Journal of Mathematical Chemistry Vol. 34, Nos. 3–4, November 2003 (© 2003)

The scaled Hermite–Weber basis still highly competitive

H. Taşeli and M. Bahar Erseçen *

Department of Mathematics, Middle East Technical University, 06531 Ankara, Turkey

Received 10 March 2003

The effectiveness of the usual harmonic oscillator basis is demonstrated on a wide class of Schrödinger Hamiltonians with various spectral properties. More specifically, it is shown numerically that an appropriately scaled Hermite–Weber basis yields extremely accurate results not only for the energy eigenvalues which differ slighly from the harmonic oscillator levels, but also for the states which reflect a purely anharmonic character.

KEY WORDS: Schrödinger equation, quantum mechanical oscillators, orthogonal expansions, Hermite–Weber functions

1. Introduction

The one-dimensional Hamiltonians

$$\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \quad x \in (-\infty, \infty) \tag{1}$$

have been the subject of many computational methods because an investigation of problems in (1) is a prerequisite for that of the more general and complex models. The so-called generalized anharmonic oscillators (GAOs) for which

$$V(x) = x^2 + v_{2k}x^{2k}, \quad v_{2k} > 0, \qquad k = 2, 3, \ldots \tag{2}$$

are the most studied systems of this kind. The divergence of the perturbation series expansion over the classical harmonic oscillator solution was first verified explicitly by Bender and Wu [1]. The aim of this paper is not the review of the anharmonic oscillators, however, after the important paper by Bender and Wu [1] concerning a quartic perturbation several modified Rayleigh–Schrödinger treatments have been proposed, which are convergent [2–4].

The harmonic oscillator eigenfunctions are considered as a basis in the Rayleigh–Ritz variational method as well. One of the first detailed variational calculations are due to Reid [5] who obtained the first 25 eigenvalues of the pure quartic oscillator, where $V(x) = x^4$, to 12 significant figures. In fact, it is not surprising that the harmonic oscillator basis yields quite satisfactory results for polynomial potentials, especially when the anharmonic interaction differs a little from the harmonic one.

* Current address: ASELSAN Inc., 06370 Ankara, Turkey.

0259-9791/03/1100-0177/0 © 2003 Plenum Publishing Corporation

Mathematically speaking, the harmonic oscillator is a symmetric single well potential which corresponds to a singular Sturm–Liouville system with an enumerable infinite set of discrete spectral points. In this paper, we use exact solutions of such an eigenvalue problem as a basis in standard variational calculations to test its numerical performance for symmetric and asymmetric single and double well polynomial potentials, as well as for certain non-polynomial potentials. Clearly, the Schrödinger operator with a polynomial well potential possesses the same spectral properties as the harmonic oscillator. However, the non-polynomial Gaussian and Morse potentials considered here have each a finite number of discrete states together with a continuous spectrum. Therefore, the present work is also motivated by this fact which makes it possible to understand how much the discrepancy in the spectral structures of the unperturbed and perturbed systems affects the accuracy of the computations.

In section 2, very general recursive relationships for the evaluation of the matrix elements are introduced. Applications to the specific problems with numerical results are presented in section 3. The discussion of the results and concluding remarks are given in a final section as usual.

2. Matrix elements

Introducing the linear transformation

$$\xi = \alpha x, \quad \alpha > 0 \tag{3}$$

we write down the Schrödinger eigenvalue problem in the form

$$\left[T + q(\xi)\right]\Psi(\xi) = \mathcal{E}(\alpha)\Psi(\xi), \quad \Psi \in L_2(-\infty, \infty) \tag{4}$$

where L_2 is the Hilbert space of the square integrable functions, and T and q are the harmonic oscillator Hamiltonian

$$T = -\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \xi^2 \tag{5}$$

and the perturbation potential

$$q(\xi) = \frac{V(\xi/\alpha)}{\alpha^2} - \xi^2, \tag{6}$$

respectively. The eigenvalues of (4) depending on the optimization parameter α, are connected with the energy eigenvalues, E say, of the original Hamiltonian $\mathcal{H}$ in (1) by the formula

