=\lambda_0$ and $\lambda=\lambda_0 Z^{1/3}$ as perturbation parameter; we used the two values of λ in order to verify the accuracy of the renormalised series for this calculation. Using two different value of screening parameter provides alternative approaches for computing energy eigenvalues. The calculated energy eigenvalues diverge at low atomic number Z, for the K-shell, whereas the series will work for zero values of the renormalising constant for Z>29.

Table (5.7). Bound-state energies (in ev) for Yukawa potential for some values of (Z) for states (1s,2s,2p,3S); First line calculation with ($\lambda=\lambda_0$) as screening parameter; Second line ($\lambda=\lambda_0 Z^{1/2}$) as screeing parameter.

Z	1s (λ_0=0.85)	N	-K	Z	2s (λ_0=0.70)	N	-K
2	-14.4020 0	33 33	1 .8	15	-258.334894 4	47 47	1 .4
3	-47.436517 7	44 48	1 .8	20	-573.2907843 3	47 50	1 .4
4	-102.0621841 1	45 39	1 .5	25	-1025.88681730 0	48 53	1 .4
5	-179.35463887 7	55 47	1 .5	30	-1621.0197521955 5	59 66	1 .4
6	-279.994172284 4	55 51	1 .5	35	-2362.10295347674 3	62 35	1 .3
7	-404.4559589484 4	56 55	1 .5	40	-3251.67227497973 3	57 45	1 .2
8	-553.0935770096 6	54 54	1 .5	45	-4291.69716256988 8	55 45	1 .2
9	-726.181984925474 4	58 62	1 .5	50	-5483.75814279113 3	56 46	1 .2
14	-1964.94154227908 8	53 60	1 .5	55	-6829.15603985114 4	56 45	1 .2
20	-4288.08295949372 2	50 62	1 .5	60	-8328.98314095929 8	59 44	1 .2
Z	2p (λ_0=0.700)	N	-K	Z	3s (λ_0=0.50)	N	-K
20	-539.26816245 5	55 58	1 .4	30	-452.6503474 5	42 46	1 .3
25	-984.29879038 8	54 59	1 .4	35	-700.34870869 9	48 48	1 .3
30	-1572.31482521041 4	65 71	1 4	40	-1007.598317730 0	49 40	1 .2
35	-2306.63603659792 2	64 50	1 .2	45	-1375.8897374470 1	52 48	1 .2
40	-3189.73523047685 5	59 45	1 .2	50	-1806.41732433816 6	54 47	1 .2
45	-4223.53651026927 7	60 50	1 .2	55	-2300.16259649132 1	54 45	1 .2
50	-5409.58629364986 6	56 46	1 .2	60	-2857.94853566594 4	52 47	1 .2
55	-6749.15887789022 2	59 47	1 .2	65	-3480.47657972057 7	55 50	1 .2
60	-8243.32537933348 8	52 45	1 .2	70	-4168.35275218268 8	50 47	1 .2
65	-9893.00079991434 4	51 45	1 .2	75	-4922.10667860021 1	50 50	1 .2

Table (5.8). Bound-state energies (in kev) for Yukawa potential for some values of (Z) with (λ_0= 0.98) for states (1s,2s,2p); First line calculation with ($\lambda=\lambda_0$) as screening parameter; Second line ($\lambda=\lambda_0 Z^{1/3}$) as screening parameter.

Z	1s	N	-K	2s	N	-K	2p	N	-K
4	-0.08903238	39	1						
	8	55	1						
9	-0.677683760928	55	1	-0.0148	30	1			
	8	56	.5	8	31	.5			
14	-1.87027785858428	62	1	-0.110653	43	1	-0.07324	41	1
	8	71	.5	3	42	.4	5	38	.3
19	-3.68841556842173	58	1	-0.3151332	48	1	-0.2614478	52	1
	3	71	.5	2	51	.4	80	48	.3
24	-6.14288507596427	57	1	-0.64100125	50	1	-0.5724722	49	1
	7	77	0	5	55	.4	2	35	.2
29	-9.24036646667202	42	0	-1.09602481	52	1	-1.013599191	59	1
	2	42	0	1	49	.3	1	43	.2
34	-12.9854756984877	27	0	-1.685525378	52	1	-1.589918464	57	1
	7	27	0	8	51	.3	4	43	.2
39	-17.3816267173904	24	0	-2.4134097691	59	1	-2.3051975508	64	1
	4	24	0	1	31	.1	8	98	.1
44	-22.4314647781598	22	0	-3.28268546803	62	1	-3.16234928891	69	1
	8	22	0	3	93	.1	1	97	.2
49	-28.1371103672585	21	0	-4.295749400340	66	1	-4.163701632626	86	1
	5	21	0	0	36	.1	6	92	.2
54	-34.5003079669106	19	0	-5.454563261700	68	1	-5.3111636380018	77	1
	6	19	0	0	84	.2	8	89	.2
59	-41.5225223945530	18	0	-6.76076657792391	79	1	-6.60633330766000	90	1
	0	18	0	1	89	.2	0	86	.2
64	-49.2050041784047	18	0	-8.21575311162935	74	1	-8.05057082149505	80	1
	7	18	0	4	83	.2	5	80	.2
69	-57.5488356173131	17	0	-9.82072448309808	72	1	-9.64505009838571	80	1
	1	17	0	8	76	.2	1	90	.3
74	-66.5549642473470	17	0	-11.5767289854157	69	1	-11.3907962117476	70	1
	0	17	0	7	65	.2	6	82	.3
79	-76.2242277931756	16	0	-13.4846904210749	66	1	-13.2887132390265	67	1
	6	16	0	9	59	.2	5	80	.3
84	-86.5573731825538	16	0	-15.5454300034009	65	1	-15.3396054458527	67	1
	8	16	0	9	59	.2	7	81	3

5.5 The energy eigenvalues for the Gaussian potential

The solution of the Schrödinger equation with an attractive radial Gaussian potential of the form $V(r)=-A\exp(-\lambda r^{2})$ is of importance in nuclear physics.It has been used as a potential model in the theory of nucleon-nucleon scattering. Bessis, et. al [40,1982] have determined its bound state energies fairly accurately using a perturbational and variational treatment on a conveniently chosen basis of transformed Jacobi functions. The results of Lai [41,1983] have been obtained by using the hypervirial-Padé scheme for various eigenstates. Chatterjee [42,1985] applied the method of 1/N expansion to obtain the bound state energy levels. The Schrödinger equation for the radial part of the attractive Gaussian potential is given by

$$-r^{-2}\frac{d}{dr}\left[r^{2}\frac{d\Psi(r)}{dr}\right]+\left[\ell(\ell+1)r^{-2}-A\exp(-\lambda r^{2})\right]\Psi(r)=E\Psi(r) \qquad (5.74)$$

where the units $2m=\hbar=1$ are used, and the function in equation (5.74) can be expressed as

$$\Psi(r)=r^{-1}\Phi(r) \qquad (5.75)$$

The potential $A\exp(-\lambda r^{2})$ can be expanded as

$$A\exp\left(-\lambda r^{2}\right)=\sum_{n=0}^{\infty}V_{n}\lambda^{n}r^{2n+2} \qquad (5.76)$$

with the potential coefficients V_n given by

$$V_{n}=A(-)^{n}[(n+1)!]^{-1} \qquad (5.77)$$

Then the equation (5.74) takes this form

$$\left[-D^{2}+\ell(\ell+1)r^{-2}+\sum_{n=0}^{\infty}V_{n}\lambda^{n}r^{2n+2}\right]\Phi(r)=E'\Phi(r) \qquad (5.78)$$

with E =E+A. The function $\Phi(r)$ must vanish at r=0. Now, applying the hypervirial theorem, the Hellmann-Feynman theorem and using equation (5.77), the relation between the coefficients B(N,M) and the energy coefficients E(M) can be expressed as

$$\left(2N+2\right)\sum_{0}^{M} E(I)B(N,M-I)=N\left[2\ell(\ell+1)\ -\ \frac{1}{2}\left(N^{2}-1\right)\right]B(N-2,M)$$

$$+\sum_{n=0}^{\infty} V_{n}\ \left[2N+2\left(n+2\right)\right]B(N+2(n+1)),M-n-1) \tag{5.79}$$

$$\left(M+1\right)E(M+1)=\sum_{n=0}^{\infty} V_{n}\left(n+1\right)B(2(n+1),M-n) \tag{5.80}$$

The unperturbed value of E is given by

$$E(0)=\left[\left(4n+2\ell+3\right)\sqrt{A}\right]-A \tag{5.81}$$

where n is the principal quantum number, ℓ the angular momentum and we set A=400 to agree with previous authors. The recurrence relations (5.79,5.80) with equation (5.81) and initial condition A(0,0)=1 can be used to evaluate the energy coefficients E(M).The success and power of the method may strongly depend on the state and the angular momentum. The convergence rate decreases noticeably as (ℓ&n) increase, as shown in table (5.9). This situation occurs in all problems involving eigenvalues in perturbation theory. The calculations show that the present procedure converges more quickly and accurately at low values of (ℓ&n). Our results are very accurate in this low range. The degree of agreement between our results and those arising from other methods is very good, both for ground and excited states. For ℓ>7 we have not found numerical results in the literature, but our results show the eigenvalues for these states. Our main goal is to show that the energy eigenvalues of the attractive radial Gaussian potential calculated from the hypervirial method are in good agreement with other numerical results. We notice from table (5.9) that for the ground state and some of the first few excited states at low value of angular momentum we find the energy values with an accuracy of 20 significant figures. Such a high degree of precision has not been obtained before by any other approach.

