

ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

44909
85-02

E4-2002-85

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ULTRA-LOW ENERGY ELASTIC SCATTERING
IN A SYSTEM OF THREE HELIUM ATOMS

Submitted to «Chemical Physics Letters»

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I. INTRODUCTION

The systems of helium atom small clusters were a subject of a number of experimental and theoretical researches during the last decades (1-19). Development of new experimental techniques (1-3) has stimulated growing interest to theoretical investigation of bound states and scattering dynamics in such systems. Availability of numerous potential models (4-10) of He-He interatomic interaction provides a good background for such theoretical researches (11-19).

Although the number of papers devoted to investigation of small helium cluster bound states, especially helium trimer, is considerable, the number of known results with respect to scattering in such systems is still very limited. There are only a few estimations for He-He₂ scattering length (21; 22) and, up to our knowledge, only one group has published results both for He-He₂ scattering length and phase shifts (14; 15). However, the accuracy of the known results for scattering length and phase shifts seems to be insufficient to resolve the details of different potential models.

The calculations presented here are performed on the base of differential Faddeev equations in configuration space in total angular momentum representation (24). This formalism was already used in our calculations of ⁴He₃ bound states (19; 20) and allowed us to obtain very accurate and detailed description for both ground and excited states of the trimer. Applying this rigorous and reliable formalism to scattering we expect to obtain benchmark-quality results for He-He₂ scattering length and phase shifts. The first presentation of these results is the subject of this Letter.

The paper is organized as follows. In Section 2 we give a brief description of the equations we solve and a short sketch on the new solution technique. The results of our calculations are provided with comments and a short discussion in Section 3. In Section 4 we give a short resume and present our view on the possible future application of the methods employed in this paper.

II. FORMALISM

According to the Faddeev formalism (23) the wave function of three particles is expressed in terms of Faddeev components Φ

$$\Psi(\mathbf{x}_1, \mathbf{y}_1) = \Phi_1(\mathbf{x}_1, \mathbf{y}_1) + \Phi_2(\mathbf{x}_2, \mathbf{y}_2) + \Phi_3(\mathbf{x}_3, \mathbf{y}_3), \quad (1)$$

where \mathbf{x}_α and \mathbf{y}_α are Jacobi coordinates corresponding to the fixed pair α

$$\begin{aligned} \mathbf{x}_\alpha &= \left(\frac{2m_\beta m_\gamma}{m_\beta + m_\gamma} \right)^{\frac{1}{2}} (\mathbf{r}_\beta - \mathbf{r}_\gamma), \\ \mathbf{y}_\alpha &= \left(\frac{2m_\alpha(m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma} \right)^{\frac{1}{2}} \left(\mathbf{r}_\alpha - \frac{m_\beta \mathbf{r}_\beta + m_\gamma \mathbf{r}_\gamma}{m_\beta + m_\gamma} \right). \end{aligned} \quad (2)$$

Here \mathbf{r}_α are the positions of the particles in the center-of-mass frame. The Faddeev components obey the set of three equations

$$\begin{aligned} (-\Delta_x - \Delta_y + V_\alpha(\mathbf{x}_\alpha) - E)\Phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha) &= \\ &= -V_\alpha(x_\alpha) \sum_{\beta \neq \alpha} \Phi_\beta(\mathbf{x}_\beta, \mathbf{y}_\beta), \end{aligned} \quad (3)$$

$$\alpha = 1, 2, 3$$

where $V_\alpha(\mathbf{x}_\alpha)$ stands for pairwise potential. To make this system of equations suitable for numerical calculations one should take into account the symmetries of the physical system. Exploiting the identity of Helium atoms one can reduce the system of equations (3) to one equation (23). Since all the model potentials are central it is also possible to factor out the degrees of freedom corresponding to the rotations of the whole cluster (24). For the case of zero total angular momentum the reduced Faddeev equation reads

$$(H_0 + V(1 + P) - E)\Phi(x, y, z) = 0, \quad (4)$$

where H_0 is the restriction of free Hamiltonian to the intrinsic space corresponding to zero total angular momentum

$$H_0 = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \left(\frac{1}{x^2} + \frac{1}{y^2} \right) \frac{\partial}{\partial z} (1 - z^2) \frac{\partial}{\partial z},$$

x , y and z are the intrinsic coordinates corresponding to the one selected partitioning of the three particles into 2+1 subsystems

$$x = |\mathbf{x}|, \quad y = |\mathbf{y}|, \quad z = \frac{(\mathbf{x}, \mathbf{y})}{xy}, \quad (5)$$

