Study of Few-Body Nuclei by Feynman's Continual Integrals and Hyperspherical Functions

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Outlook

1. **Feynman's Continual Integrals (FCI) method for solving *N*-body ground state problem was implemented using parallel computing and tested for exactly solvable models with *N*=3,4,5,6,7.**
2. **Spline approximation was applied for solving the system of hyperradial equations in Hyperspherical Functions (HSF) method. The calculation of coupling matrices was implemented using parallel computing.**
3. **3-body systems: ^{3}H, ^{3,6}He, ^{11}Li, ^{9}Be, ^{12}C with universal nucleon-nucleon, nucleon-α-cluster and α-cluster-α-cluster interactions were studied using both methods: FCI and HSF.**
4. **4-body systems ^{4}He, ^{7}Li, ^{16}O with universal nucleon-nucleon, nucleon-α-cluster and α-cluster-α-cluster interactions were studied using FCI method.**

1.1. Feynman's continual integrals (FCI) method

Feynman's continual integral [1] is propagator - probability amplitude for a particle to travel from one point to another in a given time *t*

$$K(q,t;q_0,0)=\int Dq(t')\exp\left\{\frac{i}{\hbar}S[q(t')]\right\}=\left\langle q\left|\exp\left(-\frac{i}{\hbar}\hat{H}t\right)\right|q_0\right\rangle$$

Euclidean time $t=-i\tau$

$$K_E(q,\tau;q_0,0)=\lim_{\substack{N\to\infty\\ N\Delta\tau=\tau}}\left(\frac{m}{2\pi\hbar\Delta\tau}\right)^{N/2}\times$$

$$\times\int\cdots\int\exp\left\{-\frac{1}{\hbar}\sum_{k=1}^{N}\left[\frac{m(q_k-q_{k-1})^2}{2\Delta\tau}+U(q_k)\Delta\tau\right]\right\}dq_1dq_2\ldots dq_{N-1}$$

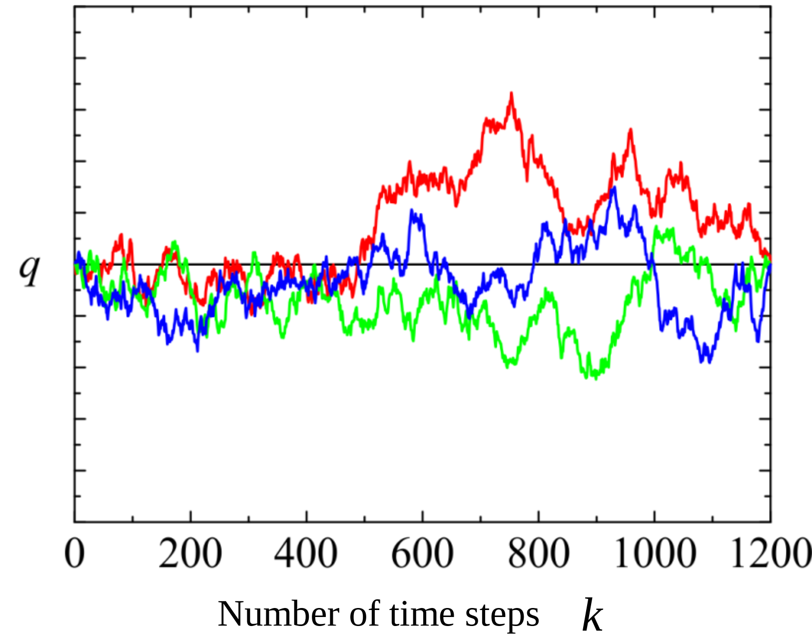
$$K_E(q,\tau;q,0)\to|\Psi_0(q)|^2\exp\left(-\frac{E_0\tau}{\hbar}\right),\ \tau\to\infty$$

Parallel calculations by Monte Carlo method [3] using NVIDIA CUDA technology were performed on cluster http://hybrilit.jinr.ru

$$K_E(q_0,\tau;q_0,0)\approx\left(\frac{m}{2\pi\hbar\tau}\right)^{1/2}\left\langle\exp\left[-\frac{\Delta\tau}{\hbar}\sum_{k=1}^{N}U(q_k)\right]\right\rangle,\qquad \langle F\rangle\approx\frac{1}{n}\sum_{i=1}^{n}F_i$$

Example of three random trajectories

$N=1200.\quad n=3.$



Algorithm is averaging over random trajectories with distribution in form of multidimensional Gaussian distribution [4, 5].

[1] R. P. Feynman, A. R. Hibbs. Quantum Mechanics and Path Integrals. New York, McGraw-Hill, 1965.
[2] D. I. Blokhintsev. Principles of Quantum Mechanics [in Russian]. Moscow, Nauka, 1976.
[3] S. M. Ermakov. Monte Carlo Method in Computational Mathematics [in Russian]. St. Petersburg, Nevskiy Dialekt, 2009.
[4] M. A. Naumenko, V. V. Samarin. Supercomp. Front. Innov. **3**, No. 2, 80. (2016).
[5] V. V. Samarin, M. A. Naumenko. Phys. Atom. Nucl., **80**, 877(2017).

1.2. Hardware, software, implementation

$$K_{\mathrm{E}}\left(q_0,\tau;q_0,0\right) \approx \left(\frac{m}{2\pi\hbar\tau}\right)^{1/2} \left\langle \exp\left[-\frac{\Delta\tau}{\hbar}\sum_{k=1}^{N} U(q_k)\right]\right\rangle$$

Calculations of K_{E} is implemented using parallel computing

- **NVIDIA Tesla K40 (for calculation)**
  NVIDIA Quadro 600, GeForce 920 (for debugging)

- **Intel® Core™ i5 (for debugging, comparing, and testing)**

- **Heterogeneous Cluster (http://hybrilit.jinr.ru/)**
  (LIT, Joint Institute for Nuclear Research)

- **Implemented in C++ language**
  (single precision)

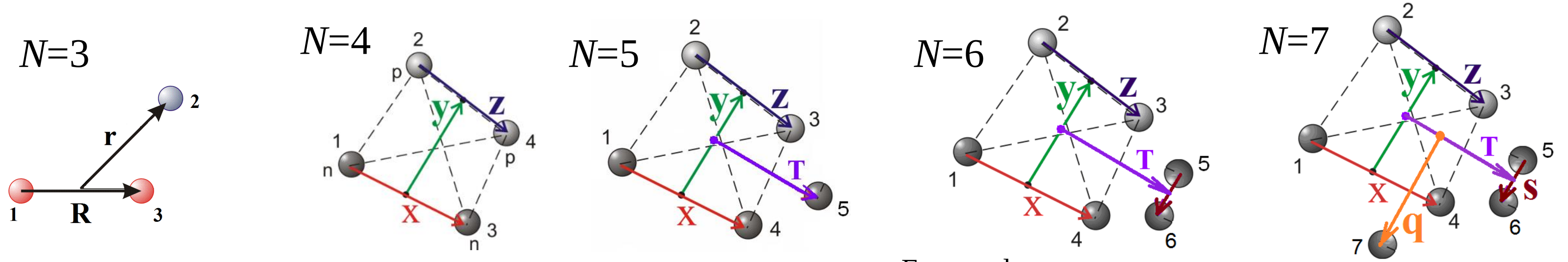
- **Code compiled**
  for architecture CUDA, CUDA Toolkit + Microsoft Visual Studio (Windows 7,10 for debugging);
  for architecture CUDA (Linux, for calculation),

- **cuRAND random number generator**

- **1 thread calculates 1 trajectory**

1.3. Calculations for exactly solvable *N*-body oscillator models

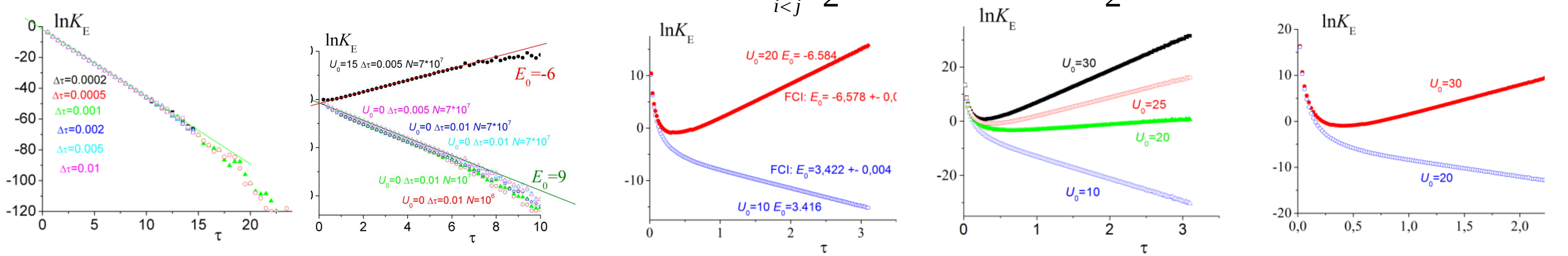
Jacobi coordinates:



Exact value:

$m_1 = m_3 = 1,\ m_2 = \infty;$

$$m_i = 1,\ i = 1,\ldots N;\ U = -U_0 + \sum_{i<j} \frac{\omega^2}{2} r_{ij}^2,\ E_0 = -U_0 + \hbar\omega \frac{3}{2}(N-1)\sqrt{N},\ \ \omega = 1,\ \hbar = 1.$$



The slope of resulting straight lines equals the energy of the ground state

$$\ln K_E(q,\tau;q,0) \approx \ln|\Psi_0(q)|^2 - E_0\tau,\ \tau\to\infty,$$

N, U_0	Exact value E_0	Calculated value E_0
N=3, U_0=0	4.098	4.117±0.006
N=4, U_0=15	– 6	–5.98±0.02
N=5, U_0=20	–6.584	6.56±0.05
N=6, U_0=20	–1.629	– 1.84±0.01
N=7, U_0=20	3.812	3.63±0.01

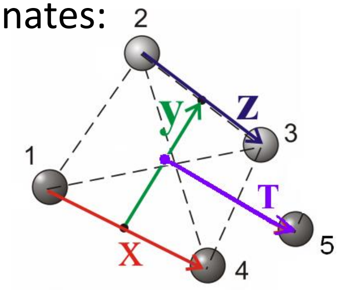
Feynman's continual integrals (FCI) Monte-Carlo calculation with statistics $n=10^7$.

FCI method reproduces exact result.

1.4. FCI calculations for "exactly" solvable 5-body nucleon model

In the system of the particles with masses $m_1 = m_2 = m_3 = m_4 = m$, $m_5 = \infty$, light particles 1, 2, 3, 4 interact only with heavy particle 5 by nucleon-nucleon potential having repulsive core.

Jacobi coordinates: **X, Y, Z, T**



$$V_{12}(r) \equiv V_{23}(r) = \sum_{k=1}^{3} u_k \exp\left(-r^2/b_k^2\right)$$

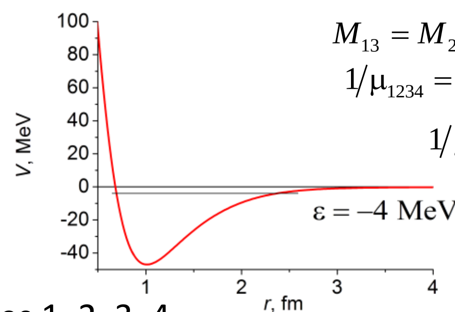
$$1/M_{13} = 1/m + 1/m = 2/m,\ 1/M_{24} = 1/m + 1/m = 2/m$$

$$M_{13} = M_{24} = m/2$$

$$1/\mu_{1234} = 1/2m + 1/2m = 1/m \qquad \mu_{1234} = m$$

$$1/\mu_{12345} = 1/4m \qquad \mu_{12345} = 4m$$

The radial Schrödinger equation was solved "exactly" by difference scheme for 2-body system 1 and 5 particles. The energy is equal to –4 MeV



The energy of the independent light particles 1, 2, 3, 4 in the field of heavy particle 5 is equal to the sum of energies of particles 1, 2, 3 and 4:

exact result

$E_0 = -16$ MeV

$$b_0^{-1} \ln K_E(q,\tau;q,0) \to \ln\left|\Psi_0(q)\right|^2 - \tilde{E}_0\tilde{\tau},\ \tilde{\tau} \to \infty$$

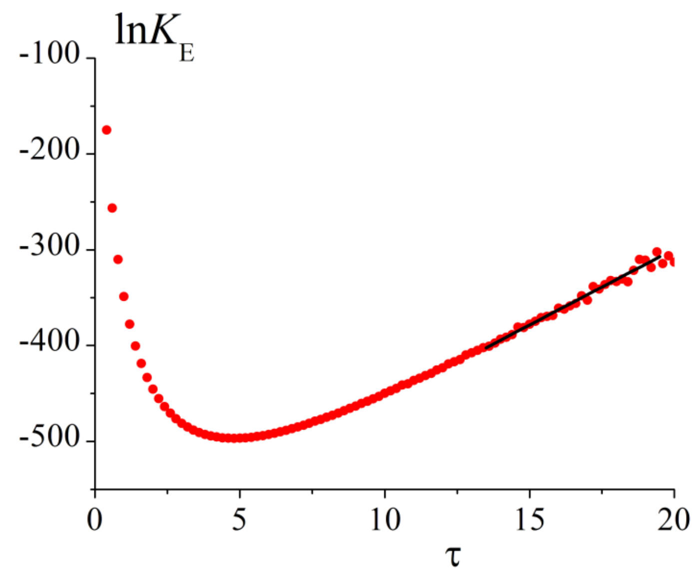
$b_0 = t_0\varepsilon_0/\hbar \approx 0.02412,\ \varepsilon_0 = 1$ MeV, $x_0 = 1$ fm,

$t_0 = m_0 x_0^2/\hbar \approx 1.57 \cdot 10^{-23}$ s,

$\tilde{\tau} = \tau/t_0,\ \ \tilde{E}_0 = E_0/\varepsilon_0,$

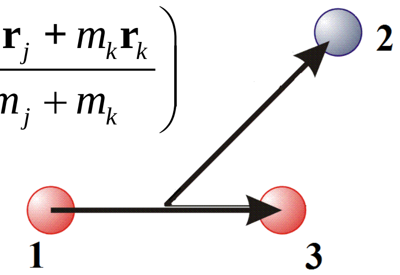
m_0 is the neutron mass

$E_0 = -15.91 \pm 0.46$



FCI calculation with statistics $N = 3 \cdot 10^7$ reproduces exact result

2.1. HSF basics: description of 3-body system



The "normalized" Jacobi coordinates $(\mathbf{x}_i, \mathbf{y}_i)$ are: $\mathbf{x}_i = \sqrt{\frac{m_j m_k}{m_j + m_k}}(\mathbf{r}_j - \mathbf{r}_k),\ \mathbf{y}_i = \sqrt{\frac{m_i(m_j + m_k)}{m_1 + m_2 + m_3}}\left(-\mathbf{r}_i + \frac{m_j \mathbf{r}_j + m_k \mathbf{r}_k}{m_j + m_k}\right)$

The hyperspherical coordinates are $\Omega = \{\theta_{\mathbf{x}}, \varphi_{\mathbf{x}}, \theta_{\mathbf{y}}, \varphi_{\mathbf{y}}, \alpha\}, \rho;$

$\rho^2 = \mathbf{x}^2 + \mathbf{y}^2,\ |\mathbf{x}| = \rho\cos\alpha,\ |\mathbf{y}| = \rho\sin\alpha$ $\quad\rho$ is the hyperradius.