Table (5.9). The eigenvalues, (-E) for Gaussian potential, as calculated by Hypervirial method, for different values of angular momentum, The empty spaces means that the corresponding eigenvalues cannot be reached by the Hypervirial method.

E_0	N	ℓ	E_1	N	ℓ
341.8952145612383126	17	0	269.64445939601828764	22	0
304.46283851873931049	20	1	235.45004237842402699	27	1
268.11073527472029733	24	2	202.43125734134946138	38	2
232.87530061640701581	30	3	170.639313715464895	36	3
198.79827015569832589	37	4	140.1351393984214	39	4
165.92819924393096815	45	5	110.992946440432	43	5
134.3225978459883659	49	6	83.3059559058	53	6
104.05115303117978	57	7	57.196331150	53	7
75.20088810228	59	8	32.8344324	60	8
47.8851109927	67	9	10.48331	62	9
22.2608608	62	10	-9.356	63	10
-14.2981	63	11			
-22.711	69	12			
E_2	N	ℓ	E_3	N	ℓ
203.98352879728788993	33	0	145.377898018770840	36	0
173.2443204775910195	37	1	118.383981222813	39	1
143.80914416451130	38	2	92.87806966475	42	2
115.754199322183	41	3	68.983554206	46	3
89.1749558925	43	4	46.86811448	53	4
64.195876773	52	5	26.777851	53	5
40.98872929	54	6	9.1257	56	6
19.812753	56	7	-5.14	57	7
1.1308	64	8			
E_4	N	ℓ	E_5	N	ℓ
94.457747566152	40	0	52.143586555	45	0
71.62355134691	44	1	34.1299347	48	1
50.567681606	49	2	18.440406	53	2
31.521072	49	3	5.6720	57	3
14.85145	56	4			
1.2909	63	5			
E_6	N	ℓ	E_7	N	ℓ
19.96628	43	0	1.3384	54	0
8.0830	51	1			
0.151	57	2			

5.6 Eigenvalues of the hydrogen atom

The problem of the perturbed hydrogen atom has received great attention in the last few years and has been attacked by various approaches. Killingbeck [43,1977] attacked the problem by using a non-perturbative finite difference method. In a subsequent work Killingbeck and Galicia [44,1980] used hypervirial relations together with the Hellmann-Feynman theorem to get the energy coefficients of the energy perturbation series. Lai and Lin [45,1981] applied the Hypervirial-Padé framework to calculate the energy eigenvalues of various eigenstates, Austin and Killingbeck [46,1982] have used a renormalised series approach to compute the energy levels of a perturbed hydrogen atom.

5.6.1 Power series approach

The power series approach to be discussed in this section allows us to compute the energy eigenvalues for the perturbed hydrogen atom. The power series approach is one of the simplest and most accurate methods for calculating eigenvalues. The Schrödinger equation for a system in which the potential depends upon the distance r (spherically symmetric potential) is taken in our calculation to have the form

$$\left[D^2+2\left(E-V(r)\right)\right]\Psi(r)=0 \tag{5.82}$$

where

$$\Psi(r)=\phi(r)Y_\ell^m(\theta,\phi) \tag{5.83}$$

In (5.83) $\phi(r)$ is the radial wavefunction, which is independent of the angles, and $Y_\ell^m(\theta,\phi)$ is a spherical harmonic, which is independent of r. If we insert equation (5.83) into equation (5.82) and rearrange, we obtain the radial equation

$$r^{-2}D\left[r^{2}D\phi(r)\right]+\left[2(E-V(r)-\ell(\ell+1)r^{-2}\right]\phi(r)=0 \qquad (5.84)$$

where (ℓ) is the angular momentum and $\phi(r)=r^{-1}R(r)$. We can express equation (5.84) with a new wavefunction R(r) as

$$D^{2}R(r)+\left[2\left(E-V(r)\right)-\ell(\ell+1)r^{-2}\right]R(r)=0 \qquad (5.85)$$

where

$$R(r)=r^{\ell+1}\Phi(r) \qquad (5.86)$$

If we insert equation (5.86) into equation (5.85) we get

$$D^{2}\Phi(r)+2(\ell+1)r^{-1}D\Phi(r)+2\left[E-V(r)\right]\Phi(r)=0 \qquad (5.87)$$

The wavefunction $\Phi(r)$ can be expressed as

$$\Phi(r)=\exp\left(-\beta r\right)\sum_{0}^{\infty}A(n)r^{n} \qquad (5.88)$$

For a perturbed hydrogen atom we take the potential V(r) as

$$V(r)=-r^{-1}+\lambda r \qquad (5.89)$$

If we substitute equations (5.88,5.89) in equation (5.87) we obtain this recurrence relation after some algebra

$$[n+1]\left[n+2\ell+2\right]S(n+1)=2\left[\left(\ell+1+n\right)\beta-1\right]rS(n)$$

$$-\left[2E+\beta^{2}\right]r^{2}S(n-1)+2\lambda r^{2}S(n-2) \qquad (5.90)$$

where

$$F(r)=\sum S(n)=\sum A(n)r^{n} \qquad (5.91)$$

To use equation (5.90), S(0) is set equal to 1 to find eigenvalues appropriate to the Dirichlet boundary conditions $\Psi(\infty)=0$. For a given (β) and two trial energies E_1 and E_2, the power series approach works out each S(n) and the sum of the S(n) at a specific r value, starting with S(0)=1 and S(-1)=S(-2)=S(-3)=0. Although it takes a little while to find an appropriate β value, there is usually quite a wide range of β over which good results can be obtained. If β is chosen reasonably the series quickly converge and lead to two values $F(r,E_1)$ and $F(r,E_2)$, from which an interpolated energy can be found which would have given F(r,E)=0. After a few repetitions the eigenvalue corresponding to the boundary condition $\Psi(r)=0$ is determined very accurately. For this radial problem we cannot use the even parity of the potential, because the coordinate range is from $0\leq r\leq\infty$.

5.6.2 Renormalised series approach

It has been shown by Killingbeck [14,1982] that the hypervirial relations yield the perturbation series for the energy E and for the expectation values $\langle r^n\rangle$ for a hydrogen atom with perturbation (λr), without the calculation of a perturbed wave function. We also use the renormalised series hypervirial approach for the perturbed hydrogen atom. The radial Schrödinger equation for this perturbed problem can be written as

$$\frac{1}{2}D^2R(r)-\left[r^{-1}-\lambda r - \frac{1}{2}\ell(\ell+1)r^{-2}\right]R(r)=ER(r) \qquad (5.92)$$

We write the potential given in equation (5.92) as

$$V(r)=-\mu r^{-1}+\lambda\left(r-Kr^{-1}\right) \qquad (5.93)$$

where

$$\mu=1-\lambda K \qquad (5.94)$$

We substitute the series expansions given by equations (2.6,2.7) into the hypervirial relation (2.3) with $V_{-2}=\frac{1}{2}\ell(\ell+1)$, $V_{-1}=(\mu+\lambda K)$, $V_1=\lambda$. Collecting terms, we find

$$\left(2N+2\right)\sum_{0}^{M}E(J)A(N,M-J)=N\left[\ell(\ell+1)-\frac{1}{4}\left(N^2-1\right)\right]A(N-2,M-1)$$

$$-\left(2N+1\right)\left[\mu A(N-1,M)+KA(N-1,M-1)\right]+\left(2N+3\right)A(N+1,M-1) \qquad (5.95)$$

The relation between the energy series and the A(N,M) series is given as follows (from the Hellmann-Feynman theorem)

$$\left(M+1\right)E(M+1)=A(1,M)-KA(-1,M) \qquad (5.96)$$

The unperturbed eigenvalue is $E(0) = -\mu^2/2n^2$ for this case, where n is the principal quantum number (1,2,3...). The equations (5.95,5.96) suffice to calculate the full set of E and A coefficients. We only need the value of E(0) given above and the starting term A(0,0) =1.

