Eigenenergies of the r^2+ lambda $r^2/(1+gr^2)$ and $1/2(r^2)$-or+$gr^4/(1+g$ alpha $r^2)$ potentials obtained by the hypervirial method

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Eigenenergies of the $r^2+\lambda r^2/(1+gr^2)$ and $\frac{1}{2}r^2 \mp gr^4/(1+g\alpha r^2)$ potentials obtained by the hypervirial method

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Abstract. The energy levels of the Schrödinger equation involving the potentials $V(r)=r^2+\lambda r^2/(1+gr^2)$ and $V^{\mp}(r)=\frac{1}{2}r^2 \mp gr^4/(1+g\alpha r^2)$ are calculated by using hypervirial and Padé approximant methods.

1. Introduction

This study has been devoted to computation of eigenvalues in the three-dimensional case by using a perturbative method for the following perturbed Hamiltonians:

$$H=P^2+r^2+l(l+1)r^{-2}+\frac{\lambda r^2}{(1+gr^2)} \tag{1}$$

$$H^{\mp}=\tfrac{1}{2}P^2+\frac{r^2}{2}+\frac{l}{2}(l+1)r^{-2}\mp\frac{gr^4}{(1+g\alpha r^2)}. \tag{2}$$

There are a variety of techniques which have been employed to calculate and to investigate the one-dimensional potential

$$V(x)=x^2+\frac{\lambda x^2}{(1+gx^2)}. \tag{3}$$

The potential given by equation (3) has recently been studied by many authors using different techniques. Mitra (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 (1979) used the finite-difference method to compute the energy eigenvalues for the three lowest even-parity states. Kaushal (1979) 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, which is valid for low values of g ($g\leqslant 2$). Bessis and Bessis (1980) have studied the same problem by taking advantage of a two-parameter (λ and g) scale transformation. Hautot (1981) has used a Hill determinant method to calculate the energy eigenvalues. A set of exact solutions has been found by Flessas (1981) under the conditions $\lambda<0$ and $\lambda=\lambda(g)$. Lai and Lin (1982) have applied the Hellmann–Feynman and hypervirial theorem and used Padé approximants to calculate the energy eigenvalues from the perturbation series. Whitehead *et al* (1982) have proved the existence of a class of exact eigenvalues, when certain algebraic relations between λ and g hold. Fack and Vanden Berghe (1985) used the finite-difference method in combination with

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matrix diagonalization for a numerical computation. Fack *et al* (1986) applied an operator method based upon the SO(1, 2) dynamic group and gave very accurate results for different values of λ and g ($0.1 \leqslant \lambda \leqslant 100$, $0.1 \leqslant g \leqslant 10$) and state number. We wish to draw attention to the fact that the dynamic group technique did not work well at larger values of g. Hodgson (1988) has applied an analytic continuation technique with a Taylor series to produce eigenvalues for wide ranges of perturbation parameters ($0.1 \leqslant g, \lambda \leqslant 10^2$) and state number n, and obtained results with very high accuracy. Witwit (1989) has used many numerical approaches, both perturbative and non-perturbative, for various eigenstates and for different values of λ and g, and obtained results with good accuracy. The interest in this type of potential arises in several areas and these have been summarized by Mitra (1978) and Kaushal (1979). In particular, this type of potential occurs when considering models in laser theory. The potential described by Hamiltonian (2) for the one-dimensional case

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

does not seem to have been widely studied; there are few references in the literature dealing with this type of potential. The potential described by equation (4) has been studied analytically by Auberson (1982), who has shown that the perturbation expansion of eigenvalues E, in terms of g at fixed α, is Borel summable. Also, Auberson and Boissiere (1983) investigated analytically and numerically the same potential: they calculated ground state energy levels for a large range of values of α and g by using many methods such as Padé, Borel–Padé, an improved Borel–Padé and Borel mapping. Flessas (1984) has investigated the same potential, and shown that there exists a class of exact eigenvalues and eigenfunctions when certain algebraic relations between g and α hold ($g > 0$, $\alpha > 0$).

However, as far as we know the other potentials given by equations (1) and (2) have not been studied to the same extent, except the potential given by equation (1) which has been studied by Varshni (1987) by using a $1/N$ expansion technique to calculate the energy eigenvalues for many eigenstates for the parameters ranges $0 \leqslant n_r \leqslant 4$, $0 \leqslant l \leqslant 4$ ($\lambda, g = 0.1$–1000). Also, Roy *et al* (1988) applied the same technique to calculate eigenvalues for various states with different values of perturbation parameters.