$$E = \alpha^2 \mathcal{E}(\alpha). \tag{7}$$

As is well known, the operator T has purely a discrete spectrum corresponding to a complete sequence of eigenfunctions

$$\phi_n(\xi) = \mathcal{N}_n \mathrm{e}^{-\xi^2/2} H_n(\xi), \quad n = 0, 1, 2, \ldots \tag{8}$$

which are called the Hermite–Weber functions [6]. The Hermite–Weber functions satisfy the equation $T\phi_n = (2n+1)\phi_n$ and become mutually orthonormal over the real line if the constants $\mathcal{N}_n$ are specified by

$$\mathcal{N}_n = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} \tag{9}$$

for each $n = 0, 1, 2, \ldots$. The matrix representation of the eigenvalue problem in (4) is then found to be

$$\boldsymbol{\mathcal{A}}(\alpha)\mathbf{c} = \mathcal{E}(\alpha)\mathbf{c} \tag{10}$$

where $\mathbf{c}$ is the column vector which consists of the coordinates of the wave function $\Psi(\xi)$ with respect to the harmonic basis under consideration. At the numerical side of this study, we assume a truncated wave function so that the matrix $\boldsymbol{\mathcal{A}}$ is a square $N \times N$ matrix with the general entry

$$\mathcal{A}_{mn} = (2n+1)\delta_{mn} + Q_{mn}, \quad m, n = 0, 1, \ldots, N-1 \tag{11}$$

in which the Q_{mn}, defined by the inner product $\langle \phi_m(\xi) \mid q(\xi)\phi_n(\xi)\rangle$, require evaluating at a number of N^2 integrals of the type

$$Q_{mn} = \int_{-\infty}^{\infty} q(\xi)\phi_m(\xi)\phi_n(\xi)\,\mathrm{d}\xi \tag{12}$$

where N is the truncation size and δ_{mn} the Kronecker's delta. Nevertheless, it can be shown that the Q_{mn} obey a recurrence relation. Indeed, we may recall the identity for the Hermite polynomials [6]

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi), \qquad H_0(\xi) = 1, \qquad H_{-1}(\xi) = 0 \tag{13}$$

to obtain an expression for the product of two Hermite–Weber functions, from which the functional relationship

$$Q_{m+1,n} = \frac{\mathcal{N}_{m+1}\mathcal{N}_n}{\mathcal{N}_m\mathcal{N}_{n+1}} Q_{m,n+1} + 2n\frac{\mathcal{N}_{m+1}\mathcal{N}_n}{\mathcal{N}_m\mathcal{N}_{n-1}} Q_{m,n-1} - 2m\frac{\mathcal{N}_{m+1}}{\mathcal{N}_{m-1}} Q_{m-1,n} \tag{14}$$

for each fixed n is derived immediately for $m = 0, 1, \ldots, N-2$ with $Q_{-1,n} \equiv 0$. It is noteworthy that such a determination of columns of the matrix $\boldsymbol{Q} = [Q_{mn}]$, in turn, is independent of the particular form of the potential function. To start using the recursions all that needs to be done is the calculation of the improper integrals

$$Q_{0,n} = \left\langle \phi_0(\xi) \;\middle|\; q(\xi)\phi_n(\xi) \right\rangle = \mathcal{N}_0\mathcal{N}_n \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2} q(\xi) H_n(\xi)\,\mathrm{d}\xi \tag{15}$$

for $n = 0, 1, \ldots, 2N-2$, which is required as an initial condition for (14). Note that the first N elements of this array are the first row entries of the matrix $\boldsymbol{Q}$. In other words, a knowledge of $2N-1$ integrals defined by (15) over a prescribed potential function suffices to form completely the $N \times N$ matrix $\boldsymbol{Q}$ and, hence, the matrix $\boldsymbol{\mathcal{A}}$ in (10). Moreover, the labor involved in such a construction may be considerably shortened by

exploiting the symmetry $Q_{mn} = Q_{nm}$ of the matrix. Note also that we assume potential functions which are at least sufficiently well behaved for large absolute values of the argument for the integrals in (15) to exist.

