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Finite difference calculations of eigenvalues for various potentials

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Abstract. The energy levels of the Schrödinger equation for the potentials $V(x) = \sum_{2N=2}^{20} \lambda_{2N} x^{2N}$, $V(x) = -Z^2 x^2 + x^{2N}$ and $V(x) = x^2 + \lambda x^{2N}/(1+gx^2)$, with $2N = 4, 6, 8, \dots, 18, 20$, have been calculated by using a finite difference method for various values of λ and the quantum number n . The obtained results are compared with previously available results.

1. Introduction

The aim of this paper is to calculate the eigenvalues for various forms of potential in one dimension by using finite difference methods. The potentials considered are

$$V(x) = \sum_{2N=2}^{20} \lambda_{2N} x^{2N} \quad 2N = 4, 6, 8, 10, \dots, 18, 20 \quad (1)$$

$$V(x) = -Z^2 x^2 + x^{2N} \quad 2N = 4, 6, 8, 10, 12 \quad (2)$$

$$V(x) = x^2 + \lambda x^{2N}/(1+gx^2) \quad 2N = 4, 6, 8, 10, \dots, 18, 20. \quad (3)$$

The study of the quantum mechanics of the anharmonic oscillator is of considerable interest from both physical and mathematical points of view, and a variety of techniques have been employed to calculate energy eigenvalues. The one-dimensional anharmonic oscillator with the potential given by equation (1) 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 (1969) calculated 75 terms of the ground state energy series. Simon (1970) studied the analytic properties of the series and its Padé approximants. Banerjee (1978) calculated energy levels for $2N=4, 6, 8$ and $10^{-5} \leq \lambda \leq 4 \times 10^4$, for various state numbers n . Schiffrer and Stanzial (1985) have reported accurate energy calculations for the ground state and first excited state for $2N=6, 8, 10, 12$ and $10^{-6} \leq \lambda \leq 10^6$ by using a gradient method. Killingbeck (1979, 1987a, b, 1988) presented several perturbative and non-perturbative numerical methods which gave results of good accuracy. Witwit (1989) applied renormalized series and power series methods for different values of λ , $2N$, n and obtained results of high accuracy.

The anharmonic oscillator (1) of the type $V(x) = \sum_{2N=2}^6 \lambda_{2N} x^{2N}$ can serve as a useful model in certain situations of physical interest. It has been used in calculations of the vibrational spectra of molecules (Lister *et al* 1978) and in a description of the behaviour of a ^3He - ^4He mixture and of metamagnets near the tricritical point (Carvalho 1977). Flessas (1979) and Flessas and Das (1980) have presented some exact solutions, valid for particular λ_n values, including positive and negative values of λ_4 . Chaudhuri and Mukherjee (1984) have found a class of exact even and odd parity solutions to

the Schrödinger equation for the same potential when $\lambda_2, \lambda_4, \lambda_6$ satisfy some specific relations. In the present work we tackle the problem in its full complexity, calculating the eigenvalues for different values of λ_{2N} , $2N = 2, 4, 6, 8, 10$ with high accuracy.

The solution of the Schrödinger equation for the asymmetric double-minimum potential given by equation (2) would be interesting and has not yet received much attention. The most studied system of this kind is the quartic double-well potential ($2N = 4$). For instance, Balsa *et al* (1983) used a matrix diagonalization method with an appropriate scaled harmonic basis to compute the energy eigenvalues for $2N = 4$, $0 \leq Z^2 \leq 100$ and $0 \leq n \leq 21$. Quick and Miller (1984) treated the case $2N = 4$, $Z^2 = 50$ and $0 \leq n \leq 79$, also using matrix diagonalization to calculate some energy levels. Fernandez *et al* (1985) applied a simple iterative solution of the Schrödinger equation for a double-well potential and produced results with very good accuracy for two state numbers ($n = 0, 1$) and different values of Z ($0 \leq Z^2 \leq 10$). Killingbeck (1988) used finite difference calculations involving the expectation values of Boolean functions, which are shown to yield detailed information about the properties of the energy levels and eigenfunctions for the double-well potential. Witwit (1989) used perturbative and non-perturbative methods to calculate the energy levels for wide ranges of parameters Z^2 , $2N$ and state number n .