In the present work we have applied the Hellmann–Feynman and hypervirial theorems to calculate the perturbation series. The perturbation series does not converge for any arbitrary values of λ and g (our method depends on the ranges of λ and g ($g/\lambda \ll 1$ or $gr^2 \leqslant 1$) if it is used to give results with good accuracy, as we will see later. Due to this setback we used the finite-difference method to calculate the energy eigenvalues for wide ranges of perturbation parameters ($0.1 \leqslant g \leqslant 10^3$, $0.1 \leqslant \lambda \leqslant 10^3$) and higher powers of the indices for perturbation ($\lambda x^{2N}/(1+gx^2)$, $2 \leqslant N \leqslant 20$) (see Witwit 1989). We also used the Padé approximants to the energy series, which was obtained from the Hellmann–Feynman theorem and the hypervirial theorem in order to improve the convergence of the perturbation series.

2. Hypervirial relations for the potentials given by equations (1) and (2)

The Schrödinger equation for the potential $V(r)$ can be written as

$$\left(\frac{d^2}{dr^2} + l(l+1)r^{-2} - V(r) + E\right)\Psi(r) = 0. \tag{5}$$

The perturbation calculation for the potential $V(r)=\lambda r^2/(1+gr^2)$ is made by expanding the factor $1/(1+gr^2)$ as a power series in gr^2 which is valid for $gr^2\leqslant 1$. As r varies ($0\leqslant r\leqslant+\infty$), the function $f(r)=1/(1+gr^2)$ runs from 1 to 0, $f(r)$ being always non-negative. For large values of g, the perturbing potential is almost entirely concentrated near $r=0$. The potentials in equations (1) and (2) can be expressed as expansions:

$$V(r)=r^2+l(l+1)r^{-2}+\lambda\sum_{m=0}^{\infty}V_m g^m r^{2(m+1)} \tag{6}$$

$$V^{\mp}(r)=\frac{r^2}{2}+\frac{l}{2}(l+1)r^{-2}\mp\frac{1}{\alpha}\sum_{m=0}^{\infty}V_m\lambda^{m+1}r^{2(m+2)} \qquad \lambda=\alpha g \tag{7}$$

where

$$V_m=(-1)^m. \tag{8}$$

The coefficient given by equation (8) alternates in sign, the coefficient takes a + sign for even m values, and a − sign for odd m values. We have expanded the potentials given by equations (6) and (7) to the limit beyond which any term makes no difference to our eigenvalues. For our calculations this limit was reached for $m=20$. The series in equations (6) and (7) are valid only for $gr^2\leqslant 1$ and $g\alpha r^2\leqslant 1$, respectively. If we apply the hypervirial relation given by Killingbeck (1985) in the form

$$2E(N+1)\langle r^N\rangle=\sum V_m(2N+m+2)\langle r^{N+m}\rangle-\frac{N}{2}(N^2-1)\langle r^{N-m}\rangle \tag{9}$$

and the Hellmann-Feynman theorem in the form

$$\frac{\partial E}{\partial\lambda}=\left\langle\frac{\partial V}{\partial\lambda}\right\rangle \tag{10}$$

and use the perturbation expansion

$$E=\sum E(I)\lambda^I \tag{11}$$

$$\langle r^N\rangle=\sum A(N,M)\lambda^M \tag{12}$$

to the potentials given by equations (6) and (7), we obtain the following recurrence relations corresponding to potentials (6) and (7), respectively, after some algebra:

$$\begin{aligned}(2N+2)\sum_{0}^{M}E(I)B(N,M-I)&\\ =2N[l(l+1)-\tfrac{1}{2}(N^2-1)]B(N-2,M)+(\lambda+1)(2N+4)B(N+2,M)&\\ +\sum_{m=0}^{\infty}V_m(2N+2m+4)B(N+2m+2,M-m-1)&\end{aligned} \tag{13}$$

$$(M+1)E(M+1)=\sum_{m=0}^{\infty}V_m(m+1)B(2m+2,M-m) \tag{14}$$

$$\begin{aligned}(2N+2)\sum_{0}^{M}E(I)B(N,M-I)&\\ =N[l(l+1)-\tfrac{1}{4}(N^2-1)]B(N-2,M)+(N+2)B(N+2,M)&\\ \mp\frac{1}{\alpha}\sum_{m=0}^{\infty}V_m(2N+2m+6)B(N+2m+4,M-m-1)&\end{aligned} \tag{15}$$

$$(M+1)E(M+1)=\mp\frac{1}{\alpha}\sum_{m=0}^{\infty}V_m(m+1)B(2m+4,M-m). \tag{16}$$

The energy of the nth unperturbed state can be written for the potential given by equation (6) as

$$E(0) = (2n+3)\sqrt{\lambda+1} \tag{17}$$

and for the potential given by equation (7) as

$$E(0) = (2n+3) \tag{18}$$

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

$$n = 2n_r + l \tag{19}$$

where n_r is called the radial quantum number and l the angular momentum, n is seen to be even or odd according to whether l is even or odd. Relations (13)–(16) and $E(0)$ with coefficient $B(0, 0) = 1$ allow us to compute the energies for different values of angular momentum and state number n. The perturbation series converges and gives satisfactory numerical results when certain relations between λ and g hold ($g/\lambda \ll 1$), as we mentioned in the introduction.