The energy spectrum of the problem can be decomposed into two subsets consisting of even and odd eigenlevels, separately, provided that the original potential has a reflection symmetry $V(x) = V(-x)$ about the origin. In such a case, the bases $\{\phi_{2n}\}$ and $\{\phi_{2n+1}\}$ can be employed, respectively, in the expansions of the even and odd wave functions to avoid large matrices. Therefore, the recursions in (14) are revised appropriately on replacing H_n in (8) by H_{2n} and H_{2n+1}, in turn, for the evaluation of the variational matrix elements representing the Schrödinger equation with a symmetric potential.

3. Applications

3.1. Symmetric potentials

We first consider the GAOs in (2) and the symmetric double well potential (SDWP)

$$V(x) = -x^2 + v_4 x^4, \quad v_4 > 0 \tag{16a}$$

which are polynomials in even powers of x. The SDWP may be taken as

$$V(x) = v_4\left(x^2 - \tfrac{1}{2}v_4^{-1}\right)^2 \tag{16b}$$

for which the Hamiltonian is positive definite. So the energy levels of (16a) shifted by the constant term in (16b) are all positive.

Thus, for non-negative integer values of s, we encounter integrals of the type

$$\mathcal{J}_n(s) = \int_{-\infty}^{\infty} \xi^{2s} \mathrm{e}^{-\xi^2} H_{2n}(\xi)\, \mathrm{d}\xi, \quad n = 0, 1, \ldots, 2N-2 \tag{17}$$

which are evaluated analytically [7],

$$\mathcal{J}_n(s) = \frac{(-4)^n}{\sqrt{\pi}} \Gamma\left(s+\tfrac{1}{2}\right)\Gamma\left(n+\tfrac{1}{2}\right) {}_2F_1\left(-n, s+\tfrac{1}{2}; \tfrac{1}{2}; 1\right), \tag{18}$$

to deal with even parity states of these potentials. Here, ${}_2F_1(a, b; c; z)$ stands for the Gauss hypergeometric function that terminates to give a polynomial of degree n in z as its first parameter a is equal to a non-positive integer $-n$. Furthermore, such a polynomial reduces to

$${}_2F_1(-n, b; c; 1) = \frac{(c-b)_n}{(c)_n} \tag{19}$$

at $z = 1$, on using the Vandermonde's theorem [6], where $(p)_n$ denotes the Pochhammer's symbol. It follows then that

$$\mathcal{J}_n(s) = \frac{\sqrt{\pi}}{4^{s-n}} \frac{(2s)!}{(s-n)!} \tag{20}$$

for $n = 0, 1, \ldots, s$ and zero, otherwise. Now, from (15), we find the initial conditions

$$Q_{0,n} = \mathcal{N}_0\mathcal{N}_{2n}\left[\alpha^{-4}\left(1-\alpha^4\right)\mathcal{J}_n(1) + \alpha^{-2k}v_{2k}\mathcal{J}_n(k)\right] \tag{21}$$

and

$$Q_{0,n} = \mathcal{N}_0\mathcal{N}_{2n}\alpha^{-2}\left[\tfrac{1}{4}v_4^{-1}\mathcal{J}_n(0) - \alpha^{-2}\left(1+\alpha^4\right)\mathcal{J}_n(1) + \alpha^{-4}v_4\mathcal{J}_n(2)\right] \tag{22}$$

for the GAOs and SDWP, respectively, for the recursive determination of the matrix elements. Note that odd parity states can be treated in a very similar fashion.

As an example of a non-polynomial symmetric potential, we test the Gaussian

$$V(x) = -\mathrm{e}^{-\beta x^2}, \quad \beta > 0 \tag{23}$$

having a finite number of discrete energy levels, which lie between $-1 < E < 0$. For the symmetric states we find that

$$Q_{0,n} = -\mathcal{N}_0\mathcal{N}_{2n}\left[\mathcal{J}_n(1) + \alpha^{-2}\mathcal{K}_n\left(\beta\alpha^{-2}\right)\right] \tag{24}$$

where the function $\mathcal{K}_n(t)$, defined by

$$\mathcal{K}_n(t) = \int_{-\infty}^{\infty} \mathrm{e}^{-(1+t)\xi^2} H_{2n}(\xi)\,\mathrm{d}\xi, \tag{25}$$

