Ultra-low energy scattering of a He atom off a He dimer

E. A. Kolganova

Laboratory of Computing Techniques and Automation, Joint Institute for Nuclear Research, Dubna, 141980, Russia

A. K. Motovilov*, S. A. Sofianos

Physics Department, University of South Africa, P.O.Box 392, Pretoria 0001, South Africa

Abstract

We present a new, mathematically rigorous, method suitable for bound state and scattering processes calculations for various three atomic or molecular systems where the underlying forces are of a hard-core nature. We employed this method to calculate the binding energies and the ultra-low energy scattering phase shifts below as well as above the break-up threshold for the three He-atom system. The method is proved to be highly successful and suitable for solving the three-body bound state and scattering problem in configuration space and thus it paves the way to study various three-atomic systems, and to calculate important quantities such as the cross-sections, recombination rates etc.

LANL E-print physics/9802016.
Published in Phys. Rev. A., 1997, v. 56, No. 3, pp. 1686–1689R.

The $^4$He trimer is of interest in various areas of Physical Chemistry and Molecular Physics, in particular such as the behavior of atomic clusters under collisions and Bose-Einstein condensation. Various theoretical and experimental works have been devoted in the past to study its ground state properties and in general the properties of the $^4$He and other noble gas droplets. From the theoretical works we mention here those using Variational and Monte Carlo type methods [1–3], the Faddeev equations [4–8] and the hyperspherical approach [9–11]. From the experimental works we recall those of Refs. [12–15] where molecular clusters consisting of a small number of noble gas atoms 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 at ultra-low energies still have not been satisfactorily addressed. In particular for scattering processes there are no works which we are aware of apart from a recent study concerning recombination rates [16]. There are various reasons for this the main one being the fact that the three-body calculations

*On leave of absence from the Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, 141980, Russia
involved are extremely difficult to perform due to the practically hard-core of the interatomic potential which gives rise to strong numerical inaccuracies that make calculations for these molecules cumbersome and unstable.

In the present work we employed a hard core version of the Boundary Condition Model (BCM) [17,18], developed in [19], [20]. The so-called hard-core potentials represent a particular variant of the BCM where one requires that the wave function vanishes when particles approach each other at a certain distance \( r = c \). Such a requirement is equivalent to an introduction of an infinitely strong repulsion between particles at distances \( r \leq c \). The standard formalism for scattering (see, for example, [21]) does not deal with hard-core interactions described by these boundary conditions. Replacement of the finite, for \( r > 0 \), but often singular at \( r = 0 \), repulsive short-range part of the potential with a hard-core interaction turns out to be a very effective way to suppress inaccuracies related to a numerical approximation of the Schrödinger operator at short distances.

In order to outline our method we start from the Schrödinger equation for bound states,

\[
H \Psi = E \Psi, \quad \text{where } \Psi \text{ is the three-body bound state wave function. We are concerned with states for which } E < 0 \text{ and that these energies are below the threshold of the continuous spectrum of } H. \]

Using the Green’s formula [22] one can show that the function \( \Psi \) satisfies the following Lippmann-Schwinger type equation

\[
\Psi(X) = - \int_{\partial \Omega} d\sigma_S G_0(X, S; E) \frac{\partial}{\partial n_S} \Psi(S) - \sum_{\alpha=1}^{3} \int_{\Omega} dX' G_0(X, X'; E) (V_{\alpha} \Psi)(X'). \quad (1)
\]

Here \( \Omega \) is the configuration space of the three-body system in the hard-core model which represents only a part of the six-dimensional space, \( \mathbb{R}^6 \), external, \( |x_\alpha| > c_\alpha \), with respect to all three cylinders \( \Gamma_\alpha, \Gamma_\alpha = \{X \in \mathbb{R}^6 : X = (x_\alpha, y_\alpha), |x_\alpha| = c_\alpha \}, \alpha = 1, 2, 3 \), where \( c_\alpha, c_\alpha > 0 \), stands for the value of \( |x_\alpha| \) when the cores of the particles in the pair \( \alpha \) contact each other. The \( x_\alpha, y_\alpha \) are the usual Jacobi coordinates [21]. By \( G_0(X, X'; z) \) we denote the free Green function of the three-body Laplacian \(-\Delta_X \) and by \( n_S \), the external unit vector (directed into \( \Omega \)) normal to the surface \( \partial \Omega \) while \( d\sigma_S \) is a surface element (five-dimensional square) on \( \partial \Omega \). By \( V_{\alpha}, V_\alpha = V_\alpha(x_\alpha) \), we denote the pair potentials acting outside the core domains, i.e. at \( |x_\alpha| > c_\alpha \).

