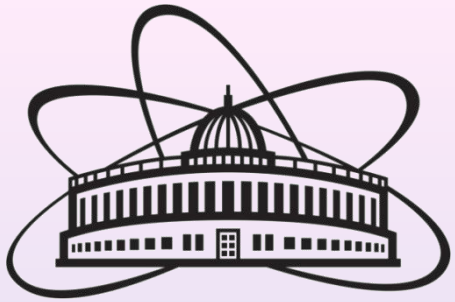
*The IVth International School and Workshop on Few-Body Systems*



# INVESTIGATION OF THE SYMMETRIC AND ASYMMETRIC THREE-ATOMIC SYSTEMS

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## *Outline:*

- ✓ ***Few –Body Systems:***
  - Dimer, Trimer and …
  - Motivation: *Why are weakly bound state problems interesting?*
  - *Efimov effect*
  - Experiments: Helium Dimers and Trimers
- ✓ ***Formalism:***
  - Solving three - body bound state problems
  - Faddeev differential equations
- ✓ ***Results:***
  - $^{4}He_3$ and $^{3}He$-$^{4}He_2$ - Helium Trimers
  - $^{20}Ne_3$ - Neon Trimers
- ✓ ***Conclusion***

# *Efimov effect*

Volume 33B, number 8 PHYSICS LETTERS 21 December 1970

## ENERGY LEVELS ARISING FROM RESONANT TWO-BODY FORCES IN A THREE-BODY SYSTEM

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Received 20 October 1970

**Resonant two-body forces are shown to give rise to a series of levels in three-particle systems. The number of such levels may be very large. Possibility of the existence of such levels in systems of three α-particles ($^{12}$C nucleus) and three nucleons ($^{3}$H) is discussed.**

The range of nucleon-nucleon forces $r_0$ is known to be considerably smaller than the scattering lengts $a$. This fact is a consequence of the resonant character of nucleon-nucleon forces. Apart from this, many other forces in nuclear physics are resonant. The aim of this letter is to expose an interesting effect of resonant forces in a three-body system. Namely, for $a \gg r_0$ a series of bound levels appears. In a certain case, the number of levels may become infinite.

Let us explicitly formulate this result in the simplest case. Consider three spinless neutral particles of equal mass, interacting through a potential $gV(r)$. At certain $g = g_0$ two particles get bound in their first s-state. For values of $g$ close to $g_0$, the two-particle scattering length $a$ is large, and it is this region of $g$ that we shall confine ourself to. The three-body continuum boundary is shown in the figure by cross-hatching. The effect we are drawing attention to is the following. As $g$ grows, approaching $g_0$, three-particle bound states emerge one after the other. At $g = g_0$ (infinite scattering length) their number is infinite. As $g$ grows on beyond $g_0$, levels leave into continuum one after the other (see fig. 1).

The number of levels is given by the equation

$$N \approx \frac{1}{\pi} \ln (|a|/r_0) \qquad (1)$$

All the levels are of the $0^+$ kind; corresponding wave functions are symmetric; the energies $E_N \ll 1/r_0^2$ (we use $\hbar = m = 1$); the range of these bound states is much larger than $r_0$.

We want to stress that this picture is valid for $a \gg r_0$. Three-body levels appearing at $a \approx r_0$ or with energies $E \approx 1/r_0^2$ are not considered.

The physical cause of the effect is in the emergence of effective attractive long-range forces of radius $a$ in the three-body system. We can demonstrate that they are of the $1/R^2$ kind; $R^2 = r_{12}^2 + r_{23}^2 + r_{31}^2$. This form is valid for $R \gtrsim r_0$. With $a \to \infty$ the number of levels becomes infinite as in the case of two particles interacting with attractive $1/r^2$ potential.

Vitaly Efimov

*Efimov Physics (1970) [1]: Nuclear Physics, Atomic Physics.*

**When one weakens the two-body potentials (supporting a single bound state) the number of 3-body bound states can increase to infinity!** And this happens at the moment when the two-body bound states disappear.

[1] *V. N. Efimov, "Energy levels arising from resonant two-body forces in a three-body system" Phys. Lett.33, 563 (1970).*

*First experimental observation in Cs atoms*

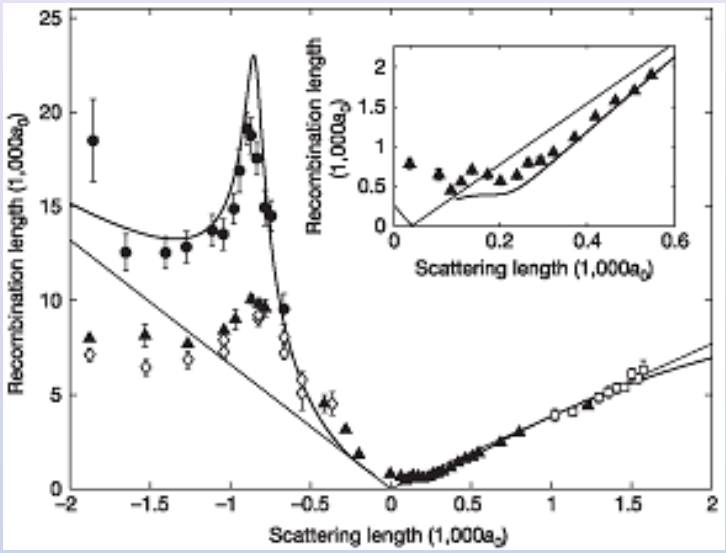
*Kraemer, et.al. Nature (2006)*

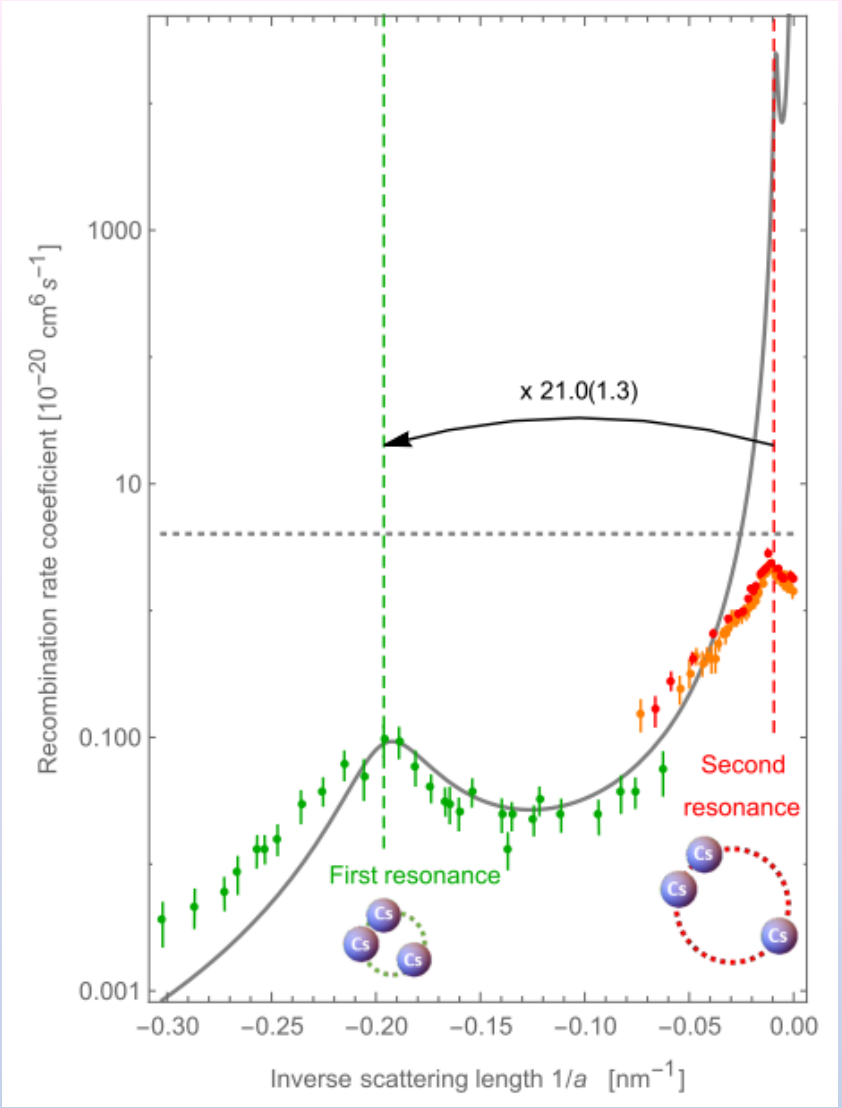
Vol 440|16 March 2006|doi:10.1038/nature04626 nature

