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Convergent method for calculating the eigenvalues of anharmonic potentials

M.A.M. de Aguiar and A.L. Xavier Jr.
Instituto de Física "Gleb Wataghin", Universidade Estadual de Campinas, 13081 Campinas, SP, Brazil

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We present a powerful and very simple method to calculate the eigenvalues of one-dimensional Hamiltonians of the form $H=\frac{1}{2}p^2+\sum_{k=1}^{m}a_k x^{2k}$. The method converges extremely fast for $m\geqslant 2$. We show that $E_n\sim n^{2m/(m+1)}$ for large n and verify it numerically for $m=2$ and 3.

The numerical solution of the eigenvalue equation $H\psi=E\psi$ for the Hamiltonian $H(p,\ x)=\frac{1}{2}p^2+\beta x^2+\lambda x^4$ has been considered as a paradigm for the failure of the usual perturbation theories in the parameter λ. In fact, the perturbation series based on harmonic oscillator eigenfunctions can be shown to be asymptotic and have zero convergence radius [1,2]. A number of methods have been developed in the past years to minimize this difficulty, from variational techniques to renormalization procedures, most directed to the calculation of the ground state energy [3]. Other methods, based again on harmonic oscillator wave functions, have been used to get the low energy part of the spectrum with good accuracy [4], but only for small enough values of λ. In this Letter we propose and test numerically a new method, based on infinite-square-well wave functions, that works very well for all Hamiltonians of the form

$$H=\tfrac{1}{2}p^2+\sum_{k=1}^{m}a_k x^{2k}\,, \tag{1}$$

independent of how large the coefficients a_k might be. Contrary to other methods, the larger the m the faster the process converges.

In order to make our procedure intuitive, let us first look at the matrix elements $H_{kn}=\langle\varphi_k|H|\varphi_n\rangle$ where $|\varphi_n\rangle$ are the wave functions for the oscillator

$$H_0=\tfrac{1}{2}p^2+a_1 x^2\,.$$

A simple calculation shows that H_{kn} is a band-diagonal matrix. A term like x^{2l} in the Hamiltonian produces several off-diagonal elements, including those proportional to $(n\hbar)^l\delta_{k,n-2l}$. Every power of x also contributes to the diagonal elements, including the $(n+\frac{1}{2})\hbar$ term from the oscillator H_0. Then it is clear that for small $\hbar$, there is always a N_0 such that the truncated matrix $N_0\times N_0$ has all off-diagonal terms smaller than the diagonal ones. However, as the matrix size increases the off-diagonal elements start to dominate and, from this point, increasing the size of the matrix affects all eigenvalues and no stabilization is obtained. From the classical point of view this corresponds to energies such that a_2x^4 dominates over a_1x^2 and, therefore, the former cannot be thought as a perturbation of the latter. In fact, for very high energies, the Hamiltonian (1) can be approximated by

$$H\simeq\tfrac{1}{2}p^2+a_m x^{2m}\,, \tag{2}$$

with classical turning points at

$$L=\left(\frac{E}{a_m}\right)^{1/2m}\,. \tag{3}$$

If m is large the potential $a_m x^{2m}$ is very steep and, therefore, an infinite square-well with width L is a

much better representation for this system than a harmonic well. This is made clearer when one realizes that the square well potential may be seen as

$$S(x)=\lim_{k\to\infty}(x/L)^{2k}.$$

Then, any power like x^{2m} is small compared to $S(x)$ and the perturbation theory should work well. In terms of matrix elements this implies that the off-diagonal terms $\langle\Psi_k|H|\Psi_n\rangle$ are always smaller than the diagonal ones if $|\Psi_n\rangle$ are the square-well wave functions.

