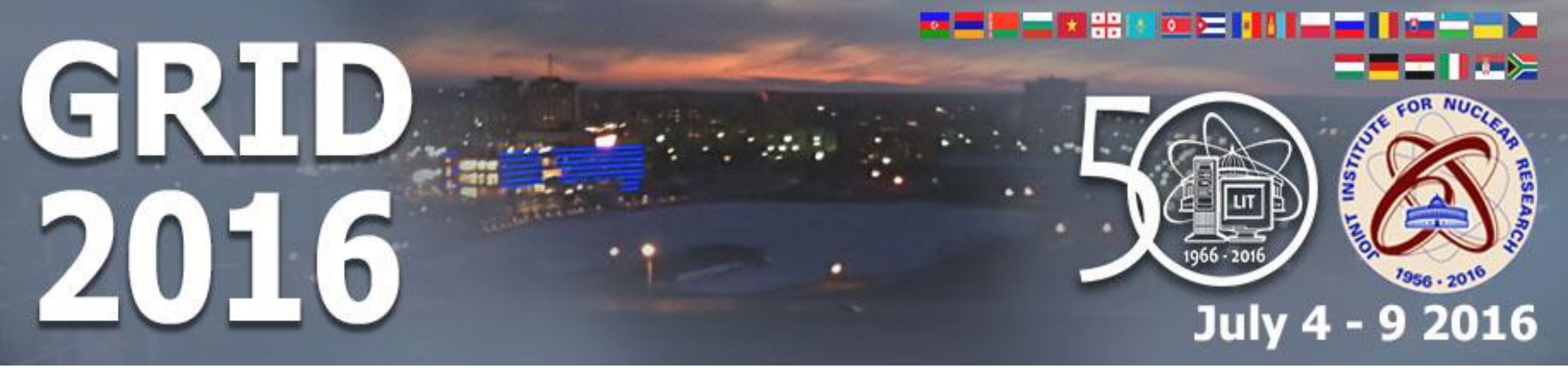

CALCULATION OF GROUND STATES OF FEW-BODY NUCLEI USING NVIDIA CUDA TECHNOLOGY

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Motivation

- ***High interest in structure and reactions with few-body nuclei from both theoreticians and experimentalists (e.g. ^{2}H, ^{3}H, ^{3}He, ^{6}He etc.)***

- ***The Feynman's continual integrals method [1] provides a mathematically more simple possibility for calculating the energy and probability density for the ground states of N-particle systems compared to other approaches (e.g. expansion on hyperspherical harmonics [2])***

- ***The choice of parameters is very simple (only nucleon-nucleon , nucleon-cluster, or cluster-cluster interaction potentials)***

- ***The method allows application of modern parallel computing solutions to speed up the calculations***

[1] Feynman R.P., Hibbs A.R. Quantum Mechanics and Path Integrals. New York, McGraw-Hill, 1965. 382 P.

[2] Dzhibuti R.I., Shitikova K.V. Metod gipersfericheskikh funktsiy v atomnoy i yadernoy fizike [Method of Hyperspherical Functions in Atomic and Nuclear Physics]. Moscow, Energoatomizdat, 1993. 269 P.

Two approaches to quantum mechanics

1) Schrödinger equation $\hat{H}\Psi = E\Psi$

2) Feynman continual (path) integral

$$K(q,t;q_0,0) = \int Dq(t)\exp\left\{\frac{i}{\hbar}S\left[q(t')\right]\right\} = \left\langle q\left|\exp\left(-\frac{i}{\hbar}\hat{H}t\right)\right|q_0\right\rangle \qquad (1)$$

is a propagator − the amplitude of the probability of propagation of the particle of mass m from the point q_0 to the point q in time t, $S[q(t)]$ and $\hat{H}$ are action and the Hamiltonian of the system, respectively, $Dq(t)$ is integration measure.

Euclidean time *t*=–*i*τ

For time-independent potential energy the transition to the imaginary (Euclidean) time $t = -i\tau$ gives the propagator

$$K_E(q,\tau;q_0,0) = \int D_E q(\tau)\exp\left\{-\frac{1}{\hbar}S_E\left[q(\tau')\right]\right\} \qquad (2)$$

Calculation of energy and wave function

$$K_E(q,\tau;q,0) = \sum_n \left|\Psi_n(q)\right|^2 \exp\left(-\frac{E_n\tau}{\hbar}\right) + \int_{E_{cont}}^{\infty} \left|\Psi_E(q)\right|^2 \exp\left(-\frac{E\tau}{\hbar}\right) g(E)dE\,. \qquad (6)$$

Here $g(E)$ is the density of states in the continuous spectrum $E \geq E_{cont}$. For a system with a discrete spectrum and finite motion of particles the square of the wave function of the ground state may also be found in the limit $\tau \to \infty$ [10] together with the energy E_0

$$K_E(q,\tau;q,0) \to \left|\Psi_0(q)\right|^2 \exp\left(-\frac{E_0\tau}{\hbar}\right),\ \tau \to \infty\,. \qquad (7)$$

[10] Shuryak E.V. Stochastic Trajectory Generation by Computer // Sov. Phys. Usp. 1984. Vol. 27. P. 448−453.

Calculation of propagator by Monte Carlo method

Feynman's continual integral may be represented as the limit of the multiple integral

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

where

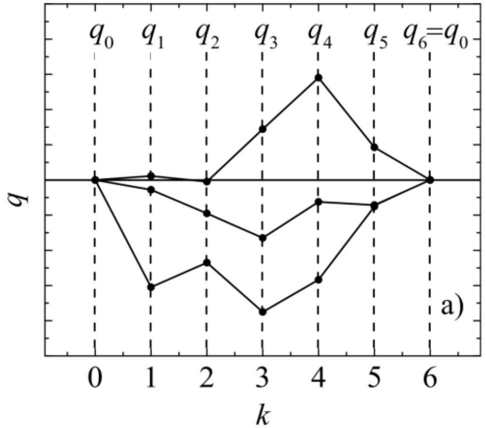
$$q_k=q(\tau_k),\ \tau_k=k\Delta\tau,\ k=\overline{0,N},\ q_N=q,\ C=\left(\frac{m}{2\pi\hbar\Delta\tau}\right)^{1/2}.$$

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

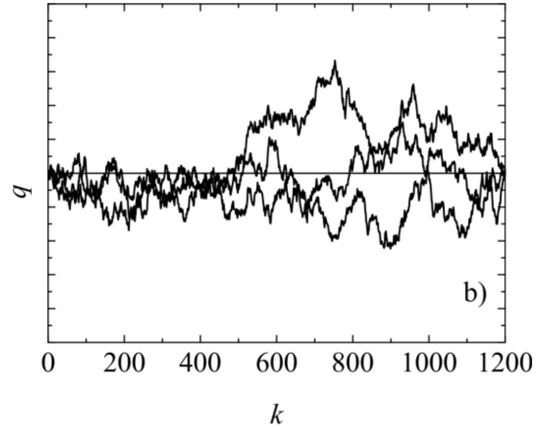
$(N-1)$-dimensional vectors $\{q_1,\ldots,q_{N-1}\}$ have the distribution law

$$W(q_0;q_1,\ldots,q_{N-1};q_N)=C^N\exp\left[-\frac{m}{\hbar}\sum_{k=1}^{N}\frac{(q_k-q_{k-1})^2}{2a}\right].$$

$N_1=6$



$N_2>>N_1$



Shuryak E.V. Stochastic Trajectory Generation by Computer // Sov. Phys. Usp. 1984. Vol. 27. P. 448−453.