LETTERS

## Evidence for Efimov quantum states in an ultracold gas of caesium atoms

T. Kraemer[1], M. Mark[1], P. Waldburger[1], J. G. Danzl[1], C. Chin[1,2], B. Engeser[1], A. D. Lange[1], K. Pilch[1], A. Jaakkola[1], H.-C. Nägerl[1] & R. Grimm[1,3]




**$^4He_3$**

*After a long and continued research, the Efimov state as the excited state of the helium trimer, was detected .*

[1] *M. Kunitski et al. // Science. 2015. V.348. P.551*.

*B. Huang et al. "Observation of the Second Triatomic Resonance in Efimov's Scenario". Phys. Rev. Lett., 112 , 190401 (2014).*

# Potential models: PRZ2010 [6] and PRZ2017 [7]

$$V(R) = V_{BO}(R) + V_{ad}(R) + V_{rel}(R) + V_{QED}(R)$$

$V_{BO}(R)$ - nonrelativistic Born - Oppenheimer (BO),
$V_{ad}(R)$ - adiabatic correction,
$V_{rel}(R)$ - relativistic correction,
$V_{QED}(R)$ - quantum electrodynamics (QED).

| $R$ | $V_{\mathrm{BO}}$ | $V_{\mathrm{ad}}$ | $V_{\mathrm{rel}}$ | $V_{\mathrm{QED}}$ | $V$ |
|---|---|---|---|---|---|
| 3.0 | 3767.681(71) | 1.387(7) | −0.2197(23) | 0.0942(2) | 3768.94(7) |
| 4.0 | 292.570(15) | 0.1080(32) | 0.0324(14) | 0.0089(2) | 292.719(15) |
| 5.0 | −0.4754(65) | −0.0075(13) | 0.0240(2) | −0.001 06(4) | −0.460(7) |
| 5.6 | −11.0006(2) | −0.0090(5) | 0.015 40(4) | −0.001 35(2) | −10.9955(5) |
| 6.0 | −9.6819(23) | −0.0072(3) | 0.011 43(5) | −0.001 20(4) | −9.6788(23) |
| 7.0 | −4.6225(6) | −0.003 33(7) | 0.005 77(3) | −0.000 74(3) | −4.6208(6) |
| 12.0 | −0.165 92(2) | −0.000 125(1) | 0.000 575(2) | −0.000 13(3) | −0.165 60(3) |

The computed values of *V(R)* were fitted to an analytic function

$$\sum_{k=1}^{M} e^{-a_k R} \sum_{i=I_0}^{I_1} P_{ik} R^i - \sum_{n=N_0}^{N_1} f_n(\zeta R) \frac{C_n}{R^n}$$

$f_{2n}(x)$ - the Tang-Toennies damping function $\quad f_{2n}(x) = 1 - e^{-x} \sum_{k=0}^{2n} \frac{x^{-k}}{k!}$

$a_k$, $P_{ik}$ and $\zeta$ are adjustable parameters, and the summation limits [$M$, $I_0$, $I_1$, $N_0$, $N_1$]

[6] Przybytek M., Cencek W., et. al. // Phys. Rev. Lett. 2010. 104. P. 183003.
[7] Przybytek M., Cencek W., et. al. // Phys. Rev. Lett. 2017. 119. P. 123401.

# $^4He_2$

***Measurements:***

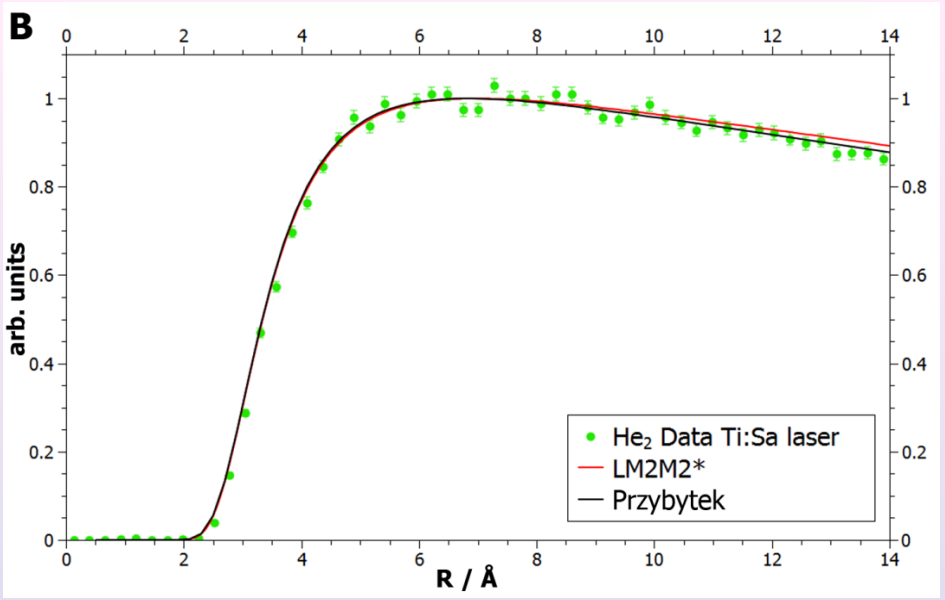
bond length [2] $\langle R \rangle = 52 \pm 4$ Å

Estimation of the binding energy and scattering length:

$\varepsilon_d = 1.1^{+0.3}_{-0.2}$ mK $\quad l_{sc} = 104^{+8}_{-18}$ Å [2]

$\varepsilon_d = 1.3^{+0.25}_{-0.19}$ mK ? $l_{sc} = 100^{+8}_{-7.9}$ Å [3]

$\varepsilon_d = 1.76^{+0.15}_{-0.15}$ mK [4]




| Potential | HFD-B [9] | LM2M2 [10] | TTY [8] | PRZ2010 [6] | PRZ2017 [7] | Exp. [2] | Exp. [2, 3] | Exp. [4] |
|---|---|---|---|---|---|---|---|---|
| $\varepsilon_d$, mK | 1.69201 | 1.30936 | 1.32103 | 1.62087 | 1.61768 | $1.1^{+0.3}_{-0.2}$ | $1.3^{+0.25}_{-0.19}$ | $1.76^{+0.15}_{-0.15}$ |
| Vloc, Å | 2.96300 | 2.96950 | 2.97207 | 2.96760 | 2.96763 | | | |
| \|Vmin\|, K | 10.9480 | 10.9700 | 10.9847 | 10.9966 | 10.9965 | | | |