Of course the wave functions $|\psi_n\rangle$ go to zero at $x=\pm L$ and those of eq. (1) do not. However, if $m\geqslant 2$ the wave functions go to zero very fast (like $\exp(-|x|^{K+1})$) and, choosing L properly, a large number of eigenvalues can be easily obtained. In fact, for high energies, a simple calculation shows that the eigenenergies of eq. (1) behave like $E_n\sim n^{2m/(m+1)}$. To see this, consider the energies of the square-well given by

$$E_n=\frac{\hbar^2\pi^2n^2}{8L^2}.$$

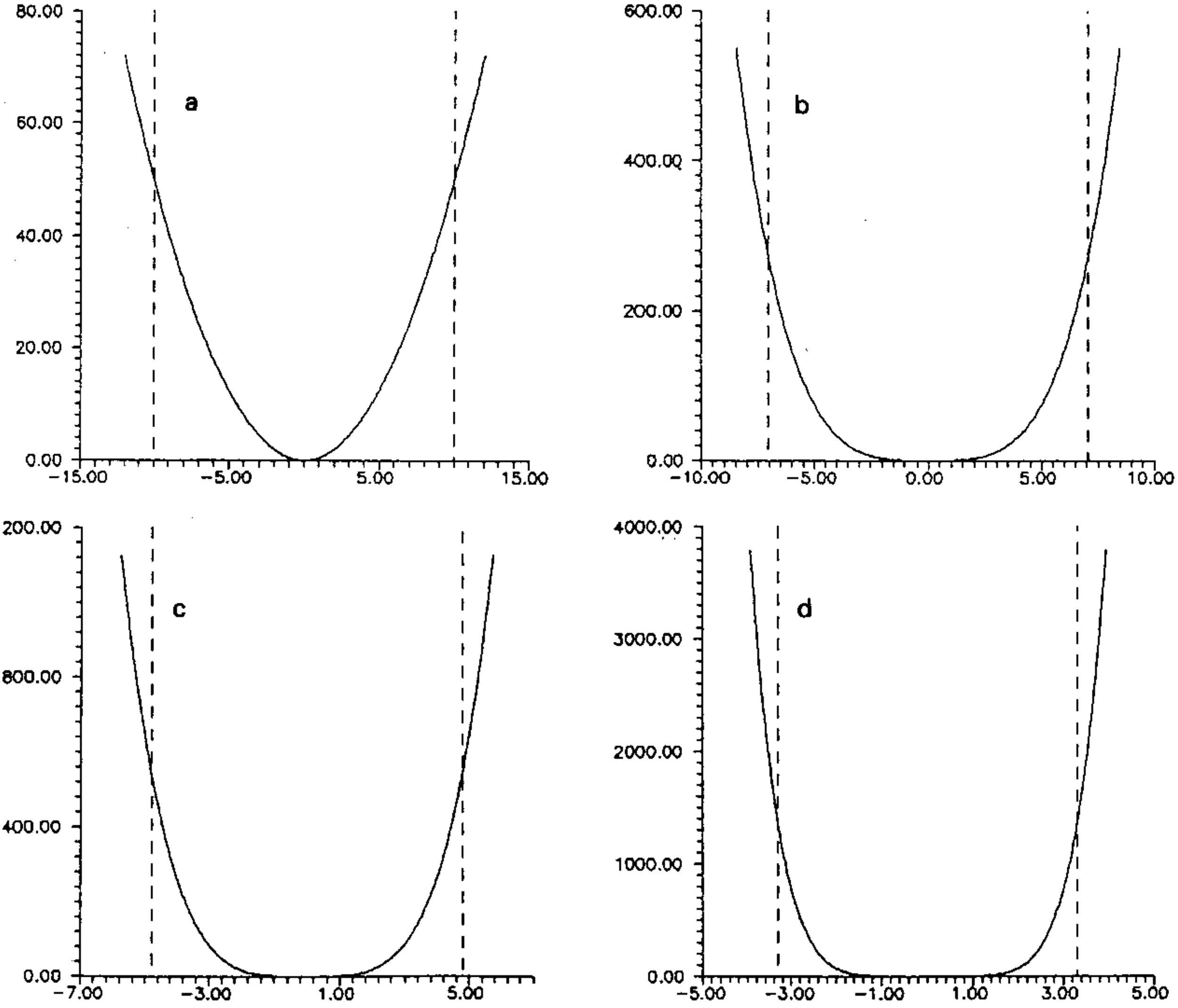

Fig. 1. The anharmonic potentials (full lines) are plotted against the square-well (dotted lines) for the cases (a) $\beta=\frac{1}{2}$, $\lambda=\delta=0$; (b) $\beta=\frac{1}{2}$, $\lambda=0.1$, $\delta=0$; (c) $\beta=\frac{1}{2}$, $\lambda=1.0$, $\delta=0$ and (d) $\beta=\lambda=\frac{1}{2}$, $\delta=0$.

