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The eigenvalues of the Schrödinger equation for spherically symmetric states for various types of potentials in two, three and N dimensions, by using perturbative and non-perturbative methods

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Abstract. The energy levels of the Schrödinger equation involving various model potentials in two, three and N-dimensional space, are calculated by using perturbative and non-perturbative methods. Our methods have been used effectively to calculate the energy eigenvalues even for high state numbers and large values of the perturbation parameters.

1. Introduction

The purpose of this paper is to compute the energy eigenvalues for the one-particle Schrödinger equation for various forms of potentials in $N = 2, 3, \ldots$ dimensions for a wide range of values of perturbation parameter λ and states number, by using perturbative numerical techniques such as the renormalized series and the inner product as well as the non-perturbative the power series technique. These potentials can be written

$$v(x, y) = \tfrac{1}{2}(x^2 + y^2) + \lambda(a_{11}x^4 + 2a_{12}x^2y^2 + a_{22}y^4) \tag{1}$$

$$v(r) = r^2 + l(l+1)r^{-2} + \lambda r^{2M} \qquad (2M = 4, 6, 8) \tag{2}$$

$$v_N(r) = r^2 + \tfrac{1}{4}[(N+2l-3)(N+2l-1)]r^{-2} + \lambda r^4 \qquad (N = 1, 2, 3, \ldots, 1000). \tag{3}$$

It is important to point out that the form of the potential given by equation (3) is a general form for the case of a spherical symmetric potentials, which can expressed the other forms of the potentials given by equations (1) and (2) in two and three dimensions. For $N = 2, 3$ the potential given by equation (3) reduces to potentials given by equations (1) and (2) respectively. For spherically symmetric states in N dimensions the Schrödinger equation generalizes to the form

$$\left(-\frac{d^2}{dr^2} + r^2 + \tfrac{1}{4}(N+2l-3)(N+2l-1)r^{-2} + \lambda r^{2M}\right)\Psi(r) = E\Psi(r) \qquad 2M = 4, 6, 8. \tag{4}$$

by studying the form of the Schrödinger equation in one and two dimensions, we found that the form of the equation (4) can be used in one, two or three dimensions by making the appropriate choice of l. In three dimensions l is the usual angular momentum value $(0, 1, 2, \ldots)$. In two dimension l is set equal to $|m| - \tfrac{1}{2}$, where m is

the magnetic quantum number. In one dimension l is set equal to $(l = 0, 1)$ and r replaced by x.

Our work also is intended to point out the flexibility of the inner product perturbation theory, which gives it an advantage over the renormalized series method.

One main difference between the two perturbative techniques is that 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. It is noteworthy that although hypervirial approach is very attractive for the one-dimensional problem, its application to a system of many dimensions has not yet been accomplished, but the inner product method deals with more general parameter values $a_{11} = a_{22} = 1, 0$; $a_{12} = 1, 0, -1$. We faced convergence difficulties in dealing with perturbative methods, but overcame this situation by using the renormalization parameter to improve the convergence of the perturbation series to give results with good accuracy.

The abundance of studies of the one-dimensional anharmonic oscillator eigenvalue problem is not matched in the case of multidimensional problems, for which there are few reported results in the literature. Many techniques have been used to obtain the energy eigenvalues for the two-dimensional potential $v(x, y)$. The work of Hioe *et al* (1978) involved matrix diagonalization. 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 together with using an appropriate scaled transformation to improve the convergence of their results, Blankenbecler *et al* (1980) used the inner product method to calculate the energy eigenvalues for the two-dimensional oscillator, involving the study of recursion relations between matrix elements of powers of the coordinate operator between the exact eigenstate and a conveniently chosen basis state. Ari and Demiralp (1985) computed the eigenvalues of a two-dimensional oscillator by using perturbation theory and Padé approximants. Killingbeck and Jones (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}).

Killingbeck (1985a) 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 $(N = 1, 2, 3, \ldots, 320)$. He computed the energy eigenvalues and expectation values such as $\langle r^2 \rangle$ for potentials $l^{-1}r^4$ and $N^{-1}r^4$ and gave results of good accuracy. We used three methods, the inner product method, the renormalized 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. The results are compared with those produced by different methods which can be used to calculate energies for the same perturbed potentials. The results showed a good agreement with each other or with those (when available) in the literature. This paper is organized as follows. Section 2 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 3 is concerned with three- and N- $(N = 1, 2, 3, 4, 5, 6, \ldots, 1000)$ dimensional oscillators and with relations which can be used to compute the energy eigenstates.

