Binding energy of the $^3\text{He}^4\text{He}_2$ trimer within the hard-core Faddeev approach$^*$

E.A. Kolganova$^*$, Y.K. Ho

Institute of Atomic and Molecular Sciences, Academia Sinica, P.O.Box 23-166, Taipei, Taiwan 10764, ROC

A.K. Motovilov

Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russia

We apply a hard-core version of the Faddeev differential equations to the $^3\text{He}^4\text{He}_2$ three-atomic system. Using these equations we calculate the binding energy of the $^3\text{He}^4\text{He}_2$ trimer with the LM2M2 potential by Aziz and Slaman and more recent TTY potential by Tang, Toennies and Yiu.

1 Introduction

There is a great number of experimental and theoretical studies of the $^4\text{He}$ three-atomic system (see, e.g., [1]–[13] and references cited therein). The non-symmetric system $^3\text{He}^4\text{He}_2$ found comparatively little attention. We can only mention the recent works [6], [8], and [13] where the $^3\text{He}^4\text{He}_2$ trimers were treated alongside with small $^4\text{He}$ clusters. Until now only the bound states of the $^3\text{He}^4\text{He}_2$ system have been studied numerically. There are still no scattering calculations reported for this system.

The $^4\text{He}$ trimer is known in particular for the Efimov's nature of its excited state (see [3, 6, 8, 14]. The binding energy of the $^4\text{He}$ dimer is extremely small (about $1 \text{ mK}$) on the molecular scale. The large spatial extension of the $^4\text{He}_2$ bound state generates a long-range effective interaction between a $^4\text{He}$ dimer and additional $^4\text{He}$ atom which results in a possibility of existence of extremely extended $^4\text{He}$ three-atomic states.

Being a more light particle than $^4\text{He}$, the $^3\text{He}$ atom supports no bound state with the $^4\text{He}$ counterpart and no $^3\text{He}$ dimer exists. Thus, the $^3\text{He}^4\text{He}_2$ is even a more loosely bound system than the $^4\text{He}$ trimer. According to the hyperspherical adiabatic calculations of [6, 8] and Monte-Carlo investigation of [13] the realistic He-He potentials such as LM2M2 [15] and TTY [16] support only one bound state of the $^3\text{He}^4\text{He}_2$ trimer with the energy of the order of $10–15 \text{ mK}$.

Notice that the $^4\text{He}/^3\text{He}$ three-atomic systems belong to the three–body systems whose theoretical treatment is quite difficult. The difficulty is mainly due to the two reasons. First, the low energy of the practically on-threshold bound states makes it necessary to consider very large domains in configuration space with a size of hundreds of Å. Second, the strong repulsive part of the He-He interaction at short distances produces large numerical errors.

Like [9, 11], the present work is based on a mathematically rigorous hard-core version of the Faddeev differential equations. This method allows to overcome the strong-repulsion

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$^*$ On leave of absence from Joint Institute for Nuclear research, 141980 Dubna, Russia
problem. The first of the problems just mentioned is tackled by choosing sufficiently large grids.

This note represents rather a first step in an extension of the numerical approach of \cite{9, 11} to the case of three-body systems including particles with different masses. In the nearest future we plan not only to continue our study of the $^3\text{He}^4\text{He}_2$ bound state but also to perform calculations of the scattering of a $^3\text{He}$ atom off a $^4\text{He}_2$ dimer. Here we only outline the method employed and report our first results for the binding energy of the $^3\text{He}^4\text{He}_2$ system.

2 Formalism

In describing the $^3\text{He}^4\text{He}_2$ three-atomic system we use the reduced Jacobi coordinates \cite{17} $x_\alpha, y_\alpha, \alpha = 1, 2, 3$, expressed in terms of the position vectors of the atoms $r_i \in \mathbb{R}^3$ and their masses $m_i$,

$$x_\alpha = \left[ \frac{2m_\beta m_\gamma}{m_\beta + m_\gamma} \right]^{1/2} (r_\beta - r_\gamma)$$
$$y_\alpha = \left[ \frac{2m_\alpha(m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma} \right]^{1/2} \left( r_\alpha - \frac{m_\beta r_\beta + m_\gamma r_\gamma}{m_\beta + m_\gamma} \right)$$

