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

# V.V. Samarin<sup>1,2</sup>

<sup>1</sup>Joint Institute for Nuclear Research, 141980 Dubna, Russia <sup>2</sup>Dubna State University, 141982 Dubna, Russia

**Abstract.** New effective method for solving of the system of hyperradial equations is proposed and testing for 3-body oscillator system and <sup>3</sup>H, <sup>3,6</sup>He nuclei. The energy of the ground states of <sup>3</sup>H, <sup>3,4,6</sup>He, <sup>6</sup>Li, <sup>9</sup>Be, <sup>12</sup>C, <sup>16</sup>O nuclei were calculated by Feynman's continual integrals method in Euclidean time. The nuclei <sup>3</sup>H, <sup>3,4</sup>He were considered as consisting of protons and neutrons, whereas the nuclei <sup>6</sup>He, <sup>6</sup>Li, <sup>9</sup>Be, <sup>12</sup>C, <sup>16</sup>O were considered as  $\alpha$ -cluster nuclei. The agreement with the experimental data on binding energies was achieved using the effective nucleon-nucleon interaction potentials similar to the M3Y potential. The superpositions of the Woods-Saxon type functions were used as nucleon- $\alpha$ -cluster and  $\alpha$ -cluster- $\alpha$ -cluster potentials.

### 1 Introduction

For description of experimental data on reactions with light nuclei we need accurate theoretical models and methods of calculation of ground states of these nuclei. It is desirable to have two (or more) complementary methods. There are two general approaches to quantum mechanics [1]. The first, and the main one is based on the Schrödinger equation [1]. For few-body systems it may be solved by expansion of the wave function into a system of functions, for example, into hyperspherical harmonics [2]. The Hyperspherical Harmonics Method (HHM) was used for calculations of nuclei <sup>3</sup>H [3], <sup>4</sup>He [4], <sup>6</sup>He [5], <sup>6</sup>He and <sup>12</sup>C [6], <sup>9</sup>Be [7]. In Ref. [8] the wave function of the three-body system was obtained using Gaussian basis and the numerical solution of the Hill-Wheeler integral equations. The Gaussian Expansion Method for few-body systems was used in Ref. [9] for calculation of the <sup>3,4</sup>He ground states. The spline approximation for solving of hyperradial equations for 3-body system is introduced in the HHM approach in *Section* 2. This modified method (HHMS) is tested for harmonic oscillator model with two sets of parameters.

The second general approach to quantum mechanics is based on Feynman's Continual Integrals (FCI) [1, 10, 11]. The FCI method was used for studying ground states of several light nuclei in Refs. [12, 13]. It is important that the FCI method may be implemented using parallel computing technologies [14].

The FCI method is tested for three- and four-body harmonic oscillator models in Section 3. Convergence of the complementary methods, HHMS and FCI, for effective nucleon-nucleon interaction is shown in Section 4. For nuclei, which may be represented as three- and four-body system, energies of ground state were also calculated in Section 4. The example of the probability density for ground state of <sup>9</sup>Be in the 3-body model is shown in the Section 5.

#### 2 Hyperspherical Harmonics Method with Spline Approximation

The basics of HHM for 3-body system [2] are described below. The "normalized" Jacobi coordinates  $(\mathbf{x}_i, \mathbf{y}_i)$  are

$$\mathbf{x}_{i} = \sqrt{\frac{m_{j}m_{k}}{m_{j} + m_{k}}} \left(\mathbf{r}_{j} - \mathbf{r}_{k}\right),\tag{1}$$

$$\mathbf{y}_{i} = \sqrt{\frac{m_{i}(m_{j}+m_{k})}{m_{1}+m_{2}+m_{3}}} \left(-\mathbf{r}_{i} + \frac{m_{j}\mathbf{r}_{j}+m_{k}\mathbf{r}_{k}}{m_{j}+m_{k}}\right),\tag{2}$$

where  $\mathbf{r}_i$  and  $m_i$  are radius vectors and masses of particles, respectively. The hyperspherical coordinates are  $\Omega = \{\theta_x, \varphi_x, \theta_y, \varphi_y, \alpha\}, x = \rho \cos \alpha, y = \rho \sin \alpha, \rho$  is the hyperradius. The hyperspherical harmonics (functions) are

$$\Phi_{KLM}^{l_x l_y}(\Omega) = \sum_{m_x m_y} (l_x l_y m_x m_y | LM) \Phi_K^{l_x l_y m_x m_y}(\Omega),$$
(3)

$$\Phi_{K}^{l_{x}l_{y}m_{x}m_{y}}(\Omega) = g_{K}^{l_{x}l_{y}}(\alpha)Y_{l_{x}m_{x}}(\hat{x})Y_{l_{y}m_{y}}(\hat{y}),$$
(4)

