Study of few-body nuclei by Feynman's continual integrals and hyperspherical functions

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Summary. — Feynman's continual integrals method for solving N-body ground state problem was implemented using parallel computing. The correctness of calculations for 3-body systems ^{6}Li, ^{12}C was checked by comparison with the results of the expansion into hyperspherical functions. New effective method for the solution of the system of hyperradial equations with cubic splines approximation is used. Feynman's continual integrals method was also used to study the ^{7}Li nucleus as a 4-body system.

1. – Spline approximation for solving hyperradial equations

There are two general approaches to studying stationary states in the quantum mechanics. The first, and the main one, is based on the Schrödinger equation. The second is Feynman's continual integral (FCI) method [1]. The Schrödinger equation was solved by expansion of wave functions into hyperspherical functions (HSF) for many three-body systems, *e.g.*, ^{3}H [2], ^{4}He [3], ^{6}He [4], ^{6}He and ^{12}C [5], ^{9}Be [6]. The main problem of this approach is the numerical solution of the so-called hyperradial equations. For the states with zero total angular momentum, the system of the hyperradial equations is

$$
\begin{aligned}
\tfrac{d^2}{d\rho^2}\varphi^{l_x l_x}_{KL}(\rho) + \left[\tfrac{2}{\hbar^2}E - \tfrac{(K+3/2)(K+5/2)}{\rho^2}\right]\varphi^{l_x l_x}_{K0}(\rho) = \\
= \sum_{K' l'_x} \tfrac{2}{\hbar^2} U^{l_x l_x; l'_x l'_x}_{K K' 00}(\rho)\varphi^{l'_x l'_x}_{K'0}(\rho)
\end{aligned}
\tag{1}
$$

with the coupling matrix

$$
U^{l_x l_x; l'_x l'_x}_{K K' 00}(\rho) = \langle l_x l_x K0|U|l'_x l'_x K'0\rangle
\tag{2}
$$

of the potential energy. In this work, we use pairwise potentials $U = V_{12} + V_{13} + V_{23}$. Here E is the energy of the system, ρ is the hyperradius, K is the hypermomentum, l_x is the angular momentum of a pair of particles of the system. There are several

laborious methods of solving hyperradial equations, *e.g.*, using the basis of the Lagrange functions [6].

New method of solving hyperradial equations using cubic spline approximation [7] was proposed in ref. [8]. The idea of this method is the simultaneous calculation of the mesh function φ_i and its second derivative m_i. The equations (1) on the mesh are

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

The matrices A and H were defined in ref. [7]. System (3) is the eigenvalue problem $B\Phi = \lambda\Phi$, where energies are eigenvalues of matrix B, and wave functions are eigenvectors of matrix B. This modified method has some advantages. The main advantage is the smooth interpolation between mesh points with natural boundary conditions $m_{l_x,n,0} = m_{l_x,n,N} = 0$. Another advantage 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. This method was tested for the exactly solvable harmonic oscillator and nuclear 3-body systems in ref. [8]. The convergence to the exact solution is fast for the pairwise parabolic interaction potential (at $K > 4$) and slow for the pairwise interaction with a repulsive core (at $K > 40$). For the exactly solvable 4-body harmonic system with equal masses m and the pairwise parabolic potentials, the convergence is also fast.

2. – Feynman's continual integrals in imaginary time

Feynman's continual integral [1] is a propagator – the probability amplitude for a particle to travel from one the point q_0 to the point q in a given time t. For a time-independent potential energy, transition to the imaginary time $t = -i\tau$ yields the propagator $K_E(q,\tau;q,0)$ with the asymptotic behavior [9]

(4)
$$K_E(q,\tau;q,0) \rightarrow |\Psi_0(q)|^2 \exp\left(-\frac{E_0\tau}{\hbar}\right), \tau \rightarrow \infty,$$

where E_0 and Ψ_0 are the energy and the wave function of the ground state of the system. The values of the propagator $K_E(q,\tau;q_0,0)$ were calculated using averaging over random trajectories with the distribution in the form of the multidimensional Gaussian distribution [10]

(5)
$$K_E(q_0,\tau;q_0,0) \approx \left(\frac{m}{2\pi\hbar\tau}\right)^{1/2}\left\langle\exp\left[-\frac{\Delta\tau}{\hbar}\sum_{k=1}^{N}V(q_k)\right]\right\rangle.$$

Parallel calculations [11] by the Monte Carlo method using NVIDIA CUDA technology [12,13] were performed on the Heterogeneous Cluster [14] of the Joint Institute for Nuclear Research.

3. – Structure of ground states of ^{6,7}Li nuclei

The experimental energies of separation of nucleons from the ^{4}He nucleus are larger than those from ^{7}Li and ^{6}Li nuclei (*e.g.*, [15]). This fact makes it possible to describe them as systems $\alpha + p + n + n$ and $\alpha + p + n$, respectively.