where $(\alpha, \beta, \gamma)$ stand for a cyclic permutation of the atom numbers $(1, 2, 3)$. The coordinates $x_\alpha, y_\alpha$ fix the six-dimensional vector $X \equiv (x_\alpha, y_\alpha) \in \mathbb{R}^6$. The vectors $x_\beta, y_\beta$ corresponding to the same point $X$ as the pair $x_\alpha, y_\alpha$ are obtained using the transformations

$$x_\beta = c_{\alpha\beta}x_\alpha + s_{\alpha\beta}y_\alpha, \quad y_\beta = -s_{\beta\alpha}x_\alpha + c_{\beta\alpha}y_\alpha,$$  

where

$$c_{\alpha\beta} = -\left( \frac{m_\alpha m_\beta}{(m_\alpha + m_\beta)(m_\beta + m_\gamma)} \right)^{1/2},$$
$$s_{\alpha\beta} = (-1)^{\beta-\alpha} \text{sign}(\beta - \alpha) \left( 1 - c_{\alpha\beta}^2 \right)^{1/2}.$$  

In the following we assume that the $^4\text{He}$ atoms are assigned the numbers 1 and 2 while the $^3\text{He}$ atom has the number 3. By $c$ we denote the hard-core radius which will be taken the same (in coordinates $x_\alpha$) for all three inter-atomic interaction potentials. A recent detail description of the Faddeev differential equations in the hard-core model which we employ can be found in \cite{9}. Nevertheless we outline here some essential characteristics of the hard-core Faddeev approach needed for understanding our numerical procedure.

Since the $^4\text{He}$ atoms are identical bosons the corresponding Faddeev component $F_3(x_3, y_3)$ is invariant under the permutations the particles 1 and 2 which implies

$$F_3(-x_3, y_3) = F_3(x_3, y_3).$$  

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The identity of the two $^4$He atoms also implies that the Faddeev components $F_1(x_1, y_1)$ and $F_3(x_2, y_3)$ are obtained from each other by a simple rotation of the coordinate space. Thus, we only have two independent Faddeev components, the one associated with the $^4$He–$^4$He subsystem, $F_3(x, y)$, and another one, say $F_1(x, y)$, associated with a pair of $^3$He and $^4$He atoms. The resulting hard-core Faddeev equations read

$$(-\Delta - E)F_\alpha(x_\alpha, y_\alpha) = \begin{cases} 0, & |x_\alpha| < c \\ -V_\alpha(x_\alpha)\Psi^{(\alpha)}(x_\alpha, y_\alpha), & |x_\alpha| > c \end{cases}, \quad (4)$$

$$\Psi^{(\alpha)}(x_\alpha, y_\alpha)\Big|_{|x_\alpha| = c} = 0, \quad \alpha = 1, 3,$$

where $\Psi^{(1)}$ and $\Psi^{(3)}$ denote the total wave function $\Psi(X)$ of the $^3$He$^4$He$_2$-system written via the Faddeev components $F_1$ and $F_3$ in different coordinates $x_1, y_1$ and $x_3, y_3$. More precisely

$$\Psi^{(1)}(x_1, y_1) = F_1(x_1, y_1) + F_1(c_{21}x_1 + s_{21}y_1, -s_{21}x_1 + c_{21}y_1) + F_3(c_{31}x_1 + s_{31}y_1, -s_{31}x_1 + c_{31}y_1)$$

and

$$\Psi^{(3)}(x_3, y_3) = F_3(x_3, y_3) + F_1(c_{13}x_3 + s_{13}y_3, -s_{13}x_3 + c_{13}y_3) + F_1(c_{23}x_3 + s_{23}y_3, -s_{23}x_3 + c_{23}y_3).$$

By $V_1$ and $V_3$ we denote the same interatomic He–He potential recalculated in the corresponding reduced Jacobi coordinates $x_1$ and $x_3$.