results in

$$\mathcal{K}_n(t) = (-4)^n\Gamma\left(n+\tfrac{1}{2}\right)(1+t)^{-1/2}{}_2F_1\left(-n, \tfrac{1}{2}; \tfrac{1}{2}; (1+t)^{-1}\right) \tag{26}$$

containing again the ordinary hypergeometric function [7]. By using the known identity

$${}_2F_1(-n, b; b; z) = (1-z)^n, \tag{27}$$

however, it is expressible as

$$\mathcal{K}_n(t) = \frac{(2n)!}{n!}\sqrt{\pi}\,(-t)^n(1+t)^{-n-1/2}, \tag{28}$$

in terms of the elementary functions.

In the numerical tables 1 and 2, we present the ground state eigenvalues of the quartic and sextic oscillators as a function of the coupling constants v_4 and v_6, respectively. Table 3 includes the first 12 nearly degenerate eigenvalues of the SDWP when $v_4 = 0.01$. Some discrete eigenvalues of the Gaussian potential (GP) are shown in table 4 as a function of the parameter β. Further results, which have not been quoted in this article, are available from the authors.

3.2. Asymmetric potentials

If we take care of a more general polynomial potential of degree $2M$ of the form

$$V(x) = \sum_{k=2}^{2M} v_k x^k, \quad v_{2M} > 0 \tag{29}$$

Table 1
Ground state energies of the quartic oscillator $V(x) = x^2 + v_4 x^4$, as a function of v_4.

v_4	E_0	N	α_{opt}
0.0001	1.000 074 986 880 200 111 122 834 155 30	8	1
0.01	1.007 373 672 081 382 460 533 843 905 98	17	1
1	1.392 351 641 530 291 855 657 507 876 62	25	2.1
10	2.499 174 072 118 386 918 268 793 906 19	26	3.1
1000	10.639 788 711 328 046 063 622 042 669 4	30	6.5
10000	22.861 608 870 272 468 891 759 867 963 5	30	9.5
100000	49.225 447 584 229 625 157 076 387 001 1	30	14

Table 2
Ground state energies of the sextic oscillator $V(x) = x^2 + v_6 x^6$, as a function of v_6.

v_6	E_0	N	α_{opt}
0.0001	1.000 187 228 153 680 768 286 355 665 62	16	1
0.01	1.016 741 363 754 732 031 671 817 981 52	32	1.8
1	1.435 624 619 003 392 315 761 272 220 54	39	3.2
10	2.205 723 269 595 632 351 009 973 387 17	40	4.2
1000	6.492 350 132 329 671 550 549 557 845 34	40	7
10000	11.478 798 042 264 543 961 289 816 038 6	39	9.5
100000	20.375 098 656 309 660 844 567 287 513 6	41	12.2

Table 3
Nearly degenerate states of the SDWP in (16b) for $v_4 = 0.01$.

n	N	α_{opt}	E_n
0	54	0.9	1.404 048 605 297 706 882 425 707 570 84
1	54	0.9	1.404 048 605 297 706 882 602 566 280 58
2	55	0.9	4.170 193 605 999 310 127 833 875 071 32
3	56	0.9	4.170 193 605 999 310 219 613 291 198 75
4	57	0.95	6.870 088 833 714 024 612 172 315 168 51
5	57	0.95	6.870 088 833 714 046 802 425 995 681 91
6	60	0.95	9.489 578 387 187 870 055 194 418 356 56
7	57	0.95	9.498 578 387 191 178 212 320 856 961 15
8	60	0.95	12.049 309 486 334 092 592 332 880 171 6
9	59	0.95	12.049 309 486 673 006 847 573 312 477 9
10	60	1	14.514 205 022 981 239 103 429 421 443 9
11	61	1	14.514 205 048 121 017 338 991 612 415 8

we have to evaluate the integrals

$$\mathcal{S}_n(k) = \int_{-\infty}^{\infty} \xi^k \mathrm{e}^{-\xi^2} H_n(\xi)\, \mathrm{d}\xi, \tag{30}$$

Table 4
Eigenvalues of the GP $V(x) = -\mathrm{e}^{-\beta x^2}$, as a function of β.

