

HELIUM TRIMER IN THE FRAMEWORK OF FADDEEV APPROACH

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Differential Faddeev equations in total angular momentum representation are used for the calculations of helium trimer system. Numerical results on binding energies of $^4\text{He}_3$ and ultracold collisions of ^4He atom on ^4He dimer are reviewed.

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INTRODUCTION

Studying the special properties of tiny molecules consisting of just two or three atoms of helium attracted considerable attention in recent years. These systems have unique quantum properties that are of greatest importance to basic research. For instance, the two atoms in a helium dimer are very weakly bonded and have an interatomic spacing of about 100 atomic radii making the helium dimer the largest known molecule that exists.

Experimentally, helium dimers have been observed for the first time in 1993 by the Minnesota group [1], and in 1994 by Schöllkopf and Toennies [2]. Later on, Grisenti et al. [3] measured a bond length of $(52 \pm 4) \text{ \AA}$ for $^4\text{He}_2$, which indicates that this dimer is the largest known diatomic molecular ground state. Based on this measurement they estimated a scattering length of $104_{-18}^{+8} \text{ \AA}$ and a dimer energy of $1.1_{-0.2}^{+0.3} \text{ mK}$ [4]. In the latter investigation [5] the trimer pair distance is found to be $1.1_{-0.5}^{+0.4} \text{ nm}$ in agreement with theoretical predictions for the ground state.

Due to the small magnitude of the dimer energy, one should expect that the $^4\text{He}_3$ trimer indeed possesses the theoretically predicted state of the Efimov type (see [6–9]). It is this property that distinguishes the ^4He atoms from the atoms of all other noble gases, and makes the ^4He clusters especially attractive objects of experiments. Because of the possibility of experimental observation of the Efimov effect [10], the ^4He trimer is undoubtedly interesting for nuclear physicists as well. In the year 2000, an interesting hypothesis [11] on the possibility of experimental observation of the Efimov state in $^4\text{He}_3$ trimers was put forward. The suggestion

was to scatter ultracold ${}^4\text{He}$ clusters on diffraction lattices with sufficiently small lattice spacing (of the order of 10 nm or less). The practical realization of this experiment, see [5], did not lead to obvious success, and at present a reliable experimental evidence on the existence of excited states in ${}^4\text{He}_3$ trimers is still missing. However, in the experiment [5], the size of the ${}^4\text{He}_3$ molecule in the ground state was estimated for the first time.

1. FORMALISM

Our previous investigation [12] (and see the ref. therein) of the ${}^4\text{He}$ three-atomic system was based on hard-core version of the Faddeev differential equations. In the exploited scheme of solving the Faddeev equations we made a partial-wave decomposition in an auxiliary (bipolar) basis in order to reduce the dimension of the Faddeev equations at the expense of dealing with an infinite set of partial equations. In such a way, we faced the problem of the slow convergence of the corresponding partial-wave expansion. As a consequence, the accuracy achieved in [12], especially for the scattering length, appeared somewhat limited [13]. A way to overcome these difficulties with taking into account higher numbers of two-body partial waves is to make use of the three-dimensional differential Faddeev equations [14] that are obtained from the original six-dimensional ones by only separating off the three angular variables (Eulerian angles) that describe the rotation of the system as a whole. Here we will apply these equations for computation of helium trimer bound state energy.

To describe the configuration of the three-body system, we introduce standard scaled Jacobi coordinates, $\mathbf{x}_\alpha, \mathbf{y}_\alpha$, $\alpha = 1, 2, 3$:

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

where \mathbf{r}_i are the position vectors of particles; m_i — the masses and (α, β, γ) are a cyclic permutation of the atom numbers (1, 2, 3).

The wave function Ψ of the system can be expressed as a sum of the three Faddeev components Ψ_α

$$\Psi(\mathbf{x}, \mathbf{y}) = \sum_{\alpha} \Psi_{\alpha}(\mathbf{x}_{\alpha}, \mathbf{y}_{\alpha})$$

which obey the Faddeev equation [15]

$$(-\Delta_{\mathbf{x}_\alpha} - \Delta_{\mathbf{y}_\alpha} + V_\alpha(|\mathbf{x}_\alpha|) - E)\Psi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = -V_\alpha(|\mathbf{x}_\alpha|) \sum_{\beta \neq \alpha} \Psi_\beta(\mathbf{x}_\beta, \mathbf{y}_\beta), \quad (2)$$

where E is the energy of the system. The potential energy of the system is invariant with respect to rotation. This makes it possible [14] to separate out the degrees of freedom corresponding to rotation of the system by expanding the Faddeev components in terms of eigenfunctions of the total angular momentum. In case of zero total angular momentum the projection of Eq. (2) takes the form

$$(H_0 + V_\alpha(x_\alpha) - E)\Phi_\alpha(x_\alpha, y_\alpha, \theta_\alpha) = -V_\alpha(x_\alpha) \sum_{\beta \neq \alpha} \Phi_\beta(x_\beta, y_\beta, \theta_\beta),$$

$$H_0 = -\frac{\partial^2}{\partial x_\alpha^2} - \frac{\partial^2}{\partial y_\alpha^2} - \left(\frac{1}{x_\alpha^2} + \frac{1}{y_\alpha^2} \right) \frac{1}{\sin \theta_\alpha} \frac{\partial}{\partial \theta_\alpha} \sin \theta_\alpha \frac{\partial}{\partial \theta_\alpha}, \quad (3)$$

where Φ_α are projections of the Faddeev components in subspace with fixed angular momentum. Equations (3) are three-dimensional partial-wave differential equations in the internal space, which is parametrized by Jacobi coordinates

$$x_\alpha = |\mathbf{x}_\alpha|, \quad y_\alpha = |\mathbf{y}_\alpha|, \quad \cos \theta_\alpha = \frac{(\mathbf{x}_\alpha, \mathbf{y}_\alpha)}{x_\alpha y_\alpha}, \quad \alpha = 1, 2, 3.$$

