JOINT INSTITUTE FOR NUCLEAR RESEARCH

Three-atomic clusters within the framework of Faddeev equations

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Two – Body Systems

INTERACTION POTENTIALS

Potential models:

– Lennard - Jones [1]: $V(r) = 4\,\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$

ε – scales the energy and σ – the length scale;

– Tang -Toennies [2]:

$$V(R) = V_{rep} + V_{att} = A\, e^{-bR} - \sum_{n=3}^{N} f_{2n}(bR)\frac{C_{2n}}{R^{2n}}$$

where A and b parameters,
the C_{2n} are the dispersion coefficient,
$f_{2n}(bR)$ - the damping function,
which is given by the following expression:

$$f_{2n}(x) = 1 - e^{-x}\sum_{k=0}^{2n}\frac{x^{-k}}{k!}$$

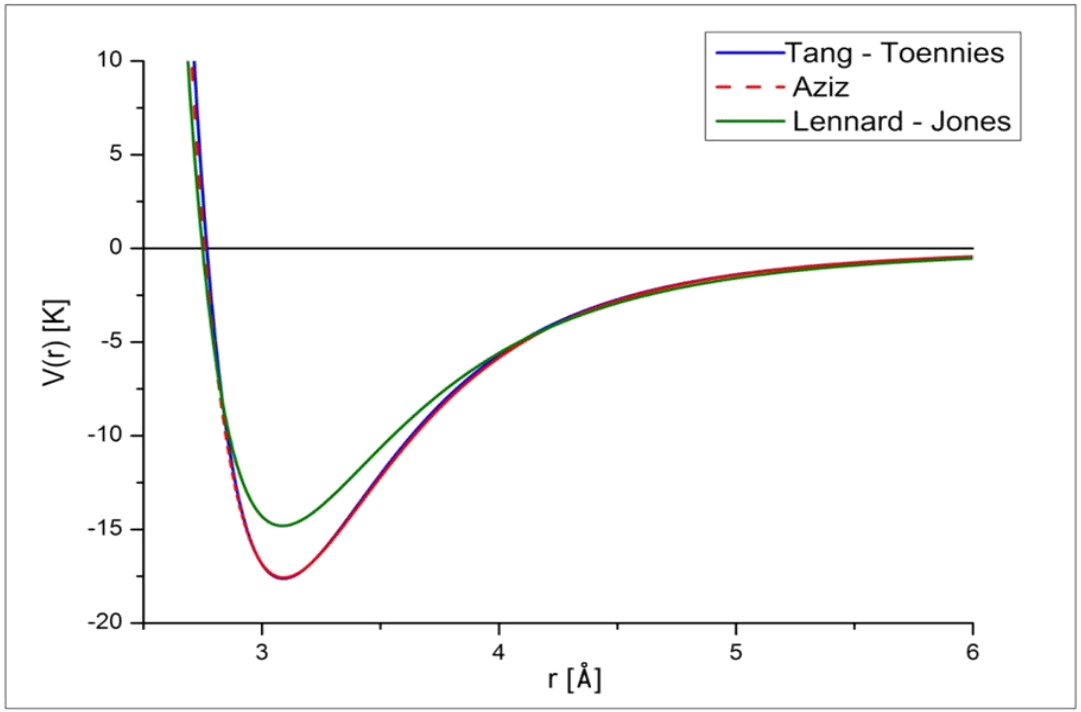
– Aziz [3]: $V(x) = \varepsilon\, V_b(\zeta)$

where $\zeta = x/r_m$, and term $V_b(\zeta)$ has the form:

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

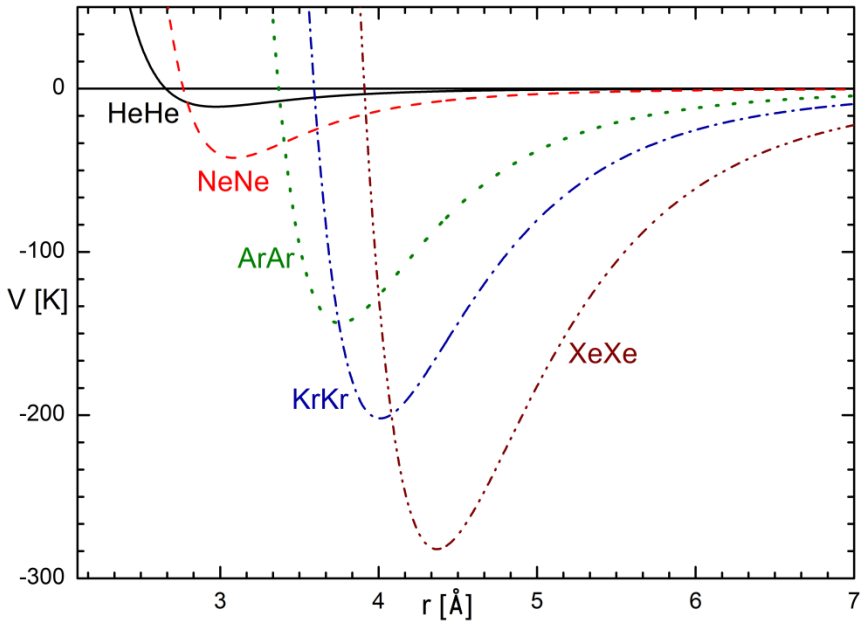
at that x is expressed in the same length units as r_m (for this case they are angstroms).
Function $F(\zeta)$ is given by the expression:

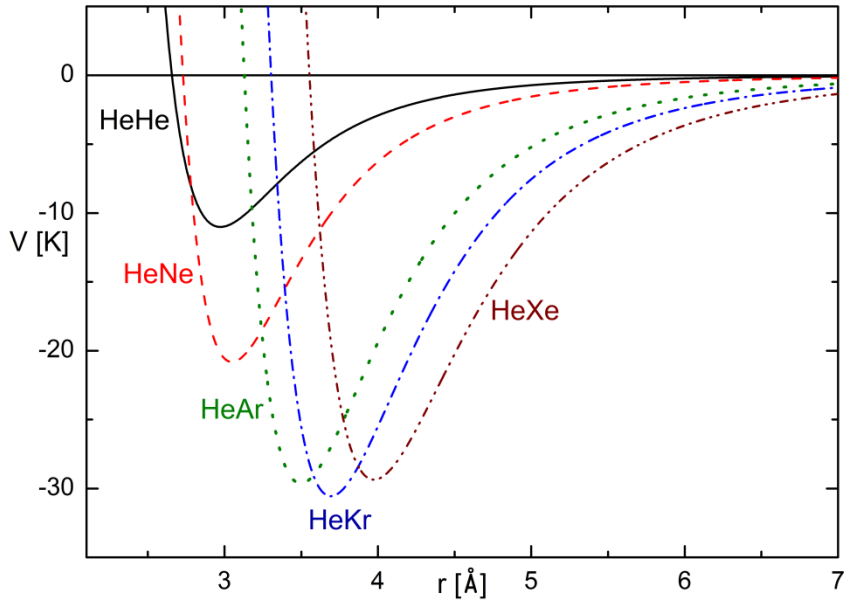
$$F(\zeta) = \begin{cases} exp[-(D/\zeta - 1)^2], & if\ \zeta \le D, \\ 1, & if\ \zeta > D. \end{cases}$$



[1] D.M. Leither, J.D. Doll, R.M.Whitnell // J.Chem.Phys. **94**, 6644 - 6659 (1991)
[2] K.T. Tang and J.P. Toennies // J.Chem.Phys. **118**, 4976 - 4983,(2003)
[3] R.A. Aziz and M.J. Slaman // J. Chem. Phys. **94**, 8047 - 8053 (1991);
D.A. Barrow, M.J. Slaman, R.A. Aziz // J. Chem. Phys. **91**, 6348-6358 (1989);
R.A. Aziz // J. Chem. Phys. **99**, 4518 - 4525 (1993)

INTERACTION POTENTIALS





System	C_6	C_8	C_{10}	A	b, $a.u.^{-1}$
He - He	1,461	14,11	183,6	41,96	2,523
Ne - Ne	6,383	90,34	1536	199,5	2,458
Ar - Ar	64,30	1623	49060	748,3	2,031
Kr - Kr	129,6	4187	155500	832,4	1,865
Xe - Xe	285,9	12810	619800	951,8	1,681
Rn - Rn	420,6	19260	1067000	5565,0	1,824

Tang –Toennies model [1]:

$$V(R) = V_{rep} + V_{att} = A\, e^{-bR} - \sum_{n=3}^{N} f_{2n}(bR)\frac{C_{2n}}{R^{2n}}$$

where A and b parameters,
the C_{2n} are the dispersion coefficient,
$f_{2n}(bR)$ - the damping function,
which is given by the following expression:

$$f_{2n}(x) = 1 - e^{-x}\sum_{k=0}^{2n}\frac{x^{-k}}{k!}$$

[1] K.T. Tang and J.P. Toennies // J. Chem. Phys. **118**, 4976-4983,(2003)

$^4He_2$

$^{20}Ne_2$

Measurements: bond length [3] $< R >= 52 \pm 4$ Å

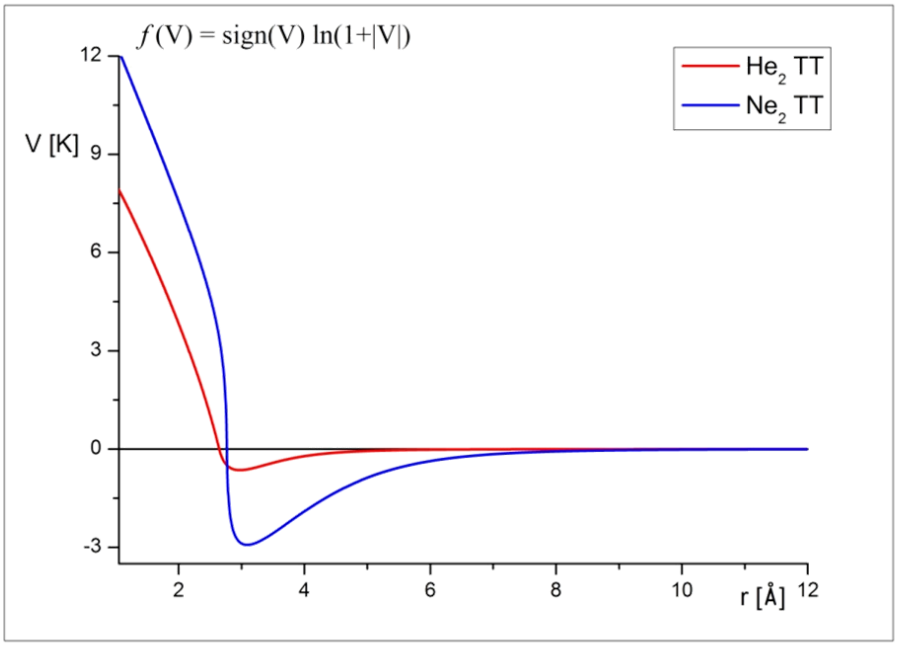
n	E (K) [5]
0	24,22 ± 0,02
1	4,405 ± 0,02
2	< 0.14