β	α_{opt}	N	n	E_n
0.001	0.2	30	0	−0.968 752 703 034 398 668 606 599 656 913
		35	2	−0.846 820 196 725 803 540 068 942 614 468
		45	4	−0.731 125 549 125 734 739 132 375 767 285
		55	6	−0.621 888 650 443 182 657 155 148 987 662
0.01	0.3	41	0	−0.903 763 987 980 773 054 539 687 567 952
		70	2	−0.550 801 670 798 557 886 254 842 935 82
		70	4	−0.267 463 693 629 351 027
		70	6	−0.068 692 251
0.1	0.4	70	0	−0.721 530 628 487 107 638 685 036 884
		70	2	−0.007 89

which are closely related to those in (17). Actually, we see that

$$\mathcal{S}_n(k) = \begin{cases} 0, & \text{if } n+k \text{ is odd,} \\ \mathcal{J}_{n/2}\left(\frac{1}{2}k\right), & \text{if } n \text{ and } k \text{ are both even,} \\ \mathcal{J}_{n+1/2}\left(k+\frac{1}{2}\right), & \text{if } n \text{ and } k \text{ are both odd} \end{cases} \tag{31}$$

from which

$$Q_{0,n} = \mathcal{N}_0\mathcal{N}_n\left[\sum_{k=2}^{2M} \alpha^{-k-2} v_k \mathcal{S}_n(k) - \mathcal{S}_n(2)\right] \tag{32}$$

is calculated immediately. Then we construct, from (14) and (11), the matrix $\boldsymbol{\mathcal{A}}$ whose eigenvalues approximate the spectrum of the asymmetric Hamiltonian in question. Specimen computations are performed for the asymmetric double well potential (ADWP)

$$V(x) = v_2x^2 + v_3x^3 + v_4x^4 \tag{33}$$

which has two minima located asymmetrically about the origin, if the parameters satisfy the inequalities $v_4 > 0$ and $9v_3^2 - 32v_2v_4 > 0$. Here, we take into account the alternative form

$$V(x) = c_1x^2(x+c_2)(x-1), \quad 0 < c_2 < 1, \quad c_1 > 0 \tag{34}$$

of the ADWPs proposed by Taşeli [11], and give results in table 5 for several values of c_1 and c_2.

These potentials are of practical interest for the protonic movement of hydrogen-bonded systems [8]. Znojil [9] constructed Hill's determinant of the problem by matching two power series valid for negative and positive values of the argument, respectively. Some numerical resuls were introduced by Diaz et. al. [10], but a more systematic numerical study of the ADWPs may be found in [11].

Finally, we revisit an asymmetric, non-polynomial potential

$$V(x) = \left(\mathrm{e}^{-\gamma x} - 1\right)^2, \quad \gamma > 0 \tag{35}$$

Table 5
Eigenvalues of ADWPs in (34) as functions of c_1 and c_2.

c_1	c_2	α_{opt}	N	n	E_n
0.001	0.25	1	54	0	0.220 496 933 551 383 181 180 584 101 238
			56	1	0.799 076 156 134 041 042 756 335 888 803
			57	2	1.579 425 872 715 042 186 839 788 277 34
			59	3	2.475 227 126 276 957 997 940 355 211 70
	0.50	1	54	0	0.218 255 536 797 065 407 353 982 485 212
			55	1	0.793 475 852 449 351 300 718 466 956 320
			58	2	1.571 726 799 166 984 751 587 449 207 98
			58	3	2.465 596 537 785 138 574 857 695 511 22
	0.75	1	55	0	0.215 207 254 047 971 748 843 624 710 389
			55	1	1.785 867 870 008 598 255 331 395 933 43
			58	2	1.561 286 635 695 375 110 776 021 304 73
			58	3	2.452 542 721 464 178 763 806 091 811 26
100	0.25	1.2	66	0	−4.277 344 849 182 474 166 847 348 848 02
			67	1	7.080 517 391 364 158 656 090 710 350 27
			67	2	19.817 761 502 618 821 399 175 325 525 3
			67	3	36.209 337 296 287 706 584 558 242 608 9
	0.50	1.2	68	0	−6.816 052 047 536 736 982 561 430 366 00
			68	1	4.675 693 930 558 290 057 997 135 848 24
			69	2	15.973 204 136 317 836 561 600 922 534 7
			67	3	31.505 546 630 519 551 260 800 075 872 1
	0.75	1.2	65	0	−9.459 479 212 224 512 858 546 562 584 41
			67	1	0.010 560 072 717 619 621 379 801 416 914
			67	2	10.866 977 233 476 768 562 653 506 503 6
			67	3	24.888 991 175 519 381 797 134 001 071 9