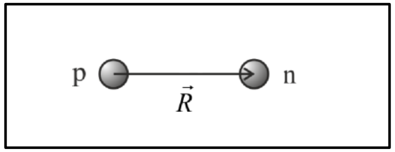
Ermakov S.M. Metod Monte-Karlo v vychislitel'noy matematike: vvodnyy kurs [Monte Carlo Method in Computational Mathematics. Introductory Course]. St. Petersburg, Nevskiy Dialekt, 2009. 192 P.

Jacobi coordinates for 2, 3, 4 - body systems

System of 2 particles (^{2}H nucleus)

$$\vec{R} = \vec{r}_2 - \vec{r}_1 \,,$$

$\vec{r}_1$ and $\vec{r}_2$ are the radius vectors of a proton and a neutron, respectively.



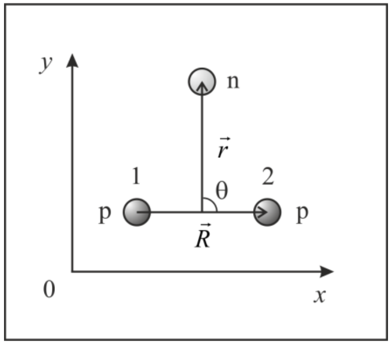
System of 3 particles two of which are identical (2 neutrons or 2 protons in ^{3}H, ^{3,6}He nuclei)

$$\vec{R} = \vec{r}_2 - \vec{r}_1 \,, \ \vec{r} = \vec{r}_3 - \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \,.$$

^{3}H nucleus: $\vec{r}_3$ is the radius vector of the proton, $\vec{r}_1$ and $\vec{r}_2$ are the radius vectors of neutrons.

^{3}He nucleus: $\vec{r}_3$ is the radius vector of the neutron, $\vec{r}_1$ and $\vec{r}_2$ are the radius vectors of protons.

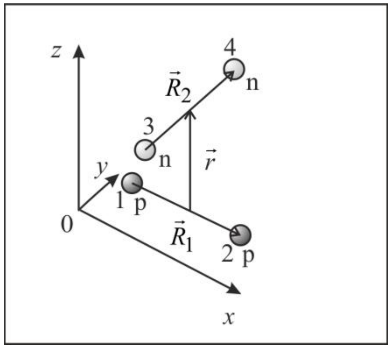
^{6}He: $\vec{r}_3$ is the radius vector of the α particle, $\vec{r}_1$ and $\vec{r}_2$ are the radius vectors of neutrons.



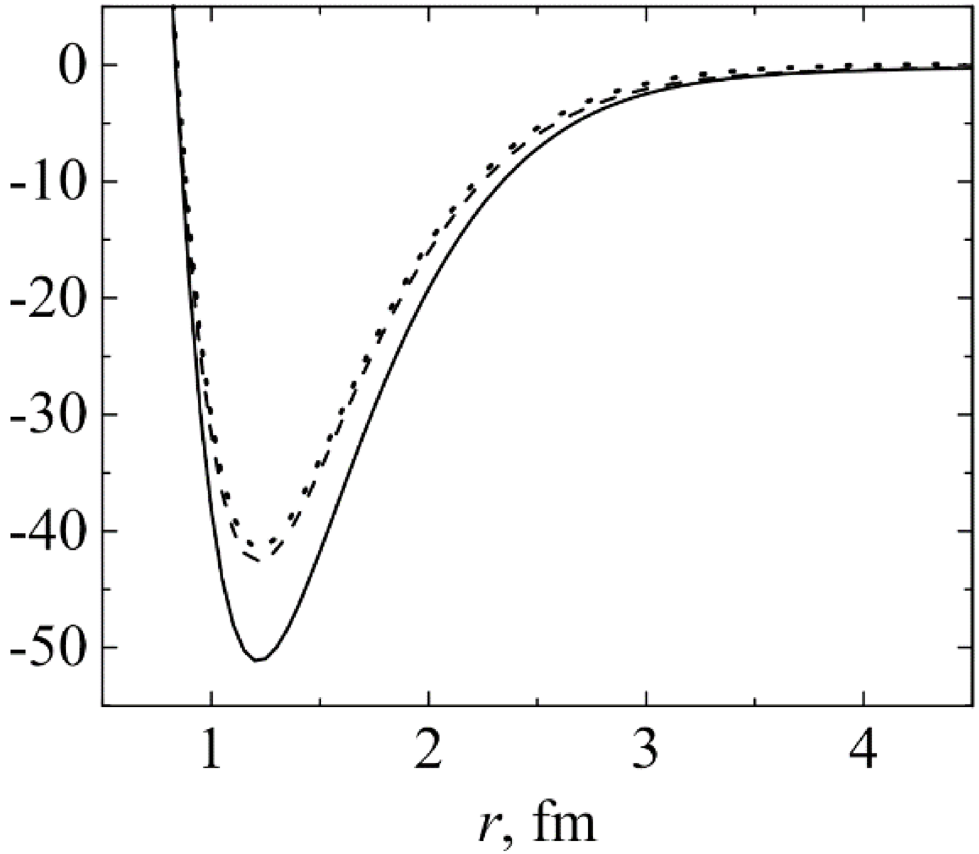
System of 4 particles with two pairs of identical particles (2 protons and 2 neutrons in the ^{4}He nucleus)

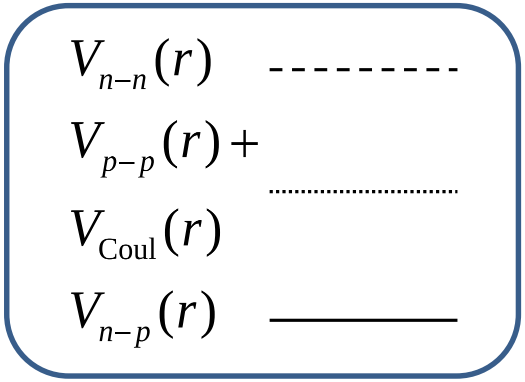
$$\vec{R}_1 = \vec{r}_2 - \vec{r}_1, \ \vec{R}_2 = \vec{r}_4 - \vec{r}_3 \,, \ \vec{r} = \frac{1}{2}(\vec{r}_3 + \vec{r}_4) - \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \,,$$

$\vec{r}_1$ and $\vec{r}_2$ are the radius vectors of protons, $\vec{r}_3$ and $\vec{r}_4$ are the radius vectors of neutrons.



