Solution of three-dimensional Faddeev equations on example of ultracold Helium trimer

Elena Kolganova
BLTP JINR, Dubna, Russia

In collaboration with

V. Roudnev and M. Cavagnero

Department of Physics and Astrophysics,

Kentucky University, USA

Outline

- Formalism (Faddeev equations)
- Computer code
- Overview - experiment and theory (two-body, three-body)
- Results
  - three-body bound states ($^4He_3$)
- Conclusion and plans for the near-term future

Faddeev Equations: Algebraic scheme

Let us deal with Hamiltonian of the form $H = H_0 + V$ with $V = V_1 + V_2 + V_3$

Equation $H\Psi = E\Psi$ is equivalent to the Lippman-Schwinger eq.

$$\Psi = -G_0(E)V\Psi \equiv -G_0(E)\sum_{\alpha=1}^{3} V_\alpha \Psi$$

We introduce the vectors

$$\Phi_\alpha = -G_0(E)V_\alpha \Psi \qquad \textit{Definition of the Faddeev components}$$

and note, $\sum_{\alpha=1}^{3} \Phi_\alpha \equiv \Psi$

Meanwhile, applying $(H_0 - E)$ to both sides of vectors definition one obtains

$$(H_0 - E)\Phi_\alpha = -V_\alpha \Psi \equiv -V_\alpha \sum_{\beta=1}^{3} \Phi_\beta$$

Or, after transfer of Φ_α from r.h.s. to l.h.s.:

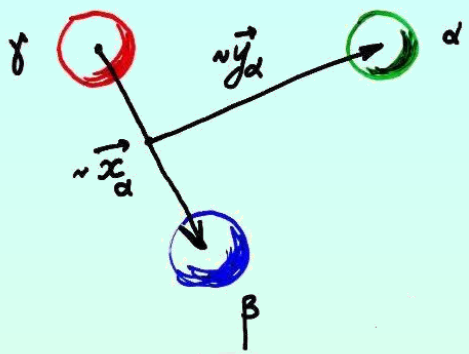
$$(H_0 + V_\alpha - E)\Phi_\alpha = -V_\alpha \sum_{\beta\neq\alpha} \Phi_\beta \qquad \textit{Faddeev equations}$$

In the form $\Phi_\alpha = -(H_0 + V_\alpha - E)^{-1} V_\alpha \sum_{\beta\neq\alpha} \Phi_\beta$ they were introduced by L.D.Faddeev in 1960

In describing the three-body system we use the standard Jacobi coordinates [4] $\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha$, $\alpha = 1, 2, 3$, expressed in terms of the position vectors of the particles $\boldsymbol{r}_i \in \mathbb{R}^3$ and their masses m_i,

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

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



where (α, β, γ) stands for a cyclic permutation of the indices $(1, 2, 3)$. The coordinates $\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha$ fix the six-dimensional vector $X \equiv (\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha) \in \mathbb{R}^6$. The vectors $\boldsymbol{x}_\beta, \boldsymbol{y}_\beta$ corresponding to the same point X as the pair $\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha$ are obtained using the transformations

$$\boldsymbol{x}_\beta = c_{\beta\alpha}\boldsymbol{x}_\alpha + s_{\beta\alpha}\boldsymbol{y}_\alpha \qquad \boldsymbol{y}_\beta = -s_{\beta\alpha}\boldsymbol{x}_\alpha + c_{\beta\alpha}\boldsymbol{y}_\alpha$$

where the coefficients $c_{\beta\alpha}$ and $s_{\beta\alpha}$ fulfil the conditions $-1 < c_{\beta\alpha} < +1$ and $s^2_{\beta\alpha} = 1 - c^2_{\beta\alpha}$ with $c_{\alpha\beta} = c_{\beta\alpha}$, $s_{\alpha\beta} = -s_{\beta\alpha}$, $\beta \neq \alpha$ and depend only on the particle masses [4]. For equal masses $c_{\beta\alpha} = -\frac{1}{2}$.

