Lecture 27: Adiabatic Projection Method and Pinhole Algorithm

Dean Lee
Facility for Rare Isotope Beams
Michigan State University
Nuclear Lattice EFT Collaboration
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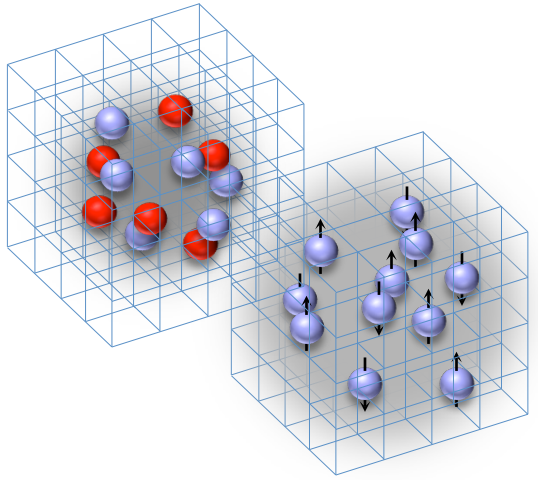


From Quarks and Gluons to Nuclear Forces and Structure

Science objectives

Ab initio calculations of scattering and reactions relevant to alpha processes in stellar evolution and Type Ia supernovae

$^4\mathrm{He} + {}^4\mathrm{He} \to {}^4\mathrm{He} + {}^4\mathrm{He}$

$^4\mathrm{He} + {}^4\mathrm{He} + {}^4\mathrm{He} \to {}^{12}\mathrm{C} + \gamma$

$^{12}\mathrm{C} + {}^4\mathrm{He} \to {}^{16}\mathrm{O} + \gamma$

$^{16}\mathrm{O} + {}^4\mathrm{He} \to {}^{20}\mathrm{Ne} + \gamma$

$^{20}\mathrm{Ne} + {}^4\mathrm{He} \to {}^{24}\mathrm{Mg} + \gamma$

$^{24}\mathrm{Mg} + {}^4\mathrm{He} \to {}^{28}\mathrm{Si} + \gamma$

$^{12}\mathrm{C} + {}^{12}\mathrm{C} \to {}^{20}\mathrm{Ne} + {}^4\mathrm{He}$

$^{16}\mathrm{O} + {}^{16}\mathrm{O} \to {}^{28}\mathrm{Si} + {}^4\mathrm{He}$

Challenges

How to reduce computational scaling with number of nucleons in participating nuclei? Can we provide useful *ab initio* input for halo or cluster EFT calculations?

Adiabatic projection method

Development inspired by progress using no-core shell model with resonating group method to describe *ab initio* scattering and reactions in light nuclei.

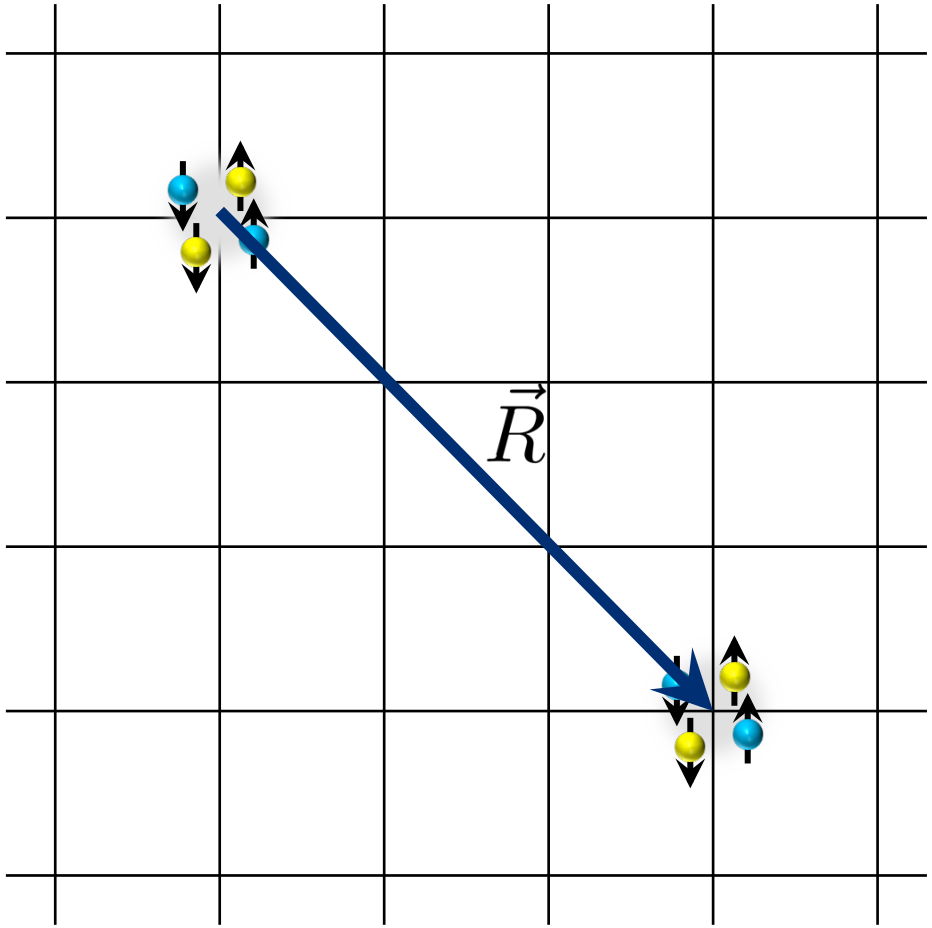
Navratil, Roth, Quaglioni, PRC 82 034609 (2010); Navratil, Quaglioni, PRC 83 044609 (2011); etc.

Strategy is to divide the problem into two parts. In the first part, we use Euclidean time projection and lattice Monte Carlo to derive an *ab initio* low-energy cluster Hamiltonian, called the adiabatic Hamiltonian (adiabatic transfer matrix for nonzero temporal lattice spacing).

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.

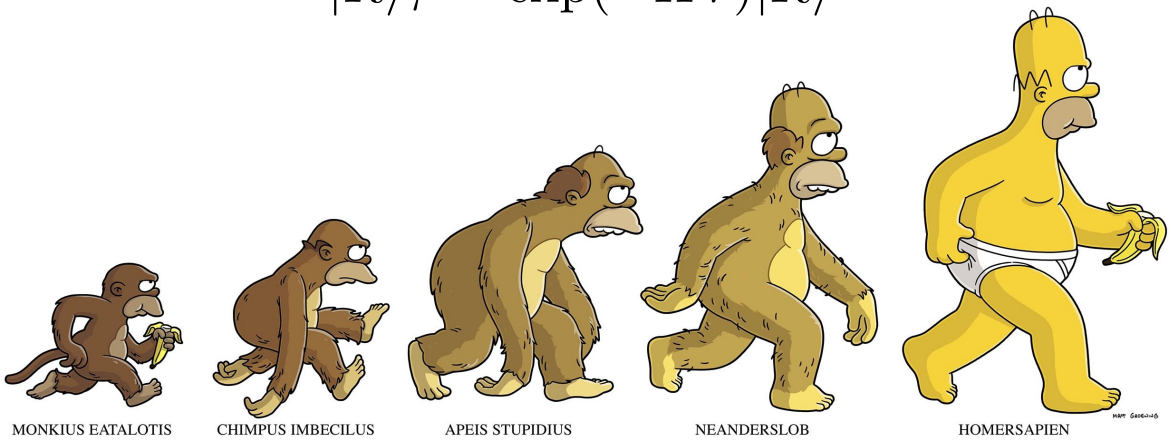
Start with localized cluster states for all possible separation vectors $\vec{R}$

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r}+\vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$



Cluster evolution with Euclidean time.

