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Stationary anharmonic oscillators in the particle-in-a-box basis: Near-exact results

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Abstract. Variational studies employing the basis functions of the quantal particle-in-a-box model are shown to lead to accurate estimates of eigenvalues, various expectation values and eigenfunctions of the stationary anharmonic oscillator problem. Calculations involve both $zx^{2\alpha}$ and $(x^2 + zx^{2\alpha})$-type oscillators, with $\alpha = 2$, 3 and 4, both in weak and strong coupling regime. Apart from its recommendable computational simplicity, convergence of the present recipe has also been demonstrated to be quite fast. Results for the first ten states are reported. A few goodness tests for the approximate wavefunctions and consistency requirements for some properties are also performed.

Keywords. Linear variations; anharmonic oscillators; eigenvalues; eigenfunctions; basis sets.

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1. Introduction

Studies on the energy-eigenvalue problem of quantum anharmonic oscillators have become important over decades. Such calculations have relevance to molecular vibrations [1], solid state and statistical physics [2] and nonlinear quantum field theory [3, 4]. Keeping aside the practical significance, strategies of obtaining accurate estimates of eigenvalues, expectation values and wavefunctions of these oscillators have attracted considerable attention recently [5–24], both from mathematical and computational standpoints, and it is here that standard quantum-theoretical methods find extensive use and their efficiencies tested. The primary reason behind a general interest on this simple problem is that the most natural choice of perturbation theory as a candidate of finding approximate but reliable results fails here miserably [4, 7]. This is because of divergence of the corresponding perturbation series that owes its origin to the more singular nature of the perturbing potential. On the other hand, variational calculations usually involve a substantially large number of basis functions and, in most cases, convergence of the process with increasing size of the matrix Hamiltonian is not quite encouraging, especially in the strong-coupling regions and for excited states.

In perturbative approaches, divergent power-series expansions are converted to convergent forms. This is accomplished in various ways, e.g. via continued fractions [5, 6], Pade' approximants [8, 9], etc. Other ways of bypassing the divergence problem, in general, also appeared [10].

Variationally, early works by using harmonic-oscillator bases [11] and the so-called Hill determinantal method [12] were poorly convergent. But, use of scaled bases [13]

has improved the accuracy remarkably. Variants of this scheme are also known [14]. A faster convergent algorithm was next put forward [15, 16] in the Bargmann representation. Other attempts to obtain reliable results include uses of Chebyshev polynomials [17], hypervirial theorems [18] and the coherent-state ansatz [19]. Variation-perturbation approaches [20] were also pursued and some kind of effective Hamiltonian scheme or renormalization is implicit in quite a few works [21–23]. A local energy method involving Wronskians [24] has recently found notable success, however. Bounds to the eigenvalues were reported in some works as well [25, 26].

While the list of works cited above is by no means complete, the intricacies, relevance of quantum-chemical methods and immense interest on this problem are very apparent now. More important, amidst such a wide variety of approaches, a question that still remains pertinent is, whether there exists any simple yet fast-convergent algorithm of obtaining gradually improved approximate solutions to this eigenvalue problem that applies to the entire coupling range. Particularly in a variationl context, such a query becomes very relevant in view of quite a few works. For example, the coupled hypervirial-WKB approach [22], matrix-folding algorithm [23] and the method based on Riccati equation [25] are all unsuitable at large coupling strengths. Moreover, well-known consistency conditions are rarely checked in most studies. Thus, one fails to gain any clear idea about the general quality of the approximate wavefunctions, the more so in small-basis computations.

That the crux of the problem lies in the choice of a suitable basis-set in variational calculations is now transparent from what has been stated above. So, in the present communication, we take the opportunity to put forward a recipe that is (i) simple, (ii) fast-convergent, (iii) applicable to both even and odd states and (iv) works over a wide coupling range with almost equal facility. To this end, a variationl route [27–28] will be chosen by employing the trigonometric bases. These are actually the particle-in-a-box (PB) eigenstates. In a very general context, the Sturm–Liouville problem, we have recently [29] noted their advantages. Pilot calculations to the ground quartic anharmonic oscillator state has also been found to be quite encouraging, though there is neither a Gaussian prefactor nor any imposed coordinate scaling. Here, we like to report a thorough investigation and extend applications to both excited states and higher anharmonicities, including property calculations and a few checks of consistency.