[4] - L.D.Faddeev,S.P.Merkuriev, 1993, *Quantum scattering theory for several particles*

The potential energy is invariant with respect to rotation and it makes possible to separate out the degrees of freedom corresponding to rotation of the system expanding the Faddeev components in term of the Wigner functions

$$\Phi(\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha) = \sum_{L,m,n} \frac{F^{Lmn}(x_\alpha, y_\alpha, z_\alpha)}{x_\alpha y_\alpha} D^L_{mn}(\boldsymbol{g})$$

When the total angular momentum L of the system is fixed, the three-body dynamics is constrained onto three-dimensional internal space [5], which can be parametrized by coordinates

$$x_\alpha = |\,\boldsymbol{x}_\alpha\,|,\ y_\alpha = |\,\boldsymbol{y}_\alpha\,|, z_\alpha = \cos\theta_\alpha = (\hat{\boldsymbol{x}}_\alpha, \hat{\boldsymbol{y}}_\alpha)$$

For zero angular momentum the Faddeev equations in internal space are given by the set of three coupled three-dimensional equations

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

$$x_\beta = \sqrt{c^2_{\beta\alpha} x_\alpha{}^2 + s^2_{\beta\alpha} y_\alpha{}^2 + 2c_{\beta\alpha}s_{\beta\alpha}x_\alpha y_\alpha z_\alpha}$$

$$y_\beta = \sqrt{s^2_{\beta\alpha} x_\alpha{}^2 + c^2_{\beta\alpha} y_\alpha{}^2 - 2c_{\beta\alpha}s_{\beta\alpha}x_\alpha y_\alpha z_\alpha}$$

$$x_\beta y_\beta z_\beta = \sqrt{(c^2_{\beta\alpha} - s^2_{\beta\alpha})x_\alpha y_\alpha z_\alpha - c_{\beta\alpha}s_{\beta\alpha}(x_\alpha{}^2 - y_\alpha{}^2)}$$

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

Asymptotic conditions

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

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

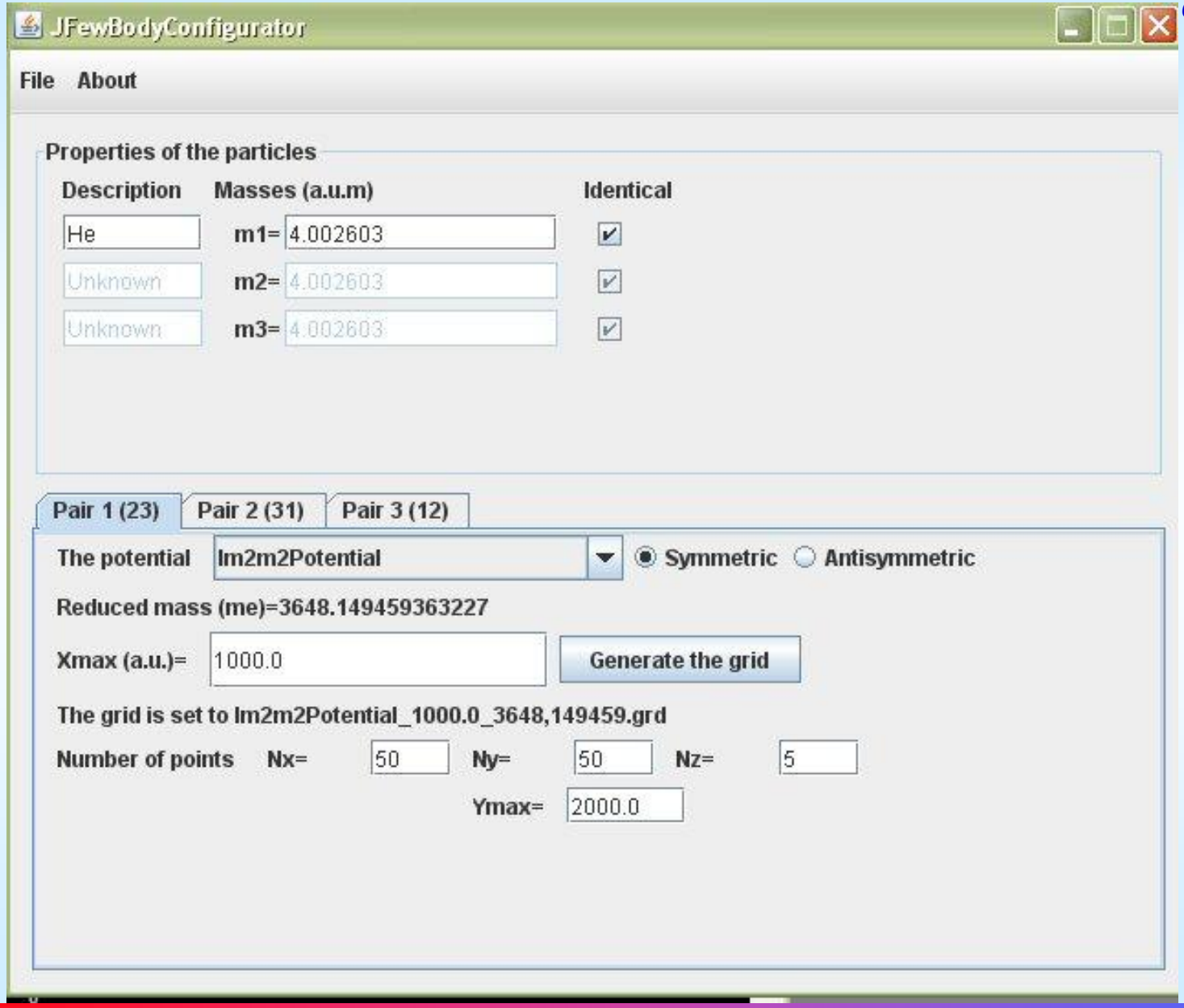
The purpose of the code is performing quantum calculation of scattering and bound states of atomic three-body systems.