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$



For notational simplicity we use the language of continuous time evolution. The actual calculations use normal-ordered transfer matrices.

$$|\vec{R}\rangle_\tau = [: \exp(-H\alpha_t) :]^{L_t} \, |\vec{R}\rangle$$

M. Groening

Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time to form dressed cluster states

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

Evaluate matrix elements of the full microscopic Hamiltonian with respect to the dressed cluster states,

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

The adiabatic Hamiltonian is defined by the matrix product

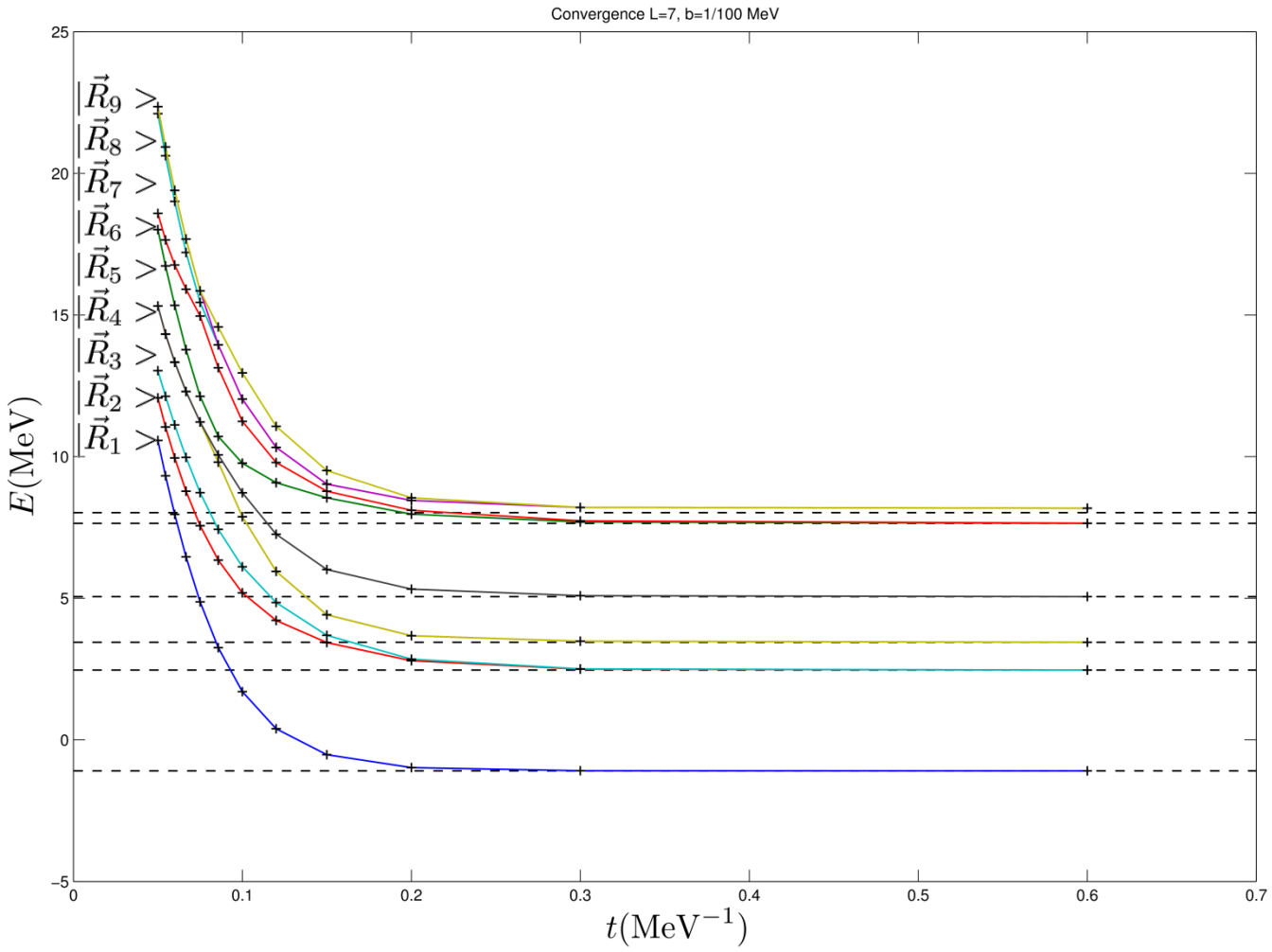
$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

One can see the similarity to no-core shell model with resonating group method. But in the adiabatic projection method we don't need to include excitations of the participating nuclei unless the energy is above the corresponding inelastic threshold.

Distortion and polarization of the nuclear wave functions are automatically produced by the Euclidean time projection.

As we increase the projection time, the adiabatic Hamiltonian exactly reproduces the low-energy spectrum of the full microscopic Hamiltonian.

Spin-quartet neutron-deuteron scattering



Pine, D.L., Rupak, EPJA 49 (2013)

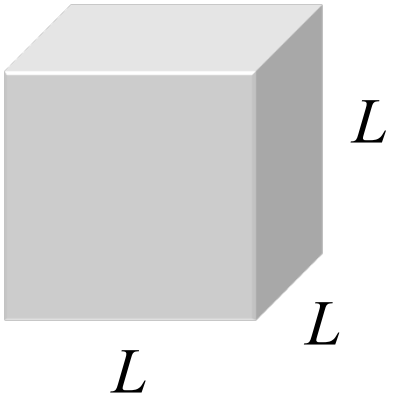
Lüscher's finite-volume formula

Lüscher, Comm. Math. Phys. 105 (1986) 153; NPB 354 (1991) 531

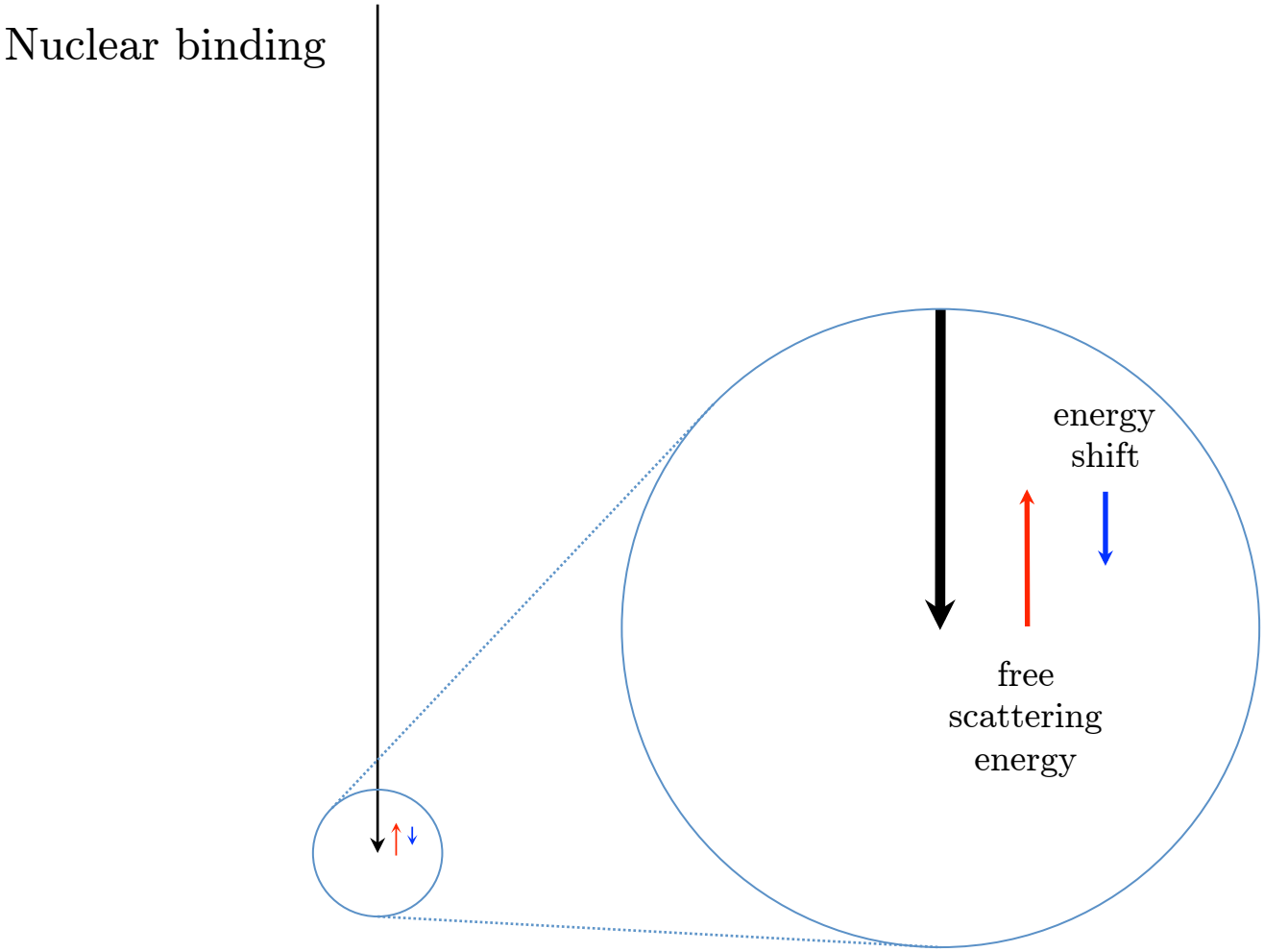
Two-particle energy levels near threshold in a periodic cube are related to the elastic phase shifts

$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta), \qquad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

$$S(\eta) = \lim_{\Lambda \to \infty} \left[\sum_{\vec{n}} \frac{\theta(\Lambda^2 - \vec{n}^2)}{\vec{n}^2 - \eta} - 4\pi\Lambda \right]$$



Signal-to-noise problems for finite-volume energy extraction



Asymptotic cluster scattering wave functions

In the far asymptotic region where our dressed clusters are widely separated, they interact only through infinite-range forces such as the Coulomb interaction.