The paper is organized as follows. The scheme is outlined in § 2. Desirable convergence properties are discussed in § 3, with attention to the character of the optimized wavefunction. Computational results are mainly summarized in § 4. Section 5 is reserved for a few goodness tests to emphasize the quality of computed data. Finally, conclusions of this survey are presented in § 6.

2. The method

We consider any 1-dimensional Hamiltonian of the form

$$H = -\nabla^2 + V(x), \tag{1}$$

with $V(x) = V(-x)$, and $V(x) = 0$ at $x = 0$, while $V(x) = \infty$ as $x \to \infty$. Also, here we shall be concerned only with positive semidifinite $V(x)$. The observations below then follow immediately. (i) For a given value of total energy (positive), there should exist classical turning points $\pm L_c$. (ii) In regions $|x| \gg L_c$, the quantal probability density

$[\rho_n(x) = \psi_n^*(x)\psi_n(x)]$ for some nth eigenstate would obey $\rho_n(x) \approx 0$. (iii) In view of the symmetry of the problem, the odd and even states can be treated separately.

Now, we choose the particle-in-a-box (PB) bases. Extending the usual domain $[0, L]$ to $[-L, L]$ by a change of variable, one finds two sets $\{\cos(2k-1)\pi x/2L\}$ and $\{\sin k\pi x/L\}$ of basis functions ($k = 1, 2, 3, \ldots$). These bases are symmetry-adapted. So, if it is ensured that $L \gg L_c$ which may be checked a posteriori, we may well choose the following trial function for even n:

$$\tilde{\psi}_n(N) = \sum_{k=1}^{N} C_{kn} \cos(2k-1)\pi x/2L \quad (-L \leqslant x \leqslant L). \tag{2}$$

For odd n, one would likewise employ

$$\tilde{\psi}_n(N) = \sum_{k=1}^{n} D_{kn} \sin k\pi x/L \quad (-L \leqslant x \leqslant L). \tag{3}$$

In (2) and (3), N refers to the number of bases employed while L appears as a non-linear variational parameter along with the linear ones (viz. the C's and D's). Optimization with respect to $L(L_0)$ is obviously based on the minimum-energy criterion for respective lowest states, $n = 0$ (even) and $n = 1$ (odd). One may further note, although such trial functions vanish for any $|x| \geqslant L$, they should be adequate in view of remark (ii) quoted above.

That there should exist some optimal L_0 is also clear from (2) or (3). This is due to the approach of the average potential energy towards infinity as $L \to \infty$; on the contrary, the average kinetic energy behaves in the same manner as $L \to 0$. Certainly then, a balanced finite estimate of each of these quantities would necessitate some nonzero finite L-value. Notably, L in (2) or (3) appears thus also as a natural scaling parameter.

Here, we concentrate on two cases. The first one $[H_1(\alpha)]$ refers to anharmonic effects on a harmonic oscillator potential:

$$H_1(\alpha) = -\nabla^2 + x^2 + zx^{2\alpha}, \quad \alpha = 2, 3, 4. \tag{4}$$

Pure anharmonic potential, defined by

$$H_2(\alpha) = -\nabla^2 + zx^{2\alpha}, \quad \alpha = 2, 3, 4 \tag{5}$$

is our other choice.

The method is simple to employ. We choose the Hamiltonian, take the appropriate bases from (2) and (3), fix the N-value, construct the Hamiltonian matrix and diagonalize it at a preassigned value of L. Then, in small steps, we change the value of L to find L_0 where the lowest eigenvalue attains a minimum. At this point, the eigenspectrum and properties of interest are recorded. The procedure is repeated by changing N. A major simplicity of the whole endeavour is provided by the integrals involved; these are extremely easy to evaluate.