If one now approximates the Hamiltonian (1) by the square-well and realizes that the "width" L depends on E like in eq. (3) one obtains

$$E_n = \frac{\hbar^2\pi^2 n^2}{8(E_n/a_m)^{1/m}} .$$

Solving for E_n gives

$$E_n = (\tfrac{1}{8}\pi^2\hbar^2 a^{1/m})^{m/(m+1)} n^{2m/(m+1)} . \qquad (4)$$

Notice that for $m=1$ eq. (3) gives $E_n = \text{const}\times n$, and for $m\to\infty$ it gives $E_n = \text{const}\times n^2$, which are the correct power laws for the harmonic oscillator and square-well respectively. For $m>1$ eq. (3) interpolates between the two. Actually, eq. (3) can also be obtained from the WKB approximation in the limit of high energies.

Therefore, we propose that the eigenvalues of (1) should be calculated by diagonalizing the Hamiltonian in a proper square-well basis. This basis is obtained as follows: given the size N of the matrix to be diagonalized, eq. (4) is used with $n=N$ to estimate a maximum energy $\bar{E}$ up to which we expect good convergence of the eigenvalues (conversely, given $\bar{E}$ we estimate N). Then, eq. (3) is used to obtain the square-well width $L=(\bar{E}/a_m)^{1/2m}$. With these definitions the basis states are simply

$$\psi_n(x) = \frac{1}{\sqrt{L}} \sin(\tfrac{1}{2}n\pi x/L - \tfrac{1}{2}n\pi) .$$

Notice that the matrix elements $\langle\psi_k|x^{2l}|\psi_n\rangle$ can be easily evaluated analytically.

We now particularize for the Hamiltonian

$$H(x,p) = \tfrac{1}{2}p^2 + \beta x^2 + \lambda x^4 + \delta x^6 \equiv \tfrac{1}{2}p^2 + U(x) \qquad (5)$$

and we present the results of numerical calculations for four situations ($\hbar=1$):

(a) $\beta=\frac{1}{2}$, $\lambda=\delta=0$,

(b) $\beta=\frac{1}{2}$, $\lambda=0.1$, $\delta=0$,

(c) $\beta=\frac{1}{2}$, $\lambda=1.0$, $\delta=0$,

(d) $\beta=\frac{1}{2}$, $\lambda=\frac{1}{2}$, $\delta=1.0$.

In figs. 1a–1d we show the potential $U(x)$ for each of the situations above and the square-well that fits in each case.

The worst case is (a). Table 1 shows the eigenenergies from the 31st to the 50th state of a 64×64 diagonalization (actually 32×32 for the even states plus 32×32 for the odd) and we see that even in this case the first 33 states are in very good agreement (9 figures) with the exact result. In table 2 we present the results for case (b) (see caption). The ground state for this set of parameters has been obtained from variational methods [#1] and agree with our results to all decimal places displayed in ref. [1]. We have diagonalized first a 100×100 matrix and then a 200×200 matrix. The first 61 eigenvalues of the former agree to 10 decimal places to those of the latter, showing a very strong convergence (60% of the total).

Table 1
Eigenenergies 31–50 for the harmonic oscillator (case (a)). The first 30 energies (not shown) agree with the exact result with all figures used in the table.

31	30.5000000	41	40.5009624
32	31.5000000	42	41.5023567
33	32.5000001	43	42.5054289
34	33.5000004	44	43.5117390
35	34.5000014	45	44.5237825
36	35.5000047	46	45.5451020
37	36.5000151	47	46.5801143
38	37.5000464	48	47.6336190
39	38.5001348	49	48.7101415
40	39.5003706	50	49.8133731

For situation (c), the convergence is even better. Fig. 2 displays a plot of $\log E_n$ versus $\log n$ for the converged eigenvalues of cases (b) and (c), showing very good agreement with the prediction of eq. (3) (for both cases a 100×100 diagonalization has been performed).

