

Efimov States for ^4He Trimers?

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Helium trimer bound states are calculated with a variational method described in terms of pair atom coordinates and distributed Gaussian functions by assuming zero total angular momentum. With the two-body interaction potential used, a weakly bound state for the dimer and only two bound states for the trimer are found. Although strictly speaking the first excited trimer state is not an Efimov state, we show that this state presents several characteristics of the Efimov behavior which are extensively discussed in the present work. Special emphasis is placed on the main geometrical configurations contributing to the two bound trimer states, and suggestions are made on the possible ways of experimentally detecting the Efimov-type state. [S0031-9007(99)08513-0]

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Small ^4He clusters (in particular, dimers and trimers) present a series of unusual quantum properties of fundamental interest. These properties can play a role not only in connection with the statistical behavior of collective modes of ^4He gas at low temperatures [1], but also with the Bose-Einstein condensation [2,3] as well as with the appearance of the so-called Efimov states in three body interactions [4]. A lot of theoretical work concerning these special states has been done in order either to confirm or to disprove their existence [5–8]. However, much of the controversy about their existence is chiefly due to uncertainties on the two-body (2B) interaction potential and only in part to the different dynamical methods applied.

In this Letter, our purpose is twofold. First, to apply a variational method based on pair coordinates leading to a more suitable way to discuss configurations and symmetrization of the ground and excited states of the trimer; and, second, to discuss whether or not Efimov states can be observed. Concerning the first point, it is obvious that even using the same 2B interaction, the theoretical model applied to solve the trimer discrete spectrum can be crucial for bound states very near to the three-body threshold, as is the case for the Efimov states. Moreover, using this kind of coordinate the weight of the different geometrical configurations can be estimated allowing one to know which of them would dominantly contribute to those special states. As far as we know, this is the first “exact” variational calculation including the proper symmetry of the problem. Finally, from our knowledge of the pair distribution function and of the main geometrical configurations, it becomes possible to determine the average size of this floppy system, and therefore to envisage different ways to observe them.

Considering a zero total angular momentum state, using atom-atom pair coordinates (R_1, R_2, R_3) and including a scale factor $(R_1 R_2 R_3)^{1/2}$ to attain the standard normalization in the total wave function, a totally symmetric Hamil-

tonian is obtained

$$H = \sum_{i=1}^3 \left\{ \frac{-\hbar^2}{m} \left[\frac{\partial^2}{\partial R_i^2} + t_i \right] + V(R_i) \right\}, \quad (1)$$

with V being the 2B-interaction potential (which corresponds in this work to that of Ref. [9]), and where the effective kinetic energy operators t_i are expressed as

$$t_i = \frac{1}{R_i} \frac{\partial}{\partial R_i} - \frac{1}{4R_i^2} + \frac{R_j^2 + R_k^2 - R_i^2}{2R_j R_k} \\ \times \left(\frac{\partial^2}{\partial R_j \partial R_k} - \frac{1}{2R_j} \frac{\partial}{\partial R_k} - \frac{1}{2R_k} \frac{\partial}{\partial R_j} + \frac{1}{4R_j R_k} \right), \quad (2)$$

with $i \neq j \neq k$. As can be clearly seen from Eq. (1), these t_i operators reflect the deviations in the total Hamiltonian from that formed by the sum of pair Hamiltonians.

The eigenfunctions of the total Hamiltonian given by Eq. (1) are expanded in terms of basis functions as

$$\Phi_k(R_1, R_2, R_3) = \sum_j a_j^{(k)} \phi_j(R_1, R_2, R_3), \quad (3)$$

where j denotes a collective index, $j = (l \leq m \leq n)$. The ϕ_j functions, in turn, are built up as symmetrized products of pair functions given by

$$\phi_j(R_1, R_2, R_3) = N_{lmn}^{-1/2} \sum_{P \in S_3} P[\varphi_l(R_1)\varphi_m(R_2)\varphi_n(R_3)], \quad (4)$$

where the coefficients

$$N_{lmn} = 6(s_{ll}s_{mm}s_{nn} + s_{ll}s_{mn}^2 + s_{mm}s_{ln}^2 \\ + s_{nn}s_{lm}^2 + 2s_{lm}s_{ln}s_{mn}) \quad (5)$$

define a normalization factor expressed in terms of the overlap integrals written as

$$s_{pq} = \langle \varphi_p | \varphi_q \rangle. \quad (6)$$

The one-dimensional functions φ_p are chosen here to be distributed Gaussian functions (DGF) [10] centered at $R_{(p)}$ positions

$$\varphi_p(R_i) = \sqrt[4]{\frac{2A_p}{\pi}} e^{[-A_p(R_i - R_{(p)})^2]}. \quad (7)$$

In order to fulfill the triangular requirement

$$|R_1 - R_2| \leq R_3 \leq R_1 + R_2, \quad (8)$$

the product $\varphi_l \varphi_m \varphi_n$ is taken into the basis set as long as the corresponding DGF centers verify that

$$R_{(n)} \leq R_{(l)} + R_{(m)}. \quad (9)$$

Because of the fact that our method provides the total wave function, averages and fluctuations of triangular magnitudes are closely related to the nature of the proper bound states.