The Faddeev components of the function \( \Psi \) are introduced via the formulas [18,19]

\[
\Phi_\alpha(X) = - \int_{\Gamma_\alpha \cap \partial \Omega} d\sigma_S G_0(X, S; E) \frac{\partial}{\partial n_S} \Psi(S) - \int_{\Omega} dX' G_0(X, X'; E) (V_\alpha \Psi)(X'). \quad (2)
\]

One can show that they satisfy the following system of differential equations

\[
\begin{cases}
(-\Delta_X + V_\alpha - E)\Phi_\alpha(X) = -V_\alpha \sum_{\beta \neq \alpha} \Phi_\beta(X), & |x_\alpha| > c_\alpha, \\
(-\Delta_X - E)\Phi_\alpha(X) = 0, & |x_\alpha| < c_\alpha. 
\end{cases} \quad (3)
\]

According to Eqs. (1) and (2) the sum \( \Phi_\alpha(X) \) outside the surface \( \partial \Omega \) coincides with the total wave function \( \Psi \), i.e., \( \sum_{\beta=1}^{3} \Phi_\beta(X) \equiv \Psi(X), \quad X \in \Omega \). At the same time, it follows from the Green’s formula that this sum vanishes inside all the core domains, \( \sum_{\beta=1}^{3} \Phi_\beta(X) \equiv 0, \quad X \in \text{core domains} \).
\[ R^6 \setminus \Omega \). In practice one can replace these, very strong, conditions with the essentially more weak ones \([19,20]\)

\[ \sum_{\beta=1}^{3} \Phi_{\beta}(X) \bigg|_{x_\alpha = c_\alpha} = 0, \quad \alpha = 1, 2, 3, \quad (4) \]

requiring that the sum of \( \Phi_{\alpha}(X) \) to be zero only on the cylinders \( \Gamma_\alpha \).

Partial version of the Faddeev equations (3) for a system of three identical bosons read (see [21,24])

\[ \left( -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \frac{l(l+1)}{x^2} + \frac{\lambda(\lambda+1)}{y^2} - E \right) \Phi_{aL}(x, y) = \begin{cases} -V(x)\Psi_{aL}(x, y), & x > c \\ 0, & x < c \end{cases} \quad (5) \]

Here, by \( x, y \) we denote absolute values of the Jacobi variables \( x, y \) and by \( c \), the core size which is now the same for all three two-body subsystems. The notation \( L \) stands for the total angular momentum, and \( l, \lambda \), for the relative angular momenta corresponding respectively to a two-body subsystem and complementary particle; \( a = \{ l, \lambda \} \). The potential \( V(x) \) is supposed to be central, acting in the same way in all the partial waves \( l \). The partial wave function \( \Psi_{aL}(x, y) \) is related to the partial Faddeev components \( \Phi_{aL}(x, y) \) by

\[ \Psi_{aL}(x, y) = \Phi_{aL}(x, y) + \sum_{a'} \int_{-1}^{+1} d\eta h_{a'a}^L(x, y, \eta) \Phi_{a'L}(x', y') \quad (6) \]

where

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

with \( \eta = \hat{x} \cdot \hat{y} \). The explicit form for the function \( h_{a'a}^L \) can be found in Ref. [21,24]. The functions \( \Phi_{aL}(x, y) \) satisfy the boundary conditions

\[ \Phi_{aL}(x, y) \big|_{x=0} = \Phi_{aL}(x, y) \big|_{y=0} = 0, \quad (7) \]

while the partial version of the hard-core condition (4) is given by

\[ \Phi_{aL}(c, y) + \sum_{a'} \int_{-1}^{+1} du h_{a'a}^L(c, y, \eta) \Phi_{a'L}(x', y') = 0. \quad (8) \]