There are a variety of techniques which have been employed to calculate and to investigate the eigenvalue problems for potential (3). Most of the calculations have been devoted to the potential given by equation (3) for $2N = 2$. However, as far as we know the other power indices ($2N = 4, 6, 8, \dots, 18, 20$) have not been widely studied. We have been unable to find a reference in the literature dealing with the other types of potentials.

The potential given by equation (3) for $2N = 2$ has recently been studied by many authors using different techniques. Mitra (1978) calculated the ground state and first two excited states using the Rayleigh-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. Fack and Vanden Berghe (1985, 1986) and Fack *et al* (1987) used the finite difference method in combination with matrix diagonalization for a numerical computation. Fack *et al* (1986) applied an operator method based upon the $SO(1, 2)$ dynamical group and gave very accurate results for different values of λ, g and the state number. Hodgson (1988) applied an analytic continuation technique with a Taylor series to produce eigenvalues for wide ranges of perturbation parameters ($0.1 \leq g, \lambda \leq 10^2$) and state number n , obtaining results of high accuracy. A set of exact solutions has been found by Flessas (1981) under the conditions $\lambda < 0$ and $\lambda = \lambda(g)$. Whitehead *et al* (1982) have proved the existence of a class of exact eigenvalues, when certain algebraic relations between λ and g hold. Gallas (1988) has shown an exact analytical eigenfunction for the potential when the relationship $\lambda = -(6g^2 + 4g)$ holds. The interest in this type of potential arises in several areas and these have been summarized by Mitra (1978). In particular, this type of potential occurs when considering models in laser theory.

2. Formulation of the finite difference method

Recent times have seen the development of various non-perturbative methods of computing energy eigenvalues. Such methods are necessary since the perturbative

methods provide insufficient information about accuracy and give convergence difficulties. Witwit (1989) has applied non-perturbative methods such as finite difference and power series methods to various eigenvalue calculations, using cross-checking of the results from various methods to establish confidence in the accuracy of the methods. The theory of the finite difference approach to find eigenvalues for the Schrödinger equation

$$\left(-\frac{d^2}{dx^2} + V(x) - E\right)\Psi(x) = 0 \tag{4}$$

with potentials given by equations (1)-(3) usually starts from the central difference operator, which can be expressed as

$$\begin{aligned} \delta &= e^{hD/2} - e^{-hD/2} \\ &= 2 \sinh(hD/2) \end{aligned} \tag{5}$$

where

$$D = \frac{d}{dx} \tag{6}$$

and h is the strip width for the numerical integration. From expression (5) it is easy to derive the relation which is used by Fack and Vanden Berghe (1985) to calculate their results. From equation (5) we obtain the following relation after squaring both sides of the expression:

$$D^2 = \frac{4}{h^2} \sinh^{-2}\left(\frac{\delta}{2}\right). \tag{7}$$

From equation (7) it is easy to obtain the result

$$h^2 D^2 = \delta^2 - \frac{\delta^4}{12} + \frac{\delta^6}{90} - \frac{\delta^8}{2560}. \tag{8}$$

The operator expansion given by equation (8) is the one applied by Fack and Venden Berghe (1985) to derive the formulae used in their approach. If we square both sides of equation (5) and multiply by the wavefunction $\psi(x)$, then equation (5) takes the form

$$\delta^2 \psi(x) = 4 \sinh^2(hD/2) \psi(x) = 2[\cosh(hD) - 1] \psi(x). \tag{9}$$

If we expand the $\cosh(hD)$ function, equation (9) takes the form

$$\delta^2 \psi(x) = h^2 D^2 \Psi(x) + \frac{1}{12} h^4 D^4 \Psi(x) + \frac{1}{360} h^6 D^6 (\Psi(x)) \dots \tag{10}$$

In order to use the Schrödinger equation (4) in equation (10), we divide equation (10) by h^2 , so that equation (10) becomes

$$h^{-2} \delta^2 \psi(x) = D^2 \Psi(x) + \frac{1}{12} h^2 D^4 \Psi(x) + \frac{1}{360} h^4 D^6 \Psi(x) \dots \tag{11}$$