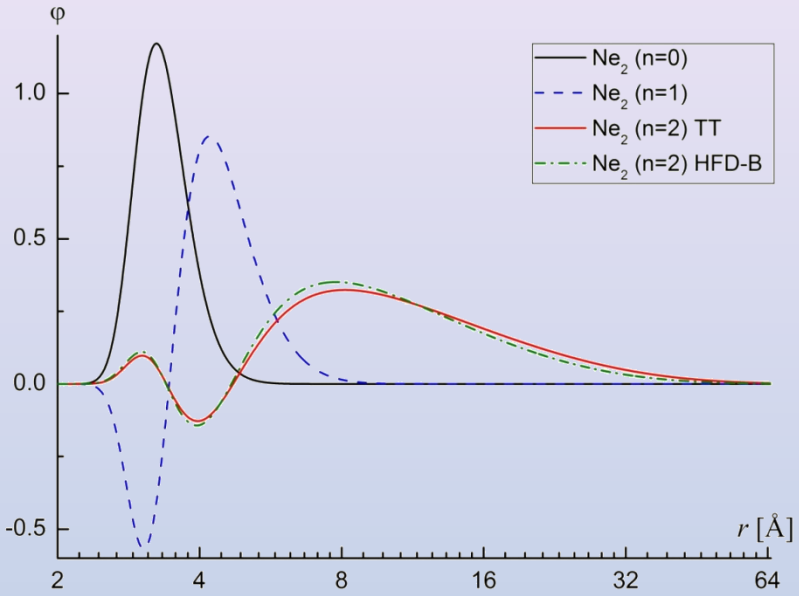

[1] F. Luo *et. al.*// J. Chem. Phys. 98 (1993) 9687.
[2] Grisenti R., Scho_llkopf W., Toennies J.P., et al. // Phys. Rev. Lett. 2000. 85. P. 2284.
[3] Cencek W., Przybytek M., Komasa J., et al. // J. Chem. Phys. 2012. 136. P. 224303.
[4] S. Zeller, *et al.* // Proc. Nat. Acad. Sci. 113 (2016) 14651
[6] Przybytek M., Cencek W., Komasa J., Lach G., Jeziorski B., Szalewicz K. // Phys. Rev. Lett. 2010. 104. P. 183003.
[7] Przybytek M., Cencek W., Jeziorski B., Szalewicz K. // Phys. Rev. Lett. 2017. 119. P. 123401.
[8] Tang K.T., Toennis J.P., Yiu C.L. // Phys. Rev. Lett. 1995. 74. P. 1546.
[9] Aziz R.A., McCourt F.R.W., Wong C.C.K. // Mol. Phys. 1987. 61. P. 1487.
[10] Aziz R.A., Slaman M.J. // J. Chem. Phys. 1991. 94. P. 8047-8053.

# $^{20}Ne_2$

| n | E (K) [1] |
|---|---|
| 0 | 24,22 ± 0,02 |
| 1 | 4,405 ± 0,02 |
| 2 | < 0.14 |

| Level | 0 | | | 1 | | | 2 | | |
|---|---|---|---|---|---|---|---|---|---|
| Potential | $E_0$ | $\langle r \rangle$ | $\sqrt{\langle r^2 \rangle}$ | $E_1$ | $\langle r \rangle$ | $\sqrt{\langle r^2 \rangle}$ | $E_2$ | $\langle r \rangle$ | $\sqrt{\langle r^2 \rangle}$ |
| TT | 24.0598 | 3.3329 | 3.3471 | 4.2049 | 4.2849 | 4.3438 | 0.0181 | 12.4793 | 13.8709 |
| HFD-B | 24.3715 | 3.3309 | 3.3452 | 4.4527 | 4.2527 | 4.3109 | 0.0276 | 11.2127 | 12.2721 |

**Table 1. Energy levels of the bound states $E_n$ (K), the average radius $\langle r \rangle$ (Å) and the root mean square radius $\sqrt{\langle r^2 \rangle}$ (Å) of Ne dimers, calculated with potentials TT [9] and HFD-B [10]. The energies are given in units of K and are relative to the three-body dissociation threshold.**



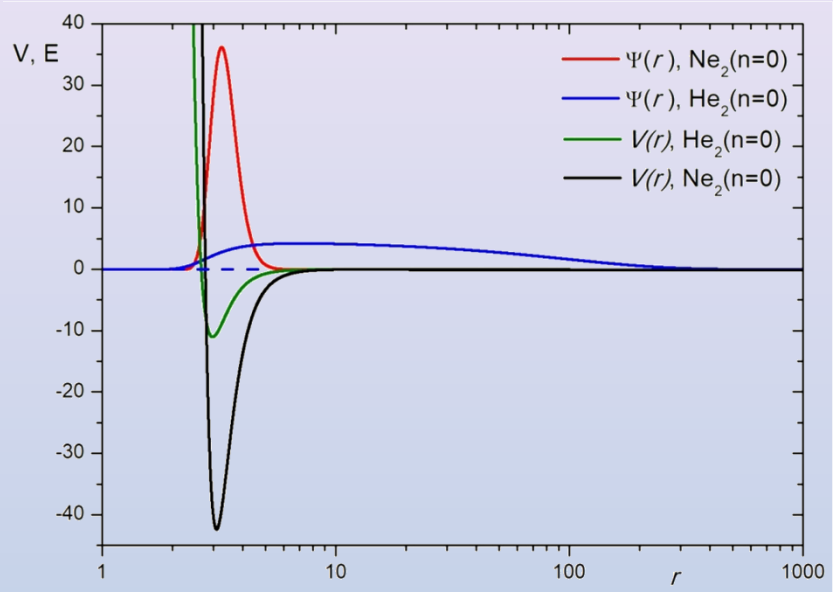
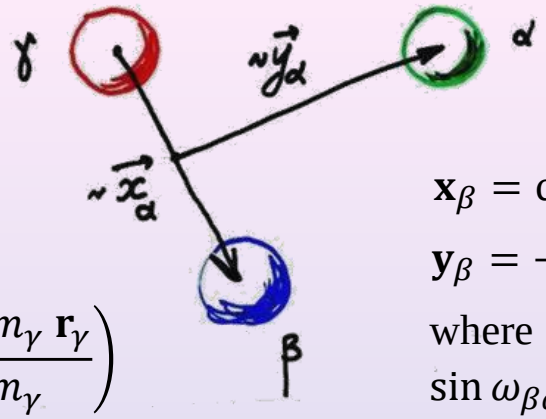




Fig. The radial wave functions φ of the ground and excited states of neon dimer, calculated with the TT [9] and HFD- B [10] potentials.


[*] A.A. Korobitsin, E.A. Kolganova et. al., Physics of Atomic Nuclei, 80, 553 (2017).
[1] A.Wüest, F.Merkt//J.Chem.Phys.118 (2003) 8807.
[9] K.T. Tang and J.P. Toennies, J. Chem. Phys. 118, 4976 (2003).
[10] R.A. Aziz and M.J. Slaman, J. Chem. Phys. 130, 187 (1989).

## *Faddeev differential equations:*

Jacobi coordinates $\mathbf{x}_\alpha$ , $\mathbf{y}_\alpha$ *($\alpha$ = 1,2,3):*




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

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

$$\mathbf{x}_\beta = \cos\omega_{\beta\alpha}\, \mathbf{x}_\alpha + \sin\omega_{\beta\alpha}\, \mathbf{y}_\alpha$$

$$\mathbf{y}_\beta = -\sin\omega_{\beta\alpha}\, \mathbf{x}_\alpha + \cos\omega_{\beta\alpha}\, \mathbf{y}_\alpha$$

where coefficients $\cos\omega_{\beta\alpha}$ and $\sin\omega_{\beta\alpha}$ depend only on the particles masses [2].

The total wave function $\Psi$ of three-body system can be written as the sum of the Faddeev components:

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

Faddeev components $F_\alpha$ satisfy the following set of equations [1]:

$$(-\Delta_x - E) F_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = \begin{cases} 0, & |\mathbf{x}_\alpha| < c \\ -V_\alpha(\mathbf{x}_\alpha)\Psi(\mathbf{x}_\alpha, \mathbf{y}_\alpha), & |\mathbf{x}_\alpha| > c \end{cases}, \quad \Psi(\mathbf{x}_\alpha, \mathbf{y}_\alpha)\big|_{|\mathbf{x}_\alpha|=c} = 0$$

$E$ – total energy of the system, $V_\alpha$ - interaction potential in the $\alpha$ pair


[1] – Kolganova E.A., Motovilov A.K., Sandhas W. // Physics of Particles and Nuclei. 2009. 40. P. 206.

