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

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In response to the criticisms raised by Taseli [preceding Comment, Phys. Rev. E **56**, 1280 (1997)], we apply the method proposed by us [Phys. Rev. E **53**, 1954 (1996)] to the confined quartic and sextic anharmonic potentials and show that our algorithm provides reasonable numerical estimates for the eigenvalues of one-dimensional quantum problems under Dirichlet's boundary conditions. The results obtained are in acceptable (ten digits) agreement with those reported by Taşeli. [S1063-651X(97)04306-7]

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Recently, we presented a method [1] to solve one-dimensional quantum problems subjected to Dirichlet's boundary conditions that is based on a matrix method proposed by Lindberg [2] and a Richardson extrapolation [3]. Taşeli [4] has shown that this algorithm is accurate up to ten digits for the confined harmonic oscillator. However, the complete algorithm was not tested in the confined quartic and sextic oscillators and thus produced eigenvalues with an unacceptable accuracy, particularly for highly excited states. This deficiency of Lindberg's approach [2] as implemented by us has been fully discussed by Taşeli [4], where he shows that indeed some results are correct only to three decimal places, and does not allow one to claim that an algorithm is adequate to produce ''exact'' results for any problem. Within the finite-differences method, there are three ways to circumvent this lack of accuracy. First, one could take the limit of vanishing step size (h); second, one could use the defect correction method originally proposed by Lindberg [2]; and, finally, one could use Richardson's extrapolation [3] as it was presented in our previous work [1]. Certainly, the ideal approach is to take the limit $h \to 0$, but this is computationally unfeasible. To show that Richardson's extrapolation provides results that are correct up to ten decimal places not only for the ''trivial'' confined harmonic oscillator but also for more general potentials such as those considered by Taşeli, in Tables I and II we present results corresponding to the quartic and sextic oscillators using the same potential parameters and confinements tested by Taşeli [4]. As can be seen, these results are in agreement with those reported in Ref. [4], confirming that the methodology proposed by us does provide reliable results not only for trivial problems, where the target is known, but also for more complicated potentials. Undoubtedly, the detailed numerical analysis performed by Taşeli for several polynomial potentials [5–7] provides benchmark eigenvalues for these systems. Thus, when testing a new algorithm attempting to solve this type of problem, one should compare the results with those reported by Taşeli. We recognize that this comparison was not done in our previous work.

It is worth noting that the computational effort involved in the calculations reported by us decreases substantially for small confining intervals, in contrast to the variational approach, which requires very large basis sets to obtain a homogeneous error for every confinement [6]. However, this situation is reversed when the confining interval is enlarged, i.e., when the system approaches the free (unbounded) problem. In principle, truly exact results are obtained when the step in a finite-differences method tends to zero or when the number of basis functions in a variational approach tends to infinity. However, both limits are computationally impossible to reach. The above comments show that with current

TABLE I. Symmetric state eigenvalues of the quartic oscillator as a function of α_2[a] and the same confining radii (R) used in Ref. [4]. The first step used in the extrapolation is $h_1 = 0.0025$ and the second is $h_2 = h_1/2$.

α_2	n	E_{2n}	R
0.0001	0	0.500 074 973 8	10.0
	1	2.500 974 232 5	10.0
	2	4.503 070 949 4	10.0
1.0	0	0.803 770 651 2	5.0
	1	5.179 291 687 6	5.0
	2	10.963 583 094 1	5.0
1000.0	0	6.694 220 850 5	1.7
	1	47.017 338 732 4	1.7
	2	102.516 157 134 2	1.7
100 000.0	0	31.008 270 778 9	0.75
	1	218.016 572 253 9	0.75
	2	475.514 422 768 3	0.75

[a]See Ref. [4] for the definition of α_2.

TABLE II. Symmetric state eigenvalues of the sextic oscillator. The first step used in the extrapolation is $h_1 = 0.01$ and the second is $h_2 = h_1/2$.

n	E_{2n}	R
0	0.874 643 498 5	3.50
1	6.197 232 644 2	3.55
2	14.206 320 179 0	3.60
3	24.129 650 493 0	3.65
4	35.637 149 199 1	3.70

technology there is no single methodology to deal with a given problem in a general situation.

The robustness claimed in our paper rests on the aforementioned statements and also on the capability of our methodology to tackle more complicated confined problems. In fact, we have applied the algorithm to confined many-electron atoms [8], where no clever or enlightened transformation either of the original problem or the basis set was necessary to solve the resulting radial equation subjected to Dirichlet's boundary conditions. At this point it is worth noting that experimental (spectroscopic) accuracy in these atomic problems is within the 10^{-1}-cm^{-1} range, which demands a 10^{-7}-a.u. accuracy in eigenvalue differences. Thus an algorithm producing ten digits is enough to deal with these problems. Finally, we would like to mention that the term ''strongly convergent'' was applied to our methodology because, as it was fully discussed in Ref. [1], it complies with the mathematical definition of a strongly convergent sequence, and has no further implications.

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