3. The Padé approximant calculation of energy eigenvalues

The Padé approximants are a particular type of rational fraction approximation to the value of a function, and the Padé approximation is a useful technique when the convergence of a series is unacceptably slow or even non-existent. The Padé approximant is in the form of one polynomial divided by another. This technique provides us with a practical method of calculating results from the energy series $E(n)$, since its use frequently accelerates convergence. The $E[M, N]$ Padé approximants to the energy series are given by

$$E[N, M] = \frac{a_0 + a_1\lambda + a_2\lambda^2 + a_3\lambda^3 \ldots a_n\lambda^N}{b_0 + b_1\lambda + b_2\lambda^2 + b_3\lambda^3 \ldots b_M\lambda^M} \tag{20}$$

$$\equiv E(0) + E(1)\lambda + E(2)\lambda^2 + \ldots + E(N+M)\lambda^{M+N} \tag{21}$$

with b_0 defined to be unity. The coefficients a_i ($i = 1, \ldots, N$) and b_i ($i = 0, \ldots, M$) in the numerator and denominator are calculated from knowledge of $E(1), E(2), \ldots, E(M+N)$, which can be computed from the hypervirial relations. Our calculated energy values E_n used the $[M, N]$ Padé approximants to the energy series for the ground and the first three excited states. However, the results of the hypervirial method can be much improved by using the Padé approximant method, particularly when $g/\lambda \simeq 1$, in which range the hypervirial method does not give reliable calculation of the energy E_n.

4. Results and discussion

Our aim in this section is to investigate and to discuss the results for the energy eigenvalues of the potentials given by equations (1) and (2). Our aim is also to push the numerical analysis as far as possible, and in this respect we go further than Varshni (1987) and Roy *et al* (1988) in our analysis, by using high values of angular momentum ($l = 1, 2, 3, 5, 10, 20$) and being able to handle higher index powers of perturbation $\mp gr^6/(1+g\alpha r^2)$.

The present work is intended to point out one feature which has not been noted in previous problems, as discussed by Witwit (1989). The hypervirial method can produce good accuracy even without use of the renormalization parameter K, which usually plays an important role in obtaining convergent perturbation series. We have computed the first four energy eigenvalues by using the hypervirial method for the potential given by equation (1), with parameter values $0.1 \leqslant g \leqslant 0.5$, $200 \leqslant \lambda \leqslant 10^4$ and angular momentum $l = 5$, 10, 20; the results are listed in table 1. The results are in good agreement with those calculated by Witwit (1989) by using the power series method. This agreement provides a check on the accuracy of our results. Also, we checked the energies for the special case $g = 0$; therefore, the potentials given by equations (1) and (2) take the forms $r^2 + l(l+1)r^{-2} + \lambda r^2$, $r^2 + (l/2)(l+1)r^{-2} \mp gr^4$, respectively, which are regarded as ordinary anharmonic oscillators in three dimensions. The test energies were obtained very easily from power series or renormalized series methods described by Witwit (1989).

We also list in table 2† the first four energy eigenvalues for the potential given by equation (1) obtained using the Padé approximant $E[6, 6]$ for the values $0.1 \leqslant g \leqslant 5$, $0.1 \leqslant \lambda \leqslant 1000$ and $l = 1$–3. We can say that the accuracy of our results listed in table 2 is very good in comparison with the results of Varshni (1987) and Roy *et al* (1988), which are the only ones available in the literature to the best of our knowledge. To compare the energy eigenvalues of our calculations with the results of Varshni's work, it is necessary to multiply his results by 2, since he used $-\frac{1}{2}\nabla^2$ in the Hamiltonian. We wish to draw attention to the fact that the present Padé approximant approach works very well even for higher values of g ($0.1 \leqslant g \leqslant 5$) and λ ($0.1 \leqslant \lambda \leqslant 10^3$), whereas the Padé approximant method of Lai and Lin (1982) is restricted to low values of g ($g \leqslant 2$). For the validity of our results it is essential that the relation between g and λ holds ($g/\lambda \ll 1$), due to the condition imposed on the expansion of the potentials (6) and (7).