Therefore we can describe everything with an effective cluster Hamiltonian H^{eff} that is nothing more than a free lattice Hamiltonian for two point particles plus any infinite-range interactions inherited from the full microscopic Hamiltonian. So in the asymptotic region we have

$$[N_\tau]_{\vec{R},\vec{R}'} = c \cdot \left[e^{-2H^{\text{eff}}\tau} \right]_{\vec{R},\vec{R}'} ,$$

$$[H_\tau]_{\vec{R},\vec{R}'} = c \cdot \left[e^{-H^{\text{eff}}\tau} H^{\text{eff}} e^{-H^{\text{eff}}\tau} \right]_{\vec{R},\vec{R}'} ,$$

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, PRC 92 (2015) 054612

Since

$$\left[N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'} = c^{-1/2} \cdot \left[e^{H^{\text{eff}}\tau}\right]_{\vec{R},\vec{R}'}$$

we conclude that the adiabatic Hamiltonian coincides with the effective cluster Hamiltonian in the asymptotic region

$$[H_\tau^a]_{\vec{R},\vec{R}'} = \left[H^{\text{eff}}\right]_{\vec{R},\vec{R}'}$$

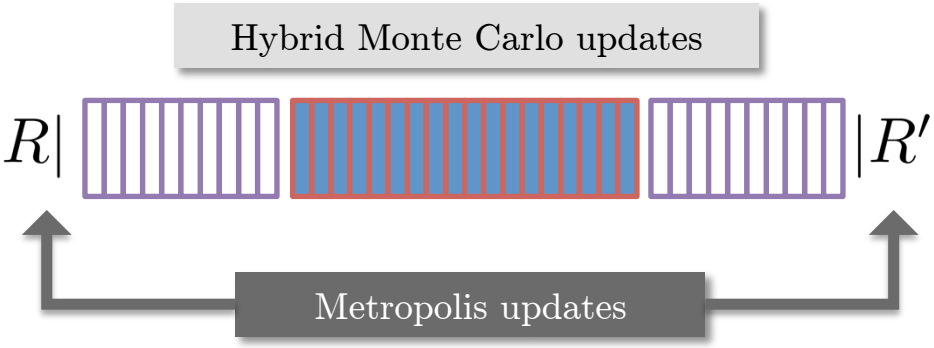
In the asymptotic region, we are inverting the diffusion process when computing the adiabatic Hamiltonian and are left with an effective cluster Hamiltonian in position space basis.

We use projections onto spherical harmonics defined on sets of lattice points with approximately the same distance from the origin.

$$|R\rangle^{L,L_z} = \sum_{||\vec{R}'|-R|<\Delta R} Y_{L,L_z}(\hat{R}')|\vec{R}'\rangle$$

New algorithm developed for auxiliary field updates and initial/final state updates

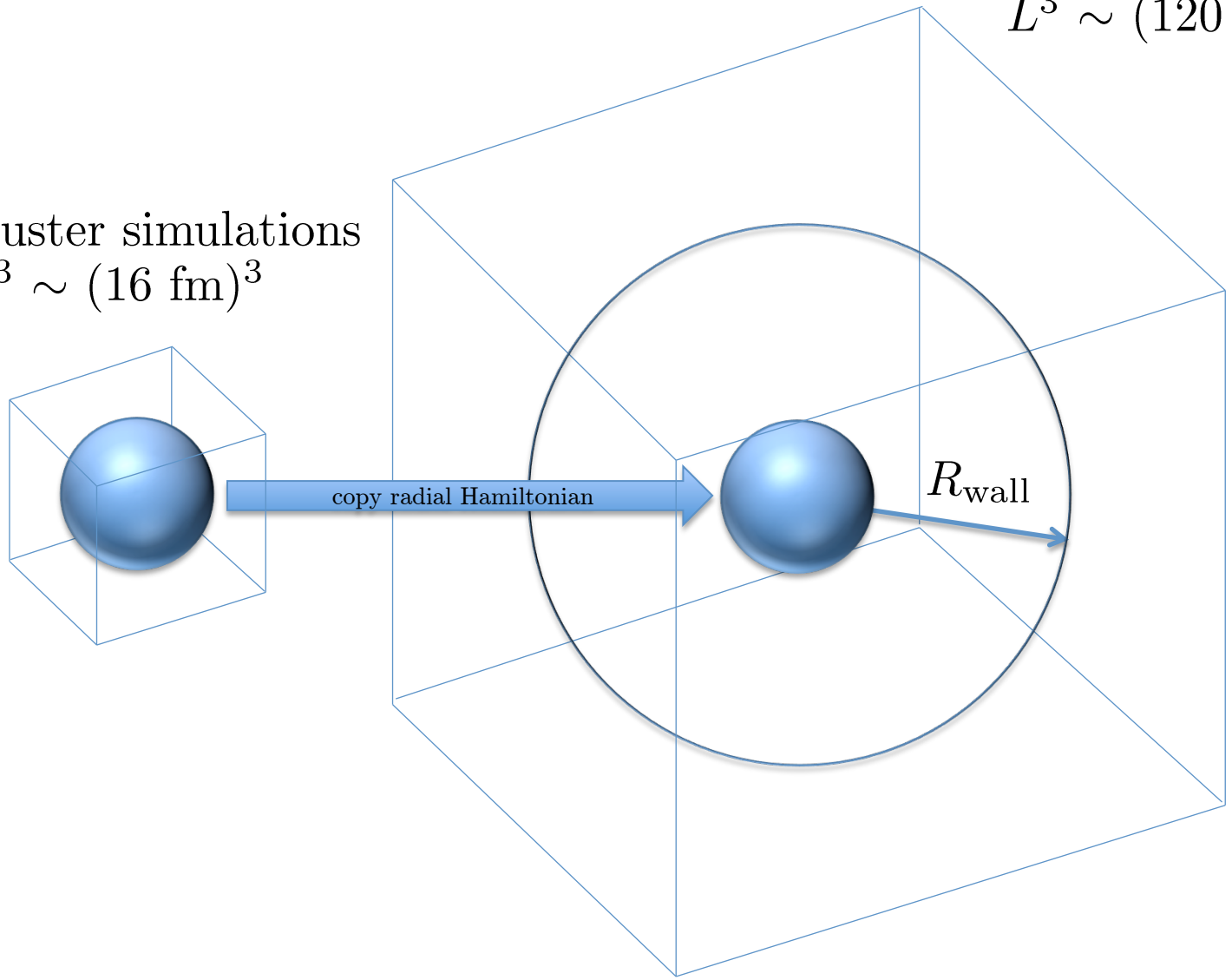
$$[Z_{n_t,\mathrm{LO}}]^{L,L_z}_{R,R'} = {}^{L,L_z}\langle R|$$