2. Two-dimensional problem

2.1. Review of the two-dimensional oscillator problem

In this section we present some extended numerical calculations using the inner product technique for a greater range of values of the perturbation parameter $0.05 \le \lambda \le 5000$, and for different values of the potential parameters (a_{11}, a_{22}, a_{12}). The inner product method to calculate eigenvalues has been investigated (Witwit 1990) to compute energy eigenvalues for the two-dimensional problem for higher powers of the perturbation $v(x, y) = \lambda(ax^6 + 3bx^4y^2 + 3cx^2y^4 + dy^6)$, and later (Witwit 1991) for three dimensions. We also used renormalized series and power series methods, for the special case $a_{11} = a_{22} = a_{12} = 1$, to calculate the energy eigenvalues for the perturbed oscillator potential in two dimensions. The potential given by equation (1) is non-separable but shows a high symmetry. The energy perturbation series is expected to be divergent, so we start by introducing a renormalization parameter (β), and write the potential in the form

$$V(x, y) = \tfrac{1}{2}\mu^2(x^2 + y^2) + \lambda[a_{11}x^4 + 2a_{12}x^2y^2 + a_{22}y^4 - \beta(x^2 + y^2)] \tag{5}$$

where

$$\mu^2 = 1 + \lambda\beta. \tag{6}$$

Setting $\beta = 0$ in the perturbation calculation gives the traditional Rayleigh–Schrödinger series for the problem and ensures that the form of the potential in (5) is the same as the original potential in (1). The use of the renormalization parameter β is helpful in improving convergence in this technique, and this parameter has played an important role in the convergence aspects of the calculations which are investigated in the work of Witwit (1989). It is interesting to point out that the effect of varying the parameter β is to allow us to obtain results of high accuracy as we will see later. In rectangular coordinates the Schrödinger equation for the renormalized potential $V(x, y)$ (5) can be written

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + V(x, y) \right]\Psi(x, y) = E\Psi(x, y). \tag{7}$$

The energy eigenvalues of the unperturbed oscillator are given by

$$E_{n1,n2} = (n_1 + n_2 + 1) \qquad n_1, n_2, = 0, 1, 2, \ldots. \tag{8}$$

In each state the energy levels depend on the pair quantum numbers (n_1, n_2). The energy levels are degenerate, because the sum

$$n_1 + n_2 = n. \tag{9}$$

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:

$$\Phi(x, y) = (x^{P1}y^{P2}) \exp[-\tfrac{1}{2}\mu(x^2 + y^2)] \tag{10}$$

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

$$A(J, M) = \langle \Phi | x^{2M} y^{2J} | \Psi \rangle \tag{11}$$

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

$$EA(M, J) = \langle \Psi | Hx^{2M}y^{2J} | \Phi \rangle \tag{12}$$

and then to substitute the perturbation expansions

$$A(M, J) = \sum_K A(M, J, K)\lambda^K \tag{13}$$

$$E = \sum_I E(I)\lambda^I \tag{14}$$

into the $A(M, J)$ recurrence relation (12). The result is the new recurrence relation

$$\sum_I^k E(I)A(M, J, K - I)$$

$$= a_{11}A(M + 2, J, K - 1) + a_{22}A(M, J + 2, K - 1)$$
$$+ a_{12}A(M + 1, J + 1, K - 1) - \beta A(M + 1, J, K - 1)$$
$$+ 4\mu(M + J - S_1 - S_2)A(M, J, K) - 2M(2M + 2P_1 - 1)A(M - 1, J, K)$$
$$- 2J(2J + 2P_2 - 1)A(M, J - 1, K). \tag{15}$$

In writing relation (15) we have moved one term $E(0)A(M, J, K)$ from the sum over I to the right of the equation, and have expressed the unpertrubed energy in the form

$$E(0) = \mu(2 + 2P_1 + 2P_2 + 4S_1 + 4S_2). \tag{16}$$

The unperturbed energy, given by equation (16), must fit with equation (8). 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

$$A(J, M, K) = (-1)^{P_3}A(M, J, K). \tag{17}$$

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

$$A(S_1, S_2, 0) = (-1)^{P_3}A(S_2, S_1, 0) = 1 \tag{18}$$

and the recurrence relation (15) 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:

