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A finite difference approach for the calculation of perturbed oscillator energies

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Abstract. A simple numerical method for calculating eigenvalues and corresponding eigenvectors of the Schrödinger equation for a perturbed oscillator is described. The derived results are compared with previously derived numerical data and with available exact values.

1. Introduction

Recently there has been a great deal of interest in the analytical as well as the numerical study of the one-dimensional anharmonic oscillator governed by the potential

$$V(x) = x^2 + \lambda x^2/(1+gx^2). \tag{1.1}$$

The solutions of the one-dimensional Schrödinger equation with a potential (1.1) are important in several areas of physics. As summarised by Mitra (1978), the potential (1.1) is related to certain specific models in laser theory (Haken 1970) and also to a zero-dimension field theory with a nonlinear Lagrangian (Risken and Vollmer 1967).

Several lines of approach have been followed in the investigation of the eigenvalues and eigenfunctions of the differential equation

$$[D^2 + (E - V(x))]y(x) \equiv \mathrm{d}^2y(x)/\mathrm{d}x^2 + (E - V(x))y(x) = 0, \tag{1.2}$$

where E denotes the eigenvalue parameter. The ground state and the first two energy levels were first computed by Mitra (1978) for a large range of λ and g ($\lambda, g = 0$ to 100) within the variational Rayleigh-Ritz framework. However, for large values of g some difficulties are encountered. Nevertheless he guarantees an accuracy of three decimal places. Kaushal (1979) has used a relatively complex perturbation algorithm in order to obtain an asymptotic expansion of the energy spectrum. He restricted his calculation to a rather small range of g ($g = 0$ to 1) and a large range of λ ($\lambda = 0$ to 100). Bessis and Bessis (1980) have reinvestigated both within a variational and a perturbational scheme the energy eigenvalues by taking advantage of a two-parameter λ and g-scale transformation. They claimed to have obtained eight significant figures. Lai and Lin (1982) have determined the ground and the first three excited energy levels by forming the [6, 6] Padé approximants to the energy perturbation series for the interaction (1.1) as obtained from the hypervirial relations. They note that their

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calculated values of E_n are closer to the results of Mitra than to those obtained by Bessis and Bessis. Their work can be considered as an improvement over the perturbative scheme of Kaushal (1979). Killingbeck (1979) and Galicia and Killingbeck (1979) combined some basic ideas of first-order perturbation theory with methods of direct numerical integration to derive accurate eigenvalues for one-dimensional Schrödinger equations. All these numerical treatments are concentrated on the $\lambda > 0$ case since they are applicable only as long as $\lambda + 1 > 0$. A set of exact solutions to the Schrödinger equation (1.2) with $V(x)$ given by (1.1) has been constructed by Flessas (1981, 1982), Varma (1981), Lai and Lin (1982) and Whitehead *et al* (1982). The existence of such exact solutions is demonstrated under the conditions $\lambda < 0$, $g > 0$ and $\lambda = \lambda(g)$, $E = E(g)$; in view of these restrictions on λ and g, these solutions do not constitute the complete set of solutions.

In this paper a direct numerical integration method will be discussed for calculating eigenvalues and eigenstates of the Schrödinger equation (1.2) by introducing a finite difference representation of $D^2y(x)$. Section 2 explains the simple mathematics which form the basis of our method. The appropriate formulae are presented. In § 3 we compare some of our results with those of previously numerical calculations and exact solutions. It will be noticed that for other potentials different from (1.1) the method is also appropriate.

2. Numerical method: theory

It is well known (Fröberg 1979) that D^2 can be expressed as a series expansion of only even powers of the central difference operator, i.e.

$$h^2D^2 = \delta^2 - \frac{\delta^4}{12} + \frac{\delta^6}{90} - \frac{\delta^8}{560} + \frac{\delta^{10}}{3150} - \frac{\delta^{12}}{16\,632} + \ldots, \tag{2.1}$$

where h is the considered step length and δ applies on a function $y(x)$ as follows:

$$\delta y(x) = y(x + \tfrac{1}{2}h) - y(x - \tfrac{1}{2}h). \tag{2.2}$$

Although the solutions of (1.2) are explicitly defined in $[-\infty, +\infty]$, it should be noted that these solutions are either of even or odd parity, i.e. $y(x) = \pm y(-x)$, so that the determination of $y(x)$ can be restricted to the region $[0, +\infty]$. Furthermore we shall suppose that the wavefunctions are restricted to obey the Dirichlet boundary condition $y(x) = 0$ at some x value R. An acceptable R value will be guessed numerically. If moreover the interval $[0, R]$ is subdivided into equal parts of length h and the second-order derivative is approximated by some terms of (2.1) the Schrödinger equation (1.2) transforms into an algebraic eigenvalue problem of the form

