Comment on "Efimov States for ^{4}He Trimers?"

In a recent Letter, González-Lezana *et al.* [1] presented a variational study of the ^{4}He trimer. Using a basis of distributed Gaussian functions (DGFs) in the pair coordinates, they found two $L = 0$ bound states of $^4He_3$. They claim that the excited state is not strictly an Efimov state although it has many of its characteristics.

In this Comment, we point out that work by a number of groups [2–4] spanning more than a decade has led to largely the same conclusions, also using "modern" He-He interaction potentials similar or identical to the one used in Ref. [1]. Contrary to a statement made in [1], at least one of these previous studies—work carried out by three of us [3]—was a variational calculation including the proper symmetry of the problem. In fact, we obtained a stricter upper bound on the excited state trimer energy using the same He-He potential.

At first glance, the calculated excited state energy [1], -1.24×10^{-3} cm^{-1}, appears to be consistent with our calculated energy of -1.472×10^{-3} cm^{-1}. A more careful inspection of Ref. [1], however, reveals probable deficiencies in the underlying numerics. For example, the trimer ground state energy in [1], -0.15 cm^{-1}, shows a significant discrepancy with published results. While it is within the bounds set in [3], it was stated there that the upper bound of -7.374×10^{-2} cm^{-1} was expected to be much more accurate. Comparison with other published results, such as the hyperspherical coupled channels value of -8.702×10^{-2} cm^{-1} [4], shows not only that the upper bound from [3] is far more accurate than the lower bound of -0.204 cm^{-1}, but also that it is the Ref. [1] result that is inconsistent. Moreover, our calculated ground state energy using the entirely different diffusion quantum Monte Carlo algorithm (see Table I of Ref. [5]) is $-0.0872(4)$ cm^{-1}.

Based on our hyperspherical calculations of the ground and excited states of $^4He_3$, it is apparent that the trial wave function adopted by González-Lezana *et al.* was not sufficiently diffuse to represent either the dimer ground state or the trimer excited state, leading to their underestimates of both the dimer binding energy and the trimer excited state binding energy. Our trimer calculations (Fig. 4 of Ref. [3]) show that the excited state wave function remains appreciable all the way out to a hyperradius of $R \approx 1000$ a.u. and peaks around $R \approx 200$ a.u. Using the definition $R^2 \equiv \rho_1^2 + \frac{4}{3}\rho_2^2$ [3], with ρ_1 and ρ_2 the magnitudes of the Jacobi vectors, one can show that $R \approx 1000$ a.u. corresponds to interparticle distances much larger than the 139 Å (263 a.u.) covered by the DGFs in [1]. In particular, already at the peak of the hyperradial function near $R \approx 200$ a.u., the nearest neighbors in a linear configuration ($\rho_2 = 0$) are separated by about 100 a.u.; in an equilateral triangle configuration ($\rho_2 = \sqrt{3}/2\rho_1$), by about 141 a.u. The converged calculations of Nielsen *et al.* [4] support these estimates: there the smallest of the He-He distances in the excited state has a mean value of 70 a.u. and the largest 219 a.u. For these reasons, the fair agreement between the excited state energies of Refs. [1] and [3] seems fortuitous.

Moreover, the abbreviated spatial extent of the trial function would explain the most serious deficiency of Ref. [1]: the fact that the exact Efimov limit was not reproduced for *any* value of the strength λ of the He-He interaction (compare Fig. 2 of [1] to Fig. 3 of [3]). Efimov's remarkable papers [6] predicted an infinite number of three-body bound states when the two-body scattering length diverges; in other words $\lambda_{2B} \equiv \lambda_{\text{Efimov}}$ if λ_{Efimov} is to indicate the value of λ at which the Efimov effect occurs. González-Lezana *et al.*, on the other hand, found only *one* three-body bound state—the ground state—at λ_{2B} and nowhere found evidence for an infinity of three-body bound states. They instead defined λ_{Efimov} to be the point at which the first excited state becomes bound and found it to be about 1% larger than λ_{2B}. We finally note that a shift of only about 0.1×10^{-3} cm^{-1} would bring the results of González-Lezana *et al.* into agreement with all of the above statements.

We thank M. Lewerenz for fruitful discussions. This work was supported partly by the National Science Foundation.

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Received 6 May 1999
DOI: 10.1103/PhysRevLett.86.4189
PACS numbers: 36.90.+f, 31.15.Ja

[1] T. González-Lezana *et al.,* Phys. Rev. Lett. **82**, 1648 (1999).
[2] T. Cornelius and W. Glöckle, J. Chem. Phys. **85**, 3906 (1986).
[3] B. D. Esry, C. D. Lin, and C. H. Greene, Phys. Rev. A **54**, 394 (1996).
[4] E. Nielsen, D. V. Fedorov, and A. S. Jensen, J. Phys. B **31**, 4085 (1998).
[5] D. Blume and C. H. Greene, J. Chem. Phys. **112**, 8053 (2000).
[6] V. Efimov, Phys. Lett. **33B**, 563 (1970); Nucl. Phys. **A210**, 157 (1973); Comments Nucl. Part. Phys. **19**, 271 (1990).