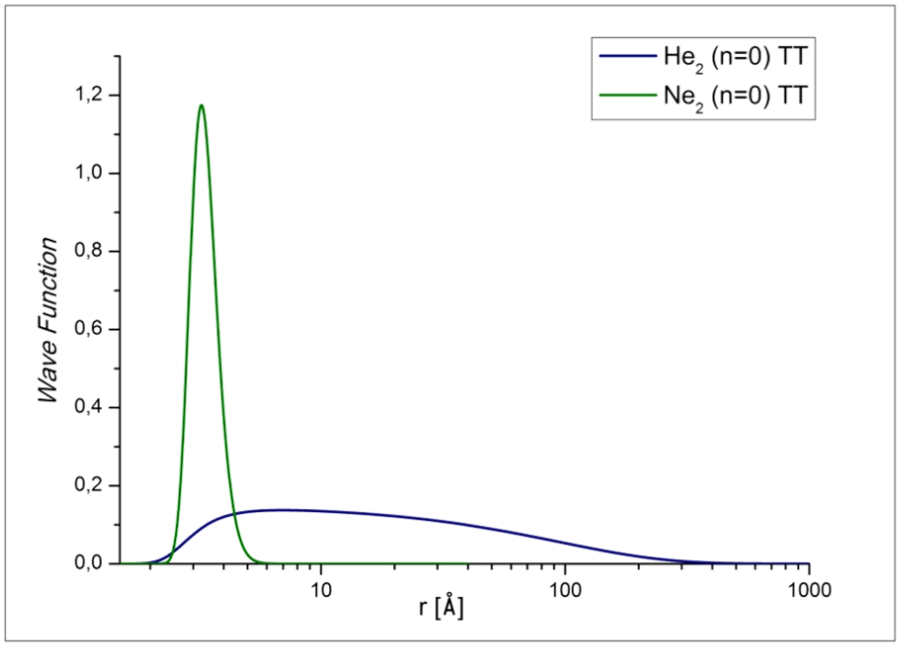
Estimation of the binding energy and scattering length

$\varepsilon_d = 1.1^{+0.3}_{-0.2}$ mK $l_{sc} = 104^{+8}_{-18}$ Å [3]

?

$\varepsilon_d = 1.3^{+0.25}_{-0.19}$ mK $l_{sc} = 100^{+8}_{-7.9}$ Å [6]

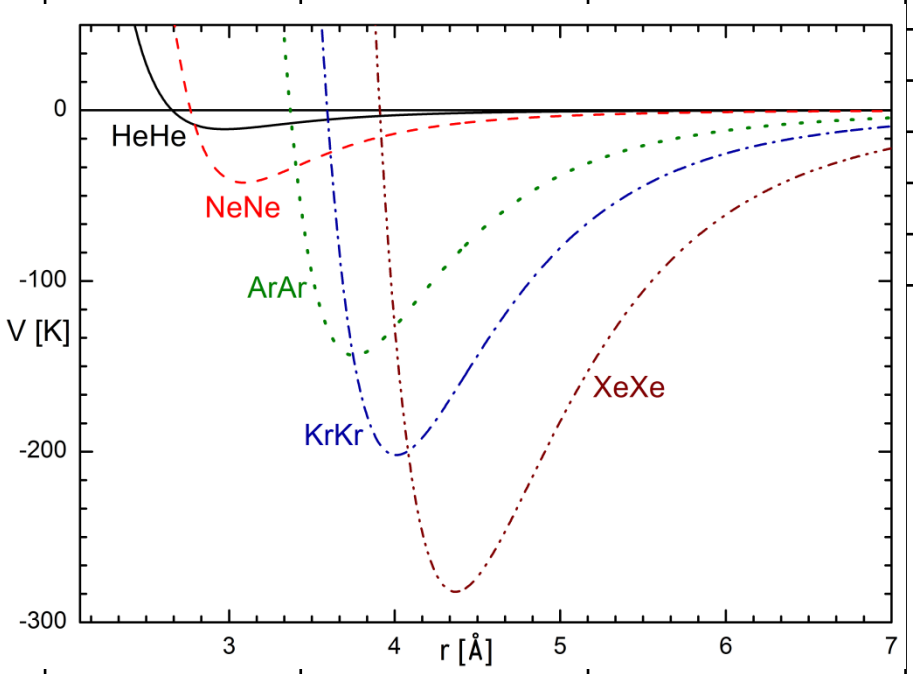




[1] F.Luo et. al.// J. Chem. Phys. 98 (1993) 9687.
[2] W.Schöllkopf et. al.// Science.266 (1994) 1345.
[3] R.Grisenti et. al. // Phys. Rev. Lett. 85 (2000) 2284.
[4] Y.Tanaka,K.Yoshino //J.Chem.Phys.57 (1972) 2964.
[5] A.Wüest, F.Merkt//J.Chem.Phys.118 (2003) 8807.
[6] W.Cencek et.al. // J.Chem.Phys., 136(2012) 224303.

Spectra of homogeneous rare gas dimers (TT potentials):

level	He_2 (K)	Ne_2 (K)	Ar_2 (K)	Kr_2 (K)	Xe_2 (K)
0	0,001309	24,1316	121,5004	184,7897	267,1759
1		4,2777	83,7284	153,1110	238,6889
2		0,02215	54,0021	124,8287	212,0169
3			31,8334	99,8756	187,1428
4			16,5115	78,1658	164,0472
5			7,0383	59,5926	142,7075
6			2,1227	44,0234	123,0977
7			0,2823	31,2940	105,1879
8				21,2031	88,9437
9				13,5088	74,3252
10				7,9285	61,2863
11				4,1441	49,7742
12				1,8129	39,7280
13				0,5801	31,0784
14				0,09122	23,7471
15				0,0001393	17,6446
16					12,6781
17					8,7381
18					5,7122
19					3,4831
20					1,9286
21					0,9256
22					0,3511
23					0,08371
24					0,004802



Weakest states of heterogeneous rare gas dimers:

Atom		He	Ne	Ar	Kr	Xe	Rn
He	E_n (K)	1.30960	3.442	9.886	0.034	0.1414	0.2749
	<R> Å	51.784	4.041	4.093	13.3545	9.8008	8.7300
	$<R^2>^{1/2}$ Å	70.618	4.138	4.137	15.0955	10.4618	9.1502
Ne	E_n (K)		0.02215	0.6890	0.2628	1.0192	0.1821
	<R> Å		11.8246	6.8575	8.5512	7.2220	9.9060
	$<R^2>^{1/2}$ Å		13.0404	6.9949	8.7115	7.3383	10.1317
Ar	E_n (K)			0.2823	0.0311	0.0262	0.0010
	<R> Å			9.6011	14.8778	16.2743	32.7279
	$<R^2>^{1/2}$ Å			9.7904	15.3308	16.7389	35.6998
Kr	E_n (K)				0.0001	0.02957	0.0006
	<R> Å				53.3392	16.6931	36.4596
	$<R^2>^{1/2}$ Å				62.4463	17.0551	39.1313
Xe	E_n (K)					0.004802	0.009926
	<R> Å					24.4651	22.0605
	$<R^2>^{1/2}$ Å					25.2103	22.5518
Rn	E_n (K)						0.001673
	<R> Å						31.1108
	$<R^2>^{1/2}$ Å						32.0870

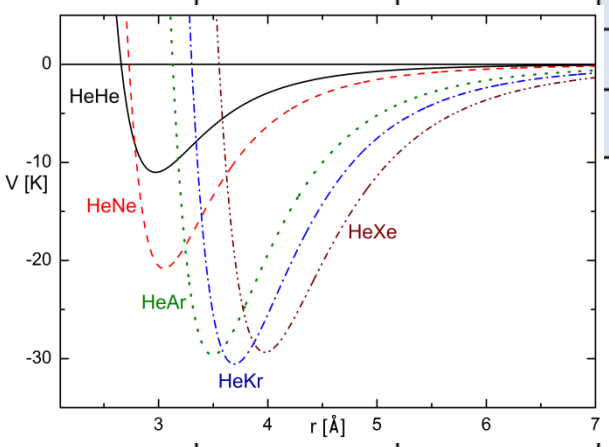
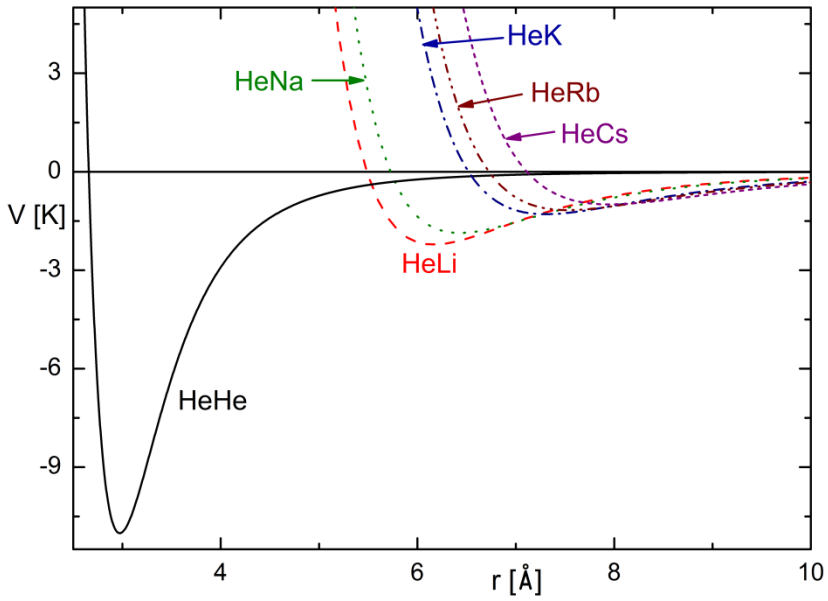
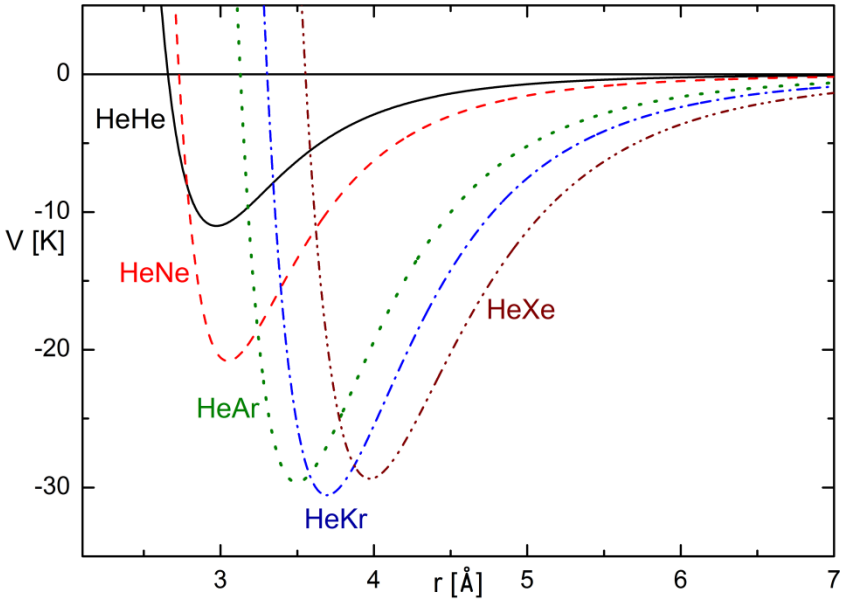


TABLE. Weakest state energy of the heterogeneous rare gases dimers (in K), average distance and mean root square radius (both in Å).