3. Adequacy of the choice

Basically, the present scheme employs at each stage, i.e. for a given L, a straightforward linear variation. The success of such a strategy is surely dependent on the choice of

k	$\alpha = 2, z = 40{,}000$	$\alpha = 4, z = 1$
1	−0·859 461 802	0·934 413 138
2	−0·493 080 486	0·355 774 948
3	−0·134 353 345	−0·006 133 336
4	0·004 500 039	−0·014 402 461
5	0·011 161 056	0·007 074 015
6	0·001 100 014	−0·000 967 240
7	−0·000 439 783	−0·000 407 236
8	−0·000 039 515	0·000 274 333
9	0·000 013 795	−0·000 086 742
10	0·000 000 073	0·000 015 606

Table 2. Behaviour of L_0 as functions of N and z for $\bar{E}_1$ (2).

z	N	L_0/π	N	z	L_0/π
1	4	0·832	10	10	0·797
	6	0·937		100	0·547
	8	1·095		1000	0·374
	10	1·129		10000	0·303
	20	1·370		100000	0·173

the trial bases and it is here that the present recipe possesses an edge over a number of other similar approaches. So, novelty of the choice (2) or (3) as variational trial functions for the problems in hand will now be briefly considered. In this respect, the first important point is, how fast the coefficients (C's or D's) decay as k increases in (2) or (3). Table 1 shows the behaviour in two selected situations. The rate of decay, one may note, is quite fast. Secondly, an extensive search for L_0 may be avoided. This is because, L_0 follows a systematic trend. Table 2 reveals the increase with N and decrease with z of L_0 by considering a specific case. While these changes are expected on physical grounds or intuitively, what table 3 shows concerning variation with α is apparently difficult to comprehend. The decrease of L_0 with increasing α is understandable here. But, this is obeyed only in the small-z regime; for large z, one observes the reverse trend. A close scrutiny on this point is hence necessary.

An explanation emerges on the obvious assumption that L_0 increases with L_c. It becomes then transparent that the potential rises more steeply as α increases, and this is why both L_c and L_0 decrease. When z is large, however, the simple picture breaks down. Primarily, this is because of the asymptotic z-dependence of $E_n(\alpha, z)$ that goes as [8].

$$E_n(\alpha, z) = e_n(\alpha) z^{1/(\alpha+1)} (z \to \infty). \tag{6}$$

Table 3. Variation of L_0/π with α at fixed $N(N = 10)$ for the two systems.

	$H_1(\alpha)$		$H_2(\alpha)$	
α	$z = 1$	$z = 40000$	$z = 1$	$z = 40000$
2	1·1416	0·1872	1·2039	0·1873
3	0·8397	0·2252	0·8470	0·2252
4	0·6980	0·2425	0·6997	0·2425

It then follows from preliminary calculations of turning points, either for $H_1(\alpha)$ or $H_2(\alpha)$, that L_c is required to satisfy at large z

$$L_{c^2} \approx e_0(\alpha)/z^{1/(\alpha+1)}. \tag{7}$$

Now, (7) explains why L_0 increases with α for large values of z.

Two more clarifications are still required. One is, whether $L_0 \gg L_c$ is valid always in the course of the present analysis. This is very easy to check. So, for brevity, these results are not displayed. A positive answer is found in every case. Indeed, had such an inequality not been followed, results would never turn out to be so impressive. Thus, success of the recipe indirectly hints satisfaction of the above starting assumption. Another point that we wish to comment on is, how the numerical optimization of L to third or, at best, fourth decimal place (see, e.g. tables 2 and 3) affects the energy or other properties, in general. A weak dependence in this respect should be computationally convenient. But, here we refrain from a thorough discussion on this aspect. As this question is intimately connected to the quality of the optimized variational function, coverage on this point will be found in § 5.

