APPLICATION OF NVIDIA CUDA TECHNOLOGY TO CALCULATION OF GROUND STATES OF FEW-BODY NUCLEI

V.V. Samarin[1,2,a], M.A. Naumenko[1]

[1] *Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, 6 Joliot-Curie, Moscow region, Dubna, 141980, Russian Federation*

[2] *Dubna State University, 19 Universitetskaya, Moscow region, Dubna, 141982, Russian Federation*

E-mail: [a] samarin@jinr.ru

The modern parallel computing solutions were used to speed up the calculations by Feynman's continual integrals method. The algorithm was implemented in C++ programming language. Calculations using NVIDIA CUDA technology were performed on the NVIDIA Tesla K40 accelerator installed within the heterogeneous cluster of the Laboratory of Information Technologies, Joint Institute for Nuclear Research, Dubna. The results for energies of the ground states of several few-body nuclei demonstrate overall good agreement with experimental data. The obtained square modulus of the wave function of the ground states provided the possibility of investigating the spatial structure of the studied nuclei. The use of general-purpose computing on graphics processing units significantly (two orders of magnitude) increases the speed of calculations.

Keywords: parallel computing, NVIDIA CUDA technology, Feynman's continual integrals method, few body systems, light atomic nuclei.

1. Introduction

There is high interest in structure and reactions with few-body atomic nuclei (e.g., ^{3}H, ^{3}He, ^{6}He, etc.) from both theoreticians and experimentalists of the Joint Institute for Nuclear Research (JINR) and other scientific centers. The development of computing and information resources of the Laboratory of Information Technologies (LIT), JINR [1] provides opportunities for high-performance computing and application of new methods for theoretical study of light nuclei. This work is devoted to application of NVIDIA CUDA technology [2, 3] to calculations within Feynman's continual integrals method [4, 5] which provides the energy and the probability densities for ground states of few body systems. This approach was already used for calculations of ^{3}H, ^{3,4,6}He nuclei [6, 7] and ^{6}Li, ^{9}Be nuclei [8, 9]. In addition to the above-listed nuclei, in this work ^{12}C and ^{16}O nuclei are considered using the same approach. The few-body nuclei ^{3}H, ^{3,4}He were described as consisting of protons and neutrons, whereas the nuclei ^{6}He, ^{6}Li, ^{9}Be, ^{12}C, and ^{16}O were described as α-cluster nuclei. The algorithm allowing us to perform calculations directly on GPU was developed and implemented in C++ programming language. The results show that the use of GPU is very effective for these calculations.

2. Theory and computing

Feynman's continual integral [4] is a propagator – the probability amplitude for a particle to travel from the point q_0 to the point q in a given time t. In the imaginary (Euclidean) time $\tau = it$ the propagator can be represented as the limit of a multiple integral [4, 5]

$$K(q,\tau;q_0,0) = \lim_{\substack{M\to\infty \\ M\Delta\tau=\tau}} \int\cdots\int \exp\left\{-\frac{1}{\hbar}\sum_{k=1}^{M}\left[\frac{m(q_k-q_{k-1})^2}{2\Delta\tau} - V(q_k)\Delta\tau\right]\right\} C^M dq_1 dq_2 \ldots dq_{M-1}, \quad (1)$$

$$q_k = q(\tau_k),\ \tau_k = k\Delta\tau,\ k = \overline{0,M},\ q_M = q,\ C = \left(\frac{m}{2\pi\hbar\Delta\tau}\right)^{1/2}. \quad (2)$$

Here m is the mass of the particle and $V(q_k)$ is its potential energy. The energy E_0 and the square modulus of the wave function $|\Psi_0|^2$ of the ground state of a system of few particles with coordinates q may be calculated using asymptotic behavior of propagator [5]

$$K_E(q,\tau;q,0) \to |\Psi_0(q)|^2 \exp\left(-\frac{E_0\tau}{\hbar}\right),\ \tau\to\infty, \quad (3)$$

or

$$\hbar \ln K_E(q,\tau;q,0) \to \hbar|\Psi_0(q)|^2 - E_0\tau,\ \tau\to\infty. \quad (4)$$