which has a composite spectrum unlike the polynomial oscillators. It is known as the Morse potential (MP) and is used to model the purely vibrational levels of diatomic molecules [12]. The number of discretely distributed spectral points of the MP, located on the energy interval $(0, 1)$, depends completely on the parameter γ and has no bound states at all if $\gamma > 2$ [13]. The MP admits exact analytical solutions on the unphysical domain of x, $x \in (-\infty, \infty)$, due to the fact that x in (35) denotes the internuclear distance which should not be negative. However, we proved numerically in [14] that Morse's original assumption of the inclusion of the unphysical portion $(-\infty, 0)$ does not cause a significant deviation from the correct eigenvalues representing the physical domain.

The numerical results for the MP are shown in table 6. It should be noted that the matrix elements are determined recursively without any trouble using the values of the array

$$Q_{0,n} = \mathcal{N}_0 \mathcal{N}_n \left\{ \alpha^{-2} \left[\mathrm{e}^{t^2} \mathcal{R}_n(t) - 2\mathrm{e}^{t^2/4} \mathcal{R}_n\left(\tfrac{1}{2}t\right) + \mathcal{R}_n(0) \right] - \mathcal{S}_n(2) \right\} \tag{36}$$

Table 6
Eigenvalues of the MP $V(x) = (\mathrm{e}^{-\gamma x} - 1)^2$, as a function of γ.

γ	α_{opt}	N	n	E_n	E_{exact}
0.02	0.1	101	0	0.019 900 000 000 000 000 000 000 000 001	199×10^{-4}
			1	0.059 100 000 000 000 000 000 000 000 001	591×10^{-4}
			2	0.097 500 000 000 000 000 000 000 000 001	975×10^{-4}
			3	0.135 100 000 000 000 000 000 000 000 001	1351×10^{-4}
			4	0.171 900 000 000 000 000 000 000 000 001	1719×10^{-4}
0.2	0.4	102	0	0.190 000 000 000 000 000 000 000 0008	19×10^{-2}
			1	0.510 000 000 000 000 005	51×10^{-2}
			2	0.750 000 000 005	75×10^{-2}
			3	0.910 000	91×10^{-2}

at $t = \gamma/\alpha$, where

$$\mathcal{R}_n(t) = \int_{-\infty}^{\infty} \mathrm{e}^{-(\xi+t)^2} H_n(\xi)\,\mathrm{d}\xi = \sqrt{\pi}(-2t)^n \tag{37}$$

with $\mathcal{R}_n(0) = \sqrt{\pi}\delta_{0,n}$.

4. Discussion

In this work, the eigenvalues of one-dimensional quantum problems are computed accurate to 30 digits in most cases. It is contented with finding lower eigenvalues since a variational method becomes forbiddingly laborious for higher excited states. Another very general disadvantage of the method is that each matrix element requires an integration. Fortunately, we overcome successfully this difficulty deriving nice recursive relationships.

The accuracy of the results is checked by increasing the truncation size N in a systematic manner. Furthermore, the results are confirmed by several values of the parameter α, whose optimum values are also included in the numerical tables. It is not surprising to deduce from tables 1 and 2 that the optimum values increase as the anharmonic interactions get stronger.

The optimality of the parameter α may be seen clearly in table 7. As an illustrative example, we list the matrix sizes N corresponding to different values of α for the quartic oscillator with a large anharmonic term. Note that, in table 7, the N denote matrix sizes at which the desired (fixed) accuracy for E_0 is reached. Therefore, as is recorded in table 1 the optimum value is $\alpha_{\mathrm{opt}} = 14$ for the ground state energy of the potential $V(x) = x^2 + 100\,000x^4$.