5.6.3 Finite difference approach

We use the finite difference method as a third method to calculate the eigenvalues for the perturbed hydrogen atom. The equation (5.87), after multiplying both side by r, takes the form

$$-\frac{1}{2}rD^2\phi(r)-(\ell+1)D\phi(r)=\left[E-V(r)\right]r\phi(r) \qquad (5.97)$$

To use the finite-difference method for this equation we make the substitutions

$$2hD\Phi(r)=\Phi(r+h)-\Phi(r-h) \tag{5.98}$$

$$h^2D^2\Phi(r)=\Phi(r+h)+\Phi(r-h)-2\Phi(r) \tag{5.99}$$

The equation (5.97) reduces to the form

$$\left[r+(\ell+1)h\right]\Phi(r+h)+\left[r-(\ell+1)h\right]\Phi(r-h)=$$

$$2r\Phi(r)+2rh^2\left[V(r)-E\right]\Phi(r) \tag{5.100}$$

The next step is the introduction of a ratio variable R(r), defined by the equation

$$\Phi(r+h)=R(r)\Phi(r)$$

$$=\left[1+h^2F(r)\right]R(r) \tag{5.101}$$

where

$$R(r)=1+h^2F(r) \tag{5.102}$$

With the substitution (5.101,5.102), the equation (5.100) is converted to a recursive equation

$$\left[r+H\right]F(r)=\left[r-H\right]\frac{F(r-h)}{R(r-h)}+2\left[V(r)-E\right]r \tag{5.103}$$

Here $H=(\ell+1)h$ is the only quantity which explicitly involves the angular momentum. If we start at $r=H$, then the first term on the right vanishes, so we can arbitrarily set $R=F=\Psi=1$ at $r=H-h$ without disturbing the rest of the calculation. The rest of the paraphernalia (use of two E values etc) is as before. By setting $\ell=0$ we get the s-state solution, which is appropriate to an odd solution for a one-dimensional problem. By setting $\ell=-1$, with $F(0)=\frac{1}{2}[V(0)-E]$, and starting at $r=h$ we get results appropriate to an even solution in one dimension. The eigenvalue associated with strip width h is related to the true eigenvalue by a perturbation-type expansion in h

$$E(h)=E+h^2E_2+h^4E_4\text{--------} \qquad (5.104)$$

To get E we do the calculation using several different strip widths, (h,2h,4h). The eigenvalues obtained are in error by a leading term of order h^2. We have applied a Richardson extrapolation process to convert them to very accurate results. To correct for the h^2 and h^4 error terms we use an extrapolation formula given in the form

$$E=\frac{1}{45}\Big[64E(h)-20E(2h)+E(4h)\Big] \qquad (5.105)$$

5.6.4 Results and discussion

The calculations reported here are for positive λ, so that well defined bound states exist, although quasi-bound states exist when (λ) is small and negative. We have used three approaches to compute the energies eigenvalues for various states and different values of perturbation parameter λ. Our main goal is to obtain accurate eigenvalues for this problem and to compare the accuracy of the results as obtained from the three approaches. The results are shown in the table (5.10) and from these results it is clear that the renormalised series method works excellently at low values of the perturbation parameter, where the series converges very quickly and certainly leads to accurate eigenvalues calculations. At $\lambda=0.1$ the accuracy is to 20 significant digits, and in fact the accuracy of this technique is crucially restricted by the choice to the value of the renormalising constant k . The rate of convergence is sensitive to the value of k . The finite difference and power series methods work very well to compute the eigenvalues, and their agreement is in general excellent. Our confidence in the accuracy of the power series approach comes from the following check; the computed eigenvalues are stable with respect to changes in β. We believe that the present results which have been calculated by the three approaches are very good compared to those of other methods which have been available for computing the eigenvalues for this problem. We have used double precision arithmetic of 20 digits.

Table (5.10). Eigenvalues of $H=P^2-r^{-1}+\ell(\ell+1)r^{-2}+\lambda r$, First line; power series calculation; Second line, renormalised series calculation; Third line, finite difference calculation.

State	λ	E	R	β	N	-K	h
1s	0.10	-0.36090007704568500 4	15	9			
		-0.360900077045685004			36	6	
		-0.3609000770456					0.005
1s	0.20	-0.235647404658515122	15	8			
		-0.2356474046585			55	6	
		-0.235647404658					0.003
1s	0.3	-0.118922615969358834	15	8			
		-0.11892261596			56	5	
		-0.1189226159693					0.0045
1s,	0.40	-0.008353654713870934	15	9			
		-0.008353654			31	2.6	
		-0.00835365471378 70					0.005
1s	0.50	0.097420543923206564	16	8			
		0.09742054			51	4	
		0.097420543932					0.005
1s	0.60	0.199284206146506018	12	8			
		0.19928420			46	3	
		0.199284206146					0.0045
1s	0.70	0.297857503274531191	12	9			
		0.29785750			47	2.6	
		0.2978575032744					0.0045
1s	0.80	0.393598890009116130	15	9			
		0.39359889			41	2	
		0.393598890009					0.0045
1s	0.90	0.486860594263223949	14	8			
		0.4868605			49	2.6	
		0.486860594263					0.004
1s	1.00	0.577921351961593598	15	9			
		0.5779213			45	1.85	
		0.5779213519615					0.004
2s	0.15	0.466659082903941026	16	9			
		0.466659			40	13	
		0.466659082904					0.005
3s	0.02	0.137084407881617	19	8			
		0.13708440			39	70	
		0.137084407881614					0.015
2p	0.10	0.222075886766612	15	9			
		0.2220758			52	20	
		0.2220758867					0.005
2p	0.15	0.358296694477485	15	8			
		0.35829			52	18	
		0.3582966944775					0.005
3d	0.02	0.092606732944116	20	8			
		0.09260673			37	70	
		0.092606732944					0.012

5.7 Polynomial perturbation of a hydrogen atom

5.7.1 Introduction

The s-wave Hamiltonian for a hydrogen atom with the perturbation term $(2\lambda r+2\lambda^2r^2)$ can be written as

$$H=-\frac{1}{2}D^2-r^{-1}+2\lambda r+2\lambda^2r^2 \tag{5.106}$$

and has been studied by Killingbeck [47,1978;48,1980]. This Hamiltonian possesses the exact ground state energy and wavefunction given respectively by

$$E_0=-\frac{1}{2}+3\lambda \tag{5.107}$$

$$\Psi_0=\exp\left(-r-\lambda r^2\right) \tag{5.108}$$

Ψ_0 correctly describes a bound ground-state only if $\lambda>0$, whereas for $\lambda<0$ the wavefunction is not normalisable. On the other hand $\Psi(-\lambda)$ is an eigenfunction of $H(-\lambda)$, not of $H(\lambda)$. Killingbeck [47,1978] calculated the first two terms for the ground state energy series $E=\sum E(n)\lambda^n$, yielding $E=-\frac{1}{2}+3\lambda$, and showing that the coefficients $E(2)$ and $E(3)$ are zero. Killingbeck [48,1980] has computed numerically the results that all coefficients $E(n)$ for $3<n<16$ vanish. Saxena and Varma [49,1982] have treated the case $(\lambda<0)$, by means of a perturbation expansion in powers of $|\lambda|^{-1/2}$. This allows a unified treatment of both positive $\lambda>0$ and negative $\lambda<0$. Their results cover a large range of values of $(-0.02\leq\lambda\leq-20480)$. Saxena and Varma [50,1982] have treated the same problem, and they have obtained an infinite number of exact solutions for the excited s states for certain specific values of (λ), corresponding to both positive and negative λ

values. Cohen and Herman [51,1982] have calculated the ground state energy by means of variational modification of Rayleigh-Schrödinger perturbation theory. They computed the energy eigenvalue over a wide range of λ $(-0.02\le\lambda\le-320)$; in spite of the large negative value of (λ), the results show satisfactory convergence for all values of (λ).