The values of the propagator $K_E(q,\tau;q,0)$ were calculated using averaging denoted by $\langle\ \rangle$ over random trajectories $q_k = f(q,k\Delta\tau)$ with the distribution in the form of the multidimensional Gaussian distribution

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

$$\langle F\rangle \approx \frac{1}{n}\sum_{i=1}^{n} F_i. \quad (6)$$

This theoretical approach to *N*-particle systems with the use of Jacobi coordinates is described in detail in Ref. [8]. Feynman's continual integrals method provides a new, mathematically simpler, possibility for calculating the energy and the probability density of the ground states of *N*-particle systems compared to other approaches, e.g., expansion into hyperspherical harmonics [10].

The Monte Carlo algorithm for numerical calculations was developed and implemented in C++ programming language using NVIDIA CUDA technology. The integration method does not require the use of any additional integration libraries. Parallel calculations (one thread calculated one

trajectory) were performed on the NVIDIA Tesla K40 accelerator installed within the heterogeneous cluster [1] of LIT, JINR, Dubna. The code was compiled with NVIDIA CUDA version 8.0 for architecture version 3.5. Calculations were performed with single precision.

To check the correctness of the calculation of the propagator the comparison with the exactly solvable *N*-body ($N = 3-7$) oscillatory systems has been performed. For particles with equal masses $m_i = m$ interacting with each other by oscillator potentials

$$V_{ij}(r_{ij}) = \frac{m\omega^2}{2} r_{ij}^2, \qquad V = -U_0 + \sum_{i<j} V_{ij}(r_{ij}), \tag{7}$$

the exact value of the ground state energy is

$$E_0 = -U_0 + \hbar\omega \frac{3}{2}(N-1)\sqrt{N}. \tag{8}$$

Assuming $\omega = 1, \hbar = 1$, we obtain $E_0 = -U_0 + 1.5(N-1)\sqrt{N}$. The Monte Carlo calculations were carried out with statistics $n = 10^7$. For values of the logarithm of the propagator, linear smoothing according to formula (4) was performed and the ground state energies were found. The results in Table 1 demonstrate satisfactory accuracy of calculations.

Table 1. Comparison of exact and calculated ground state energies the exactly solvable *N*-body oscillatory systems

Number of particles *N*	U_0	Exact value of E_0	Calculated value of E_0
3	0	4.098	4.11 ± 0.006
4	15	–6	–5.98 ± 0.02
5	20	–6.584	–6.56 ± 0.05
6	20	–1.629	–1.84 ± 0.1
7	20	3.812	3.63 ± 0.1

3. Results for 3 and 4 body nuclei

The same effective pairwise nucleon-nucleon, nucleon-cluster and cluster-cluster interaction potentials $V(r)$ were used for all the studied nuclei, where r is the distance between nucleons. In Refs. [6–9] the calculation of the propagator for the nuclei ^{2,3}H, ^{3,4}He neutron-neutron, proton-proton and neutron-proton two-body effective strong interaction potentials $V_{i-j}(r)$ ($i, j = n, p$) similar to the M3Y potential [11, 12] have been used

$$V_{i-j}(r) = \sum_{k=1}^{3} u_k \exp\left(-r^2/b_k^2\right). \tag{9}$$

The values of parameters are given in Ref. [8]. The calculations were performed in the center of mass system using the usual Jacobi coordinates. For a system of three particles, two of which have equal masses $m_1 = m_2 = m$ (two neutrons in ^{3}H and ^{6}He, a proton and a neutron in ^{6}Li, two α-clusters in ^{9}Be and in ^{12}C)

$$\mathbf{q} = \{\mathbf{x}, \mathbf{y}\}, \ \mathbf{x} = \mathbf{r}_2 - \mathbf{r}_1, \ \mathbf{y} = \mathbf{r}_3 - \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2). \tag{10}$$

The theoretical binding energies $E_B = -E_0$ obtained using formula (4) are listed in Table 2 together with the experimental values taken from the NRV web knowledge base [13]. It is clear that the theoretical values are close enough to the experimental ones. The observed difference between the calculated binding energies of ^{3}H and ^{3}He is also in agreement with the experimental values.

