Comment on “Weakly bound states of the He-He-Ca triatomic system”

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We discuss the computational results on the energetics and features of the bound states of one and two He atoms attached to a Ca atom, which have been presented by Gou and Li in a recently published paper in *Phys. Rev. A* **85**, 012510 (2012). We show that, given their choice for the interaction potential-energy surface, the energy they found for the three-particle complex’s ground state must be incorrect. We also point out that a large number of their excited states for the same system do not really exist since they are located above either of the two-atom components’ bound-state energies.

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Gou and Li have published [1] a computational paper which deals with the CaHe_2 complex, using hyperspherical coordinates in an adiabatic approximation to obtain the weakly bound states of the complexes of one Ca atom with one and two He atoms, both bosons and fermions. There are several aspects of the discussion which are physically unclear, but we mostly intend to point out the unphysical results given by the data in Table II; there are at least three features of those data which cannot be correct:

(i) The lowest bound-state energy of the He-He-Ca complex with bosons given in the last two columns of Table II is shown to be lower in energy than the sum of the three well depths for the atom-atom potentials used by the authors (see their Fig. 1): This is unphysical since the authors use a sum-of-potentials approximation so that no extra features are present other than the simple sum of the three wells so that the strongest interaction (deepest minimum energy value) comes to about -41 K. Even if one accepts the potential curve given by their Fig. 2 as the lowest hyperspherical potential curve, it is certainly incorrect that the deepest well depth of that figure reaches -60 K versus the -41 K of the sum-of-potential value of their V_{tot} since the additional potential term in their Eq. (6) is given by the grand angular momentum contribution that is

expected to be repulsive, such as the conventional centrifugal potential in Jacobi coordinates.

(ii) The bound-state energy of the ^4He -Ca dimer is given by their Table I to be -5.63 K, whereas, that of He-He is given by -4.74 K. Hence, any trimer’s state with a bound-state energy of less than the smaller of the above values must be unbound with respect to both the He_2 and the HeCa asymptotic states and, therefore, does not exist as a bound state relative to its physical asymptotes. This means that, of the numerous bound states of the trimer listed in the last two columns of Table II, only the first four are physically acceptable, all the others being unbound with respect to one or the other asymptotic state for the two-body partners: When one excludes the first of those four as being unphysical [see our point (i) above], then only three other bound-state energies are physically acceptable, whereas, all the others have to be rejected as unphysical.

As a comparison, the earlier paper using this very method [e.g., see Esry *et al.* *Phys. Rev. A* **54**, 394 (1996)] invariably finds bound-state energies of ground states which are less than the deepest value of the well of their V_{tot} .

(iii) Furthermore, if the whole series of bound-state energies in Table II are to be referred to as the global zero of the three-body breakup, then all values in that table also need to be increased in magnitude by -5.63 K, the bound-state energy of the HeCa partner.

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[1] Q. Gou and Y. Li, *Phys. Rev. A* **85**, 012510 (2012).