INTERACTION POTENTIALS





Kleinkathöfer, Tang, Toennies, Yiu model [2,3]

$$V(r) = A\exp(-b_1 r - b_2 r^2) - \sum_{n=3}^{8} f_{2n}(b'(r), r)\frac{C_{2n}}{r^{2n}},$$

$$b'(r) = b_1 + 2b_2 r$$

Tang –Toennies model [1]:

$$V(R) = V_{rep} + V_{att} = A\,e^{-bR} - \sum_{n=3}^{N} f_{2n}(bR)\frac{C_{2n}}{R^{2n}}$$

where A and b parameters,
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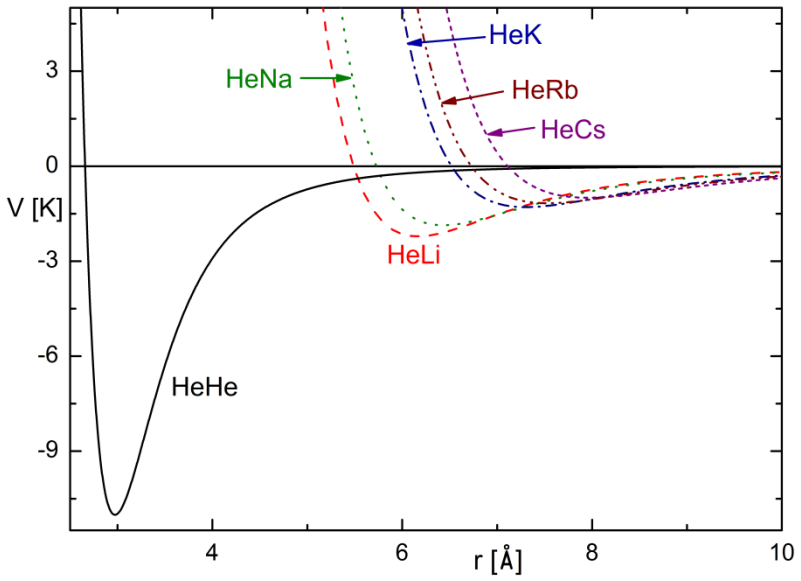
which is given by the following expression:

$$f_{2n}(x) = 1 - e^{-x}\sum_{k=0}^{2n}\frac{x^{-k}}{k!}$$

[1] K.T. Tang and J.P. Toennies // J. Chem. Phys. **118**, 4976-4983,(2003)
[2] U. Klenkathöfer, K.T. Tang, J.P. Toennies, C.I.Yiu // Chem.Phys.Lett. **249**, 257-263 (1996)
[3] U. Klenkathöfer, M. Lewerenz, M.Mladenoc // Phys.Rev.Lett**. 83**, 4717-4720 (1999)

INTERACTION POTENTIALS

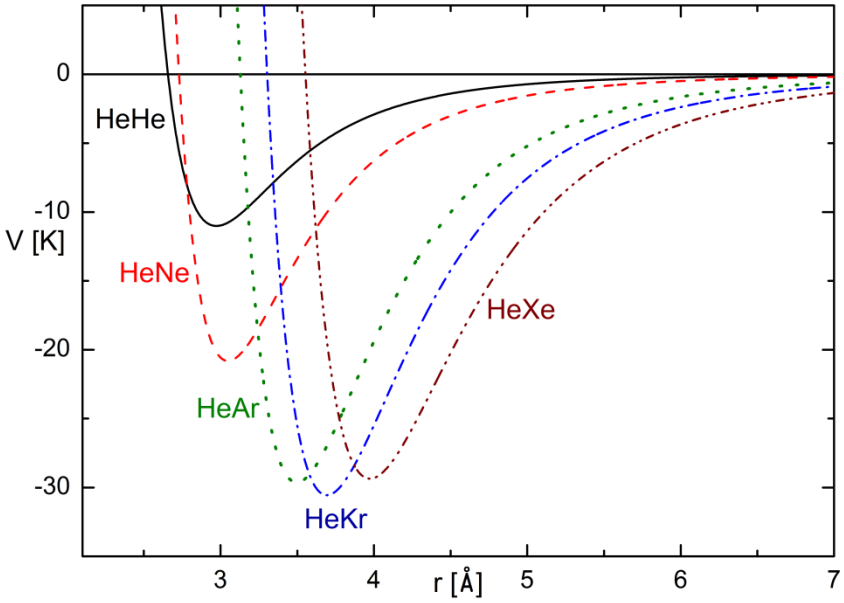


Dimer	$\|E\|$ (mK)	Dimer	$\|E\|$ (mK)
^{4}He ^{4}He	1,3096[a]	^{4}He ^{23}Na	28.97
^{4}He ^{4}He	1,728[b,c]	^{4}He ^{39}K	11.20[c]
^{4}He ^{6}Li	1,512	^{4}He ^{85}Rb	10.27[c]
^{4}He ^{7}Li	5,617	^{4}He ^{133}Cs	4.945[c]

[a] potential model LM2M2

[b] potential model from M. Jeziorska *et al.*, J. Chem. Phys. **127**, 124303 (2007)

[c] data taken from H.Suno and B.D.Esry, Phys. Rev. A **80**, 062702 (2009)



Dimer	$\|E\|$ (K)	Dimer	$\|E\|$ (K)
^{4}He ^{4}He	0.0013	^{4}He ^{84}Kr	11.540
^{4}He ^{20}Ne	3,442	^{4}He ^{131}Xe	11.978
^{4}He ^{40}Ar	9,886	^{4}He ^{222}Rn	13.224

[1] K.T. Tang and J.P. Toennies // J. Chem. Phys. **118**, 4976-4983,(2003)

[2] U. Klenkathöfer, K.T. Tang, J.P. Toennies, C.I.Yiu // Chem.Phys.Lett. **249**, 257-263 (1996)

[3] U. Klenkathöfer, M. Lewerenz, M.Mladenoc // Phys.Rev.Lett**. 83**, 4717-4720 (1999)

INTERACTION POTENTIALS

Experiment ^{7}Li ^{4}He

$$0.0024 \pm 0.025 \text{ cm}^{-1}$$

$$0.0039 \text{ cm}^{-1}$$

Dimer	$\|E\|$ (mK)	Dimer	$\|E\|$ (mK)
^{4}He ^{4}He	1,3096[a]	^{4}He ^{23}Na	28.97
^{4}He ^{4}He	1,728[b,c]	^{4}He ^{39}K	11.20[c]
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^{4}He ^{7}Li	5,617	^{4}He ^{133}Cs	4.945[c]

N.Tariq, N.A.Taisan, V.Singh, and J.D. Weinstein,
Phys. Rev .Lett. **110**, 153201 (2013).

[a] potential model LM2M2

[b] potential model from M. Jeziorska *et al.*, J. Chem. Phys. **127**, 124303 (2007)

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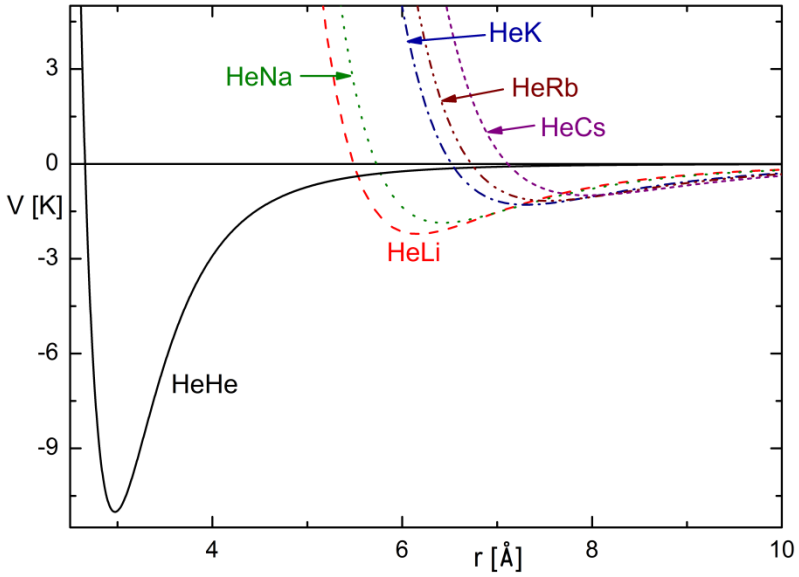


[1] U. Klenkathöfer, K.T. Tang, J.P. Toennies, C.I.Yiu // Chem.Phys.Lett. **249**, 257-263 (1996)

[2] U. Klenkathöfer, M. Lewerenz, M.Mladenoc // Phys.Rev.Lett**. 83**, 4717-4720 (1999)

Three – Body Systems

Faddeev Equations: Algebraic scheme

Let us deal with Hamiltonian of the form

$$H = H_0 + V \qquad \text{with} \qquad V = V_1 + V_2 + V_3$$

We consider the bound-state problem

$$H\Psi = E\Psi$$

where E does not belong to the spectrum of H_0. Thus $G_0(E) = (H_0 - E)^{-1}$ is well defined. Equation $H\Psi = E\Psi$ is equivalent to the Lippman-Schwinger eq.

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

Further we introduce the vectors

$$\Phi_\alpha = -G_0(E)V_\alpha \Psi$$

So, we have

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

Faddeev Equations: Algebraic scheme

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

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

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.:

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

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

Faddeev Equations

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

can be written in the matrix form

$$\begin{pmatrix} H_0 + V_1 & V_1 & V_1 \\ V_2 & H_0 + V_2 & V_2 \\ V_3 & V_3 & H_0 + V_3 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{pmatrix} = E \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{pmatrix}$$

Even the number of equation became tripled, in many respects these equations are more convenient then the initial equation

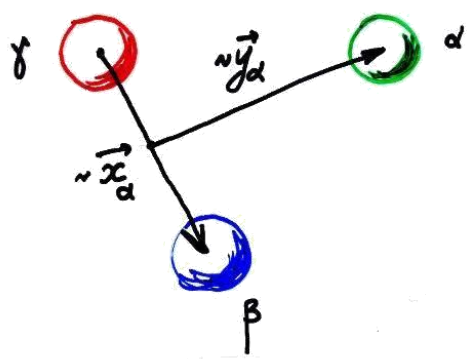
$$H\Psi = E\Psi$$

In case of a three-body problem this is especially true in the scattering case since the Faddeev operator decouples two-body channels

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,

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

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



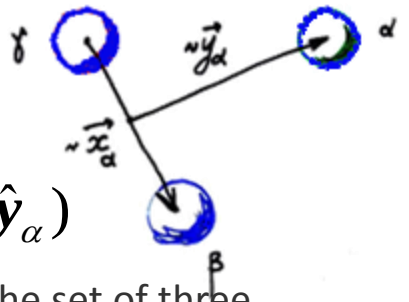
where (α, β, γ) stands for a cyclic permutation of the indices $(1, 2, 3)$. The coordinates $\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha$ fix the six-dimensional vector $X \equiv (\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha) \in \mathbb{R}^6$. The vectors $\boldsymbol{x}_\beta, \boldsymbol{y}_\beta$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

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

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

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

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

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

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

or in hyperspherical coordinates $\rho = \sqrt{x_\alpha^2 + y_\alpha^2}, \tan\vartheta_\alpha = y_\alpha / x_\alpha, \eta_\alpha = (\hat{\boldsymbol{x}}_\alpha, \hat{\boldsymbol{y}}_\alpha)$

$$(H_0 + V_\alpha - E)\Phi_\alpha(\rho, \vartheta_\alpha, \eta_\alpha) = -V_\alpha \sum_{\beta\neq\alpha} \Phi_\beta(\rho, \vartheta_\beta, \eta_\beta)$$

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

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

16

$^4He_3$

E (mK)	present	[11]	[12]	[13]	[14]	[15]	[16]	[17]	[18]	[19]
$\|E_{^4He_3}\|$	126.50	126.499	126.499	126.41	126.2	126.39	125.9	126.40	126.40	125.9
$\|E^*_{^4He_3}\|$	2.277	2.2784	2.2779	2.271		2.268	2.282	2.265	2.271	2.28

Table 3. Calculations for binding energies of the trimer $^4He_3$ with LM2M2 potential in mK.