The code consists of two parts. The first part is a configurator that simplifies composing the necessary configuration files.

The second part is the 3-body computational kernel that performs the actual calculations.

$^4He_3$

Three-body, theory computer code



Java code
by V.Roudnev

- Potential models: Aziz et al. – HFD-B (1987), LM2M2 (1991),Tang et al. – TTY (1995)

$$V(r) = \varepsilon V_b(\zeta) + V_a(\zeta),$$

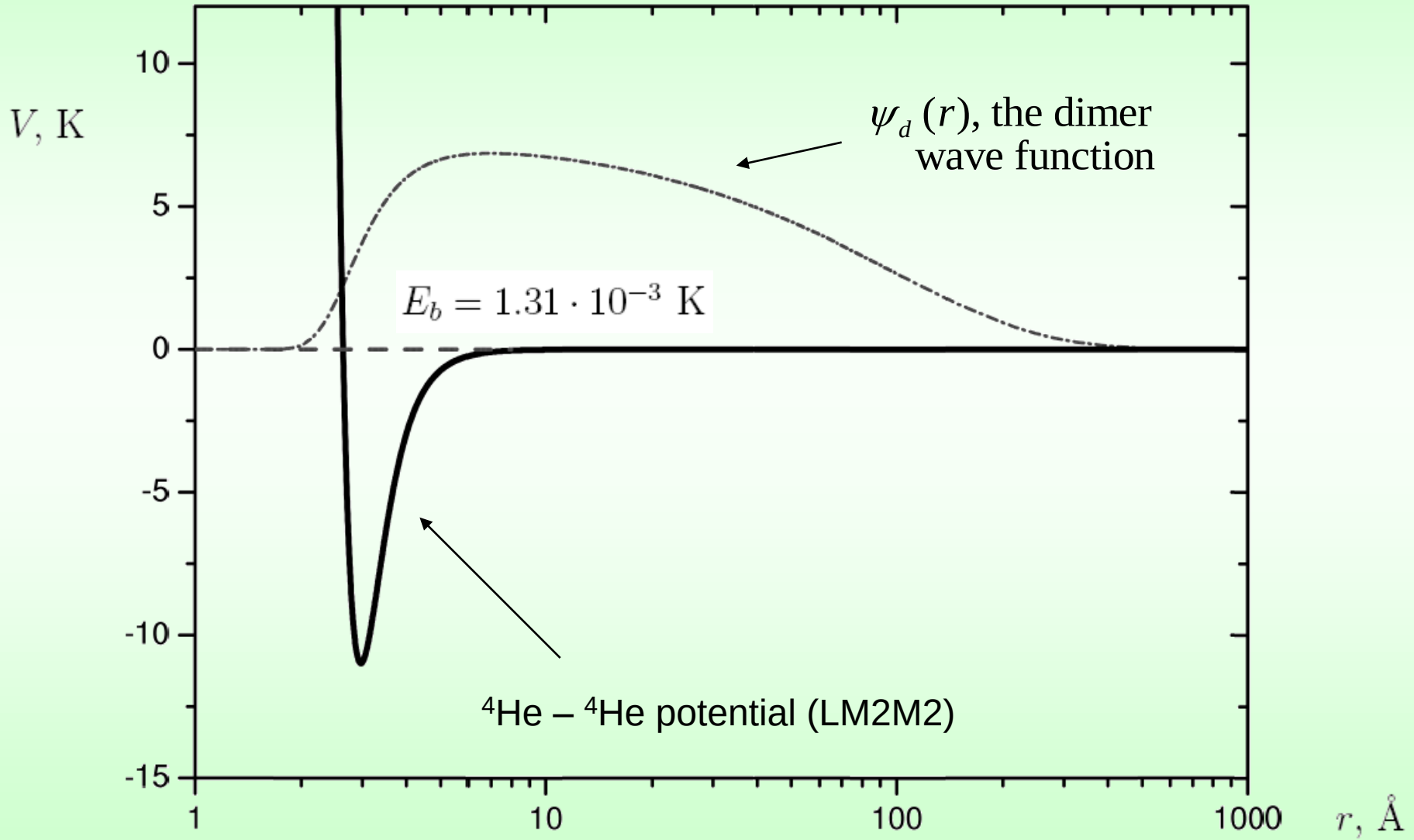
where $\zeta = x/r_m$.

$$V_b(\zeta) = A\exp(-\alpha\zeta + \beta\zeta^2) - \left[\frac{C_6}{\zeta^6} + \frac{C_8}{\zeta^8} + \frac{C_{10}}{\zeta^{10}}\right] F(\zeta),$$

$$V_a(\zeta) = \begin{cases} A_a\left\{\sin\left[\frac{2\pi(\zeta-\zeta_1}{\zeta_2-\zeta_1} - \frac{\pi}{2}\right] + 1\right\}, & \zeta_1 \le \zeta \le \zeta_2 \\ 0, & \zeta < \zeta_1, \zeta > \zeta_2 \end{cases}$$

$$F(\zeta) = \begin{cases} \exp\left[-\left(D/\zeta - 1\right)\right]^2, & \text{if } \zeta \le D \\ 1, & \text{if } \zeta > D\,. \end{cases}$$