 $(l_{x_i}l_{y_i}m_{x_i}m_{y_i}|LM)$  are the Clebsch-Gordon coefficients,  $Y_{l_xm_x}(\hat{x})$ ,  $Y_{l_ym_y}(\hat{y})$ , are spherical harmonics. The orbital angular momentum for ground state equals zero, L = 0, therefore  $l_y = l_x$  and

$$g_{K0}^{l_x l_x}(\alpha) = N_K^{l_x l_x}(\cos \alpha)^{l_x} (\sin \alpha)^{l_x} P_n^{l_x + 1/2, \, l_x + 1/2}(\cos 2\alpha),\tag{5}$$

 $P_n^{l_y+1/2, l_x+1/2}(t)$  are the Jacobi polynomials,  $K = 2n + 2l_{x_i}$  is hypermoment,  $n = 0, 1, 2 \dots$  Expansion into hyperspherical functions of the ground state wave function  $\Psi_0$  for L = 0 is

$$\Psi_{0}(x, y, \cos \theta) = \tilde{\Psi}_{0}(\alpha, \theta, \rho) = \sum_{l_{xn}} \frac{\varphi_{K0}^{l_{x}l_{x}}(\rho)}{\rho^{5/2}} \Phi_{K00}^{l_{x}l_{x}}(\Omega)$$
$$= \sum_{l_{xK}} f_{K0}^{l_{x}l_{x}}(\rho) g_{K0}^{l_{x}l_{x}}(\alpha) \left(2l_{x}+1\right) P_{l_{x}}\left(\cos \theta\right), \qquad (6)$$

$$\varphi_{KL}^{l_x l_x}(\rho) = \rho^{5/2} f_{K0}^{l_x l_x}(\rho) \left(2l_x + 1\right),\tag{7}$$

where  $\theta$  is the angle between the Jacobi vectors. The main problem is the solution of the system of hyperradial equations

$$\frac{d^2}{d\rho^2} \varphi_{KL}^{l_x l_x}(\rho) + \left[\frac{2}{\hbar^2} \varepsilon - \frac{(K+3/2)(K+5/2)}{\rho^2}\right] \varphi_{K0}^{l_x l_x}(\rho) \\
= \sum_{K' l'_x} U_{KK'00}^{l_x l_x; l'_x l'_x}(\rho) \varphi_{K'0}^{l'_x l'_x}(\rho) \tag{8}$$

with coupling matrix of the potential energy  $U = V_{12} + V_{13} + V_{23}$ :

$$U_{KK'00}^{l_xl_x;l'_xl'_x}(\rho) = \langle l_x l_x K0 | U | l'_x l'_x K'0 \rangle.$$
(9)

There are several laborious methods of solving hyperradial equations: power expansion [15], artificial hyperradial basis [16, 17], basis of Lagrange functions [6].

### 2.1 Solution of System of Hyperradial Equations Using Splines

New method of solving hyperradial equations using cubic spline approximation is proposed. The idea of this method is simultaneous calculation of the mesh function  $\varphi_i$  and its second derivative  $m_i$ . The cubic spline interpolation expression [18]

$$\varphi_{K0}^{l_x l_x}(\rho) \equiv \varphi_{l_x,n}(\rho) = m_{l_x,n,i-1} \frac{(\rho_i - \rho)^3}{6h_i} + m_{l_x,n,i} \frac{(\rho - \rho_{i-1})^3}{6h_i} \\
+ \left(\varphi_{l_x,n,i-1} - \frac{m_{l_x,n,i-1}h_i^2}{6}\right) \frac{\rho_i - \rho}{h_i} \\
+ \left(\varphi_{l_x,n,i} - \frac{m_{l_x,n,i}h_i^2}{6}\right) \frac{\rho - \rho_{i-1}}{h_i}, \quad (10) \\
\rho \in [\rho_{i-1}, \rho_i], h_i = \rho_i - \rho_{i-1}, i = 1, 2, \dots N$$