The hyperspherical harmonics (functions) [1] are $\Phi^{l_x l_y}_{KLM}(\Omega)$,

$\Phi^{l_x l_y}_{KLM}(\Omega) = \sum_{m_x m_y} (l_x l_y m_x m_y \mid LM)\Phi^{l_x l_y m_x m_y}_{K}(\Omega),\ (l_{x_i} l_{y_i} m_{x_i} m_{y_i} \mid LM)$ are the Clebsch-Gordon coefficients

$\Phi^{l_x l_y m_x m_y}_{K}(\Omega) = g^{l_x l_y}_{K}(\alpha) Y_{l_x m_x}(\hat{\mathbf{x}}) Y_{l_y m_y}(\hat{\mathbf{y}}),\ g^{l_x l_x}_{K0}(\alpha) = N^{l_x l_x}_{K}(\cos\alpha)^{l_x}(\sin\alpha)^{l_x} P^{l_x+1/2, l_x+1/2}_{n}(\cos 2\alpha),$

$Y_{l_x m_x}(\hat{\mathbf{x}}),\quad Y_{l_y m_y}(\hat{\mathbf{y}})$ are spherical harmonics, $\quad P^{l_y+1/2, l_x+1/2}_{n}(t)$ are the Jacobi polynomials

$K = 2n + l_{x_i} + l_{y_i}$ is hypermoment, n=0,1,2…. $\Phi^{l_x l_x}_{K00}(\Omega) \equiv | l_x l_x K0\rangle = \sum_{m_x} (l_x l_x m_x - m_x \mid 00)\Phi^{l_x l_x m_x, -m_x}_{K}(\Omega)$

Expansion into hyperspherical functions for L=0

$$\Psi_0(x, y, \cos\theta) = \tilde{\Psi}_0(\alpha, \theta, \rho) = \sum_{l_x n} \frac{\varphi^{l_x l_x}_{K0}(\rho)}{\rho^{5/2}} \Phi^{l_x l_x}_{K00}(\Omega) =$$

$$= \sum_{l_x K} f^{l_x l_x}_{K0}(\rho) g^{l_x l_x}_{K0}(\alpha)(2l_x + 1) P_{l_x}(\cos\theta),\ \varphi^{l_x l_x}_{KL}(\rho) = \rho^{5/2} f^{l_x l_x}_{K0}(\rho)(2l_x + 1),$$

$$U = V_{12} + V_{13} + V_{23}$$

$$U^{l_x l_x; l'_x l'_x}_{KK'00}(\rho) = \langle l_x l_x K0 | U | l'_x l'_x K'0\rangle$$

coupling matrix

$$\frac{d^2}{d\rho^2}\varphi^{l_x l_x}_{KL}(\rho) + \left[\frac{2}{\hbar^2}\varepsilon - \frac{(K+3/2)(K+5/2)}{\rho^2}\right]\varphi^{l_x l_x}_{K0}(\rho) = \frac{2}{\hbar^2}\sum_{K' l'_x} U^{l_x l_y; l'_x l'_x}_{KK'00}(\rho)\varphi^{l'_x l'_x}_{K'0}(\rho)$$

hyperradial equations

[1] R.I. Dzhibuti and K.V. Shitikova. Method of Hyperspherical Functions in Atomic and Nuclear Physics. (Energoatomizdat, Moscow. 1993, in Russian).

2.2. HSF basics: methods of solving hyperradial equations [1]

$$\frac{d^2}{d\rho^2}\varphi_{KL}^{l_x l_x}(\rho)+\left[\frac{2}{\hbar^2}\varepsilon-\frac{(K+3/2)(K+5/2)}{\rho^2}\right]\varphi_{K0}^{l_x l_x}(\rho)=\frac{2}{\hbar^2}\sum_{K' l'_x}U_{KK'00}^{l_x l_x;l'_x l'_x}(\rho)\varphi_{K'0}^{l'_x l'_x}(\rho)$$

$$U_{KK'00}^{l_x l_x;l'_x l'_x}(\rho)=\langle l_x l_x K0\,|\,U\,|\,l'_x l'_x K'0\rangle$$

$$U=V_{12}+V_{13}+V_{23}$$

There are several methods for solving hyperradial equations: power expansion [2], artificial hyperradial basis [3, 4], basis of Lagrange functions [5].

New method using cubic spline approximation [6] is proposed.

[1] R.I. Dzhibuti and K.V. Shitikova. Method of Hyperspherical Functions in Atomic and Nuclear Physics. (Energoatomizdat, Moscow. 1993, in Russian).

[2] M.I. Haftel, V.B. Mandelzweig, Ann. Phys. **150,** No 1, 48−91 (1983).

[3] J.A. Mignaco, I. Roditi. J. Phys. Atom. And Mol. Phys. B14 N 2 L161−L166 (1981).

[4] V.D. Efros, A.M. Frolov, M.I. Mikhtarova, J. Phys. Atom. And Mol. Phys. B15 N 2 L819−L825 (1982).

[5] P. Descouvemont C. Daniel and D. Baye, Three-body Systems with Lagrange-mesh Techniques in Hyperspherical Coordinates, Phys. Rev. C **67**, 044309 (2003).

[6] G. I. Marchuk, Methods of Computational Mathematics (Nauka, Moscow, 1980, in Russian).

2.3. New in HSF: solving hyperradial equations using cubic splines

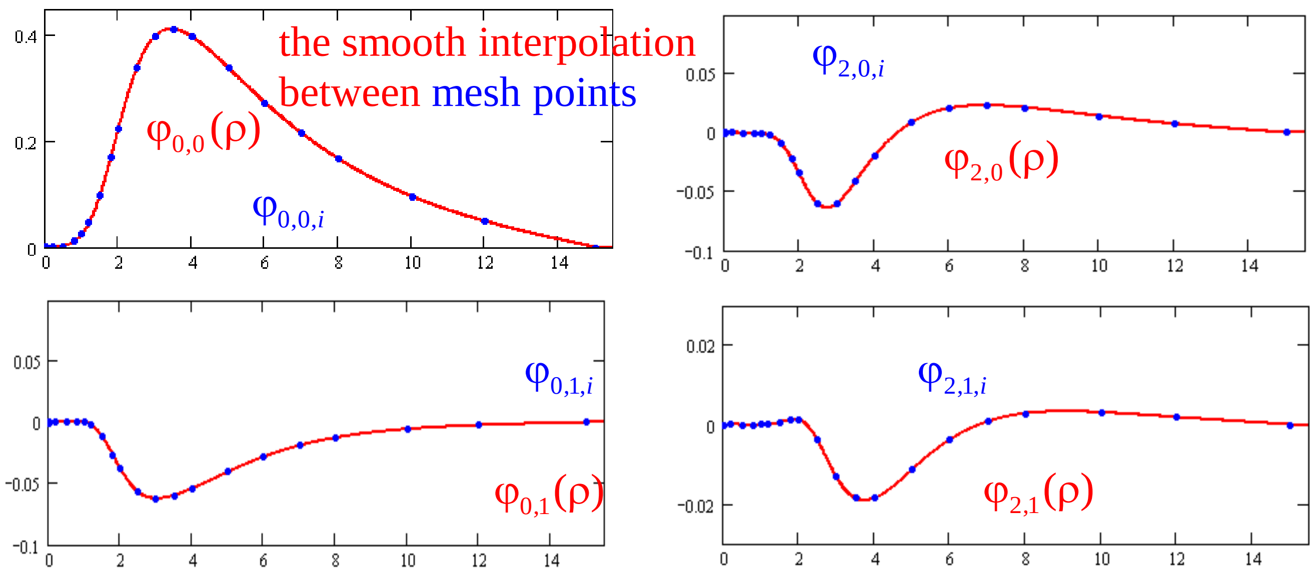
$$\varphi_{K0}^{l_x l_x}(\rho) \equiv \varphi_{l_x,n}(\rho) = m_{l_x,n,i-1}\frac{(\rho_i-\rho)^3}{6h_i} + m_{l_x,n,i}\frac{(\rho-\rho_{i-1})^3}{6h_i} + \left(\varphi_{l_x,n,i-1} - \frac{m_{l_x,n,i-1}h_i^2}{6}\right)\frac{\rho_i-\rho}{h_i} + \left(\varphi_{l_x,n,i}-\frac{m_{l_x,n,i}h_i^2}{6}\right)\frac{\rho-\rho_{i-1}}{h_i}, \quad \rho\in[\rho_{i-1},\rho_i], \quad \mathbf{[1]}$$

$$K = 2n + 2l_{x_i}, \quad n = 0,1,2,\dots,$$

$$m_{l_x,n,i} = \varphi''_{l_x,n}(\rho_i), \quad \varphi''_{l_x,n}(\rho) = m_{l_x,n,i-1}\frac{\rho_i-\rho}{h_i} + m_i\frac{\rho-\rho_{i-1}}{h_i},$$

$$h_i = \rho_i - \rho_{i-1}, \quad i = 1,2,\dots N, \quad m_{l_x,n,0} = m_{l_x,n,N} = 0$$

The idea of this method is simultaneous calculation of the mesh function φ_i and its second derivative m_i .



Advantages (+) and disadvantages (–):

In the general case for arbitrary mesh;

(+) small size of matrix for special mesh choice and fast calculation for ground state only,
(–) unsymmetric matrix B.

$$-A^{-1}H\varphi_{KL} + \frac{1}{\rho_i^2}(K+3/2)(K+5/2)\varphi_{KL} + \varphi_{KL'}(\rho_i)\frac{2}{\hbar^2}U_{KK}^{LL}(\rho) + \sum_{K'\neq K, L'\neq L}\varphi_{K'L'}(\rho_i)\frac{2}{\hbar^2}U_{KK'}^{LL'}(\rho) = \frac{2}{\hbar^2}E\varphi_{KL}$$

$$B\Phi = \lambda\Phi$$

Energies are eigenvalues of matrix B [2].
Wave functions are eigenvectors of matrix B [2].

For equidistant mesh
(+) symmetric matrix B,
(+) for ground and exited states calculation,
(–) large size of matrix.

1. G. I. Marchuk, Methods of Computational Mathematics (Nauka, Moscow, 1980).
2. J.H. Wilkinson, C. Reinsch. Handbook for Automatic Computation. Linear Algebra.

2.4. HSF test: Exactly solvable 3-Body harmonic oscillator (HO) models

Three particles with masses $m_1 = m_3 = m$, $m_2 = \infty$ interact with each other by oscillator potentials:

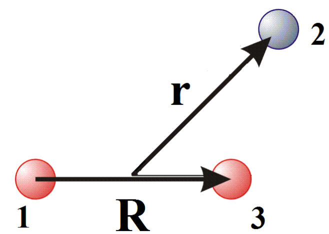
$$V_{13}(r) = \frac{m\omega_{13}^2}{2} r^2 \quad V_{12}(r) = \frac{m\omega_{12}^2}{2} r^2 \quad V_{23}(r) = \frac{m\omega_{23}^2}{2} r^2$$

Normalized Jacobi coordinates {**x**,**y**}:

$$1/\mu = 1/m + 1/m = 2/m \qquad 1/M = 1/\infty + 1/2m = 1/2m$$

$$\mu = m/2 \qquad M = 2m$$

$$\mathbf{R} = \mathbf{r}_3 - \mathbf{r}_1 = \sqrt{2}\mathbf{x} \qquad \mathbf{r} = \frac{1}{\sqrt{2}}\mathbf{y}$$



$$m = 1,\ \hbar = 1$$

The frequencies of the normal modes are equal to Ω_1, Ω_2.

$$\Omega_{1,2}^2 = \frac{\omega_{12}^2 + \omega_{23}^2 + 2\omega_{13}^2 \pm \sqrt{\left(\omega_{12}^2 + \omega_{23}^2 + 2\omega_{13}^2\right)^2 - 4\left(\omega_{13}^2\omega_{23}^2 + \omega_{13}^2\omega_{12}^2 + \omega_{12}^2\omega_{23}^2\right)}}{2}$$

In the case of $\omega_{23} = \omega_{12}$

$$E_0 = \hbar\Omega_1 \frac{3}{2} + \hbar\Omega_2 \frac{3}{2}$$

$$\Omega_1 = \sqrt{\omega_{12}^2 + 2\omega_{13}^2},\ \Omega_2 = \omega_{12}$$

For instance:

$$\omega_{12} = \omega_{23} = \omega_{13} = 1$$

$$\Omega_1 = \sqrt{1+2} = \sqrt{3},\ \Omega_2 = 1$$

$$E_0 = \frac{3}{2}\left(1 + \sqrt{3}\right) = 4{,}098$$

$$\omega_{12} = \sqrt{2};\ \omega_{23} = \frac{1}{\sqrt{2}};\ \omega_{13} = 1 \qquad E_0 = 4.306$$