The convergence for the sextic oscillator, case (d), is, as expected, even stronger. Table 3 presents the results of a 200×200 and 300×300 diagonalization (only the first 10 and the 110th to 140th states are shown). It is seen that the first 119 states of both calculations agree up to 14 decimal places, and the first 150 agree up to 6 decimal places. Fig. 3 shows again $\log E_n$ versus $\log n$ for this case, confirming again the power law of eq. (3).

We have also computed the eigenvalues of Hamiltonian (5) in cases where $\beta<0$ and $\lambda>0$ and found again very fast convergence.

[#1] See for instance ref. [1]. Notice that our energies are twice as large as those in ref. [1] due to a different definition of the Hamiltonian.

Table 2
First 20 and 60th–80th energies for $\beta=\frac{1}{2}$, $\lambda=0.1$, $\delta=0$ (case (b)). The second column shows the results of a 100×100 diagonalization and the third column the results of a 300×300 diagonalization. Again, the energies 21–59 (not shown) of both calculations coincide up to 9 figures.

1	0.5591463	0.5591463	60	157.0994258	157.0994257
2	1.7695026	1.7695026	61	160.5327704	160.5327704
3	3.1386243	3.1386243	62	163.9840018	163.9840017
4	4.6288828	4.6288828	63	167.4529313	167.4529312
5	6.2203009	6.2203009	64	170.9393753	170.9393749
6	7.8997672	7.8997672	65	174.4431548	174.4431540
7	9.6578400	9.6578400	66	177.9640958	177.9640940
8	11.4873156	11.4873156	67	181.5020287	181.5020246
9	13.3824748	13.3824748	68	185.0567890	185.0567801
10	15.3386420	15.3386420	69	188.6282177	188.6281983
11	17.3519076	17.3519076	70	192.2161622	192.2161212
12	19.4189434	19.4189434	71	195.8204799	195.8203945
13	21.5368743	21.5368743	72	199.4410402	199.4408674
14	23.7031866	23.7031866	73	203.0777362	203.0773926
15	25.9156598	25.9156598	74	206.7304941	206.7298259
16	28.1723150	28.1723150	75	210.3993293	210.3980266
17	30.4713752	30.4713752	76	214.0842404	214.0818570
18	32.8112340	32.8112340	77	217.7861708	217.7811823
19	35.1904307	35.1904307	78	221.5040597	221.4958706
20	37.6076303	37.6076303	79	225.2402283	225.2257929
			80	228.9946399	228.9708228