[2] – L.D. Faddeev, S.P. Merkuriev // Quantum scattering theory for several particles (1993)

# *Three-dimensional Faddeev differential equations*

Faddeev equations in the representation of zero total angular momentum:

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

$$x_\alpha = |\mathbf{x}_\alpha|, \qquad y_\alpha = |\boldsymbol{y}_\alpha|, \qquad z_\alpha = \frac{(\mathbf{x}_\alpha, \boldsymbol{y}_\alpha)}{x_\alpha\, y_\alpha}$$

where the kinetic energy operator $H_0$ is of the form:

$$H_0 = -\frac{\partial^2}{\partial {x_\alpha}^2} - \frac{\partial^2}{\partial {y_\alpha}^2} - \left(\frac{1}{{x_\alpha}^2} + \frac{1}{{y_\alpha}^2}\right)\frac{\partial}{\partial z_\alpha}(1 - {z_\alpha}^2)\frac{\partial}{\partial z_\alpha}$$

Asymptotic boundary conditions for the Faddeev component:

$$F(x, y, z) \underset{\rho\to\infty}{=} \varphi_2(x)\exp(ipy)\, a_0(z; E) + \frac{\exp(i\sqrt{E}\rho)}{\rho^{1/2}} A\left({}^{y}/_{x}, z; E\right),$$

where $\varphi_2(x)$ - bound state wave function of the two-body subsystem,
$E = E_2 + p^2$, $E_2$- two - body bound state energy,
$E$- energy of the three body system, $\rho = \sqrt{x^2 + y^2}$
$a_0(z; E)$ - amplitude of the rearrangement,
$A(x/y, z; E)$ - amplitude decay into three separate particles.

[1] - V.V. Kostrykin, A.A. Kvitsinsky, S.P. Merkuriev // Few-Body Syst. 6 (1989) 97

Faddeev differential equations in the hyperspherical coordinates [1-3]:

$$(H_0 + V_\alpha - E)\, F_\alpha(\rho, \chi_\alpha, \theta_\alpha) = -V_\alpha \sum_{\beta \neq \alpha} F_\beta(\rho, \chi_\beta, \theta_\beta) \qquad (1)$$

The kinetic energy operator $H_0$ is of the form:

$$H_0 = -\rho^{-5}\partial_\rho \rho^5 \partial_\rho - \frac{4}{\rho^2}\sin^{-2}\chi_\alpha \left(\partial_{\chi_\alpha} \sin^2\chi_\alpha\, \partial_{\chi_\alpha} + \sin^{-1}\theta_\alpha\, \partial_{\theta_\alpha} \sin\theta_\alpha\, \partial_{\theta_\alpha}\right)$$

where $\rho$, $\chi_\alpha$ and $\theta_\alpha$ are the hyperspherical coordinates expressed through standard Jacobi variables $\mathbf{x}_\alpha, \mathbf{y}_\alpha$, $\alpha$ = 1,2,3:

$$\rho = \sqrt{{x_\alpha}^2 + {y_\alpha}^2}, \qquad \tan\left(\frac{\chi_\alpha}{2}\right) = y_\alpha / x_\alpha, \qquad \cos\theta_\alpha = \frac{(\mathbf{x}_\alpha, \mathbf{y}_\alpha)}{x_\alpha y_\alpha}$$

$$x_\alpha = |\mathbf{x}_\alpha|, \quad y_\alpha = |\boldsymbol{y}_\alpha|, \quad \rho \in [0, \infty], \quad \{\chi_\alpha, \theta_\alpha\} \in [0, \pi] \otimes [0, \pi].$$

The hyperradius $\rho$ is invariant in $\alpha$, whereas the hyperspherical angles are related by:

$$\cos\chi_\beta = \cos\omega_{\beta\alpha}\cos\chi_\alpha + \sin\omega_{\beta\alpha}\sin\chi_\alpha\cos\theta_\alpha$$

$$\cos\theta_\beta \sin\chi_\beta = -\sin\omega_{\beta\alpha}\cos\chi_\alpha + \cos\omega_{\beta\alpha}\sin\chi_\alpha\cos\theta_\alpha$$

for three identical particles:

$$\sin\omega_{\beta\alpha} = \pm\frac{\sqrt{3}}{2}$$

$$\cos\omega_{\beta\alpha} = -\frac{1}{2}$$

[1] - V.V. Kostrykin, A.A. Kvitsinsky, S.P. Merkuriev // Few-Body Syst. 6 (1989) 97,
[2] - A.A. Kvitsinsky and C.-Y. Hu // Few-Body Syst. 12 (1992) 7,
[3] - V.A. Roudnev, S.L. Yakovlev, and S.A. Sofianos // Few-Body Syst. 37 (2005) 179.

For numerical solution it is suitable to substitute:

$$\phi_\alpha = \rho^{5/2} \sin\chi_\alpha \sin\theta_\alpha F_\alpha$$

The differential operator $\widetilde{H}_0$ is given by

$$\widetilde{H}_0 = -\partial_\rho^2 - \frac{4}{\rho^2}\left[\partial_\chi^2 + \sin^{-2}\chi\left(\partial_\theta^2 - \cot\theta\,\partial_\theta + \sin^{-2}\theta\right) + \frac{1}{16}\right]$$

where $\chi \equiv \chi_\alpha, \theta \equiv \theta_\alpha,\ x = \rho\cos(\chi_\alpha/2).$

The Faddeev equations (1) in terms $\phi_\alpha$ of and the hard-core boundary conditions are written as [1]:

$$(\widetilde{H}_0 + V_\alpha(x) - E)\,\phi_\alpha(\rho,\chi,\theta) = -V_\alpha(x)(P^+ + P^-)\,\phi_\alpha(\rho,\chi,\theta),\ x > core$$
$$(\widetilde{H}_0 - E)\,\phi_\alpha(\rho,\chi,\theta) = 0, \qquad x < core$$

and

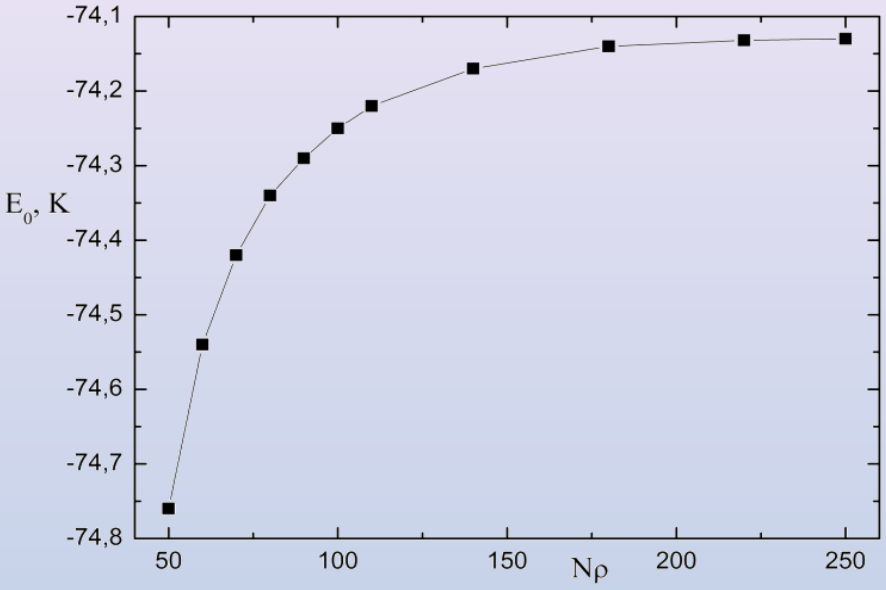
$$\phi_\alpha(\rho,\chi,\theta) = -(P^+ + P^-)\,\phi_\alpha(\rho,\chi,\theta),\ x = core.$$