K_{max} (ρ_{max} =5, $\Delta\rho$=0.05)	E_0
6	4.1082
8	4.0992
14	4.0988
16	4.0988

HSF+spline algorithm has fast converge for increasing K_{max} value

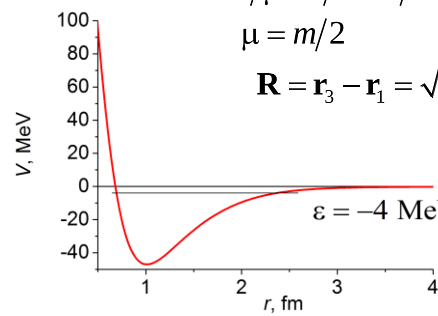
K_{max} (ρ_{max} =10, $\Delta\rho$=0.05)	E_0
6	4.31187
8	4.3071
12	4.3070
16	4.3070

3.1. FCI & HSF calculations for “exactly” solvable 3-Body nucleon model: algorithm convergence

In the system of the particles with masses $m_1=m_3=m$, $m_2=\infty$, light particles 1, 3 interact only with heavy particle 2 by nucleon-nucleon potential having repulsive core.

$$V_{12}(r) \equiv V_{23}(r) = \sum_{k=1}^{3} u_k \exp\left(-r^2/b_k^2\right)$$

The radial Schrödinger equation was solved “exactly” by difference scheme for 2-body system 1 and 2 particles. The energy is equal to –4 MeV

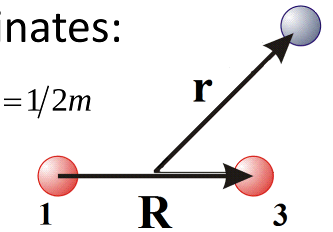


Normalized Jacobi coordinates:

$$1/\mu = 1/m + 1/m = 2/m \qquad 1/M = 1/\infty + 1/2m = 1/2m$$

$$\mu = m/2 \qquad M = 2m$$

$$\mathbf{R} = \mathbf{r}_3 - \mathbf{r}_1 = \sqrt{2}\mathbf{x} \qquad \mathbf{r} = \frac{1}{\sqrt{2}}\mathbf{y}$$



Hyperspherical functions (HSF+spline):

K_{max} (ρ_{max} =10, $\Delta\rho$=h=0.1)	E_0
6	-6.350
16	-7.616
24	-7.861
32	-7.942
40	-7.970
48	-7.973
56	-7.981

The energy of the independent light particles 1, 3 in the field of heavy particle 2 is equal to the sum of energies of particles 1 and 2,

exact result

$$E_0 = -8 \text{ MeV}$$

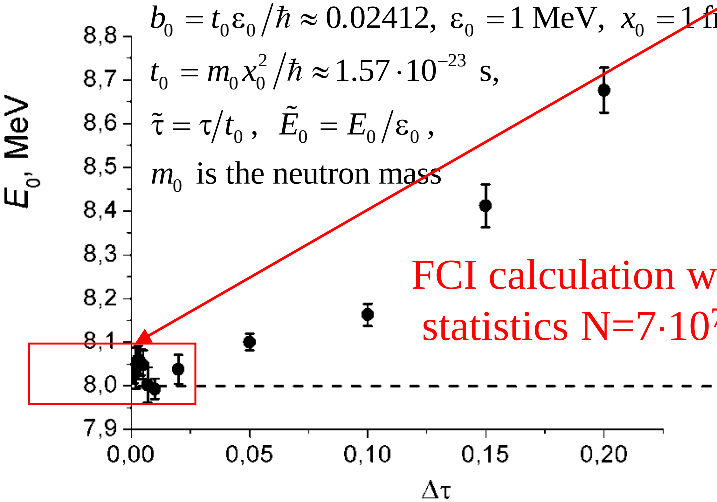
$$b_0^{-1} \ln K_E(q,\tau;q,0) \to \ln\left|\Psi_0(q)\right|^2 - \tilde{E}_0\tilde{\tau},\ \tilde{\tau} \to \infty$$

$b_0 = t_0\varepsilon_0/\hbar \approx 0.02412$, $\varepsilon_0 = 1$ MeV, $x_0 = 1$ fm,

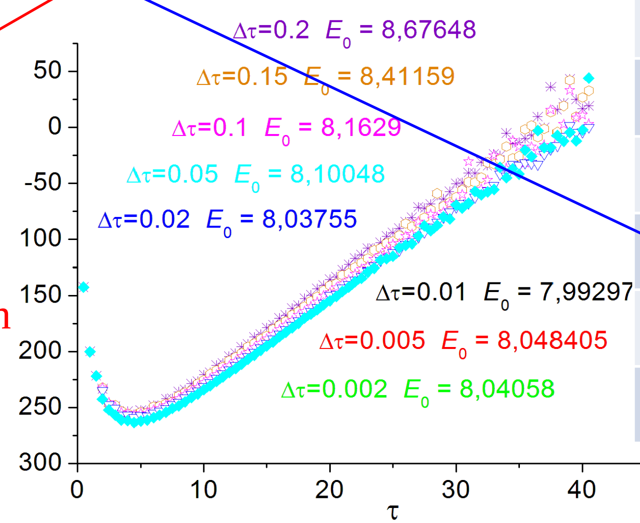
$t_0 = m_0 x_0^2/\hbar \approx 1.57\cdot 10^{-23}$ s,

$\tilde{\tau} = \tau/t_0$, $\tilde{E}_0 = E_0/\varepsilon_0$,

m_0 is the neutron mass



FCI calculation with statistics N=7·10^7

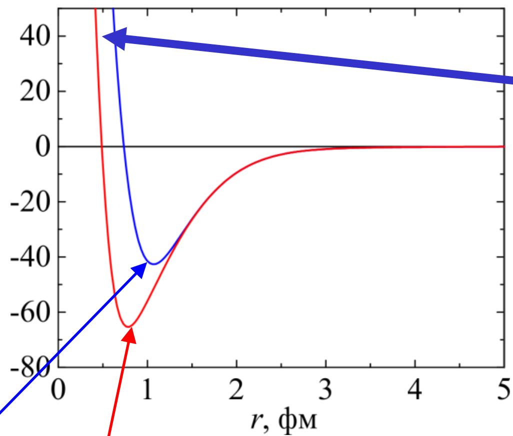


Both methods reproduce exact result

3.2. Unified set of effective two-body central potentials

Nucleon-nucleon

$V_{p-n}(r),\ V_{n-n}(r) \equiv V^{(\mathrm{N})}_{p-p}(r)$, MeV



The repulsive core is the typical property of nucleon-nucleon, nucleon-cluster and cluster-cluster potentials

$$V_{n-n}(r) \equiv V^{(\mathrm{N})}_{p-p}(r) = \sum_{k=1}^{3} u'_k \exp\left(-r^2/b'^2_k\right)$$

$$V_{p-n}(r) = \sum_{k=1}^{3} u_k \exp\left(-r^2/b^2_k\right),$$

$$V_{p-p}(r) = V^{(\mathrm{N})}_{p-p}(r) + V^{(\mathrm{C})}_{p-p}(r), \qquad V^{(\mathrm{C})}_{p-p}(r) = \frac{e^2}{\sqrt{r^2+\delta^2}},\ \delta = 0.01\ \mathrm{fm}$$

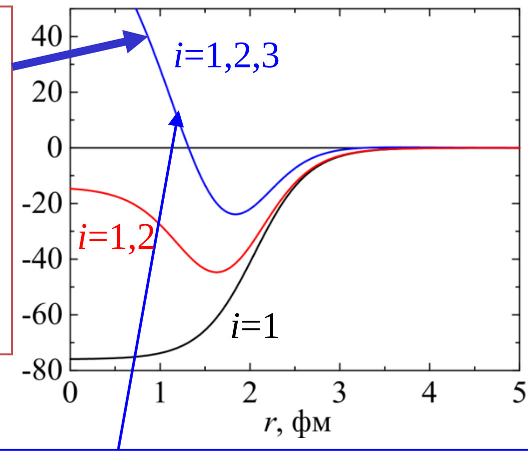
Model parameters

$u'_1 = u_1 = 500,\ u'_2 = u_2 = -102,\ u'_3 = u_3 = -2,$

$b'_1 = 0.53,\ b_1 = 0.37,\ b'_2 = b_2 = 1.26,\ b'_3 = b_3 = 2.67.$

Nucleon-alpha-cluster

$V_{n-\alpha}(r) = V^{(\mathrm{N})}_{p-\alpha}(r)$, MeV



$$V_{n-\alpha}(r) = V^{(\mathrm{N})}_{p-\alpha}(r) = \sum_{i=1}^{3} U_i \left[1+\exp\left((r-R_i)/a_i\right)\right]^{-1}$$

$$V_{p-\alpha}(r) = V^{(\mathrm{N})}_{p-\alpha}(r) + V^{(\mathrm{C})}_{p-\alpha}(r)$$

$$V^{(\mathrm{C})}_{p-\alpha}(r) = \begin{cases} \dfrac{2e^2}{2R_\alpha}\left[3-\left(\dfrac{r}{R_\alpha}\right)^2\right], & r \le R_\alpha \\[2ex] \dfrac{2e^2}{r}, & r > R_\alpha \end{cases}$$

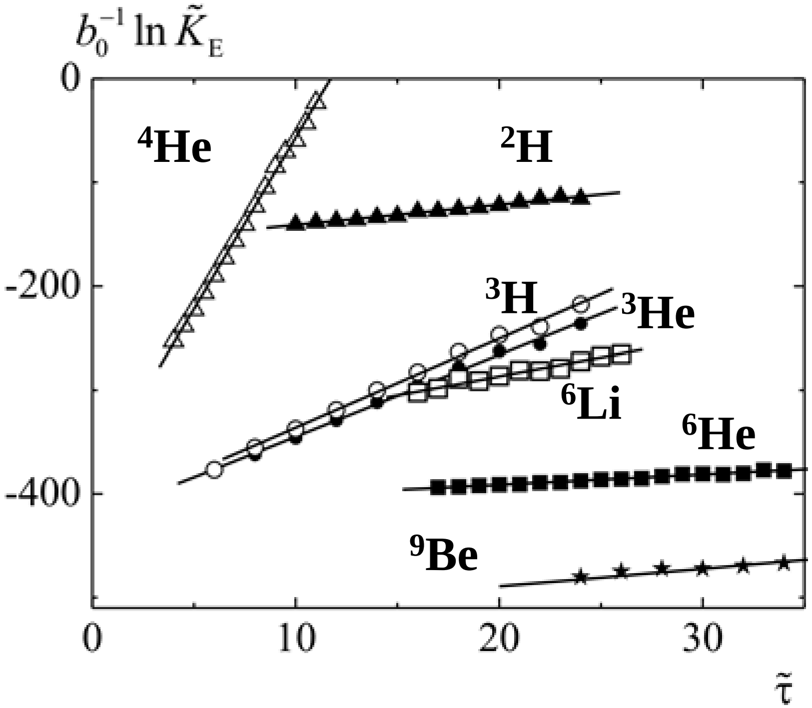
R_α = 1.6755 fm;

U_1 = -76 MeV, R_1 = 2.05 fm, a_1 = 0.3 fm;
U_2 = 62 MeV, R_2 = 1.32 fm, a_2 = 0.3 fm;
U_3 = 112 MeV, R_3 = 1 fm, a_3 = 0.5 fm.

3.3. Results of calculation of binding energies for nuclei ^{2}H, $^{3,4,6}He$, ^{6}Li, ^{9}Be with unified set of effective two-body central potentials

$$b_0^{-1} \ln K_E\left(q,\tau;q,0\right) \rightarrow \ln\left|\Psi_0(q)\right|^2 - \tilde{E}_0\tilde{\tau},\ \tilde{\tau}\rightarrow\infty$$

slope coefficient gives ground state energy



Comparison of theoretical and experimental binding energies in unified set of potentials

(*for alpha-cluster nuclei ^{6}He, ^{9}Be energy of separation into alpha particles and nucleons is given).

Atomic nucleus	Theoretical value, MeV	Experimental value [1], MeV
^{2}H	2.22 ± 0.15	2.225
^{3}H	8.21 ± 0.3	8.482
^{3}He	7.37 ± 0.3	7.718
^{4}He	30.60 ± 1.0	28.296
^{6}He*	0.96 ± 0.05	0.97542
^{6}Li*	3.87 ± 0.2	3.637
$^{9}Be^{*}$	1.573	1.7 ± 0.1

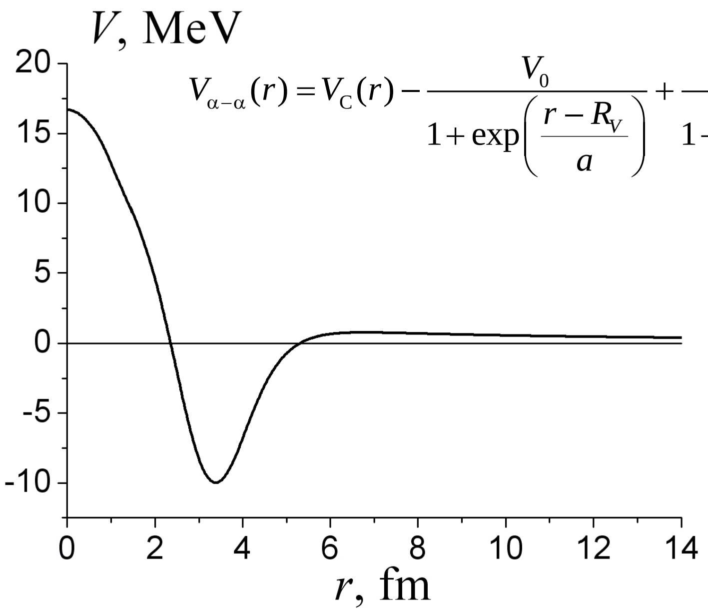
Good agreement with experimental data

[1] NRV web knowledge base on low-energy nuclear physics. URL: http://nrv.jinr.ru/

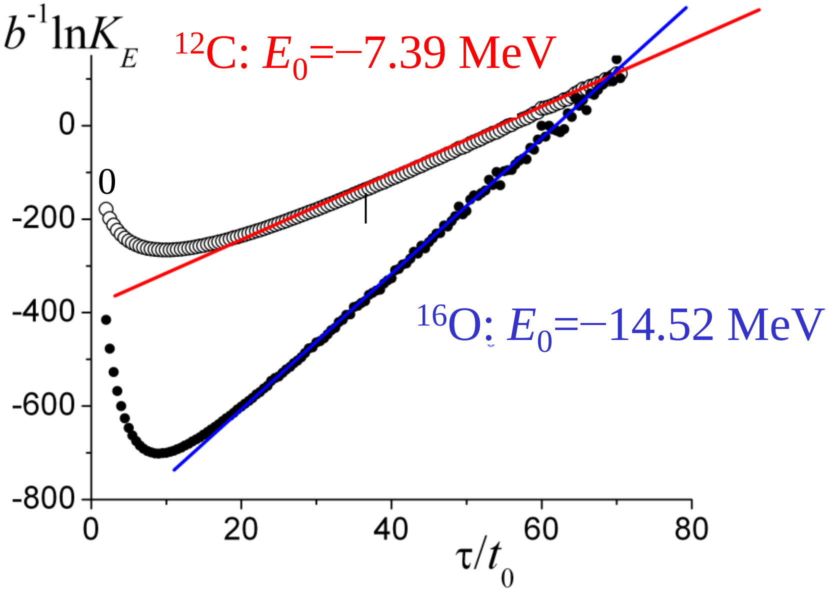
3.4. α–α potential $V_{\alpha-\alpha}(r)$ and ground state energy E_0 of ^{12}C (α + α + α) and ^{16}O (α + α + α + α)

Energy of breakup into α-particles is equal to $-E_0$, where E_0 is the energy of the ground state of α-cluster system.