$$|R'\rangle^{L,L_z}$$

single cluster simulations
$L^3 \sim (120 \text{ fm})^3$

two cluster simulations
$L^3 \sim (16 \text{ fm})^3$

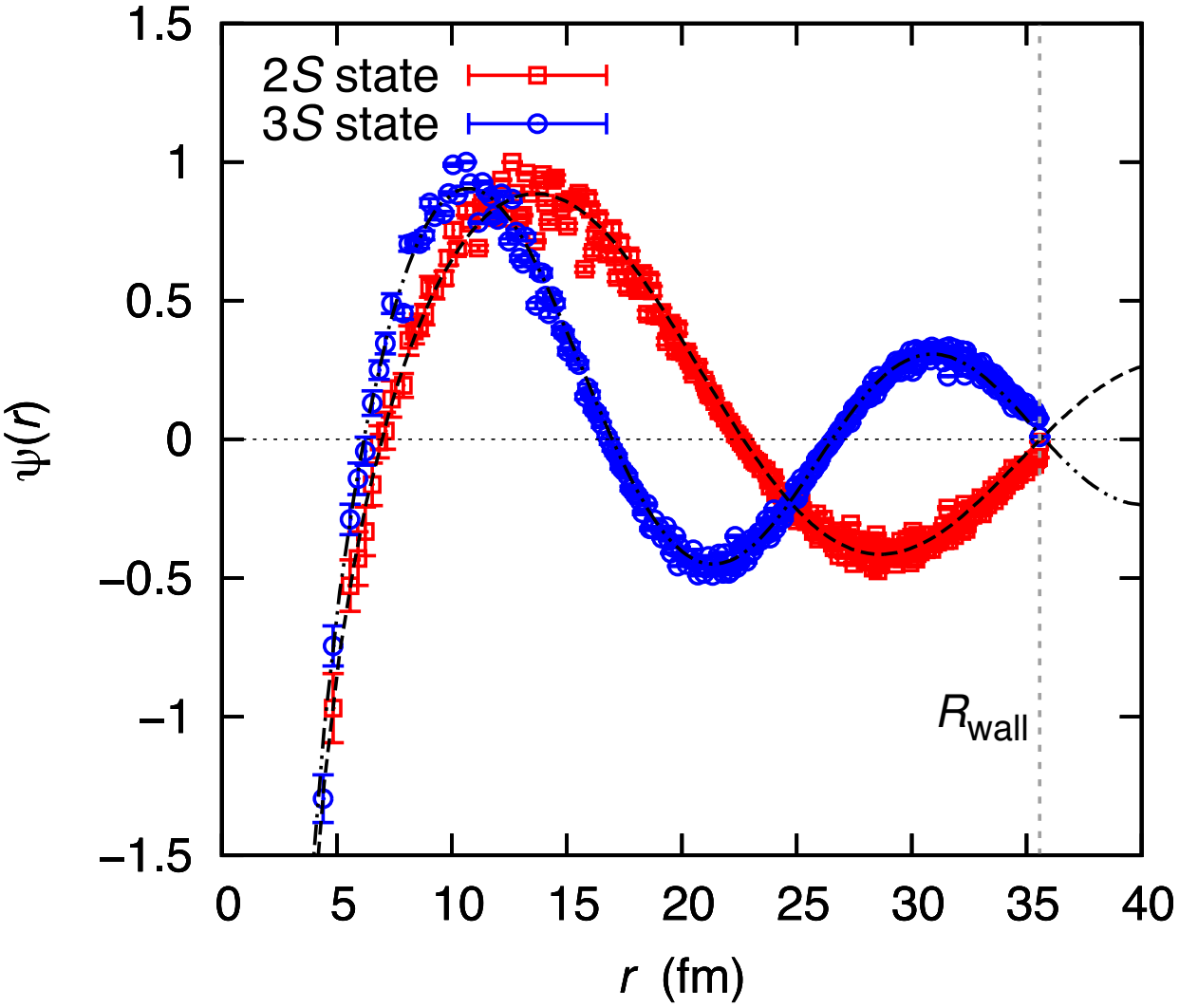


$$\underline{{}^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}}$$

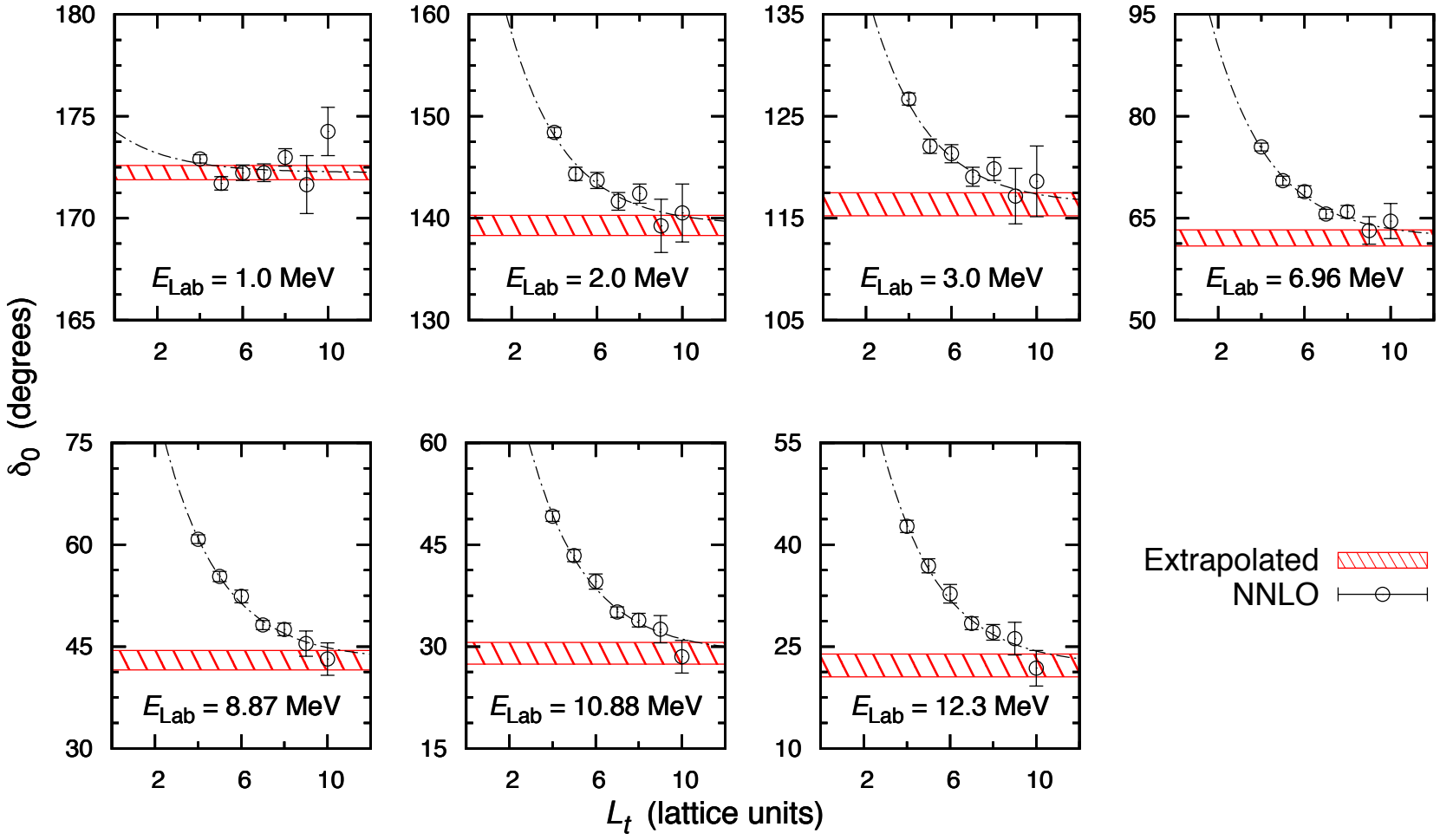
We now present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

Using the adiabatic projection method, we performed lattice simulations for the S-wave and D-wave channels.

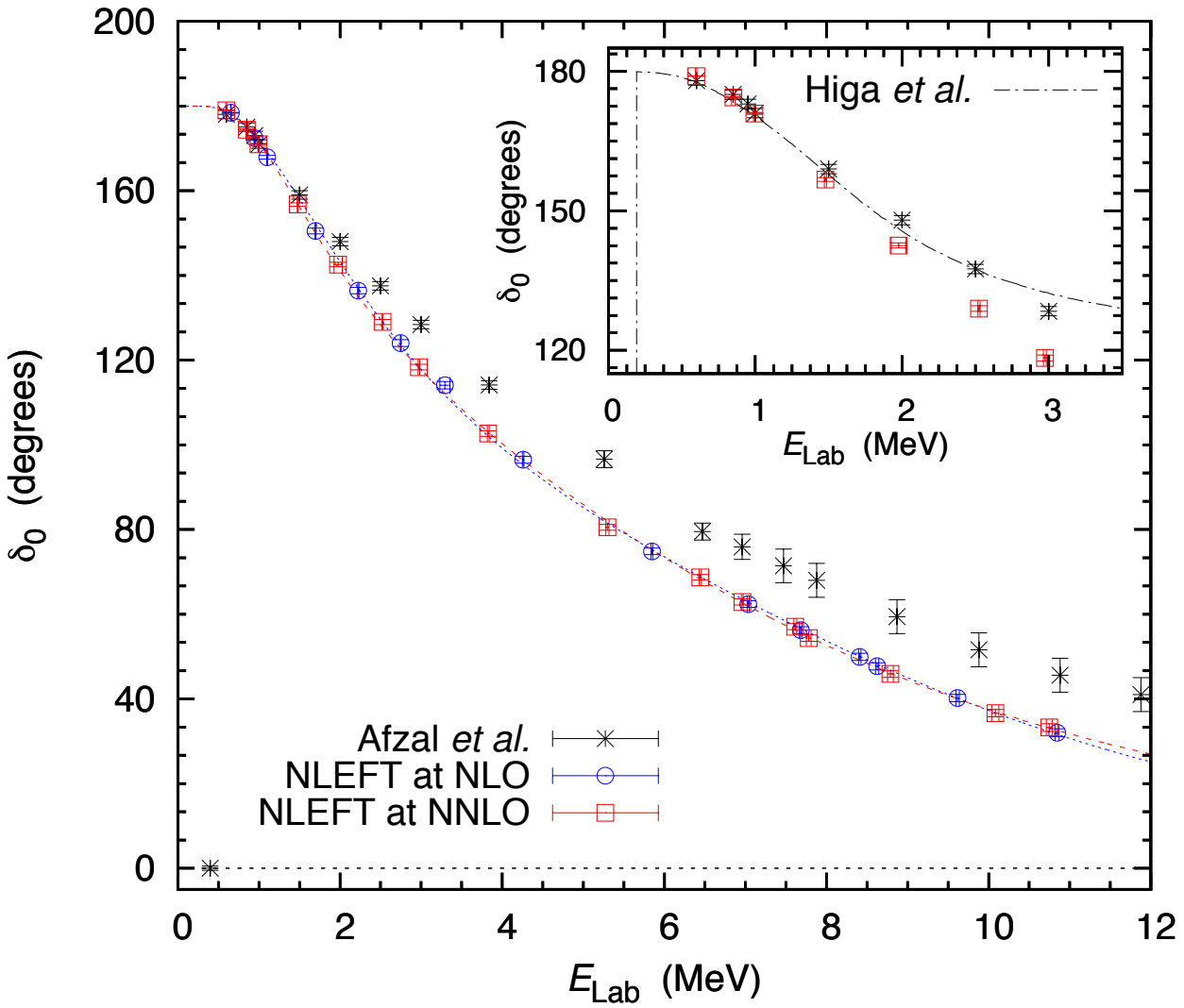
Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)