[11] V. ROUDNEV, M. CAVAGNERO *J. Phys. B* **45**,025101 (2012).

[12] E. HIYAMA, M. KAMIMURA, *Phys. Rev. A* **85**, 062505 (2012); *Phys. Rev. A* **85**, 022502 (2012).

[13] V. A. ROUDNEV, S. L. YAKOVLEV, S. A. SOFIANOS, *Few-Body Systems* **37**, 179 (2005).

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[15] R. LAZAUSKAS, J. CARBONELL, *Phys. Rev. A* **73**, 062717 (2006).

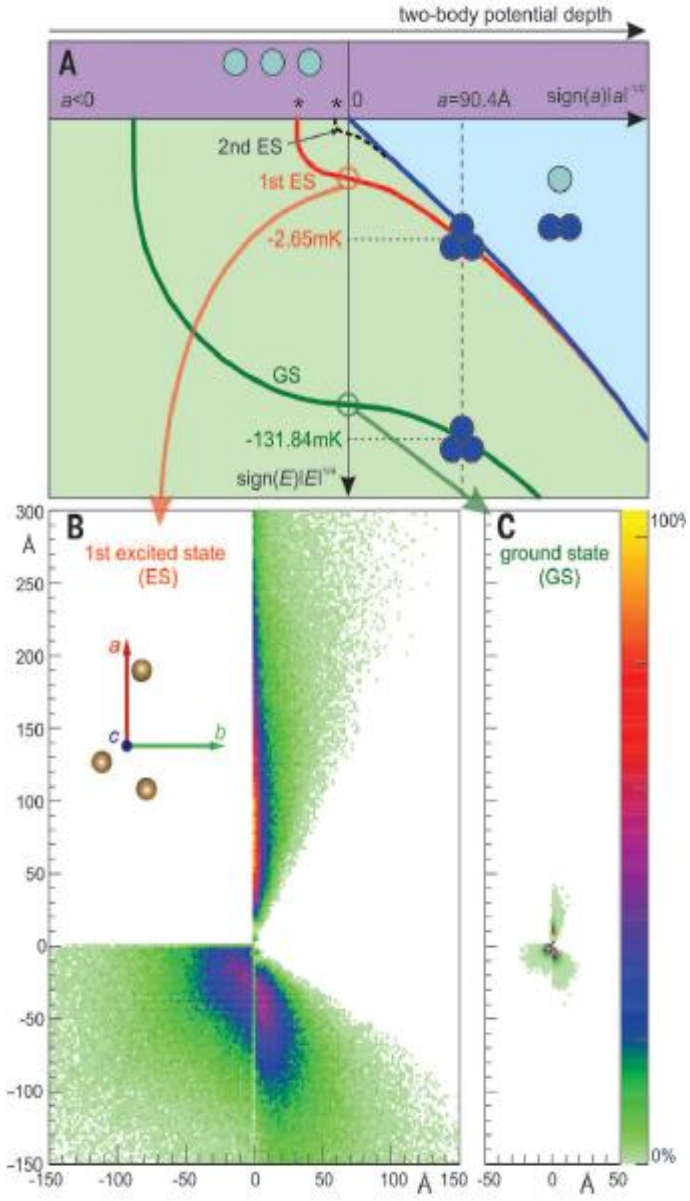
[16] E. A. KOLGANOVA, A. K. MOTOVILOV, W.SANDHAS, *Few-Body Syst.* **51**, 249 (2011).

[17] A. KIEVSKY *et al.*, *Few-Body Systems* **51**, 259 (2011).

[18] A. DELTUVA, *Few-Body Systems* **56**, 897 (2015).

[19] A. K. MOTOVILOV, W.SANDHAS, S. A. SOFIANOS AND E. A. KOLGANOVA, *Eur. J. Phys. D* **13**, 33 (2001).

$^4He_3$



Three-Body Efimov States

Measurements:

$$|E^*_{1ES} - \varepsilon_d| = 0.98 \pm 0.2\text{mK}$$

Kunitski M. et. al. // *Science* **348** (2015) 551.

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

Grisenti R. et. al. // *Phys. Rev. Lett.* **85** (2000) 2284.

Calculations:

$$|E^*_{1ES} - \varepsilon_d| = 0.972\text{mK}$$

$$\varepsilon_d = -1.3035\text{mK} \qquad l_{sc} = 100.23\,\text{Å}$$

$$E_{GS} = -126.507\text{mK} \qquad E^*_{1ES} = -2.276\text{mK}$$

Kolganova E.A., Motovilov A.K., Sandhas W. al. // *Few-Body Systems* **51** (2011) 249.

A Dependence of the binding energies of the ground (GS) and first excited (1ST) states of the He trimer on the scattering length calculated by scaling He-He potential.

B and **C** Structure of the excited and ground states of $^4He_3$

$^4He_3$

TABLE I: Dimer energy ε_d, bond length $< R >$, ^{4}He$-^4$He scattering length $\ell_{sc}^{(1+1)}$ energy of excited state of trimer E^*_{1ES} and difference $|E^*_{1ES} - \varepsilon_d|$ for the different potentials, as compared to the experimental values of Ref. [1] and [2].

	ε_d (mK)	$\ell_{sc}^{(1+1)}$ (Å)	$< R >^a$ (Å)	E^*_{1ES} (mK)	$\lvert E^*_{1ES} - \varepsilon_d \rvert$ (mK)
HFDHE2	-0.830	124.65	-	1.67	0.84
HFD-B	-1.685	88.50	46.46	2.74	1.05
LM2M2	-1.303	100.23	51.84	2.27	0.97
TTY	-1.309^b	100.01	51.65	2.28	0.97
PCKLJS [3]	-1.615	90.42	47.09	2.65	1.03
SAPT96 [3]	-1.744		45.45	2.80	1.06
CCSAPT07 [3]	-1.564		47.78	2.59	1.02
Jeziorska [4]	-1.728	87.53		2.78	1.06
Exp. [1]	$1.1^{+0.3}_{-0.2}$	104^{+8}_{-18}	52^{+4}_{-4}		0.98 ± 0.2 [2]

[a]Results from Ref. [5].

[1] GRISENTI R. *et al.*, *Phys. Rev. Lett.* **85** (2000) 2284.

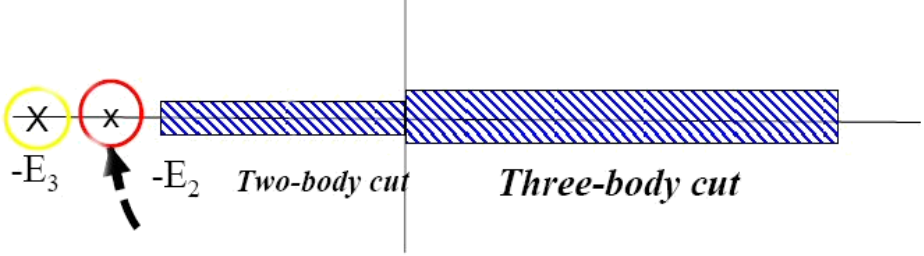
[2] KUNITSKI M. *et al.*, *Science* **348** (2015) 551.

[3] E. HIYAMA, M. KAMIMURA, *Phys. Rev. A* **85**, 062505 (2012); *Phys. Rev. A* **85**, 022502 (2012).

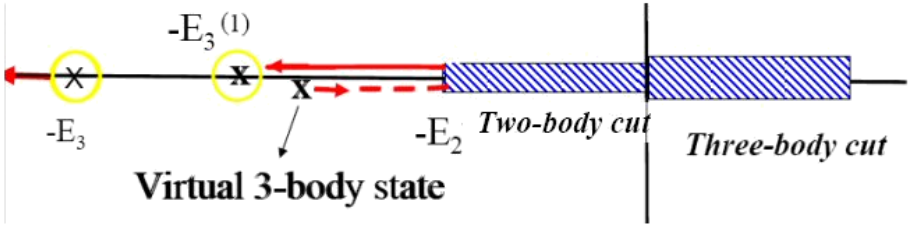
[4] H.SUNO, B.D.ESRY, *Phys. Rev. A* **78**, 062701 (2008).