Experimental breakup energy is equal to 7.37 MeV for ^{12}C and 14.53 MeV for ^{16}O.



$$V_{\alpha-\alpha}(r) = V_C(r) - \frac{V_0}{1+\exp\left(\frac{r-R_V}{a}\right)} + \frac{U_0}{1+\exp\left(\frac{r-R_W}{b}\right)}$$



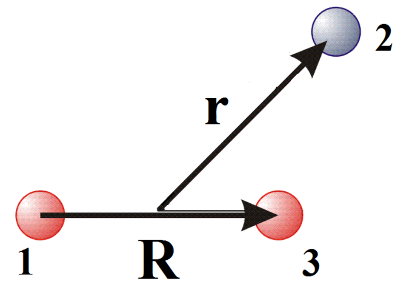
The slope of resulting straight lines equals the energy of the ground state

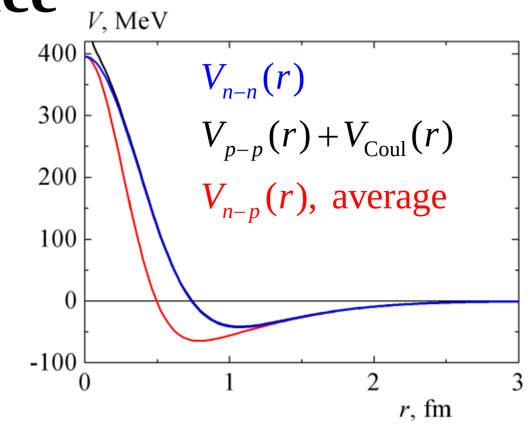
$$\frac{1}{b_0}\ln\tilde{K}_E(q,\tau;q,0) \to \frac{1}{b_0}\ln|\Psi_0(q)|^2 - E_0\tilde{\tau},\ \tilde{\tau}\to\infty$$

$b_0 = t_0\varepsilon_0/\hbar \approx 0.02412,\ \varepsilon_0 = 1$ MeV, $x_0 = 1$ fm, $t_0 = m_0 x_0^2/\hbar \approx 1.57\cdot 10^{-23}$ s,

$\tilde{\tau} = \tau/t_0$, $\tilde{E}_0 = E_0/\varepsilon_0$, m_0 is the neutron mass

3.5. Calculations for ^3H nucleus: FCI & HSF algorithms convergence



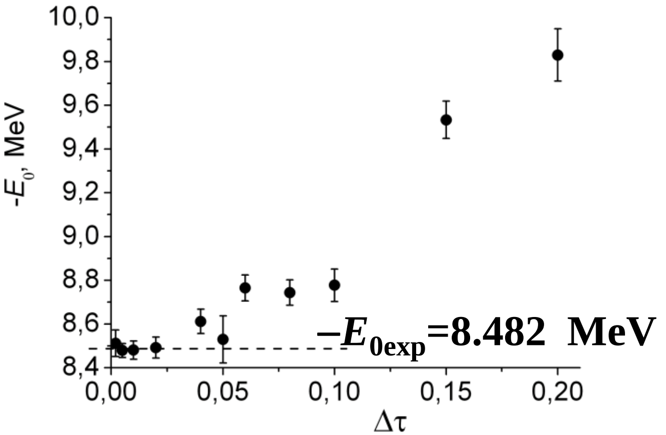


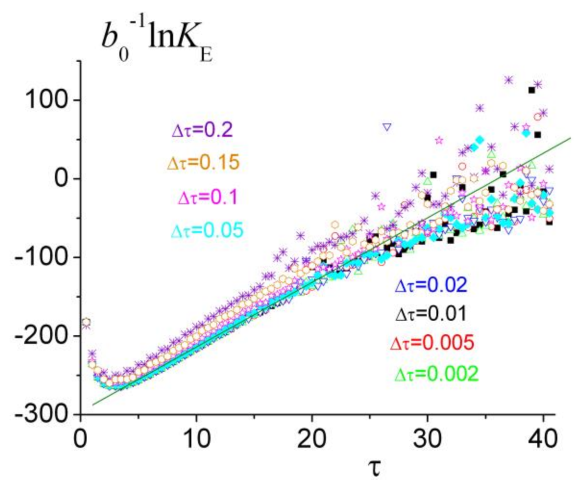
FCI: Monte-Carlo calculation with statistics $N=7\cdot10^7$

$$b_0=t_0\varepsilon_0/\hbar\approx0.02412,\ \varepsilon_0=1\text{ MeV},\ x_0=1\text{ fm},$$
$$t_0=m_0x_0^2/\hbar\approx1.57\cdot10^{-23}\text{ s},\ \tilde{\tau}=\tau/t_0,\ \ \tilde{E}_0=E_0/\varepsilon_0,$$

m_0 is the neutron mass

$$b_0^{-1}\ln K_E(q,\tau;q,0)\to\ln\left|\Psi_0(q)\right|^2-\tilde{E}_0\tilde{\tau},\ \tilde{\tau}\to\infty$$





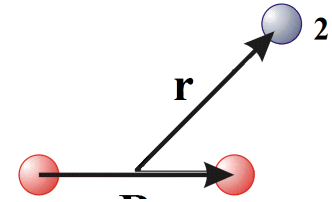
$-E_{0\text{exp}}$=8.482 MeV

Hyperspherical Functions (HSF+spline):

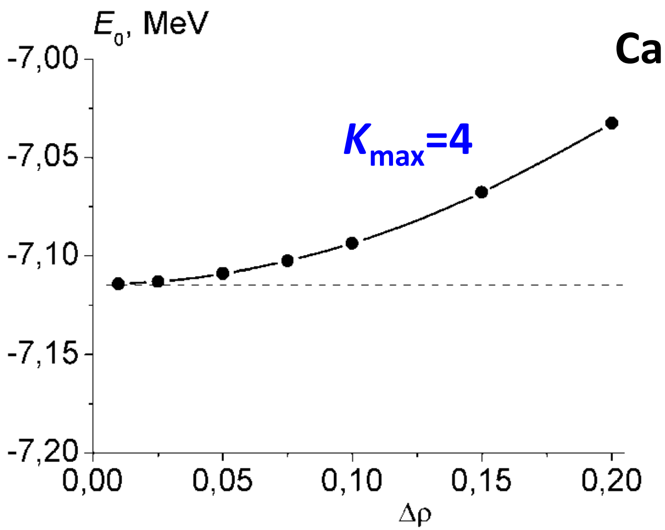
K_{max} (ρ_{max} =10, $\Delta\rho$=0.05)	E_0
6	-7,153
8	-8,480
16	-8,134
24	-8,330
32	-7.384
40	-8.407
48	-8.417

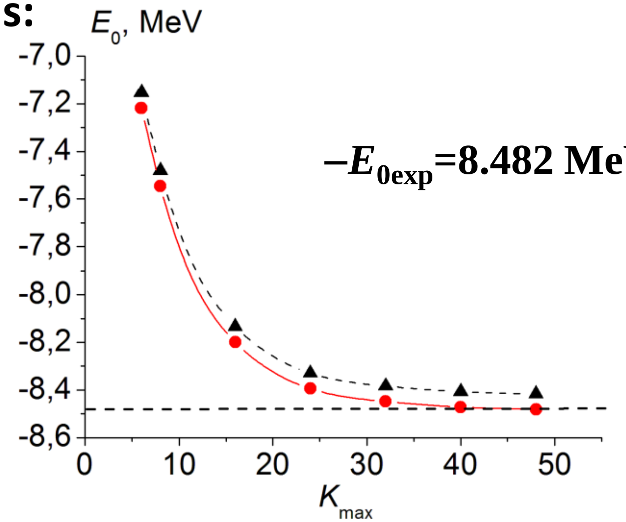
Both methods reproduce the experimental result

3.6. HSF algorithm convergence



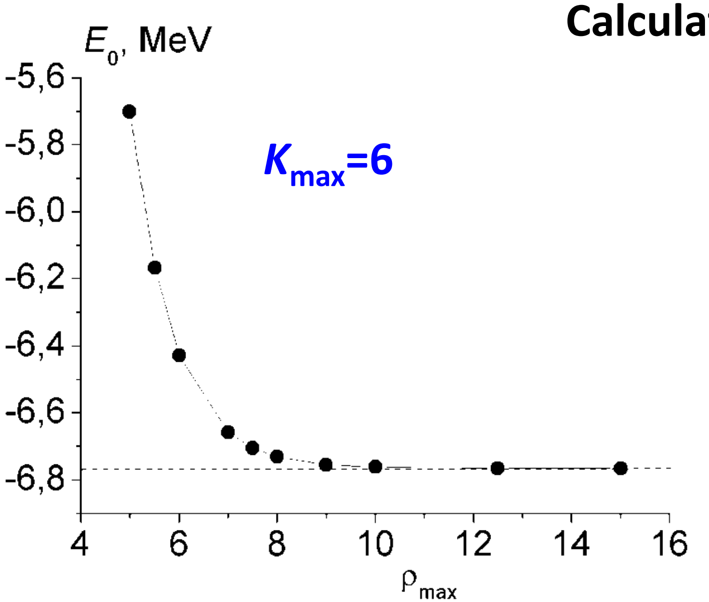
Calculations for ³H nucleus:

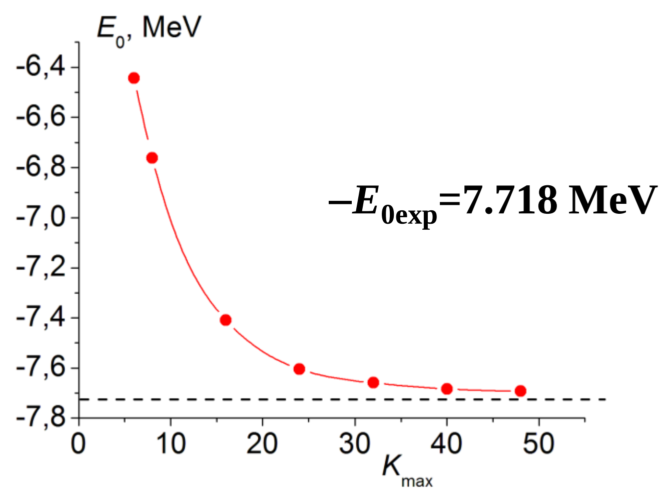




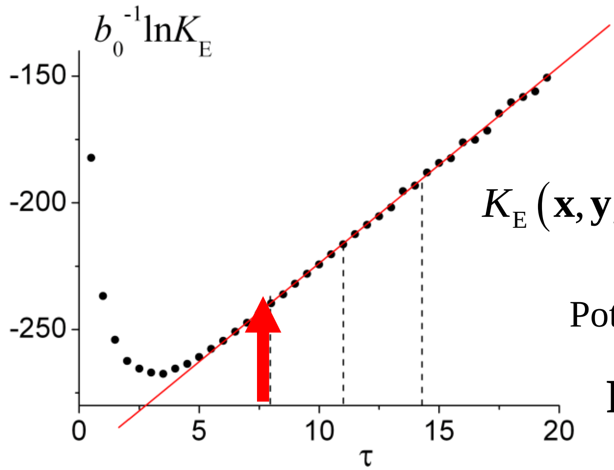
HSF+spline method reproduces the experimental result

Calculations for ³He nucleus





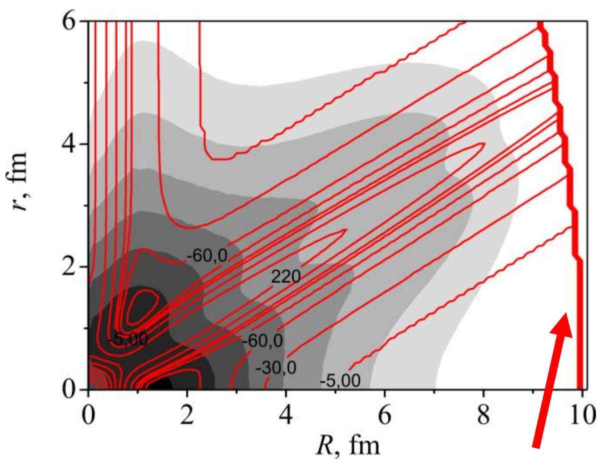
3.7. FCI: Propagator K_E and probability density $|\Psi_0|^2$ for ground state of ^{3}He ($p + p + n$)