- Potential models: Aziz et al. – HFD-B (1987), LM2M2 (1991),Tang et al. – TTY (1995)



^{4}He - ^{4}He

- First observation by Luo et al. (1993) and Schöllkopf, Toennies (1994)
- First measurement of the bond length by Grisenti et al.(2000)

$$< R >= 52 \pm 4\,\text{Å}$$

- Estimation of the binding energy and scattering length

$$\varepsilon_d = 1.1^{+0.3}_{-0.2}\,\text{mK} \qquad l_{sc} = 104^{+8}_{-18}\,\text{Å}$$

^{4}He - ^{4}He - ^{4}He

$1\,\text{mK} \approx 10^{-7}\ eV$

Experiment – Toennies et al. JCP 104, 1155 (1996), JCP 117, 1544 (2002)

Trimer pair distance $d = 1.1^{+0.4}_{-0.5}\,\text{nm}$

Theory – variational, hyperspherical, Faddeev equations (integral, differential)

$$E_{gs} = 126\,\text{mK} \qquad E_{ex} = 2.28\,\text{mK}$$

^{4}He - ^{4}He

Two-body, theory results

- Potential models: Aziz et al. – HFD-B (1987), LM2M2 (1991)
  Tang et al. – TTY (1995)

TABLE I. Dimer energy ε_d, wave length $1/\varkappa^{(2)}$, and ^{4}He–^{4}He scattering length $\ell_{sc}^{(2)}$ for the potentials used, as compared to the experimental values of Ref. [5].