The basis set given by Eq. (4) is not orthonormal but the pseudoeigenvalue problem can be transformed to a standard eigenvalue problem by using the method developed originally by Löwdin [11]. Starting with 39 Gaussian functions φ_p , 17 of them equally spaced in the region of the 2B potential well (say, between 3–11 Å) and the rest ranging up to 139 Å with increasingly larger spacings, a number of about 3000 symmetrized Φ_k functions is included. This is equivalent to considering a basis set of approximately 18000 nonsymmetrized functions. The quality of the numerical calculations is controlled via the moments of the radial and angular distributions. Moreover, this method has been also successfully applied to the trimer systems Ar_3 and Ne_3 [12].

In Fig. 1 we present the 2B interaction potential (dashed line, and expressed in cm^{-1}) together with the two-pair distribution functions corresponding to the ground ($k = 0$) and first ($k = 1$) excited trimer states (solid lines) as well

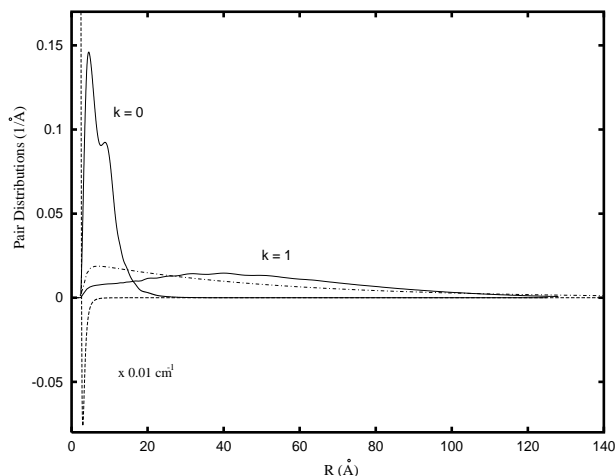


FIG. 1. Pair distribution functions (in Å^{-1}) for the ground ($k = 0$) and first ($k = 1$) excited trimer states (solid lines) together with the square modulus of the dimer wave function (dot-dashed line) and the two-body interaction potential (dashed line) multiplied by a factor of 0.01 and expressed in cm^{-1} . R (in Å) stands for any of the three-pair distances.

as the square value of the diatomic wave function (dot-dashed line). As can be seen, for the ground state, the pair distribution function is mainly located in the region limited by the 2B interaction potential and presents an average distance of 7.88 Å and standard deviation of 3.72 Å. The relative magnitude of the spread of this pair distribution function about the mean value is therefore 47% indicating that the fluctuation is quite important. Two maxima are also found, the first one more pronounced than the second in a ratio of about 2 to 1. This bimodal distribution can be interpreted as being due to the presence of quasilinear configurations, as will be discussed below. Concerning the pair distribution function for the excited state, the average distance is 50 Å with a standard deviation of 28 Å. Here the fluctuation is even larger, of the order of 60%. In Table I, some statistical quantities extracted from the total wave functions for the ground and first excited trimer states are collected. Furthermore, the percentage of the pair distribution function in the excited state inside the 2B potential well is about 3% when taking an effective radius of the 2B-interaction potential of $r_0 = 7.35$ Å and a scattering length of $a = 100.13$ Å. Compared to the square modulus of the 2B wave function, both behaviors are quite similar at very large distances where the interaction potential is now negligible. Therefore, this excited state could be considered as a good candidate for an Efimov state.

According to the 2B interaction potential which we have employed [9], the dimer presents, through the DGF method, a weakly bound state at $-0.8 \times 10^{-3} \text{ cm}^{-1}$ versus $-0.91 \times 10^{-3} \text{ cm}^{-1}$ obtained from a direct numerical integration of the Schrödinger equation. The bound energy values found for the trimer are -0.15 cm^{-1} (ground state) and $-1.24 \times 10^{-3} \text{ cm}^{-1}$ (first excited state). These energy values are quite close to those reported in the literature (see, for example, Ref. [8] which utilizes the same 2B-interaction potential but an approximate adiabatic method). Recently, quantum Monte Carlo (DMC) methods have been also applied to the trimer ground state [13,14]. Very similar results have been obtained for the ground state by using slightly different 2B interactions. As it is well known, the DMC method does not yield excited states. However, some discrepancies have been found about the main geometrical configurations contributing to the ground state. Moreover, after the formula to estimate the number of Efimov states

TABLE I. Average $\langle x \rangle_k$ and root mean square $\langle x^2 \rangle_k^{1/2}$ of several magnitudes, x , obtained from the ground ($k = 0$) and Efimov-type ($k = 1$) trimer states. The $\cos \theta$ is any of the three cosines of a triangle.