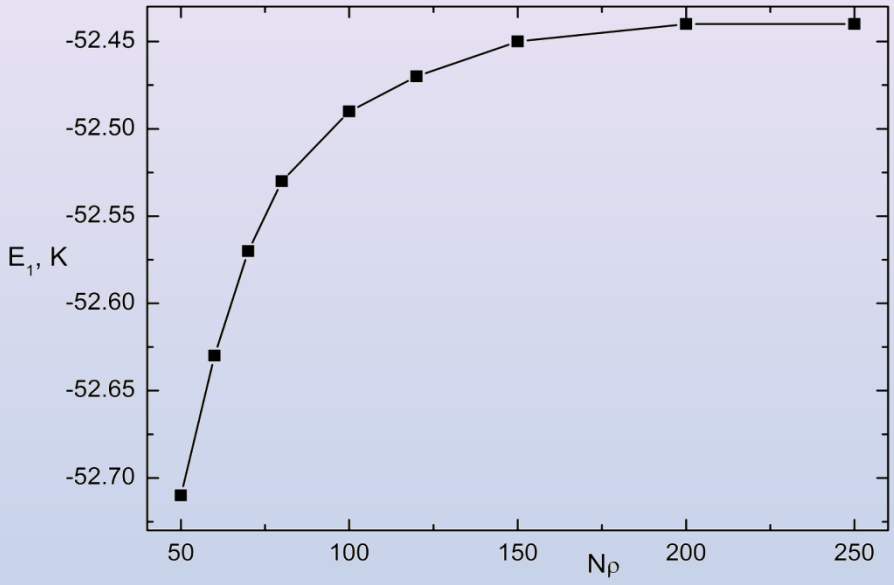
$\phi_\beta = P^+\phi_\alpha, \qquad \phi_\gamma = P^-\phi_\alpha, \quad P^+(123) = (312), P^-(123) = (231)$

where $P^\pm$ stand for operators of cyclic permutation of particles.

[1] - E.A. Kolganova, A.K. Motovilov, S.A. Safianos // J. Phys.B. 31 (1998) 1279

# Eigen (C++ library)




Convergence of the neon trimer ground and first excited states energy on the grid points $N_\rho$ for fixed value of $N_\theta$ = 100 and $N\chi$ = 10.

$^{20}Ne_3$

| $E$ (K) | HFD-B [1] | TT [1] | [13]$^a$ | [14]$^a$ |
|---|---|---|---|---|
| $E_0$ | 74,13 | 74,07 | 74,10 | 74,11 |
| $E_1$ | 52,44 | 52,37 | 52,41 | 52,43 |
| $E_2$ | 49,25 | 49,19 | 49,23 | 49,24 |
| $E_3$ | 45,53 | 45,49 | 45,51 | 45,52 |
| $E_4$ | 40,37 | 40,31 | 40,34 | 40,35 |
| $E_5$ | 34,67 | 34,62 | 34,65 | 34,66 |
| $E_6$ | 32,33 | 32,27 | 32,3 | 32,31 |
| $E_7$ | 31,54 | 31,48 | 31,51 | 31,52 |
| $E_8$ | 27,66 | 27,61 | 27,64 | 27,65 |
| $E_9$ | 26,20 | 26,16 | 26,17 | 26,18 |
| $E_{10}$ | 24,95 | 24,92 | 24,93 | 25,02 |

a – HFD-B potential model used.

[1] A.A. Korobitsin, E.A. Kolganova, Physics of Elementary Particles and Atomic Nuclei, Letters, **14**, 971, (2017).
[13] M. Salci, S. B. Levin, N. Elander, and E. Yarevsky, J. Chem. Phys. **129**, 134304 (2008).
[14] H. Suno, J. Chem. Phys. **135**, 134312 (2011); *ibid*, J. Phys. B **49**, 014003 (2016).

## *Two-dimensional Faddeev differential equations* $^4He_3$

*Expanding the Faddeev components F in a series of bispherical harmonics we have*

$$x=|\mathbf{x}|,\ \ y=|\mathbf{y}|,\ \ \hat{x}=\mathbf{x}/x,\ \ \hat{y}=\mathbf{y}/y \qquad F(\mathbf{x},\mathbf{y})=\sum_l \frac{F_l(x,y)}{xy}\mathcal{Y}_{ll0}(\hat{x},\hat{y}),$$

The Faddeev differential equations are transformed to the following partial integro-differential equations

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

and partial boundary conditions $F_l(x,y)|_{x=0}=F_l(x,y)|_{y=0}=0, \quad \Psi_l(x,y)|_{x=c}=0.$

The asymptotic boundary condition for a $^4He_3$ bound state reads as follows

$$F_l(x,y)=\delta_{l0}\psi_d(x)exp(i\sqrt{E-\varepsilon_d}\,y)\left[a_0+o(y^{-1/2})\right]+\frac{exp(i\sqrt{E}\rho)}{\sqrt{\rho}}\left[A_l(\theta)+o(\rho^{-1/2})\right],$$

where $E$- energy of the three body system, $E=\varepsilon_d+p^2$, $\varepsilon_d$ - two - body bound state energy, $\psi_d(x)$ - bound state wave function of the two-body subsystem, $\rho=\sqrt{x^2+y^2}$, $a_0$ - amplitude of the rearrangement, $A_l(\theta)$ - amplitude decay into three separate particles.

# The finite - difference approximation

The grid knots were chosen to be the points of intersection of the arcs $\rho = \rho_i,\ \ i = 1,2,..N_\rho$ and the rays $\chi = \chi_j, j = 1,2,..N_\chi$

$$\rho_i = \frac{i}{N_c^{(\rho)} + 1} c, \qquad i = 1,2,\dots, N_c^{(\rho)},$$

$$\rho_{i+N_c^{(\rho)}} = \sqrt{c^2 + y_i^2}, \qquad i = 1,2,\dots, N_\rho - N_c^{(\rho)}$$

where $N_c^{(\rho)}$ stands for the number of arcs inside of the core domain and

$$y_i = f(\tau_i)\sqrt{\rho_{N_\rho}^2 - c^2},\ \ \tau_i = \frac{i}{N_\rho - N_c^{(\rho)}}.$$

The nonlinear monotonously increasing function $f(\tau)$, $0 \le \tau \le 1$, satisfying the conditions $f(0) = 0$ and $f(1) = 1$ was chosen in the form

$$f(\tau) = \frac{(1+a)\tau^2}{1 + a\tau}$$

A typical value of the acceleration $a$, $a > 0$, which is satisfactory in ground-state calculations is $a = 0.4$ (for $\rho_{N_\rho} < 100$ Å ).

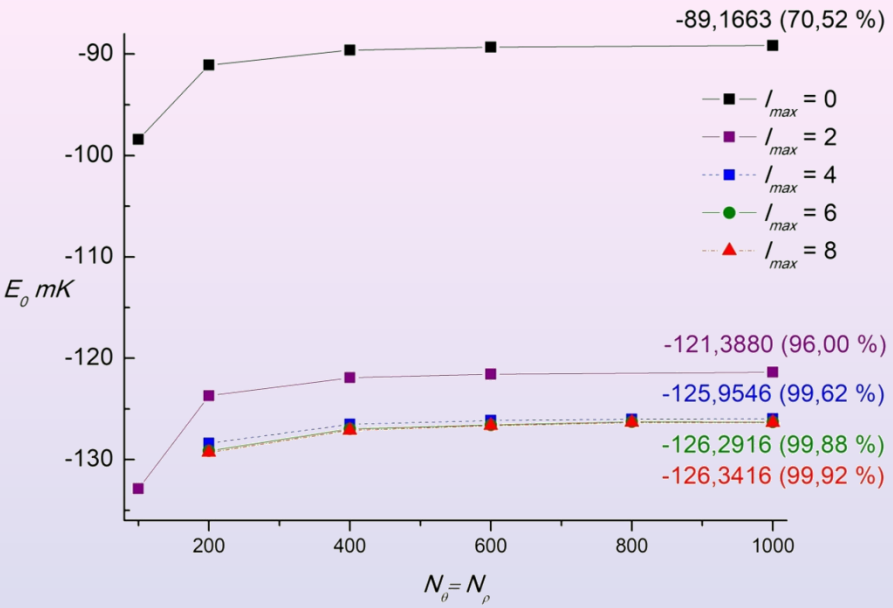
The knots $\chi_j$ for $j = 1,2,\dots, N_\rho - N_c^{(\rho)}$ were taken according to $\chi_j = \arctan(y_i/c)$

The rest knots $\chi_j,\ j = N_\rho - N_c^{(\rho)} + 1 \dots N_\chi$, were chosen equidistantly.