Nucleon-nucleon interaction potentials





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

$$V_{n-p}(r) = \eta V_{n-n}(r)$$

The values of the parameters $u_1 = 500$ MeV, $u_2 = -102$ MeV, $u_3 = 2$ MeV, $b_1 = 0.59$ fm, $b_2 = 1.40$ fm, $b_3 = 2.94$ fm and $\eta = 1.2$ were determined from the condition of the absence of bound states of two identical nucleons as well as the approximate equality of the binding energy $E_b = -E_0$ to the experimental values of the binding energies for the nuclei ^{2}H, ^{3}H, ^{3}He, ^{4}He.

Hardware, software, implementation

- NVIDIA Tesla K40
  (for calculation)

- Intel® Core™ i5-3470 (up to 3.60 GHz)
  (for comparison)

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

- Implemented in C++ language
  (single precision)

- Code compiled for architecture 3.5, CUDA version 7.5

- cuRAND random number generator

- 1 thread calculates 1 trajectory

hYBRILIT http://hybrilit.jinr.ru/ Heterogeneous cluster | LIT/JINR

Characteristics of a HybriLIT cluster

Number of compute nodes	**7**
The total amount of RAM	**896 Gb**
The total amount of disk space	**57.6 Tb**

Number of cores available for computations

Blade hostname	CPU	GPU	PHI
blade01	24	-	-
blade02	24	2688	60
blade03	24	-	122
blade04	24	8640	-
blade05	24	8640	-
blade06	24	8640	-
blade07	24	8640	-
Total cores	**168**	**37248**	**182**

Software	
OS:	Scientific Linux 6.6. Kernel: 2.6.32-504
File system:	NFS4
Scheduler	SLURM-14.11.6-3 [1]
Modules:	MODULES 3.2.10 [2]
Technologies	
MPI:	OpenMPI 1.6.5, 1.8.1; [3]
CUDA:	CUDA 5.5, 6.0, 7.0; [4]
OpenMP:	GNU 4.4.7 [5], Intel 14.0.2 [6], PGI 15.3 [7];
OpenCL:	Intel 14.0.2, CUDA 6.0, 7.0.
Compilers (C/C++, Fortran):	
GNU:	gcc, g++, gfrortran;
PGI:	pgcc, pgc++, pgf77, pgf90;
Intel:	icc, icpc, ifort, mpiicc, mpiicpc, mpiifort;
CUDA:	nvcc;
OpenMPI:	mpicc, mpicxx, mpif77, mpif90;

Each node 2 x Intel Xeon E5-2695 v2 (2,40 GHz, 12 cores)

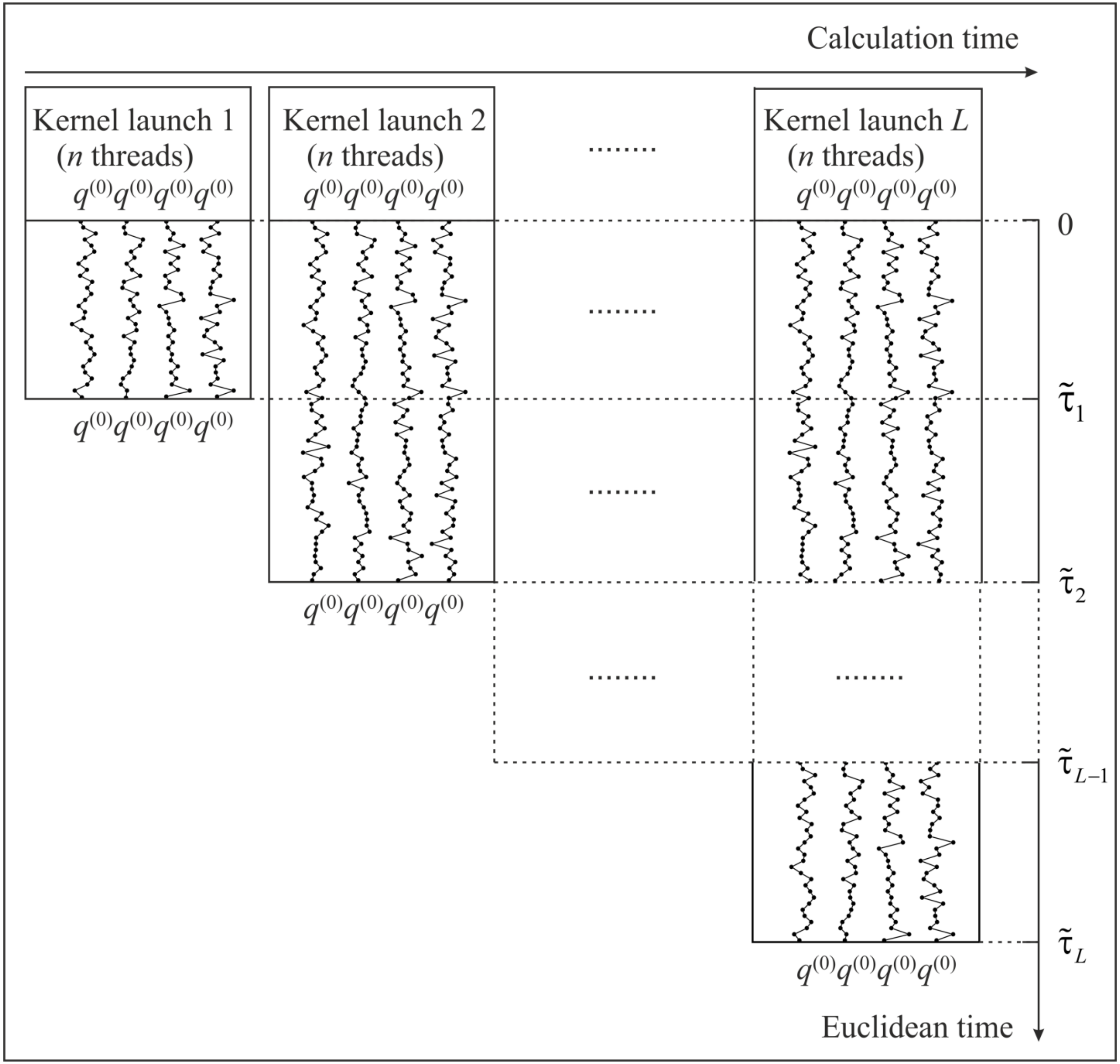
1 node NVIDIA Tesla K20X
2 nodes 3 x NVIDIA Tesla K40
2 nodes 2 x NVIDIA Tesla K80
1 node Intel Xeon Phi 5110P
1 nodes 2 x Intel Xeon Phi 7120P