4. Results

Tables 4 and 5 display the energy-eigenvalues $\bar{E}_n(\alpha)$ for the two classes of potentials (4) and (5). Results are remarkably accurate and comparable with the oft-quoted near-exact values of Ref. [13]. As the accuracy gradually decreases with increasing n, characteristic of linear variations, we report here data up to which agreement with standard [13] results are obtained. In all cases, however, stability to approximately 10 decimal places is always retained though we employ only 20 basis functions. For further accuracy, one only needs to increase the size of the Hamiltonian matrix—a routine numerical job.

Values for properties like $\langle x^2 \rangle$ and $\langle -\nabla^2 \rangle$ are presented in tables 6 and 7. They also agree with literature values, wherever obtained [13]. But, such results are not generally available. So, we have quoted here estimates up to 13 to 14 digits. The efficiency of our simple variational scheme is pretty apparent now. We hope, these results may be important as standard benchmark work.

5. Goodness tests

A few goodness tests are now in order. These would indicate correctness of data displayed in tables 4 to 7. Also, one would find here an opportunity to assess how

Table 4. Computed $\bar{E}_n(\alpha)$ values of anharmonic oscillators $[H_1(\alpha)]$ at $N = 20$.

n	$\alpha = 2$	$\alpha = 3$	$\alpha = 4$
$(z = 1)$			
0	1·392 351 641 530 291 856	1·435 624 619 003 392 316	1·491 019 895 662 205 17
1	4·648 812 704 212 077 536	5·033 395 937 720 266 477	5·368 778 061 748 130 171
2	8·655 049 957 759 309 688	9·966 621 999 718 110 285	10·993 737 335 502 964 04
3	13·156 803 898 049 875 08	15·989 440 787 825 731 07	18·191 100 018 514 932 45
4	18·057 557 436 303 252 90	22·910 180 430 728 544 76	26·743 448 558 041 7
5	23·297 441 451 223 189 09	30·622 590 570 533 258 64	36·509 236 308 241 9
6	28·835 338 459 504 248 87	39·051 906 854 386 110 73	47·393 379 092 02
7	34·640 848 321 111 332 59	48·141 305 571 449 512 35	59·323 544 225 67
8	40·690 386 082 106 446 90	57·845 728 456 325 8	72·241 637 072 8
9	46·965 009 505 675 533 54	68·128 291 836 139	86·099 541 860 5
$(z = 40000)$			
0	36·274 458 133 736 835 47	16·211 718 264 749 243 62	10·238 868 235 479 041 60
1	129·973 351 403 293 737 9	61·407 828 604 359 446 05	39·670 505 945 098 289 20
2	255·017 677 289 573 991 3	128·376 742 015 189 214 9	85·384 995 313 355 091 00
3	398·290 246 956 059 026 2	211·290 344 511 508 045 9	144·492 517 309 256 575 7
4	556·200 474 630 525 35	307·169 772 116 720 73	214·986 131 730 878
5	726·403 686 448 354 09	414·453 587 749 839 37	295·660 523 015 272
6	907·329 749 584 430 3	532·031 545 974 230 4	385·708 384 533 62
7	1097·832 281 319 199	659·065 528 349 994 5	484·514 056 324 43
8	1297·030 657 029 7	794·894 932 499 66	591·584 145 929 7
9	1504·223 045 054 7	938·981 406 361 52	706·511 061 163 9

Table 5. Computed $\bar{E}_n(\alpha)$ values for pure oscillators $[H_2(\alpha)]$ at $N = 20$.