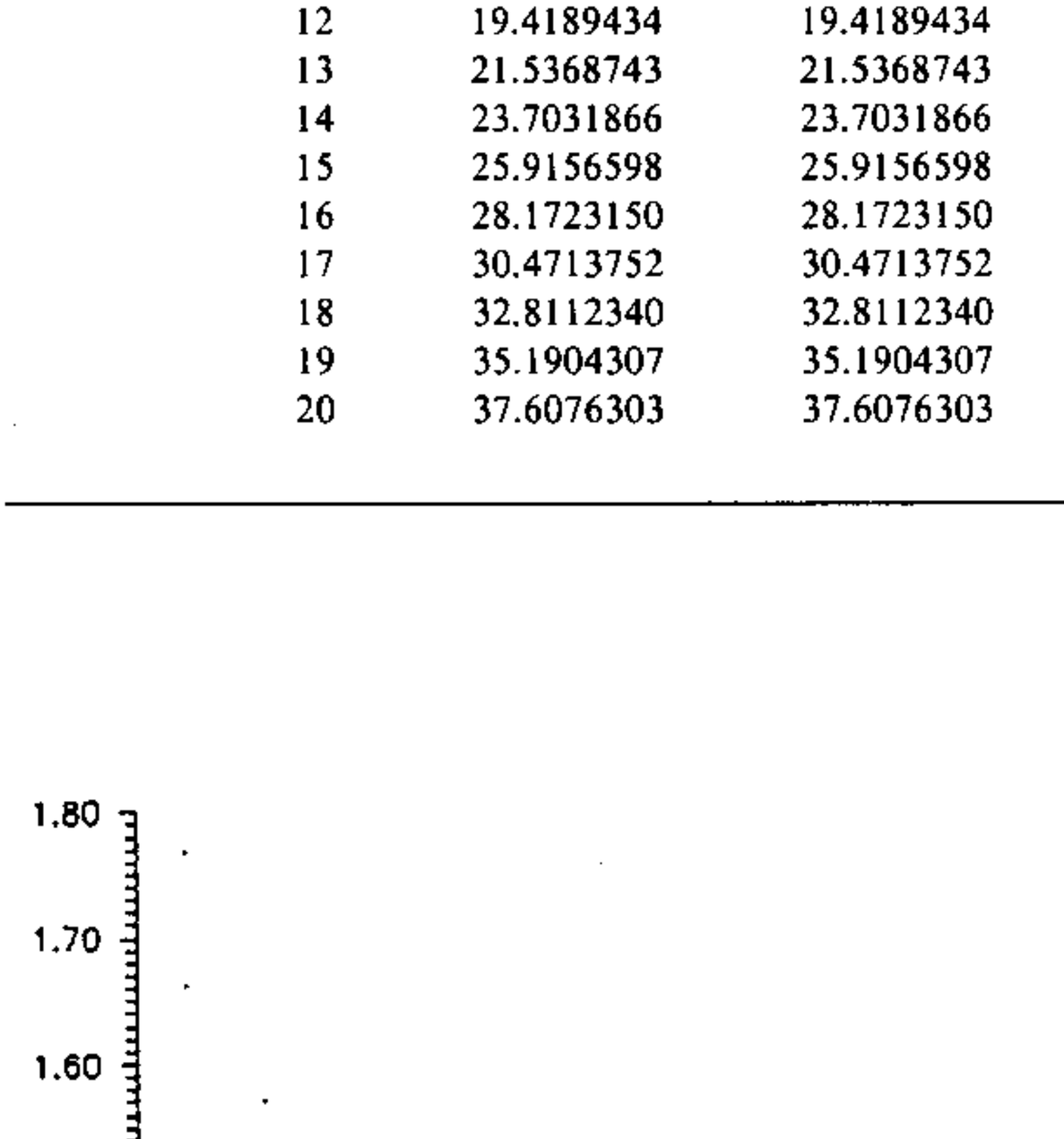

Fig. 2. Log E_n versus log n for cases (b) (lower curve) and (c) (upper curve). The dashed line indicates the asymptotic behavior $\frac{4}{3}$ according to eq. (4).