$V = V(x)$ is the two-body potential and P is an operator defined as

$$P\Phi(x, y, z) = xy\left(\frac{\Phi(x^+, y^+, z^+)}{x^+y^+} + \frac{\Phi(x^-, y^-, z^-)}{x^-y^-}\right).$$

Here x^\pm , y^\pm and z^\pm are Jacobi coordinates corresponding to other partitionings of three particles into subsystems. Explicit expressions for these coordinates in the case of particles with equal masses are given by the following formulae

$$\begin{aligned} x^\pm &= \left(\frac{x^2}{4} + \frac{3y^2}{4} \mp \frac{\sqrt{3}}{2}xyz\right)^{1/2}, \\ y^\pm &= \left(\frac{3x^2}{4} + \frac{y^2}{4} \pm \frac{\sqrt{3}}{2}xyz\right)^{1/2}, \\ z^\pm &= \frac{\pm \frac{\sqrt{3}x^2}{4} \mp \frac{\sqrt{3}y^2}{4} - \frac{1}{2}xyz}{x^\pm y^\pm}. \end{aligned}$$

In this paper we concentrate our attention on the case of elastic scattering only. In this case the solution of the Faddeev equation (4) can be presented as a sum of two terms

$$\Phi(x, y, z) = \chi(x, y, z) + \tilde{\Phi}(x, y, z). \quad (6)$$

The function $\chi(x, y, z)$ corresponds to the initial state of the system, i.e. free motion of the atom and the dimer, the second term $\tilde{\Phi}(x, y, z)$ corresponds to the scattered state of the atom and the dimer. Explicit expression for $\chi(x, y, z)$ reads

$$\chi(x, y, z) = \varphi_2(x) \frac{\sin ky}{k},$$

where $\varphi_2(x)$ is the two-body bound state wave function, $k = \sqrt{E - E_2}$, E_2 is the energy of the two-body bound state and E is the total energy of the three-body system in the center of mass frame. The asymptotic boundary condition for the function $\tilde{\Phi}(x, y, z)$ is defined by

$$\tilde{\Phi}(x, y, z) \xrightarrow{y \rightarrow \infty} \frac{a(k)}{k} \varphi_2(x) \cos ky, \quad (7)$$

where $a(k)$ stands for the elastic scattering amplitude. Substituting the representation (6) to the equation (4) we get the equation for the function $\tilde{\Phi}(x, y, z)$

$$(H_0 + V(1 + P) - E)\tilde{\Phi}(x, y, z) = -VP\chi(x, y, z). \quad (8)$$

To calculate the low-energy scattering characteristics of the system one has to solve the equation (8) with the asymptotic boundary condition (7). The scheme of numerical solution of the equation is not the subject of the Letter, but we would like to mention some features of the method we employ that seem to be original or at least that were not applied for few-body calculations previously.

The general scheme of the problem discretization reproduces the one used in our helium trimer calculations (19; 20). However, the way we use tensor-trick preconditioning (26) is changed, that allowed us to reduce the dimension of the corresponding linear problem almost twice. Due to the structure of the Faddeev equations, in the case of potentials decreasing sufficiently fast, the region in configuration space where an interaction between atoms vanishes has a simple geometric shape of a hypercylinder $x > x_{max}$ exterior. Therefore, outside of the hypercylinder the Faddeev component $\tilde{\Phi}(x, y, z)$ satisfy an equation for free particles. At the same time, for large values of y , where the component meets the asymptotic boundary conditions, it satisfies the equation

$$(H_0 + V(x) - E)\tilde{\Phi}(x, y, z) \approx 0, y > y_{max}. \quad (9)$$

Taking into account the aforementioned observations one can find that a new component defined as