The spectral properties of the SDWPs in (16) are virtually the same as the quartic oscillator for large enough values of v_4. However, the lower eigenvalues are closely bunched in pairs if the two wells are sufficiently separated. This situation corresponds to weak couplings when $v_4 \ll 1$ and implies the tunneling through the potential barrier.

Table 7
Convergence rate of the ground state of the quartic oscillator $V(x) = x^2 + v_4 x^4$, where $v_4 = 100\,000$, as a function of α.

α	8	10	12	13	14	15	17	20	23
N	69	41	33	31	30	31	37	47	69

In such a case, the determination of the gaps between pseudodegenerate eigenvalues becomes more important. We infer from table 3 that the scaled Hermite–Weber basis has the capability of giving those eigenvalues without any loss of accuracy. This may be regarded as quite an impressive result if we recall the fact that many methods fail for potentials with degenerate minima [15–18].

The last example of problems with a reflection symmetry is the GP in (23) whose radial form received more attention in the literature [19–21]. It is known that there exists a threshold value of the parameter β, say β_{thr}, beyond which the particular bound state being considered can no longer survive. We notice, from table 4, that as β approaches β_{thr} a remarkable slowing down of convergence occurs for very weakly bound states, with E just below zero.

In the case of an asymmetric operator, the matrix sizes N are relatively larger since there is no characterization of the energy spectrum of being even or odd parity. Therefore, we include all basis elements in our formulation without any decomposition. Nevertheless, we achieve the same accuracy as the symmetric cases, as shown from tables 5 and 6. We observe again, from table 6, that the method fails in computing the eigenvalues of the MP at the near border of the continuum as E tends toward one.

As a final remark, we could not get success in stating an analytic estimation for the optimum values of α. However, we perceive that the experimental optimum values determined here, for instance, for the quartic oscillator are in good agreements with some WKB estimates [22]. Furthermore, it seems that it is straightforward to extend such a scaled basis to two-dimensional Schrödinger equation as well.

References

[1] C.M. Bender and T.T. Wu, Phys. Rev. 184 (1969) 1231.
[2] P.K. Patnaik, Phys. Rev. D 33 (1986) 3145.
[3] M. Znojil, Phys. Rev. A 35 (1987) 2448.
[4] G.S. Tschumper and M.R. Hoffmann, J. Math. Chem. 31 (2002) 105.
[5] C.E. Reid, J. Mol. Spectr. 36 (1970) 183.
[6] I.N. Sneddon, *Special Functions of Mathematical Physics and Chemistry* (Oliver and Boyd, Edinburgh, 1966).
[7] I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series, and Products* (Academic Press, New York, 1980).
[8] R.L. Somorjai and D.F. Hornig, J. Chem. Phys. 36 (1962) 1980.
[9] M. Znojil, J. Math. Phys. 35 (1992) 213.
[10] C.G. Diaz, F.M. Fernandez and E.A. Castro, J. Phys. A 21 (1988) L11.
[11] H. Taşeli, Int. J. Quantum Chem. 60 (1996) 641.
[12] P.M. Morse, Phys. Rev. 34 (1929) 57.

[13] H. Taşeli, J. Comput. Appl. Math. 115 (2000) 535.
[14] H. Taşeli, J. Phys. A 31 (1998) 779.
[15] E. Gildener and A. Patrascioui, Phys. Rev. D 16 (1977) 423.
[16] K. Banerjee and S.P. Bhatnagar, Phys. Rev. D 18 (1978) 4767.
[17] C.S. Hsue and J.L. Chern, Phys. Rev. D 29 (1984) 643.
[18] J. Killingbeck, J. Phys. A 20 (1987) 601.
[19] N. Bessis, G. Bessis and B. Joulakian, J. Phys. A 15 (1982) 3679.
[20] C.S. Lai, J. Phys. A 16 (1983) L181.
[21] M. Cohen, J. Phys. A 17 (1984) L101.
[22] K. Banerjee, S.P. Bhatnagar, V. Choudhry and S.S. Kanwal, Proc. Roy. Soc. London Ser. A 360 (1978) 575.