Tesla K40

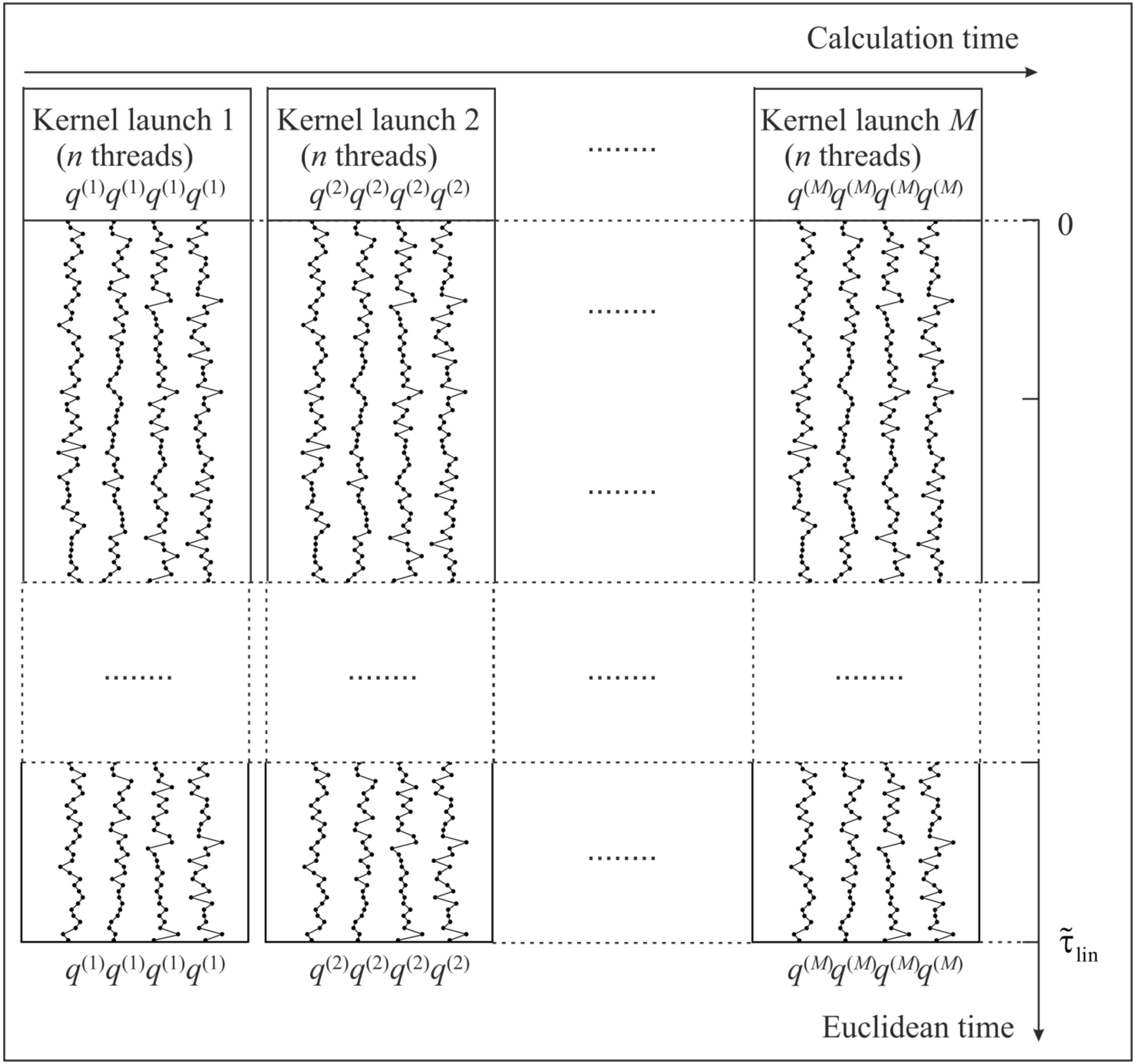
TESLA K40 Module - PRODUCT SPECIFICATIONS

CUDA PARALLEL PROCESSING CORES	2880
FRAME BUFFER MEMORY	12 GB GDDR5
PEAK DOUBLE PRECISION FLOATING POINT PERFORMANCE	1.43 Tflops
PEAK SINGLE PRECISION FLOATING POINT PERFORMANCE	4.29 Tflops
INTERFACE	384-bit
MEMORY BANDWIDTH	288 GB/s
DISPLAY CONNECTORS	None
MAX POWER CONSUMPTION	235 W
PROCESSOR CORE CLOCK	745 MHz
POWER CONNECTORS	1 × 6-pin PCI Express power connectors 1 × 8-pin PCI Express power connectors
GRAPHICS BUS	PCI Express 3.0 x16
FORM FACTOR	110 mm (H) × 265 mm (L) - Dual Slot, Full-Height
THERMAL SOLUTION	Passive

Scheme of calculation of ground state energy



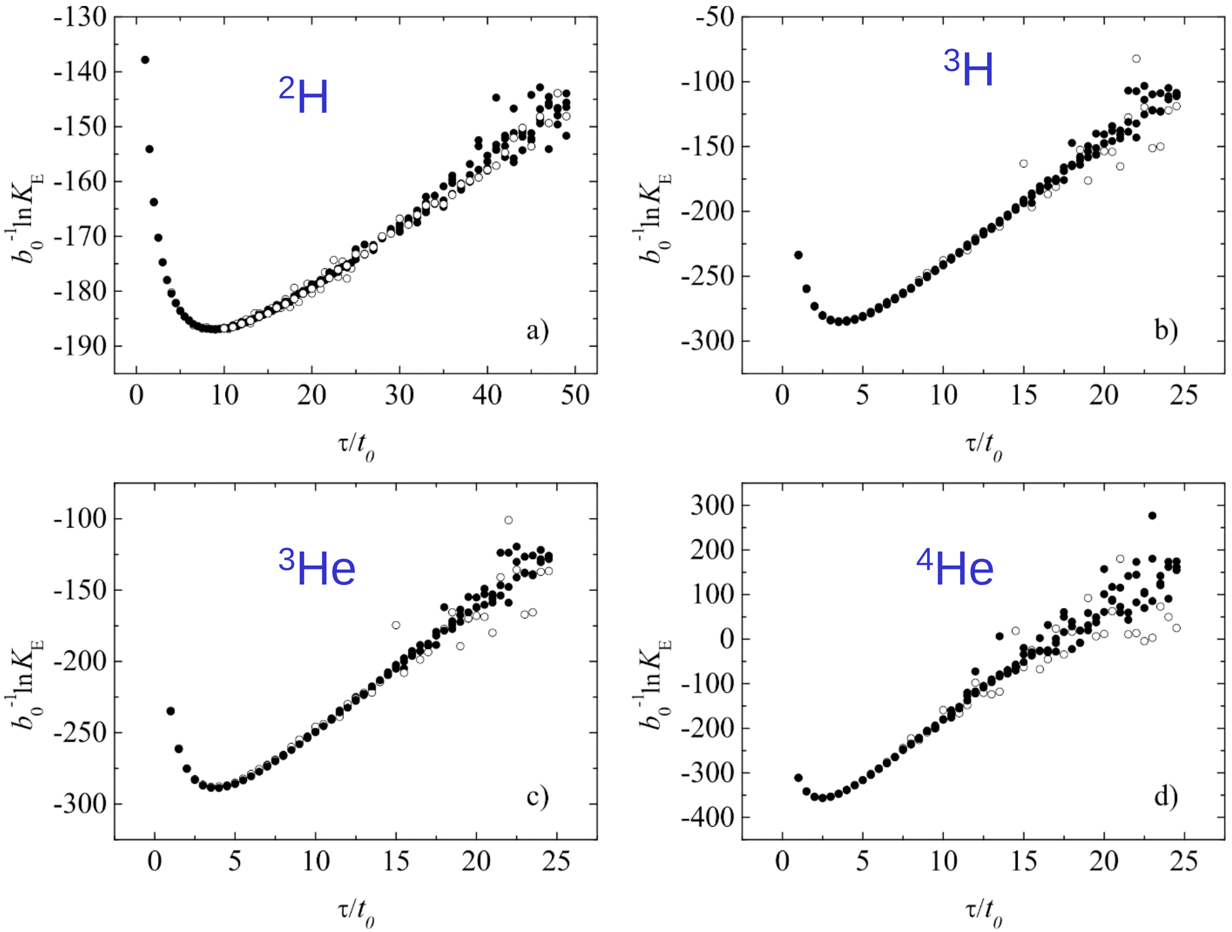
Scheme of calculation of ground state wave function