Magnitude (x)	$\langle x \rangle_0$	$\langle x^2 \rangle_0^{1/2}$	$\langle x \rangle_1$	$\langle x^2 \rangle_1^{1/2}$
Distance (Å)	7.9	8.7	50	57.3
$\cos \theta$	0.396	0.82	0.398	0.789
Area (Å ²)	15	26	684	994
Diameter (Å)	6.7	7.4	44.7	50.3

($N \approx (1/\pi) \ln |a/r_0|$), we obtain in our case $N \approx 0.8$. Therefore, as the number of Efimov states is very sensitive to the 2B binding energy [15], the usual way to characterize such states is to carry out an analysis of the discrete spectrum by varying the strength of the 2B interaction potential through a factor λ . In Fig. 2, the bound states (in cm^{-1}) for the dimer (solid line) and trimer (dashed lines; He3(0) for $k=0$ and He3(1) for $k=1$) are plotted as a function of λ covering the range $[0.8, 1.15]$. Several regions in λ can be considered: (i) Between $\lambda_{\text{halo}} = 0.8942$ and $\lambda_{2B} = 0.9755$, where only a trimer bound state exists but not a dimer state; this type of trimer bound states are usually called halo states; (ii) between $\lambda_{2B} = 0.9755$ and $\lambda_{\text{Efimov}} = 0.9849$, where the first excited state for the trimer begins to appear; this state could be characterized as a virtual state since it becomes a bound state as the interaction increases; (iii) between $\lambda_{\text{Efimov}} = 0.9849$ and $\lambda_{\text{ghost}} = 1.0256$, where the Efimov-type state is below the 2B continuum threshold and finally is overrun by this threshold; and (iv) $\lambda_{\text{ghost}} > 1.0256$ where the first excited state for the trimer is above the 2B continuum threshold and is generally called a ghost state.

In the inset of Fig. 2 an enhancement of the critical λ region is shown. The limiting values of the parameter

λ are slightly different from those estimated in Ref. [8]. However, the ratio $\lambda_{\text{halo}}/\lambda_{2B} = 0.92$ is quite close in both methods and should be independent on the shape of the pairwise potential (in nuclear physics this ratio is instead of ~ 0.8 , probably due to the different nature of nuclear and molecular interactions). It should be stressed at this point that in region (iii) only one Efimov-type state appears (according to the estimate $N \approx 0.8$) but no more. The striking result in our case is that this region includes $\lambda = 1$, i.e., the case for which we consider the 2B interaction to be the actual physical interaction. This fact implies that the Efimov states must be quite elusive because very small fluctuations or uncertainties in the 2B interaction potential can lead to different conclusions about their existence.

In the coordinates used here the kinetic energy operators of the total Hamiltonian, Eq. (2), *do not present* a clear behavior of an effective attractive long-range interaction of the $1/R^2$ type, with R being one of the given coordinates. It would be instead the balance among all the terms involved in these kinetic operators which should be responsible for the long-range interaction, at least for distances larger than r_0 .

An additional advantage of the coordinates used in this work is that they permit us to make a quantitative analysis