$$(A - KI)y = 0 \tag{2.3}$$

where $y = (y(0), y(h), y(2h), \ldots, y(R))^T$, K is proportional to E, I is the unity matrix and the structure of the matrix A depends on the number of terms which are withheld in the series expansion (2.1). Taking into account one, two, or three terms in the expansion (2.1) results respectively in a tridiagonal, pentadiagonal or heptadiagonal form for the matrix $(A - KI)$. Denoting $x = kh$ $(k = 0, 1, \ldots, n;\ nh = R)$ $y(x) = y(kh) = y_k$ and considering that $y_{-k} = \pm y_k$, depending on the parity of the considered eigenfunc-

tion, the tridiagonal form of $(A-KI)$ reads

$$\begin{pmatrix} \alpha_0-K & \beta_0 & 0 & 0 & \dots & 0 \\ 1 & \alpha_1-K & 1 & 0 & \dots & 0 \\ 0 & 1 & \alpha_2-K & 1 & \dots & 0 \\ & & & \ddots & & \\ 0 & & \dots & 1 & \alpha_{n-1}-K & 1 \\ 0 & \dots & & 0 & 1 & \alpha_n-K \end{pmatrix}, \tag{2.4}$$

with $\alpha_k=-(2+V(kh))$, $K=-Eh^2$, and (2.5)

$$\begin{aligned} \beta_0=2 \quad & \text{for even-parity solutions,} \\ 0 \quad & \text{for odd-parity solutions.} \end{aligned} \tag{2.6}$$

In an analogous way the pentadiagonal form of $(A-KI)$ can be denoted as

$$\begin{pmatrix} \gamma_0-K & \delta_0 & \varepsilon_0 & 0 & 0 & 0 & \dots & 0 \\ 16 & \gamma_1+\delta_1-K & 16 & -1 & 0 & 0 & \dots & 0 \\ -1 & 16 & \gamma_2-K & 16 & -1 & 0 & \dots & 0 \\ 0 & -1 & 16 & \gamma_3-K & 16 & -1 & \dots & 0 \\ & & & & \ddots & & & \\ 0 & \dots & -1 & 16 & \gamma_{n-2}-K & 16 & & -1 \\ 0 & \dots & 0 & -1 & 16 & \gamma_{n-1}-K & & 16 \\ 0 & \dots & 0 & 0 & -1 & 16 & & \gamma_n-K \end{pmatrix}, \tag{2.7}$$

with

$$\gamma_k=-12(5/2+V(kh)), \qquad K=-12Eh^2, \tag{2.8}$$

and

$$\begin{aligned} \delta_0=32,\ \varepsilon_0=-2,\ \delta_1=-1 \quad & \text{for even-parity solutions,} \\ \delta_0=0,\ \varepsilon_0=0,\ \delta_1=1 \quad & \text{for odd-parity solutions.} \end{aligned} \tag{2.9}$$

For the heptadiagonal case one obtains in a similar way for $(A-KI)$

$$\begin{pmatrix} \eta_0-K & \mu_0 & \tau_0 & \sigma_0 & 0 & 0 & 0 & 0 \dots 0 \\ 270 & \eta_1+\mu_1-K & \tau_1 & -27 & 2 & 0 & 0 & 0 \dots 0 \\ -27 & \mu_2 & \eta_2-K & 270 & -27 & 2 & 0 & 0 \dots 0 \\ 2 & -27 & 270 & \eta_3-K & 270 & -27 & 2 & 0 \dots 0 \\ 0 & 2 & -27 & 270 & \eta_4-K & 270 & -27 & 2 \dots 0 \\ & & & & & \ddots & & \\ 0 & & \dots & 2 & -27 & -270 & \eta_{n-1}-K & 270 \\ 0 & & \dots & 0 & 2 & -27 & 270 & \eta_n-K \end{pmatrix} \tag{2.10}$$

with

$$\eta_k=-180(49/18+V(kh)), \qquad K=-180Eh^2, \tag{2.11}$$

and

$$\mu_0 = 540,\ \tau_0 = -54,\ \sigma_0 = 4,\ \mu_1 = -27,\ \tau_1 = 272,\ \mu_2 = 272 \qquad \text{for even-parity solutions,}$$

$$\mu_0 = 0,\ \tau_0 = 0,\ \sigma_0 = 0,\ \mu_1 = 27,\ \tau_1 = 268,\ \mu_2 = 268 \qquad \text{for odd-parity solutions.} \tag{2.12}$$