Replacing D^2 by $V(x) - E$ in equation (11) gives

$$h^{-2} \delta^2 \psi(x) = (V(x) - E) \Psi(x) + \frac{1}{12} h^2 D^4 \Psi(x) + \frac{1}{360} h^4 D^6 \Psi(x) \dots \tag{12}$$

If we expand the wavefunctions $\Psi(x + h)$ and $\Psi(x - h)$ by using Taylor series we obtain

$$\begin{aligned} \psi(x + h) &= \Psi(x) + hD\Psi(x) + \frac{1}{2}h^2 D^2\Psi(x) + \frac{1}{6}h^3 D^3\Psi(x) + \frac{1}{24}h^4 D^4\Psi(x) \\ &\quad + \frac{1}{120}h^5 D^5\Psi(x) + \frac{1}{720}h^6 D^6\Psi(x) \end{aligned} \tag{13}$$

$$\psi(x-h) = \Psi(x) - hD\Psi(x) + \frac{1}{2}h^2D^2\Psi(x) - \frac{1}{6}h^3D^3\Psi(x) + \frac{1}{24}h^4D^4\Psi(x) - \frac{1}{120}h^5D^5\Psi(x) + \frac{1}{720}h^6D^6\Psi(x). \quad (14)$$

Adding equations (13) and (14) and using equation (10) we obtain

$$\begin{aligned} \delta^2\Psi(x) &= \Psi(x+h) + \Psi(x-h) - 2\Psi(x) \\ &= h^2D^2\Psi(x) + \frac{1}{12}h^4D^4\Psi(x) + \frac{1}{360}h^6D^6\Psi(x) + \dots \end{aligned} \quad (15)$$

Equation (12) differs from the Schrödinger equation in the form $D^2\Psi(x) = (V(x) - E)\Psi(x)$ by having perturbing terms $V_1 = \frac{1}{12}h^2D^4\Psi(x)$ and $V_2 = \frac{1}{360}h^4D^6\Psi(x)$. The first term produces an energy shift and this shift would be the expectation value

$$\Delta E_1 = \int_{-\infty}^{+\infty} \Psi(x) V_1 \Psi(x) dx = \frac{1}{12}h^2 \int_{-\infty}^{+\infty} \Psi(x) D^4\Psi(x) dx. \quad (16)$$

The integral can easily be evaluated by parts to yield

$$\frac{1}{12}h^2\langle (E - V)^2 \rangle = \frac{1}{12}h^2\langle V(x) - E \rangle^2 \quad (17)$$

which means that the local operator $(V(x) - E)^2$ gives the same effect on the energy as the operator D^4 . The calculation of the effect of $V_2 = \frac{1}{360}h^4D^6\Psi(x)$ is more difficult than the perturbation V_1 term

$$\Delta E_2 = \frac{1}{360}h^4 \int_{-\infty}^{+\infty} \Psi(x) D^6\Psi(x) dx. \quad (18)$$

However, for Dirichlet boundary conditions and non-singular potential the term ΔE_2 can be expressed as

$$\Delta E_2 = V_2 = \frac{1}{360}h^4(V(x) - E)^3 + \frac{1}{240}h^4(DV(x))^2. \quad (19)$$

Our results show that the term involving h^4D^6 is not easy. However, for our calculations we used a very small value of h ($h = 10^{-4}$) for which the higher terms $h^{2N}D^{2(N+1)}$ ($N = 2, 4, \dots$) in the expansion do not make any appreciable difference to the accuracy.

If we use the quantity $S(x)$ which is defined as

$$\Psi(x+h) = (1 + h^2S(x))\Psi(x) \quad (20)$$

in equation (15) and combine equations (9) and (15), the following equation is obtained:

$$S(x) = \frac{S(x-h)}{1 + h^2S(x-h)} + \frac{2}{h^2}[\cosh(h|D|) - 1] \quad (21)$$

where $D = \sqrt{V(x) - E}$. If $D < 0$, equation (21) takes the form

$$S(x) = \frac{S(x-h)}{1 + h^2S(x-h)} + \frac{2}{h^2}[\cos(h|D|) - 1]. \quad (22)$$