5.7.2 Renormalised series

We treat this problem by using renormalised perturbation series. The potential can be written as follow

$$V(r)=-\mu r^{-1}+\left[2\lambda r+ 2\lambda^{2}r^{2}-Kr^{-1}\right] \qquad (5.109)$$

where

$$\mu=1-K\lambda \qquad (5.110)$$

The first step is to insert the series expansion for E and $\langle r^{n}\rangle$, as given in previous sections, into the hypervirial relation, with $V_{-1}=(\mu-K\lambda)$, $V_{1}=2\lambda$ and $V_{2}=2\lambda^{2}$. The following relations is obtained

$$\begin{aligned}\left(2N+2\right)\sum_{0}^{M} E(I)A(N,M-I) = & -\frac{N}{4}\left(N^{2}-1\right)A(N-2,M)\\ & -\left(2N+1\right)\left[\mu A(N-1,M)+KA(N-1,M-1)\right]\\ & +\left(4N+6\right)A(N+1,M-1)+\left(4N+8\right)A(N+2,M-2) \qquad (5.111)\end{aligned}$$

Using the Hellmann-Feynman theorem in order to get the relation between the energy series E(M) coefficients and the series coefficients A(N,M), we obtain

$$\left(M+1\right)E(M+1)=-KA(-1,M)+2A(1,M)+4A(2,M) \qquad (5.112)$$

From the recurrence relations (5.111,5.112) together with the unperturbed energy $E(0)=-\mu^{2}/2n^{2}$ and the initial coefficient $A(0,0)=1$, we can calculate the perturbation series for the energy. The potential given by equation (5.109) can be expressed in the form

$$V(r)=-\mu r^{-1}-2\lambda r+2\lambda^{2}r^{2}-K\lambda r^{-1} \qquad (5.113)$$

Therefore the equations (5.111&5.112) take the form

$$\left(2N+2\right)\sum_{0}^{M} E(I)A(N,M-I)=-\frac{N}{4}\left[N^{2}-1\right]A(N-2,M)$$

$$-\left(2N+1\right)\left[\mu A(N-1,M)+KA(N-1,M-1)\right]$$

$$-\left(4N+6\right)A(N+1,M-1)+\left(4N+8\right)A(N+2,M-2) \qquad (5.114)$$

$$\left(M+1\right)E(M+1)=-KA(-1,M)-2A(1,M)+4A(2,M) \qquad (5.115)$$

We use a modified renormalised technique where (μ) takes the form

$$\mu=1-\lambda^{2}K \qquad (5.116)$$

where

$$\underline{\lambda}=\sqrt{\lambda} \qquad (5.117)$$

and the equations (5.111&5.112) take the form

$$\left(2N+2\right)\sum_{0}^{M} E(I)A(N,M-I)=-\frac{N}{4}\left[N^{2}-1\right]A(N-2,M)$$

$$-\left(2N+1\right)\left[\mu A(N-1,M)+KA(N-1,M-1)\right]$$

$$-\left(4N+6\right)A(N+1,M-2)+\left(4N+8\right)A(N+2,M-4) \qquad (5.118)$$

$$\left(M+1\right)E(M+1)=-KA(-1,M)-4A(1,M-1)+8A(2,M-3) \qquad (5.119)$$

5.7.3 Results and discussion

We have used three renormalised series approaches to compute the energy eigenvalue for this problem, and the results are shown in table (5.10) for the ground state. and for a range of perturbation parameter from $(-0.01 \leq \lambda \leq -0.1)$. The accuracy of these approaches decrease as (λ) increases. The agreement between the results of these three approaches is very good. While no one of the three approaches offers particular advantages to improve the accuracy or increase the range of (λ), the agreement of the three gives us confidence that our results are correct. We believe that the results which are found from these approaches are good in comparison with these of other methods have been used to compute the eigenvalues for this problem. The renormalised series approach works well for small values of λ, the perturbation series convergence being satisfactory for these values. For larger values of (λ), this approach does not work because the perturbation series does not converge. Thus the renormalised series approach is limited to low ranges of the perturbation parameter λ. Also we have been used a finite difference approach to compute the eigenvalues for this problem and the results produced are in good agreement with those results obtained by Saxena and V.S.Varma by using Hill determinants. In table (5.11) we list the energies eigenvalues for the range $(-0.01 \leq \lambda \leq -24080)$ and compare them with numerical computations of the ground state energy which were obtained by Saxena.

Table (5.11). The energy result of $\frac{1}{2}p^2-r^{-1}+2\lambda r+2\lambda^2r^2$, perturbation by using renormalised series method, Ea calculation from equations (5.104 & 5.105); Eb calculation from equations (5.107 & 5.108); Ec calculation from equations (5.111 & 5.112)

λ	-Ea	N	K	-Eb	N	-K	-Ec	N	-K
0.01	0.5299999999999	34	24	0.5299999999999	31	20	0.5299999999999	44	2
0.02	0.55999999	44	22	0.55999999	39	20	0.5599999983	87	2
0.03	0.5899966	46	16	0.589996	45	20	0.5899966	96	6
0.04	0.6198821	46	16	0.6198820	46	18	0.6198820	98	8
0.05	0.649106	41	15	0.649106	45	16	0.649106	105	8
0.06	0.67681	43	15	0.67681	46	16	0.67681	104	9
0.07	0.7024	39	14	0.7024	41	15	0.7024	73	9
0.08	0.7258	47	15	0.7258	45	14	0.7258	90	15
0.09	0.7468	49	15	0.746	45	14	0.746	80	15
0.10	0.765	47	15	0.765	44	14	0.765	85	18

Table (5.12). The energy result of $(\frac{1}{2}P^2-r^{-1}+2\lambda r+2\lambda^2r^2)$ perturbation by using finite difference method.

λ	E	h	r	Hill determinant
0.01	-0.529999999981	0.0075	22.5	
0.02	-0.559999995328	0.0075	22.5	-0.559999983
0.03	-0.589996652925	0.007	21.0	
0.04	-0.619881802714	0.008	24.0	
0.05	-0.649106898032	0.0075	22.5	-0.64910689805
0.06	-0.676826124753	0.0075	22.5	
0.07	-0.702453360505	0.0075	22.5	
0.08	-0.725787829886	0.005	15.0	
0.09	-0.746865801124	0.005	15.0	
0.10	-0.765826903961	0.005	15.0	-0.76582690396
1	-0.226772769861	0.003	9.00	-0.22677276986
2	1.452916838112	0.0025	7.50	1.45291683811
5	7.831279461467	0.002	6.00	7.831279614
40	99.78407751379	0.0008	2.40	99.784077513
320	902.8776177169	0.0001	0.30	902.877617716
2560	7518.489264286	0.00005	0.15	7.518489264276
20480	60983.23402645	0.00004	0.12	60983.234026772

5.8 The exponential cosine screened coulomb (ECSC) potential

The radial Schrödinger equation for the exponential cosine screened Coulomb (ECSC) potential is not solvable analytically and can be expressed as

$$D^2\Psi(r)+2\left[E+V(r)\ -\ \frac{1}{2}\ell(\ell+1)r^{-2}\right]\Psi(r)=0 \qquad (5.120)$$

where

$$V(r)=-r^{-1}\exp\left(-\lambda r\right)\cos(\lambda r) \qquad (5.121)$$

This potential is of importance in solid-state physics. It is used in describing the potential between an ionized impurity and an electron in a metal or a semiconductor . It has also been used to represent the effective interaction between an electron and a positronium atom in a solid. The (ECSC) potential has been treated by several approximation methods. Aparna and Pirtamp [52,1980] applied the generalized virial theorem and Hellmann-Feynman theorem to calculate perturbatively the bound state energy levels without using perturbed wavefunction. C.S.Lai [53,1982] has treated this potential by using the hypervirial relations and the Padé approximant E [10,10] and E [10,11] for different eigenstates. In this section we set out to calculate the bound-state energies of the ECSC potential for different eigenstates, by applying the hypervirial and Hellmann-Feynman theorems to calculate perturbatively the bound-state energy levels without using perturbed wave functions. The ECSC potential can be expanded in a power series of the screening parameter by the Taylor expansion

$$F(x)=F(0)+xF'(0)+\frac{x^{2}}{2!}F''(0)+\ldots.\frac{x^{n}}{n!}F^{n}(0) \qquad (5.122)$$