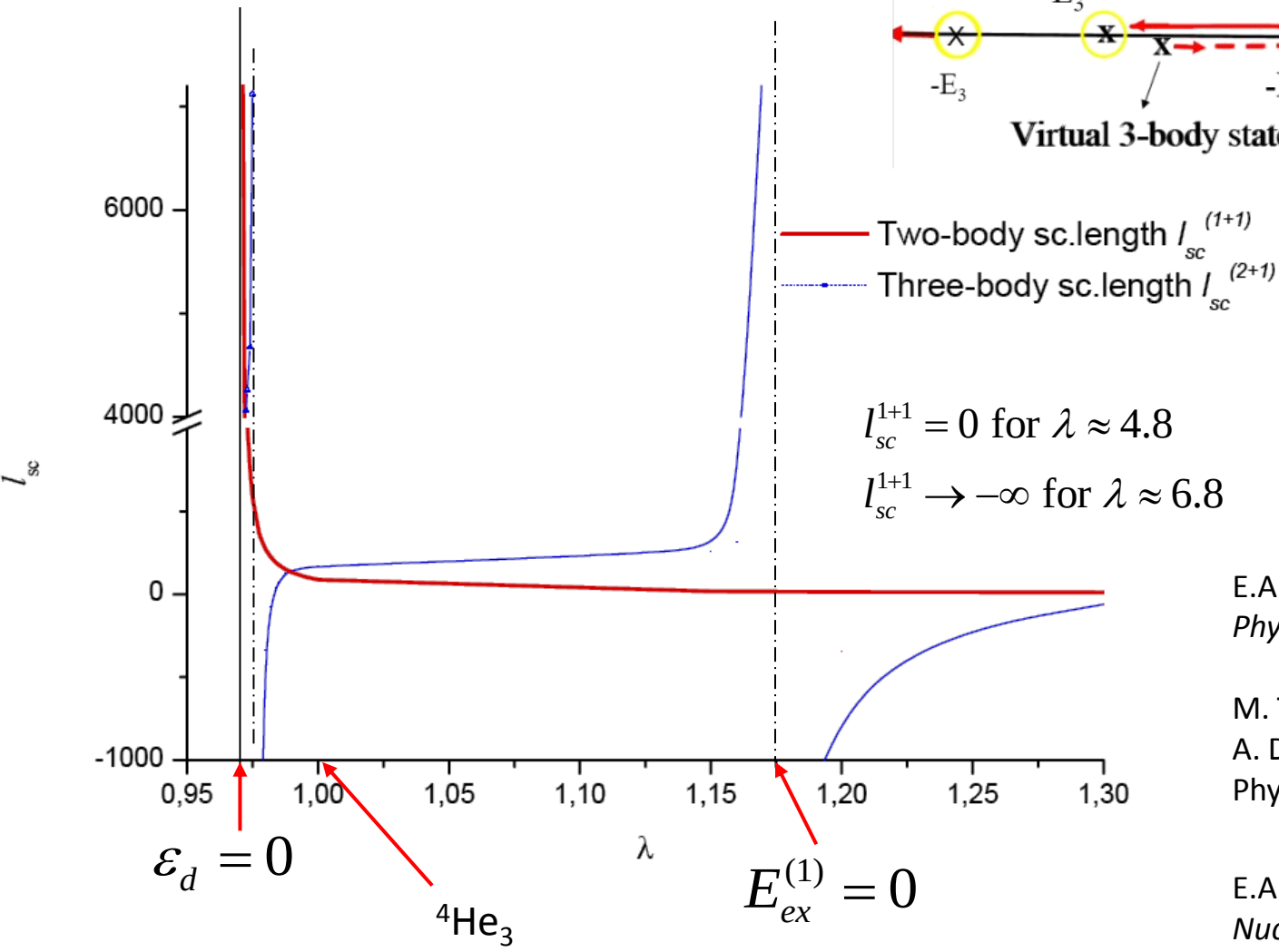
[5] A. KIEVSKY *et al.*, *Few-Body Systems* **51**, 259 (2011).

$^4He_2$ - ^4He



$$V(x) = \lambda V_{HFD-B}(x)$$





$l_{sc}^{1+1} = 0$ for $\lambda \approx 4.8$

$l_{sc}^{1+1} \to -\infty$ for $\lambda \approx 6.8$

$\varepsilon_d = 0$

$^4He_3$

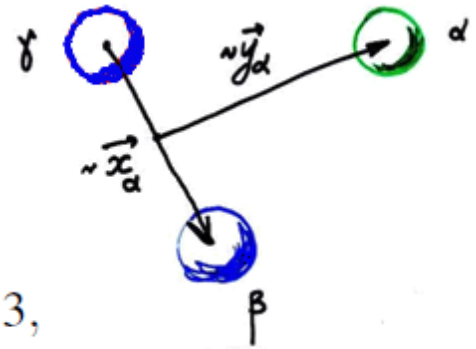
$E_{ex}^{(1)} = 0$

E.A.K, A.Motovilov,
Phys. At. Nucl. **62**, 1179 (1999)

M. T. Yamashita, T. Frederico,
A. Delfino, L. Tomio ,
Phys. Rev. A 66, 052702 (2002)

E.A.K, A.Motovilov, W.Sandhas
Nucl.Phys. A **790**, 752 (2007)

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

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

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

Expanding Faddeev components in a series of bispherical harmonics we have

$$F_\alpha(\boldsymbol{x}, \boldsymbol{y}) = \sum_l \frac{f_l^{(\alpha)}(x, y)}{xy} \mathscr{Y}_{ll0}(\hat{x}, \hat{y}), \quad \alpha = 1, 3, \quad x = |\boldsymbol{x}|, y = |\boldsymbol{y}|, \hat{x} = \boldsymbol{x}/x, \text{ and } \hat{y} = \boldsymbol{y}/y.$$

As a results we obtain the partial integro-differential equations

$$\left(-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+l(l+1)\left(\frac{1}{x^2}+\frac{1}{y^2}\right)-E\right)f_l^{(\alpha)}(x,y)=-V_\alpha(x)\psi_l^{(\alpha)}(x,y),\qquad \alpha=1,3,$$

$$\begin{aligned}
\psi_l^{(1)}(x,y) &= f_l^{(1)}(x,y)+\sum_{l'}\int_0^1 d\eta\left[h^0_{(1;ll0)(2;l'l'0)}(x,y,\eta)f_{l'}^{(1)}(x_{21}(\eta),y_{21}(\eta))\right.\\
&\quad\left.+h^0_{(1;ll0)(3;l'l'0)}(x,y,\eta)f_{l'}^{(3)}(x_{31}(\eta),y_{31}(\eta))\right],\\
\psi_l^{(3)}(x,y) &= f_l^{(3)}(x,y)+\sum_{l'}\int_0^1 d\eta\left[h^0_{(3;ll0)(1;l'l'0)}(x,y,\eta)f_{l'}^{(1)}(x_{13}(\eta),y_{13}(\eta))\right.\\
&\quad\left.+h^0_{(3;ll0)(2;l'l'0)}(x,y,\eta)f_{l'}^{(1)}(x_{23}(\eta),y_{23}(\eta))\right]
\end{aligned}$$

$$
\begin{aligned}
&h^{L}_{(\alpha;l\lambda L)(\beta;l'\lambda' L)}(x,y,\eta) \\
&= \frac{xy}{x_{\beta\alpha}(\eta)y_{\beta\alpha}(\eta)}(-1)^{l+L}\frac{(2\lambda+1)(2l+1)}{2^{\lambda+l}}\left[(2\lambda)!(2l)!(2\lambda'+1)(2l'+1)\right]^{1/2} \\
&\quad\times\sum_{k=0}^{k_{max}}(-1)^{k}(2k+1)P_k(\eta)\sum_{\substack{\lambda_1+\lambda_2=\lambda,\\ l_1+l_2=l}}\frac{y^{\lambda_1+l_1}x^{\lambda_2+l_2}}{[y_{\beta\alpha}(\eta)]^{\lambda}[x_{\beta\alpha}(\eta)]^{l}}(-1)^{\lambda_1}\mathsf{c}_{\beta\alpha}{}^{\lambda_1+l_2}\mathsf{s}_{\beta\alpha}{}^{\lambda_2+l_1} \\
&\quad\times[(2\lambda_1)!(2l_1)!(2\lambda_2)!(2l_2)!]^{-1/2}\sum_{\lambda''l''}(2\lambda''+1)(2l''+1)\begin{pmatrix}\lambda_1 & l_1 & \lambda''\\ 0 & 0 & 0\end{pmatrix} \\
&\quad\times\begin{pmatrix}\lambda_2 & l_2 & l''\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}k & \lambda'' & \lambda'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}k & l'' & l'\\ 0 & 0 & 0\end{pmatrix} \\
&\quad\times\begin{Bmatrix}l' & \lambda' & L\\ \lambda'' & l'' & k\end{Bmatrix}\begin{Bmatrix}\lambda_1 & \lambda_2 & \lambda\\ l_1 & l_2 & l\\ \lambda'' & l'' & L\end{Bmatrix}, \\
&\quad k_{max}=\frac{1}{2}(l+\lambda+l'+\lambda').
\end{aligned}
$$

Here $P_k(\eta)$ is the Legendre polynomial of order k. The standard notation for the 3-j, 6-j, and 9-j Wigner symbols is used. We also use the notation

$$
\begin{aligned}
x_{\beta\alpha}(\eta) &= \sqrt{\mathsf{c}^2_{\beta\alpha}x^2+2\mathsf{c}_{\beta\alpha}\mathsf{s}_{\beta\alpha}xy\eta+\mathsf{s}^2_{\beta\alpha}y},\\
y_{\beta\alpha}(\eta) &= \sqrt{\mathsf{s}^2_{\beta\alpha}x-2\mathsf{c}_{\beta\alpha}\mathsf{s}_{\beta\alpha}xy\eta+\mathsf{c}^2_{\beta\alpha}y}.
\end{aligned}
$$

The asymptotic boundary condition for a bound state reads as follows

$$f_l^{(\alpha)}(x,y) = \delta_{l0}\psi_d(x)\exp(\mathrm{i}\sqrt{E-\varepsilon_d}\,y)\left[\mathrm{a}_0 + o\left(y^{-1/2}\right)\right] + \frac{\exp(\mathrm{i}\sqrt{E}\rho)}{\sqrt{\rho}}\left[A_l^{(\alpha)}(\theta) + o\left(\rho^{-1/2}\right)\right]$$

as $\rho = \sqrt{x^2+y^2} \to \infty$ and/or $y \to \infty$.

The asymptotic boundary condition for the partial-wave Faddeev components of the $(2+1 \to 2+1\,;\,1+1+1)$ scattering wave function for $\rho \to \infty$ and/or $y \to \infty$ reads

$$f_l^{(\alpha)}(x,y,p) = \delta_{l0}\psi_d(x)\left\{\sin(py) + \exp(\mathrm{i}py)\left[\mathrm{a}_0(p) + o\left(y^{-1/2}\right)\right]\right\} + \frac{\exp(\mathrm{i}\sqrt{E}\rho)}{\sqrt{\rho}}\left[A_l^{(\alpha)}(E,\theta) + o\left(\rho^{-1/2}\right)\right],$$

where p is the momentum conjugate to the coordinate y, E the scattering energy given by $E = \varepsilon_d + p^2$, and $\mathrm{a}_0(p)$ the elastic scattering amplitude. The functions $A_l(E,\theta)$ provide us for $E > 0$ with the corresponding partial-wave Faddeev breakup amplitudes.

$$\ell_{\mathrm{sc}} = -\frac{1}{2}\sqrt{1+2\frac{\mathrm{m}_{^4\mathrm{He}}}{\mathrm{m}_{\mathrm{X}}}}\lim_{p\to 0}\frac{\mathrm{a}_0(p)}{p}, \qquad \delta_0(p) = \frac{1}{2}\,\mathrm{Im}\ln \mathrm{S}_0(p).$$

INTERACTION POTENTIALS

Experiment ^{7}Li ^{4}He

$$0.0024 \pm 0.025 \text{ cm}^{-1}$$

$$0.0039 \text{ cm}^{-1}$$

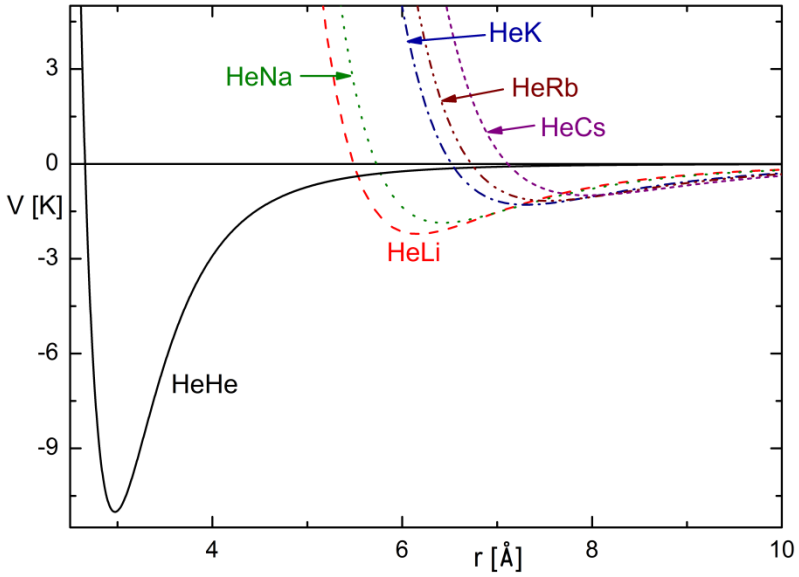
Dimer	$\|E\|$ (mK)	Dimer	$\|E\|$ (mK)
^{4}He ^{4}He	1,3096[a]	^{4}He ^{23}Na	28.97
^{4}He ^{4}He	1,728[b,c]	^{4}He ^{39}K	11.20[c]
^{4}He ^{6}Li	1,512	^{4}He ^{85}Rb	10.27[c]
^{4}He ^{7}Li	5,617	^{4}He ^{133}Cs	4.945[c]

N.Tariq, N.A.Taisan, V.Singh, and J.D. Weinstein,
Phys. Rev .Lett. **110**, 153201 (2013).