for function  $\varphi_{l_x,n}(\rho)$  may be written with its values  $\varphi_{l_x,n,i}$  and values of its second derivative  $m_{l_x,n,i}$  in the points of mesh. This modified method (HHMS) has some advantages. The main one is the smooth interpolation between mesh points with natural boundary conditions

$$m_{l_x,n,0} = m_{l_x,n,N} = 0. (11)$$

The hyperradial equations on the mesh are

$$-A^{-1}H\varphi_{KL} + \frac{1}{\rho_i^2}(K+3/2)(K+5/2)\varphi_{KL} + \varphi_{KL'}(\rho_i)\frac{2}{\hbar^2}U_{KK}^{LL}(\rho) + \sum_{K'\neq K,L'\neq L}\varphi_{K'L'}(\rho_i)\frac{2}{\hbar^2}U_{KK'}^{LL'}(\rho) = \frac{2}{\hbar^2}E\varphi_{KL}.$$
 (12)

The matrix A was determined in Ref. [18]. The system (12) represents the eigenvalue problem  $B\Phi = \lambda \Phi$ . Energies are eigenvalues of matrix B and wave functions are eigenvectors of matrix B [19]. The other advantage of HHMS is a small size of the matrix for a special choice of the non-uniform mesh and fast calculations, but only for the ground state. A disadvantage of HHMS in the general case of an arbitrary mesh is that matrix B is unsymmetric. For the equidistant mesh, B is symmetric, and the method may be used for calculation of both ground and exited states, but a disadvantage is that matrix B has a large size.

#### 2.2 Exactly solvable harmonic oscillator systems

For verification testing HHMS approach we used 3-body harmonic oscillator system. Three particles with masses  $m_1 = m_3 = m, m_2 = \infty$  interact with each other by oscillator potentials:

$$V_{ij}(r) = \frac{m\omega_{ij}^2}{2}r^2.$$
 (13)

The frequencies of the normal modes are equal to  $\Omega_1, \Omega_2$  and energy of the ground state is

$$E_0 = \hbar \Omega_1 \frac{3}{2} + \hbar \Omega_2 \frac{3}{2}.$$
 (14)

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

$$\Omega_1 = \sqrt{\omega_{12}^2 + 2\omega_{13}^2}, \Omega_2 = \omega_{12}.$$
(15)

Two sets of parameters were used in calculations. In the case of

$$\omega_{12} = \omega_{23} = \omega_{13} = 1, \tag{16}$$

$$\Omega_1 = \sqrt{1+2} = \sqrt{3}, \Omega_2 = 1. \tag{17}$$

In the system of units with  $\hbar = 1$  energy of the ground state is

$$E_0 = \frac{3}{2} \left( 1 + \sqrt{3} \right) = 4.098, \tag{18}$$

and  $E_0 = 4.306$  in the case of

$$\omega_{12} = \sqrt{2}; \omega_{23} = \frac{1}{\sqrt{2}}; \omega_{13} = 1.$$
<sup>(19)</sup>

HHMS calculations were performed for  $\rho_{max} = 5, \Delta \rho = 0.05, K_{max} = 8$ . Exact values were obtained and the relative errors were not greater than 0.3%. In both cases HHMS leads to fast convergence to exact values of the ground state energy.

