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# The energy levels of the Schrödinger equation for various types of potentials using a renormalized method

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**Abstract.** A perturbative method is used to compute energy levels for many different forms of potentials. Results of high accuracy are produced for various eigenstates.

## 1. Introduction

The aim of this work is to use numerical techniques to compute the energy eigenvalues for one-particle Schrödinger equations in one and three dimensions, for different forms of potentials. We face convergence difficulties in dealing with the perturbation method. However, there is an extensive range of techniques in the mathematical literature to deal with the divergence problem, e.g. renormalized 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 renormalization parameter ( $K$ ) which has been used widely by Witwit (1989). The renormalization parameter  $K$  plays an important role in the convergence aspects of the calculations which are investigated in this work. Also, Padé approximants have been used to calculate the energy eigenvalues for some problems.

This work is organized as follows. In section 2 we investigate the Gaussian potential

$$V(r) = -A e^{-\lambda r^2}. \quad (1)$$

This potential has been studied by Bessis *et al* (1982) and they have computed the bound state energies of the Gaussian potential, 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 ( $l, n$ ). Lai (1983) calculated the bound state energies of the same potential for various eigenstates ( $l, n = 0-7$ ) by using the hypervirial Padé scheme. Also Chatterjee (1985) has applied the  $1/N$  expansion method to obtain the bound state energy levels of a Gaussian potential. The  $1/N$  expansion method yields energy values which are in good agreement with those results which are available in the literature. In this work, we use the hypervirial method to calculate the energy eigenvalues for various bound states. We extend our calculation to highly excited states ( $0 \leq l \leq 12$ ) and ( $0 \leq n \leq 7$ ), and our method achieves 20-digit accuracy. Such a high degree of precision has not been obtained before by any other method.

In section 3 we investigate the Yukawa potential:

$$V(r) = Zr^{-1} e^{-\lambda r} \quad Z = 1, 2, 3, \dots \quad (2)$$

Grant and Lai (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  $\lambda$  up to order  $\lambda^{20}$ ; Lai (1981) 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. Vrscay (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 attack this problem by using a renormalized series, and perform our calculation for many eigenstates. The renormalized series yields energy eigenvalues with excellent accuracy (more than 15 digits).

In section 4 the energy eigenvalues are calculated for the exponential cosine screened Coulomb potential

$$V(r) = -r^{-1} e^{-\lambda r} \cos(\lambda r) \quad (3)$$

and this potential has been treated by several approximate methods. For instance, Aparna and Pirtam (1980) applied the generalized virial theorem and Hellmann-Feynman theorem to calculate perturbatively the bound state energy levels without using a perturbed wavefunction. Lai (1982) has calculated the energy eigenvalues of potential for various eigenstates within the framework of the hypervirial Padé scheme. We used a renormalized series to calculate the energy eigenvalues for various states and different values of screening parameter. Our method yields 15 digit accuracy, and the results are given in table 5†.

Section 5 deals with an eigenvalue calculation for the Hulthen potential

$$V(r) = -\lambda \left[ \frac{e^{-\lambda r}}{1 - e^{-\lambda r}} \right]. \quad (4)$$

Lai and Lin (1980) have applied the Padé approximant technique to a perturbation series obtained by use of hypervirial and Hellmann-Feynman theorems. They computed the energies of 2p, 3p, 4p, 4d and 4f states. Also, this potential has been treated by Dutt and Mukherji (1982) they 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. We use the renormalized series to calculate the energy eigenvalues for potential (4) for various values of  $\lambda$  and for highly excited states (2p to 8h). The renormalized series gives high accuracy (15 digits).

Finally, we calculate the energy eigenvalues for potentials in (one and three dimensions):

$$V(x) = -2 \left[ \frac{e^{-2\lambda x^2}}{1 + e^{-2\lambda x^2}} \right] \quad (5)$$

$$V(r) = -2 \left[ \frac{e^{-2\lambda r^2}}{1 + e^{-2\lambda r^2}} \right]. \quad (6)$$

We used the Padé approximant and the hypervirial method to compute the energy eigenvalues for different values of  $\lambda$  and excited states ( $n = 0-5$ ;  $l = 0-5$ ).

† This table and all others in this paper have been deposited in the British Library Supplementary Publications Scheme, document no. SUP70042.

