Bound States and Scattering Processes in the $^4\text{He}_3$ Atomic System

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Abstract

We present a mathematically rigorous method for solving three-atomic bound state and scattering problems. The method is well suited for applications in systems where the inter-atomic interaction is of a hard-core nature. It has been employed to obtain the ground- and excited-state energies for the Helium trimer and to calculate, for the first time, the scattering phase shifts and wave-functions for the He atom–He dimer at ultra-low energies.

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The $^4\text{He}$ triatomic system is of interest in various areas of physical chemistry and molecular physics. The study of the Helium dimer and trimer properties is the first step towards the understanding of the Helium liquid drops, superfluidity in $^4\text{He}$ films, finite pores etc. Various theoretical and experimental works have been devoted in the past to study the ground state properties of the $^4\text{He}$ clusters. From the theoretical works we mention here those using Variational and Monte Carlo type methods [2, 3], the Faddeev equations [7, 8], and the hyperspherical approach [10, 12]. From the experimental works we recall those of Refs. [13–16] where the Helium dimer and trimer clusters were investigated.

Despite the efforts made to solve the He-trimer problem various questions such as the existence of Efimov states and the study of scattering processes still have not been satisfactorily addressed. In particular for scattering processes there are no works which we are aware of apart from a zero-energy calculation of Ref. [7] and a recent study [17] concerning recombination rates. There are various reasons for this, the main one being that the three-body calculations involved are extremely difficult to perform due to the practically hard-core

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of the interatomic interaction which gives rise to strong numerical inaccuracies that make calculations cumbersome and unstable.

In this work we employed a mathematically rigorous method based on a hard-core version [18,19] of the boundary-condition model to calculate the binding energies and the ultralow energy scattering phase shifts below as well as above the breakup threshold. Such an approach takes into account, from the beginning, the hard-core nature of the He–He interatomic interaction. We show that this method is highly successful and suitable for solving three-body bound state and scattering problems in configuration space when the two-body interactions have a hard-core.

In the present investigation we consider that the $^4\text{He}_3$ molecule has a total angular momentum $L = 0$. In this case one has to solve the following, two-dimensional, integrodifferential Faddeev equations [20]

$$\left[ -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + l(l + 1) \left( \frac{1}{x^2} + \frac{1}{y^2} \right) - E \right] \Phi_l(x,y) = \begin{cases} -V(x)\Psi_l(x,y), & x > c \\ 0, & x < c. \end{cases} \quad (1)$$

Here, $x,y$ stand for the standard Jacobi variables and $c$, for the core range. The angular momentum $l$ corresponds to a dimer subsystem and a complementary atom; for the $S$-state three-boson system $l$ is even, $l = 0, 2, 4, \ldots$. $V(x)$ is the He-He central potential acting outside the core domain. The partial wave function $\Psi_l(x,y)$ is related to the Faddeev components $\Phi_l(x,y)$ by

$$\Psi_l(x,y) = \Phi_l(x,y) + \sum_{l'} \int_{-1}^{+1} d\eta h_{l'l}(x,y,\eta) \Phi_{l'}(x',y') \quad (2)$$

where

$$x' = \sqrt{\frac{1}{4} x^2 + \frac{3}{4} y^2 - \sqrt{3} x y \eta}, \quad y' = \sqrt{\frac{3}{4} x^2 + \frac{1}{4} y^2 + \sqrt{3} x y \eta},$$

and $1 \leq \eta \leq 1$. The explicit form of the function $h_{l'l}$ can be found in Refs. [20,21].

The functions $\Phi_l(x,y)$ satisfy the boundary conditions

$$\Phi_l(x,y) \big|_{x=0} = \Phi_l(x,y) \big|_{y=0} = 0. \quad (3)$$

In the hard-core model these functions satisfy also the condition

$$\Phi_l(c,y) + \sum_{l'} \int_{-1}^{+1} d\eta h_{l'l}(c,y,\eta) \Phi_{l'}(x',y') = 0 \quad (4)$$

requiring the wave function $\Psi_l(x,y)$ to be zero on the core boundary $x = c$. In fact, one can show that, in general, the condition (4) causes the wave functions (2) to vanish inside the core domains as well. Moreover, for the helium trimer bound-state problem the functions $\Phi_l(x,y)$ satisfy as $\rho \to \infty$ and/or $y \to \infty$ the asymptotic condition

$$\Phi_l(x,y) = \delta_{l0} \psi_d(x) \exp(i\sqrt{E} - \epsilon_d y) \left[ a_0 + o\left(y^{-1/2}\right) \right]$$

$$+ \frac{\exp(i\sqrt{E} \rho)}{\sqrt{\rho}} \left[ A_l(\theta) + o\left(\rho^{-1/2}\right) \right] \quad (5)$$
where $\epsilon_d$ is the dimer energy and $\psi_d(x)$, the dimer wave function. The $\rho, \rho = \sqrt{x^2 + y^2}$, and $\theta, \theta = \arctan \frac{y}{x}$, are the hyperradius and hyperangle for the trimer. The coefficients $a_0$ and $A_l(\theta)$ describe contributions into $\Phi_l$ from the $(2 + 1)$ and $(1 + 1 + 1)$ channels respectively. It should be noted that both the $E - \epsilon_d$ and $E$ in (5) for a bound state are strictly negative. This implies that for any $\theta$ the function $\Phi_l$ is exponentially decreasing in $\rho$ as $\rho \to \infty$.