$$\tau(x, y, z) \equiv (H_0 + V(x) - E)\tilde{\Phi}(x, y, z) \quad (10)$$

is localized much better in coordinate x than the original component $\tilde{\Phi}(x, y, z)$ and can be approximated using much less grid points. One can even prove that unlike the original component $\tilde{\Phi}(x, y, z)$ such component is square integrable for scattering states even above the break-up threshold (square integrability of a similar object was briefly discussed in (27)). The equation for $\tau(x, y, z)$ reads

$$\tau(x, y, z) = -VP\chi(x, y, z) - VP(H_0 + V - E - i0)^{-1}\tau(x, y, z). \quad (11)$$

This is the equation which we solve numerically using Krylov subspace projection techniques. The operator $(H_0 + V - E - i0)^{-1}$ entering the equation is a resolvent of so called cluster Hamiltonian which corresponds to a system of

one free and two interacting particles. In our approach this operator is constructed by solving the corresponding differential equation with appropriate asymptotic boundary conditions, what is made using tensor-trick technique. Having the equation (11) solved, we recover the original component $\tilde{\Phi}(x, y, z)$ according to the definition (10), using the same tensor-trick.

As a result of numerical procedure we get an approximate solution $\tilde{\Phi}(x, y, z)$. To recover the scattering amplitude we compare the numerical solution with the asymptotic representation (7) pointwise. This way we define the function

$$a(k; x, y, z) \equiv \frac{k\tilde{\Phi}(x, y, z)}{\phi_2(x) \cos ky} .$$

Stability of this function with respect to variations of x , y and z coordinates indicates, that the asymptotic region is reached in the calculations and the function approaches the scattering amplitude. Such simple test for an asymptotic region is made possible by use of Cartesian coordinates (17). Another advantage provided by the usage of Cartesian coordinates is a simple test for the quality of a grid taken in x coordinate: this grid should support the correct value of the dimer binding energy (17; 19).

III. RESULTS

In this section we describe our calculations of He-He₂ elastic scattering and give a brief comparison of our calculations with other published results.

On the preliminary stage of the calculations we have verified, that our code reproduces the known properties of helium trimer ground and excited states for a particular potential model. To do it, a special version of the code using exactly the same procedures as the ones involved in scattering calculations was developed. All the known figures of trimer ground and excited state energies (19) were successfully reproduced. After that we have performed a set of calculations with maximal values of x and y taken at 2500 Å. The analysis of the results has allowed us to conclude that for small values of atom-dimer kinetic energy the asymptotic region starts approximately from 1000 Å in y coordinate. For all the values of y taken in the region $y > 1000$ Å and for all $x > 2$ Å (outside of the repulsive core region) the value of scattering

amplitude was stable up to 5 figures. The most of the subsequent calculations were performed with maximal values of x and y fixed at 1200 Å. To ensure that our results are stable and accurate we have performed the calculations of the He-He₂ scattering length, phase shifts and scattering amplitude using different sets of grids. The stability of the scattering length and scattering amplitude with respect to the number of grid points is demonstrated in the Tables I and II. The presented data allows to estimate the accuracy of our scattering length calculations as low as 0.1% what is comparable with the accuracy of the used physical constants.

In the Table III we present the results of scattering length and phase shifts calculations for six different potential models. The potentials HFD-B, LM2M2 and TTY were already used in atom-dimer scattering calculations (14; 15; 22). The estimations of scattering observables for more recent SAPT, SAPT1 and SAPT2 potentials are presented here for the first time. The potentials SAPT1 and SAPT2 (10) are constructed taking into account retardation effects that lead to the change of the highest term from $O(x^{-6})$ to $O(x^{-7})$ at large interatomic distances (28). All other potentials have $O(x^{-6})$ long-distance asymptotic behavior.

To prove the correctness of our calculations we must compare our results with known published results and to explain the differences between our results and results of other authors if possible. Unfortunately, only small number of independent results were published with respect to He-He₂ scattering problem. The number of calculations that take into account the interatomic interactions in the states with non-spherical symmetry is limited, up to our knowledge, only by the results of Motovilov et al. (14; 15) and recent calculations of Blume et al. (22). Our results for scattering length are brought together with the results known from literature in the Table IV. Obviously, the difference between our results and other results is far from negligible and requires an explanation.