[a] potential model LM2M2

[b] potential model from M. Jeziorska *et al.*, J. Chem. Phys. **127**, 124303 (2007)

[c] data taken from H.Suno and B.D.Esry, Phys. Rev. A **80**, 062702 (2009)



[1] U. Klenkathöfer, K.T. Tang, J.P. Toennies, C.I.Yiu // Chem.Phys.Lett. **249**, 257-263 (1996)

[2] U. Klenkathöfer, M. Lewerenz, M.Mladenoc // Phys.Rev.Lett**. 83**, 4717-4720 (1999)

$^{6;7}Li\,^{4}He_2$

E (mK) He-He potential He-Li potental	present LM2M2 KTTY	[11] LM2M2 KTTY	[12] Jeziorska KTTY	[12] LM2M2 Cvetko	[13] LM2M2 Cvetko	[14] KTTY KTTY	[15]
$\lvert E_{^7Li^4He_2}\rvert$	51.11	78.73	81.29	64.26	73.3	45.7	45.7
$\lvert E^*_{^7Li^4He_2}\rvert$	5.618	5.685	5.67	3.01	12.2		2.31
$\lvert E_{^6Li^4He_2}\rvert$	35.45				51.9	31.4	31.4
$\lvert E^*_{^6Li^4He_2}\rvert$	1.719				7.9		-

Table 3. Calculations for binding energies of the trimer Li^4He_2 in mK.

[11] M-S. WU, H-L. HAN, CH-B. LI, AND T-Y. SHI *Phys. Rev. A* **90**,062506 (2014).

[12] H.SUNO, B.D.ESRY, *Phys. Rev. A* **80**, 062702 (2009).

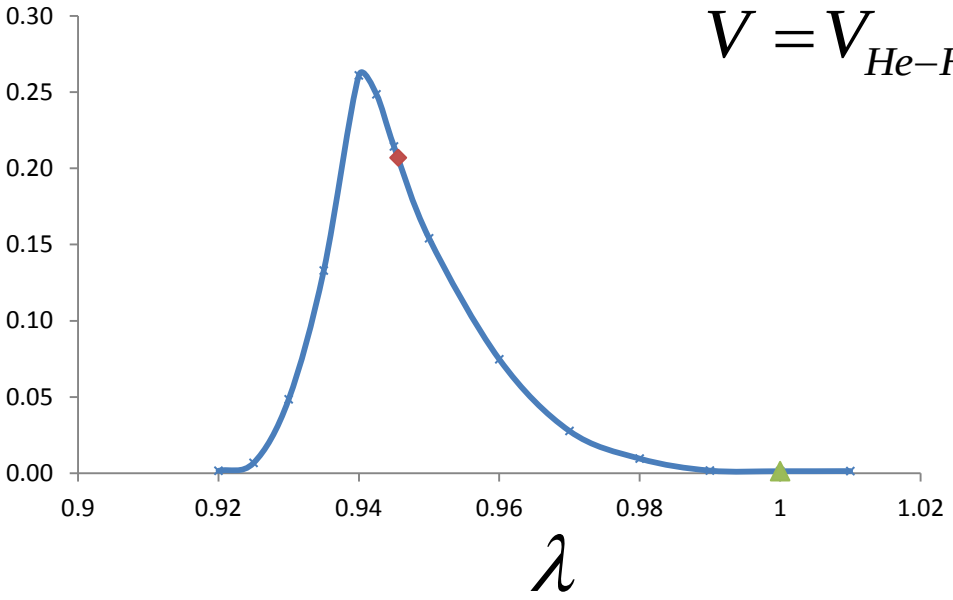
[13] I. BACCARELLI, G. DELGADO-BARRIO, F. A. GIANTURCO, T. GONZALEZ- LEZANA, S. MIRET-ARTES, AND P. VILLARREAL, *Europhys. Lett.* **50**, 567 (2000).

[14] J.M. YUAN AND C.D.LIN, *J. Phys. B* **31**, L637 (1998).

[15] A. DELFINO, T. FEDERICO, L. TOMIO, *J. Chem. Phys.* **113**, 7874 (2000).

$^{7}Li\,^{4}He_2$

$$|E_1^* - \varepsilon_d|$$



$$V = V_{He-He}(r_{12}) + \lambda[V_{He-Li}(r_{13}) + V_{He-Li}(r_{23})]$$

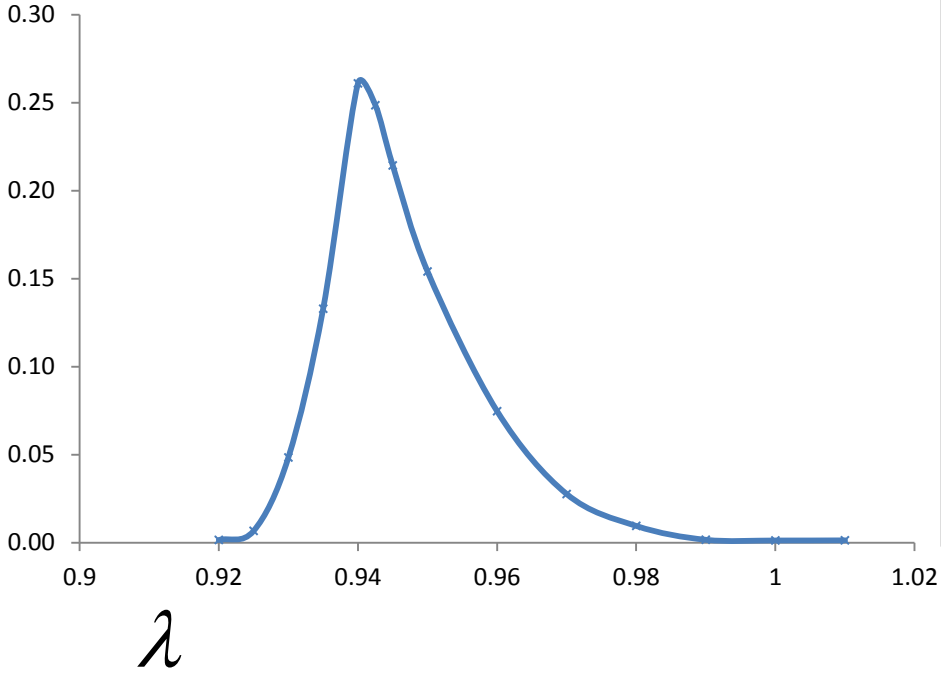
$$|E^*_{^{7}Li\,^{4}He_2} - \varepsilon_d| = 0.013\text{mK}$$

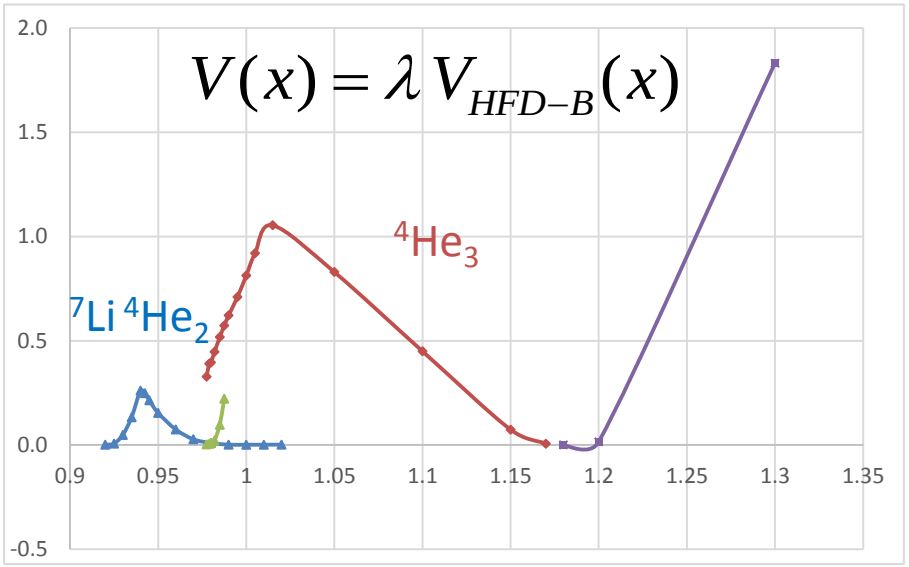
$$|E^*_{^{6}Li\,^{4}He_2} - \varepsilon_d| = 0.207\text{mK}$$

$^7Li\,^4He_2$

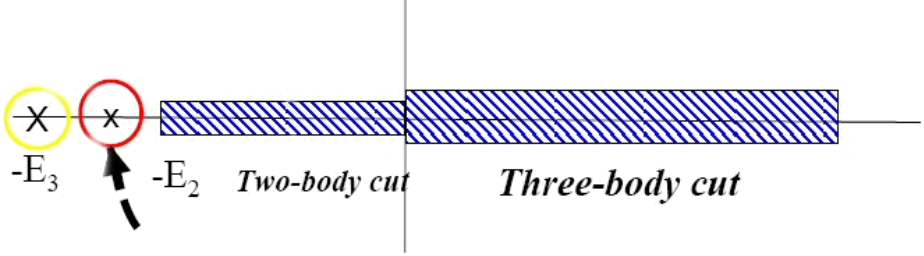
$$V = V_{He-He}(r_{12}) + \lambda[V_{He-Li}(r_{13}) + V_{He-Li}(r_{23})]$$