n	$\alpha = 2$	$\alpha = 3$	$\alpha = 4$
$(z = 1)$			
0	1·060 362 090 484 182 900	1·144 802 453 797 052 764	1·225 820 113 800 492 589
1	3·799 673 029 801 394 169	4·338 598 711 513 981 192	4·755 874 413 960 760 520
2	7·455 697 937 986 738 392	9·073 084 560 921 433 861	10·244 946 977 236 870 80
3	11·644 745 511 378 162 02	14·935 169 634 910 736 03	17·343 087 970 585 609 98
4	16·261 826 018 850 225 94	21·714 165 422 196 722 80	25·809 006 751 297 9
5	21·238 372 918 235 940 03	29·299 645 937 401 893 78	35·497 898 805 171 8
6	26·528 471 183 682 518 27	37·613 086 560 895 194 00	46·312 770 495 05
7	32·098 597 710 968 326 86	46·595 211 448 551 772 09	58·179 649 949 71
8	37·923 001 027 033 986 79	56·199 300 852 500 4	71·039 257 676 3
9	43·981 158 097 289 736 50	66·387 281 706 593	84·842 624 592 7
$(z = 40000)$			
0	36·263 873 389 915 441 73	16·189 951 563 977 905 42	10·205 604 674 423 291 48
1	129·946 989 723 931 049 7	61·357 051 395 175 074 53	39·595 184 973 435 355 93
2	254·981 282 792 887 419 8	128·312 792 386 130 299 1	85·294 634 655 606 736 20
3	398·244 694 592 561 819 1	211·215 194 540 335 894 0	144·390 435 161 638 914 9
4	556·146 626 825 504 84	307·084 672 356 835 09	214·873 713 506 492
5	726·342 136 734 665 83	414·359 566 574 035 14	295·538 895 062 724
6	907·260 952 524 099 9	531·929 371 371 311 8	385·578 456 193 11
7	1097·756 600 156 166	658·955 799 721 840 2	484·376 541 711 32
8	1296·948 391 643 0	794·778 134 614 92	591·439 618 295 2
9	1504·134 449 069 7	938·857 941 585 47	706·359 992 287 2

Table 6. Mean square displacements and average kinetic energies for the first ten states of $H_1(\alpha)$ at $N = 20$.

		$\langle x^2 \rangle$		$\langle -\nabla^2 \rangle$	
α	n	$z = 1$	$z = 40000$	$z = 1$	$z = 40000$
2	0	0·305 813 650 718	0·010 583 881 287	0·826 296 544 114	24·179 444 128 73
	1	0·801 250 595 541	0·026 360 242 520	2·832 124 937 628	86·640 114 188 02
	2	1·155 440 519 200	0·036 393 331 691	5·384 886 465 440	169·999 653 749 2
	3	1·467 523 215 391	0·045 551 185 855	8·282 028 193 570	265·511 647 575 4
	4	1·750 939 501 761	0·053 846 632 183	11·454 725 123 62	370·782 367 542 9
	5	2·014 067 745 278	0·061 548 542 567	14·860 271 719 06	484·248 608 118 0
	6	2·261 703 958 855	0·068 795 890 247	18·469 657 653 38	604·863 567 758 6
	7	2·496 957 081 437	0·075 679 993 598	22·261 579 853 60	731·862 960 881 1
	8	2·721 984 850 987	0·082 264 217 733	26·219 595 771 08	864·659 683 287 5
	9	2·938 362 108 797	0·088 594 816 340	30·330 552 300 85	1002·785 831 762
3	0	0·275 058 719 125	0·021 760 150 814	0·939 189 104 690	12·147 908 623 15
	1	0·672 320 074 176	0·050 768 587 541	3·438 886 916 202	46·030 487 159 50
	2	0·882 083 484 881	0·063 946 002 760	7·033 924 757 348	96·250 583 510 01
	3	1·045 462 539 517	0·075 147 043 401	11·469 349 321 11	158·430 184 861 9
	4	1·188 346 123 442	0·085 097 160 029	16·588 462 261 32	230·334 780 507 5
	5	1·316 082 578 838	0·094 018 831 047	22·308 901 638 48	310·793 181 396 9
	6	1·432 555 255 303	0·102 172 450 727	28·572 652 513 14	398·972 573 255 3
	7	1·540 292 104 466	0·109 726 627 310	35·335 833 126 35	494·244 282 948 8
	8	1·640 998 542 235	0·116 796 007 033	42·563 797 071 13	596·112 801 371 2
	9	1·735 889 945 138	0·123 463 001 099	50·228 273 904 52	704·174 323 270 5
4	0	0·253 957 749 812	0·033 241 708 529	1·040 441 266 642	8·171 149 563 27
	1	0·598 857 545 807	0·075 295 431 260	3·935 707 921 914	31·691 227 497 32
	2	0·744 787 196 663	0·090 355 310 117	8·348 117 550 403	68·253 783 064 62
	3	0·845 935 134 230	0·102 079 152 686	14·045 318 934 27	115·532 766 355 79
	4	0·932 834 785 354	0·112 415 736 233	20·835 057 975 23	171·921 455 943 03
	5	1·009 985 263 283	0·121 625 795 626	28·601 397 888 63	236·455 442 934 85
	6	1·079 440 668 553	0·129 926 447 414	37·267 038 872 59	308·488 751 759 53
	7	1·142 863 779 829	0·137 512 924 652	46·773 117 112 73	387·528 737 304 96
	8	1·201 454 698 458	0·144 526 104 338	57·072 436 839 68	473·180 601 086 89
	9	1·256 076 644 509	0·151 067 479 828	68·125 987 501 79	565·118 208 446 54