For the bound-state problem one requires that the functions \( \Phi_{aL}(x, y) \) are square integrable in the quadrant \( x \geq 0, y \geq 0 \). A more detailed and useful in bound state calculations is the asymptotic condition

\[ \Phi_{aL} = \sum_{\nu} \psi_{l,\nu}(x) h_\lambda(\sqrt{E - \epsilon_{l,\nu}} y) \left[ a_{aL,\nu} + o(y^{-1/2}) \right] \\
+ \frac{\exp(i\sqrt{E}\rho + i\pi L/2)}{\sqrt{\rho}} \left[ A_{aL}(\theta) + o(\rho^{-1/2}) \right] \quad (9) \]

where \( E \) is the bound-state energy, \( \rho = |X|, \ \theta = \arctan y/x \), and \( \psi_{l,\nu}(x) \) is the two-body partial wave function corresponding to a \( \nu \)-th bound state \( \epsilon_{l,\nu} \) for the angular momentum
value \( l \). The notation \( h_\lambda \) is used for the spherical Hankel function. The coefficients \( a_{aL,\nu} \) and \( A_{aL}(\theta) \) describe contributions into \( \Phi_{aL} \) from the \((2+1)\) and \((1+1+1)\) channels respectively. The corresponding asymptotic boundary conditions for the partial Faddeev components of the \((2+1 \rightarrow 2+1;\ 1+1+1)\) scattering wave function as \( \rho \rightarrow \infty \) and/or \( y \rightarrow \infty \) read as

\[
\Phi_{aL}^{[a,\nu]}(x, y, p) = \delta_{a, a'} \psi_{l, \nu}(x) j_\lambda(p y) + \sum_{\nu'} \psi_{l', \nu}(x) h_\lambda(\sqrt{E - \epsilon_{l', \nu'}} y) \left[ a_{a', L, \nu'}^{[a, \nu]}(p) + o(y^{-1/2}) \right] \\
+ \frac{\exp(i \sqrt{E} \rho + i \pi L/2)}{\sqrt{\rho}} \left[ A_{a', L}^{[a, \nu]}(p, \theta) + o(\rho^{-1/2}) \right]
\]

where \( p = |p| \) is the relative moment conjugate to the variable \( y \) and the scattering energy \( E \) is given by \( E = \epsilon_{l, \nu} + p^2 \). The \( j_\lambda \) stands for the spherical Bessel function. The value \( a_{a', L, \nu'}^{[a, \nu]} \) represents, at \( E > \epsilon_{l', \nu'} \), the partial amplitude of an elastic scattering, \( a' = a \) and \( \nu' = \nu \), or rearrangement, \( a' \neq a \) or \( \nu' \neq \nu \), process. The functions \( A_{a', L}^{[a, \nu]}(\theta) \) provide us, at \( E > 0 \), the corresponding partial Faddeev breakup amplitudes.

We employed the Faddeev equations (4) and the hard-core, (8), and asymptotic, (9,10), boundary conditions to calculate the binding energies of the Helium at omic trimer and the estimation of corresponding partial Faddeev breakup amplitudes. A rearrangement, represents, at \( E > \epsilon \), where \( \epsilon \) is given by the (2 + 1 \rightarrow 2 + 1) process. The functions \( A_{a', L}^{[a, \nu]}(\theta) \) provide us, at \( E > 0 \), the corresponding partial Faddeev breakup amplitudes.

In the present work we restrict ourselves to calculations for \( S \)-state only. The partial components \( \Phi_{1\lambda 0} \) can be obtained in this case from the addition of even partial waves \( l \) and \( \lambda \) with \( l = \lambda \). 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. \cite{10} but in disagreement with the statement made in Ref. \cite{4}. It should be further noted that most of the contribution to the binding energy stems from the \( l = \lambda = 0 \) and \( l = \lambda = 2 \) partial component the latter being more than 35%. The contribution from the \( l = \lambda = 4 \) partial wave was shown in \cite{8} 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. \cite{3,4,11}. Note that in the papers \cite{4,11} this state is interpreted as an Efimov one \cite{27}. Our excited state results are given in Table II.