In table 3 we present the first nine energy levels for potential (1) for different values of λ and g ($\lambda = 0.1$–1000, $g = 0.1$–1); our results have been compared with the previous results of Varshni (1987) and the agreement between the results is very good. For large g and small λ it is found that the hypervirial method underestimates the eigenenergies because it violates the condition $g/\lambda \ll 1$, which imposes on the expansion given by potential (6). Therefore, we restricted our calculation to a rather small range of g and a large range of λ.

Also, we have calculated the first five energy eigenvalues for the potential given by equation (2) by using the hypervirial method for different sets of $10^{-3} \leqslant g \leqslant 5 \times 10^{-3}$, $0.25 \leqslant \alpha \leqslant 10$ and $1 \leqslant l \leqslant 10$. The results are given in tables 4 and 5. However, the hypervirial method works very well and gives results of good accuracy. We have performed various numerical checks on the obtained energy eigenvalues for potential (2), e.g. for these values at $l = -1$ and $l = 0$ the problem reduces to a one-dimensional problem and our results agree with those obtained by Auberson and Boissiere (1983) in the one-dimensional case. In this paper, we would like to point out that there exists another set of exact solutions to the Schrödinger equation from potential (4), which has been obtained by Flessas (1984):

$$E = 5\alpha^{-1}\sqrt{\alpha^2\omega^2 + \alpha} - g^{-1}\alpha^{-2} \tag{22}$$

† Tables 2–6 of this paper have been deposited in the British Library Supplementary Publications Scheme, document SUP70045

Table 1. Eigenvalues of $H = P^2 + r^2 + l(l+1)r^{-2} + \lambda r^2/(1+gr^2)$ for the first four energy levels obtained using the hypervirial method.

g=0.1, λ=500, ℓ=5	N	g=0.1, λ=1000, ℓ=10	N
286.130764905274	9	406.4431319290257	9
371.220429074117	9	528.5360761160119	9
455.147483320689	11	649.4547569735891	8
537.920332236231	11	769.2050328634557	8
g=0.1, λ=500, ℓ=20	N	g=0.1, λ=1000, ℓ=20	N
914.36631099435	15	1312.251674809389	13
990.80662152100	15	1425.586001638665	12
1066.14830339382	14	1537.790459039524	13
1140.40019428154	15	1648.871122885173	13
g=0.1, λ=200, ℓ=5	N	g=0.1, λ=200, ℓ=10	N
179.483113218955	10	311.8608808927604	14
231.793477703205	12	361.3087886245920	14
282.966326293934	12	409.6535649976535	15
333.015394380859	12	456.9093231268753	15
g=0.5, λ=10^4, ℓ=5	N	g=0.5, λ=10^4, ℓ=10	N
1275.78396774570	9	2228.518434524944	11
1653.57546408975	9	2591.730583013077	11
2025.56190179117	9	2949.254575011444	11
2391.79003752214	10	3301.138048089259	11
g=0.4, λ=10^4, ℓ=5	N	g=0.4, λ=10^4, ℓ=10	N
1280.62552249442	9	2242.794175885625	10
1662.81939206438	9	2613.256672479269	10
2040.33773798231	10	2979.117911998585	11
2413.21026716282	11	3340.408059097673	11
g=0.2, λ=10^3, ℓ=5	N	g=0.2, λ=10^3, ℓ=10	N
401.608033488556	10	699.105622574512	13
519.308447108056	10	811.026062535263	13
634.710381177172	12	920.708010354177	13
747.837820161021	12	1028.176013499331	14

where

$$g=(2\alpha^3)^{-1}[4\alpha\omega+5-2(2(2\alpha\omega^2+3)(\alpha\omega^2+1))^{1/2}]. \tag{23}$$

Equation (23) yields real and positive α-values if g is fixed and solved for α; at $\omega=1$, $g=0.5$, the real α-value lies between the limits $4\leqslant\alpha\leqslant5$. It is interesting to compare our results with the exact one given by equation (22). At $\omega=1$, $g=0.5$ and $\alpha=4$. Equation (22) gives $E^-=5.465\,169\,9$; our method for $g=2$, $\alpha=10$, $\omega=1$, $n=2$ yielded $E^+=5.464\,870\,4$. As can be seen, both values are approximately the same.

If we take $g\alpha$ as the perturbation parameter instead of g, it does not make any difference to the accuracy of our calculations. 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 l

The Padé approximant method $[M, N]$ has been applied to eigenvalues for the case V^+ to different sets of parameters ($0.01\leqslant g\leqslant0.2$, $2\leqslant\alpha\leqslant50$, $1\leqslant l\leqslant4$), and results for the ground state are given in table 6. The accuracy decreases as g and α increase, as is clear from our results in tables 4–6 The present calculations in table 6 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.

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