$|E_1^* - \varepsilon_d|$

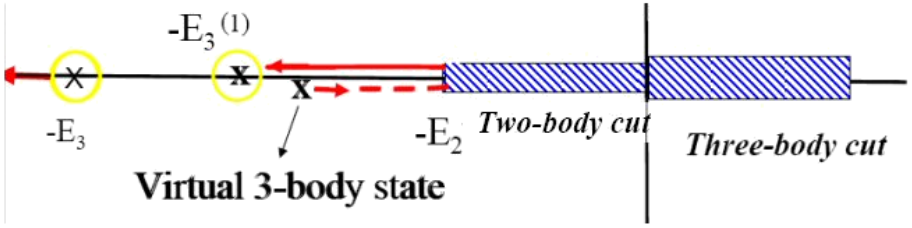


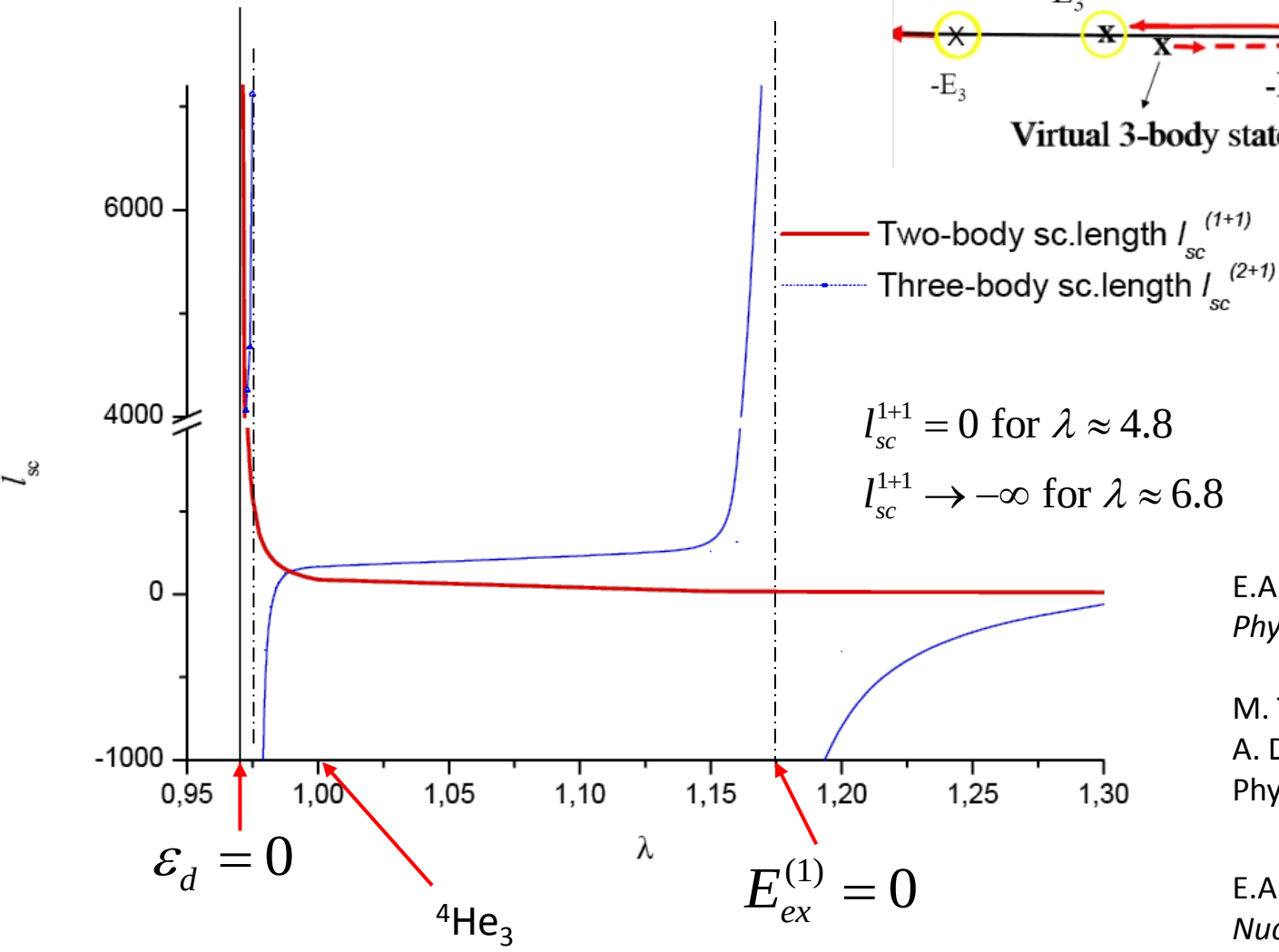


$^4He_2$ - ^4He



$$V(x) = \lambda V_{HFD-B}(x)$$





$l_{sc}^{1+1} = 0$ for $\lambda \approx 4.8$

$l_{sc}^{1+1} \to -\infty$ for $\lambda \approx 6.8$

$\varepsilon_d = 0$

$^4He_3$

$E_{ex}^{(1)} = 0$

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M. T. Yamashita, T. Frederico,
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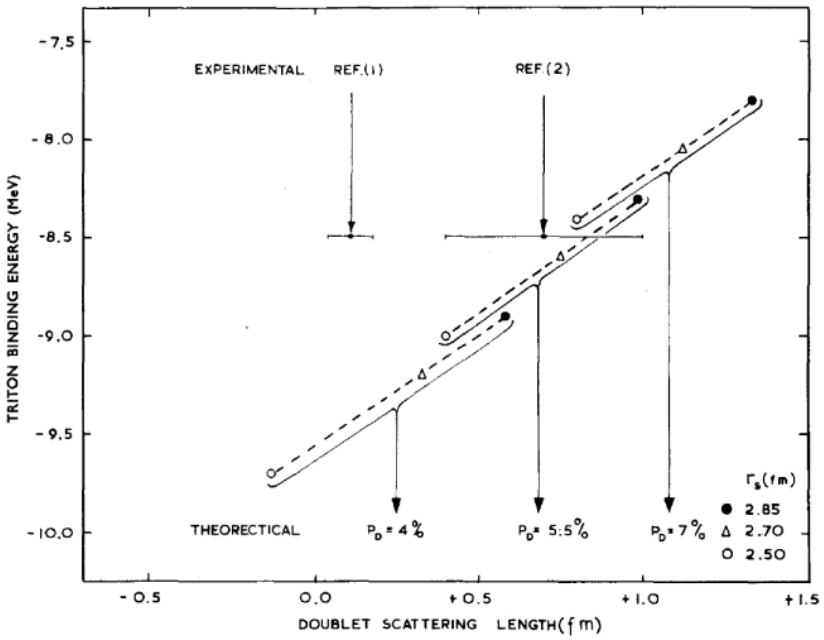
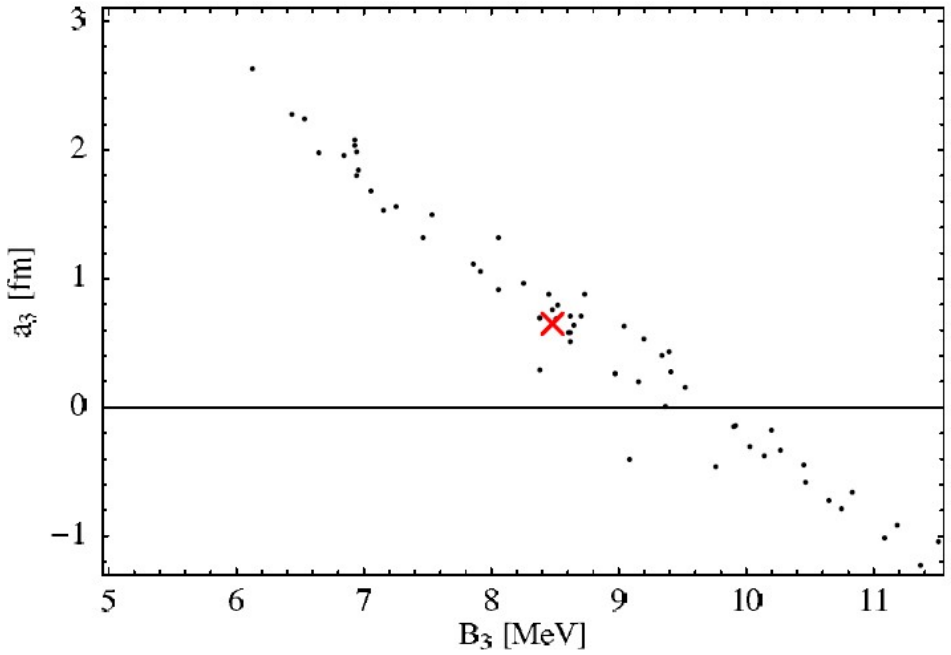
Phys. Rev. A 66, 052702 (2002)

E.A.K, A.Motovilov, W.Sandhas
Nucl.Phys. A **790**, 752 (2007)