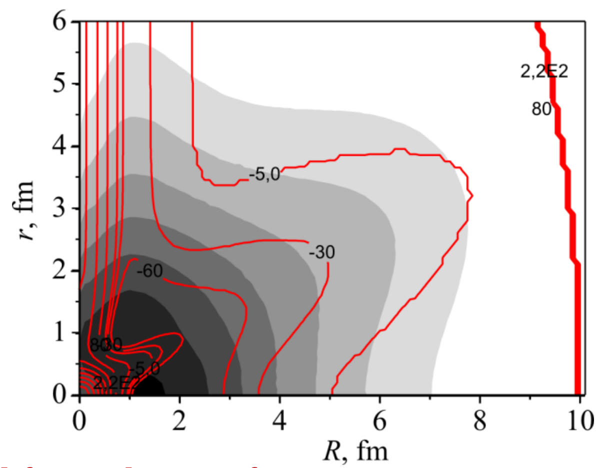


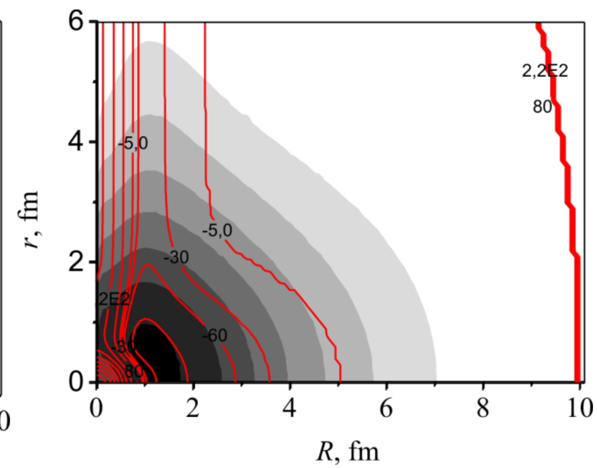
$$K_E(\mathbf{x},\mathbf{y},\tau;\mathbf{x},\mathbf{y},0) \to |\Psi_0(\mathbf{x},\mathbf{y},)|^2 \exp\left(-\frac{E_0\tau}{\hbar}\right) + |\Psi_1(\mathbf{x},\mathbf{y},)|^2 \exp\left(-\frac{E_1\tau}{\hbar}\right) + \ldots,\ \tau \to \infty$$

Potential wall at r_i =5 fm for excluding excitation of breakup states.

Probability density $|\Psi|^2$ is consistent with potential landscape

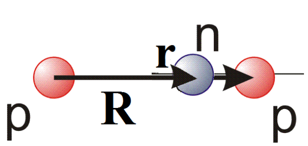


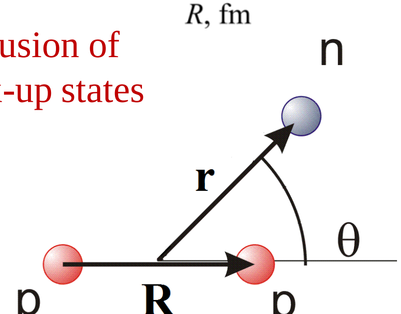


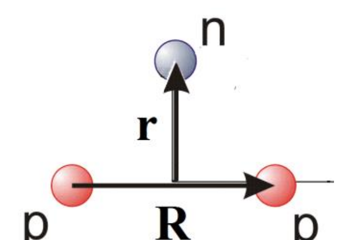


Potential wall for exclusion of the excitation of break-up states

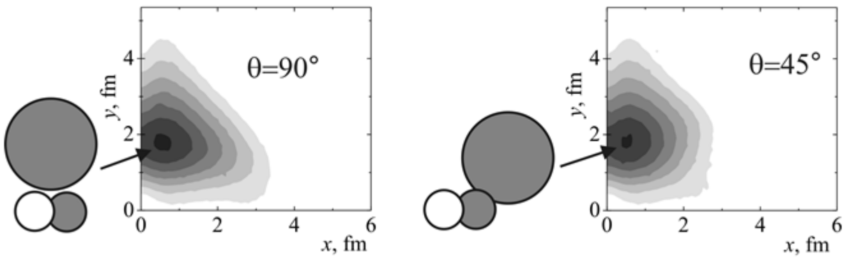
Logarithmic scale



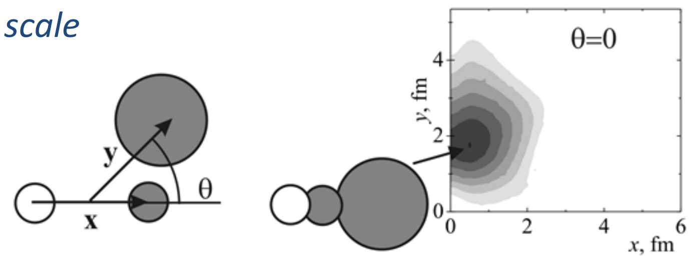


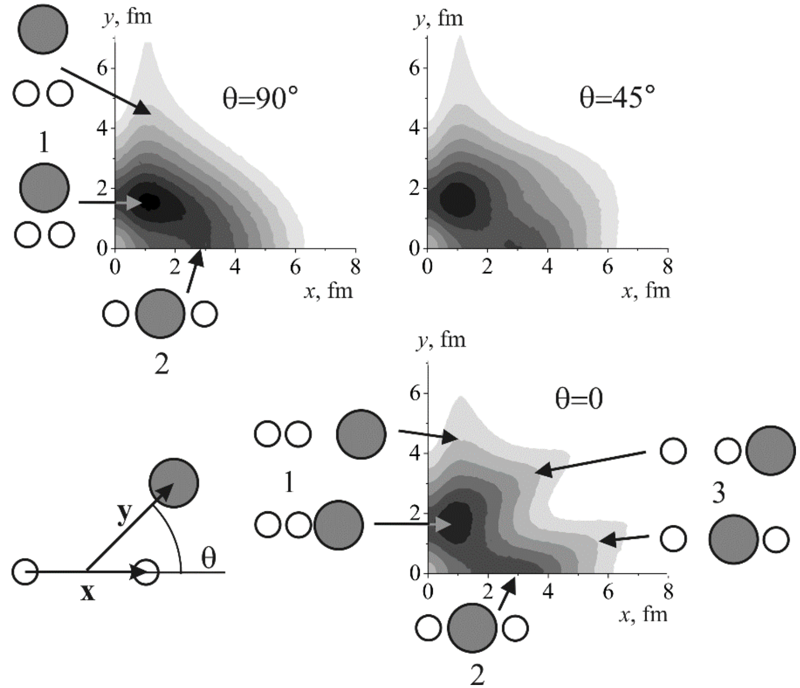


3.8. FCI 3-body: Comparison of the probability densities $|\Psi|^2$ for ground states of ^{6}Li ($\alpha + n + p$) and ^{6}He ($\alpha + n + n$)



Logarithmic scale





The probability density $|\Psi_0|^2$ for the ^{6}Li nucleus and the vectors in the Jacobi coordinates; neutrons and α-clusters are denoted as small empty circles and large filled circles, protons are denoted as small filled circles. The only one possible configuration is α-cluster + deuteron-cluster [1,2]; $E_{\alpha+n+p,\mathrm{sep}}$=3.64 MeV.

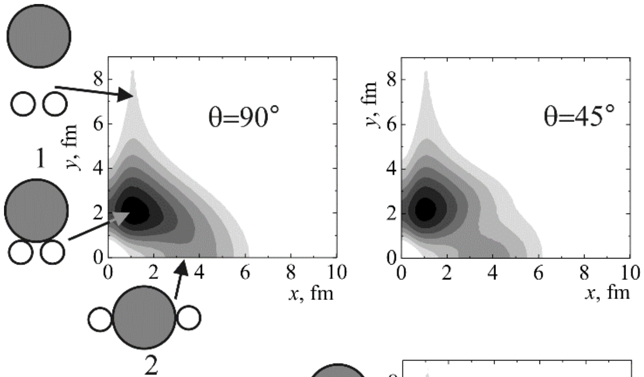
The probability density $|\Psi_0|^2$ for the ^{6}He nucleus and the vectors in the Jacobi coordinates; neutrons and α-clusters are denoted as small empty circles and large filled circles, respectively. The most probable configurations are α-cluster + dineutron (1) and the cigar configuration (2). The configuration n + ^{5}He (3) has low probability [1,2]; $E_{\alpha+n+n,\mathrm{sep}}$=0.98 MeV.

Feynman's Continual Integrals (FCI) method [1,2] was used.

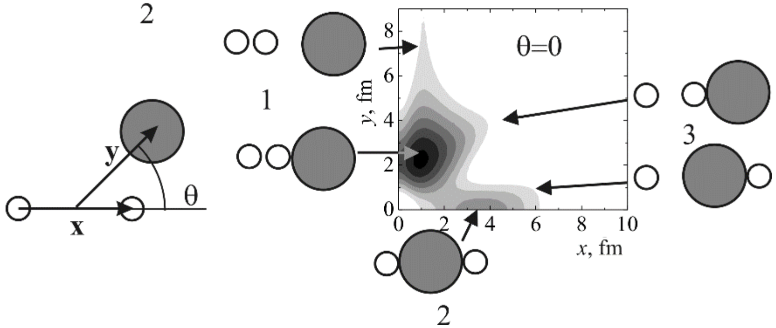
[1] V. Samarin *et al.*, Proc. Int. Symp. on Exotic Nuclei. (Kazan, Russia, Sept. 2016) World Scientific. Singapore. p. 93 (2017).

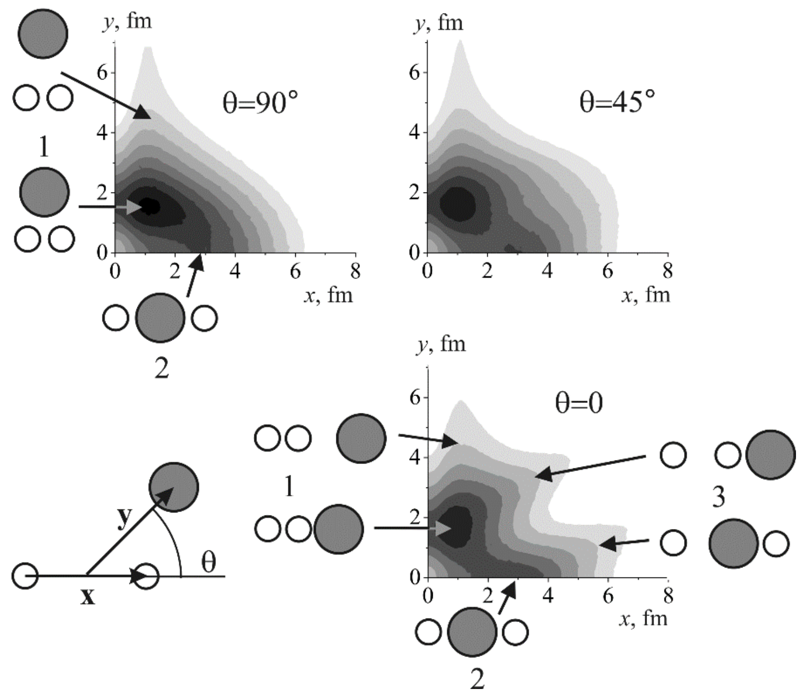
[2] V. Samarin *et al.*, Phys. Atom. Nucl., **80**, 928 (2017).

3.9. Comparison of the probability densities $|\Psi|^2$ for ground states of ^{11}Li ({^{9}Li } + n + n) and ^{6}He (α + n + n)



Central and far parts of halo are mainly composed of loose di-neutron cluster.





The probability density $|\Psi_0|^2$ for the ^{11}Li nucleus (configuration {^{9}Li} + n + n) and the vectors in the Jacobi coordinates; neutrons and ^{9}Li-core are denoted as small empty circles and large filled circles, respectively. The most probable configurations are {^{9}Li} + di-neutron (1) and the cigar configuration (2).

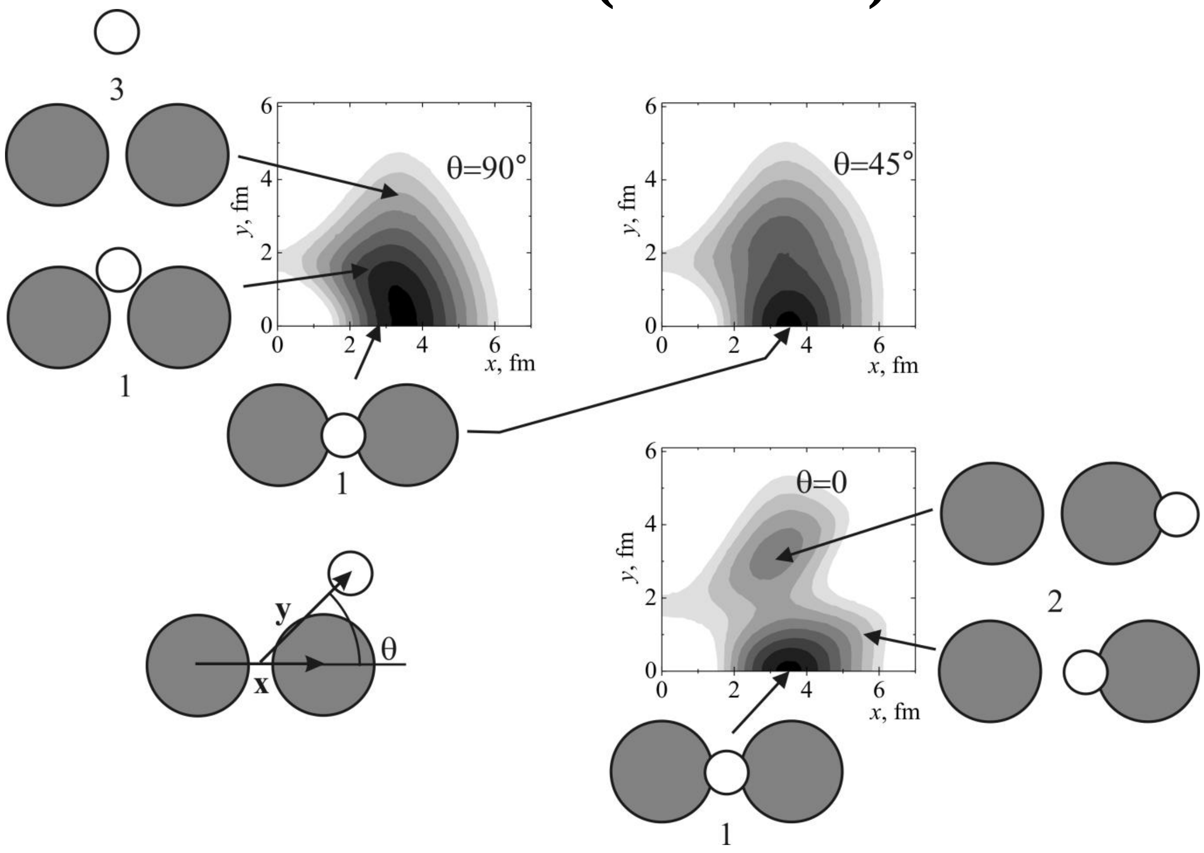
The configuration ^{10}Li + n (3) has low probability; $E_{\{9\mathrm{Li}\}+n+n,\mathrm{sep}}$=0.37 MeV [1].