far the accuracy in estimating L_0 affects the computed data for observables, a question that has been raised towards the end of § 3.

The virial theorem [30] will be considered first. For $H_1(\alpha)$, it states that

$$\langle -\nabla^2 \rangle = \langle x^2 \rangle + \alpha z \langle x^{2\alpha} \rangle, \tag{8}$$

by virtue of which the average energy for any state would satisfy

$$\langle H \rangle = 2\langle x^2 \rangle + (\alpha + 1) z \langle x^{2\alpha} \rangle = E_v. \tag{9}$$

So, if $\bar{E}_n$ refers to the eigenvalue of the matrix problem and E_v is the energy obtained from (9) by computing the relevant moments for state n, we should have

$$|\bar{E}_n(\alpha)/E_v(\alpha) - 1| = 0. \tag{10}$$

Table 7. Mean square displacements and average kinetic energies for the first ten states of $H_2(\alpha)$ at $N = 20$.

		$\langle x^2 \rangle$		$\langle -\nabla^2 \rangle$	
α	n	$z = 1$	$z = 40000$	$z = 1$	$z = 40000$
2	0	0·362 022 648 789	0·010 585 606 467	0·706 908 060 323	24·175 915 593 28
	1	0·901 605 895 820	0·026 363 116 323	2·533 115 353 201	86·631 326 482 62
	2	1·244 714 121 511	0·036 395 661 703	4·970 465 291 991	169·987 521 861 9
	3	1·557 909 193 537	0·045 553 541 164	7·763 163 674 252	265·496 463 061 7
	4	1·841 609 138 552	0·053 848 977 879	10·841 217 345 90	370·764 417 883 7
	5	2·105 010 651 065	0·061 550 884 828	14·158 915 278 82	484·228 091 156 4
	6	2·352 866 384 212	0·068 798 230 431	17·685 647 455 79	604·840 635 015 1
	7	2·588 299 362 716	0·075 682 332 484	21·399 065 140 65	731·837 733 437 0
	8	2·813 476 631 178	0·082 266 555 751	25·282 000 684 69	864·632 261 102 2
	9	3·029 980 037 256	0·088 597 153 750	29·320 772 064 86	1002·756 299 377
3	0	0·307 920 303 733	0·021 773 253 483	0·858 601 840 348	12·142 463 672 98
	1	0·718 220 132 308	0·050 785 832 594	3·253 949 033 635	46·017 788 546 38
	2	0·904 435 592 147	0·063 953 254 035	6·804 813 420 691	96·234 594 289 59
	3	1·062 822 482 158	0·075 152 898 433	11·201 377 226 18	158·411 395 905 3
	4	1·203 529 109 137	0·085 102 359 443	16·285 624 066 65	230·313 504 267 6
	5	1·329 693 376 533	0·094 023 520 345	21·974 734 453 05	310·769 674 930 5
	6	1·444 997 526 013	0·102 176 754 944	28·209 814 920 66	398·947 028 528 5
	7	1·551 825 435 504	0·109 730 628 866	34·946 408 586 41	494·216 849 791 4
	8	1·651 798 079 925	0·116 799 762 347	42·149 475 639 39	596·083 600 961 1
	9	1·746 080 708 075	0·123 466 550 918	49·790 461 279 93	704·143 456 189 0
4	0	0·277 118 934 339	0·033 285 432 315	0·980 656 091 040	8·164 483 739 54
	1	0·627 299 876 815	0·075 346 520 948	3·804 699 531 169	31·676 147 978 75
	2	0·752 344 968 196	0·090 365 992 408	8·195 957 581 785	68·235 707 724 48
	3	0·849 913 091 187	0·102 085 138 058	13·874 470 376 47	115·512 348 129 31
	4	0·935 962 229 723	0·112 420 710 340	20·647 205 401 05	171·898 970 805 21
	5	1·012 635 366 092	0·121 630 108 093	28·398 319 044 14	236·431 116 050 19
	6	1·081 738 316 981	0·129 930 232 371	37·050 216 396 17	308·462 764 954 66
	7	1·144 896 373 375	0·137 516 300 845	46·543 719 959 89	387·501 233 369 27
	8	1·203 282 142 484	0·144 529 158 241	56·831 406 141 69	473·151 694 638 50
	9	1·257 740 403 671	0·151 070 273 055	67·874 099 674 36	565·087 993 833 11