# $^4He_3$ - ground and excited state

$\hbar^2/m = 12.11928$ KÅ$^2$

| LM2M2 | | | | |
|---|---|---|---|---|
| $l_{max}$ | $\|E_0\|$ | % | $\|E_1\|$ | % |
| 0 | 89,1663 | 70,52 | 2,0252 | 88,86 |
| 2 | 121,3880 | 96,00 | 2,2466 | 98,57 |
| 4 | 125,9546 | 99,62 | 2,2752 | 99,83 |
| 6 | 126,2916 | 99,88 | 2,2780 | 99,95 |
| 8 | 126,3416 | 99,92 | 2,27905 | 100,00 |
| ∞ | 126,4397 | 100,00 | 2,27910 | 100,00 |

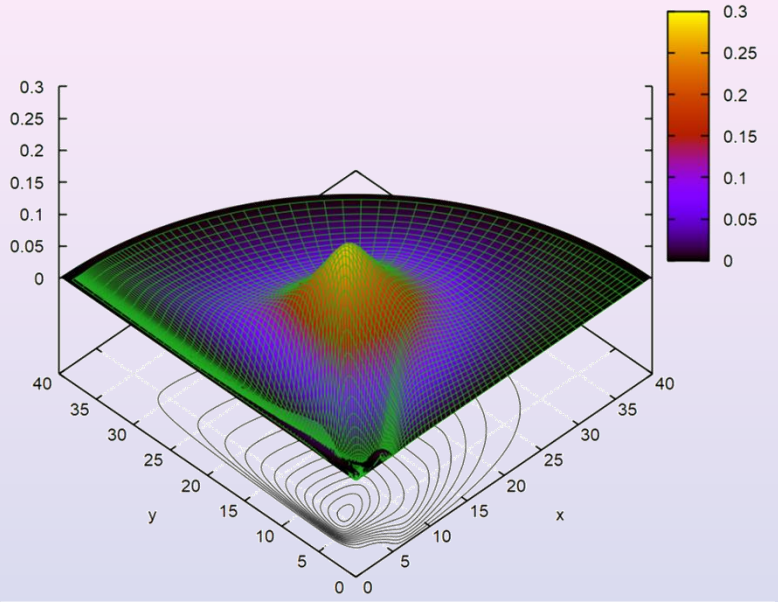


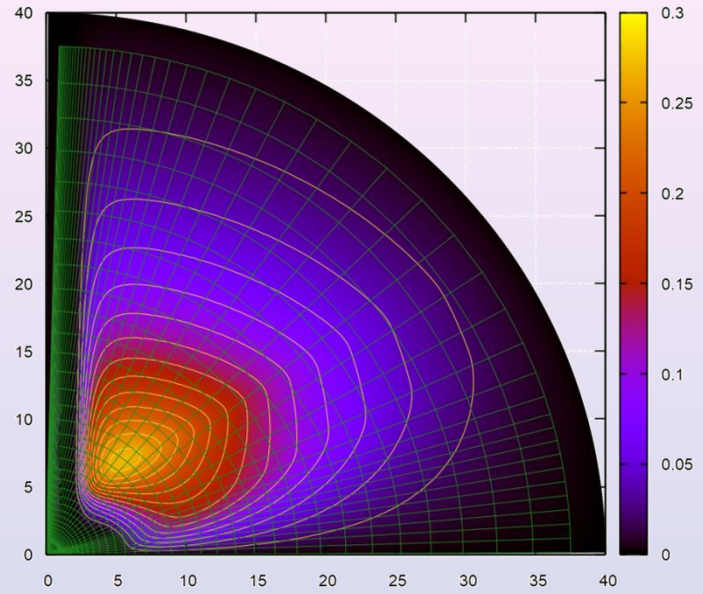

| Potential | $\|E\|$ | * | [7]† | [11]† | [12]† | [12] | [13] |
|---|---|---|---|---|---|---|---|
| HFD-B [6] | $\|E_0\|$ | 133,199 | 132,5 | 133,0 | 132,968 | 133,075 | 133,24 |
| | $\|E_1\|$ | 2,741 | 2,74 | 2,73 | 2,734 | 2,742 | |
| TTY [5] | $\|E_0\|$ | 126,549 | 125,8 | 126,4 | 126,431 | 126,537 | 126,36 |
| | $\|E_1\|$ | 2,291 | 2,28 | 2,28 | 2,284 | 2,292 | |

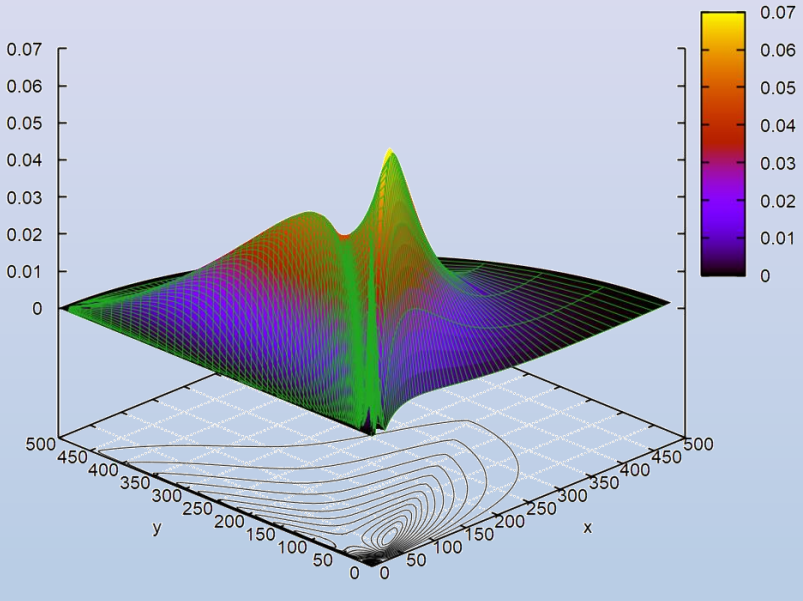
† $\hbar^2/m = 12.12$ KÅ$^2$

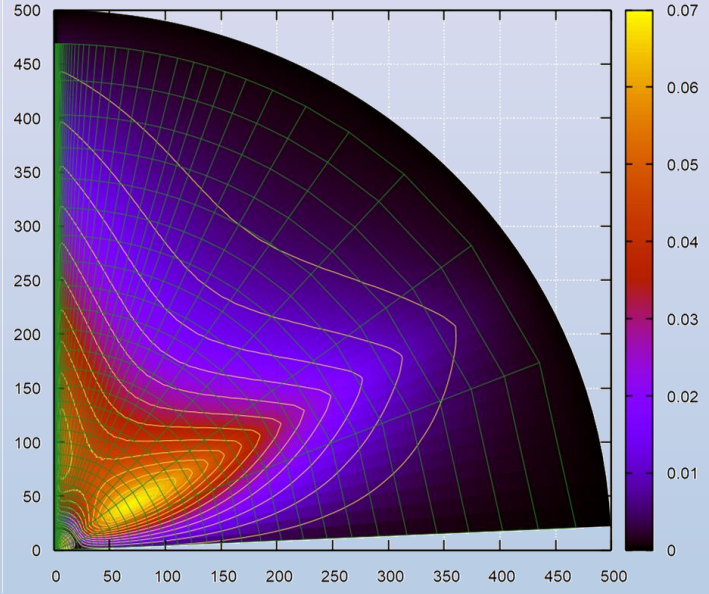

LM2M2 - Aziz R.A., Slaman M.J. // J. Chem. Phys. 1991. 94. P. 8047-8053.
[5] Tang K.T., Toennis J.P., Yiu C.L. // Phys. Rev. Lett. 1995. 74. P. 1546
[6] Aziz R.A., McCourt F.R.W., Wong C.C.K. // Mol. Phys. 1987. 61. P. 1487.
[7] Motovilov A.K., Sandhas W., Sofianos S.A., Kolganova E.A. // Eur. Phys. J. D. 2001. 13. P. 33.
[11] Roudnev V., Yakovlev S. // Chem. Phys. Lett. 2000. 328. P. 97-106.
[12] Roudnev V., Cavagnero M. // J. Phys. B. 2012. 45. P. 025101.
[13] Stipanović P., Markić L.V., Boronat J. // J. Phys. B. 2016. 49. P. 185101.