For even states we have

$$\Psi(-h) = \Psi(h) \quad (23)$$

which leads to the starting conditions

$$S(0) = \frac{1}{2}(V(0) - E). \quad (24)$$

To apply equations (21) and (22) we need some initial value for $S(x)$ and can then calculate successive $S(x)$ values along the x -axis, with some test energy E . The

wavefunction $\Psi(x)$ is calculated using equation (21) or equation (22) for two trial energies E_a and E_b . We suppose that $E_b > E_a$, so that (Ψ_b) has its nodes earlier than Ψ_a . Then the calculation of the projected energy is given as

$$E_p = E_b + \frac{E_b - E_a}{1 - \Psi_b/\Psi_a} \quad (25)$$

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 $E_b - E_a$ 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 h by a formula of the type

$$E(h) = E_0 + h^2 E_2 + h^4 E_4 + \dots \quad (26)$$

The results for E as obtained using three values ($h, 2h, 4h$) can be treated by the Richardson extrapolation process, giving the results

$$E_0 = \frac{1}{45}(64E(h) - 20E(2h) + E(4h)). \quad (27)$$

Here $E(h)$ is the energy calculated using strip width h and E_0 is the exact energy (for $h \rightarrow 0$). In the present eigenvalue calculated using strip width h and E_0 is the exact energy (for $h \rightarrow 0$). In the present eigenvalue calculations, we used the above relations. The error of the method used here should be smaller when a smaller h (step length) is used. 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 $x = kh$ ($k = 0, 1, 2, \dots, n; nh = R$).

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

In the present paper we have found a further application for the energy eigenvalues by calculating the expectation values without using wavefunctions. To find expectation values of the type $\langle x^{2N} \rangle$ for potential (1) for the case $2N = 4$,

$$V(x) = x^2 + \lambda x^4 \quad (28)$$

we need to have the eigenfunction $\Psi(x)$ for all x if we wish to apply the definition

$$\langle x^{2N} \rangle = \int \Psi^2(x) x^{2N} dx \quad (29)$$

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

$$\langle x^{2N} \rangle = \lim_{\epsilon \rightarrow 0} \frac{1}{2\epsilon} (E(H + \epsilon x^{2N}) - E(H - \epsilon x^{2N})). \quad (30)$$

This algorithm demonstrates 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 $\mp \epsilon x^{2N}$ included in the potential:

$$E_+ = x^2 + \lambda x^4 + \epsilon x^{2N} \quad (31)$$

$$E_- = x^2 + \lambda x^4 - \epsilon x^{2N} \quad (32)$$

where ϵ is a very small number, typically $10^{-8} \leq \epsilon \leq 10^{-3}$. The value of $\langle x^{2N} \rangle$ is then given by

$$\langle x^{2N} \rangle = \frac{1}{2\epsilon} (E_+ - E_-). \quad (33)$$

We have performed various numerical checks on the obtained energy and the expectation values; for example, hypervirial theory gives the $\langle x^{2N} \rangle$ directly.

4. Results and discussion

In the present work we have studied the one-dimensional potentials (1)–(3) over wide ranges of parameters (g, λ, Z^2), various state numbers and high indices ($2N = 2, 4, \dots, 20$) of the perturbation, demonstrating that accurate energies and also expectation values such as $\langle x^{2N} \rangle$ can be calculated without storing explicit values of the wavefunction Ψ .

The energy eigenvalues of the generalized anharmonic oscillator defined by potential (1) have been calculated for various values of λ . Table 1† gives the values of the ground energies of the anharmonic oscillator ($2N = 6, 8, \dots, 20$) for wide ranges of λ ($0.1 \leq \lambda \leq 50\,000$) and for $\mu = 1, 0$. We have computed 10 eigenvalues in this range. The results obtained by the present method are compared with those reported by Banerjee (1978) and Schiffrer and Stanzial (1985), the agreement between them and our results being very good. Also, we did some checks for our results by applying the power series method for $2N = 6, \dots, 18, 20$, yielding eigenvalues agreeing to 16 digits. As can be seen from these calculations, the accuracy of our results is around 16 significant digits. The energies quoted in table 1 agree nearly to all the number of digits given with those obtained by Banerjee (1978) and Schiffrer and Stanzial (1985).