The probability density $|\Psi_0|^2$ for the ^{6}He nucleus and the vectors in the Jacobi coordinates; neutrons and α-clusters are denoted as small empty circles and large filled circles, respectively. The most probable configurations are α-cluster + dineutron (1) and the cigar configuration (2). The configuration n + ^{5}He (3) has low probability; $E_{\alpha+n+n,\mathrm{sep}}$=0.98 MeV

Approximation of independent outer neutrons of ^{9}Li and ^{11}Li was used.

[1] V. Samarin *et al*., Book of Abstracts of LXVIII Int. Conf. Nucleus-2018 (Voronezh, Russia, July 2018). Saint-Petersburg (2018).

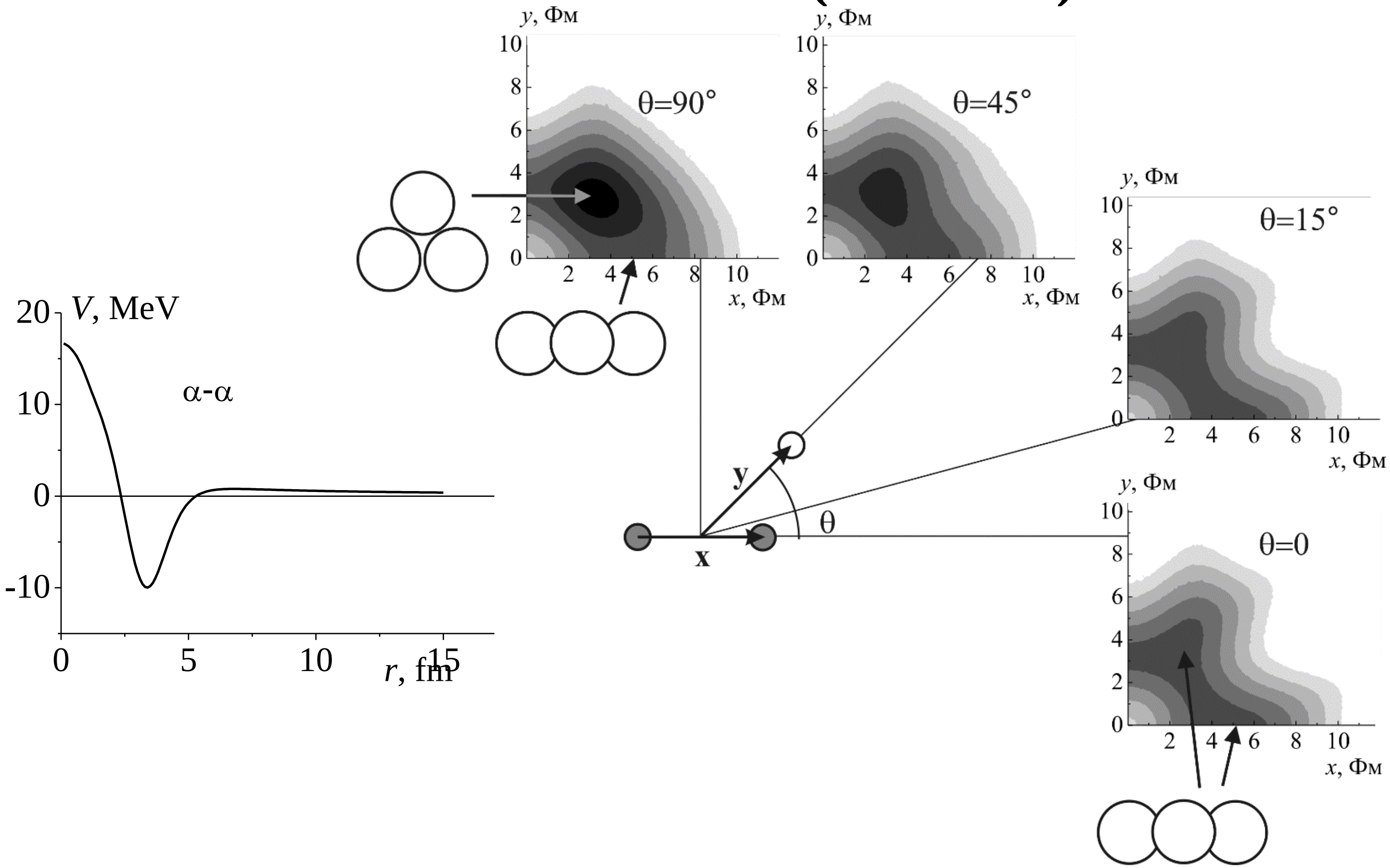
3.10. FCI 3-body: Probability density $|\Psi|^2$ for ground state of ^{9}Be ($\alpha + \alpha + n$)



The probability density $|\Psi_0|^2$ for the ^{9}Be nuclei and the vectors in the Jacobi coordinates. The most probable configuration is $\alpha + n + \alpha$ (1). The configurations $\alpha + {}^5$He (2) and $n + {}^8$Be (3) are less probable.

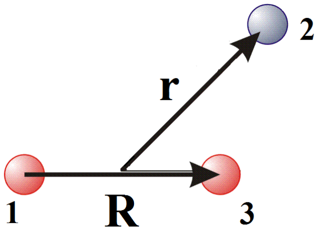
Logarithmic scale

3.11. FCI 3-body: Probability density $|\Psi|^2$ for ground state of ^{12}C ($\alpha + \alpha + \alpha$)

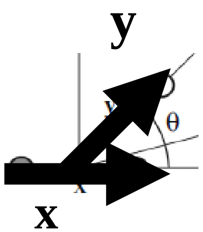


Logarithmic scale

The probability density $|\Psi_0|^2$ for the ^{12}C nucleus and the vectors in the Jacobi coordinates. The alpha-particle clusters being considered are represented by circles of radius equal to the root-mean-square radius of the ^4He nucleus (1.7 fm). A regular triangle configuration is the most probable, a linear configuration having a low probability.



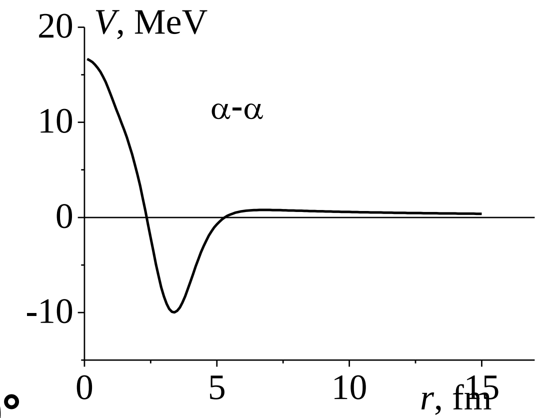
3.12. Calculations for ^{12}C (α+α+α) nucleus: probability density for ground state



Jacobi coordinates:

$$\mathbf{R} = \mathbf{r}_3 - \mathbf{r}_1$$

$$\mathbf{r} = \mathbf{r}_2 - \frac{\mathbf{r}_1 + \mathbf{r}_3}{2}$$

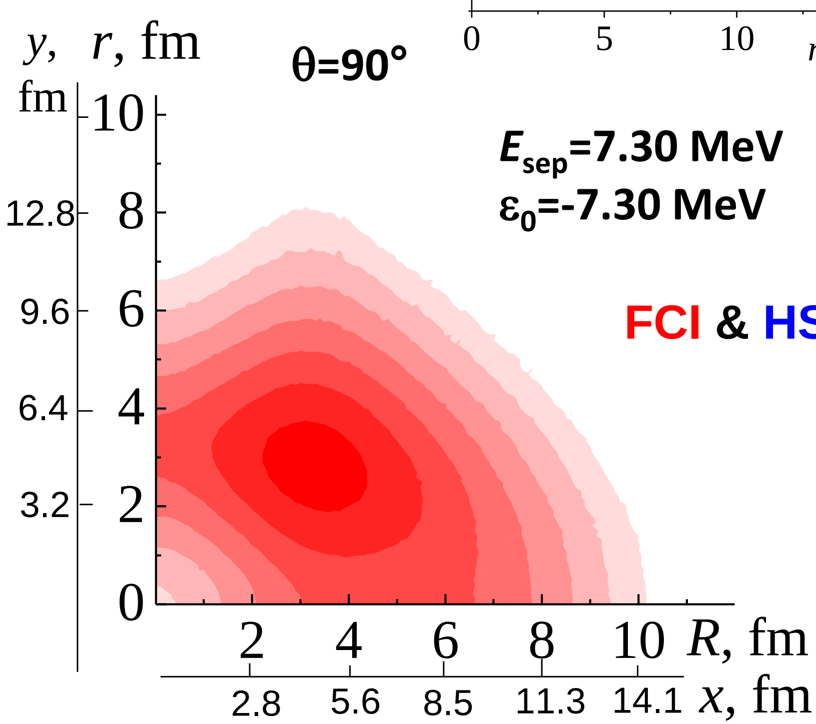


Normalized Jacobi coordinates:

$$\mathbf{x} = \sqrt{2m}\left(\mathbf{r}_3 - \mathbf{r}_1\right) = \mathbf{R}\sqrt{2m} \approx 1.4\mathbf{R}\sqrt{m}$$

$$\mathbf{y} = \sqrt{\frac{8m}{3}}\left(\mathbf{r}_2 - \frac{\mathbf{r}_1 + \mathbf{r}_3}{2}\right) = \mathbf{r}\sqrt{\frac{8m}{3}} \approx 1.6\mathbf{r}\sqrt{m}$$

in the system of units with m=1

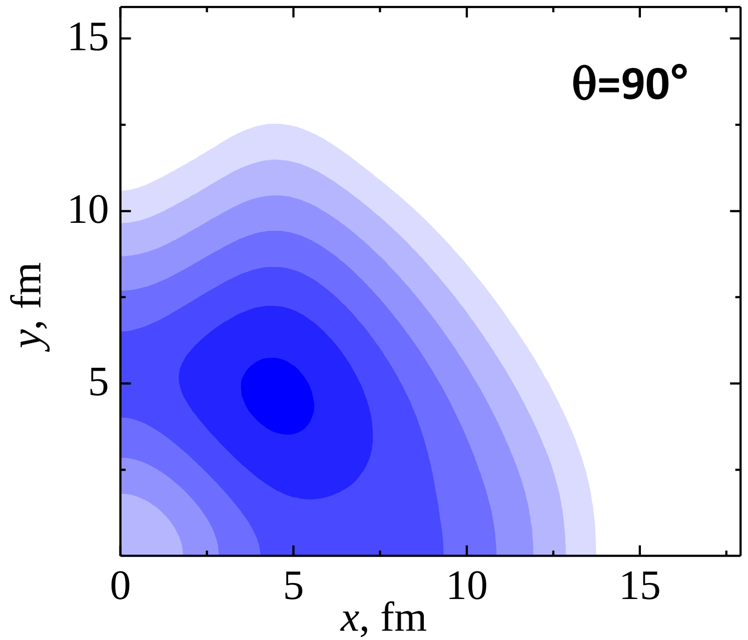


E_{sep}=7.30 MeV

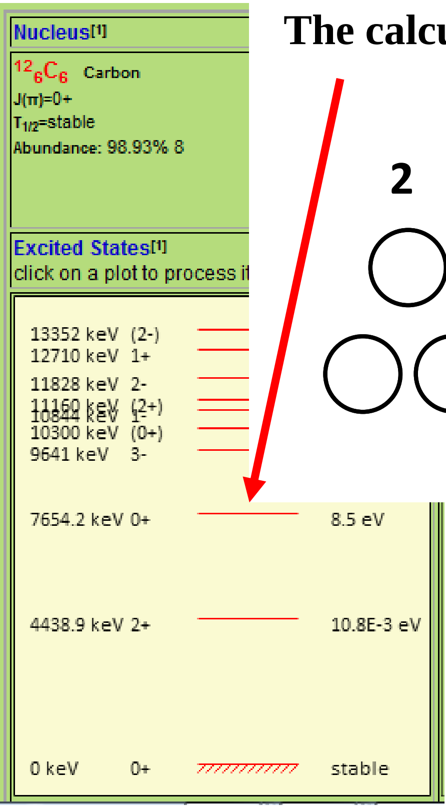
ε_0=-7.30 MeV

FCI & HSF

Hyperspherical functions (HSF+spline):