# $^4He_3$ - ground and excited state wave function



## $^4He_3$ - ground and excited state

$\hbar^2/m = 12.11928$ KÅ$^2$

| Potential | $\lvert E\rvert$ | * | Faddeev equations | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | [7]† | [11]† | [17]† | [12]† | [12] | [20]† | [21]† |
| LM2M2 [14] | $\lvert E_0\rvert$ | 126,440 | 125,9 | 126,4 | 126,41 | 126,394 | 126,499 | 126,2 | 126,39 |
| | $\lvert E_1\rvert$ | 2,279 | 2,28 | 2,271 | 2,271 | 2,271 | 2,278 | | 2,268 |

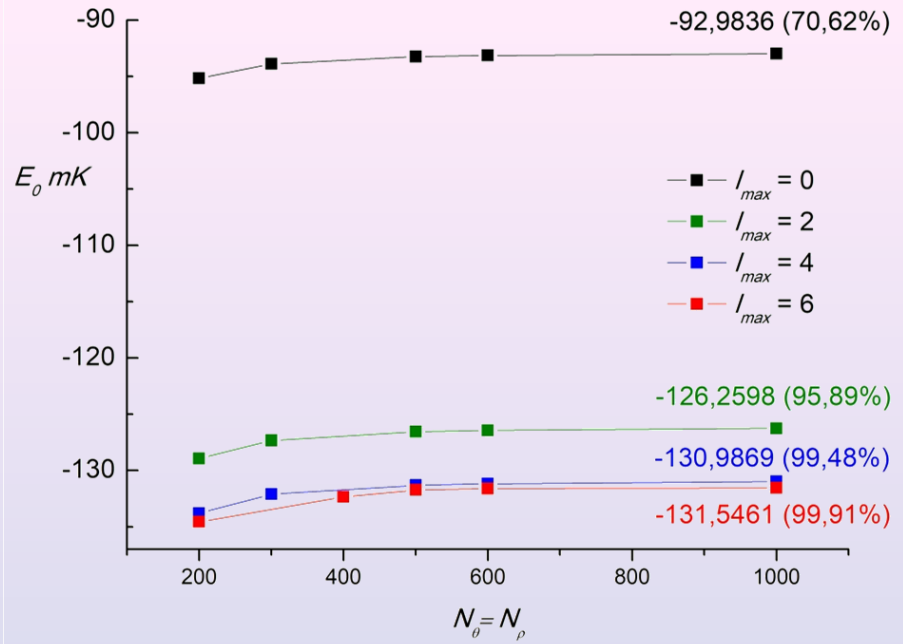
| Potential | $\lvert E\rvert$ | * | Variational methods | | | Adiabatic approach |
|---|---|---|---|---|---|---|
| | | | [16] † | [18]† | [19]† | [15]† |
| LM2M2 [14] | $\lvert E_0\rvert$ | 126,440 | 125,52 | 126,39 | 126,15 | 125,2 |
| | $\lvert E_1\rvert$ | 2,279 | | | 2,274 | 2,269 |

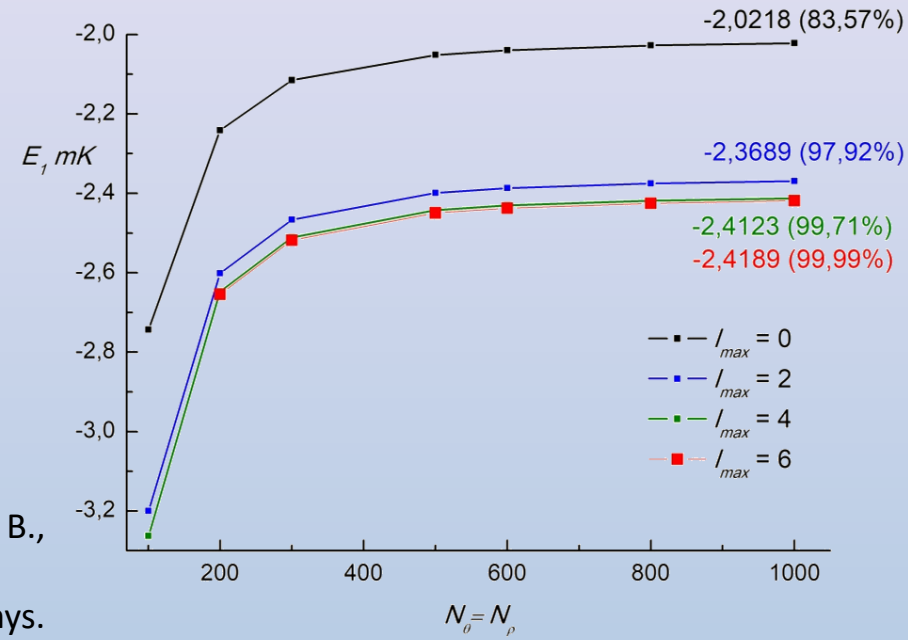
† $\hbar^2/m = 12.12$ KÅ$^2$


[7] Motovilov A.K., Sandhas W., Sofianos S.A., Kolganova E.A. // Eur. Phys. J. D. 2001. 13. P. 33.
[11] Roudnev V., Yakovlev S. // Chem. Phys. Lett. 2000. 328. P. 97-106.
[12] Roudnev V., Cavagnero M. // J. Phys. B. 2012. 45. P. 025101.
[14] Aziz R.A., Slaman M.J. // J. Chem. Phys. 1991. 94. P. 8047-8053.
[15] Nielsen E., Fedorov D.V., Jensen A.S. // J. Phys. B. 1998. 31. P. 4085-4105.
[16] Blume D., Greene C.H. // J. Chem. Phys. 2000. 112. P. 8053-8067.
[17] Roudnev V.A., Yakovlev S.L., Sofianos S.A. // Few-Body Syst. 2005. 37. P. 179-196.
[18] Bressanini D. et al. // J. Chem. Phys. 2000. 112. P. 717-722.
[19] Barletta P., Kievsky A. // Few-Body Syst. 2009. 45. P. 123-125.
[20] Salci M. et al. // Intern. J. Quant. Chem. 2007. 107. P. 464-468.
[21] Lazauskas R., Carbonell J. // Phys. Rev. A. 2006. 73. P. 062717(11).

# $^4He_3$ - ground and excited state

| Potential model | PRZ2010 [3] | | PRZ2017 [4] | |
|---|---|---|---|---|
| $l_{max}$ | $\|E_0\|$ | $\|E_1\|$ | $\|E_0\|$ | $\|E_1\|$ |
| 0 | 93.023 | 2.0257 | 92.984 | 2.0218 |
| 2 | 126.310 | 2.3728 | 126.260 | 2.3689 |
| 4 | 131.039 | 2.4166 | 130.987 | 2.4123 |
| 6 | 131.599 | 2.4235 | 131.546 | 2.4189 |
| 8 | 131.670 | 2.4238 | 131.620 | 2.4192 |
| $\infty$ | 131.721 | 2.4239 | 131.669 | 2.4193 |





[3] Przybytek M., Cencek W., Komasa J., Lach G., Jeziorski B., Szalewicz K. // Phys. Rev. Lett. 2010. 104. P. 183003.