From the listed numerical results in table 1, we can study the crossing of the levels $E_{n=0}^{2N}(\lambda)$ as a function of λ . The crossing points between the levels $E_{n=0}^{2N}(\lambda)$ were located by finding these eigenvalues for various λ . From our results we observed the order of levels,

$$E^4(\lambda) < E^6(\lambda) < E^8(\lambda) < E^{10}(\lambda) < E^{12}(\lambda) < E^{14}(\lambda) < E^{16}(\lambda) < E^{18}(\lambda) < E^{20}(\lambda)$$

for small values of λ ($\lambda = 0.1, 1, \dots, 5$), but for large values of λ ($\lambda = 10, 50, \dots, 50\,000$) we observed the reversed order

$$E^4(\lambda) > E^6(\lambda) > E^8(\lambda) > E^{10}(\lambda) > E^{12}(\lambda) > E^{14}(\lambda) > E^{16}(\lambda) > E^{18}(\lambda) > E^{20}(\lambda).$$

The crossings between energy levels were discussed and analysed analytically by Bender (1969) and Simon (1970). Also, Banerjee (1978) has studied the energy level crossings with extensive numerical calculations. It seems from our eigenvalue results for $E^{2N}(\lambda)$

† Tables 2-9 of this paper have been deposited in the British Library Supplementary Publications Scheme, document SUP70046.

λ	2N=6		2N=8	
	$\mu=1$	$\mu=0$	$\mu=1$	$\mu=0$
0.1	1.109087078465584 <u>1.10908707846558</u>	0.643769728949398	1.168970453245986 <u>1.16897045324599</u>	0.773440203813966
1	1.435624619003392 <u>1.43562461900339</u>	1.144802453797053	1.49101989566221 <u>1.491019895662205</u>	1.225820113800492
5	1.912453832222856	1.711878954024485	1.887487143032062	<u>1.691300370626301</u>
10	2.205723269595632 <u>2.20572326959563</u>	2.035778632149334	2.114544621942129 <u>2.11454462194213</u>	1.942793953544308
50	3.159021201059654	3.044199096420710	2.806065089316286	2.680530443812583
100	3.716974729208620 <u>3.71697472920862</u>	3.620183224948363	3.188654346492268 <u>3.188654346492268</u>	3.079120911326986
500	5.478379090462791	5.413436573224043	4.328012380250563	4.248354452583329
10 ³	6.492350132329672 <u>6.49235013232967</u>	6.437697289493980	4.949487440032743 <u>4.94948744003274</u>	4.880077771126800
10 ⁴	11.47879804226454 <u>11.4787980422645</u>	11.44802453797053	7.778272214311099 <u>7.77827221431110</u>	7.734402038139668
5×10 ⁴	17.13937586886189	17.11878954024485	10.70319738012488	10.67138390568737
λ	2N=10		2N=12	
	$\mu=1$	$\mu=0$	$\mu=1$	$\mu=0$
0.1	1.233888970608270	0.884891912218169	1.297825599507269	0.981479602247295
1	1.546263512572346 <u>1.546263512572346</u>	1.298843700678521	1.597990499275997 <u>1.597990499275997</u>	1.363761485141757
5	1.890504964852582	1.698446584882680	1.904581416085660	1.716292397976640
10	2.078302786974826	1.906441832611472	2.066095016976872	1.894940439004090
50	2.625342516665687	2.492978653386003	2.521614348137108	2.384780554015410
100	2.916442269358709	2.798273925671195	2.757179800598476	2.633011202101639
500	3.749860472753474	3.659192241637428	3.412622122439136	3.313641834873087
10 ³	4.188159234093666	4.107304418706113	3.748294589104394	3.658557201954226
10 ⁴	6.083894977292836 <u>6.083894977292836</u>	6.028698417677723	5.148272347405043 <u>5.148272347405043</u>	5.083548748021790
5×10 ⁴	7.925731446518450	7.883490702879206	6.449114472836206	6.397640764921995
λ	2N=14		2N=16	
	$\mu=1$	$\mu=0$	$\mu=1$	$\mu=0$
0.1	1.358260097208969	1.065928788394754	1.414362993380629	1.140391627412878
1	1.645427301667530	1.421438884484289	1.688644355400802	1.472872424370881
5	1.923094061080720	1.738198785933759	1.943134116363347	1.761280249421046
10	2.065584866993021	1.895519216970127	2.071102069825460	1.902287886305871
50	2.457745391569692	2.317925334402937	2.416622648346604	2.274780916137083
100	2.656152748781866	2.527715500907106	2.588434696119420	2.456899282320219
500	3.196353882040352	3.091003111580656	3.048304497176280	2.937992530219101
10 ³	3.467464357512808	3.370762794871078	3.275439884385238	3.173207445055988
10 ⁴	4.567664896385973	4.494984429699328	4.177691914410590	4.098355012684797
5×10 ⁴	5.556160251167479	5.496667189690124	4.967281266904783	4.900866917948242
λ	2N=18		2N=20	
	$\mu=1$	$\mu=0$	$\mu=1$	$\mu=0$
0.1	1.466051107940292	1.206561190366403	1.513551983259983	1.265776428650721
1	1.727982665235992	1.518970543436885	1.763848060090803	1.560508342924665
5	1.963339575048171	1.784211574313667	1.983057870600219	1.806378778736560
10	2.079784762725154	1.912270616899490	2.090092595021987	1.923867622446815
50	2.389407087844083	2.246189290920753	2.371139171663949	2.226988187562709
100	2.541227162797541	2.407406073842077	2.507363140468163	2.371833925451716
500	2.942019458371235	2.827784778040057	2.862914498435694	2.745535125812682
10 ³	3.137427615949501	3.030744682867415	3.034416484690723	2.924107721491224
10 ⁴	3.900417102469582	3.815481497921844	3.694653961275296	3.604976670217825
5×10 ⁴	4.554124076231136	4.481736844460848	4.250526051587301	4.172969266359273