Also $V(r)$ can be expanded as

$$V(r)=-r^{-1}\exp\left(-\lambda r\right)\mathrm{Cos}\left(\lambda r\right)=-r^{-1}\sum_{n=0}^{\infty}V_{n}(\lambda r)^{n} \qquad (5.123)$$

$$=-V_{0}\left[\mu+\lambda K\right]r^{-1}-r^{-1}\sum_{n=1}^{\infty}V_{n}(\lambda r)^{n}$$

Comparing (5.122 & 5.123), we obtain the coefficients

$V_{0}=1$, $V_{1}=-1$, $V_{2}=0$, $V_{3}=\frac{2}{3!}$, $V_{4}=-\frac{4}{4!}$, $V_{5}=\frac{4}{5!}$, ... $V_{20}=-\frac{1024}{20!}$,

$V_{21}=\frac{1024}{21!}$

The coefficients V_{n} in equation (5.123) also can be expressed as

$$V_{n}=(-1)^{n}\left(2\right)^{n/2}\mathrm{Cos}\left(\frac{\pi n}{4}\right)\frac{1}{n!} \qquad (5.124)$$

Here, we use atomic units. The hypervirial relation for the (ECSC) potential is given as

$$\left(2N+2\right)\sum_{0}^{M}E(I)B(N,M-I)=N\left[\frac{1}{4}\left(N^{2}-1\right)-\ell(\ell+1)\right]B(N-2,M)$$

$$+V_{0}\left(2N+1\right)\left[\mu B(N-1,M)+kB(N-1,M-1)\right]$$

$$+\sum_{n=0}^{\infty}V_{n}\left(2N+1+n\right)B(N+n-1,M-n) \qquad (5.125)$$

The Hellmann-Feynman theorem

$$\frac{\partial E}{\partial\lambda}=\langle\frac{\partial V}{\partial\lambda}\rangle \qquad (5.126)$$

gives

$$\left(M+1\right)E(M+1)=KV_0\ B(-1,M)+\sum_{n=1}^{\infty} nV_n B\ (n-1,M+1-n) \qquad (5.127)$$

The recurrence relations (5.125 & 5.127)can be used to calculate the energy coefficients from a knowledge of $B(0,0)=1$ and $E(0)=-\mu^2/2n^2$. The energy eigenvalues can be evaluated by using equations (5.125,5.127) using the appropriate values of renormalised constant k; results for this calculation are given in table (5.13). Our calculated values of the energy levels are excellent as compared with the results obtained from the hypervirial -Padė approximant scheme of Lai. From our results it can be seen that the Hypervirial method with a renormalised constant k is sufficient to calculate the energy eigenvalue without using Padė approximants. Although the renormalised series method has calculational elegance, it suffers from two major drawbacks. First, the accuracy of the numerical results for bound states falls off very rapidly with increasing value of the screening parameter λ. Second the calculations become progressively more difficult as the state number n increases. The ECSC potential differs from $\exp(-\lambda r)r^{-1}$ by a cosine factor (Cosλr), which leads to an oscillatory behaviour. It is of obvious interest to compare the result for the ECSC potential with those for SÇCP. Generally speaking the binding of the electron is weaker in the ESCS potential than in the SSCP potential.

Table (5.13). The energy eigenvalues of $V(r)=-r^{-1}\exp(-\lambda r)\cos(\lambda r)$, as function of screening parameter for various eigenstates, by using renormalised series

λ	state	Energy	N	K
0.05	1S	-0.4501174664206873	16	-2
0.10	1S	-0.4008847746394779	27	-2
0.20	1S	-0.3063344884577977	62	-3
0.25	1S	-0.2617680856978	66	-3
0.30	1S	-0.21941569190	64	-3
0.40	1S	-0.14243903	62	-3
0.05	1S	-0.077663	72	-4
0.02	2S	-0.1051035876922210	16	-3
0.04	2S	-0.0857689988968006	30	-3
0.06	2S	-0.0674211051489110	49	-6
0.08	2S	-0.0503865619256	67	-8
0.1	2S	-0.03494131191	76	-8
0.15	2S	-0.005264	89	-10
0.02	2P	-0.1050746383061889	17	-4
0.04	2P	-0.0855591372187105	28	-4
0.06	2P	-0.0667775205247901	50	-6
0.08	2P	-0.0489972478082	68	-8
0.10	2P	-0.032468804	69	-10
0.02	3S	-0.0360251051130600	32	-6
0.04	3S	-0.01882306333	45	-10
0.05	3S	-0.011575563	49	-10
0.06	3S	-0.0054619	57	-12
0.02	3P	-0.0359676034335847	30	-5
0.04	3P	-0.018453352988	49	-10
0.05	3P	-0.01092932	44	-12
0.06	3P	-0.004471	49	-16
0.02	3d	-0.0358506623108868	27	-6
0.04	3d	-0.01768206425	50	-12
0.05	3d	-0.00955487	47	-12
0.06	3d	-0.002309	54	-16
0.01	4S	-0.0214374651555588	27	-6
0.02	4S	-0.01257177731	30	-10
0.03	4S	-0.00527039	39	-16
0.01	4P	-0.0214243745995200	28	-6
0.02	4P	-0.012485752309	41	-10
0.03	4P	-0.00503284	42	-16
0.01	4d	-0.0213979776324376	27	-6
0.02	4d	-0.0123102664765	38	-12
0.03	4d	-0.0045392	32	-16
0.01	4f	-0.0213578402687837	23	-8
0.02	4f	-0.0120381878144	42	-12
0.03	4f	-0.0037481	38	-18
0.01	5S	-0.01042417006702	33	-12
0.01	5P	-0.01040587713648	35	-12
0.01	5d	-0.010368961255624	35	-12
0.01	5f	-0.010312749318579	35	-12
0.01	5g	-0.010236214244166	30	-12
0.01	6S	-0.0046993015	32	-16
0.01	6P	-0.0046763149	32	-16
0.01	6d	-0.0046298602	32	-16
0.01	6f	-0.0045589530	28	-16
0.01	6g	-0.0044620593	26	-16
0.01	6h	-0.00433701680	28	-16

5.9 Hulthen potential

The radial Schrödinger equation for the Hulthen potential can be written in atom units as

$$D^2\Psi(r)+2\left[E+V_H(r) - \frac{1}{2}\ell(\ell+1)r^{-2}\right]\Psi(r)=0 \qquad (5.128)$$

where

$$V_H(r)=-\lambda\exp\left(-\lambda r\right)\left[1-\exp\left(-\lambda r\right)\right]^{-1} \qquad (5.129)$$

where (λ) is a screening parameter. The Hulthen potential at small values of r behaves like a Coulomb potential, whereas for large values of r it decreases exponentially, so that its "capacity" for bound states is smaller than that of the Coulomb potential. The energy levels always lie lower in the Coulomb case than in the Hulthen case. The Hulthen potential, apart from its initial interest in a number of areas of physics ranging from nuclear physics (as a possible form of nuclear interaction) to scattering theory to atomic physics, has recently been shown to be a judicious choice of starting point for the perturbation theoretic treatment of screened Coulomb potentials. The Hulthen potential has been treated numerically by Lai and Lin [54,1980], who applied the Padė approximant technique to the analytic perturbation series obtained through the use of hypervirial and Hellmann-Feynman theorems. Also Dutt and Mukherji [55,1980] proposed a new approximation scheme to obtain analytic expressions for the bound-state energies and eigenfunctions for any arbitrary bound (ℓ,n) state of the Hulthen potential. The purpose of this section is to study the bound-state energies of the Hulthen potential for $\ell \neq 0$. The Hulthen potential $V_H(r)$ in eq (5.129) can be rewritten in the form

$$V_H(r)=-\lambda\exp\left(-\lambda r\right)\left[1-\exp\left(-\lambda r\right)\right]^{-1}=-r^{-1}\left(\lambda r\right)\left[\exp(\lambda r)-1\right]^{-1}$$

$$=-r^{-1}\sum_{n=0}^{\infty}V_n(\lambda r)^n \tag{5.130}$$

where

$$V_n=\frac{B_n}{n!} \tag{5.131}$$

$$V_0=1,\ V_1=-\frac{1}{2},\ V_2=\frac{1}{6}\ \frac{1}{2!},V_4=-\frac{1}{30}\ \frac{1}{4!}\ ,\dots V_{30}=\frac{861\ 58421\ 76005}{14322}\ \frac{1}{30!}$$

and B_n are the Bernoulli numbers. The Hulthen potential $V_H(r)$ in equation (5.130) can be rewritten in another form