In the present investigation we apply the above formalism to the $^3$He$^4$He$_2$ three-atomic system with total angular momentum $L = 0$. Expanding the functions $F_1$ and $F_3$ in a series of bispherical harmonics we have

$$F_\alpha(x, y) = \sum_l f_l^{(\alpha)}(x, y) \gamma_{l0}(\tilde{x}, \tilde{y}), \quad \alpha = 1, 3,$$

where $x = |x|$, $y = |y|$, $\tilde{x} = x/x$, and $\tilde{y} = y/y$. (Notice that by (6) only the terms $f_l^{(3)}(x, y)$ with even momenta $l$ are nonzero.) As a result the equations (4) and boundary conditions (5) are transformed to the following partial integro-differential equations

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + l(l+1)\left(\frac{1}{x^2} + \frac{1}{y^2}\right) - E\right)f_l^{(\alpha)}(x, y) = \begin{cases} 0, & x < c \\ -V_\alpha(x)\psi_l^{(\alpha)}(x, y), & x > c \end{cases}, \quad \alpha = 1, 3,$$

where $x = |x|$, $y = |y|$, $\tilde{x} = x/x$, and $\tilde{y} = y/y$. (Notice that by (6) only the terms $f_l^{(3)}(x, y)$ with even momenta $l$ are nonzero.) As a result the equations (4) and boundary conditions (5) are transformed to the following partial integro-differential equations

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The partial wave functions \( \psi^{(\alpha)}_j(x,y) \), \( \alpha = 1,3 \), read as follows

\[
\psi^{(1)}_j(x,y) = f^{(1)}_j(x,y) + \sum_{l'} \int_0^1 d\eta \left[ h^{(0)}_{(1J0)(2J'0)}(x,y,\eta)f^{(1)}_{l'}(x_{21}(\eta),y_{21}(\eta)) \right.
\]
\[
\left. + h^{(0)}_{(1J0)(3J'0)}(x,y,\eta)f^{(3)}_{l'}(x_{31}(\eta),y_{31}(\eta)) \right],
\]
\[
\psi^{(3)}_j(x,y) = f^{(3)}_j(x,y) + \sum_{l'} \int_0^1 d\eta \left[ h^{(0)}_{(3J0)(1J'0)}(x,y,\eta)f^{(1)}_{l'}(x_{13}(\eta),y_{13}(\eta)) \right.
\]
\[
\left. + h^{(0)}_{(3J0)(2J'0)}(x,y,\eta)f^{(1)}_{l'}(x_{23}(\eta),y_{23}(\eta)) \right]
\]

where (cf. [17])

\[
\begin{align*}
  h^{(0)}_{(\alpha J Kl')(\beta J' k'l')} \quad &
  h^{(0)}_{(1J0)(2J'0)}(x,y,\eta) \\
  &\quad = \frac{xy}{x_{\beta\alpha}(\eta) y_{\beta\alpha}(\eta)} \left[ (2\lambda + 1)(2I + 1) \right]^{1/2}
  \left[ (2\lambda + 1)(2I + 1) \right]^{1/2}
  \sum_{k=0}^{k_{\text{max}}} (-1)^k (2k + 1) \prod_{l=1}^{l_{\text{max}}} \frac{\gamma_{\beta\alpha}(\eta) \lambda_{l_{\text{max}}}^{\lambda_{l_{\text{max}}}+l_{\text{max}}}}{\gamma_{\beta\alpha}(\eta) \lambda_{l_{\text{max}}}^{\lambda_{l_{\text{max}}}+l_{\text{max}}}}
  \times \left[ (2\lambda + 1)(2I + 1) \right]^{1/2}
  \left. \sum_{l'_{\text{max}}} (2\lambda_{l'+1} + 1)(2I_{l'+1} + 1) \right]
\end{align*}
\]

Here \( P_k(\eta) \) is the Legendre polynomial of order \( k \). In the above, the standard notation for the 3-\( j \), 6-\( j \), and 9-\( j \) Wigner symbols, as defined in [18], is used. We also use the notation

\[
  x_{\beta\alpha}(\eta) = \sqrt{c_{\beta\alpha}^2 + 2c_{\beta\alpha}s_{\beta\alpha}\eta + s_{\beta\alpha}^2},
\]
\[
  y_{\beta\alpha}(\eta) = \sqrt{s_{\beta\alpha}^2 - 2c_{\beta\alpha}s_{\beta\alpha}\eta + c_{\beta\alpha}^2}.
\]