Benefits:

1) **Accumulation of data points**
2) **Low memory consumption (no grid)**

Results of calculation the energy of ground state

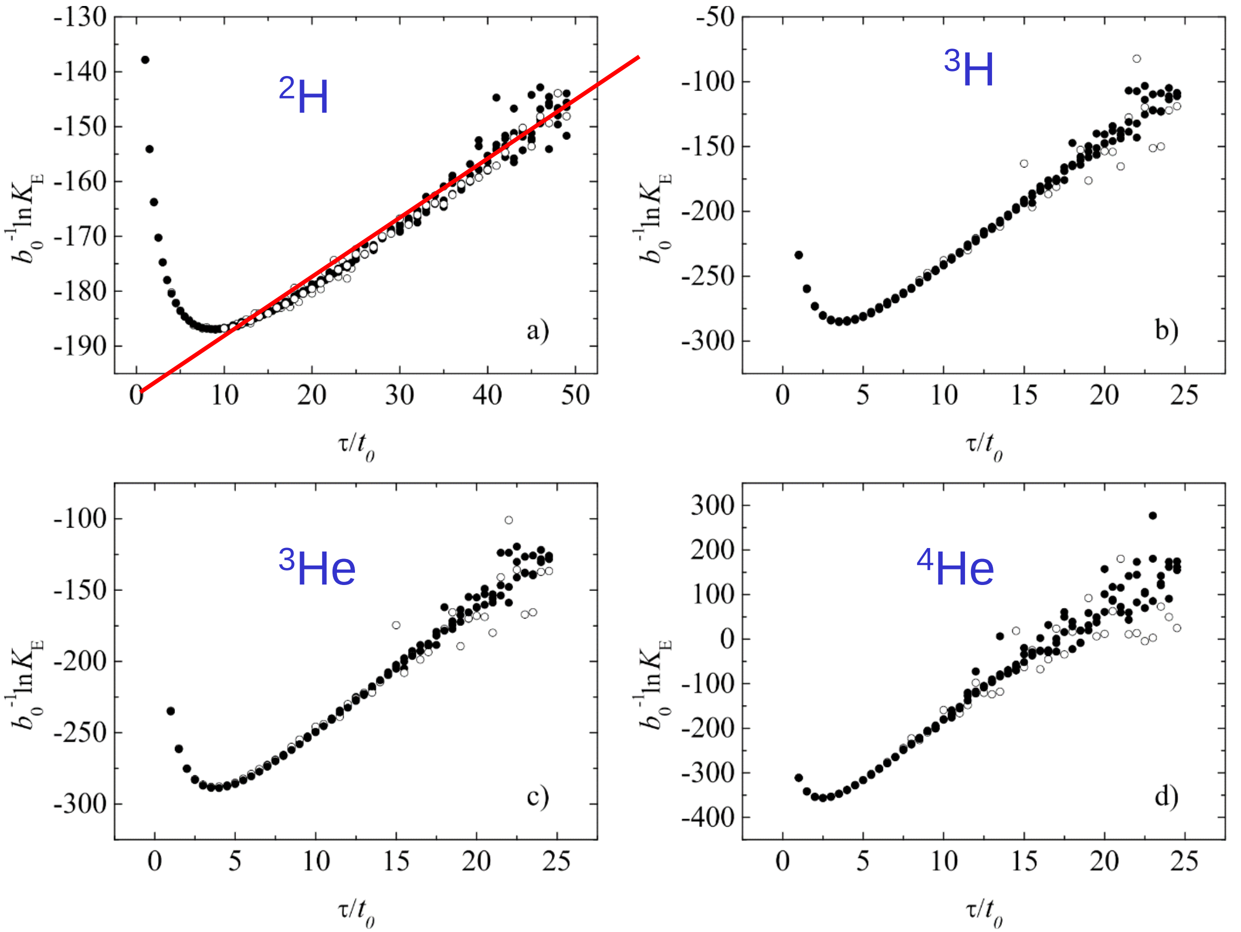


Statistics, *n*	Symbol
10^5	○
10^6	●
$5{\cdot}10^6$	●
10^7	●

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

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

Results of calculation the energy of ground state

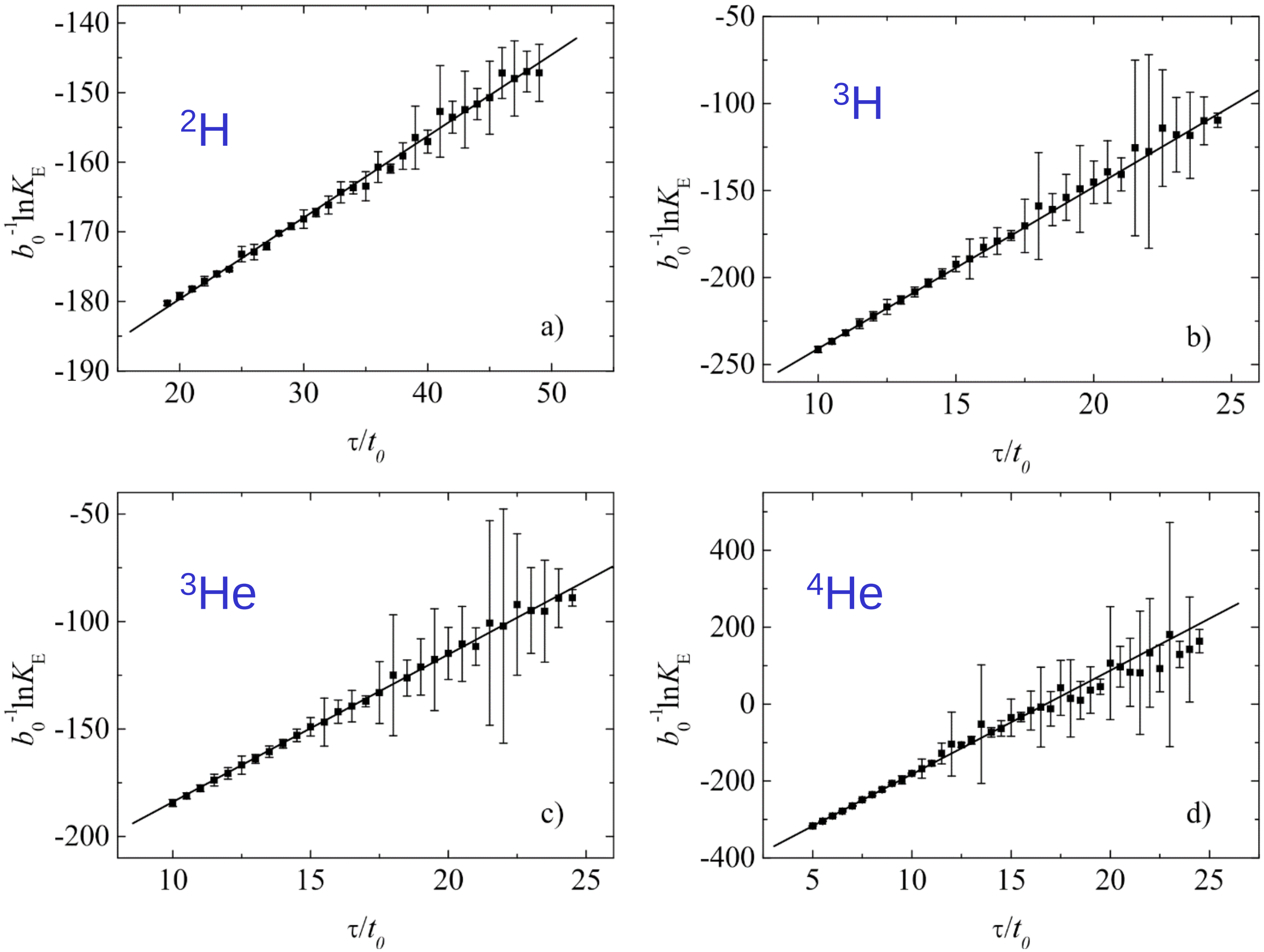


Statistics, n	Symbol
10^5	○
10^6	●
$5\cdot10^6$	●
10^7	●

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

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

