Comment on ''Strongly convergent method to solve one-dimensional quantum problems''

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Vargas *et al.* [Phys. Rev. E **53**, 1954 (1996)] presented a numerical matrix method to solve the one-dimensional Schrödinger equation subject to Dirichlet boundary conditions. It is a well-known fact that the eigensolutions of such a confined system converge asymptotically to those of the corresponding unbounded problem as the boundary value increases. However, it is verified computationally that the results given by Vargas *et al.* are inaccurate, especially for the excited states of the perturbed oscillator Hamiltonian. [S1063-651X(97)03606-4]

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In a recent article by Vargas *et al.* [1], Lindberg's matrix approach was used to solve the Schrödinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+\sum_{k=1}^{M}\alpha_k x^{2k}\right)\Psi(x)=E\Psi(x),$$

$$\Psi\in L_2(-R,R), \tag{1}$$

where

$$\Psi(-R)=\Psi(R)=0 \tag{2}$$

and $L_2(-R,R)$ is the Hilbert space of square-integrable functions. Such a modification of the usual asymptotic boundary conditions at $\pm\infty$ and the consideration of the Dirichlet problem, in which the boundary value R is regarded as a nonlinear optimization parameter, was realized previously by the present author as well [2–4]. The eigenvalues of the Dirichlet problem so defined are upper bounds to the eigenvalues of the usual unbounded system. Moreover, we deduced that the von Neumann boundary-value problem, for which the wave function obeys the conditions

$$\Psi'(-R)=\Psi'(R)=0, \tag{3}$$

generates lower-bound eigenvalues in this context [2,3].

Unfortunately, however, it appears that the authors in [1] were completely unaware of our earlier studies. Therefore, the main purpose of this comment is to show that the well-founded variational methods using the matrix representation of the Hamiltonian are superior to numerical matrix methods.

We sketch briefly here some of the findings of our recent articles. Introducing the coordinate transformation

$$\xi=\frac{\pi}{R}x, \quad \xi\in[-\pi,\pi], \tag{4}$$

the Schrödinger equation may be rewritten in the form

$$\left[-\frac{d^2}{d\xi^2}+\frac{2R^2}{\pi^2}V(\xi)\right]\Psi(\xi)=\frac{2R^2}{\pi^2}E\Psi(\xi),$$

$$\Psi\in L_2(-\pi,\pi), \tag{5}$$

with a rescaled potential function $V(\xi)$. Now the limiting case $R\to 0$ leads to the simple boundary-value problem

$$-\frac{d^2\Psi}{d\xi^2}=\lambda\Psi, \quad \Psi(-\pi)=\Psi(\pi)=0, \tag{6}$$

having the normalized sequences of eigenfunctions

$$\phi_j^{(\mathrm{even})}(\xi)=\frac{1}{\sqrt{\pi}}\cos\left(j-\frac{1}{2}\right)\xi, \quad j=1,2,\ldots \tag{7}$$

and

$$\phi_j^{(\mathrm{odd})}(\xi)=\frac{1}{\sqrt{\pi}}\sin j\xi, \quad j=1,2,\ldots. \tag{8}$$

Therefore, for a problem with a reflection symmetry as in Eq. (1), $\phi_j^{(\mathrm{even})}$ and $\phi_j^{(\mathrm{odd})}$ may be used to determine the symmetric and antisymmetric states, respectively, in a variational scheme. Actually, postulating the wave function $\Psi(\xi)$ as the linear combination of Eq. (7) or (8) then yields the standard matrix eigenvalue problem

TABLE I. Symmetric state eigenvalues of the harmonic oscillator as a function of the boundary parameter R.

R	n	E_{2n}	N
4	0	0.500 000 490	6
	1	2.500 201	6
	4	9.091	10
6	0	0.500 000 000 000 001	15
	1	2.500 000 000 003	15
	4	8.500 008	15
8	0	0.500 000 000 000 000 000 000 000 001	22
	1	2.500 000 000 000 000 000 000 000 011	22
	4	8.500 000 000 000 001	22
10	0	0.500 000 000 000 000 000 000 000 000 000	27
	1	2.500 000 000 000 000 000 000 000 000 00	29
	4	8.500 000 000 000 000 000 000 000 000 01	32

TABLE II. Lower and upper bounds for the symmetric state eigenvalues of the quartic oscillator as a function of α_2.

α_2	n	E_{2n}	N	R_{cr}
0.0001	0	0.500 074 973 770 778 406 839 704 533 744/5	27	10
	1	2.500 974 232 502 151 027 841 135 559 010/1	29	10
	2	4.503 070 949 409 913 913 484 032 094 841/2	30	10
1.0	0	0.803 770 651 234 273 769 354 085 964 732/3	32	5
	1	5.179 291 687 639 390 959 022 862 864 20/1	33	5
	2	10.963 583 094 127 472 925 799 051 713 4/5	34	5
1000.0	0	6.694 220 850 504 030 969 503 088 451 37/8	33	1.7
	1	47.017 338 732 427 724 313 680 975 622 0/1	35	1.7
	2	102.516 157 134 231 472 937 324 175 680/1	36	1.7
100 000.0	0	31.008 270 778 878 314 051 297 662 933 6/7	33	0.75
	1	218.016 572 253 841 491 646 153 774 153/4	34	0.75
	2	475.514 422 767 858 784 048 384 890 305/6	35	0.75

$$\sum_{j=1}^{\infty}\left(H_{ij}-\frac{2R^2}{\pi^2}E\delta_{ij}\right)c_j=0,\quad i=1,2,\ldots, \tag{9}$$

where the c_j are the expansion coefficients. Furthermore, the matrix elements H_{ij} can be evaluated analytically with simple and nice mathematical expressions. In the same way, similar trigonometric bases can be derived for a formulation of the von Neumann problem [2,3]. Another very important advantage of this approach is that it can be extended to multidimensional nonseparable problems [5,6].