#### 3 Feynman's Continual Integrals in Euclidean Time

Feynman's continual integral [1, 10] is a propagator - the probability amplitude for a particle to travel from one point  $(q_0)$  to another (q) in a given time t

$$K(q,t;q_0,0) = \int Dq(t') \exp\left\{\frac{i}{\hbar}S\left[q(t')\right]\right\} = \left\langle q \left| \exp\left(-\frac{i}{\hbar}\hat{H}t\right) \right| q_0 \right\rangle.$$
(20)

Here S[q(t)] and  $\hat{H}$  are, respectively, the action and the Hamiltonian of the system, and Dq(t) is the integration measure [20]. For a time-independent potential energy a transition to the imaginary (Euclidean) time  $t = -i\tau$  yields the propagator  $K_E(q, \tau; q_0, 0)$  with the asymptotic behavior

$$K_E(q,\tau;q,0) \to |\Psi_0(q)|^2 \exp\left(-\frac{E_0\tau}{\hbar}\right), \tau \to \infty$$
 (21)

or

$$\hbar \ln K_{\rm E}\left(q,\tau;q,0\right) \to \hbar \left|\Psi_0(q)\right|^2 - E_0\tau, \tau \to \infty.$$
(22)

Equation (22) can be used to obtain the energy  $E_0$  as the slope of the linear part of the graph representing  $\ln K_E(q,\tau;q,0)$  as a function of  $\tau$ . The squared modulus of the ground-state wave function,  $|\Psi_0(q)|^2$  in the points q of the finite region corresponding to finite motion can be determined based on expression (21) at  $\tau$  values in the linear part of the graph representing the dependence  $\ln K_E(q,\tau;q,0)$ .

The propagator  $K_E(q, \tau; q_0, 0)$  can be represented as the limit of a multiple integral [1, 10, 11]

$$K_{\rm E}(q_0,\tau;q_0,0) = \lim_{\substack{N \to \infty \\ N \Delta \tau = \tau}} \left(\frac{m}{2\pi\hbar\Delta\tau}\right)^{N/2} \\ \times \int \cdots \int \exp\left\{-\frac{1}{\hbar} \sum_{k=1}^{N} \left[\frac{m\left(q_k - q_{k-1}\right)^2}{2\Delta\tau} + V\left(q_k\right)\Delta\tau\right]\right\} dq_1 dq_2 \dots dq_{N-1}.$$
(23)

#### 3.1 Calculation of Feynman's continual integrals by Monte-Carlo method

The values of the propagator  $K_E(q, \tau; q0, 0)$  were calculated using averaging over random trajectories with the distribution in the form of the multidimensional Gaussian distribution [12, 14]

$$K_{\rm E}(q_0,\tau;q_0,0) \approx \left(\frac{m}{2\pi\hbar\tau}\right)^{1/2} \left\langle \exp\left[-\frac{\Delta\tau}{\hbar}\sum_{k=1}^N V(q_k)\right] \right\rangle, \tag{24}$$

$$\langle F \rangle \approx \frac{1}{n} \sum_{i=1}^{n} F_i.$$
 (25)

Parallel calculations by Monte Carlo method [21] using NVIDIA CUDA [22] technology were performed on the Heterogeneous Cluster of LIT, JINR [23].

#### 3.2 Exactly solvable harmonic oscillator systems

The verification testing of the FCI method for 3-dimensional harmonic oscillator which is equivalent to 2-body system was made in Ref. [12]. In addition, for verification testing of the FCI method we used 3-body harmonic oscillator system (13)-(15). The FCI method with Monte-Carlo statistics  $n = 7 \times 10^7$ reproduces the exact result  $E_0 = 4.117 \pm 0.006$  for the system with parameter values (16)-(18) and  $E_0 = 4.36 \pm 0.03$  for the system with parameter values (19).

For extended verification testing of the FCI method we used 4-body harmonic oscillator system. Four particles with masses  $m_1 = m_2 = m_3 = m_4 = 1$ interact with each other by oscillator potentials (13). The expression for total potential energy in terms of "normalized" Jacobi coordinates (**x**, **y**, **z**) is

$$V = -U_0 + \frac{1}{2} (2\omega)^2 \left(x^2 + y^2 + z^2\right)$$
(26)

and the energy of the ground state for  $\omega = 1$ ,  $\hbar = 1$  is

$$E_0 = -U_0 + 9. (27)$$

The FCI method with Monte-Carlo statistics  $n = 7 \times 10^7$  reproduces the exact results with a satisfactory uncertainty:  $E_0 = 9.05 \pm 0.1$  for  $U_0 = 0$  and  $E_0 = -5.98 \pm 0.02$  for  $U_0 = 15$ . The FCI method leads to fast convergence to exact values of the ground state energy.