R. Grisenti, W. Schöllkopf, J. P. Toennies, G. C. Hegerfeld, T. Köhler, and M. Stoll, Phys. Rev. Lett. **85**, 2284 (2000).

	ε_d (mK)	$\ell_{sc}^{(2)}$(Å)	Potential	ε_d (mK)	$1/\varkappa^{(2)}$ (Å)	$\ell_{sc}^{(2)}$ (Å)
			LM2M2	−1.30348	96.43	100.23
Expt.	$1.1^{+0.3}_{-0.2}$	104^{+8}_{-18}	TTY	−1.30962	96.20	100.01
			HFD-B	−1.68541	84.80	88.50

Helium dimer

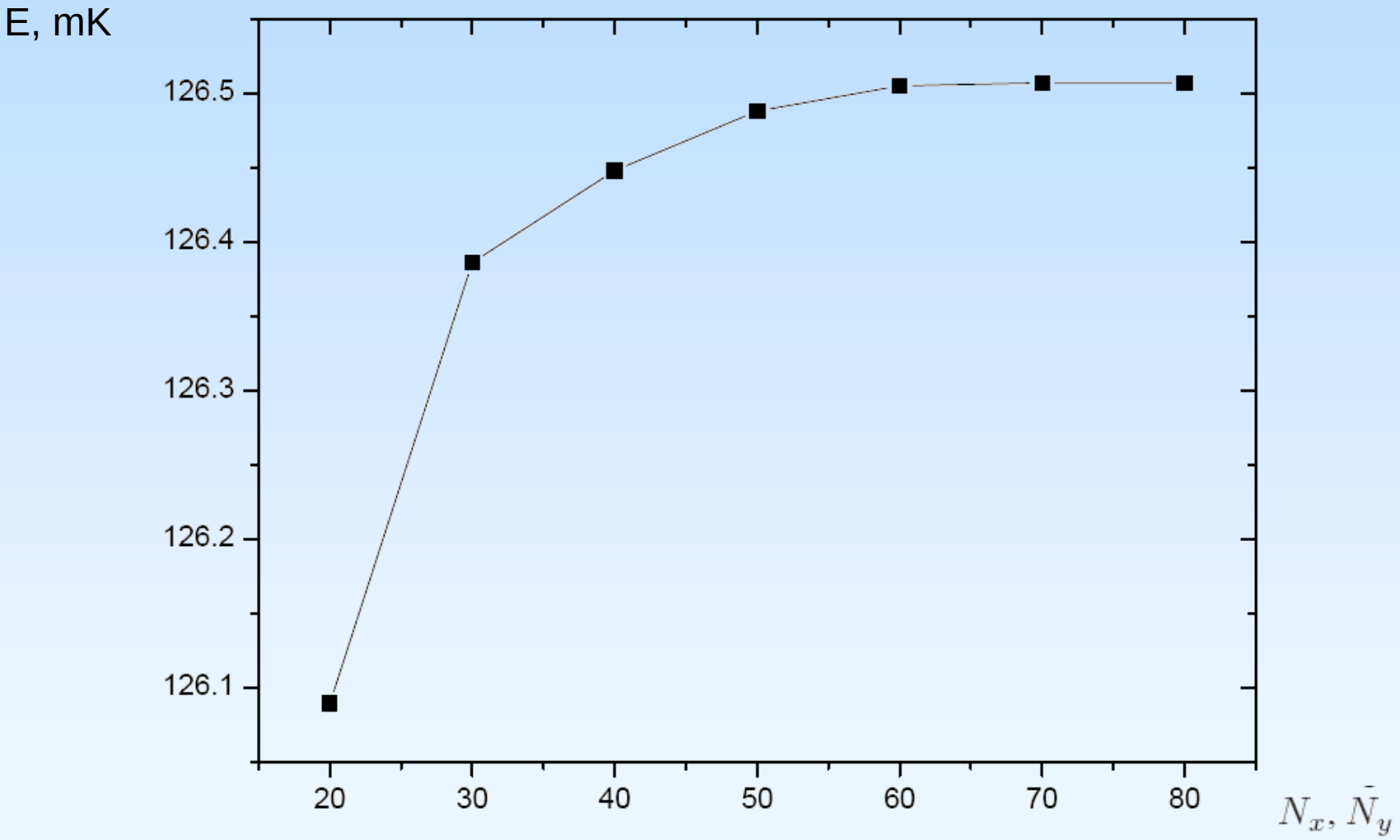
Two-body, theory results

Potentials	HFD-B [16]			HFDHE2 [17]			[6]
	*	[28]	[29]	*	[28]	[29]	эксп.
$\lvert\varepsilon_d\rvert$, мК	1,685	1,685	1,685	0,830	-	0,830	$1,1^{+0,3}_{-0,2}$
$< R >$, Å	46,178	46,466	46,18	64.201	-	64,21	52±4
$\sqrt{< R^2 >}$, Å	62,706	62,971	62,71	88.160	-	88,18	-

Potentials	LM2M2 [18]			TTY [19]			[6]
	*	[28]	[29]	*	[28]	[29]	эксп.
$\lvert\varepsilon_d\rvert$, мК	1,304	1,303	1,304	1,310	1,313	1,312	$1,1^{+0,3}_{-0,2}$
$< R >$, Å	52.001	51,838	52,00	51.889	51,658	51,84	52±4
$\sqrt{< R^2 >}$, Å	70.926	70,327	70,93	70.768	70,115	70,70	-

[28] Barletta P. Kievsky A. // Phys. Rev. A. 2001. V. 64. P. 042514(9).
[29] Roudnev V., Yakovlev S.// Chem. Phys. Lett. 2000. V. 328. P. 97.

Convergence of the binding energy on number of grids x,y



$^4He_3$

Three-body, theory results

Таблица 1: Results for binding energies of the $^4He_3$ trimer. LM2M2 Potential.

	*	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]