$$K = 0, 1, 2, \ldots Q$$

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

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

The indices are scanned in the order given above and the relation (15) is used to work out $A(M, J, K)$ in term of lower-order elements which are already known. Then we can get $A(J, M, K)$ from the symmetry relation (17). $E(K)$ is found from the equation (15) for the special case $M = S_1$, $J = S_2$, because in this case relation (15) is used differently and the sum on the left-hand side becomes $E(K)$, because of the intermediate normalization convention $A(S_1, S_2) = 1$ which we impose on the algorithm, this gives the value of the energy coefficient $E(K)$ in terms of already calculated elements of the $A(J, M, K)$ array. The sum of the energy perturbation series can then be calculated term by term, and β is varied to give the best possible convergence of the perturbation series.

2.3. The recurrence relation for the renormalized series approach

The renormalized series method has been found to work very well in previous work and has produced highly accurate results for the problems investigated by Witwit (1989). As indicated previously the renormalized series can be used to compute the energy eigenvalues for equation (7) in some cases. When the relationship $a_{12} = a_{11} = a_{22} = 1$ holds, the equation (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 (7) is

$$\left[\frac{1}{2} \left(-\frac{d^2}{dr^2} - r^{-1} \frac{d}{dr} + \frac{m^2}{r^2} + r^2 \right) + \lambda r^4 \right] \Psi(r) = E \Psi(r). \tag{19}$$

If we set

$$\Psi(r) = [r]^{-1/2} \Phi(r) \tag{20}$$

we get

$$\left(-\frac{1}{2} \frac{d^2}{dr^2} + \frac{1}{2} V_m \right) \Phi(r) = E \Phi(r) \tag{21}$$

$$V_m = (m^2 - \tfrac{1}{4}) r^{-2} + r^2 + 2\lambda r^4 \tag{22}$$

$$\equiv (m^2 - \tfrac{1}{4}) r^{-2} + (\mu - \lambda\beta) r^2 + 2\lambda r^4 \qquad \mu = 1 + \lambda\beta. \tag{23}$$

The Schrödinger equation (21) and V_m can written directly from the equation (4) for the case $N = 2$ as indicated previously in the beginning of the introduction. If we use the perturbation expansions

$$E = \sum E(I) \lambda^I \tag{24}$$

$$\langle x^J \rangle = \sum A(J, M) \lambda^M \tag{25}$$

in the hypervirial relation given by Killingbeck (1985b) in the form

$$2E(J+1)\langle x^J \rangle = \sum V_I (2J + 2 + I)\langle x^{J+I} \rangle - \frac{J}{2} (J^2 - 1)\langle x^{J-2} \rangle \tag{26}$$

and apply the Hellmann–Feynman theorem in the form

$$\frac{\partial E}{\partial \lambda} = \left\langle \frac{\partial V}{\partial \lambda} \right\rangle \tag{27}$$

to the potential given by (23), we get the following recurrence relation after some algebra:

$$(2J+2) \sum_0^M E(I) A(J, M - I)$$

$$= J[(m^2 - \tfrac{1}{4}) - \tfrac{1}{4}(J^2 - 1)] A(J - 2, M) + (J + 4)$$

$$\times [\mu A(J + 2, M) - \beta A(J + 2, M - 1)] + (2J + 6) A(J, M - 1) \tag{28}$$

$$(M + 1) E(M + 1) = A(4, M) - \beta A(2, M). \tag{29}$$

From the recurrence relations (28) and (29), we can find the energy coefficients with the help of the unperturbed energy $E(0)$ and the initial coefficient $B(0,0) = 1$. The unperturbed energy is

$$E(0) = (n+1)\sqrt{\mu}. \tag{30}$$

As in (8) we find again the degeneracy of the same multiplicities, where n is the principal quantum number, which can be expressed as

$$n = 2n_r + |m|$$
$$\equiv n_1 + n_2$$
$$n_r = 0, 1, 2, 3, \ldots$$
$$m = 0, \mp 1, \mp 2, \ldots$$

where n_r and m are the radial quantum number and the magnetic quantum number. The expression $(2n_r + |m| + 1)$ shows 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 $E_{2,0}$ have the same quantum numbers $(n_r = 0, m = 2)$ and have the same perturbed energy eigenvalues when the relationship $a_{12} = a_{11} = a_{22} = 1$ *holds*, but this degeneracy removed when $a_{11} = a_{22} = 0$ and $a_{12} = 1$ and this is confirmed by our results and the results given by Hioe *et al* (1978) and Killingbeck and Jones (1986) that perturbation energies for these two eigenstates have the same perturbed energy eigenvalues ($E_{1,1}$ (even) $= E_{2,0}$ (odd)), which means that the energy levels for these eigenstates crosses at $a_{12} = a_{11} = a_{22} = 1$, but when $a_{11} = a_{22} = 0$, $a_{12} = 1$ the doubly degenerate level splits into two levels.