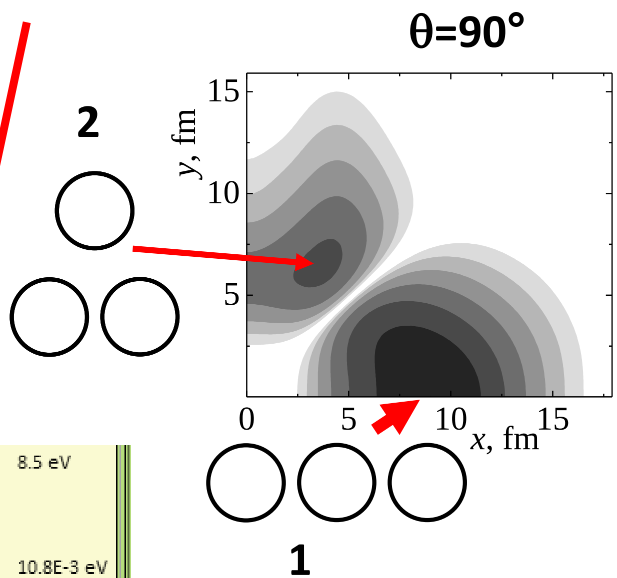


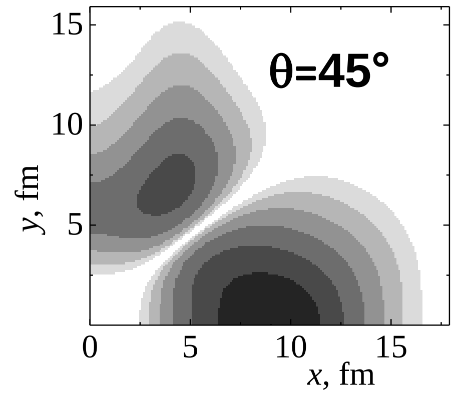
3.13. HSF calculations for ^{12}C ($\alpha+\alpha+\alpha$) nucleus: probability density for excited state with L=0 (Hoyle state)

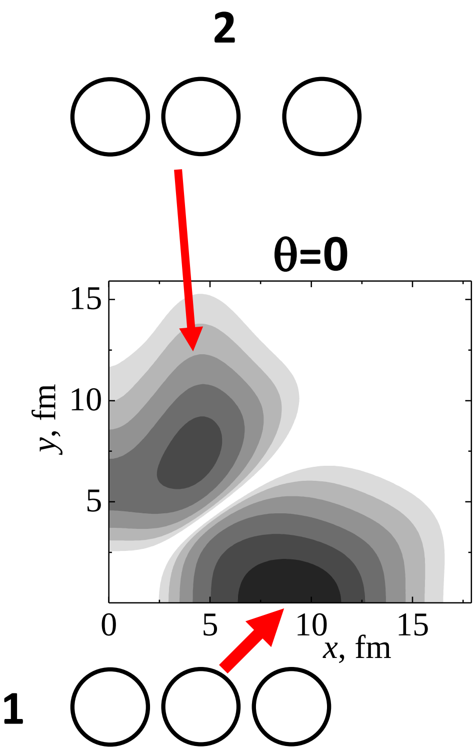


The calculated value of $\varepsilon_1 - \varepsilon_0$=5.38 MeV is less then experimental value 7.65 MeV

Hyperspherical functions (HSF+spline):

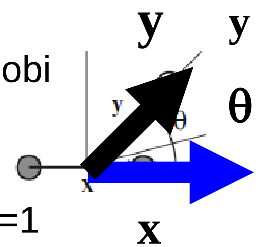






Normalized Jacobi coordinates:

in the system of units with m=1



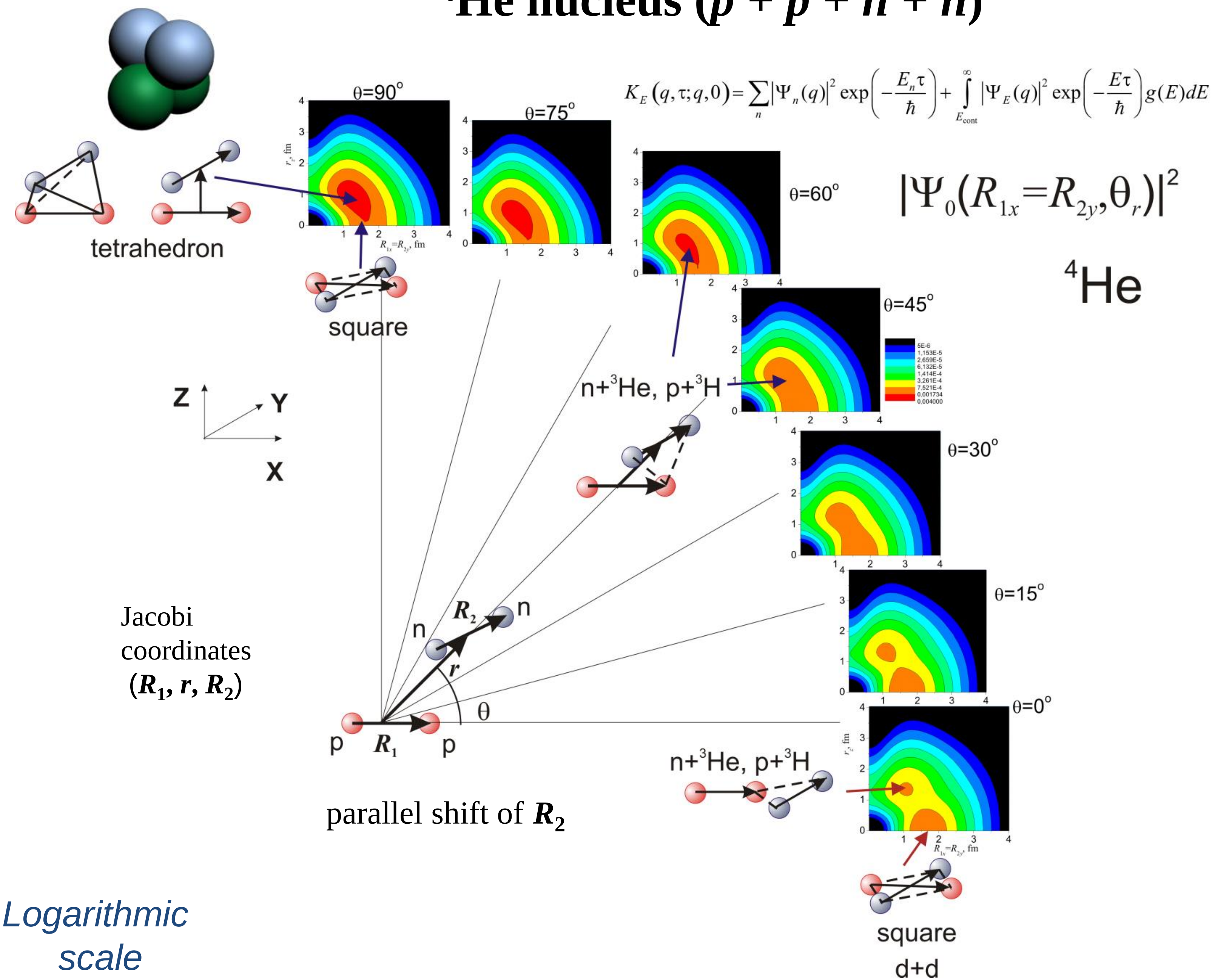
$$\mathbf{y} = \sqrt{\frac{8m}{3}}\left(\mathbf{r}_2 - \frac{\mathbf{r}_1 + \mathbf{r}_3}{2}\right)$$

$$\mathbf{x} = \sqrt{2m}\left(\mathbf{r}_3 - \mathbf{r}_1\right)$$

The probability density $|\Psi|^2$ for the first excited state with total orbital angular momentum L=0 (Hoyle state) of the ^{12}C nucleus and the normalized vectors in the Jacobi coordinates. The alpha-particle clusters being considered are represented by circles of radius equal to the root-mean-square radius of the ^{4}He nucleus (1.7 fm). A linear configuration (1) is the most probable, a triangle configuration (2) (^{8}Be + ^{4}He) has a low probability.

4.1. FCI 4-body: Probability density for ground state of ^4He nucleus ($p + p + n + n$)

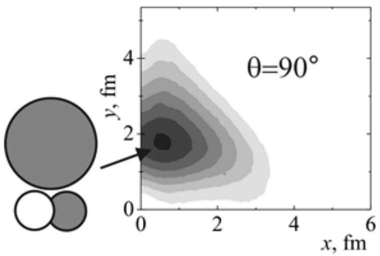
$$K_E(q,\tau;q,0)=\sum_n |\Psi_n(q)|^2 \exp\left(-\frac{E_n\tau}{\hbar}\right)+\int_{E_{\mathrm{cont}}}^{\infty}|\Psi_E(q)|^2 \exp\left(-\frac{E\tau}{\hbar}\right)g(E)dE$$

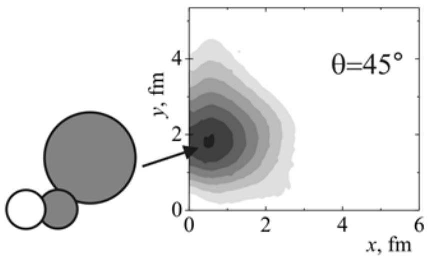


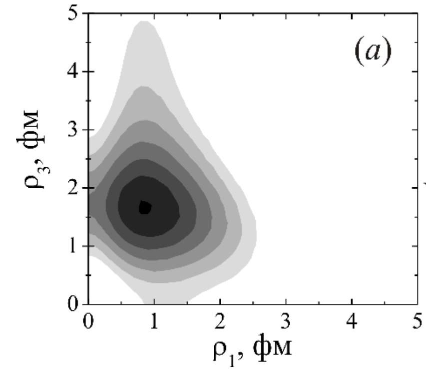
Logarithmic scale

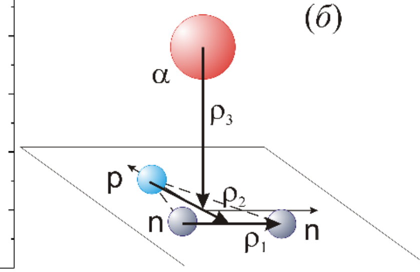
4.2. Comparison of the probability densities $|\Psi|^2$ for ground states of ^{6}Li ($\alpha + n + p$) and ^{7}Li ($\alpha + n + n + p$)

Feynman's Continual Integrals (FCI) method [1-4] was used.

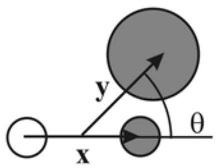


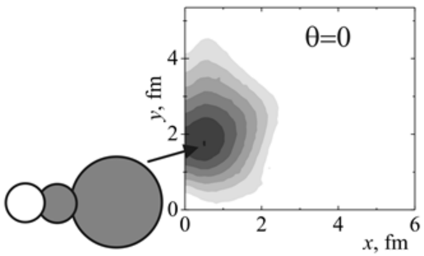


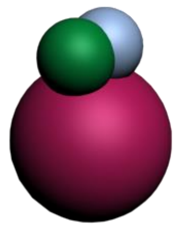




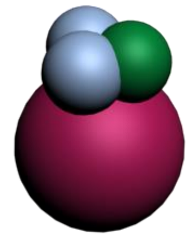
Logarithmic scale



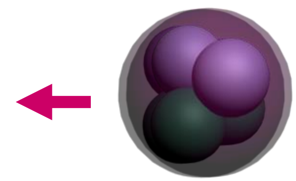




^{6}Li



^{7}Li



^{4}He and α-cluster

The probability density $|\Psi_0|^2$ for the ^{6}Li nucleus and the vectors in the Jacobi coordinates; neutrons and α-clusters are denoted as small empty circles and large filled circles, protons are denoted as small filled circles. The only one possible configuration is α-cluster + deuteron-cluster [1];
$E_{\alpha+n+\boldsymbol{p},\mathrm{sep}}$=3.64 MeV, $E_{\alpha+\boldsymbol{d},\mathrm{sep}}$=1.47 MeV.

The probability density $|\Psi_0|^2$ for the ^{7}Li nucleus and the vectors in the Jacobi coordinates. The most probable configurations are α-cluster + triton [2] ;
$E_{\alpha+n+n+\boldsymbol{p},\mathrm{sep}}$=10.95 MeV, $E_{\alpha+t,\mathrm{sep}}$=2.47 MeV

The outer neutrons in ^{6}Li and ^{7}Li are bound in the positively-charged deuteron and triton clusters.

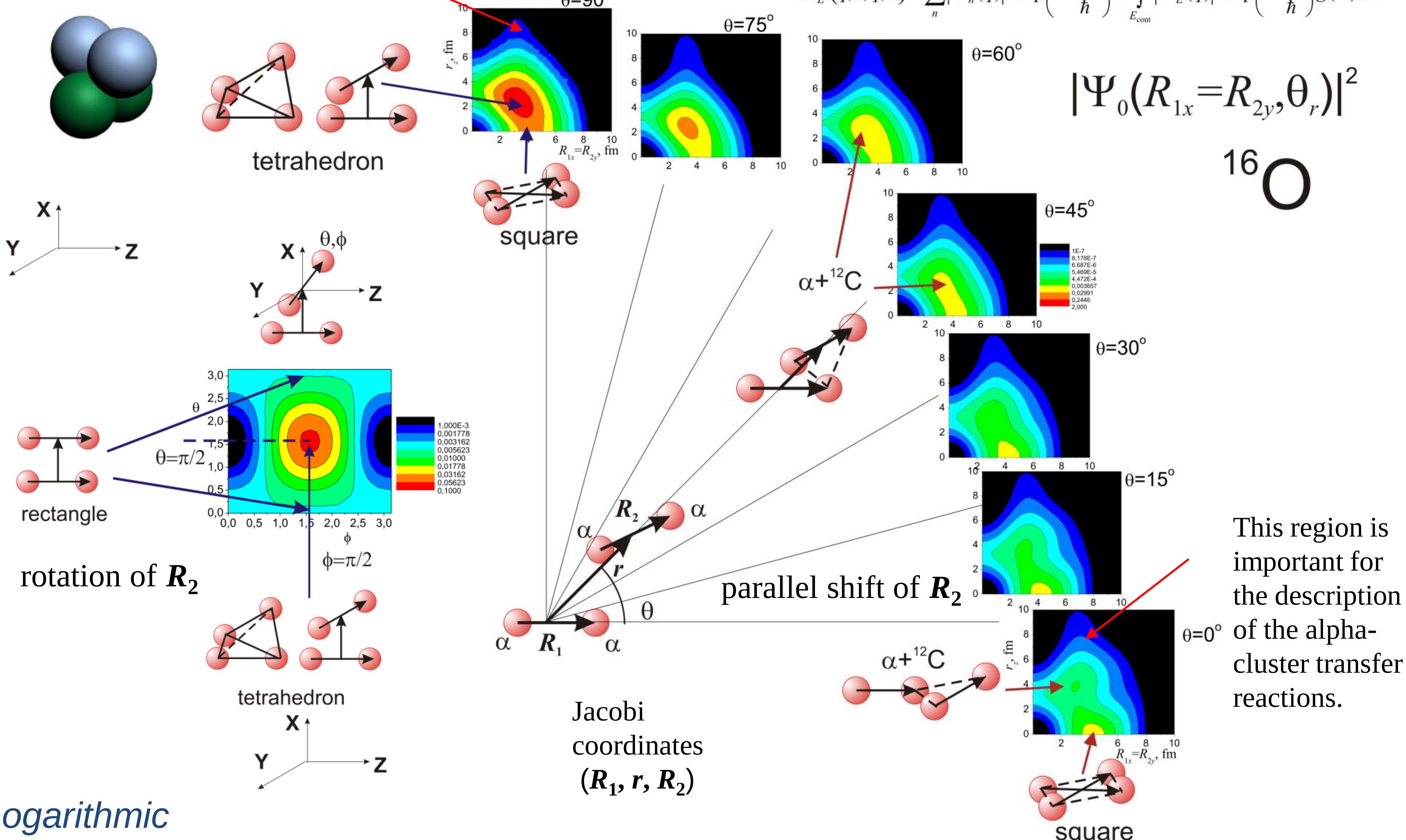
[1] V. Samarin *et al.*, Proc. Int. Symp. on Exotic Nuclei. (Kazan, Russia, Sept. 2016) World Scientific. Singapore. p. 93(2017).
[2] V. Samarin *et al.*, Book of Abstracts of LXVIII Int. Conf. Nucleus-2018 (Voronezh, Russia, July 2018). Saint-Petersburg (2018).
[3] V. Samarin NUCLEAR THEORY, Vol. 36 (2017) eds. M. Gaidarov, N. Minkov, Heron Press, Sofia p. 233.
[4] V. Samarin *et al.*, Phys. Atom. Nucl., **80**, 928 (2017).