2S state
3S state
1.5
1
0.5
0
−0.5
−1
−1.5
ψ(r)
0
5
10
15
20
25
30
35
40
r (fm)
R_wall

S-wave scattering



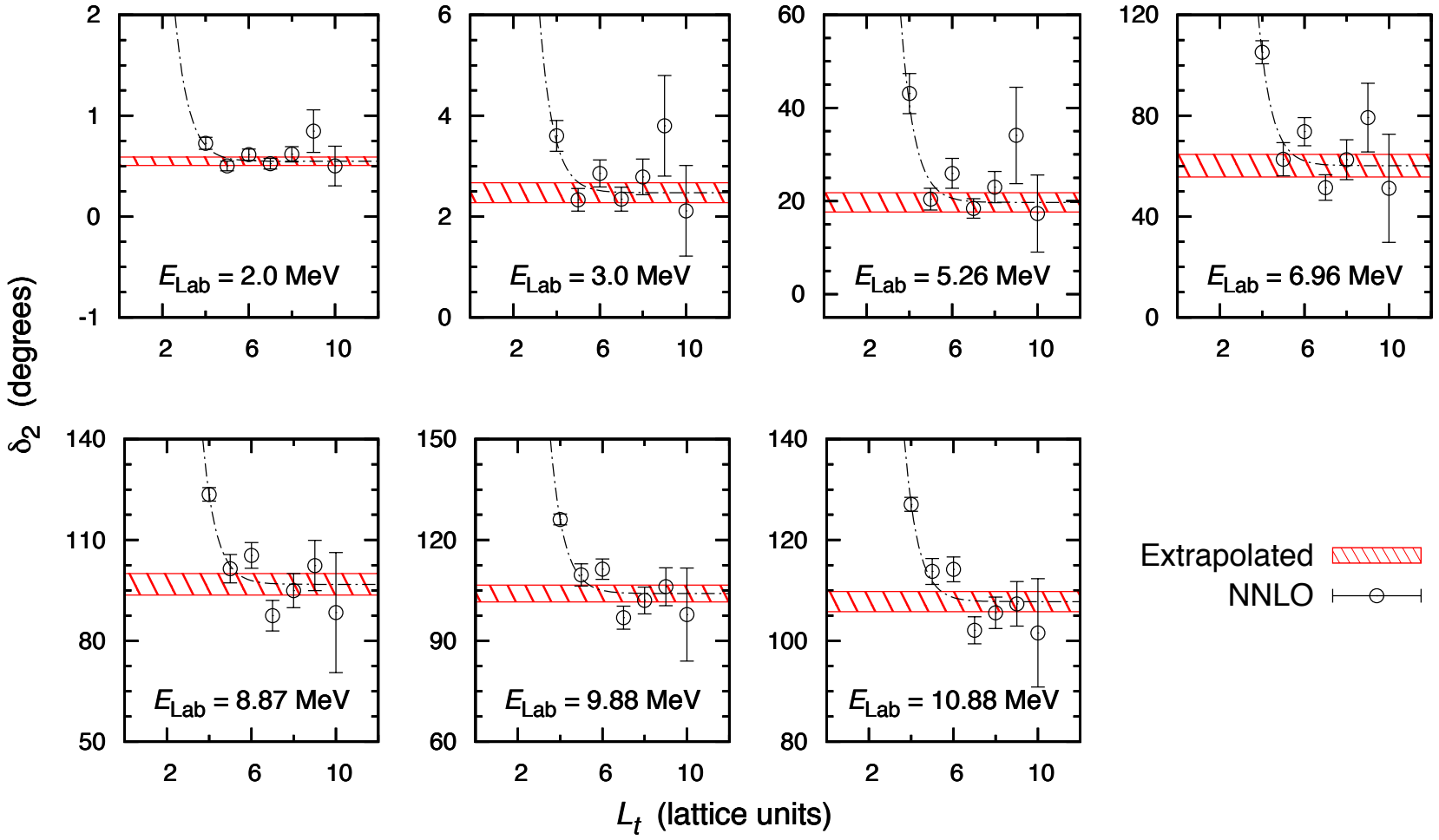
S-wave scattering



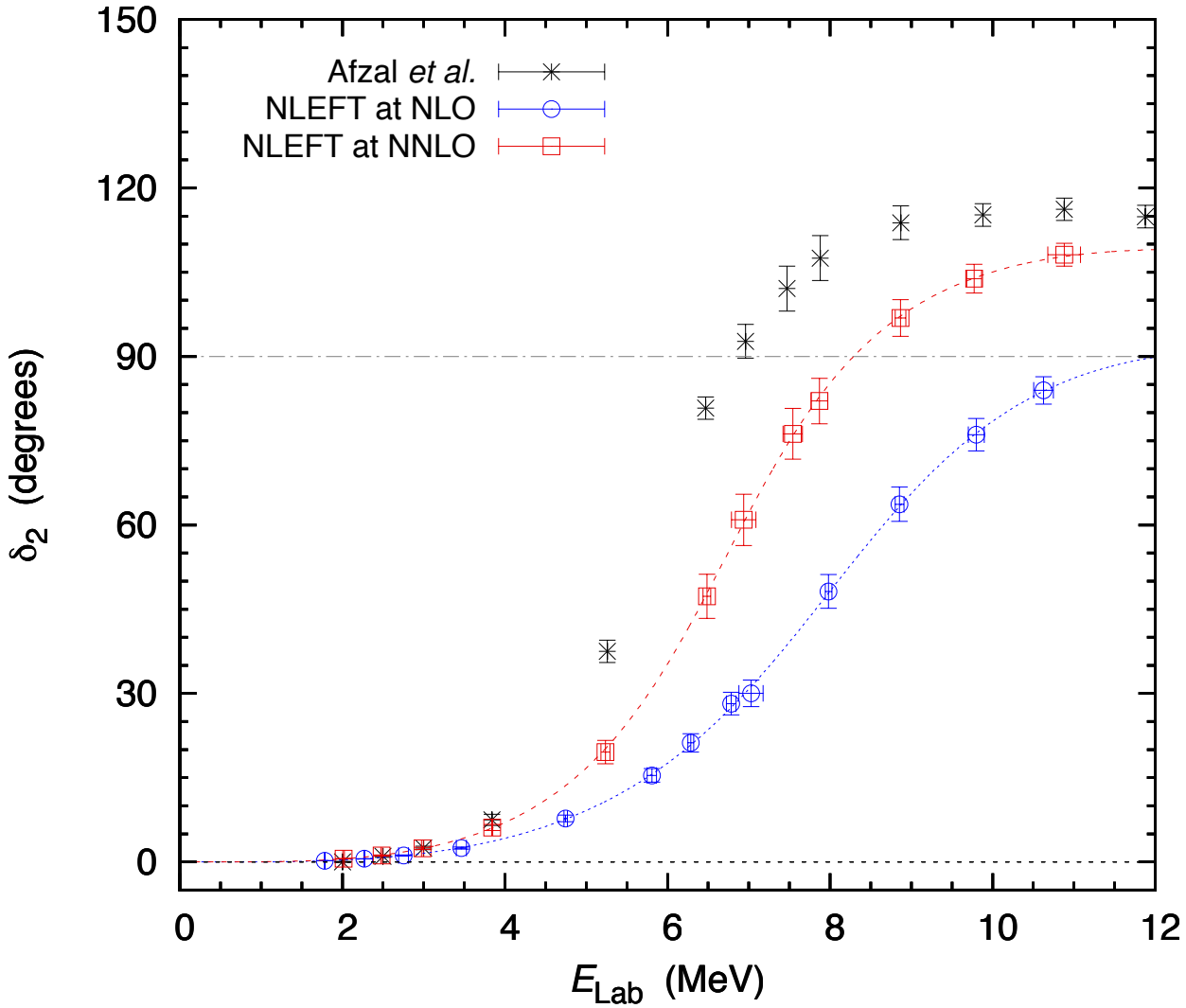
Afzal, Ahmad, Ali, RMP 41 247 (1969)