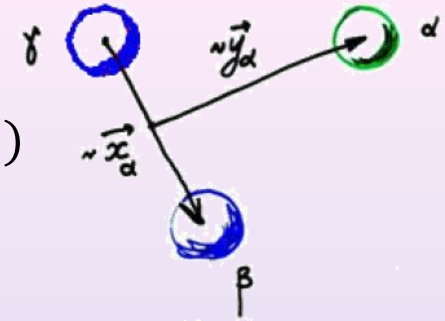
[4] Przybytek M., Cencek W., Jeziorski B., Szalewicz K. // Phys. Rev. Lett. 2017. 119. P. 123401.

The energy of the excited state of helium trimer with respect to the two-particle threshold $|E_1 - \varepsilon_d|$, calculated for different potentials and experimental results from [2].

| Potential | HFD-B [6] | LM2M2 [14] | TTY [5] | PRZ2010 [3] | PRZ2017 [4] | Exp. [2] |
|---|---|---|---|---|---|---|
| $\lvert E_1 - \varepsilon_d \rvert$ | 1.049 | 0.972 | 0,970 | 0.803 | 0.802 | $0.98 \pm 0.2$ |


[2] Kunitski M., Zeller S., Voigtsberger J., Kalinin A., Schmidt L.Ph.H., Schoeffler M., Czasch A., Scho¨llkopf W., Grisenti R.E., Jahnke T., Blume D., Doerner R. // Science. 2015. 348. P. 551.
[3] Przybytek M., Cencek W., Komasa J., Lach G., Jeziorski B., Szalewicz K. // Phys. Rev. Lett. 2010. 104. P. 183003.
[4] Przybytek M., Cencek W., Jeziorski B., Szalewicz K. // Phys. Rev. Lett. 2017. 119. P. 123401.
[5] Tang K.T., Toennis J.P., Yiu C.L. // Phys. Rev. Lett. 1995. 74. P. 1546
[6] Aziz R.A., McCourt F.R.W., Wong C.C.K. // Mol. Phys. 1987. 61. P. 1487.
[14] Aziz R.A., Slaman M.J. // J. Chem. Phys. 1991. 94. P. 8047-8053.

# $^3He\,^4He_2$




For two $^4$He atom the corresponding Faddeev component $F_3(\boldsymbol{x}_3, \boldsymbol{y}_3)$ is invariant under the permutation of the 1 and 2 particles

$$(-\Delta_X - E)\, F_\alpha(\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha) = -V_\alpha(\boldsymbol{x}_\alpha)\, \Psi^{(\alpha)}(\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha),\ \alpha = 1,3,$$

where $\Psi^{(1)}(\boldsymbol{x}_1, \boldsymbol{y}_1)$ and $\Psi^{(3)}(\boldsymbol{x}_3, \boldsymbol{y}_3)$ denote the total wave function in terms of the Faddeev components

$$\begin{aligned}\Psi^{(1)}(\boldsymbol{x}_1, \boldsymbol{y}_1) = {} & F_1(\boldsymbol{x}_1, \boldsymbol{y}_1) \\ & + F_1(c_{21}\boldsymbol{x}_1 + s_{21}\boldsymbol{y}_1, -s_{21}\boldsymbol{x}_1 + c_{21}\boldsymbol{y}_1) \\ & + F_3(c_{31}\boldsymbol{x}_1 + s_{31}\boldsymbol{y}_1, -s_{31}\boldsymbol{x}_1 + c_{31}\boldsymbol{y}_1)\end{aligned}$$

$$\begin{aligned}\Psi^{(3)}(\boldsymbol{x}_3, \boldsymbol{y}_3) = {} & F_3(\boldsymbol{x}_3, \boldsymbol{y}_3) \\ & + F_1(c_{13}\boldsymbol{x}_3 + s_{13}\boldsymbol{y}_3, -s_{13}\boldsymbol{x}_3 + c_{13}\boldsymbol{y}_3) \\ & + F_1(c_{23}\boldsymbol{x}_3 + s_{23}\boldsymbol{y}_3, -s_{23}\boldsymbol{x}_3 + c_{23}\boldsymbol{y}_3).\end{aligned}$$

As a results we obtain the partial integro-differential equations

$$\left(-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+l(l+1)\left(\frac{1}{x^2}+\frac{1}{y^2}\right)-E\right)F_l^{(\alpha)}(x,y)=$$

$$=\begin{cases}0, & x<c,\\ -V_\alpha(x)\Psi_l^{(\alpha)}(x,y), & x>c,\end{cases}\qquad \alpha=1,3,$$

$$\Psi_l^{(\alpha)}(x,y)\Big|_{x=c}=0,\qquad \alpha=1,3.$$

$$\Psi_l^{(1)}(x,y)=F_l^{(1)}(x,y)+\sum_{l'}\int_0^1 d\eta\left[h^0_{(1;ll)(2;l'l')}(x,y,\eta)F_{l'}^{(1)}(x_{21}(\eta),y_{21}(\eta))+\right.$$

$$\left.+\,h^0_{(1;ll)(3;l'l')}(x,y,\eta)F_{l'}^{(3)}(x_{31}(\eta),y_{31}(\eta))\right],$$

$$\Psi_l^{(3)}(x,y)=F_l^{(3)}(x,y)+\sum_{l'}\int_0^1 d\eta\left[h^0_{(3;ll)(1;l'l')}(x,y,\eta)F_{l'}^{(1)}(x_{13}(\eta),y_{13}(\eta))+\right.$$

$$\left.+\,h^0_{(3;ll)(2;l'l')}(x,y,\eta)F_{l'}^{(1)}(x_{23}(\eta),y_{23}(\eta))\right],$$

# $^3He\,^4He_2$

| Potential | | LM2M2 [14] | | | | TTY [5] | | | | PRZ2010 [3] | PRZ2017 [4] |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $\lvert E_0\rvert$, mK | $l_{max}$ | * | [7] | [15] | [20] | * | [7] | [18] | [20] | * | * |
| | 0 | 7.321 | 7.30 | | | 7,271 | 7.25 | | | 7,482 | 7,477 |
| | 2 | 13.198 | 13.15 | | | 13.137 | 13.09 | | | 13.277 | 13.270 |
| | 4 | 13.952 | 13.84 | | | 13.891 | 13.78 | | | 14.117 | 14.110 |
| | 6 | 14.039 | | | | 13.957 | | | | 14.171 | 14.169 |
| | ∞ | 14.057 | | 13.66 | 13.3 | 13.982 | | 14.165 | 13.2 | 14.214 | 14.210 |


[3] Przybytek M., Cencek W., Komasa J., Lach G., Jeziorski B., Szalewicz K. // Phys. Rev. Lett. 2010. 104. P. 183003.
[4] Przybytek M., Cencek W., Jeziorski B., Szalewicz K. // Phys. Rev. Lett. 2017. 119. P. 123401.
[5] Tang K.T., Toennis J.P., Yiu C.L. // Phys. Rev. Lett. 1995. 74. P. 1546
[7] Motovilov A.K., Sandhas W., Sofianos S.A., Kolganova E.A. // Eur. Phys. J. D. 2001. 13. P. 33.
[14] Aziz R.A., Slaman M.J. // J. Chem. Phys. 1991. 94. P. 8047-8053.
[15] Nielsen E., Fedorov D.V., Jensen A.S. // J. Phys. B. 1998. 31. P. 4085-4105.
[18] Bressanini D. et al. // J. Chem. Phys. 2000. 112. P. 717-722.
[20] Salci M. et al. // Intern. J. Quant. Chem. 2007. 107. P. 464-468.

# *Conclusion*

- Numerical algorithm for solving the two-dimensional differential Faddeev equations in the hard-core model – has been improved. This algorithm is applied to study the properties of the $^4He_3$ and $^3He^4He_2$ three-atomic systems using recently constructed realistic potentials. The calculated results we compare with the results obtained by other authors using different methods and with the experiment.

- It is shown that all modern potential models well reproduce the ground and excited states binding energy of the helium trimer.

- It is demonstrated that all modern potentials reproduce well the difference between the binding energies of the excited helium trimer state and the helium dimer ground state, although the absolute values of the energies are differ significantly.

***Thank you for your attention***