$$V_H(r)=-\frac{\lambda e^{-\lambda r}}{[1-e^{-\lambda r}]}$$

$$=-\frac{\lambda}{2}\left[\frac{e^{\lambda r/2}+e^{-\lambda r/2}}{e^{\lambda r/2}-e^{-\lambda r/2}}-1\right]=-\frac{1}{2}\lambda\left[\mathrm{Coth}\left(\frac{\lambda r}{2}\right)-1\right] \tag{5.132}$$

where

$$\mathrm{Coth}(Z)=\frac{1}{Z}+\frac{Z}{3}-\frac{Z^3}{45}+\frac{2Z^5}{945}\dots+\frac{2^{2n}}{2n!}B_{2n}Z^{2n-1} \tag{5.133}$$

where $|Z|<\frac{\pi}{2}$

Furthermore, we use the hypervirial relation as used in previous sections, assuming that the energy and the expectation values $\langle r^M\rangle$ can be expanded as

$$E=\sum E(I)\lambda^I \tag{5.134}$$

$$\langle r^M\rangle=\sum B(M,N)\lambda^N \tag{5.135}$$

Then the hyperviral relation for the Hulthen potential can be expressed as

$$\left(2N+2\right)\sum_{0}^{M} E(I)B(N,M-I)=N\left[\left(N^{2}-1\right)-\ell(\ell+1)\right]B(N-2,M)$$

$$-V_{0}\left(2N+1\right)\left[\mu B(N-1,M)+KB(N-1,M-1)\right]$$

$$+\sum_{n=1}^{\infty} V_{n}\left(2N+n+1\right)B(N+n-1,M-n) \qquad (5.136)$$

Applying the Hellmann-Feynman theorem

$$\frac{\partial E}{\partial \lambda}=\langle\frac{\partial V}{\partial \lambda}\rangle \qquad (5.137)$$

with the use of (5.134,5.135) and (5.130) equation (5.137) leads to

$$\left(M+1\right)E(M+1)=-KV_{0}B(-1,M)+\sum_{n=1}^{\infty} B(n-1,M+1-n) \qquad (5.138)$$

With unperturbed energy $E(0)=-\mu^{2}/2n^{2}$ and initial condition $B(0,0)=1$, we use the recurrence relations (5.136) and (5.138) to compute the energy coefficient E(I). Energies of many eigenstates of the Hulthen potential are listed in table (5.14). It is apparent from table (5.14) that the energy series is a converging very quickly at low values of the screening parameter (λ). We wish here to make a few comments summarising the advantage of using the renormalised series approach. It is important, however to remember that our results has been calculated directly from the hypervirial approach with a renormalised constant (k), without use of Padé approximants, which were used by Lai to improve a convergent series. It is necessary to point out that the agreement of our calculated energy eigenvalues with the results of Lai is good. The renormalised series approach works very well even for higher excited states with higher value of angular momentum. We believe that the accuracy of our results may be improved even further with a better choice of renormalised constant k, the approach gives well converged eigenvalues for the best values of the renormalised constant k.

Table (5.14). Eigenvalues of $H=\frac{1}{2}P^2+\frac{1}{2}\ell(\ell+1)r^{-2}-\lambda\exp(-\lambda r)[1-\exp(-\lambda r)]^{-1}$ by using renormalised series, where $\lambda o=\lambda x10^{-3}$

λo	S	Energy	N	-K	λo	S	Energy	N	-K
10	2P	-0.1200416667916930	8	2	10	5f	-0.01526278330223 1	14	1
20	2P	-0.1151666686683576	9	1	20	5f	-0.011054635886584	19	1
30	2P	-0.110375101442916	11	1	30	5f	-0.007386926302296	30	1
40	2P	-0.105666987752976	12	1	40	5f	-0.00428217970	27	0.1
50	2P	-0.101042452072357	14	1	50	5f	-0.00178354	28	0.1
100	2P	-0.079179439105145	29	2	10	5g	-0.001522951337927	12	1
200	2P	-0.041886049217	26	0.1	20	5g	-0.010922364141886	21	1
250	2P	-0.026611051	27	0.1	30	5g	-0.007092765581779	33	1
300	2P	-0.0137899	24	0.1	40	5g	-0.00377001650	33	0.1
350	2P	-0.00377	19	0.1	50	5g	-0.0010158	27	0.1
10	3P	-0.050659729727901	9	1	10	6P	-0.009330688020377	13	1
20	3P	-0.045972342587020	12	1	20	6P	-0.005657737604454	24	1
30	3P	-0.041493667236800	14	1	30	6P	-0.002875554754	27	0.1
40	3P	-0.037224165923463	17	1	40	6P	-0.000996120	26	0.1
50	3P	-0.033164501183867	21	1	10	6d	-0.009314259653815	15	1
100	3P	-0.016053726638	26	0.25	20	6d	-0.005595029146250	26	1
150	3P	-0.0044662	23	0.2	30	6d	-0.002747059427	27	0.1
10	3d	-0.050643071323050	8	1	40	6d	-0.00080663	27	0.1
20	3d	-0.045905808680886	11	1	10	6f	-0.009289550080574	15	1
30	3d	-0.041344344233043	16	1	20	6f	-0.005499922860413	28	1
40	3d	-0.036959661072211	19	1	30	6f	-0.0025492694	29	0.1
50	3d	-0.032753184225127	21	1	40	6f	-0.0005112	27	0.1
100	3d	-0.0144842268	23	0.2	10	6g	-0.009256477595909	13	1
150	3d	-0.001394	27	0.1	20	6g	-0.005371080584005	30	1
10	4P	-0.026441691717959	10	1	30	6g	-0.00227574087	34	0.1
20	4P	-0.022017069984944	15	1	40	6g	-0.0000918	35	0.1
30	4P	-0.017977063497853	19	1	10	6h	-0.009214931077266	16	1
40	4P	-0.014323288816487	25	1	20	6h	-0.005206558419113	30	1
50	4P	-0.011058170219449	27	0.1	30	6h	-0.00191444888	42	0.1
75	4P	-0.0046219264	28	0.2	40	6h	+0.000493	33	0.1
100	4P	-0.000754	23	0.2	10	7p	-0.005808497437053	16	1
10	4d	-0.026425063173532	10	1	20	7p	-0.002624962332237	32	1
20	4d	-0.021951019249727	14	1	30	7P	-0.00665641	27	0.05
30	4d	-0.017830233991680	19	1	10	7d	-0.005792293327495	17	0.05
40	4d	-0.014066888018391	28	1	20	7d	-0.002566214565 04	33	0.05
50	4d	-0.01066740417256	32	0.6	30	7d	-0.00056219	29	0.05
75	4d	-0.003834532	28	0.1	10	7f	-0.005767897038536	16	0.05
80	4d	-0.00277264	27	0.1	20	7f	-0.0024767684844	29	0.05
10	4f	-0.026400090317113	10	1	30	7f	-0.00040273	31	0.05
20	4f	-0.021851460627588	15	1	10	7g	-0.005735198054619	19	0.05
30	4f	-0.017607531625427	21	1	20	7g	-0.0023548775690	31	0.05
40	4f	-0.013674454773534	29	1	30	7g	-0.0001808	29	0.05
50	4f	-0.0100619645509	33	0.1	10	7h	-0.005694044936944	19	0.05
75	4f	-0.00255629	33	0.1	20	7h	-0.0021979059566	36	0.05

Table (5.14 continued)

10	5P	-0.01530422945661 3	11	1	30	7h	+0.000115	29	0.05
20	5P	-0.011217685705423	17	1	10	7i	-0.005644241524433	19	0.05
30	5P	-0.007742789398949	27	1	20	7i	-0.00200195002	29	0.05
40	5P	-0.0048840333379	27	0.1	30	7i	+0.00051	23	0.05
50	5P	-0.0026490107	25	0.1	10	8P	-0.003604598802576	19	0.05
10	5d	-0.015287669725778	12	1	20	8P	-0.00098683270	25	0.05
20	5d	-0.011152764259769	19	1	10	8d	-0.003588750898457	19	0.05
30	5d	-0.007601938776343	28	1	20	8d	-0.0009349530	25	0.05
40	5d	-0.004647881641	31	0.1	10	8f	-0.003564863870506	20	0.05
50	5d	-0.002313111	26	0.1	20	8f	-0.0008556948	27	0.05
10	8i	-0.003443266962011	23	0.05	10	8g	-0.003532795494148	21	0.05
20	8i	-0.00042742	27	0.05	20	8g	-0.000747090	25	0.05
10	8k	-0.003385220760661	23	0.05	10	8h	-0.003492349118332	23	0.05
20	8k	-0.0002027	27	0.05	20	8h	-0.00060601	27	0.05