The α-cluster-nucleon and α-cluster-α-cluster strong interaction potentials $V_{i-j}(r)$ ($i, j = n, p, \alpha$) were used in the form of the combination of Woods–Saxon potentials

$$V_{\alpha-j}(r) = \sum_{i=1}^{s} U_i \left\{1 + \exp\left[(r - R_i)/a_i\right]\right\}^{-1}, \tag{11}$$

where $s = 2,3$. The values of parameters are given in Ref. [8]. The obtained theoretical energies of separation into cluster(s) and nucleon(s) $E_S = -E_0$ are listed in Table 2 together with the experimental values taken from the NRV web knowledge base [13]. It can be seen that the theoretical values are close enough to the experimental ones.

Table 2. Comparison of theoretical and experimental energies of separation of light nuclei into constituent particles

Atomic nucleus	Constituent particles	Experimental value [13], MeV	Theoretical value, MeV
^{3}H	$n + n + p$	8.482	8.21 ± 0.3
^{3}He	$n + n + p$	7.718	7.37 ± 0.3
^{4}He	$n + n + p + p$	28.296	30.60 ± 1.0
^{6}He	$n + n + \alpha$	0.97542	0.96 ± 0.05
^{6}Li	$n + p + \alpha$	3.637	3.87 ± 0.2
^{9}Be	$n + \alpha + \alpha$	1.573	1.7 ± 0.1
^{12}C	$\alpha + \alpha + \alpha$	7.37	7.39 ± 0.1
^{16}O	$\alpha + \alpha + \alpha + \alpha$	14.53	14.52 ± 0.1

The probability density distribution $\Psi_0(x, y, \cos\theta)$ for the configurations of nuclei ^{6}He ($\alpha + n + n$) and ^{6}Li ($\alpha + n + p$) with the angle θ between the vectors **x** and **y** is shown in Figures 1 and 2, respectively.

It can be seen that the most probable configurations of ^{6}He nucleus are α-cluster + dineutron and the cigar configuration, whereas the configuration $n + {}^5$He has low probability. The only one possible configuration of ^{6}Li nucleus is α-cluster + deuteron-cluster.

The probability density distribution $\Psi_0(x, y, \cos\theta)$ for the configurations of nucleus ^{9}Be ($\alpha + n + \alpha$) with the angle θ between the vectors **x** and **y** is shown in Figure 3. The most probable configuration is $\alpha + n + \alpha$, whereas the configurations $\alpha + {}^5$He and $n + {}^8$Be are less probable.

