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REPLY TO COMMENT

Reply to Comment on 'Coupled anharmonic oscillators: the Rayleigh–Ritz approach versus the collocation approach'

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Abstract
The Comment by Amore *et al* (2011 *Phys. Scr.* **83** 047003) proves only that the results of the collocation approach become upper bounds for bound-state energies in the limit of an infinite number of grid points N. We point out that the results obtained at finite N may lie below the exact results and should be taken with care.

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The aim of our paper 'Coupled anharmonic oscillators: the Rayleigh–Ritz approach versus the collocation approach' [1] was not to question the validity of the collocation method based on little sinc functions or its variational improvement [2, 3], but rather to show that the application of the method requires some care. In the collocation approach, the Hamiltonian matrix is calculated only approximately; therefore the method does not have a variational character [4, 5]. Recovery of a variational behavior is expected when the number of points in the grid N is sufficiently high [5], and such an expectation has been also expressed for the optimized collocation method based on little sinc functions by Amore *et al* [2]. This paper does not provide a convergence proof but only shows that the method yields accurate approximations for some one-dimensional (1D) potentials. In the Comment by Amore *et al* [6], the authors prove that the variational character is recovered but only in the limit of infinite N. We want to point out that the results obtained at finite N are not necessarily upper bounds.

In a paper on the 2D Pullen–Edwards problem [3], Amore and Fernández presented the results of the optimized collocation method obtained at finite N. The eigenenergies, given with a precision of 17 digits, were lower than the results reported in the literature, which caused our doubts [1] about their accuracy. In [6], Amore *et al* explain that the results were in error since their calculations were performed to 12 digit accuracy. By repeating the calculations with a numerical precision of 24 digits, they obtained more accurate results; however, the computational cost had to be quite high. Our comparison of the convergence rate of the optimized collocation method with that of the optimized Rayleigh–Ritz method [1] shows that for the Pullens–Edwards Hamiltonian, the computational cost of the collocation method is higher and rapidly grows with the desired accuracy. Of course, in solving problems with a greater number of degrees of freedom and/or more complicated potentials, the advantages of the collocation approach over the Rayleigh–Ritz approach can be seen. However, in any case, discussion of the accuracy of the collocation approach is more complicated and has to be carefully performed.

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