The phase shift \( \delta_0(E) \) results, for a Helium atom scattered off a Helium dimer at \( L = 0 \), are given in Table III. 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 \( l = \lambda = 2 \) partial wave is essential to describe the scattering correctly.

Our estimation for the scattering length, based on the phase shift results, with the HFD-B interactions is \( 170 \pm 5 \text{Å} \) in the case where only the \( l = \lambda = 0 \) are taken into account and \( 145 \pm 5 \text{Å} \) when both the \( l = \lambda = 0 \) and \( l = \lambda = 2 \) are considered. We mention here that an estimation of \( \ell_{sc} = 195 \text{Å} \) for the \(^4\text{He} \) atom. \(^4\text{He} \) dimer scattering length was previously made.
by Nakaichi-Maeda and Lim [6] via zero-energy scattering calculations and by employing a separable approximation for the HFDHE2 potential.

The results obtained with two realistic $^4\text{He}–^4\text{He}$ potentials clearly demonstrate the reliability of our method in three-body bound state and scattering calculations. The effectively hard-core inter-atomic potential together with other characteristics of the system, make such calculations extremely tedious and numerically unstable. The numerical advantage of our approach is already obvious from the structure of Eqs. (3): When a potential with a strong repulsive core is replaced with the hard-core model, one approximates, inside the core domains, only the Laplacian $-\Delta X$, instead of the sum of the Laplacian and a huge repulsive term, and in this way a much better numerical approximation can be achieved. Thus the present formalism paves the way to study various three-atomic systems, and to calculate important quantities such as the cross-sections, recombination rates etc.

ACKNOWLEDGMENTS

Financial support from the University of South Africa, the Joint Institute for Nuclear Research, Dubna, and the Russian Foundation for Basic Research (Projects No. 96-01-01292, No. 96-01-01716 and No. 96-02-17021) is gratefully acknowledged. The authors are indebted to Dr. F. M. Penkov for a number of useful remarks and to Prof. I. E. Lagaris for allowing us to use the computer facilities of the University of Ioannina, Greece, to perform scattering calculations.
REFERENCES

[1] W. L. McMillan, Phys. Rev. A 138, 442 (1983).
[2] V. R. Pandharipande, J. G. Zaboliwzky, S. C. Pieper, R. B. Wiringa, and U. Helmbrecht, Phys. Rev. Lett., 50, 1676 (1983).
[3] N. Usmani, S. Fantoni, and V. R. Pandharipande, Phys. Rev. B, 26, 6123 (1983).
[4] S. C. Pieper, R. B. Wiringa, and V. R. Pandharipande, Phys. Rev. B, 32, R3341 (1985).
[5] S. W. Rick, D. L. Lynch, J. D. Doll, J. Chem. Phys. 95, 3506 (1991).
[6] S. Nakai-Maeda and T. K. Lim, Phys. Rev. A, 28, 692 (1983).
[7] Th. Cornelius, W. Glöckle, J. Chem. Phys., 85, 3906 (1986).
[8] J. Carbonell, C. Gignoux, S. P. Merkuriev, Few–Body Systems 15, 15 (1993).
[9] J. S. Levinger, Yad. Fiz. 56, 106 (1993).
[10] M. Braun, S. A. Sofianos, D. G. Papageorgiou, and I. E. Lagaris, Preprint UNISA-NP-96/12 (1996).
[11] B. D. Esry, C. D. Lin, and C. H. Greene, Phys. Rev. A 54, 394 (1996).
[12] U. Buck, H. Meyer, J. Chem. Phys. 84, 4854 (1986).
[13] O. Echt, K. Sattler, and E. Recknagel, Phys. Rev. Lett. 47, 1121 (1981).
[14] F. Luo, G. C. McBane, G. Kim, C. F. Giese, and W. R. Gentry, J. Chem. Phys. 98, 3564 (1993).
[15] W. Schöllkopf and J. P. Toennies, Science 266, 1345 (1994).
[16] P. O. Fedichev, M. W. Reynolds, and G. V. Shlyapnikov, Phys. Rev. Lett., 77, 2921 (1996).
[17] V. N. Efimov, H. Schulz, Sov. J. Part. Nucl. 7, 349 (1976).
[18] S. P. Merkuriev, A. K. Motovilov, and S. L. Yakovlev, Theor. Math. Phys. 94, 306 (1993) (also see LANL E-print nucl-th/9606022).
[19] S. P. Merkuriev, A. K. Motovilov, Lett. Math. Phys. 7, 497 (1983).
[20] A. K. Motovilov, Vestnik Leningradskogo Universiteta, 22, 76 (1983).
[21] L. D. Faddeev, S. P. Merkuriev, Quantum scattering theory for several particle systems (Doderecht: Kluwer Academic Publishers, (1993)).
[22] B. Schulze, G. Wildenhain, Methoden der Potentialsforie für elliptische differential gleichungen beliebiger Ordnung (Academie–Verlag, Berlin, 1977.)
[23] A. A. Kvitsinsky, Yu. A. Kuperin, S. P. Merkuriev, A. K. Motovilov, and S. L. Yakovlev, Sov. J. Part. Nucl. 17, 113 (1986).
[24] S. P. Merkuriev, C. Gignoux, and A. Laverne, Ann. Phys. (N.Y.) 99, 30 (1976).
[25] R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor, and G. T. McConville, J. Chem. Phys. 79, 4330 (1979).
[26] R. A. Aziz, F. R. W. McCourt, and C. C. K. Wong, Mol. Phys. 61, 1487 (1987).
[27] V. Efimov, Nucl. Phys. A, 210, 157 (1973).
### TABLE I. Bound state energy (in K) results for the Helium trimer.