In our model, neutrons (n) and protons (p) in the nuclei interact with each other by nucleon-nucleon potentials with repulsive cores, *e.g.*,

$$(6) \qquad V_{p-n}(r) = \sum_{k=1}^{3} u_k \exp(-r^2/b_k{}^2), u_1 > 0, u_2 < 0, u_3 < 0.$$

The nuclear parts of the α-nucleon potentials used for ^{6}He, ^{6}Li nuclei (see [10]) have a repulsive core for excluding the forbidden (internal) $1s$ state, *e.g.*,

$$(7) \qquad V_{\alpha-n}(r) = \sum_{i=1}^{3} U_i \left[1 + \exp\left((r - R_i)/a_i\right)\right]^{-1}, U_1 > 0, U_2 < 0, U_3 < 0.$$

The values of parameters of potentials (6), (7), and others are given in ref. [10].

Examples of the probability density for the ground state of the ^{6}Li nucleus calculated as a 3-body system and of the ^{7}Li nucleus calculated as a 4-body system by the FCI method are shown in fig. 1 and fig. 2, respectively.

The HSF method yields a similar result for the ^{6}Li nucleus. The most probable configurations are α + deuteron for the ^{6}Li nucleus and α + triton for the ^{7}Li nucleus. These pictures are consistent with small separation energies of a triton from the ^{7}Li nucleus (2.5 MeV) and of a deuteron from the ^{6}Li nucleus (1.5 MeV) [15].
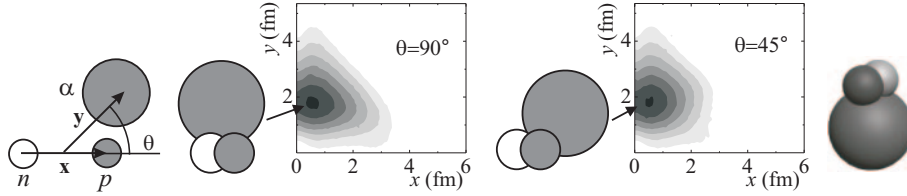

Fig. 1. – The Jacobi vectors $\mathbf{x}$, $\mathbf{y}$ (left), the probability density (centre), and the 3D model for the ^{6}Li nucleus (right); neutrons are denoted as small empty circles; protons and α-clusters are denoted as small filled circles and large filled circles, respectively. The only possible configuration is α + deuteron.
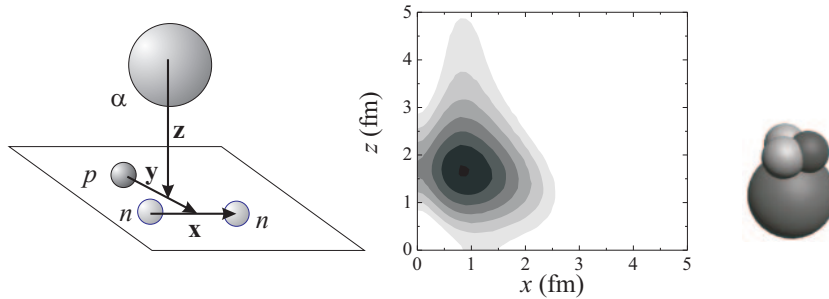

Fig. 2. – The Jacobi vectors $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$ (left), the probability density (centre), and the 3D model for the ^{7}Li nucleus (right) in the model $\alpha + p + n + n$ with regular triangle configuration of nucleons; nucleons and α-cluster are denoted as small and large spheres, respectively. The most probable configuration is α + triton.
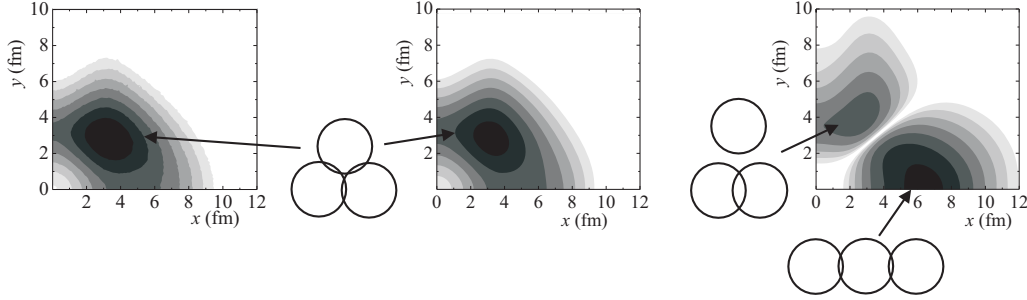
Fig. 3. – The probability density for the ^{12}C nucleus in the model $\alpha + \alpha + \alpha$ for the ground state calculated by the FCI method (left), by the HSF method (centre), and for the Hoyle state (right) calculated by the HSF method; x and y are the Jacobi coordinates, angle between vectors $\mathbf{x}$, $\mathbf{y}$ is $\theta = 90°$; α-clusters are denoted as circles.

4. – Structure of ground state and Hoyle state of ^{12}C nucleus

The nuclear part of the α-α potential used for ^{9}Be, ^{12}C, ^{16}O nuclei has form (7) with parameters given in ref. [10]. An example of the probability density in the 3-body model for the ground state of ^{12}C and for the first excited state with total angular momentum $L = 0$ (the Hoyle state) is shown in fig. 3. For the ground state, the most probable configuration is a regular triangle of α-clusters. For the Hoyle state, the result of the HSF method demonstrates two possible configurations: linear (the most probable) and ^{8}Be $+ \alpha$-cluster (less probable).

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