We conclude the section with the asymptotic boundary condition for a \(^4\text{He}^3\text{He}_2\) bound
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$$f_l^{(a)}(x,y) = \delta_{\alpha \delta_0} \delta_0 \psi_d(x) \exp\left(i \sqrt{E - \epsilon_d} y\right) \left[a_0 + o\left(y^{-1/2}\right)\right]$$

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

(10)

as $\rho = \sqrt{x^2 + y^2} \to \infty$ and/or $y \to \infty$. Here we use the fact that the helium dimer $^4$He$_2$ has a bound state and this state only exists for $l = 0$; $\epsilon_d$ stands for the $^3$He$_2$ dimer energy while $\psi_d(x)$ denotes the $^3$He$_2$ dimer wave function which is assumed to be zero within the core, that is, $\psi_d(x) \equiv 0$ for $x \leq c$.

3 Results

We employed the Faddeev equations \cite{1}, the hard-core boundary condition \cite{8}, and the asymptotic condition \cite{10} to calculate the binding energy of the helium trimer $^3$He$^4$He$_2$. As He-He interaction we used the semi-empirical LM2M2 potential of Aziz and Slaman \cite{15} and the latest theoretical potential TTY of Tang, Toennies and Yiu \cite{16}. In our present calculations we used the value $\hbar^2/m = 12.1192 \, \text{KÅ}^2$ where $m$ stands for the mass of a $^4$He atom. (Notice the difference between this more precise value and the value $\hbar^2/m = 12.12 \, \text{KÅ}^2$ which was used in the previous calculations \cite{9}.) Both the LM2M2 and TTY potentials produce a weakly bound state for the $^4$He dimer. We found that the $^4$He-dimer energy is 1.309 mK in case the LM2M2 interaction and 1.316 mK for the TTY potential. Both LM2M2 and TTY support no bound state for the $^4$He$^3$He two-atomic system.

As in \cite{9,11} we considered a finite-difference approximation of the boundary-value problem \cite{2,5,10} in the polar coordinates $\rho = \sqrt{x^2 + y^2}$ and $\theta = \arctan(y/x)$. The grids were chosen such that the points of intersection of the arcs $\rho = \rho_i$, $i = 1, 2, \ldots, N_\rho$ and the rays $\theta = \theta_j$, $j = 1, 2, \ldots, N_\theta$ with the core boundary $x = c$ constitute the knots. The value of the core radius was chosen to be $c = 1 \, \text{Å}$ by the same argument as in \cite{11}. Also the method for choosing the grid radii $\rho_i$ (and, thus, the grid hyperangles $\theta_j$) was the same as described in \cite{11}.

In the present investigation we were restricted to considering only the two lowest partial components $f_0^{(1)}(x,y)$ and $f_0^{(3)}(x,y)$ and therefore we only dealt with the two partial equations of the system \cite{7} corresponding to $l = 0$. We solved the block three-diagonal algebraic system, arising as a result of the finite-difference approximation of \cite{7,8,10}, on the basis of the matrix sweep method \cite{19}. This method makes it possible to avoid using disk storage for the matrix during the computation.

The best possible dimensions of the grids which we employed in this investigation were $N_\rho = 600$ and $N_\theta = 605$. We found that on the $600 \times 605$ grid with $\rho_{\text{max}} = 200 \, \text{Å}$ the LM2M2 potential supports the bound state of the $^3$He$^4$He$_2$ with the energy $E_i = 7.33 \, \text{mK}$ while the corresponding binding energy produced by the TTY potential is $E_i = 7.28 \, \text{mK}$.

Our figures for $E_i$ correspond to the lowest possible dimension of the system \cite{7}. We consider this as reason why our results show a significant underboundedness of the $^3$He$^4$He$_2$ trimer as compared to the available results for $E_i$ obtained for the TTY potential on the basis of the variational VMC (9.585 mK \cite{14}) and DMC (14.165 mK \cite{13}) methods and for the LM2M2 potential on the basis of a one-channel hyperspherical adibatic
approximation of the Faddeev differential equations \((9.682 \text{ mK} \ [8])\) and \((10.22 \text{ mK} \ [6])\). We think the situation will change when more partial waves in \((7)\) will be employed. A certain (but rather small) deepening of the binding energy \(E_t\) may also be expected due to choosing the grids with larger \(N_\theta\) and \(N_\rho\).

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