2.4. The power series method

The use of non-perturbative methods of computing energy eigenvalues is necessary because the perturbative method provides insufficient information about accuracy and has convergence difficulties. Recently Witwit (1989) has applied the power series and finite difference methods to various eigenvalue problems. In the present problem we use 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 (21). The regular solution to equation (21) will behave as r^l near the origin, so we postulate $\Phi(r)$ to be of the form:

$$\Phi(r) = \exp(-\tfrac{1}{2}\beta r^2) \sum_0^\infty A(J) r^{J+l} \tag{31}$$

and use the notation

$$\sum T(J) = \sum A(J) r^J. \tag{32}$$

Inserting these relations (31) and (32) into equation (21) yields the recurrence relation

$$(J+2)[J+2l+3]T(J+2)$$
$$= [(2J+2l+3)\beta - E]r^2 T(J) + [\mu - \beta^2]r^4 T(J-2) + \lambda r^6 T(J-4) \tag{33}$$

where $l = |m| - \tfrac{1}{2}$.

The calculation starts at $J = 0$, with $T(0) = 1$ and with all lower coefficients zero. The power series approach works out each $T(J)$ and the sum of the $T(J)$ at a specific

r value. The method works out the sum $\Sigma\, T(J)$ for two neighbouring energies E and $E + H$, and finds the energy which would make the sum zero. The calculation as set out above finds eigenvalues appropriate to the Dirichlet boundary conditions $\Psi(r) = 0$, with r approaching infinity (or sometimes for some finite r). H is typically $\simeq 10^{-4}$. In this approach we also have a convergence factor $\exp(-\beta x^2)$, and the choice of the β parameter helps to achieve or improve convergence.

2.5. Results and discussion

In this subsection we investigate and discuss the results of the numerical calculations for the two-dimensional systems. It is clear from our results which are calculated by perturbative methods and listed in tables 1-4† that the accuracy can be expected to decrease as λ increases. Let us now turn to the renormalization parameter β 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 renormalized parameter β. One continues to change the renormalized parameter until energy eigenvalues of the best required accuracy are obtained. The values of energy in table 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 $0.05 \leqslant \lambda \leqslant 5000$. The three approaches work very well for the two-dimensional oscillator, and the results obtained by these methods are in good agreement with each other. We observe that the three approaches yield the eigenvalues at low values of λ with 14-digit accuracy. For higher values of the perturbation parameter λ the power series method gives greater accuracy than the inner product method and a renormalized series method.

One main difference between the two perturbative techniques lies in the values of the renormalization parameter. For the hypervirial approach the values of β increase as the perturbation parameter increase, while for the inner product method the values of β decrease as the perturbation parameter 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 exploits this symmetry to reduce computation. To get the energy eigenvalues of Killingbeck and Jones (1986) in table 1 it is necessary to multiply 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 this was relatively insensitive to the choice of the state number. We can summarize our results as follows:

(i) We succeeded in finding the energy eigenvalues for eight eigenstates $E_{0,0}$, $E_{1,0}$, $E_{0,1}$, $E_{1,1}$, $E_{0,2}$, $E_{2,0}$, $E_{1,3}$, $E_{3,1}$, with excellent accuracy in two dimensions even for high values of λ $(0.05 \leqslant \lambda \leqslant 5000)$ and for different values of the potential parameters $(a_{12} = 1, -1, 0)$, $(a_{11} = a_{22} = 1, 0)$. The set of tables 1-4 covers a wide range of values of λ.

(ii) 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 and Jones (1986), Ari and Demiralp (1985) and Hioe *et al* (1978).

† Tables 1 and 3-9 of this paper have been deposited in the British Library Supplementary Publications Scheme, document no SUP70044.

Table 2. Energy eigenstates for the potential $V(x, y) = \lambda x^2 y^2$, calculated using the inner product method.