The low-lying symmetric energy levels of the harmonic

$$V(x)=\frac{1}{2}x^2, \tag{10}$$

quartic

$$V(x)=\frac{1}{2}x^2+\alpha_2x^4,\quad \alpha_2>0, \tag{11}$$

and the sextic

$$V(x)=\frac{1}{2}x^2+\alpha_2x^4+\alpha_3x^6,\quad \alpha_2,\alpha_3>0 \tag{12}$$

oscillators considered by Vargas *et al.* [1] are recalculated in this work with some of their parameters for comparison. In Table I the upper-bound eigenvalues yielded by the Dirichlet problem are presented as a function of R for the harmonic oscillator whose exact unbounded eigenvalues are given by the formula $E_{2n}=2n+\frac{1}{2}$ in terms of the quantum number n. It is observed that the eigenvalues of the enclosed harmonic oscillator start to behave like the eigenvalues of the unbounded potential when $R>4$. At $R=8$, 27 significant figures are obtained for the ground-state energy diagonalizing a matrix of size $N=22$. The ground-state eigenvalue becomes accurate to more than 30 digits if $R=10$. On the other hand, Vargas *et al.* were able to calculate the same eigenvalue only to 10 digits at the cost of using a step size $h=0.0025$, which results in a generalized matrix eigenvalue problem of order $N=6400$. In [1], even this huge matrix size is not sufficient for the excited states and 10-digit accuracy could be achieved by an additional extrapolation procedure.

In Table II, we report extremely accurate two-sided eigenvalue bounds for the asymptotic energies of the quartic oscillator. In the terminology of our previous papers, the boundary value at which the required precision for a specific state being considered is reached is defined as the critical distance R_{cr}. To denote lower and upper bound energies, i.e., the eigenvalues of the von Neumann and Dirichlet problems, we employ the notation in which, for instance, 0.500 074$\cdots$533 744/5 means that

$$0.500\,074\cdots533\;\;744\leqslant E\leqslant 0.500\,074\cdots533\;\;745, \tag{13}$$

so that there is no uncertainty in our results. Comparing the results with those of Vargas *et al.* tabulated in their Table III, we see that theirs are not correct. As an example, the last 7 decimal points of $E_4=475.514\,382\,764\,8$ for $\alpha_2=100\;\;000.0$ are wrong. Clearly, if 7 decimals of a number recorded to 10 decimal points are wrong, then one should not conclude that the method used in this calculation gives a high degree of accuracy.

A careful inspection of our Table III and of Table 4 in [1] shows that the situation is virtually the same in the case of the sextic perturbation with $\alpha_2=0.5$ and $\alpha_3=1$. Most likely, the numerical algorithm would be much more unsatisfactory if they had tried for larger values of the coupling constants. Note also that the results of Aguiar *et al.* and Hioe *et al.*

TABLE III. Lower and upper bounds for the symmetric state eigenvalues of the sextic oscillator $V(x)=\frac{1}{2}x^2+\frac{1}{2}x^4+x^6$.

n	E_{2n}	N	R_{cr}
0	0.874 643 498 551 409 790 738 727 559 981/2	35	3.50
1	6.197 232 644 187 403 534 437 688 611 75/6	38	3.55
2	14.206 320 178 955 759 565 493 479 622 0/1	39	3.60
3	24.129 650 492 953 797 984 095 127 483 8/9	40	3.65
4	35.637 149 199 063 125 326 089 351 457 1/2	42	3.70

(Refs. 6 and 11 in [1]) given by Vargas *et al.*, for comparison, are correct up to their last digits quoted.

Consequently, Vargas *et al.* solved solely the simple and trivial harmonic oscillator correctly, with the aforementioned reservations. There are, however, a number of serious objections about the results of the perturbed cases, implying evidently that the method therein is not a robust and strongly convergent one as claimed by the authors. First of all, since the eigenvalues of the Dirichlet problem provide upper bounds, they cannot go below the asymptotic energies. On the contrary, most of the results in [1] are less than the exact unbounded eigenvalues. Moreover, everybody knows the theoretical argument that the $h \rightarrow 0$ limit gives the exact results. In practice, however, nobody can reach this limiting case, and it is important to have a rapidly convergent and stable method that uses a reasonable value of h giving satisfactory results. Otherwise, the smaller the h, the larger the dimension of the matrix required. The diagonalization of a matrix beyond a certain size is, unfortunately, intractable. The reported inaccurate numerical results show that this is exactly the case for the algorithm proposed by Vargas *et al.* For the harmonic oscillator the target is known, so that the algorithm may be forced to give the correct results by further computational effort such as Richardson's extrapolation. For the anharmonic cases, however, where the target is unknown, the stability of the method should have been checked by applying different step sizes. By this way, the confirming digits of two consecutive approximations could be recorded as significant digits for the energy levels.

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