It has to be noted that in each of the three cases considered, one can easily deduce the error τ, introduced by replacing $D^2y(x)$ by one, two or three terms of (2.1) respectively, acting on $y(x)$, i.e. for

$$h^2D^2y(x) = \delta^2y(x), \qquad \tau = -\tfrac{1}{12}h^2D^4y(\xi) \tag{2.13}$$

$$h^2D^2y(x) = (\delta^2 - \tfrac{1}{12}\delta^4)y(x), \qquad \tau = \tfrac{1}{90}h^4D^6y(\xi) \qquad \xi \in [0, R] \tag{2.14}$$

$$h^2D^2y(x) = (\delta^2 - \tfrac{1}{12}\delta^4 + \tfrac{1}{90}\delta^6)y(x), \qquad \tau = -\tfrac{1}{560}h^6D^8y(\xi). \tag{2.15}$$

By this it is clear that the accuracy of our solutions increases roughly by a factor h^2 by adding one more term in the approximation for D^2.

There exist a lot of algorithms to deduce the lowest eigenvalues and their corresponding eigenvectors for matrices of the form (2.4), (2.7) and (2.10). Since each of the constructed matrices have, with the exception of some of the first rows, a symmetric structure, it seems favourable in the first instance to transform them by means of one similarity transformation to complete symmetric ones. Following Wilkinson (1965) it is interesting for the calculation of eigenvalues of band symmetric matrices to reduce them to a tridiagonal form by preliminary transformations. We have applied this idea to the matrices (2.7) and (2.10) by using Rutishauser's (1963) method based on plane rotations. Once the matrices are reduced to a symmetric tridiagonal band form we have used the F02BEF-subroutine of the NAG library (NAG 1981) especially developed for the calculation of selected eigenvalues and corresponding eigenvectors of such matrices. The obtained eigenvectors are then afterwards normalised to unity by requiring $\int_{-R}^{R} y^2(x)\,dx = 1$. To reproduce these eigenvectors in a clear way, we finally have developed them in terms of an orthonormal set $\{u_n | n = 0, \ldots, N_{\max}\}$, the harmonic oscillator eigenfunctions defined by

$$u_n = [2^n n!\,\pi^{1/2}]^{-1/2}\,e^{-x^2/2}H_n(x), \tag{2.16}$$

with H_n the Hermite polynomials. In fact the normalised y solutions are given by

$$y(x) = \sum_{n=0}^{N_{\max}} a_n u_n(x). \tag{2.17}$$

The upper limit in this sum is fixed by the condition that $\Sigma_{n=0}^{N_{\max}} a_n^2$ approximates unity within a given accuracy.

3. Numerical method: applications

To study the importance of the several terms in the series expansion (2.1), we have applied the three above derived approximations for $(A - KI)$, i.e. (2.4), (2.7) and (2.10), for two specific choices of λ and g values for which either exact or a lot of numerical values for the energy values of the low-lying states are available in the literature. For this comparison we have kept $R = 10.0$ and $h = 0.05$. The influence of the R value on the final results will be discussed later. Note that by the above choices

for h and R the maximum dimension of the occurring matrices is 200×200. The obtained energy values (E_n, $n = 1, 5$) for the case ($\lambda = 1.0$, $g = 1.0$) are given in table 1 and compared with the previously calculated values of Mitra (1978), Bessis and Bessis (1980), Galicia and Killingbeck (1979) (corrected results mentioned in Lai and Lin (1982)) and Lai and Lin (1982). By comparing the results derived in the tri-, penta- and hepta-diagonal approaches respectively, one observed approximately an improvement of accuracy of three significant figures, a value which is of the same order of magnitude as predicted by the theory, i.e. $h^2 = (0.05)^2$. It is clear that our results are in better agreement with those of Mitra and of Galicia and Killingbeck than with those of Bessis and Bessis in the considered (λ, g) region; this fact has also been observed by Lai and Lin (1982). Our results in the heptadiagonal approach (for $\lambda = 1.0$ and $g = 1.0$ as well as for $\lambda = g = 0.0$) have an overall accuracy of eight significant figures.