Table 1. The eigenvalues of the ground state for $H = P^2 + \mu x^2 + \lambda x^{2N}$; the results without an underline are the present calculations, and those with continuous lines and cut lines correspond to [3] and [24] respectively. The empty spaces mean the corresponding results are not reported.

that the crossing occurs approximately at the same value ($\lambda \approx 5$) for various indices $2N$. It is noteworthy that the wkb formula, which can be expressed as

$$E_n^{2N}(\lambda) = A(N)(\lambda)^{1/(N+1)}(n + \frac{1}{2})^{2N/(N+1)} \quad (34)$$

with

$$A(N) = \left(\frac{\pi N \Gamma(\frac{3}{2} + 1/2N)}{\Gamma(\frac{3}{2})\Gamma(1/2N)} \right)^{2N/(N+1)} \quad (35)$$

implies such crossings, and predicts the correct order of levels in the large- λ limit. For two anharmonic oscillator specified by N_1 and N_2 ($N_1 < N_2$) the wkb condition for crossing of $E_n^{2N_1}(\lambda)$ and $E_n^{2N_2}(\lambda)$ is

$$A(N_1)(\lambda_{\text{cross}})^{1/(N_1+1)}(n + \frac{1}{2})^{2N_1/(N_1+1)} = A(N_2)(\lambda_{\text{cross}})^{1/(N_2+1)}(n + \frac{1}{2})^{2N_2/(N_2+1)}. \quad (36)$$

We wish to stress that the finite difference method works very well for any value of the index ($2N = 4, 6, \dots, 20$), and has obvious advantages over the perturbative renormalized series method (Witwit 1989), which can only handle the values $2N = 4, 6, 8$. For $2N > 12$ we have not found numerical results in the literature. Our 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 $2N \rightarrow \infty$ the potential becomes a square-well potential and our methods should allow this limit to be studied.

In the present work we applied the finite difference method to calculate the energy eigenvalues for polynomial perturbations as given by equation (1) for $0 \leq \lambda_{2N} \leq 10^6$, $2N = 2, 4, 6, 8, 10$, and different state numbers n . The results listed in tables 2-4 show that the finite difference method works extremely well for potential (1) with polynomial perturbation. Our results appear to show that the perturbation term $\lambda_4 x^4$ is the more effective one to contribute to the value of the perturbed energy, with contributions of the other terms of the perturbation being smaller. We checked our listed results by applying the power series and renormalized series methods; the results produced by these methods agree quite well with those given by the finite difference method and this agreement confirms that our results are accurate in the absence of other reported results in the literature.