#### 4 Energy of Ground State for Three and Four Body Nuclei

#### 4.1 Exactly Solvable Nuclear Systems

For verification testing of the FCI method for nuclear interactions we used 3body system of the particles with masses  $m_1 = m_3 = m_0, m_2 = \infty$ , where  $m_0$  is the mass of a nucleon. The light particles 1, 3 interact only with infinitely heavy particle 2 by nucleon-nucleon potential having repulsive core. The nucleon-nucleon interaction potentials similar to the M3Y potential (*e.g.*, [24]) was used

$$V_{12}(r) \equiv V_{23}(r) = \sum_{k=1}^{3} u_k \exp\left(-r^2/b_k^2\right).$$
 (28)

The radial Schrödinger equation was solved "exactly" by difference scheme for 2-body system of particles 1 and 2. The energy is equal to -4 MeV for parameters values:  $u_1 = 500$  MeV,  $u_2 = -102$  MeV,  $u_3 = -2$  MeV,  $b_1 = 0.5$  fm,  $b_2 = 1.26$  fm,  $b_3 = 2.67$  fm. 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,  $E_0 = -8$  MeV. The convergence of HHMS and FCI algorithms is shown in Figure 1. Hyperspherical harmonics calculations were made on the equidistant mesh  $\rho \leq \rho_{max} = 10$  fm with step h = 0.1 fm. The results show slow



Figure 1. The convergence of HHMS (a) and FCI (b) algorithms for the model of a 3body system with nuclear interaction (28); the exact value of the ground state energy is  $E_0 = -8$  MeV.

convergence with increase of the value of maximum hypermoment  $K_{max}$  (see Figure 1). FCI calculations were made with statistics  $n = 7 \times 10^7$ . The results show fast convergence with decrease of the dimensionless Euclidean time step  $\Delta \tilde{\tau}$  (see Figure 1). The dimensionless Euclidean time is  $\tilde{\tau} = \tau/t_0$ , where  $t_0 = m_0 x_0^2/\hbar \approx 1.57 \times 10^{-23}$ s,  $x_0 = 1$  fm.

In addition, the FCI method was tested for a 4-body system of the particles with masses  $m_1 = m_2 = m_3 = m_0, m_4 = \infty$ . Light particles 1, 2, 3 interact only with infinitely heavy particle 4 by nucleon-nucleon potential (28). The energy of the independent light particles 1, 2, 3 in the field of infinitely heavy particle 4 is equal to the sum of energies of particles 1, 2, and 3,  $E_0 = -12$  MeV. The FCI calculation with statistics  $n = 7 \times 10^7$  and  $\Delta \tilde{\tau} = 0.01$  yields the following result of linear regression of dependence (22):  $E_0 = 12.16 \pm 0.05$  MeV, *i.e.*, the absolute uncertainty is small.

# 4.2 <sup>3</sup>H, <sup>3,4,6</sup>He, <sup>6</sup>Li, <sup>9</sup>Be, <sup>12</sup>C, <sup>16</sup>O nuclei

In the used model in the <sup>3</sup>H, <sup>3,4</sup>He nuclei neutrons (n) and protons (p) interact with each other by nucleon-nucleon potentials having repulsive core

$$V_{n-n}(r) \equiv V_{p-p}^{(N)}(r) = \sum_{k=1}^{3} u'_k \exp(-r^2/b'_k{}^2),$$
(29)

$$V_{p-n}(r) = \sum_{k=1}^{3} u_k \exp(-r^2/b_k^2).$$
(30)

The parameters u (in MeV) and b (in fm) are

$$u'_1 = u_1 = 500, \quad u'_2 = u_2 = -102, \quad u'_3 = u_3 = -2,$$
  
 $b'_1 = 0.53, \quad b_1 = 0.38, \quad b'_2 = b_2 = 1.26, \quad b'_3 = b_3 = 2.67.$ 



Figure 2. Logarithm of the propagator  $b_0^{-1} \ln \tilde{K}_E$  as a function of the Euclidean time  $\tilde{\tau}$  for nuclei <sup>3</sup>H (open circles), <sup>3</sup>He (solid circles), <sup>6</sup>He (solid squares), <sup>6</sup>Li (open squares), <sup>9</sup>Be (stars) <sup>12</sup>C (solid triangles) and <sup>16</sup>O (open triangles). The lines on display stand for the results of a linear regression (calculation by the Monte Carlo method for  $n = 7 \times 10^7$  trajectories with a grid step  $\Delta \tilde{\tau} = 0.01$ ).