Table 8 shows how far (10) is obeyed in our scheme. We happily note, accuracy to 10 decimal places always persists. This implies, dependence of results on accuracy in L_0 is very feeble, as wanted. Also, it is now clear that if we compute $\langle x^{2\alpha} \rangle$ on the basis of (8) and table 6, results should be correct up to 10 decimal places at least. This is precisely why we have not separately displayed data for the said property. A similar error level is likely when $\langle x^{2\alpha} \rangle$ will be estimated through the virial theorem and table 7 for $H_2(\alpha)$. So, these values also are not tabulated, for brevity.

In the above context, let us finally notice that satisfaction of (8) does not follow directly on the ground that (2) or (3) is ultimately optimally scaled. This assertion [30] is true only when one optimizes the scale parameter analytically. As we have performed a numerical optimization here, which is partial, significance of goodness test via (8) or (9) is still retained.

Another criterion of accuracy of data is provided by (6). Table 9 presents demonstrative calculations in this regard for ground states. With $N = 10$, we already obtain stability

Table 8. Satisfaction of the virial theorem for $H_1(\alpha)$ in the form $|\bar{E}_n(\alpha)/E_v(\alpha) - 1| = 0$. Results refer to the lhs in 20-basis calculations. Values beyond $10^{-14}(\equiv E\text{-}14)$ are considered zero.

	$\alpha = 2$		$\alpha = 3$		$\alpha = 4$	
n	$z = 1$	$z = 40000$	$z = 1$	$z = 40000$	$z = 1$	$z = 40000$
0	0·0	0·0	0·0	0·0	0·0	0·0
1	0·0	0·0	0·0	0·0	0·0	0·0
2	0·0	0·0	6·0 E-13	1·9 E-13	6·3 E-13	1·0 E-13
3	0·0	0·0	1·6 E-14	0·0	2·5 E-13	9·9 E-14
4	0·0	1·0 E-13	2·7 E-12	1·9 E-13	1·4 E-12	1·5 E-12
5	0·0	6·8 E-14	1·1 E-13	0·0	2·5 E-13	1·3 E-13
6	0·0	3·3 E-12	1·0 E-13	1·0 E-13	1·1 E-11	1·4 E-11
7	0·0	1·3 E-12	3·0 E-13	2·3 E-14	2·0 E-12	2·2 E-12
8	0·0	1·6 E-11	8·0 E-13	3·9 E-13	3·6 E-11	4·9 E-11
9	0·0	8·0 E-12	6·4 E-13	2·9 E-13	7·7 E-12	2·3 E-11