| Potential | Faddeev equations | Variational methods | Adiabatic approach |
|-----------|-------------------|---------------------|-------------------|
|           | $l$               | This work           | 6                | 7                | 11               | 10                |
| HFDHE2    | 0                 | 0.084               | 0.082            | 0.092            | 0.1173           |
|           | 0.2               | 0.114               | 0.107            | 0.11             | 0.1193           |
| HFD-B     | 0                 | 0.096               |                  | 0.096            |                  |
|           | 0.2               | 0.131               |                  | 0.130            |                  |

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

| Potential | $l$ | This work | 6 | 7 | 10 |
|-----------|-----|-----------|---|---|----|
| HFDHE2    | 0   | 1.54      | 1.46| 1.04| 1.517 |
|           | 0.2 | 1.74      |    | 1.6 |      |
| HFD-B     | 0   | 2.56      |    |    |      |
|           | 0.2 | 2.83      |    |    |      |

### TABLE III. The $S$-state Helium atom–Helium dimer scattering phase shifts $\delta_0^{(0)}$ and $\delta_0^{(0,2)}$ obtained with the HFD-B $^4$He–$^4$He potential. The shifts $\delta_0^{(0)}$ correspond to the case where only the partial wave $l = \lambda = 0$ was included while the shifts $\delta_0^{(0,2)}$ were obtained with inclusion of both partial waves $l = \lambda = 0$ and $l = \lambda = 2$. The values of $\delta_0^{(0)}$, $\delta_0^{(0,2)}$ are given in degrees and $E$, in mK.

| $E$     | $\delta_0^{(0)}$ | $\delta_0^{(0,2)}$ | $E$     | $\delta_0^{(0)}$ | $\delta_0^{(0,2)}$ | $E$     | $\delta_0^{(0)}$ | $\delta_0^{(0,2)}$ |
|---------|------------------|--------------------|---------|------------------|-------------------|---------|------------------|-------------------|
| $-1.685$| 177.5            | 177.8              | $-1.1$  | 123.6            | 132.6             | $0.7$   | 88.9             | 98.7              |
| $-1.68$ | 172.3            | 173.3              | $-0.8$  | 115.0            | 124.6             | $1.0$   | 85.7             | 95.4              |
| $-1.60$ | 153.4            | 156.4              | $-0.4$  | 105.7            | 115.5             | $1.4$   | 81.8             | 91.5              |
| $-1.5$  | 142.3            | 148.0              | $-0.1$  | 99.9             | 109.7             | $1.8$   | 78.4             | 88.0              |
| $-1.4$  | 135.8            | 143.0              | $+0.3$  | 93.9             | 103.7             | $2.4$   | 74.2             | 83.5              |