4.3. FCI 4-body: Probability density for ground state of ^{16}O ($\alpha + \alpha + \alpha + \alpha$)

This region is important for the description of the one- and two-alpha-cluster transfer reactions and resonances.

$$K_E(q,\tau;q,0)=\sum_n|\Psi_n(q)|^2\exp\left(-\frac{E_n\tau}{\hbar}\right)+\int_{E_{\rm cont}}^{\infty}|\Psi_E(q)|^2\exp\left(-\frac{E\tau}{\hbar}\right)g(E)dE$$

$$|\Psi_0(R_{1x}=R_{2y},\theta_r)|^2$$

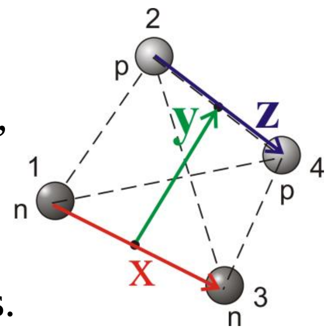


Logarithmic scale

4.4. HSF basics: description of 4-body system

The "normalized" Jacobi coordinates $(\mathbf{x}_i,\mathbf{y}_i)$ are:

$$\mathbf{x}=\sqrt{\frac{m_1m_3}{m_1+m_3}}(\mathbf{r}_3-\mathbf{r}_1),\quad \mathbf{y}_i=\sqrt{\frac{m_i(m_j+m_k)}{m_1+m_2+m_3}}\left(-\mathbf{r}_i+\frac{m_j\mathbf{r}_j+m_k\mathbf{r}_k}{m_j+m_k}\right)\quad z=\sqrt{\frac{m_2m_4}{m_2+m_4}}(\mathbf{r}_4-\mathbf{r}_2),$$



The hyperspherical coordinates are: $\Omega=\{\theta_\mathbf{x},\varphi_\mathbf{x},\theta_\mathbf{y},\varphi_\mathbf{y},\theta_\mathbf{z},\varphi_\mathbf{z},\alpha,\beta\},\rho;$

$$\rho^2=\mathbf{x}^2+\mathbf{y}^2+\mathbf{z}^2,\ |\mathbf{x}|=\rho\sin\beta\cos\alpha,\ |\mathbf{y}|=\rho\sin\beta\sin\alpha, |\mathbf{z}|=\rho\cos\beta$$

ρ is the hyperradius.

The hyperradial equations are:

They are solved using cubic spline approximation

$$\frac{d^2}{d\rho^2}\chi^{l_xl_yl_{xy}l_z}_{\mu KL}(\rho)-\left[\kappa^2+\frac{(\mu+3)(\mu+4)}{\rho^2}\right]\chi^{l_xl_yl_{xy}l_z}_{\mu KL}(\rho)=\sum_{\mu'K'l'_xl'_yl'_{xy}l'_z}W^{l_xl_yl_{xy}l_z;l'_xl'_yl'_{xy}l'_z}_{\mu K\mu'K'}(\rho)\chi^{l'_xl'_yl'_{xy}l'}_{\mu KL}(\rho)$$

$K=l_x+l_y+2n, \mu+3/2=l_z+K+3/2+2m$

$\mu=l_z+K+2m$ is hypermoment, n,m=0,1,2….

The calculation of coupling matrices was implemented using parallel computing.

The coupling matrix is

$$W^{l_xl_yl_{xy}l_z;l'_xl'_yl'_{xy}l'_z}_{\mu K\mu'K'}(\rho)=\frac{2m}{\hbar^2}\int\Psi^{*l_xl_yl_{xy}l_z}_{\mu KLM}(\omega)U_{1234}\Psi^{l'_xl'_yl'_{xy}l'_z}_{\mu'K'LM}(\omega)d\omega$$

$$U=V_{12}+V_{13}+V_{14}+V_{23}+V_{24}+V_{34}$$

The hyperspherical functions are: $\Psi^{l_xl_yl_{xy}l_z}_{\mu KLM}(\omega)=\sum_{m_xm_ym_{xy}m_z}(l_xl_ym_xm_y\,|\,l_{xy}m_{xy})(l_{xy}l_zm_{xy}m_z\,|\,LM)\Phi^{l_xl_yl_zm_xm_ym_z}_{\mu K}(\omega)$

$$\Phi^{l_xl_yl_zm_xm_ym_z}_{\mu K}=N^{l_xl_y}_K(\cos\alpha)^{l_x}(\sin\alpha)^{l_y}P^{l_y+1/2,l_x+1/2}_n(\cos2\alpha)N^{l_zK+3/2}_{\mu+3/2}(\cos\beta)^{l_z}(\sin\beta)^K P^{K+2,l_z+1/2}_m(\cos2\beta)\times$$
$$\times Y_{l_xm_x}(\hat{\mathbf{x}})Y_{l_ym_y}(\hat{\mathbf{y}})Y_{l_zm_z}(\hat{\mathbf{z}})$$

[1] R.I. Dzhibuti and K.V. Shitikova. Method of Hyperspherical Functions in Atomic and Nuclear Physics. (Energoatomizdat, Moscow. 1993, in Russian).

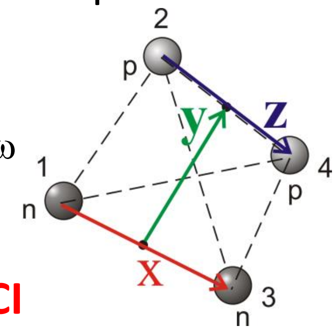
4.5. Test for exactly solvable 4-body oscillator model: HSF & FCI

Four particles with masses $m_1=m_2=m_3=m_4=m$ interact each with other by oscillator potentials:

Energies:

$$V_{ij}(r_{ij})=\frac{m\omega^2}{2}r_{ij}^2,\; V=-U_0+\sum_{i<j}V_{ij}(r_{ij})=-U_0+\frac{m\omega^2}{2}\left(r_{12}^2+r_{13}^2+r_{14}^2+r_{23}^2+r_{24}^2+r_{34}^2\right),$$

$$T=\frac{m}{2}\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right),\; V=-U_0+\frac{m}{2}(2\omega)^2\left(x^2+y^2+z^2\right),\; E_0=-U_0+\hbar(2\omega)\left(\frac{3}{2}+\frac{3}{2}+\frac{3}{2}\right)=-U_0+9\hbar\omega$$



For instance: $m=1, \omega=1, \hbar=1$ $\quad E_0=-U_0+9$

HSF **HSF+spline and FCI method reproduce accurate results.**

FCI

$$U=-U_0+\frac{\omega^2}{2}4\left(x^2+y^2+z^2\right)=-U_0+\frac{1}{2}(2\omega)^2\rho^2=U(\rho)$$

Exact value $U_0=0$, $E_0=9$; $U_0=15$, $E_0=-15+9=-6$

$$\ln K_E(q,\tau;q,0)\approx\ln\left|\Psi_0(q)\right|^2-E_0\tau,\; T_1<\tau$$

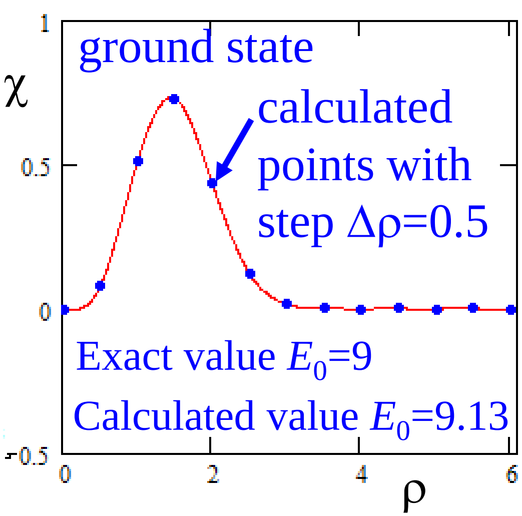
$$W_{\mu K\mu' K'}^{l_x l_y l_{xy} l_z; l'_x l'_y l'_{xy} l'_z}=\frac{2m}{\hbar^2}U(\rho)\delta_{\mu\mu'}\delta_{KK'}\delta_{l_x l'_x}\delta_{l_y l'_y}\delta_{l_{xy} l'_{xy}}\delta_{l_z l'_z}$$

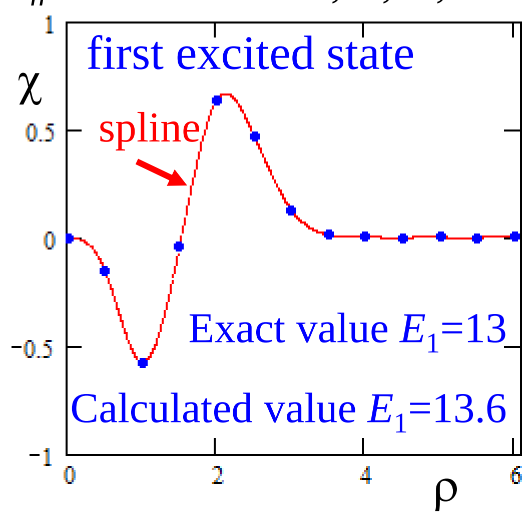
$$\frac{d^2}{d\rho^2}\chi_{\mu K0}^{l_x l_y l_{xy} l_z}(\rho)-\left[\kappa^2+\frac{(\mu+3)(\mu+4)}{\rho^2}\right]\chi_{\mu K0}^{l_x l_y l_{xy} l_z}(\rho)=U(\rho)\chi_{\mu K0}^{l_x l_y l_{xy} l_z}(\rho)$$

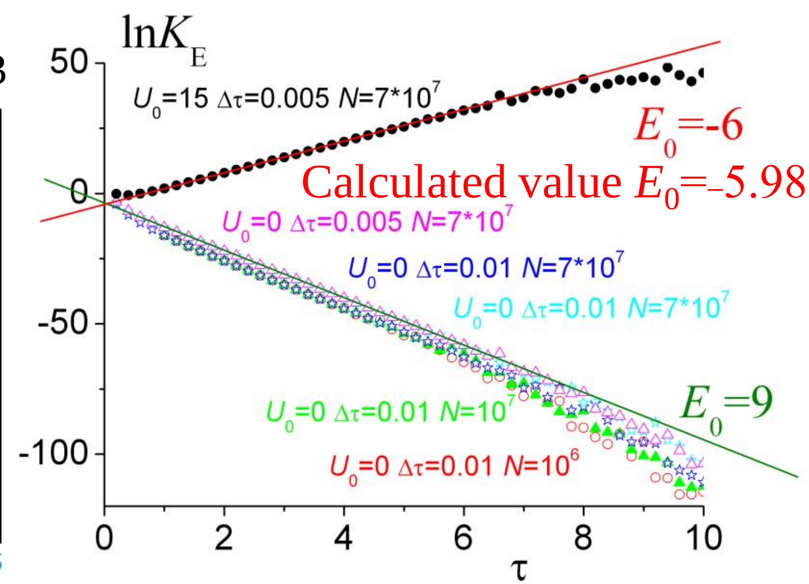
$$\frac{d^2}{d\rho^2}\chi_{000}^{0000}(\rho)-\left[\kappa^2+\frac{(3)(4)}{\rho^2}\right]\chi_{000}^{0000}(\rho)=U(\rho)\chi_{000}^{0000}(\rho)\quad \kappa^2=\frac{2}{\hbar^2}E,\; E=\frac{\hbar^2\kappa^2}{2}$$

Exact value $E_n=4n+2l+3=9,13,\ldots; l=3$

Feynman's continual integrals (**FCI**)
Monte-Carlo calculation with statistics $N=7\cdot10^7$.







Summary

1. Feynman's continual integrals method in Euclidean time was used for calculation of energies and wave functions of the ground states of light nuclei ^{3}H, ^{3,4}He ^{6}He,^{6,7,11}Li, ^{9}Be, ^{12}C, ^{16}O.
2. The agreement with the experimental data on binding energies was achieved using the nucleon-nucleon interaction potentials similar to the M3Y potential and nucleon-cluster and cluster-cluster potentials in the forms of the superposition of the Woods-Saxon type functions.
3. The correctness of calculations was checked by comparison with the results of the expansion in hyperspherical functions.
4. New effective method for the solution of the system of hyperradial equations using cubic splines is proposed.

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