Table 9. Convergence of $\bar{E}_0(\alpha)/z^{1/(\alpha+1)}$ towards a constant value for $H_1(\alpha)$ at $N = 10$.

z	$\alpha = 2$	$\alpha = 3$	$\alpha = 4$
10000	1·061	1·148	1·233
20000	1·060 9	1·147	1·231
40000	1·060 7	1·146 3	1·229 8
60000	1·060 60	1·146 1	1·229 2
80000	1·060 56	1·145 89	1·228 85
100000	1·060 53	1·145 78	1·228 59

to 3rd or 4th decimal place. Naturally, results would converge better for $N = 20$. The actual relation

$$E_n(\alpha)/z^{1/(\alpha+1)} = e_n(\alpha) + O(z^{-2/(\alpha+1)}) \quad (z \to \infty), \tag{11}$$

obtained by Symanzik scaling argument [8], also implies that neglected terms are likely to affect 3rd place of decimal or beyond for the region of z considered. So, our results are quite accurate.

While the credibility of energy-eigenvalues is thus justified above, now we shall see whether the average values also obey the asymptotic (large-z) behaviour properly. Noting for $H_1(\alpha)$ that

$$\langle x^{2\alpha} \rangle = \mathrm{d}E_n(\alpha)/\mathrm{d}z, \tag{12}$$

we use (11) to arrive at the following relation

$$z\langle x^{2\alpha} \rangle / E_n(\alpha) = 1/(\alpha + 1) + O(z^{-2/(\alpha+1)}) \quad (z \to \infty). \tag{13}$$

Table 10 shows how well (13) is satisfied. Here, we see betterment for smaller α-value. This is expected. Generally, accuracy decreases as α increases. Of interest is to also

Table 10. Verification of $z\langle x^{2\alpha}\rangle/\bar{E}_n(\alpha) = 1/(1+\alpha)$ at $z = 40000$ with different N for a few even states.

		n		
α	N	0	2	4
2	5	0·333 139	0·334 125	0·370 553
	10	0·333 139	0·333 238	0·333 269
	20	0·333 139	0·333 238	0·333 269
4	5	0·198 703	0·198 290	0·192 076
	10	0·198 701	0·199 577	0·199 789
	20	0·198 701	0·199 577	0·199 791

Table 11. Dependence of $z\langle x^{2\alpha}\rangle/\bar{E}_n(\alpha)$ on n at $\alpha = 3$, $N = 20$, $z = 40000$.

n	$z\langle x^{2\alpha}\rangle/\bar{E}_n(\alpha)$
0	0·249 329
1	0·249 587
2	0·249 751
3	0·249 822
4	0·249 861
5	0·249 887
6	0·249 904
10	0·249 941
15	0·249 960

note that, while results become worse with n for smaller N, a gradual betterment is observed with increasing n at large N. Since small-N data are not dependable because of inherent errors in both $\langle x^{2\alpha}\rangle$ and $\bar{E}_n(\alpha)$, we value the latter part more and presume that results would improve systematically with n for accurate data. This is exactly what a sample calculation in table 11 reveals. Thus, a sort of classicality, i.e. better results for larger n, may be hidden in the present scheme.

6. Final remarks

Summarizing, we have put forward a very simple scheme of obtaining quite accurate results of various anharmonic oscillators. Major advantages of the present endeavour are fast convergence and simplicity. Energies and important average values of the first ten states are reported here for all the anharmonic oscillators usually considered in the literature. These tabulated data satisfy a number of criteria which the 'exact' results should obey, providing additional testimony of the reliability of our computations. Still more accuracy may be gained just by increasing N.

Only anharmonic oscillators are chosen here as examples. But, our recipe is likely to be equally efficient in solving any bound-state 1-dimensional polynomial potential problem which may correspond to physically relevant situations, e.g. double wells. Here lies its generality. Further work along this direction is in progress.

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