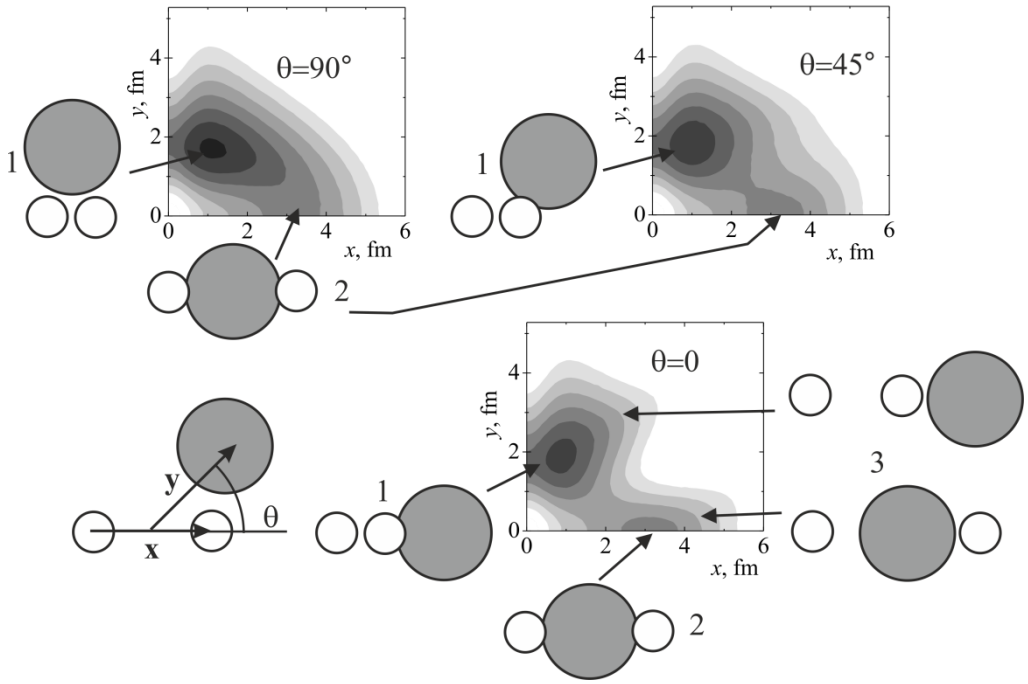

Figure 1. The probability density $|\Psi_0|^2$ for the ^{6}He nucleus and the vectors in the Jacobi coordinates; neutrons and α-clusters are denoted as small empty circles and large filled circles, respectively. The most probable configurations are α-cluster + dineutron (1) and the cigar configuration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

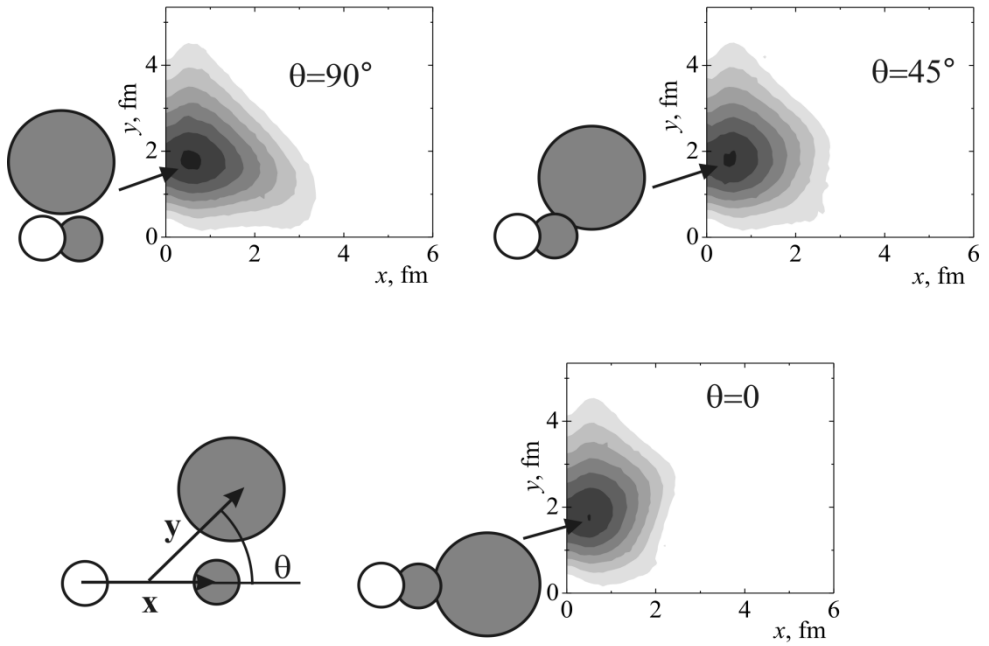

Figure 2. The probability density $|\Psi_0|^2$ for the ^{6}Li nucleus and the vectors in the Jacobi coordinates; notations are the same as in Figure 1, protons are denoted as small filled circles. The only one possible configuration is α-cluster + deuteron-cluster.