Assuming that each two-body subsystem has only one bound state, one can write the asymptotic boundary condition for the Faddeev components of the $(2 + 1 \rightarrow 2 + 1; 1 + 1 + 1)$ scattering processes, as $\rho \rightarrow \infty$ and/or $y \rightarrow \infty$,

$$\Phi(x, y, \theta; p) = \delta_{l_0} \psi_d(x) \left\{ \sin(py) + \exp(ipy) \left[a_0(\theta; p) + o(y^{-1/2}) \right] \right\} + \frac{\exp(i\sqrt{E}\rho)}{\sqrt{\rho}} \left[A(y/x, \theta; p) + o(\rho^{-1/2}) \right]. \quad (4)$$

Here, $\psi_d(x)$ is the wave function of the two-body bound state in the two-body subsystem, E stands for scattering energy $E = \epsilon_d + p^2$ with ϵ_d being the two-body bound state energy, and p for the relative momentum conjugates to the variable y , $\rho = \sqrt{x^2 + y^2}$. The coefficients $a_0(\theta; p)$ and $A(y/x, \theta; p)$ are the amplitudes of the rearrangement and break-up processes.

To overcome the strong-repulsion problem we use the hard-core modification of the Faddeev differential equations [16–18].

2. RESULTS

We have applied developed numerical algorithm for solving the above-mentioned equations to the ${}^4\text{He}_3$ three-atomic system. Number of grid points was taken up to 300 on each variable. As He–He interaction we used the LM2M2 potentials by Aziz and co-workers [19]. For the explicit form of these polarization potentials we refer to the Appendix of [20]. We choose $\hbar^2/m_{4\text{He}} = 12.12 \text{ K} \cdot \text{\AA}^2$

Table 1. Dimer energy ϵ_d , bond length $\langle R \rangle$ and ${}^4\text{He}-{}^4\text{He}$ scattering length $\ell_{\text{sc}}^{(1+1)}$ for the potentials used, as compared to the experimental values of [4]

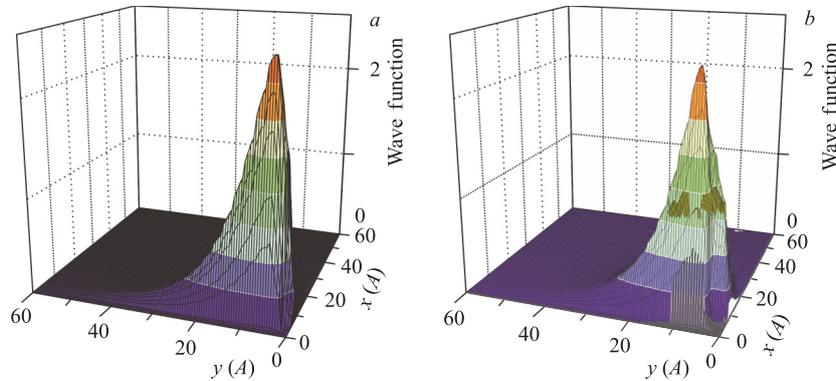
Potential model	ϵ_d , mK	$\ell_{\text{sc}}^{(1+1)}$, Å	$\langle R \rangle^*$, Å
LM2M2	-1.30348	100.23	51.84
Exp. [4]	$1.1^{+0.3}_{-0.2}$	104^{+8}_{-18}	52^{+4}_{-4}

*Results from [21].

Table 2. Results for binding energies of the ${}^4\text{He}_3$ trimer and the ${}^4\text{He}-{}^4\text{He}_2$ scattering lengths

$ E , \ell_{\text{sc}}$	Pres. work	[22]	[23]	[24]	[25]	[26]	[27]	[28]	[29]
$ E_{4\text{He}_3} $, mK	126.45	125.2	125.52^1	126.41	$126.3(9)^1$	126.15	126.2	126.39	125.6^1
$ E_{4\text{He}_3}^* $, mK	2.282^2	2.269		2.271		2.274		2.268	2.245^1
$\ell_{\text{sc}}^{(4\text{He}-4\text{He}_2)}$, Å	116^3			115.8^4		120.91			

¹In original paper the energy value is given in cm^{-1} ($1 \text{ cm}^{-1} = 1.4387752 \text{ K}$).
²This value was rounded in [20].
³Result of extrapolation, see [13].
⁴Result from [30].



Surface of the wave function of the ${}^4\text{He}_3$ ground state (sections at $z = 0.025$ (a) and $z = 0.769$ (b) for the LM2M2 interaction

for comparison with the results of other authors. The ${}^4\text{He}$ dimer binding energies and ${}^4\text{He}-{}^4\text{He}$ scattering lengths obtained with the LM2M2 potential are shown in Table 1.

Table 2 summarizes the results on trimer binding energies and He–He₂ scattering lengths. The binding energies of the ⁴He trimer ground state ($E_{4\text{He}_3}$) and excited state ($E_{4\text{He}_3}^*$) are presented in the first two rows. These results demonstrate good agreement between the different methods. The third row contains values of the ⁴He–⁴He₂ scattering lengths.

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