The group of Motovilov has been solving differential Faddeev equations in bispherical harmonics representation, and they have taken into account the contribution of first three terms of the bispherical expansion. It can be shown, that this approach corresponds to the simplest grid in z coordinate that can be used within our method. This grid consists of the only one interval and the

corresponding spline basis contains 6 basic polynomial functions. However, as one can see from the Table I, restriction of our basis to the simplest case can not cover the observed difference of 10% in scattering length. The source of the observed discrepancy can be found in the cutoff distances used in the numerical calculations. The values reported in (15) are obtained for the cutoff radius of 460 Å. According to (25) the choice of this cutoff radius was forced by the limitations of the available computer facilities. To check the version about strong influence of the cutoff radius to the result we have performed calculations with cutoff parameters $x_{max} = 800$ Å and $y_{max} = 460$ Å. The results of these calculations are also presented in the Table IV. Evidently, they are in perfect agreement with the results of (15). Therefore we can confidently confirm the consistency of our results and the results published by Motovilov et al. (15). However, we must note, that for such reduced cutoff parameters the scattering amplitude varies within 30% interval even outside of the core region what indicates that such small cutoff distance is not enough to obtain stable results. As one can see from the Fig. 1, the asymptotic region where the scattering amplitude is rather stable with respect to variations of coordinates starts approximately from $y \sim 1000$ Å.

Even though the results for scattering length published in (15), considerably differs from the results presented in this Letter, the discrepancy between the results for phase shifts, as one can see from the Fig. 2, is not so big. The difference grows towards 2-body threshold, however in the vicinity of 3-body threshold ($E = 0$) the difference is rather small.

Unfortunately, the estimations of numerical error for the calculations performed by Blume et al. (22) are not available. Being aimed to calculation of larger clusters, their technique differs much from the one employed in this work. It makes detailed comparison of our results difficult, and we can only mention that their result for He-He₂ scattering length is in better agreement with the our one than the result of (15).

IV. CONCLUSIONS

New results for He-He₂ scattering length and elastic scattering phase shifts are presented for six different potential models. Being based on a rigorous

Table I Convergence of the He-He₂ scattering length with respect to the number of grid points (HFD-B potential)

Grid	$\times 6_z$	$\times 9_z$	$\times 15_z$
$56_x \times 86_y$	122.31	121.91	121.93
$68_x \times 101_y$	122.32	121.91	121.92
$77_x \times 116_y$	122.34	121.94	-
$86_x \times 131_y$	122.32	121.90	-
$98_x \times 146_y$	122.31	-	-

Table II Convergence of the He-He₂ scattering amplitude with respect to the number of grid points (HFD-B potential) at $E_{rel} = E - E_2 = 1.515$ mK

Grid	$\times 6_z$	$\times 9_z$	$\times 15_z$
$56_x \times 86_y$	-3.023	-2.996	-2.997
$68_x \times 101_y$	-3.036	-3.009	-3.009
$77_x \times 116_y$	-3.041	-3.014	-
$86_x \times 131_y$	-3.041	-3.013	-
$98_x \times 146_y$	-3.039	-	-

theoretical approach suitable for atom-dimer scattering calculations (Faddeev equations in total angular momentum representation, Cartesian coordinates) and an original numerical technique, these results improve the reference results of Motovilov et al.(15) by two orders of magnitude. The results for SAPT, SAPT1 and SAPT2 potential models are new.