It is evident that the heptadiagonal form yields the most accurate results. All further calculations are performed in that approach. To show the dependence of the results on the choice of the R value, we present in table 2, again for $\lambda = 1.0$ and $g = 1.0$, the

Table 1. Comparison of the results respectively derived in the tri-, penta- and hepta-diagonal approach for the potential (1.1) with exact and previously derived data for the case ($\lambda = 1.0$, $g = 1.0$) and ($\lambda = 0$, $g = 0$).

	$\lambda = 1.0$ $g = 1.0$				
	E_1	E_2	E_3	E_4	E_5
tridiagonal	1.232 140 98	3.506 474 73	5.587 538 98	7.644 011 85	9.677 291 11
pentadiagonal	1.232 350 51	3.507 387 16	5.589 775 07	7.648 191 96	9.684 023 56
heptadiagonal	1.232 350 72	3.507 388 35	5.589 778 92	7.648 201 21	9.684 041 95
Mitra (1978)	1.232 35	3.507 38	5.589 77	—	—
Bessis and Bessis (1980)	1.232 372 05	3.507 420 53	5.589 860 86	7.648 316 81	—
Galicia and Killingbeck (1979)†	1.232 350 72	—	5.589 778 94	—	—
Lai and Lin (1982)	1.232 353 53	3.507 397 06	5.589 833 55	7.649 068 99	—
	$\lambda = 0$ $g = 0$				
	E_1	E_2	E_3	E_4	E_5
tridiagonal	0.999 843 73	2.999 218 53	4.997 967 89	6.996 091 53	8.993 589 13
pentadiagonal	0.999 999 87	2.999 999 09	4.999 996 75	6.999 991 81	8.999 983 24
heptadiagonal	1.000 000 00	3.000 000 00	4.999 999 99	6.999 999 98	8.999 999 94
exact	1	3	5	7	9

† Corrected results reported in Lai and Lin (1982).

Table 2. The dependence of the results on the choice of the R value.

R	E_1	E_2	E_3	E_4	E_5
4.0	1.232 351 55	3.507 424 42	5.590 273 52	7.652 784 69	9.708 479 44
6.0	1.232 350 72	3.507 388 35	5.589 778 92	7.648 201 21	9.684 041 96
10.0	1.232 350 72	3.507 388 35	5.589 778 92	7.648 201 21	9.684 041 95

results obtained with step length $h = 0.05$ but with three different R values, i.e. $R = 4.0$, 6.0 and 10.0. This shows that for this particular (λ, g) combination the first eight figures of the E_n $(n = 1, 5)$ results do not change anymore whenever $R \geq 6.0$. Of course one should control for each parameter choice the influence of the chosen R value on the results. Further in this paper we shall keep R fixed at 10.0 and $h = 0.05$.

In order to have an idea about the accuracy of the described method we compare in table 3 our results for different typical (λ, g) combinations with previous results. For small values of λ we certainly reproduce seven significant digits, while for large λ values our results are a little less accurate, which should be attributed to our particular choice for the R parameter. For each of the mentioned energies we also have derived the corresponding eigenvectors. The coefficients a_n as defined in (2.17) are not given here, but are available on request to the authors.

Table 3. Calculated values of the energy E_n $(n = 1, 5)$ for the potential (1.1) obtained from five different methods: (a) the present work, (b) Mitra (1978), (c) Bessis and Bessis (1980), (d) Lai and Lin (1982), (e) Killingbeck (1979).

		$\lambda = 0.1$ $g = 0.1$	$\lambda = 0.1$ $g = 100.0$	$\lambda = 100.0$ $g = 0.1$	$\lambda = 100.0$ $g = 100.0$	$\lambda = 10.0$ $g = 10.0$
E_1	a	1 043 173 71	1.000 841 10	9.976 178 31	1.836 334 44	1.580 022 33
	b	1.043 17	1.000 84	9.976 18	1.836 4	1.580 02
	c	1.043 173 71	1.000 841 1	9.976 180 09	1.836 385 0	1.580 024 9
	d	1.043 173 71	—	9.976 180 09	—	—
	e	1.043 174 08	1.000 841 43	9.976 180	1.836 337 3	—
E_2	a	3.120 081 86	3.000 983 18	29.781 175 75	3.983 098 36	3.879 036 83
	b	3.120 08	3.000 98	29.781 19	3.983 1	3.879 03
	c	3.120 081 86	3.000 983 1	29.781 191 1	3.983 099 2	3.879 037 2
	d	3.120 081 86	—	29.781 191 11	—	—
E_3	a	5.181 094 78	5.000 927 54	49.292 623 58	5.928 327 90	5.832 767 52
	b	5.181 09	5.000 93	49.292 69	5.928	5.832 77
	c	5.181 094 79	5.000 925 7	49.292 690 5	5.928 352 5	5.832 769 2
	d	5.181 094 79	—	49.292 690 50	—	—
	e	5.181 095 06	5.000 927 8	49.292 69	5.928 329 3	—
E_4	a	7.231 009 95	7.000 984 47	68.512 861 08	7.984 443 54	7.903 154 13
	c	7.231 009 98	7.000 984 5	68.513 052 2	7.984 444 8	7.903 154 9
	d	7.231 009 98	—	68.513 062 23	—	—
E_5	a	9.272 816 91	9.000 948 53	87.444 233 67	9.949 160 38	9 882 298 66
	e	9.272 818	9.000 948	87.444 7	9.949 162	—