The asymptotic boundary condition of the partial Faddeev components for the $(2 + 1 \rightarrow 2 + 1; 1 + 1 + 1)$ scattering wave function as $\rho \to \infty$ and/or $y \to \infty$ reads

$$\Phi_l(x, y; p) = \delta_{l0} \psi_d(x) \left\{ \sin(py) + \exp(iy) \left[ a_0(p) + o(y^{-1/2}) \right] \right\}$$

$$+ \frac{\exp(i\sqrt{E}\rho)}{\sqrt{\rho}} \left[ A_l(\theta) + o(\rho^{-1/2}) \right]$$

where $p$ is the relative momentum conjugate to the variable $y$, $E$ is the scattering energy given by $E = \epsilon_d + p^2$, and $a_0$ is the elastic scattering amplitude. The $S$-state elastic scattering phase shifts $\delta_0(p)$ are then given by

$$\delta_0(p) = \frac{1}{2} \Im \ln S_0(p)$$

where $S_0(p) = 1 + 2ia_0(p)$ is the $(2+1\rightarrow2+1)$ partial component of the scattering matrix. The functions $A_l(\theta)$ provide us, at $E > 0$, the corresponding partial Faddeev breakup amplitudes.

We employed the Faddeev equations [1], the hard-core condition (4), and the asymptotic expressions (5, 6), to calculate the binding energies of the Helium trimer and the ultra-low energy phase shifts of the Helium atom scattered by the Helium diatomic molecule. In our calculations we used $\hbar^2/m = 12.12$ KÅ². Our finite-difference algorithm was closed in essential to that described in [20,21]. As a $^4$He$^-^4$He interaction we employed the HFDHE2 [22] and HFD-B [23] potentials of Aziz and co-workers which we found that they sustain a dimer bound state at $-0.8301$ mK and $-1.6854$ mK respectively. The corresponding $^4$He atom$^-^4$He atom scattering length was found to be $124.7$ Å for the HFDHE2 and $88.6$ Å for the HFD-B potential.

The results of the Helium trimer ground-state energy calculations are presented in Table I. Although the two potentials used differ only slightly, they produce important differences in the ground-state energy. This is in agreement with the finding of Ref. [11] but in disagreement with the statement made in Ref. [3]. It should be further noted that most of the contribution to the binding energy stems from the $l = 0$ and $l = 2$ partial component the latter being more than 35%. The contribution from the $l = 4$ channel was shown in [3] to be of the order of a few per cent. We have found that the Helium trimer can form an excited state with both the HFDHE2 and HFD-B potentials in agreement with the findings of Refs. [7,8,12]. Note that in Refs. [8,12] this state was interpreted as an Efimov one [24]. Our excited state results are given in Table II.

The phase shift results for a Helium atom scattered by a Helium dimer are plotted in Fig. 1. We considered incident energies below as well as above the breakup threshold, i.e., for the $(2 + 1 \rightarrow 2 + 1)$ and the $(2 + 1 \rightarrow 1 + 1 + 1)$ processes. It is seen that, similarly to the bound state results, the inclusion of the $l = 2$ partial wave is essential to describe the scattering correctly. The relevant partial wave functions $\Psi_l(x, y; p), l = 0, 2$, calculated at $E = 4.1$ mK with the inclusion of both channels $l = 0$ and $l = 2$ are plotted in Figs. 2–5.
Further to the bound and scattering calculations we endeavour to estimate the scattering length

\[ \ell_{sc} = \frac{-\sqrt{3}}{2} \lim_{p \to 0} \frac{a_0(p)}{p} \]

from the phase shifts. For the HFD-B potential we found \( \ell_{sc} = 170\pm5 \text{Å} \) when only the \( l = \lambda = 0 \) are taken into account and \( \ell_{sc} = 145\pm5 \text{Å} \) when both the \( l = \lambda = 0 \) and \( l = \lambda = 2 \) are considered. We note here that previous estimate made by Nakaichi-Maeda and Lim via zero-energy scattering calculations and by employing a separable approximation for the HFDHE2 potential gave the value of \( \ell_{sc} = 195 \text{Å} \).