λ	$E_{0,0}$ (even)	J	β	$E_{1,1}$ (even)	J	β
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
50.0	4.4766	24	1.3	19.21721	29	2
100	5.4611	31	1.2	23.86291	27	1.4
1000	11.23	17	0.5	50.39	14	1.1
5000	19.04	12	0.2	85.85	18	0.8
λ	$E_{0,1}$ mixed e-o	J	β	$E_{1,0}$ mixed e-o	J	β
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 2. (continued)

λ	$E_{0,2}$ (even)	J	β	$E_{2,0}$ (odd)	J	β
0.1	6.15928575075223	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	6.557803326	51	3.2
2.0	7.620032	47	2.5	6.9506339	39	5
3.0	8.06620	48	2.4	7.271682	38	4
4.0	8.4360	45	2.2	7.549157	39	3.8
5.0	8.7568	49	2	7.79644	35	3.4
20.0	11.61	15	2	10.1304	39	2.2
50.0	14.59	32	2	12.685	38	2
100	17.72	30	2	15.37	30	2
1000	36.3	17	1.2	31.6	20	1.2
5000	61.4	12	0.5	54.	12	0.6
λ	$E_{1,3}$ (odd)	J	β	$E_{3,1}$ (even)	J	β
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
20.0	23.7604	22	2.2	27.1386	24	2.1
50.0	31.1268	32	2.1	35.657	26	1.6
100	38.582	31	2	44.249	27	1.4
1000	81.29	22	1.2	93.2	19	0.8
5000	138.39	16	0.4	158.8	17	0.4

(iii) We avoid the phenomenon of false convergence by computing the energy eigenvalues for different values of the renormalization parameter β. We believe that some of our results may be improved in accuracy with a better choice of β.

(iv) 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-digit accuracy and the results are presented in table 4. We mention that the results yielded by the inner product were improved by using Aitken extrapolation; it seems that such extrapolation improves the convergence of the perturbation series and gives extra digits of accuracy.

3. Three and N dimensional problems

We used two methods to produce our results for this problem, the renormalized series method and the power series method. We extended our numerical calculations for higher powers of the perturbation index $(2M = 4, 6, 8)$, and for a wide range of values of angular momentum, perturbation parameter and state number. The radial part of the three-dimensional Schrödinger equation can be written conventionally in the form

$$\left[-\frac{d^2}{dr^2} + v(r) \right] \Psi(r) = E\Psi(r) \tag{34}$$

where $v(r)$ is given by equation (2), or insert $N = 3$ in the potential given by equation (3). We can write $v(r)$ in another form by using the renormalization parameter β

$$V(r) = \mu r^2 + l(l+1)r^{-2} + \lambda(r^{2M} - \beta r^2) \qquad (2M = 4, 6, 8) \qquad \mu = 1 + \lambda\beta \tag{35}$$

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

$$E(0) = (2n + 3)\sqrt{\mu} \tag{36}$$

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

$$n = (2n_r + l). \tag{37}$$

Here n_r is called the radial quantum number. The energy values include a zero-point energy of 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 term. We have presented two methods to compute energy eigenvalues. The first approach uses a hypervirial scheme based on the formulation of appropriate recurrence relations, and the second approach uses a power series, based on relations derived by using wavefunctions.

3.1. Renormalized series to calculate energy eigenvalues for
$H = P^2 + r^2 + l(l+1)r^{-2} + \lambda r^{2M}$ (2M = 4, 6, 8)

We used renormalized series to calculate the energy eigenvalues for the potential given by equation (35). Using the hypervirial recurrence relations (26), the Hellmann–Feynman theorem (27) and the perturbation expansions (24) and (25) with the potential terms

$$V_{-2} = l(l+1) \tag{38}$$

$$V_2 = (\mu - \lambda\beta) \tag{39}$$

$$V_{2l} = \lambda \qquad 2l = 4, 6, 8 \tag{40}$$

we obtain the following recurrence relations after some algebra

$$(2J+2) \sum_0^M E(J)A(J, M-J)$$

$$= J[2l(l+1) - \tfrac{1}{2}(J^2-1)]A(J-2, M) + (2J+4)$$

$$\times [\mu A(J+2, M) - \beta A(J+2, M-1)]$$

$$+ [2J+2I+2]A(J+2I, M-1) \tag{41}$$

$$(M+1)E(M+1) = A(2I, M) - \beta A(2, M) \qquad (2I = 4, 6, 8). \tag{42}$$

The recurrence relations (41) and (42) suffice to compute the coefficients of energy $E(M)$ and $A(J, M)$ and this procedure allows us to calculate the expectation values of powers (r^J) without the explicit use of eigenfunctions. The input for our calculations are the renormalized parameter β, the angular momentum l and the state number n. The values of $\mu = 1 + \lambda\beta$, $E(0) = (4n_r + 2l + 3)\sqrt{\mu}$, are worked out by the program. The renormalized series approach seems to give results of excellent accuracy, whereas at $\beta = 0$ the perturbation series diverge and do not give satisfactory numerical results.