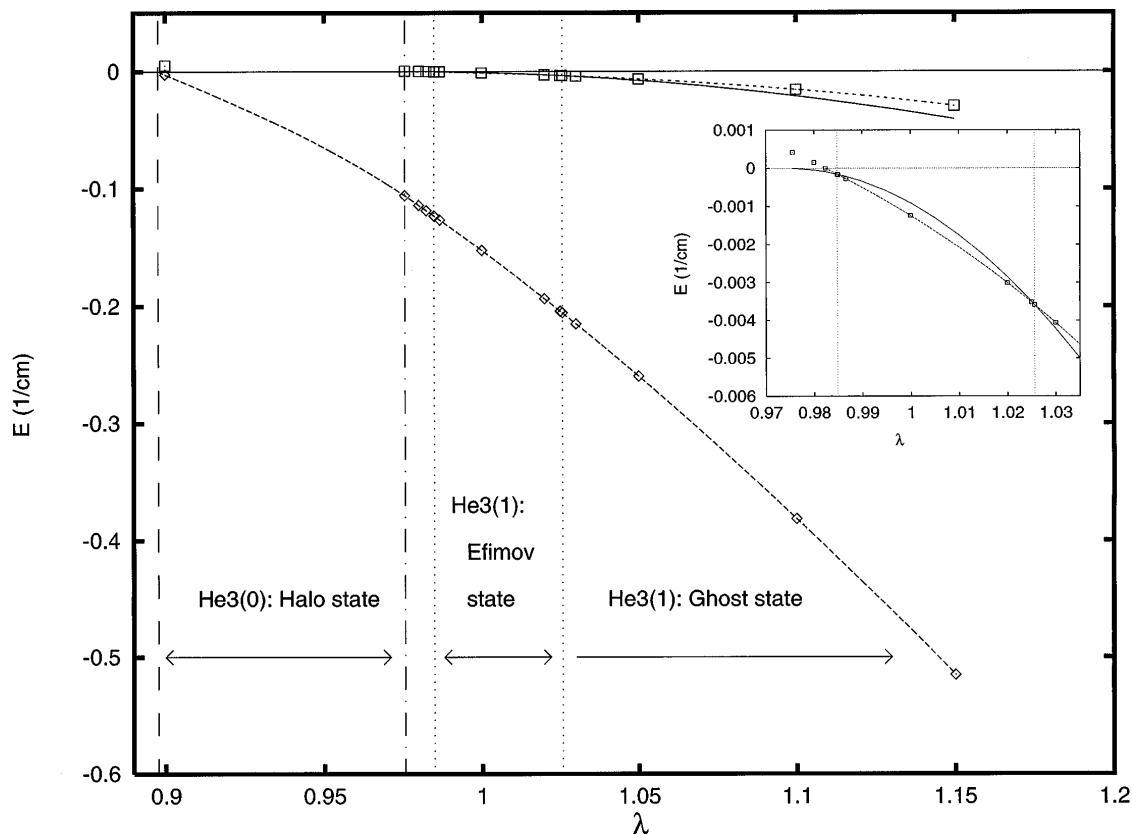


FIG. 2. Evolution of the bound states for the dimer and trimer (in cm^{-1}) as a function of the factor strength λ . The solid line corresponds to the two-body bound state and the dashed lines to the two-trimer bound states. In each region of λ values (see text) the character of the bound states [He3(0), ground state and, He3(1), first excited state] is marked: halo, Efimov-type, and ghost states. The inset shows an enhancement of the critical region.

of the different geometrical configurations contributing to each triatomic bound state. Thus, averages and root mean squares of the area and cosine of any of the three angles for both trimer states can be easily obtained from the total wave function via the Heron formula and the cosine theorem, respectively (see Table I). The following considerations can be made from the present analysis: the ground state is formed by about 30% of quasilinear configurations and a negligible contribution from equilateral triangles. Moreover, if these quasilinear configurations are not taken into account in the total wave function the ground level disappears. According to the ground pair distribution function plotted in Fig. 1, the two peaks placed at 4.53 and 8.81 Å can be understood as quasilinear configurations presenting two sides of about 4.5 Å and the third side of about 9 Å resulting in a ratio between the two maxima of nearly two. The existence of quasilinear structures was also pointed out in an earlier DMC calculation [14] and we interpret such an existence as due to intermediate configurations among all the possible triangular ones. Concerning the Efimov-type state, a preference of scalene configurations (about 70%) is found, with negligible contributions of quasilinear and equilateral configurations.

Finally, our next point here is to suggest possible ways of observing Efimov-type states. Recently, He dimers and trimers have been detected by diffraction from a transmission grating [16]. The signal corresponding to He trimers has not been resolved in terms of the two different bound states of this system which we found here. The diffraction grating was built with a period of 200 nm with bars and slits of equal size. According to our estimates trimers can pass through this kind of gratings independently of the bound states which are populated in the experiment. The question now is to envisage a way to select or discriminate one of these two bound states. Moreover, the average diameter of the circumscribed circumference for all of the triangular configurations (see Table I) is ~ 7 Å for the ground state and ~ 45 Å for the first excited state. Because of this difference, if the grating is tilted with respect to the incident orientation of the He beam, the effective slit can be smaller than the average diameter of the Efimov-type state and therefore it would be possible to filter it. From the different populations (and if the experimental resolution in intensity is good enough) it could therefore be possible to discriminate it. Alternative ways to isolate such states could also come from the kinetics of formation of dimers and trimers in He beams [17], three-body recombination of ultracold atoms [18], and from the

properties of liquid helium. In this last case, a complete different dynamics could be developed by considering that the He dimer interaction potential is affected by the surroundings in many ways similar to what we have simulated by varying the λ value and, therefore, dimers and trimers could play a very important role when one analyzes the well known properties of liquid He.

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