Results of calculation of ground state energy



The slopes were obtained for the straight parts of curves and data points with statistics 10^6, $5\cdot10^6$, 10^7

Comparison of the theoretical and experimental binding energy $E_b = - E_0$

Atomic nucleus	Theoretical value, MeV	Experimental value, MeV
^{2}H	1.17 ± 1	2.225
^{3}H	9.29 ± 1	8.482
^{3}He	6.86 ± 1	7.718
^{4}He	26.95 ± 1	28.296

Experimental data was taken from the NRV Knowledge Base

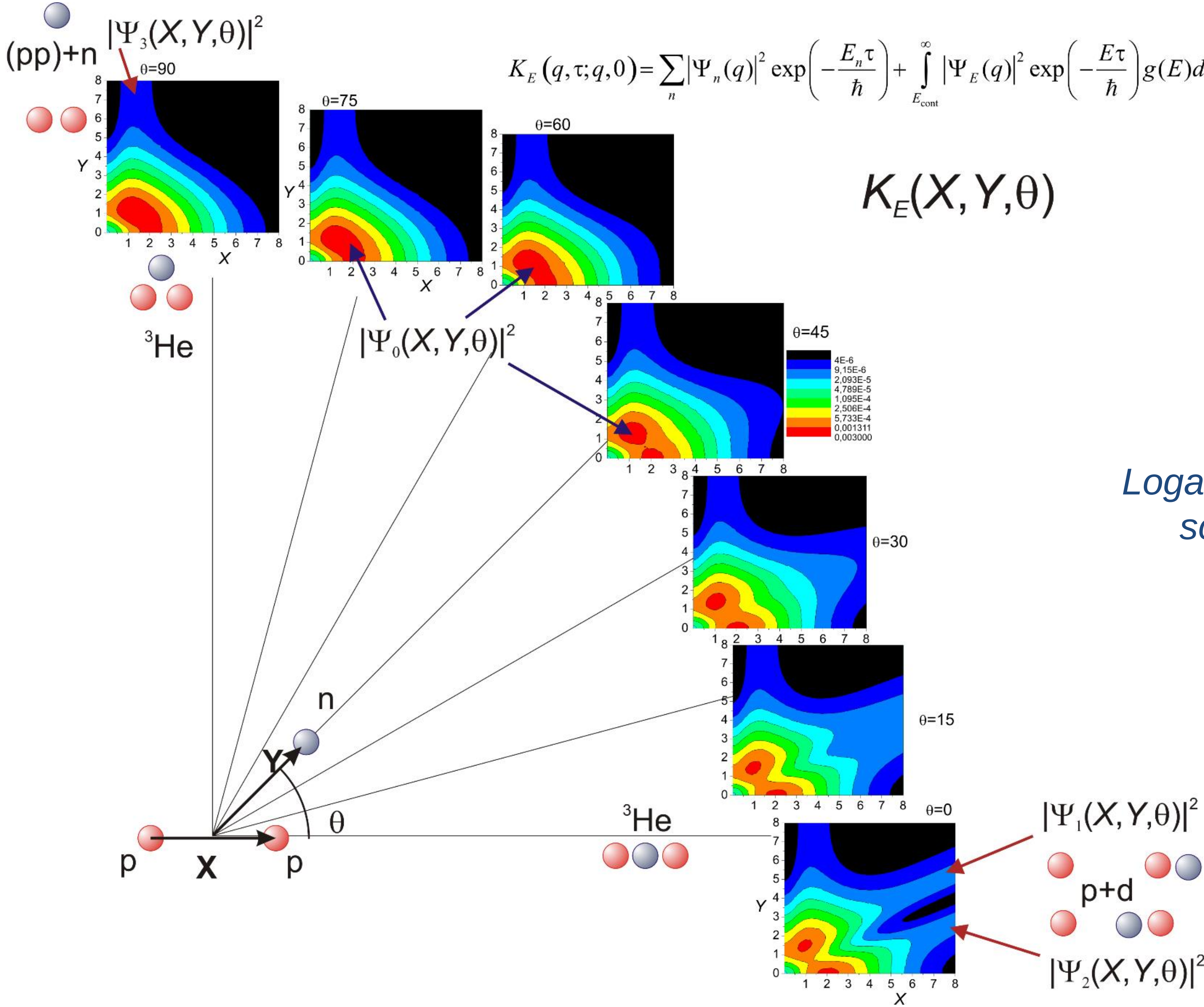
http://nrv.jinr.ru/nrv/

Reasonable agreement with experimental data without any fitting

Propagator for ^{3}He (p + p + n)