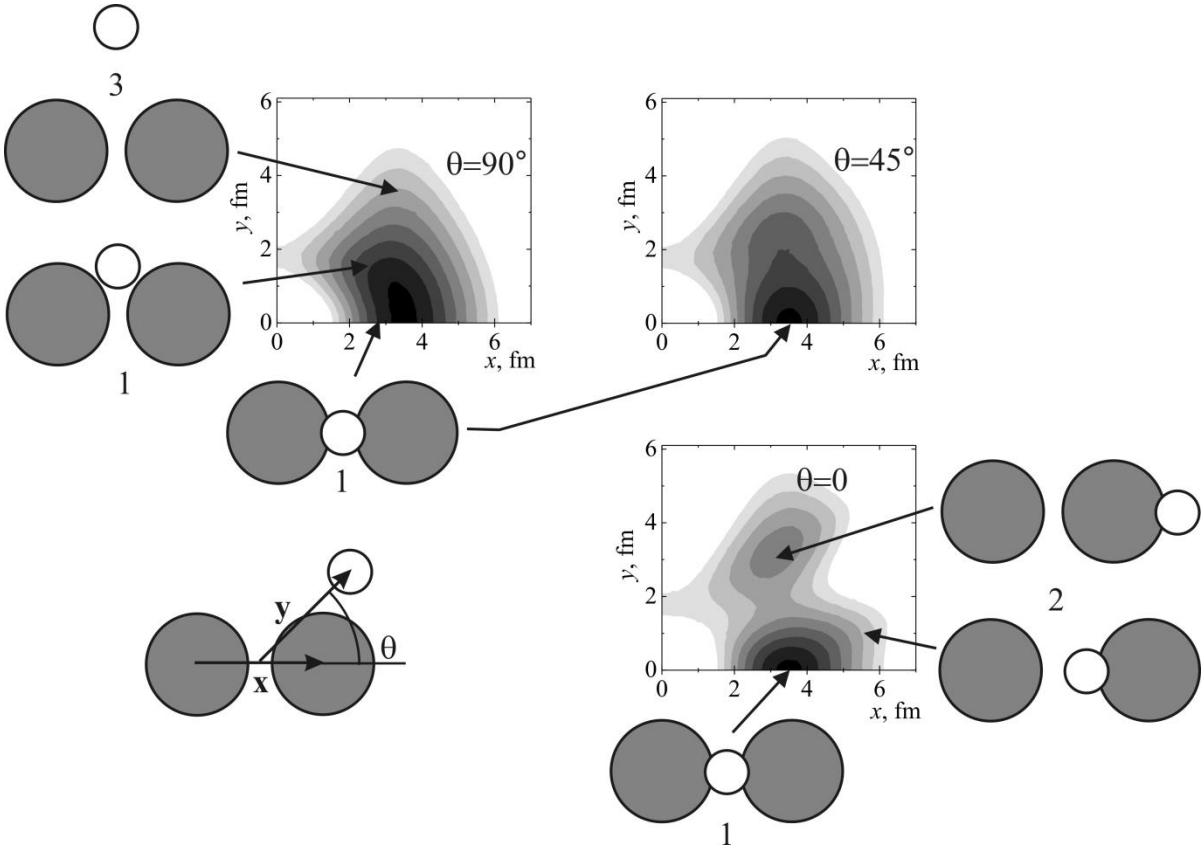

Figure 3. The probability density $|\Psi_0|^2$ for the ^{9}Be nuclei and the vectors in the Jacobi coordinates; notations are the same as in Figures 1, 2. The most probable configuration is α + *n* + α (1). The configurations α + ^{5}He (2) and *n* + ^{8}Be (3) are less probable.

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5. Conclusions

In this work an attempt is made to use modern parallel computing solutions to speed up the calculations of ground states of few-body nuclei by Feynman's continual integrals method. The developed parallel algorithm provided significant increase of the speed of calculations. The method was applied to the nuclei consisting of nucleons and cluster nuclei. The results of calculations demonstrate that the obtained theoretical values are close enough to the experimental ones for the studied nuclei. The obtained probability densities may be used for the correct definition of the initial conditions in the time-dependent calculations of reactions with the considered nuclei [14]. The results may also serve as a useful addition to the results obtained by the expansion in hyperspherical functions [15].

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