**2. Hypervirial method of calculating energy eigenvalues for a 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. The Schrödinger equation for the radial part of the attractive Gaussian potential is given by

$$-r^{-2} \frac{d}{dr} \left[ r^2 \frac{d\Psi(r)}{dr} \right] + [l(l+1)r^{-2} - A \exp(-\lambda r^2)]\Psi(r) = E\Psi(r) \quad (7)$$

where the units  $2m = \hbar = 1$  are used, and the function in equation (7) can be expressed as

$$\Psi(r) = r^{-1}\Phi(r). \quad (8)$$

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

$$A \exp(-\lambda r^2) = \sum_{m=0}^{\infty} V_m \lambda^m r^{2m+2} \quad (9)$$

with the potential coefficients  $V_m$  given by

$$V_m = (-1)^m A [(m+1)!]^{-1}. \quad (10)$$

Then the equation (7) takes this form

$$\left[ -D^2 + l(l+1)r^{-2} - \sum_{m=0}^{\infty} V_m \lambda^m r^{2m+2} \right] \Phi(r) = \mathcal{E} \Phi(r) \quad (11)$$

where  $\mathcal{E} = E + A$ . If we use the perturbation expansions

$$E = \sum E(I) \lambda^I \quad (12)$$

$$\langle x^N \rangle = \sum A(N, M) \lambda^M \quad (13)$$

in the hypervirial relation given by Killingbeck (1982) in the form

$$2E(N+1)\langle x^N \rangle = \sum V_m (2N+2+m)\langle x^{N+m} \rangle - \frac{N}{2} (N^2-1)\langle x^{N-2} \rangle. \quad (14)$$

We obtain recurrence relations corresponding to the Gaussian potential case as follows:

$$\begin{aligned} (2N+2) \sum_0^M E(I) A(N, M-I) &= N[2l(l+1) - \frac{1}{2}(N^2-1)]A(N-2, M) \\ &- \sum_{m=0}^{\infty} V_m [2N+2m+4]A(N+2m+2, M-m-1). \end{aligned} \quad (15)$$

Applying the Hellmann-Feynman theorem in the form

$$\frac{\partial E}{\partial \lambda} = \left\langle \frac{\partial V}{\partial \lambda} \right\rangle \quad (16)$$

we obtain a recurrence relation for the energy coefficients of the form

$$(M+1)E(M+1) = - \sum_{m=0}^{\infty} V_m (m+1)A(2m+2, M-m). \quad (17)$$

The unperturbed value of  $E$  is given by

$$E(0) = [(4n + 2l + 3)\sqrt{A}] - A \quad (18)$$

where  $n$  is the principal quantum number,  $l$  the angular momentum quantum number and we set  $A = 400$  to agree with previous authors. The recurrence relations (15) and (17) with equation (18) 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  $l$  and  $n$  increase, as shown in table 1. 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  $l$  and  $n$ . 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 produced by other methods, 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 1 that for the ground state and some of the first few excited states at low values of angular momentum we find the energy values with an accuracy of 20 significant figures.

### 3. Renormalized series method for computing eigenvalues for the hydrogen atom with a Yukawa potential

The general screened Coulomb potential given by (2) for hydrogen-like atoms may be written in the form

$$V(r) = -Zr^{-1} \sum_{m=0}^{\infty} V_m(\lambda r)^m \quad (19)$$

where  $Z$  is the nuclear charge and  $\lambda$  represents the screening parameter. 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. We employ the Hellmann–Feynman theorem and the hypervirial theorems to calculate the energy eigenvalues of various energy eigenvalues to high accuracy. In our work we wish to show that the renormalized series method can be used to calculate the bound state energies of a screened Coulomb potential to very high accuracy. This study was motivated by the work of Lai (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 renormalized series method can give 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 renormalized series method for this problem is complicated by the presence of the renormalization parameter  $K$ . A proper treatment would necessarily involve the choice of an ideal value for the renormalization parameter  $K$ . The Hamiltonian for the Yukawa potential can be written as

$$\begin{aligned} H &= -\frac{1}{2}D^2 + \frac{1}{2}l(l+1)r^{-2} - Zr^{-1}e^{-\lambda r} \\ &\equiv -\frac{1}{2}D^2 + \frac{1}{2}l(l+1)r^{-2} - Z(\mu + \lambda K)r^{-1} - Zr^{-1} \sum_{m=1}^{\infty} V_m(\lambda r)^m \end{aligned} \quad (20)$$