Higa, Hammer, van Kolck, NPA 809 171(2008)

D-wave scattering



D-wave scattering



Pinhole Algorithm

Consider the density operator for nucleon with spin i and isospin j

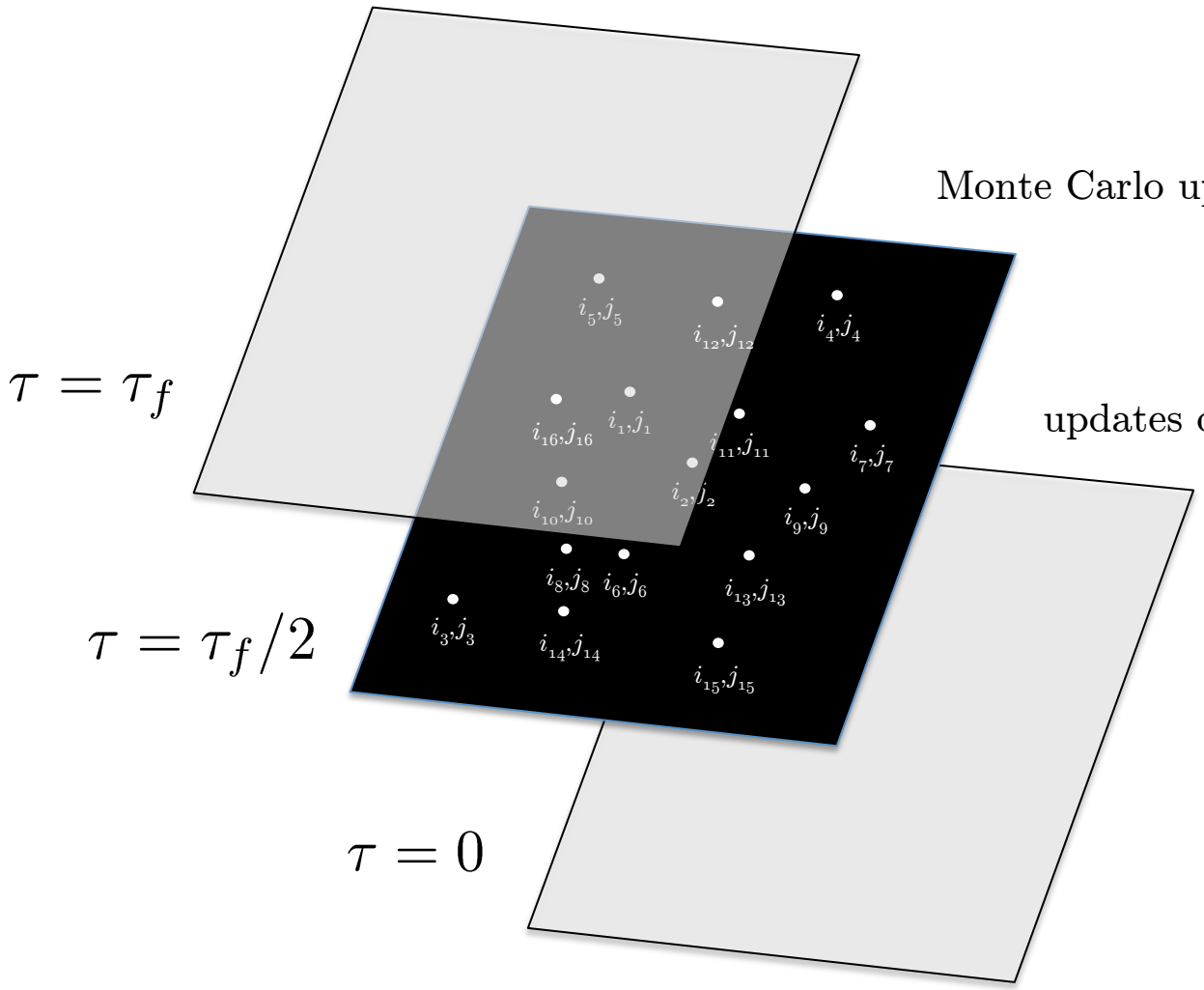
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

We construct the normal-ordered A-body density operator

$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = :\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$

In the simulations we do Monte Carlo sampling of the amplitude

$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A,t) = \langle\Psi_I|e^{-Ht/2}\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A)e^{-Ht/2}|\Psi_I\rangle$$