5.10 Eigenvalue calculations for some potentials

5.10.1 Hypervirial method to calculate energy eigenvalues for $H=P^2+x^2-2e^{-2\lambda x^2}\left[1+e^{-2\lambda x^2}\right]^{-1}$

The Schrödinger equation in atomic unit for the potential which is given as:

$$V(x)=-2e^{-2\lambda x^2}\left[1+e^{-2\lambda x^2}\right]^{-1} \qquad (5.139)$$

takes the form

$$-D^2\Psi(x)+x^2\Psi(x)-2e^{-2\lambda x^2}\left[1+e^{-2\lambda x^2}\right]^{-1}\Psi(x)=E\Psi(x) \qquad (5.140)$$

The potential given in equation (5.139) can be expressed as

$$V(x)=\left[\frac{e^{\lambda x^2}-e^{-\lambda x^2}}{e^{\lambda x^2}+e^{-\lambda x^2}}-1\right]=\mathrm{Tanh}(\lambda x^2)-1 \qquad (5.141)$$

We let

$$\lambda x^2=y \qquad (5.142)$$

The perturbation calculation by using Hypervirial relations for the interaction given by (5.139) is made by expanding $\tanh(\lambda x^2)$ in a power series in (λx^2) which is valid for $\lambda x^2<\frac{\pi}{2}$. Then $\tanh(y)$ can be express as

$$\tanh\left(y\right)= y - \frac{y^3}{3} + \frac{2y^5}{15} + ----- \frac{2^{2n}[2^{2n-1}-1]y^{2n-1}}{2n!}B_{2n} \qquad (5.143)$$

As x varies from $(-\infty\le x\le+\infty)$ the potential runs from $(0\le V(x)\le 0)$ through (-1) at $x=0$. We can use the Hypervirial relation as we have used it in previous problem. The Hypervirial relation for potential (5.139) leads to the recurrence relation

$$\left(2N+2\right)\sum_{0}^{M} E(I)A(N,M-I)=-\frac{N}{2}\left[N^{2}-1\right]B(N-2,M)$$

$$+\left(1+\lambda\right)\left[2N+4\right]B(N+2,M)$$

$$+\sum_{n=0}^{\infty} V_{n}\left[2N+2+2\left(2n+1\right)\right]B(N+2(2n+1),M-2n-1) \qquad (5.144)$$

If we apply the Hellmann-Feynman theorem using the energy and the expectation value $\langle x^{M}\rangle$ series as given by equations (5.134) and (5.135) we obtain the following recurrence relation

$$\left(M+1\right)E(M+1)=\sum_{n=1}^{\infty}\left[2n+1\right]V_{n}B(2(2n+1),M-2n) \qquad (5.145)$$

where

$$V_{n}=\frac{2^{2n}(2^{2n-1}-1)y^{2n-1}}{2n!}B_{2n} \qquad (5.146)$$

Here B_{2n} is the nth Bernoulli number. The unperturbed energy E(0)

$$E(0)=\left(2n+1\right)\sqrt{(1+\lambda)}-1 \qquad (5.147)$$

allows us to use the recurrence relations to compute the energy coefficient E(M),with initial condition B(0,0)=1.

5.10.2 Hypervirial method to calculate energy eigenvalues for $H=P^{2}+r^{2}+\ell(\ell+1)r^{-2}-2e^{-2\lambda r^{2}}\left[1+e^{-2\lambda r^{2}}\right]^{-1}$

In this subsection we extend the numerical calculation from one dimension to three dimensions. The main difference between one and three dimensional potential lies in the angular momentum term. We have applied the same two methods which were used to compute energies for one- dimensional potentials. Using Hypervirial and Hellmann-Feynman theorems as used for one dimensional problems, and we following the same route leads to recurrence relations (5.144) and (5.145) with an additional potential term due to the angular momentum. With $V_{-2}=\ell(\ell+1)$, $V_2=(1+\lambda)$ we obtain the following recurrence relation after some algebra

$$\left(2N+2\right)\sum_{0}^{M} E(I)A(N,M-I)=N\left[2\ell(\ell+1) - \frac{N}{2}\left(N^2-1\right)\right]B(N-2,M)$$

$$+\left(1+\lambda\right)\left(2N+4\right)B(N+2,M)$$

$$+\sum_{n=1}^{\infty} V_n \left[2N+2+2\left(2n+1\right)\right]B(N+2(2n+1),M-2n-1) \qquad (5.148)$$

$$\left(M+1\right)E(M+1)=+\sum_{n=1}^{\infty}\left[2n+1\right]V_n \; B(2(2n+1),M-2n) \qquad (5.149)$$

5.10.3 Results and discussion

Tables (4.15) and (5.16) show the eigenvalues for potentials

$$V(x)=\left[\frac{e^{\lambda x^2}-e^{-\lambda x^2}}{e^{\lambda x^2}+e^{-\lambda x^2}}-1\right]=\mathrm{Tanh}(\lambda x^2)-1$$

$$V\ (r)=\left[\frac{e^{\lambda r^2}-e^{-\lambda r^2}}{e^{\lambda r^2}+e^{-\lambda r^2}}-1\right]=\mathrm{Tanh}(\lambda r^2)-1$$

It is clear from our results that the energy series convergence very quickly at low values of λ, but the convergence decreases as λ increase. It is important to point out that the accuracy of results for this problem which have been obtained without use of renormalised constant k, also we used the Padé approximants as second method to compute the energy eigenvalue. The agreement between the two methods are very good for low values of λ, but for high values of λ the Padé approximants give more accurate eigenvalues. We have computed many energy eigenvalues of the potential given by equation (5.141), for different values of $(0.01\leq\lambda\leq0.1)$ and for the ground and first four excited state. We list our results for this calculation in table (5.15) for one dimension and in table (5.16) for three dimensions, for different values of $(0.01\leq\lambda\leq0.05)$, different values of $(\ell=0,2,5,10)$ and state number n.

Table (5.15). Eigenvalues of $H=P^2+x^2-2\exp(-2\lambda x^2)[1+\exp(-2\lambda x^2)]^{-1}$, upper lines Hypervirial calculation, lower lines, Padé approximants E [M,M] calculation

λ	$E_0+\lambda$	N M , M	$E_1+\lambda$	N M , M	$E_2+\lambda$	N M , M
0.01	2.00999938054028 8	7 7 , 7	4.02999564470961 1	9 7 , 7	6.04998442433791 1	9 7 , 7
0.02	2.01999509362435 5	9 7 , 7	4.05996537741999 2000	13 7 , 7	6.09987614412735 5	15 8 , 8
0.03	2.02998362238362 2	13 7 , 7	4.08988408082744 4	15 8 , 8	6.14958560182659 9	19 8 , 8
0.04	2.03996164005009 9	19 8 , 8	4.11972783885644 5	24 10, 10	6.19902856159832 61	31 15, 15
0.05	2.04992603057096 6	27 8 , 8	4.14947421386347 4	36 16, 16	6.2481276287439 8	38 15, 15
0.06	2.05987390105514 631	42 16, 16	4.179102426517 6	48 16, 16	6.296813169 72	32 15, 15
0.07	2.0698025869 9	29 16, 16	4.20859344 49	27 15, 15	6.345023 3731	24 15, 15
0.08	2.0797096 651	9 15, 15	4.237930 003	15 15, 15	6.39270 0602	13 15, 15
0.09	2.089592 2879	9 15, 15	4.26709 9666	9 14, 14	6.4398 8146	7 15, 15
0.10	2.099450 027	11 15, 15	4.2960 07952	5 14, 14	6.486 63117	7 15, 15

λ	$E_3+\lambda$	N M , M	$E_4+\lambda$	N M , M	$E_5+\lambda$	N M , M
0.01	8.06996075033870 0	10 8 , 8	10.0899196844155 5	9 8 , 8	12.1098563311365 5	11 8 , 8
0.02	8.13968835575794 4	15 8 , 8	10.1793639200018 8	15 8 , 8	12.2188660401912 2	15 8 , 8
0.03	8.20896023323394 4	23 14, 14	10.2678868075600 0	24 12, 12	12.3262532243041 5	27 12, 12
0.04	8.27757226957313 6	36 14, 14	10.3550940822281 6	36 14, 14	12.4313636124165 82	43 13, 13
0.05	8.345344055874 6	46 14, 14	10.4406563192 278	44 14, 14	12.533690623 714	46 13, 13
0.06	8.41212155 6089	44 14, 14	10.524313 4022	36 12, 12	12.63287 8024	46 12, 12
0.07	8.47777 7801	34 14, 14	10.6059 87633	15 12, 12	12.728 871940	13 12, 12
0.08	8.542 22126	7 14, 14	10.685 5215	11 12, 12	12.82 21117	7 12, 12
0.09	8.605 8146	7 15, 15	10.760 22611	13 12, 12	12.9 910084	11 12, 12
0.10	8.66 67133	5 13, 13	10.84 836988	11 12, 12	13.0 12.99570	11 12, 12

Table (5.16). Eigenvalues of $H=P^2+r^2+\ell(\ell+1)r^{-2}-2e^{-2\lambda r^2}/(1+e^{-2\lambda r^2})$ for many eigenstates, upper lines Hypervirial calculation, lower lines Padé approximant E [M,M] calculation, The two numbers in brackets correspond to state number and angular momentum respectively.