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

$K_E(X,Y,\theta)$



Logarithmic scale

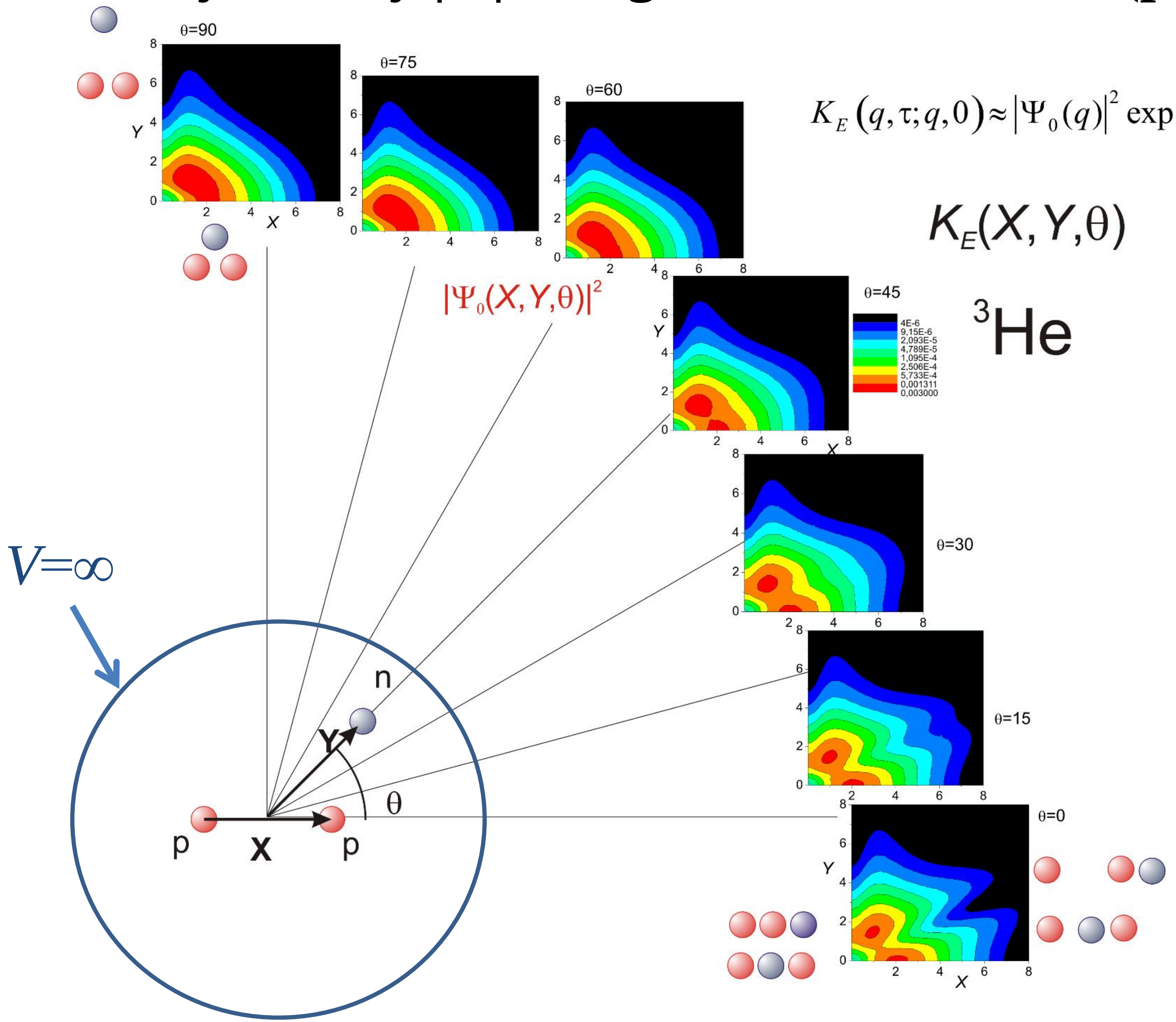
Probability density $|\Psi|^2$ for ground state of ^{3}He (p + p + n)

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

$K_E(X,Y,\theta)$

^{3}He

Logarithmic scale



Results for ground state of ^{3}He nucleus (p + p + n)