It is interesting to compare the results for \( \ell_{sc} \) with the inverse wave numbers \( \kappa^{-1} \) for the trimer excited state energies, \( \kappa = \frac{2}{\sqrt{3}} \sqrt{\epsilon_d - E_t} \), where the trimer excited state and dimer bound state energies \( E_t \) and \( \epsilon_d \) are measured in \( \text{Å}^{-2} \). For the HFD-B interaction we find \( \kappa^{-1} \approx 102 \text{Å} \) with \( l = \lambda = 0 \) and \( \kappa^{-1} \approx 89 \text{Å} \) with \( l = \lambda = 0 \) and \( l = \lambda = 2 \). These are about 1.7 times smaller than the above estimates for \( \ell_{sc} \). This is compared with the \( ^4\text{He} \) two-atomic scattering results where the inverse wave number \( (\kappa^{(2)})^{-1} = 84.8 \text{Å} \) is a good approximation for the \( ^4\text{He}--^4\text{He} \) scattering length, \( \ell_{sc}^{(2)} = 88.6 \text{Å} \). Such a significant difference between \( \kappa^{-1} \) and \( \ell_{sc} \) can be attributed to the Efimov properties of the trimer system which imply that the effective range \( r_0 \) of the interaction between \( ^4\text{He} \) atom and \( ^4\text{He} \) dimer is very large as compared to the \( ^4\text{He} \) two-atomic problem. Unfortunately, insufficient accuracy of our results for the amplitude \( a_0(p) \) at \( p \approx 0 \) which we have at the moment does not allow us to extract the values for the \( r_0 \).

It should be noted that the \( ^4\text{He}_3 \) system is probably one of the most challenging problems for any three-body scattering calculation, not only because of the hard-core of the pair forces, but also in view of its pre-Efimov nature. The latter manifests itself in a very slow falling off of the dimer wave function and then, as a consequence, in very large hyperradius values for the asymptotical boundary conditions (5) and (6) for the trimer excited state and scattering wave functions were fulfilled. In our finite-difference calculations we had to increase the cut-off radius \( \rho_{\text{max}} \) up to 400 – 600 Å while we had to use grids with up to 600 knots in both hyperradius \( \rho \) and hyperangle \( \theta \) variables until the converged results were obtained. All this required for storage of the resulting matrices up to 5 Gb of a (hard-drive) memory. Calculation of each phase shift point was also very expensive in time requiring in the case of the two equations \( (l, \lambda = 0, 2) \) up to ten or more hours. We plan to describe more details of our technics in an extended article which is under preparation.

Our results clearly demonstrate the reliability of our method in three-body bound state and scattering calculations in system where the inter-atomic potential contains a hard-core which makes such calculations extremely tedious and numerically unstable. Thus the present formalism paves the way to study various three-atomic systems, and to calculate important quantities such as cross-sections, recombination rates etc.

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### TABLE I. Bound state energy (in K) results for the Helium trimer.

| Potential | Faddeev equations | Variational methods | Adiabatic approach |
|-----------|-------------------|---------------------|-------------------|
|           | $l$ This work     | $l$ $l$ $l$         | $l$ $l$ $l$       |
| HFDHE2    | 0 0.084           | 0.082 0.092         | 0.098             |
|           | 0.2 0.114         | 0.107 0.11          | 0.1173            |
| HFD-B     | 0 0.096           | 0.096               |                   |
|           | 0.2 0.131         | 0.130               | 0.1193            |

### TABLE II. Excited state energy (in mK) results for the Helium trimer.

| Potential | $l$ | This work | $l$ | $l$ | $l$ |
|-----------|-----|-----------|-----|-----|-----|
| HFDHE2    | 0   | 1.5       | 1.46| 1.04| 1.517|
|           | 0.2 | 1.7       | 1.6 |     |     |
| HFD-B     | 0   | 2.5       |     |     |     |
|           | 0.2 | 2.8       |     |     |     |
FIG. 1. S-wave Helium atom – Helium dimer scattering phase shifts \( \delta_0 (E_{\text{lab}}) \), \( E_{\text{lab}} = \frac{3}{2} (E + |\epsilon_d|) \), for the HFD-B \(^4\text{He}-^4\text{He}\) potential. The lower curve corresponds to the case where only \( l = 0 \) are taken into account while for the upper both \( l = 0 \) and \( l = 2 \).

FIG. 2. Absolute value of the wave function component \( \Psi_0 (x, y, p) \) for the HFD-B \(^4\text{He}-^4\text{He}\) potential at \( E = +1.4 \text{ mK} \). Values of \( x \) and \( y \) are in \( \AA \).
FIG. 3. Detail of the $|\Psi_0(x, y, p)|$ surface shown in Fig. 2.

FIG. 4. Absolute value of the wave function component $\Psi_2(x, y, p)$ for the HFD-B $^4$He-$^4$He potential at $E = +1.4$ mK. Values of $x$ and $y$ are in Å.

FIG. 5. Detail of the $|\Psi_2(x, y, p)|$ surface shown in Fig. 4.