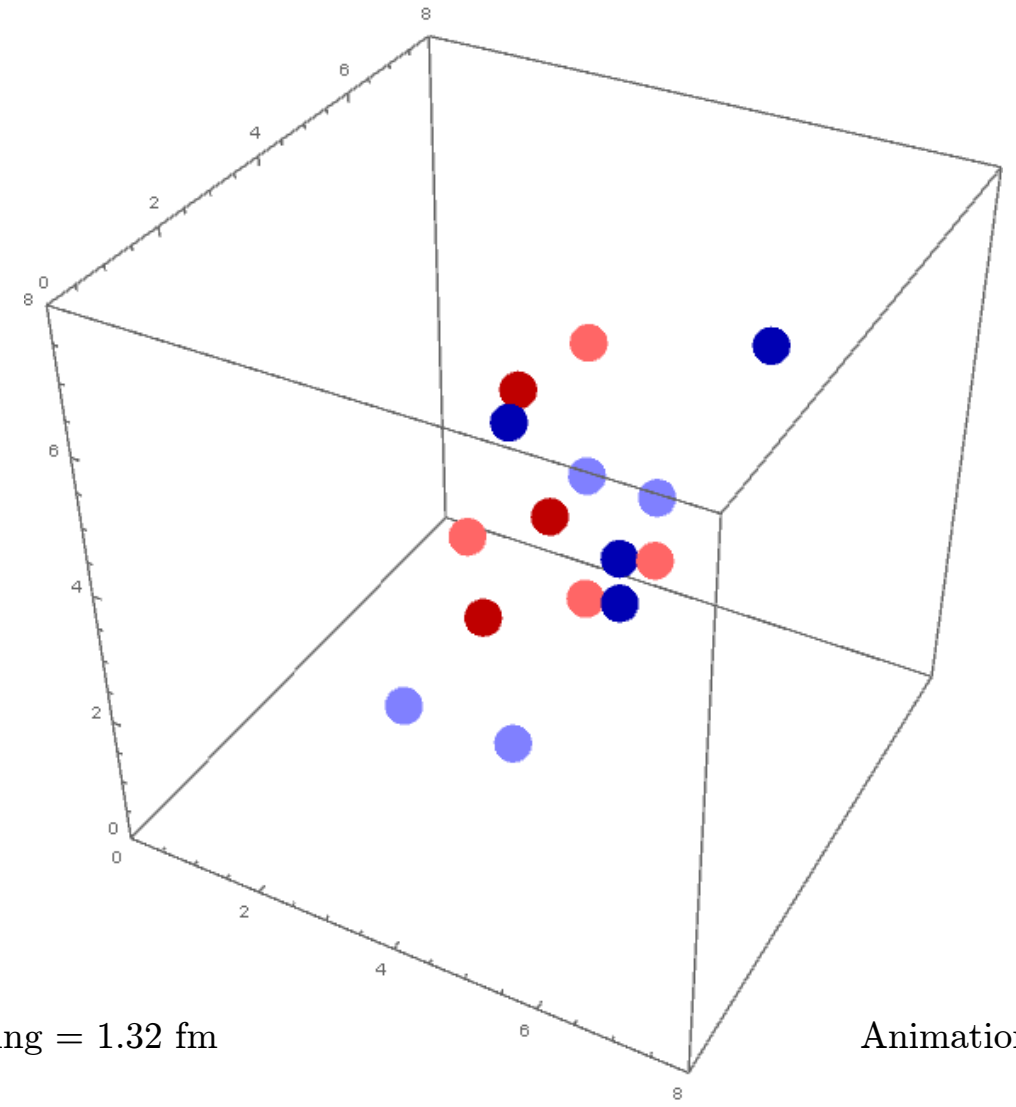


Monte Carlo updates of pinholes

Monte Carlo
updates of auxiliary/pion fields

Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

Oxygen-16



$p_\uparrow$

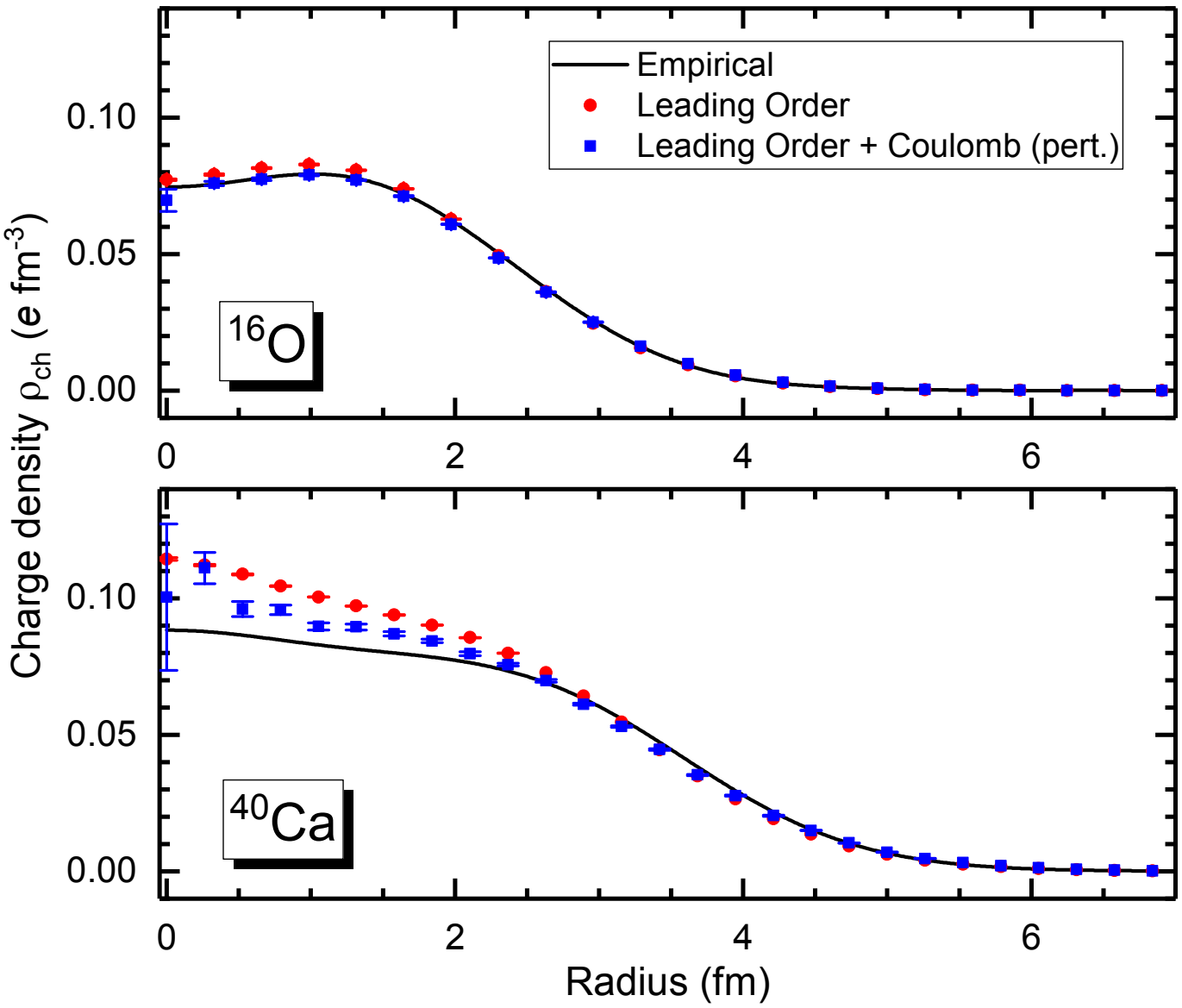
$p_\downarrow$

$n_\uparrow$

$n_\downarrow$

lattice spacing = 1.32 fm

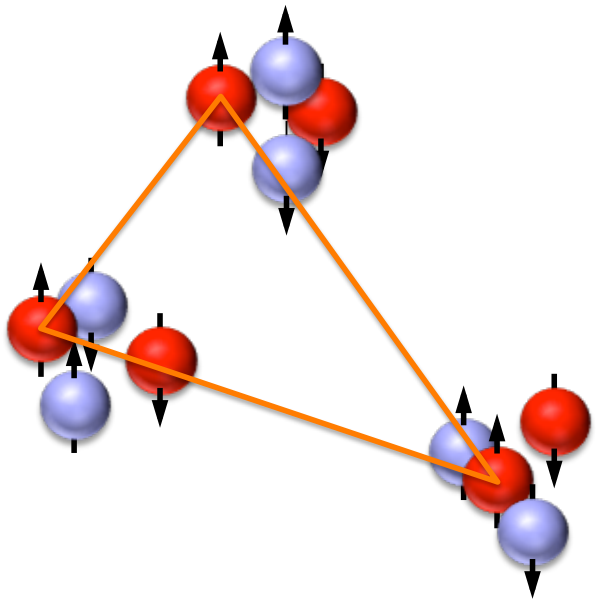
Animation by Gabriel Given



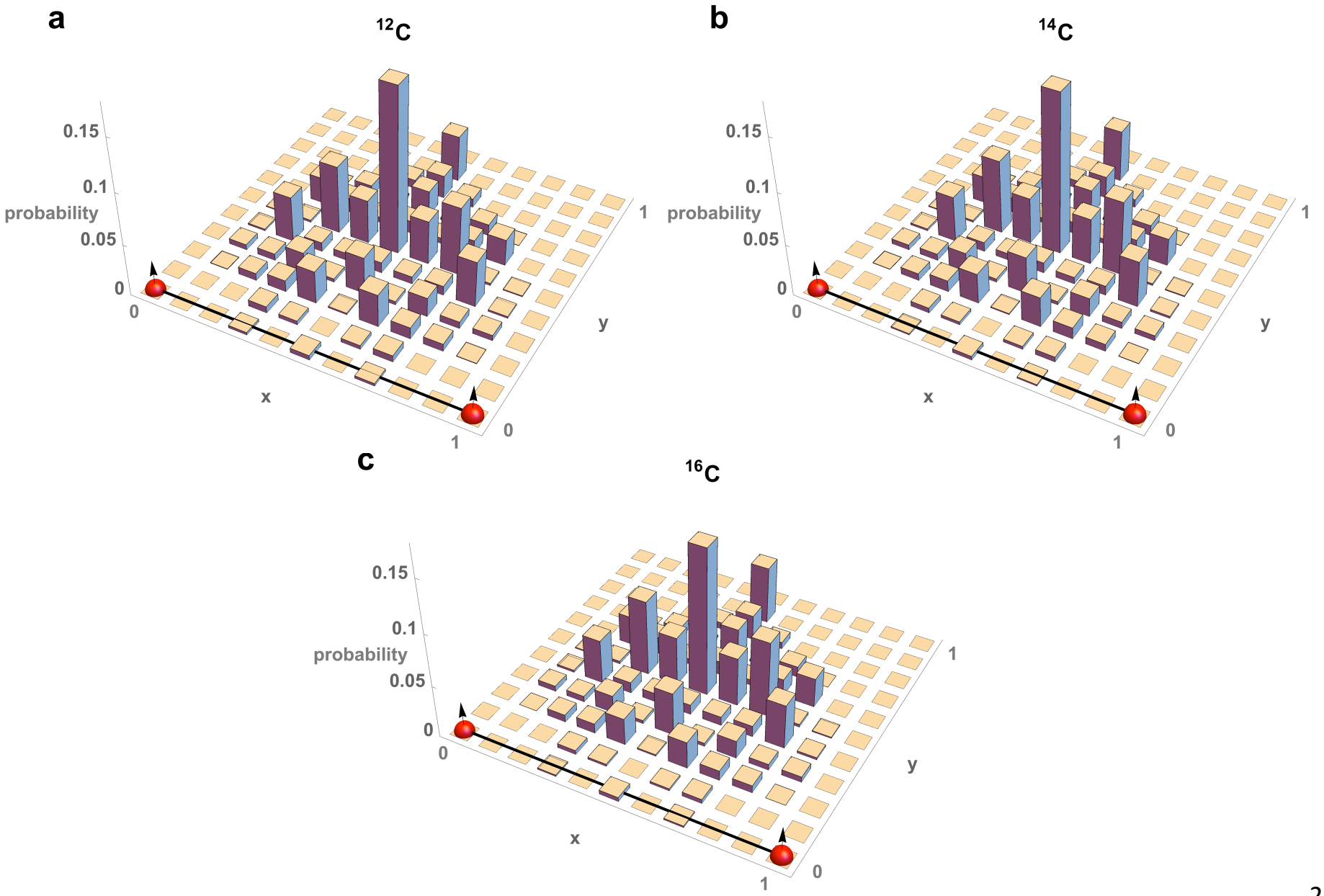
Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, arXiv:1812.10928

Model-independent measure of alpha cluster geometry

For the carbon isotopes, we can map out the alpha cluster geometry by computing the density correlations of the three spin-up protons. We compute these density correlations using the pinhole algorithm.