The propagator  $K_E$  was calculated using dimensionless variables

$$b_0^{-1} \ln \tilde{K}_{\rm E}(q, \tilde{\tau}; q, 0) \approx b_0^{-1} \ln |\Psi_0(q)|^2 - E_0 \tilde{\tau}, \tilde{\tau} \gg 1,$$
 (31)

where  $b_0 = t_0 \varepsilon_0 / \hbar = 0.02412$ ,  $\varepsilon_0 = 1$  MeV. The results are shown in Figure 2. The values of ground state energy are in Table 1.

In the <sup>6</sup>He, <sup>6</sup>Li, <sup>9</sup>Be nuclei neutrons (and proton) interact with  $\alpha$ -cluster. In the used model the nuclear part of  $\alpha$ -nucleon potential has repulsive core for excluding the forbidden (internal) 1s state in the <sup>6</sup>He, <sup>6</sup>Li nuclei.

$$V_{\alpha-n}(r) = \sum_{i=1}^{3} U_i f_i [1 + \exp((r - R_i)/a_i)]^{-1}.$$
 (32)

Table 1. Energies of splitting of light nuclei to constituent particles

Atomic nucleus	Constituent particles	Experimental values, MeV [25]	Theoretic: FCI	al values, MeV HHMS
<sup>3</sup> H	n+n+p	8.482	8.5	8.42
<sup>3</sup> He	p + p + n	7.718	7.7	7.69
<sup>6</sup> He	$n + n + \alpha$	0.975	0.83	0.98
<sup>6</sup> Li	$n + p + \alpha$	3.64	3.1	
<sup>9</sup> Be	$\alpha + \alpha + n$	1.573	1.58	
$^{12}$ C	3lpha	7.37	7.39	
$^{16}$ O	4lpha	14.53	14.52	
<sup>4</sup> He	n+n+p+p	28.296	30.6	

The values of parameters are given in Ref. [12]. The results of the calculations of the propagator are shown in Figure 2. The values of the ground state energy are in Table 1.

In the used model in the <sup>9</sup>Be, <sup>12</sup>C, <sup>16</sup>O nuclei  $\alpha$ -clusters interact with  $\alpha$ clusters by potential having repulsive core

$$V_{\alpha-\alpha}(r) = \sum_{i=1}^{2} U_i \left[1 + \exp\left((r - R_i)/a_i\right)\right]^{-1}.$$
 (33)

The values of parameters are given in Ref. [12]. The results of the calculations of the propagator are shown in Figure 2. The values of the ground state energy are given in Table 1.

## 5 Probability Density for Ground State of Three-Body Nuclei

The calculations of the ground state probability density  $|\Psi_0|^2$  were made based on expression (21) at  $\tau$  values in the linear part of the graph representing the dependence  $\ln K_E(q,\tau;q,0)$ . An example of the probability density for the ground state of <sup>9</sup>Be in the 3-body model is shown in Figure 3.



Figure 3. The probability density  $|\Psi_0|^2$  for the <sup>9</sup>Be nucleus 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.

#### 6 Conclusion

Feynman's continual integrals method in Euclidean time and expansion in Hyperspherical Harmonics Method with Splines were used for calculations of ground state properties of nuclei <sup>3</sup>H, <sup>3,4,6</sup>He, <sup>6</sup>He, <sup>6</sup>Li, <sup>9</sup>Be, <sup>12</sup>C, and <sup>16</sup>O. The different iterative convergence of FCI and HHMS approaches provided the possibility of obtaining more accurate results in the complementary calculations. Both methods may be useful for calculations of ground state properties of light few-body nuclei, *e.g.*, <sup>7,8,9</sup>Li, <sup>10</sup>Be, and  $\alpha$ -cluster nuclei, *e.g.*, <sup>20</sup>Ne. The HHMS approach may be used for calculation of the excited states of few-body nuclei both in the discrete and continuous spectra.

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