where

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

where  $l$  is the orbital angular momentum quantum number. Here we are using atomic units,  $\hbar = e = m = 1$ . By employing the hypervirial recurrence relation given by (14) and applying the Hellmann-Feynman theorem (16), together with the perturbation expansions (12) and (13), as in the previous section the following two recurrence relations are obtained after some algebra:

$$\begin{aligned} (2N+2) \sum_0^M E(I)A(N, M-I) \\ = N[l(l+1) - \frac{1}{4}(N^2-1)]A(N-2, M) \\ - Z(2N+1)[\mu A(N-1, M) + KA(N-1, M-1)] \\ - Z \sum_{m=0}^{\infty} V_m(2N+m+2)A(N+m, M-m-1) \end{aligned} \quad (21)$$

$$(M+1)E(M+1) = -KA(-1, M) - Z \sum_{m=0}^{\infty} V_m(m+1)A(m, M-m). \quad (22)$$

The coefficients  $V_m$  in (21) and (22) can be written as

$$V_m = \frac{(-1)^{m+1}}{(m+1)!}. \quad (23)$$

The coefficients  $V_m$  in general alternate in sign and decrease with increasing ( $m$ ). Where the energy of the unperturbed  $n$ th state  $E(0) = -Z^2\mu^2/2n^2$  is known, the equations (21) and (22) suffice to calculate the full set of  $E(M)$  and  $A(N, M)$  coefficients, with the aid of equation (23) and the starting term  $A(0, 0)$  which is obtained from the condition of normalization  $\langle r^0 \rangle = \langle 1 \rangle = 1$ . Our numerical results, presented in table 2, reveal that at low values of ( $\lambda$ ) for states (1s, 2s, 2p) we have excellent agreement with the values of Vrscay (1985). Our approach provides extremely accurate eigenvalues at low  $\lambda$ . These values are accurate to all the digits shown and agree to over 19 digits with those of Vrscay. The power of this renormalized series techniques at low values of  $\lambda$  has thus been demonstrated. However, at larger values of  $\lambda$ , the accuracy decreases as expected from our previous renormalized series calculations, although the accuracy is better than that of Lai (1984), who used the hypervirial theorem and Padé approximants. In the preceding case we have calculated the bound state energy eigenvalues for a Yukawa potential with  $Z = 1$ , but we will extend our discussion of the Yukawa potential given by (2), to the case  $Z > 1$ , where the screening parameter  $\lambda = \lambda_0[Z]^{1/3}$ , corresponding to the  $Z$  dependence of the reciprocal of the Thomas-Fermi radius of the atom. Grant and Lai (1979) have recently evaluated the energy levels for atoms with ( $4 \leq Z \leq 84$ ) using Padé approximants [6, 6] and [6, 7], for K- and L-shell electrons with ( $\lambda_0 = 0.98$ ). 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 2 Ryd = 27.212 eV. The coefficients  $V_m$  can be written for  $\lambda = \lambda_0 Z^{1/3}$  as given by (23), and for  $\lambda = \lambda_0$  as

$$V_m = [-Z^{1/3}]^{m+1} [(m+1)!]^{-1}. \quad (24)$$

The two coefficients (23) and (24) in general alternate in sign and the coefficients (23) decrease with increasing  $m$ , but the coefficients (24) decrease less quickly than the

coefficients (23). For the case  $Z > 1$ , in table 3 we list the energies of states (1s, 2s, 2p, 3s) for different values of  $\lambda_0$  and different values of  $Z$  ( $2 \leq Z \leq 65$ ). Our results are summarized in table 4, ranging from  $4 \leq Z \leq 84$  in 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 renormalized series approach as used by Witwit (1989) is a very elegant and powerful approach to compute the energy eigenvalues with high accuracy. The approach achieved an accuracy of 15 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. We wish to draw attention to the fact that the renormalized series works equally well for  $\lambda = \lambda_0$  and  $\lambda = \lambda_0 Z^{1/3}$  as perturbation parameter; we used the two values of  $\lambda$  in order to verify the accuracy of the renormalized series for this calculation. Using two different values 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 renormalization parameter for  $Z > 29$ .