λ	(0,0)	N M , M	(0,10)	N M , M
0.01	4.02999564470961 1	9 8 , 8	24.2293527633224 4	13 8 , 8
0.02	4.05996537741999 2000	13 8 , 8	24.4549077417207 8	24 11,11
0.03	4.08988408082744 4	15 8 , 8	24.6733540527698 32	41 12,12
0.04	4.11972783885644 5	24 12,12	24.8822703 890	36 12,12
0.05	4.14947421386347 48	36 13,13	25.080 02636	15 12,12
λ	(1,5)	N M , M	(1,10)	N M , M
0.01	18.1696087390894 4	11 8 , 8	28.2686914441029 9	15 8 , 8
0.02	18.3369301930818 8	19 11,11	28.5299326355848 8	28 11,11
0.03	18.4999694159148 56	34 11,11	28.7780940527698 3	41 11,11
0.04	18.652290705 116	45 11,11	29.01021 490	48 11,11
0.05	18.80776 7669	34 11,11	29.2 2259304	4 11,11
λ	(2,5)	N M , M	(3,5)	N M , M
0.01	22.2091905530535 5	13 8 , 8	26.2485711955362 2	15 10,10
0.02	22.4137398414062 3	24 12,12	26.4891257776520 44	29 11,11
0.03	22.6099690784326 8027	43 12,12	26.7159935463 959	45 11,11
0.04	22.7956646 6766	45 12,12	26.9266 7165	31 11,11
0.05	22.970 00558	15 12,12	26.1 121485	4 11,11
λ	(4,5)	N M , M	(5,2)	N M , M
0.01	30.2877167815098 8	15 10,10	28.2680213586179 9	15 10,10
0.02	30.5629312865129 55	33 11,11	28.5251440396900 708	31 11,11
0.03	30.817919 207	28 11,11	28.76438912 50	43 11,11
0.04	31.05 50788	11 11,11	28.983 3691	36 11,11
0.05	31. 31.26357	10 11,11	29.1 18448	9 11,11

CONCLUSION

In the preceding chapters of this work we have seen, without being concerned with any specific application, how perturbation and non-perturbation methods can be used for solving the eigenvalue problem. The numerical methods presented in this work have been tested for Schrödinger equation involving several perturbed and unperturbed potentials. These methods have been shown to be very effective and to be more simple and accurate than the widely used matrix calculations. We would like to emphasize the following aspects of the present eigenvalue calculations:.

1.The methods which have been used all yielded highly accurate results. These results showed good agreement with each other or with those (when available) in the literature. Our methods proved to be very effective in dealing with one, two, three and N dimensional radial problems.

2.It is interesting to note that the renormalised series method can be extended to compute the energy eigenvalues for quasi-bound states of potentials such as

I. $V(x)=x^2+\lambda x^3$

II. $V(x)=x^2+\lambda x^5$

The renormalised series converge well for sufficiently small values of λ.

3.We studied a double well potential $V(x)=-Z^2x^2+x^{2N}$, for various values of 2N, Z^2 and state number n, by using perturbative and non-perturbative methods. All methods yielded highly accurate results except that the renormali series gave poor accuracy at low values of Z^2, although it works very well for high values of Z^2.

4.It has been shown, (section 2.4), that expectation values such as $\langle x^{2N}\rangle$ can be calculated without storing explicit values of the wavefunction Ψ. The relevant difference equation

$$\langle x^{2N}\rangle = \mathrm{Lt}_{\varepsilon\longrightarrow 0}\ \frac{1}{2\varepsilon}\left[E(H+\varepsilon x^{2N})-E(H-\varepsilon x^{2N})\right]$$

involves the use of energy calculations, which can be performed by many methods (e.g renormalised series, finite difference and power series). In numerical work one or more finite values of ε are used to estimate the value of the limit. For double precision calculations, we found that $\varepsilon = 10^{-8}$ gives reasonably accurate results.

5.In the case of perturbation methods (both hypervirial and inner product) we have shown how one may avoid divergence problem, by using the renormalising constant k and (when necessary) Padé approximants and the Aitken procedure.

6.In the present work, we have compared various methods, with respect to their accuracy and divergence properties and changing behaviour with respect to variation of

I.perturbation parameters (e.g λ, g, α).

II.state number n.

III.power index (x^{2N}) of a perturbing potential.

It is worth pointing out that perturbation methods are sensitive to points (I,II,III), but nonperturbation method in general are less sensitive (except that the simple pow series method in the case $V=\lambda x^2/(1+gx^2)$ requires $gx^2<1$).

7.Our results allow us to study the numerical behaviour of energy levels for the potentials

$$\text{I. } \mu x^2+\lambda x^{2N},\ \mu=0,1;\ 2N=4,6,8....18,20$$

$$\text{II. } V(x)=x^2+\frac{\lambda x^{2N}}{1+gx^2}\ ;2N=4,6,8....18,20$$

for different index 2N, perturbation parameters λ&g and state number n. We have seen how the order of the energy levels varies with these parameters. We determined the value of λ at which a crossing point occurs for potential (I) (i.e $\lambda\cong5$).

8.In chapter four we investigated the eigenvalue problem

$$\text{I.} \qquad V^{\pm}(x)=\frac{1}{2}x^2\pm\frac{gx^{2N}}{1+g\alpha x^2} \qquad ;2N=4,6$$

$$\text{II.} \qquad V^{\pm}(x)=\frac{1}{2}r^2\pm\frac{gr^6}{1+g\alpha x^2}$$

We have not observed any fundamental difference in behaviour between the V^- and V^+ cases as we vary the perturbation parameters (α,g) and index (2N). We used $(g\alpha)$ and (g) as perturbation parameters.

9.We have discovered that the renormalised series method does not work so well for the perturbed potential

$$\text{I.} V=\mu x^2+\lambda(x^{2N}-Kx^2);\ \mu=1+\lambda K;\ 2N=6,8$$

and gives reduced accuracy. However, we partly overcame this difficulty by introducing higher powers of λ

$$\text{II.}\ V=\mu x^2+\underline{\lambda}^I(x^{2N}-Kx^2);\ \mu=1+\underline{\lambda}^I K;\ \underline{\lambda}=\lambda^{\frac{1}{I}};2N=6,8$$

We illustrated the effect of use of the $\underline{\lambda}^I$ technique on the convergence rate in tables (2.3) and (2.4).

We use this modified technique with other eigenvalue problems for instance

$$V(r)=r^2+\ell(1+\ell)r^{-2}+\lambda r^{2N}\ ;2N=6,8$$

$$V(r)=-r^{-1}+\frac{\ell}{2}(1+\ell)r^{-2}+A(\ell,m)\gamma^2r^2$$

10.It should also be mentioned that a large part of our results are not available in the literature. Accordingly, we used more than one method to compute the energy eigenvalues as an internal check on the accuracy and to make sure our results are correct.

11.In the case of the renormalised series approach, we achieved results with very high accuracy as a result of a lengthy study of the effects of changing the value of the overflow parameter (2^N, N=1,2,3,..), of increasing the dimension of B(N,M) and of varying the value of the renormalising constant K....etc. We also obtained much experience at dealing with other eigenvalue methods which involve optimum choice of parameters e.g Padé approximant, finite difference, inner product and power series methods.

The present work gives us good grounds for believing that in future work the methods tested can be used to study other more complicated eigenvalue problems. The many numerical results which are reported in this work enrich considerably the stock of information available in the literature.

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