Several authors have studied a class of exact solutions for eigenvalues and eigenvectors of the Schrödinger equation (1.2). These solutions all correspond to negative λ values. They yield interesting material for testing the validity and accuracy of our numerical method. Let us compare some of these exact even-parity solutions as deduced by Flessas (1981) with our numerical results. His lowest-lying solution is given in terms of g as follows:

$$\lambda = -2g(2+g), \tag{3.1}$$

$$E_1(g) = 1 - 2g, \tag{3.2}$$

$$y(x) = \exp(-x^2/2)a(1+gx^2) = \alpha u_0(x) + \beta u_2(x),$$

where a is a normalisation factor and the u_n $(n = 0, 2)$ are defined in (2.16). The ratio α/β can also be expressed in terms of g, i.e.

$$\alpha/\beta = (2+g)/(\sqrt{2}g). \tag{3.3}$$

Flessas' second energy level corresponds with

$$\lambda = -7g^2 - 6g \pm g(25g^2 - 12g + 4)^{1/2}, \tag{3.4}$$

$$E_2(g) = 9 + \lambda/g = 3 - 7g \pm (25g^2 - 12g + 4)^{1/2}, \tag{3.5}$$

$$y(x) = \exp(-x^2/2)a'[1 - (8g+\lambda)/(2g)x^2 + 2g(8g+\lambda)/(12g^2+\lambda)x^4]$$
$$= \alpha' u_0(x) + \beta' u_2(x) + \gamma' u_4(x),$$

where a' is again a normalisation factor and

$$\alpha'/\beta' = (\lambda + 6g^2 + 4g)/[\sqrt{2}(8g+\lambda)], \tag{3.6}$$

$$\beta'/\gamma' = -\lambda/(4\sqrt{3}g^2). \tag{3.7}$$

For the odd-parity levels Varma (1981) obtains the following relations

$$\lambda = -2g(2+3g), \tag{3.8}$$

$$E_1'(g) = 7 + \lambda/g = 3(1-2g), \tag{3.9}$$

$$y(x) = \exp(-x^2/2)ax(1+gx^2) = \alpha'' u_1(x) + \beta'' u_3(x),$$

with

$$\alpha''/\beta'' = (2+3g)/(\sqrt{6}g) \tag{3.10}$$

and

$$\lambda = -13g^2 - 6g \pm g(49g^2 - 4g + 4)^{1/2} \tag{3.11}$$

$$E_2'(g) = 11 + \lambda/g = 5 - 13g \pm (49g^2 - 4g + 4)^{1/2} \tag{3.12}$$

$$y(x) = \exp(-x^2/2)a'x\{1 - (8g+\lambda)/(6g)x^2 + 2g(8g+\lambda)/[3(20g^2+\lambda)]x^4\}$$
$$= \alpha''' u_1(x) + \beta''' u_3(x) + \gamma''' u_5(x)$$

with

$$\alpha'''/\beta''' = \sqrt{6}(\lambda + 4g + 10g^2)/2(8g+\lambda) \tag{3.13}$$

$$\beta'''/\gamma''' = -\lambda/(4\sqrt{5}g^2). \tag{3.14}$$

In table 4 we compare for $g = 0.1$ the exact results (3.1)-(3.14) with the calculated values. As well for the energies as for the eigenstates we obtain an accuracy of at least eight significant figures. Moreover one has to realise that besides the energy value(s) which correspond for a particular g and corresponding $\lambda = \lambda(g)$ with an exactly expressible eigenstate of the polynomial type, we obtain numerically a lot more other eigenvalues, which have no exact counterparts. For example for $g = 0.1$ and $\lambda = -0.42$ we reproduce (as can be seen in table 4) quite nicely Flessas' exact solution $E_1(g)$, but we also find levels at 4.197 895 89, 7.820 097 62, 11.548 628 92, ... etc, whose eigenstates have a complex structure in the sense that at least twelve $u_n(x)$ $(n = 0, 2, \ldots, 22)$ are present in the expansion of the type (2.17). Note also that for this

Table 4. Comparison of certain exact energies and eigenvectors associated with the potential (1.1) as derived by Flessas (1981) and Varma (1981) with our numerical predictions.