#### 4. Renormalized series for calculating the eigenvalues for the exponential cosine screened Coulomb potential

The radial Schrödinger equation for the exponential cosine screened Coulomb potential given by (3) is not solvable analytically and can be expressed as

$$D^2\Psi(r) + 2[E + V(r) - \frac{1}{2}l(l+1)r^{-2}]\Psi(r) = 0. \quad (25)$$

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. In this section we set out to calculate the bound state energies of the (cos) potential for different eigenstates, by applying the hypervirial and Hellmann-Feynman theorems to calculate perturbatively the bound state energy levels without using perturbed wavefunctions. The (cos) potential can be expanded in a power series of the screening parameter by the Taylor expansion

$$F(x) = F(0) + xF'(0) + \frac{x^2}{2!}F''(0) + \dots + \frac{x^m}{n!}F^{(m)}(0). \quad (26)$$

Also  $V(r)$  can be expanded as

$$\begin{aligned} V(r) &= -r^{-1} \exp(-\lambda r) \cos(\lambda r) = -r^{-1} \sum_{m=0}^{\infty} V_m(\lambda r)^m \\ &= -V_0[\mu + \lambda K]r^{-1} - r^{-1} \sum_{m=1}^{\infty} V_m(\lambda r)^m \quad \mu = 1 - \lambda K. \end{aligned} \quad (27)$$

Comparing (26) and (27), we obtain the coefficients

$$\begin{aligned} V_0 &= 1 & V_1 &= -1 & V_2 &= 0 & V_3 &= \frac{2}{3!} \\ V_4 &= -\frac{4}{4!} & V_5 &= \frac{4}{5!} \dots & V_{20} &= -\frac{1024}{20!} & V_{21} &= \frac{1024}{21!}. \end{aligned}$$

The coefficients  $V_m$  in equation (27) also can be expressed as

$$V_m = (-1)^m (2)^{m/2} \cos\left(\frac{\pi m}{4}\right) \frac{1}{m!}. \quad (28)$$

Here, we use atomic units. If we insert the expansion of potential (33) in the hypervirial relation (14), we obtain the following relation

$$\begin{aligned} (2N+2) \sum_0^M E(I)A(N, M-I) \\ = N[I(I+1) - \frac{1}{4}(N^2-1)]A(N-2, M) \\ - V_0(2N+1)[\mu A(N-1, M) + KA(N-1, M-1)] \\ - \sum_{m=1}^{\infty} V_m(2N+1+m)A(N+m-1, M-m). \end{aligned} \quad (29)$$

Applying the Hellmann-Feynman theorem to the expansion of the potential given by (33), we obtain the following relation

$$(M+1)E(M+1) = -KV_0A(-1, M) - \sum_{m=1}^{\infty} mV_mB(m-1, M-m+1). \quad (30)$$

The recurrence relations (35) and (36) can be used to calculate the energy coefficients from a knowledge of  $A(0, 0) = 1$  and  $E(0) = -\mu^2/2n^2$ . The energy eigenvalues can be evaluated by using equations (35) and (36) using appropriate values of the renormalization parameter  $K$ ; the results of this calculation are given in table 5. Our calculated values of the energy levels are good as compared with the results obtained from the hypervirial Padé approximant scheme of Lai (1982). From our results it can be seen that the hypervirial method with a renormalization parameter  $K$  is sufficient to calculate the energy eigenvalue without using Padé approximants. Although the renormalized 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  $\lambda$ . Second, the calculations become progressively more difficult as the state number  $n$  increases. The Yukawa potential given by (2) differs from the cos potential given by (3) by a cosine factor ( $\cos \lambda r$ ), which leads to an oscillatory behaviour. It is of obvious interest to compare the result for the cos potential with those for Yukawa. Generally speaking the binding of the electron is weaker in the cos potential than in the Yukawa potential and this is clear from our results in tables 2 and 5.

## 5. Renormalized series for calculating the energy eigenvalues for the Hulthen potential

The radial Schrödinger equation for the Hulthen potential (4) can be written in atomic units as

$$D^2\Psi(r) + 2[E + \lambda \exp(-\lambda r)\{1 - \exp(-\lambda r)\}^{-1} - \frac{1}{2}I(I+1)r^{-2}]\Psi(r) = 0 \quad (31)$$

where  $\lambda$  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 purpose of this section is to study the bound state energies of the Hulthen potential for  $l \neq 0$ . The Hulthen potential  $V_H(r)$  in (37) can be rewritten in the form

$$\begin{aligned} V_H(r) &= -\lambda \exp(-\lambda r)[1 - \exp(-\lambda r)]^{-1} \\ &= -r^{-1}(\lambda r)[\exp(\lambda r) - 1]^{-1} \\ &= -V_0[\mu + \lambda K]r^{-1} - r^{-1} \sum_{m=1}^{\infty} V_m(\lambda r)^m \end{aligned} \quad (32)$$