^{3}H - system

Three-body, theory

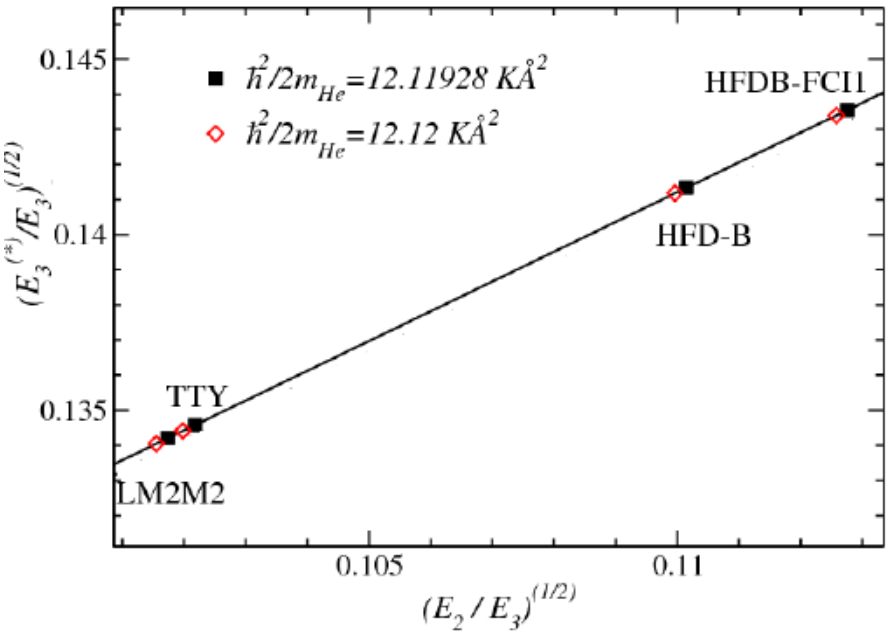




Phillips line from the original paper, showing the unexpected linear correlation

A.C. Phillips, *Nucl. Phys. A* ***107****, 209 (1968).*

$^4He_3$



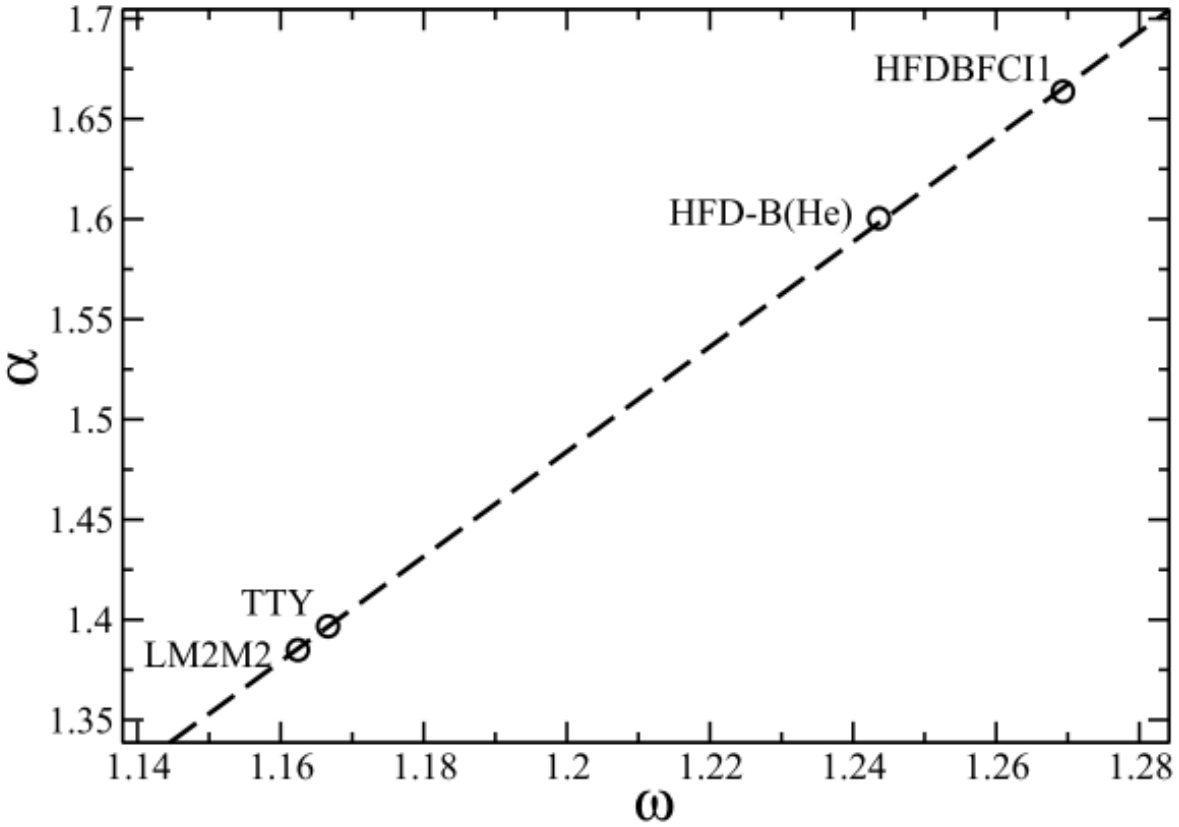
V. Roudnev and M. Cavagnero //*J. Phys. B* **45,** 025101 (2012)

$^4He_3$

Three-body, theory

$$E_2 - E_3 \approx 1/(2m_{12}a_3^2)$$

V.Efimov, E.G.Tkachenko,
Phys.Lett. B **157**, 108 (1985)



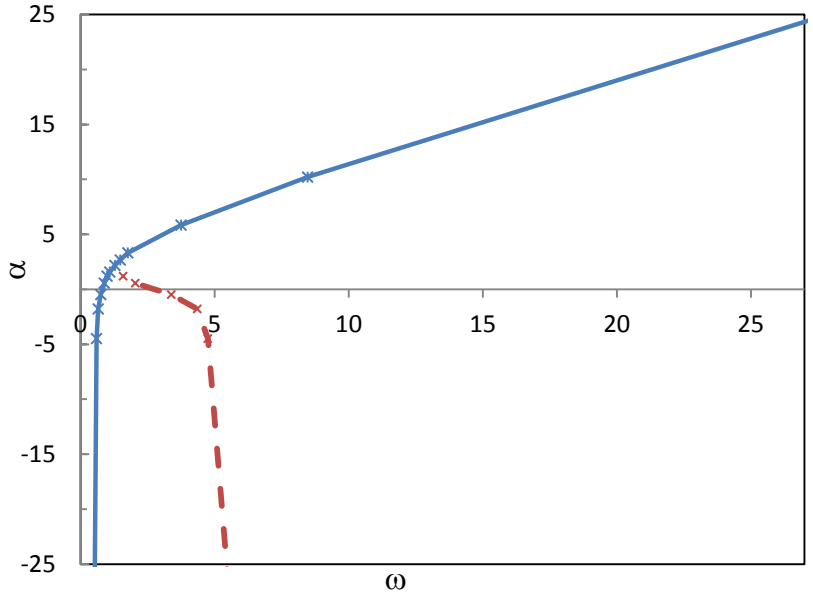
$$\alpha \equiv a_3\sqrt{-\mu E_2} \propto 1/\sqrt{E_3/E_2 - 1} \equiv \omega$$

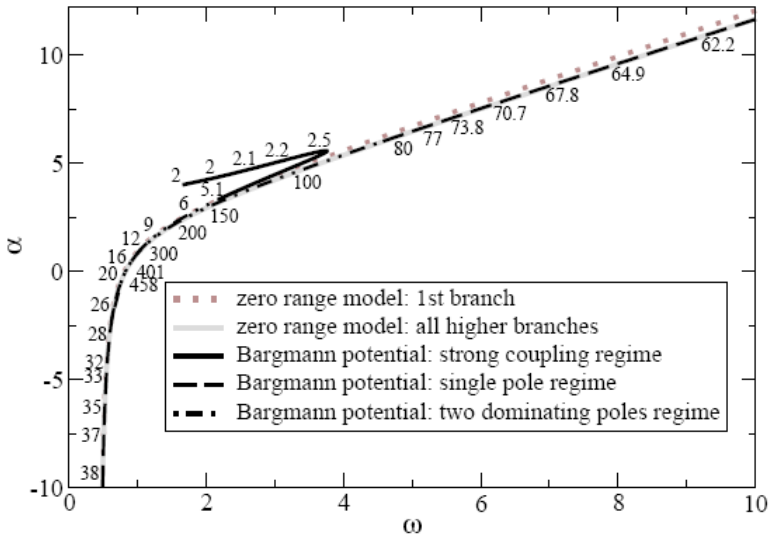
V.Roudnev, M.Cavagnero
Phys.Rev.Lett. **108**, 110402 (2012)

$^4He_2$ - ^4He

Three-body, theory

$$V(x) = \lambda V_{HFD-B}(x)$$





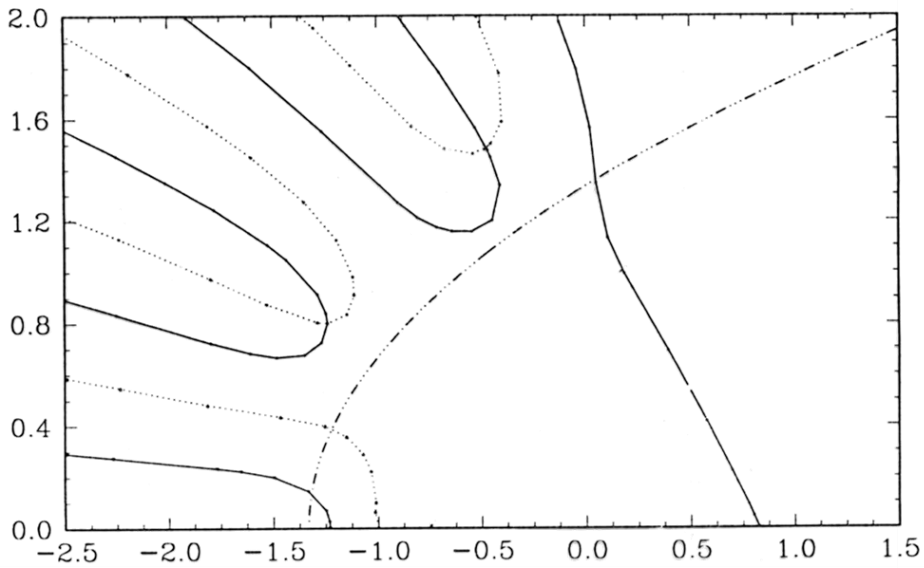
$$\alpha \equiv a_3\sqrt{-\mu E_2} \propto 1/\sqrt{E_3/E_2 - 1} \equiv \omega$$

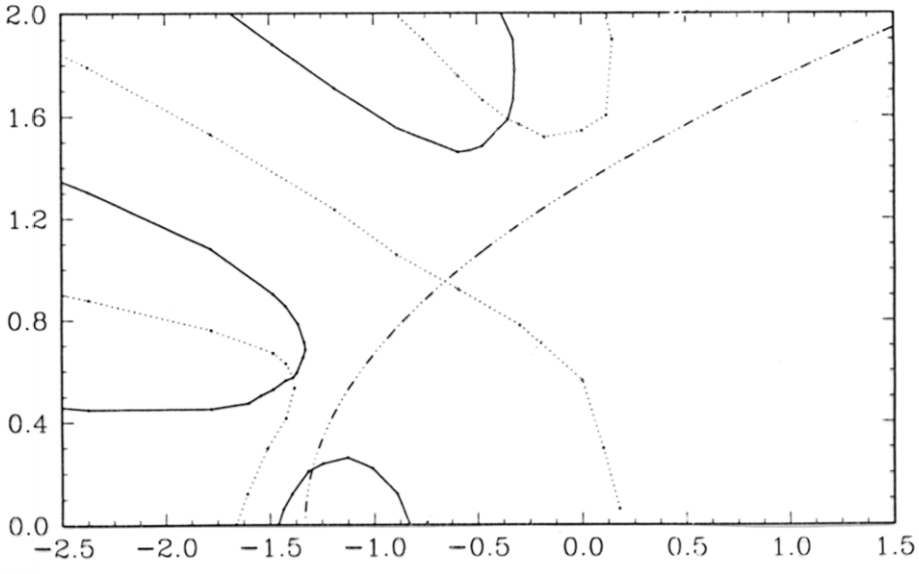
E.A.K, *Few-Body Syst.* **55**, 957 (2014)

V.Roudnev, M.Cavagnero
Phys.Rev.Lett. **108**, 110402 (2012)

Root locus curve of scattering matrix

$\mathrm{Im}\, z / |\varepsilon_d|$





^{3}H

$\mathrm{Re}\, z / |\varepsilon_d|$

^{4}He$_3$

S-matrix root lines in nnp system

S-matrix root lines in ^{4}He$_3$ system

Solid line - Re(S)=0, tiny dashed line – Im(S)=0

E.A.K, *Few-Body Syst.* **55**, 957 (2014)

Some consequences

- There are correlations between two-body and three-body parameters at the two-body threshold

- Similar structure of S-matrix for atomic and nuclear systems

Conclusions

- We employed formalism which is suitable for three-body atomic systems interacted via hard-core potential. This method let us calculate bound states and scattering observables.
- Further experiments with better accuracy are necessary!

Thank you !

Thank you !

- Olga Klimenko (Dubna Univ.)
- Artem Korobitsin (JINR)
- Alexander Motovilov (JINR)
- Werner Sandhas (PI Bonn Univ.)