3.2. The power series approach

We use 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. The regular solution to equation (34) will behave as r^l near the origin. Inserting the relations (31) and (32) into equation (34) yields the recurrence relation

$$(J+2)[J+2l+3]T(J+2)$$

$$= [(2J+2l+3)\beta - E]r^2 T(J) + [\mu - \beta^2]r^4 T(J-2)$$

$$+ \lambda T(J-2M)r^{2M+2} \qquad (2M = 4, 6, 8). \tag{43}$$

The calculation starts at $J = 0$, with $T(0) = 1$, and all lower coefficients zero.

3.3. N-dimensional calculation by using renormalized series

We used the renormalized series approach to calculate the energy eigenvalues. If we apply the hypervirial recurrence relation given by equation (26), the Hellmann-Feynman theorem (27) and the perturbation series given by equations (24 & 25) to the potential given by equation (3) we get the following recurrence relations:

$$(2I+2) \sum_0^M E(J)A(I, M-J)$$

$$= \frac{I}{2}[(N+2l-3)(2N+2l-1) - (I^2-1)]A(I-2, M) + (2I+4)$$

$$\times [\mu A(I+2, M) - \beta A(I+2, M-1)] + (2I+6)A(I+4, M-1) \tag{44}$$

$$(M+1)E(M+1) = A(4, M) - \beta A(2, M). \tag{45}$$

Here N is number of dimensions. The recurrence relations (41) and (42) for three dimensions reduce to the recurrence relations (44) and (45) if we insert $l = (N + 2l - 3)/2$. It is clear now that from relations (44) and (45) we obtain the full set of A and E coefficients starting from the unperturbed energy

$$E(0) = (4n + 2l + N)\sqrt{\mu} \tag{46}$$

and the initial condition $A(0, 0) = 1$. The convergence properties of the perturbation series are controlled by varying β. We also used the power series method to calculate energy eigenvalues for the N-dimensional problem; by inserting $l = (N + 2l - 3)/2$ in relation (33) we obtain the relation corresponding to N dimensions:

$$(J + 2)[J + N + 2l]T(J + 2)$$
$$= [(2J + N + 2l)\beta - E]r^2 T(J) + [\mu - \beta^2]r^4 T(J - 2) + \lambda r^6 T(J - 4). \tag{47}$$

3.4. Results and discussion

We have used the techniques described in this work, the renormalized series and power series methods, to compute the energy eigenvalues for spherically symmetric states in three and N dimensions. The results are given in tables 5–9. Our energy eigenvalues cover a large range of values of angular momentum, perturbation parameter 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 $l = -1$. At these values the problem reduces to a one-dimensional problem for odd- and even-parity states respectively. 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 5 for different values of angular momentum and state number. We note particularly that in the case of high values of angular momentum the renormalized series approach works well. We notice from table 5 that for ($\lambda = 100$, $l = 100$, $n = 20$) 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 renormalized 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 as 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 renormalized series and power series methods are displayed in table 6 for different values of angular momentum and state number n. These methods lead to very accurate results. We have also calculated the energy eigenvalues for higher power of the perturbation index ($2M = 6, 8$). The renormalized series method was used to compute the energy eigen-values for ($2M = 6$), n, $l = 0, 1, 2, 3, 4$ and $\lambda = 0.1$. This method achieved six-digits accuracy; the renormalized series method has limited capability to deal with high powers (r^{2M}, $2M = 8$) and we could 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 (see Witwit 1989). However, the power series method works excellently and gives results with 16-digits accuracy. We also computed the energy eigenvalues for s-states in ($N = 1, 2, 3, \ldots, 1000$) dimensions for potentials $V(r) = Nr^4$, $N^{-1}r^4$. The renormalized series work very well for calculating the energy eigenvalues even for higher values of M. The energy eigenvalues are

compared with corresponding ones obtained by the power series method and listed in table 8. The agreement of our results with those of Killingbeck (1985) is good.

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