The energies E_- , E_+ and the expectation values for $\langle x^{2N} \rangle$ ($2N = 2, 4$) for state number $0 \leq n \leq 10$ and for $\lambda = 0.1, 1, 10, 100$ with the value $\varepsilon = 10^{-3}$ have been calculated by using the finite difference method and the results are listed in table 5. This value of ε seems appropriate to give 10-digit accuracy. We checked some of our results which are given in table 5 by using the power series and the renormalized series methods, which give the same accuracy as that achieved by the finite difference method.

We calculated the energy levels of a double-well potential given by equation (2) for various values of Z^2 , $2N$, n . We compared our results with those produced by Balsa *et al* (1983) and Fernandez *et al* (1985); the agreement between the results is very good. It is clear from table 6 that there is agreement between our results and the results of Fernandez *et al* (1985) to about 16 digits and the results of Balsa *et al* (1983) to about 12 digits. Also, we have calculated the energy levels of potential (2) for various values of parameters ($2N = 4$; $Z^2 = 100, 200$; $0 \leq 10 \leq 100$), and the results are listed in table 6. We have observed good agreement between these results and results yielded by the renormalized perturbation series (Witwit 1989). In the present work we have not only considered $2N = 4$, but have extended the work to higher powers ($2N = 6, 8, 10, 12$). We list in table 7 the results for the ground state for $10 \leq Z^2 \leq 5000$. It is clear from the listed results that the finite difference method achieves very high accuracy.

For potential (3) we have computed the first four even energy eigenvalues for the index $2N = 2, 4, \dots, 20$, with perturbation parameter values $0.1 \leq \lambda \leq 1000$ and $0.1 \leq g \leq 1000$. The accuracy of our results in general is more than 12 significant digits, as shown in table 8.

However, it is obvious that for certain limiting parameter values (e.g. $g = 0$) the differential equations corresponding to potential (3) reduce to the differential equations of the harmonic oscillator for potential (1). On the other hand, the two potentials (1) and (3), with their perturbation terms λx^{2N} , $\lambda x^{2N}/(1+gx^2)$, respectively, differ only by the denominator $1+gx^2$, so that we expect that the value of the perturbed energy corresponding to potential (1) is higher than that for potential (3), and this is confirmed by our listed results in tables 1 and 8. In table 9, comparing the sample from our results for $V(x) = x^2 + \lambda x^{2N}/(1+gx^2)$ for the case $2N = 2$ and for state numbers $n = 0, 2, 4$ with those given by Hodgson (1988) and Fack *et al* (1986), we can say that the accuracy of our listed results is very good in comparison with their results. For higher values ($2N = 4, 6, 8, \dots, 18, 20$) we are unable to find any results in the literature.

If we study the energy level crossings for the type of perturbations given by potential (3), the picture is more complicated than that for potential (1) because there are two perturbation parameters (g, λ). Many energy levels have been calculated ($n = 0, 2, 4, 6$). Briefly, we have seen from our results that some energy eigenvalues for various values of g and λ decrease or increase with increasing index ($2N = 2, 4, \dots, 20$). For example, at $g = \lambda = 0.1$ the energy eigenvalues increase as $2N$ increases, as is clear from our listed results in table 8. The ordering of the eigenvalues can be expressed as below:

$$E_n^2(\lambda) < E_n^4(\lambda) < E_n^6(\lambda) < E_n^8(\lambda) < E_n^{10}(\lambda) < E_n^{12}(\lambda) < E_n^{14}(\lambda) < E_n^{16}(\lambda) < E_n^{20}(\lambda)$$

where $n = 0, 2, 4, 6$ and $g = \lambda = 0.1$. With another set of values of the perturbation parameters g and λ the order of levels have a different behaviour, as indicated by the listed results in table 8.

The numerical results obtained show that the finite difference method produces accurate energy values and expectation values when used in the shooting mode, and represents an effective alternative to the standard matrix diagonalization methods.

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