where

$$\begin{aligned} V_m &= \frac{B_m}{m!} \\ V_0 &= 1 \quad V_1 = -\frac{1}{2} \quad V_2 = \frac{1}{6} \frac{1}{2!} \\ V_4 &= -\frac{1}{30} \frac{1}{4!}, \dots, V_{30} = \frac{8615\ 842\ 176\ 005}{14\ 322} \frac{1}{30!} \end{aligned} \quad (33)$$

and  $B_m$  are the Bernoulli numbers. The Hulthen potential  $V_H(r)$  in equation (37) can be rewritten in another form:

$$\begin{aligned} V_H(r) &= -\frac{\lambda e^{-\lambda r}}{[1 - e^{-\lambda r}]} \\ &= -\frac{\lambda}{2} \left[ \frac{e^{\lambda r/2} + e^{-\lambda r/2}}{e^{\lambda r/2} - e^{-\lambda r/2}} - 1 \right] \\ &= -\frac{\lambda}{2} \left[ \coth\left(\frac{\lambda r}{2}\right) - 1 \right] \end{aligned} \quad (34)$$

where

$$\coth(Z) = \frac{1}{Z} + \frac{Z}{3} - \frac{Z^3}{45} + \frac{2Z^5}{945} + \dots + \frac{2^{2m}}{2m!} B_{2m} Z^{2m-1} \quad (35)$$

where  $|Z| < \pi/2$ .

Furthermore, we use the hypervirial relation (14) as used in previous sections, and using the energy and the expectation values  $\langle r^M \rangle$  given by (12) and (13). Then the hypervirial relation for the Hulthen potential can be expressed as

$$\begin{aligned} (2N+2) \sum_0^M E(I) A(N, M-I) \\ &= N[l(l+1) - \frac{1}{4}(N^2-1)] A(N-2, M) \\ &\quad - V_0(2N+1)[\mu A(N-1, M) + K A(N-1, M-1)] \\ &\quad - \sum_{m=1}^{\infty} V_m(2N+m+1) A(N+m-1, M-m). \end{aligned} \quad (36)$$

Applying the Hellmann-Feynman theorem given by (16) with the use of (12) and (13) we obtain the following relation

$$(M + 1)E(M + 1) = -KV_0A(-1, M) - \sum_{m=1}^{\infty} mV_m A(m - 1, M + 1 - m). \tag{37}$$

With unperturbed energy  $E(0) = -\mu^2/2n^2$  and initial condition  $A(0, 0) = 1$ , we use the recurrence relations (36) and (37) to compute the energy coefficient  $E(M)$ . Energies of many eigenstates (2p to 8h) of the Hulthen potential are listed in table 6. It is apparent from table 6 that the energy series is converging very quickly at low values of the screening parameter  $\lambda$ . We wish here to make a few comments summarizing the advantage of using the renormalized series approach. It is important, however to remember that our results have been calculated directly from the hypervirial approach with a renormalization parameter  $K$ , without the use of Padé approximants, which were used by Lai (1980) 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 renormalized series approach works very well even for higher excited states with higher values of angular momentum. We believe that the accuracy of our results may be improved even further with a better choice of renormalization parameter  $K$ ; the approach gives well converged eigenvalues for the best values of the renormalization parameter  $K$ .

**6. Hypervirial and the Padé approximant methods for calculating energy eigenvalues for potentials which are given by (5) and (6)**

In this section we study the two potentials which are given by (5) and (6). The potential given in equation (5) can be expressed as

$$V(x) = -2 \left[ \frac{e^{-2\lambda x^2}}{1 + e^{-2\lambda x^2}} \right] = \left[ \frac{e^{\lambda x^2} - e^{-\lambda x^2}}{e^{\lambda x^2} + e^{-\lambda x^2}} - 1 \right] = \tanh(\lambda x^2) - 1. \tag{38}$$

We let

$$\lambda x^2 = y. \tag{39}$$

The perturbation calculation by using hypervirial relations for the interaction given by (38) is made by expanding  $\tanh(\lambda x^2)$  in a power series in  $(\lambda x^2)$  which is valid for  $\lambda x^2 < \pi/2$ . Then  $\tanh(y)$  can be expressed as

$$\tanh(y) = y - \frac{y^3}{3} + \frac{2y^5}{15} + \dots + \frac{2^{2m}[2^{2m-1} - 1]y^{2m-1}}{2m!} B_{2m}. \tag{40}$$