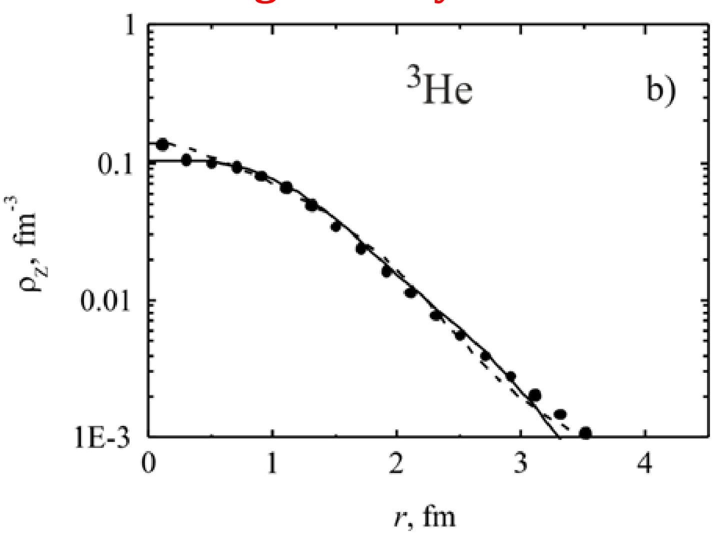
Binding energy, MeV

Theory	Experiment
6.86 ± 1	7.718

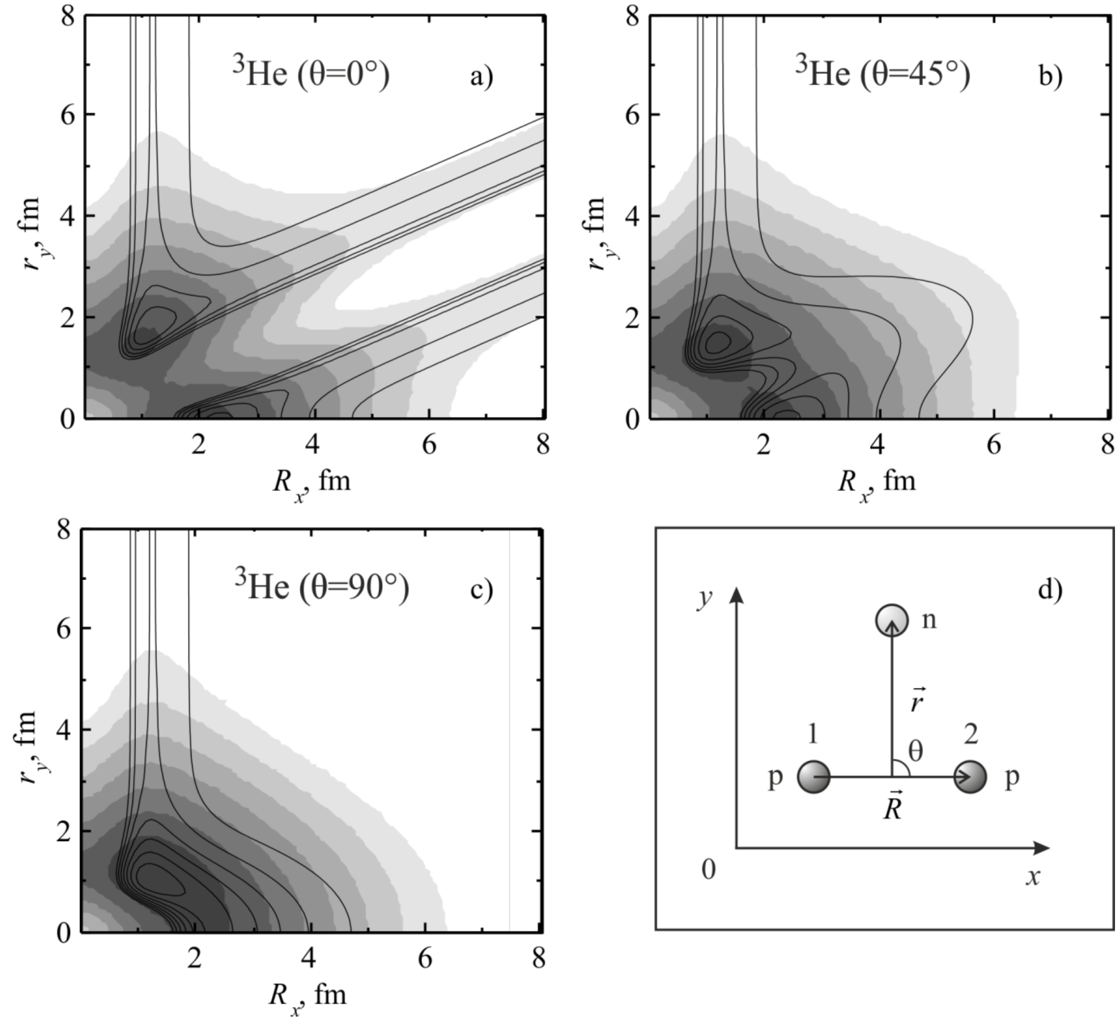
Charge radius, fm

Theory	Experiment
1.94	1.9664

Charge density



Probability density $|\Psi|^2$



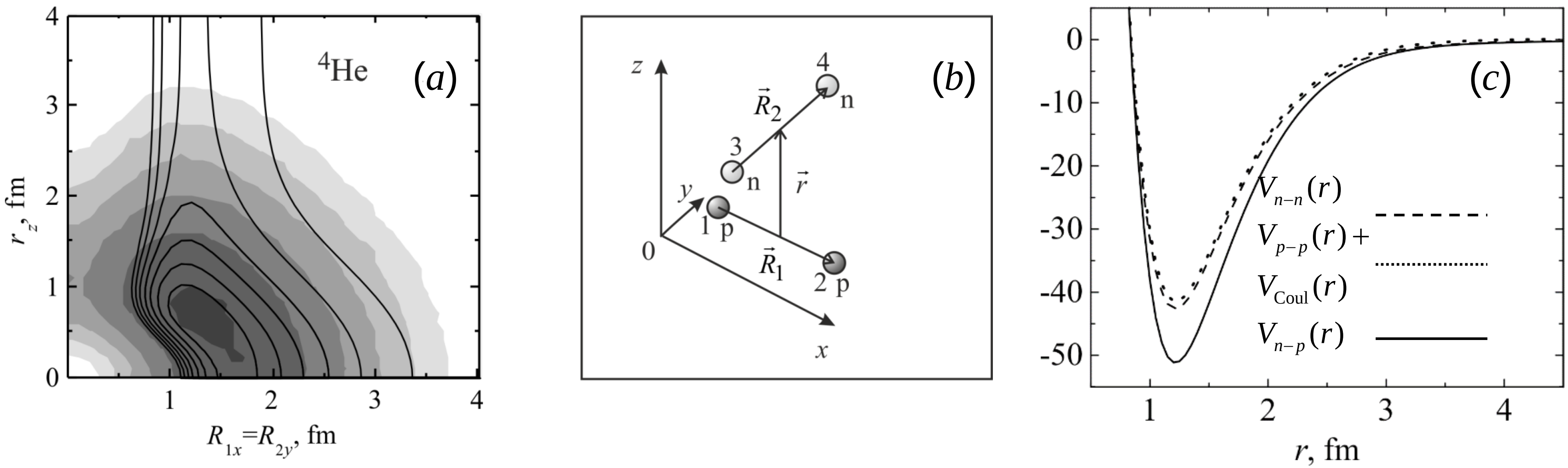
Reasonable results and good agreement with experimental data

Probability density for ^{4}He nucleus ($p + p + n + n$)

$$\left|\Psi_0\left(\vec{R}_1;\vec{r};\vec{R}_2\right)\right|^2 = \left|\Psi_0\left(R_{1x},0,0;0,0,r_z;0,R_{2y}=R_{1x},0\right)\right|^2$$

for symmetric tetrahedral configuration of four nucleons:

$$\vec{R}_1 \perp \vec{r} \perp \vec{R}_2,\ \left|\vec{R}_1\right| = \left|\vec{R}_2\right|,\ \vec{R}_1 = \left(R_{1x},0,0\right),\ \vec{r} = \left(0,0,r_z\right),\ \vec{R}_2 = \left(0,R_{2y}=R_{1x},0\right)$$



(a) The probability density distribution for the configurations of ^{4}He nucleus together with the potential energy surface (linear scale, lines).

(b) The vectors in the Jacobi coordinates.

(c) Nucleon-nucleon potentials in the model [1].

[1] V. V. Samarin, M. A. Naumenko. Bull. Russ. Ac. of Sci. Phys, **80**. 283 (2016). http://link.springer.com/article/10.3103/S1062873816030278

Comparison of calculation time for ^{3}He nucleus (p + p + n)

Ground state energy

Statistics, *n*	Intel Core i5 3470 (1 thread), sec	Tesla K40s, sec	Performance gain, times
10^5	≈1854	≈8	≈241
10^6	≈18377	≈47	≈389
$5 \cdot 10^6$	–	≈221	–
10^7	–	≈439	–

Probability density $|\Psi|^2$ in 43200 points

Statistics, *n*	Intel Core i5 3470 (1 thread), estimation	Tesla K40
10^6	~ 177 days	≈ 11 hours

Method enables calculations impossible before

Conclusions

- *The algorithm of calculation of ground states of few-body nuclei by Feynman's continual integrals method allowing us to perform calculations directly on GPU using NVIDIA CUDA technology was developed and implemented on C++ language;*

- *The energy and the square modulus of the wave function of the ground states of several few-body nuclei have been calculated; the method may also be applied to the calculation of cluster nuclei;*

- *Correctness of the calculations was justified by comparison with*
  - *the wave function obtained using the shell model*
  - *experimental binding energies*
  - *experimental charge radii and charge distributions*

- *The results show that the use of GPGPU significantly increases the speed of calculations. This allows us to*
  - *increase the statistics and accuracy of calculations*
  - *reduce the space step in the calculation of the wave functions*
  - *simplifies the process of debugging and testing*
  - *enables calculations impossible before*

Additional information

- *The results are submitted to the international journal*

SUPERCOMPUTING FRONTIERS AND INNOVATIONS

An International Journal

[*http://superfri.org/*](http://superfri.org/)

- *International Workshop on Few-Body Systems (FBS-Dubna-2016)*
  [*http://theor.jinr.ru/~fbs2016/index.html*](http://theor.jinr.ru/~fbs2016/index.html)

  BLTP, July 7, Thursday, 16:50-17:20
  V.V. Samarin, M.A. Naumenko (Presented by Vyacheslav SAMARIN)
  Study of ground states of few body nuclei by Feynman's continual integrals method

Thank You