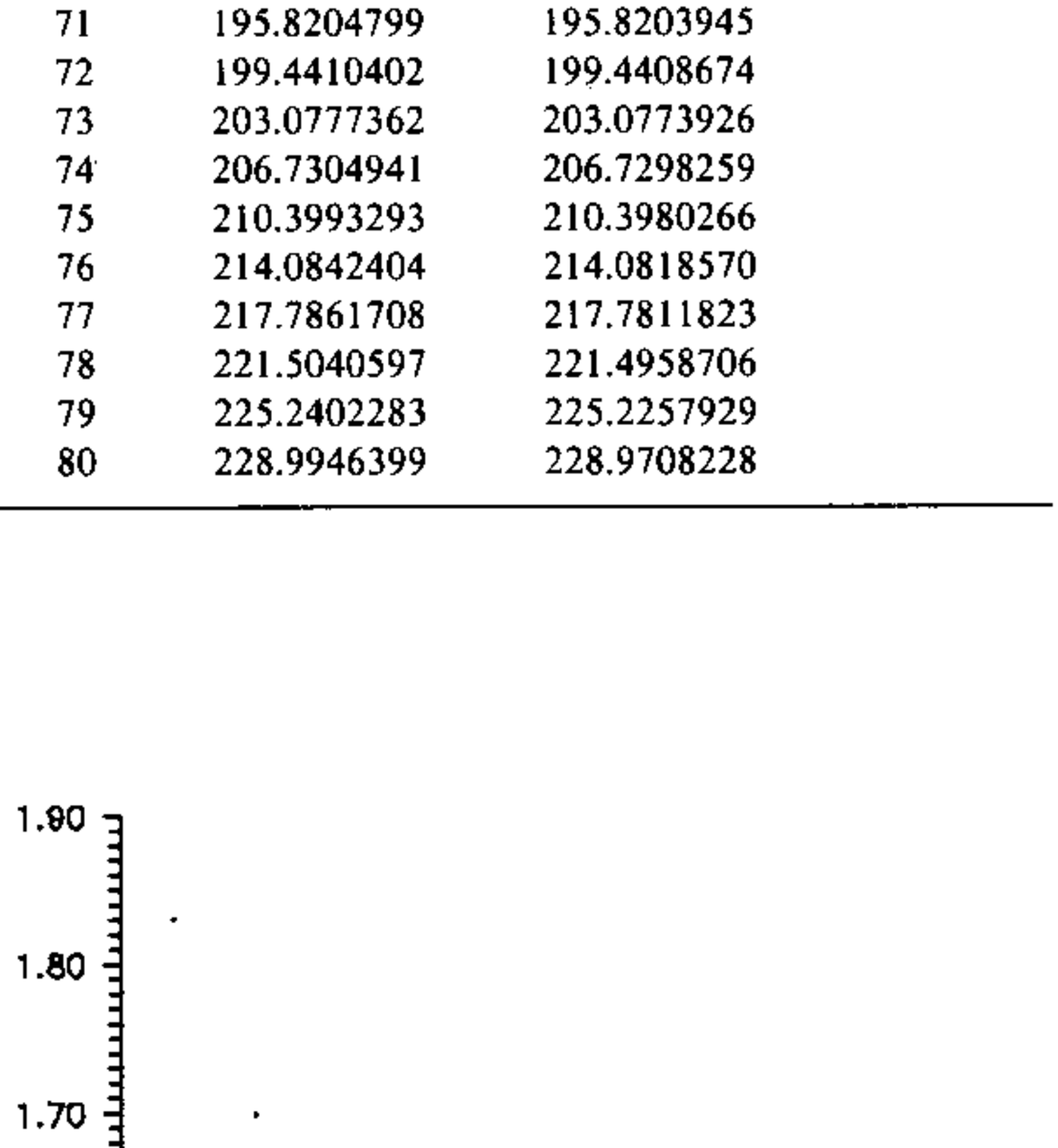

Fig. 3. Log E_n versus log n for case (d). The dashed line indicates the asymptotic behavior $\frac{3}{2}$.

Table 3
First 10 and 115th–140th energies for $\beta=\lambda=\frac{1}{2}$, $\delta=1.0$ (case (d)). The results are for a 200×200 matrix (second column) and a 300×300 matrix (third column). The energies 11–114 (not shown) also coincide up to 14 figures.

1	0.8746434986	0.8746434986	122	1828.9697254472	1828.9697254469
2	3.1113928416	3.1113928416	123	1851.4815436300	1851.4815436295
3	6.1972326442	6.1972326442	124	1874.0845872640	1874.0845872631
4	9.9327731892	9.9327731892	125	1896.7784865797	1896.7784865780
5	14.2063201790	14.2063201790	126	1919.5628762683	1919.5628762651
6	18.9537131297	18.9537131297	127	1942.4373953925	1942.4373953865
7	24.1296504930	24.1296504930	128	1965.4016873005	1965.4016872893
8	29.6998402405	29.6998402405	129	1988.4553995421	1988.4553995215
9	35.6371491991	35.6371491991	130	2011.5981837877	2011.5981837501
10	41.9194016778	41.9194016778	131	2034.8296957496	2034.8296956813
			132	2058.1495951065	2058.1495949835
115	1673.9733516661	1673.9733516661	133	2081.5575454316	2081.5575452113
116	1695.8358435615	1695.8358435615	134	2105.0532141242	2105.0532137325
117	1717.7922822205	1717.7922822205	135	2128.6362723480	2128.6362716566
118	1739.8422639326	1739.8422639326	136	2152.3063949767	2152.3063937650
119	1761.9853901477	1761.9853901477	137	2176.0632605514	2176.0632584431
120	1784.2212673670	1784.2212673669	138	2199.9065512559	2199.9065476147
121	1806.5495070370	1806.5495070368	139	2223.8359529194	2223.8359466770
			140	2247.8511550606	2247.8511444382

To conclude, the infinite square-well basis works very well for anharmonic potentials and results in a strongly convergent algorithm. Although extremely simple, this method seems to solve the old quantum mechanical challenge of computing the spectrum of such systems and may be of value for computational calculations in several fields of physics.

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