As  $x$  varies from  $(-\infty \leq x \leq +\infty)$  the potential runs from  $(0 \leq V(x) \leq 0)$  through  $(-1)$  at  $x = 0$ . We can use the hypervirial relation (14) as in previous problems together with the perturbation expansions given by (12) and (13) for potential (38), leading to the recurrence relation

$$\begin{aligned} (2N + 2) \sum_0^M E(I)A(N, M - I) \\ = -\frac{N}{2} [N^2 - 1]A(N - 2, M) + (1 + \lambda)[2N + 4]A(N + 2, M) \\ + \sum_{m=1}^{\infty} V_m [2N + 4m + 4]A(N + 4m + 2, M - 2m - 1). \end{aligned} \tag{41}$$

If we apply the Hellmann-Feynman theorem which is given by (16) and use the energy and the expectation value  $\langle x^M \rangle$  series as given by equations (12) and (13) we obtain the following recurrence relation

$$(M+1)E(M+1) = \sum_{m=1}^{\infty} [2m+1]V_m A(4m+2, M-2m) \quad (42)$$

where

$$V_m = \frac{2^{2m}(2^{2m-1}-1)y^{2m-1}}{2m!} B_{2m}. \quad (43)$$

Here  $B_{2n}$  is the  $n$ th Bernoulli number. The unperturbed energy  $E(0)$

$$E(0) = (2n+1)\sqrt{(1+\lambda)} - 1 \quad (44)$$

allows us to use the recurrence relations (41) and (42) to compute the energy coefficient  $E(M)$ , with initial condition  $A(0,0) = 1$ . Also we extend the numerical calculation from one dimension to three dimensions. The main difference between the one- and three-dimensional potential lies in the angular momentum term. Then there is an additional potential term due to the angular momentum with its coefficient value  $V_{-2} = l(l+1)$ ; therefore the first term on the right-hand side takes the form  $[2Nl(l+1) - (N/2)(N^2-1)]A(N-2, M)$  and other terms in the recurrence relations (41) and (42) remain the same, and the unperturbed energy  $E(0)$  becomes

$$E(0) = (4n+2l+3)\sqrt{(1+\lambda)} - 1. \quad (45)$$

We also used the Padé approximants to calculate the eigenvalues for potentials (5) and (6). Padé approximation is a useful technique when the convergence of the series is unacceptably slow or even non-existent. The Padé approximant is in the form of one polynomial divided by another polynomial. This technique provides 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 are given by

$$E[N, M] = \frac{a_0 + a_1\lambda + a_2\lambda^2 + a_3\lambda^3 \dots a_n\lambda^N}{b_0 + b_1\lambda + b_2\lambda^2 + b_3\lambda^3 \dots b_M\lambda^M} \quad (46)$$

$$\equiv E(0) + E(1)\lambda + E(2)\lambda^2 + \dots + E(N+M)\lambda^{M+N} + \dots \quad (47)$$

with  $b_0$  defined to be unity. The coefficients  $(a_i, i = 1, \dots, N)$  and  $(b_i, i = 0, \dots, M)$  in the numerator and denominator are calculated from the knowledge of  $E(1), E(2), \dots, E(M+N)$ , which can be computed from the hypervirial relations. The energy series for the potentials (5) and (6) appears to be convergent for  $0.01 \leq \lambda \leq 0.1$ . Our calculated energy values  $E_n$  used the  $E[N, N]$  Padé approximants to the energy series for the ground and the first five excited states. Tables 7 and 8 show the eigenvalues for potentials (5) and (6). It is clear from our results that the energy series converges very quickly at low values of  $\lambda$ , but the convergence decreases as  $\lambda$  increases. It is important to point out that the accuracy of results for this problem has been achieved without the use of the renormalization parameter  $K$ ; also we have used Padé approximants as a second method of computing the energy eigenvalue. The agreement between the two methods is very good for low values of  $\lambda$ , but for high values of  $\lambda$  the Padé approximants give more accurate eigenvalues. We have computed many energy eigenvalues of the potential given by equation (5), for different values of

( $0.01 \leq \lambda \leq 0.1$ ) and for the ground and first four excited states. We list our results for this calculation in table 7 for one dimension and in table 8 for three dimensions, for different values of ( $0.01 \leq \lambda \leq 0.05$ ), different values of ( $l=0, 2, 5, 10$ ) and state number  $n$ .

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