Flessas (1981) $g = 0.1$			
Formula		Exact values	Calculated values
(3.1)	λ	-0.42	-0.42
(3.2)	E_1	0.8	0.800 000 00
(3.3)	α/β	$21/\sqrt{2} \simeq 14.849\,242\,41$	14.849 242 64
(3.4) (plus sign)	λ	$-0.67 + 0.1\sqrt{3.05} \simeq -0.495\,357\,51$	$-0.495\,357\,51$
(3.5) (plus sign)	E_2	$2.3 + \sqrt{3.05} \simeq 4.046\,424\,92$	4.046 424 92
(3.6)	α'/β'	$\simeq -0.082\,068\,44$	$-0.082\,068\,44$
(3.7)	β'/γ'	$\simeq 7.149\,869\,76$	7.149 869 93
Varma (1981) $g = 0.1$			
Formula		Exact values	Calculated values
(3.8)	λ	-0.46	-0.46
(3.9)	E_1'	2.4	2.400 000 00
(3.10)	α''/β''	$23/\sqrt{6} \simeq 9.389\,710\,68$	9.389 710 80
(3.11) (plus sign)	λ	$-0.73 + 0.1\sqrt{4.09} \simeq -0.527\,762\,52$	$-0.527\,762\,52$
(3.12) (plus sign)	E_2'	$3.7 + \sqrt{4.09} \simeq 5.722\,374\,84$	5.722 374 83
(3.13)	α'''/β'''	$\simeq -0.124\,898\,30$	$-0.124\,898\,30$
(3.14)	β'''/γ'''	$\simeq 5.900\,564\,31$	5.900 564 56

special class of solutions with $\lambda < -1$ the possibility exists to obtain finally negative energy values.

It is evident that the presented method can be used for a variety of potential forms. As an example we consider the potential

$$V(x) = \mu x^2 + \lambda x^4, \tag{3.15}$$

Table 5. Calculated values of the energies E_n $(n = 1, 5)$ for the potential (3.15) obtained from four different methods: (a) the present work, (b) Chan and Stellman (1963), (c) Killingbeck (1985), (d) Biswas *et al* (1973).

		$\mu = 0.0\ \lambda = 1.0$		$\mu = 1.0\ \lambda = 1.0$
E_1	a	1.060 362 09	a	1.392 351 64
	b	1.060 362	d	1.392 351 641 530 29
	c	1.060 362 09	c	1.392 351 64
E_2	a	3.799 673 02	a	4.648 812 68
	b	3.799 657	d	4.648 812 70
	c	3.799 673 03	c	4.648 812 70
E_3	a	7.455 697 86	a	8.655 049 85
	b	7.455 702	d	8.655 049 9
E_4	a	11.644 745 16	a	13.156 803 42
	b	11.644 75	d	13.156 803 8
E_5	a	16.261 824 85	a	18.057 555 89
		—	d	18.057 557 4

which is of particular interest in molecular physics. Biswas *et al* (1973) have derived its ground state as well as the excited energy levels using the Hill determinants. By using the Hellmann-Feynman theorem combined with power series expansion and finite difference approaches Killingbeck (1985) also derived some very accurate eigenvalues. In table 5 we compare our results for two typical (μ, λ) values, i.e. (0.0, 1.0) and (1.0, 1.0) with previously derived results. Again we have chosen $h = 0.05$, $R = 10.0$ and we have considered the heptadiagonal approach. As can be observed we obtain at least an accuracy of seven significant figures.

4. Summary

In this paper we have presented a purely numerical method for the determination of the solutions of a Schrödinger equation. We have paid special attention to the potential $V(x) = x^2 + \lambda x^2/(1 + gx^2)$ and have shown that our method is applicable as well for positive λ values as negative ones. In the heptadiagonal approach we globally obtain seven to eight significant figures. In the cases where exact eigenvalues and eigenvectors are known we reproduce both quantities very satisfactorily. We have noted that the method can be used for other potentials as well.

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