$\lvert E_{^4He_3}\rvert$ (мК)	126.507	125.2	126.45	125.52[a]	126.41	126.3(9)[a]	126.15	126.2	126.39	125.6[a]
$\lvert E^*_{^4He_3}\rvert$ (мК)	2.277	2.269	2.28		2.271		2.274		2.268	2.245[a]

[a] In original paper the energy value is given in cm^{-1} ($1\ cm^{-1} = 1.4387752$ K).

[1] *Nielsen E., Fedorov D. V., Jensen A. S.* // J. Phys. B. 1998. V. 31. P. 4085–4105.

[2] *Kolganova E.A.* // PEPAN. 2010. V. 41 (7).

[3] *Blume D., Greene C. H.* // J. Chem. Phys. 2000. V. 112. P. 8053–8067.

[4] *Roudnev V. A., Yakovlev S. L., Sofianos S. A.* // Few-Body Syst. 2005. V. 37. P. 179–196.

[5] *Bressanini D., Zavaglia M., Mella M., Morosi G.* // J. Chem. Phys. 2000. V. 112. P. 717–722.

[6] *Barletta P., Kievsky A.* // Few-Body Syst. 2009. V. 45. P. 123–125.

[7] *Salci M., Yarevsky E., Levin S. B., Elander N.* // Int. J. Quant. Chem. 2007. V. 107. P. 464–468.

[8] *Lazauskas R., Carbonell J.* // Phys. Rev. A. 2006. V. 73. P. 062717(11).

[9] *Orlandini S., Baccarelli I., Gianturco F.A.* // Comp. Phys. Comm. 2009. V. 180. P. 384–391.

Outgoing results and future directions

- To test the program for scattering calculations
- To test the program for calculation of other three-body systems

Acknowledgements

- Diploma student – A.Korobitsin
- Alexander von Humboldt foundation

Thank you!