Comparison of elastic scattering parameters calculated for the available potential models shows, that difference between the parameters is rather small and can hardly reveal the fine details of the He-He interatomic interaction. It gives promise that low-energy properties of He-He interaction can be repro-

Table III Scattering lengths and phase shifts for different potential models

Potential	l_{sc} (Å)	δ (degrees) for different values of $E_{rel} = E - E_2$ (mK)						
		0.01212	0.1212	0.303	0.606	0.909	1.212	1.515
HFD-B	121.9	353.01	337.95	325.37	311.86	302.2	294.6	288.3
LM2M2	115.4	353.38	338.79	326.19	312.54	302.7	294.8	288.3
TTYPT	115.8	353.35	338.73	326.13	312.47	302.6	294.3	286.5
SAPT	123.7	352.91	337.72	325.10	311.66	302.0	294.4	288.2
SAPT1	122.4	352.99	337.90	325.30	311.84	302.2	294.6	288.3
SAPT2	123.1	352.95	337.81	325.20	311.75	302.1	294.5	288.3

Table IV Comparison of calculated scattering length with the results known from literature

Potential	(15)	(22)	This work	
			$x_{max} = y_{max} = 1200\text{Å}$	$x_{max} = 800\text{Å},$ $y_{max} = 460\text{Å}$
HFD-B	135 ± 5	N/A	121.9 ± 0.1	132
LM2M2	131 ± 5	126	115.4 ± 0.1	134

duced within much simpler model than realistic potential models employed in this work.

The numerical technique developed and applied in this work can be further applied in investigation of bound states and scattering of other exotic systems. For instance, it can be applied to calculate bound states and scattering in the systems of other rare gas atoms. Four-body calculations based on Faddeev-Yakubovsky differential equations (29) can also be performed within our approach.

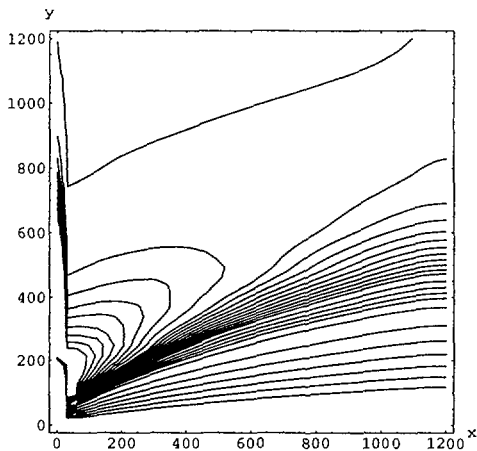


Figure 1 Contour plot of $\lim_{k \rightarrow 0} a(k; x, y, 0)/k$, the values of x and y are given in Å

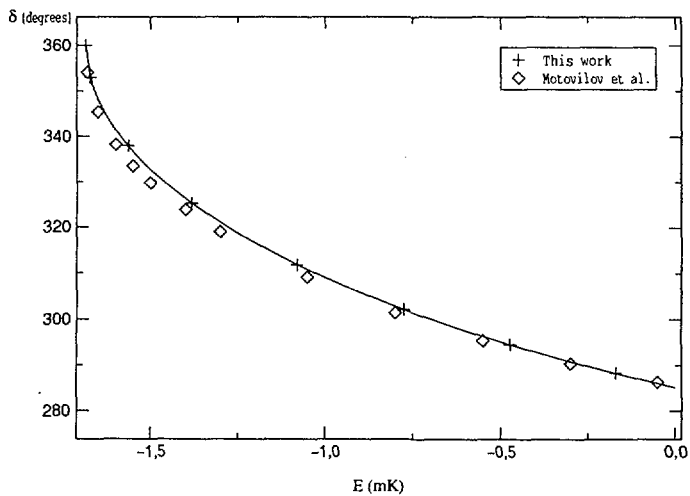


Figure 2 He-He₂ scattering phase shifts for HFD-B potential. The energy E is the energy of the system in the center of mass frame.

Acknowledgements

The author is like to express his special gratitude to Dr. A.K.Motovilov for attracting his attention to the subject and for a recommendation to visit the Bogolubov Laboratory of Theoretical Physics, JINR, Dubna, where the final part of this work was performed in the framework of JINR-UNESCO agreement. The author is grateful to Prof. S.L.Yakovlev for constant moral support and useful practical advises, to Dr. D.E.Monakhov for organising the visit to Dubna, to Dr. F.M.Pen'kov for encouraging discussions and to I.M.Alexandrovitch for inspiration and warm hospitality during the stay in Dubna.

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Received on April 19, 2002.