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## Comment on “Ritz variational treatment of the $^4\text{He}$ trimer” by Geltman S.

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In this Comment we show that the recent suggestion [1] that many published calculations of the ground-state energy of the  $^4\text{He}$  trimer might be wrong is not substantiated. We show that the proposed [1] functional form of the trial wave function for  $^4\text{He}_3$  can indeed provide a variational energy in agreement with the literature.

In his recent paper Geltman [1] developed a trial wave function for the  $^4\text{He}$  dimer. Using the recently developed accurate TTY interaction potential [2] he optimized the variational parameters and, using a numerical integration scheme, he obtained an upper bound to the exact ground-state energy of  $-3.548 \times 10^{-9}$  a.u., recovering 85% of the binding energy, compared to the supposedly exact value computed by the author himself with a numerical solution of the Schrödinger equation. This is a good result for such a peculiar system described with a very compact trial wave function with only four adjustable parameters. The computed energy is in agreement both with the known experimental value and other theoretical works.

The author then used his newly developed functional form to construct a wave function for  $^4\text{He}_3$ , built as a product of three two-body wave functions. The four variational parameters have been optimized and a final energy of  $-1.391 \times 10^{-7}$  a.u. has been estimated using a numerical integration scheme. Comparing his value with other published calculations on the ground state of  $^4\text{He}_3$  with the same or similar potential Geltman finds a large disagreement, recovering only half the energy of the averaged published calculations. Trying to explain this large discrepancy Geltman pointed out that some of the quoted calculations were based on the Faddeev approach, which does not necessarily result in an upper bound, and some others were diffusion Monte Carlo (DMC) calculations

Table 1: Ground-state energy of  $^4\text{He}_3$  with the TTY potential computed using different methods.

Energy <sup>(a)</sup>	Method employed	Reference
$-4.003 \times 10^{-7}$	Correlated hyperspherical harmonics	[3]
$-3.997 \times 10^{-7}$	Finite elements method	[4]
$-4.002(3) \times 10^{-7}$	DMC	[5]
$-3.973(18) \times 10^{-7}$	DMC	[6]
$-3.991(23) \times 10^{-7}$	DMC	[7]
$-4.003 \times 10^{-7}$	Faddeev equations	[8]

<sup>(a)</sup>Energies are in a.u. In parentheses the uncertainty on the last digits.

which are stochastic in nature. Trusting his numerical procedure Geltman concluded that “a real discrepancy appears to exist between our present results and those of other calculations. We hope this may stimulate new laboratory efforts to determinate the trimer binding energy, which has not yet been experimentally measured”.

In this Comment we wish to point out that the DMC calculations quoted by Geltman estimate the exact ground-state energy of  $^4\text{He}_3$ , within the statistical error, and agree with all other recent calculations carried out using different approaches, including a variational estimate [3] computed using the hyperspherical approach quoted by Geltman.

In table 1 we report a few modern literature estimates of the ground-state energy of  $^4\text{He}_3$ , all using the TTY potential. Some calculations are variational, including the DMC results, and provide an upper bound to the exact energy while others are not variational but are considered

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well converged. All quoted DMC calculations have a small statistical error and provide essentially the same value of the ground-state energy, in complete agreement with all other calculations and in disagreement with Geltman calculation [1]. From table 1 it is clear that there is a general consensus on the energy of the ground state of  ${}^4\text{He}_3$  so it is Geltman's calculation to be in error. We now try to explain the reason of this discrepancy.

We have implemented Geltman's wave function for the  ${}^4\text{He}$  dimer in our variational Monte Carlo (VMC) computer code. The VMC computer code computes the variational energy of a given trial function using the Metropolis algorithm, while the DMC method used in the calculations quoted in table 1 estimates the exact ground-state energy of a boson system. For  ${}^4\text{He}_2$  we used Geltman's variational parameters obtaining a VMC estimate of  $-3.560(4) \times 10^{-9}$  a.u. (in parentheses the uncertainty on the last digits) in good agreement with Geltman's value. VMC estimates of the ground-state energy are variational, within the statistical error that can be made as small as desired. Having checked our correct implementation of the functional form and its validity to describe the helium dimer, we then proceeded to estimate, using Geltman's parameters, the variational trial energy for  ${}^4\text{He}_3$ . Our estimate of Geltman's wave function energy is  $-2.805(2) \times 10^{-7}$  a.u., in disagreement with his own calculation and recovering a larger amount of the total energy. His paper does not provide enough details to exactly reproduce the employed numerical integration method; however, we suspect that some numerical error has been made at this stage. Computationally the helium trimer is quite a challenging problem. Its hard-core potential combined with the very diffuse nature of its wave function makes numerical methods prone to introduce numerical errors if not properly tuned, and special methods are needed [4,8].

Assuming, from table 1, an exact ground-state energy of  $-4.003 \times 10^{-7}$  a.u. Geltman's wave function recovered 35% of the total energy, a much worse performance

than for  ${}^4\text{He}_2$ . It is known [6] that wave functions for  ${}^4\text{He}_2$  are less accurate than those for the trimer and higher clusters so it is possible that, by careful optimization of the parameters, an even better variational energy could be recovered. We optimized the variational parameters using the VMC computer code [9]. The resulting optimized wave function provides a variational energy of  $-3.414(2) \times 10^{-7}$  a.u. for the parameters value:  $\alpha = 0.009492$ ,  $\beta = 1.0411$ ,  $\delta = 7.4154$ , and  $\gamma = 0.8453$ , recovering 85% of the total energy, in much better agreement with the literature results. This value is comparable to other variational results from similar compact wave functions, like Lewerenz's  $-3.631(22) \times 10^{-7}$  a.u. [6].

In conclusion, we showed that there is no disagreement, as was suggested by Geltman, between different calculations on the ground state of  ${}^4\text{He}_3$  and that treated with a proper numerical integration method, like the variational Monte Carlo one, the wave function developed in ref. [1] can provide energies in agreement with the literature and with the current estimate of the exact energy of the helium trimer.

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