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)


a
^{12}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1
b
^{14}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1
c
^{16}C
0.15
0.1
probability
0.05
0
0
x
1
0
y
1

Nuclear thermodynamics

In order to compute thermodynamic properties of finite nuclei, nuclear matter, and neutron matter, we need to compute the partition function

$$\mathrm{Tr}\exp(-\beta H)$$

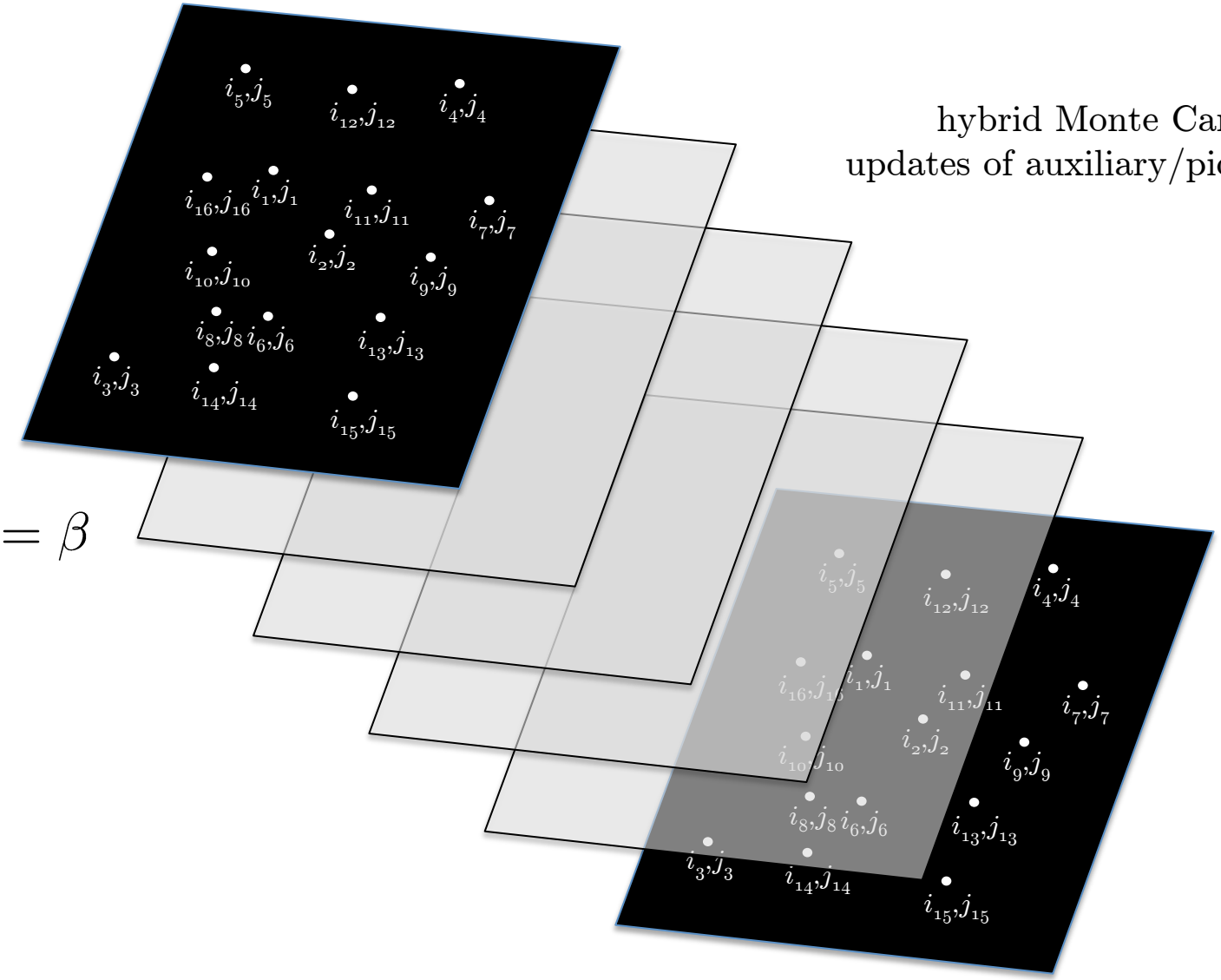
We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

$$\mathrm{Tr}\,O = \frac{1}{A!}\sum_{i_1\cdots i_A, j_1\cdots j_A, \mathbf{n}_1\cdots\mathbf{n}_A} \langle 0|a_{i_A,j_A}(\mathbf{n}_A)\cdots a_{i_1,j_1}(\mathbf{n}_1)\,O\,a^\dagger_{i_1,j_1}(\mathbf{n}_1)\cdots a^\dagger_{i_A,j_A}(\mathbf{n}_A)|0\rangle$$

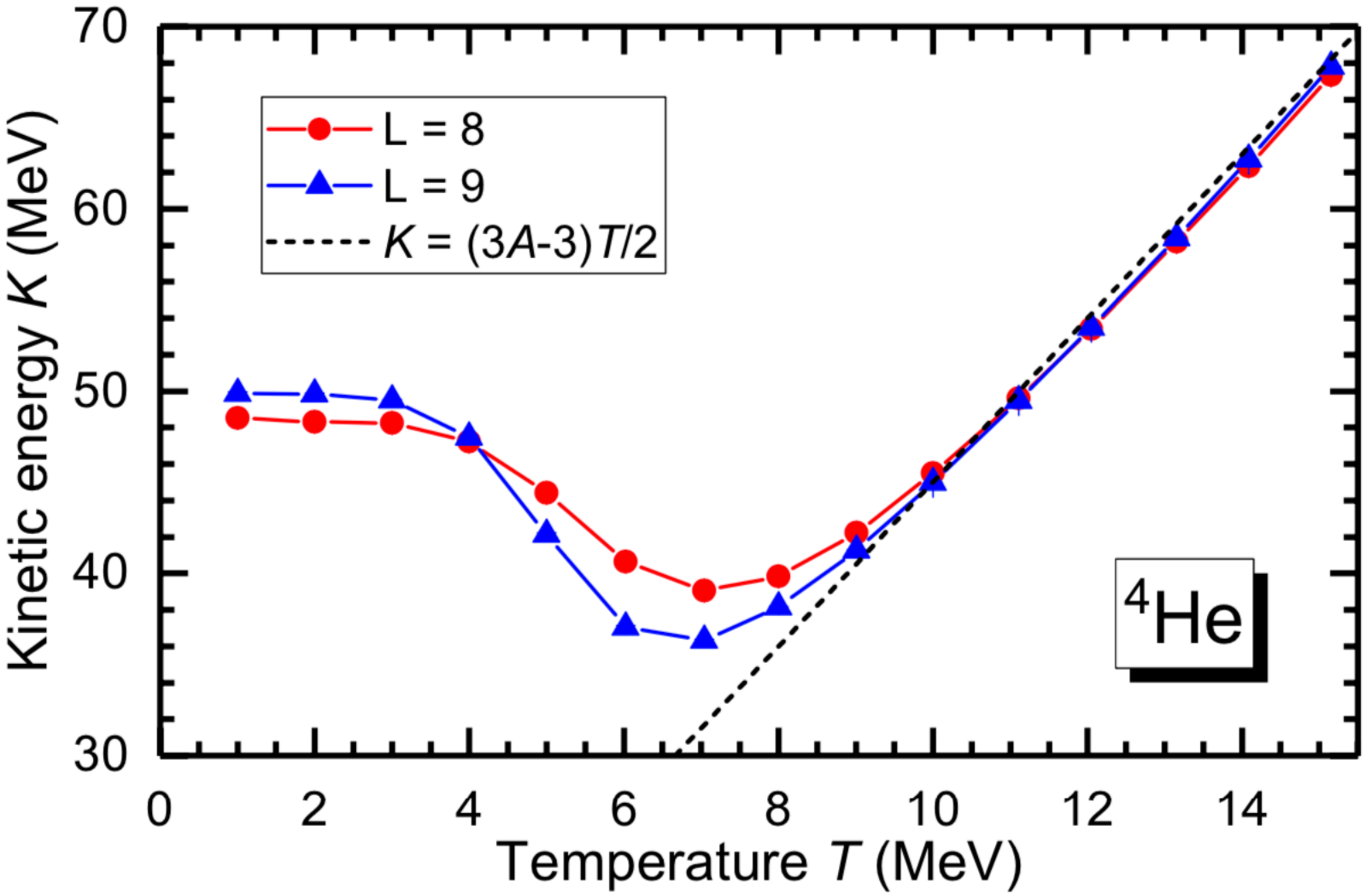
This can be used to calculate the partition function in the canonical ensemble.

Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, work in progress

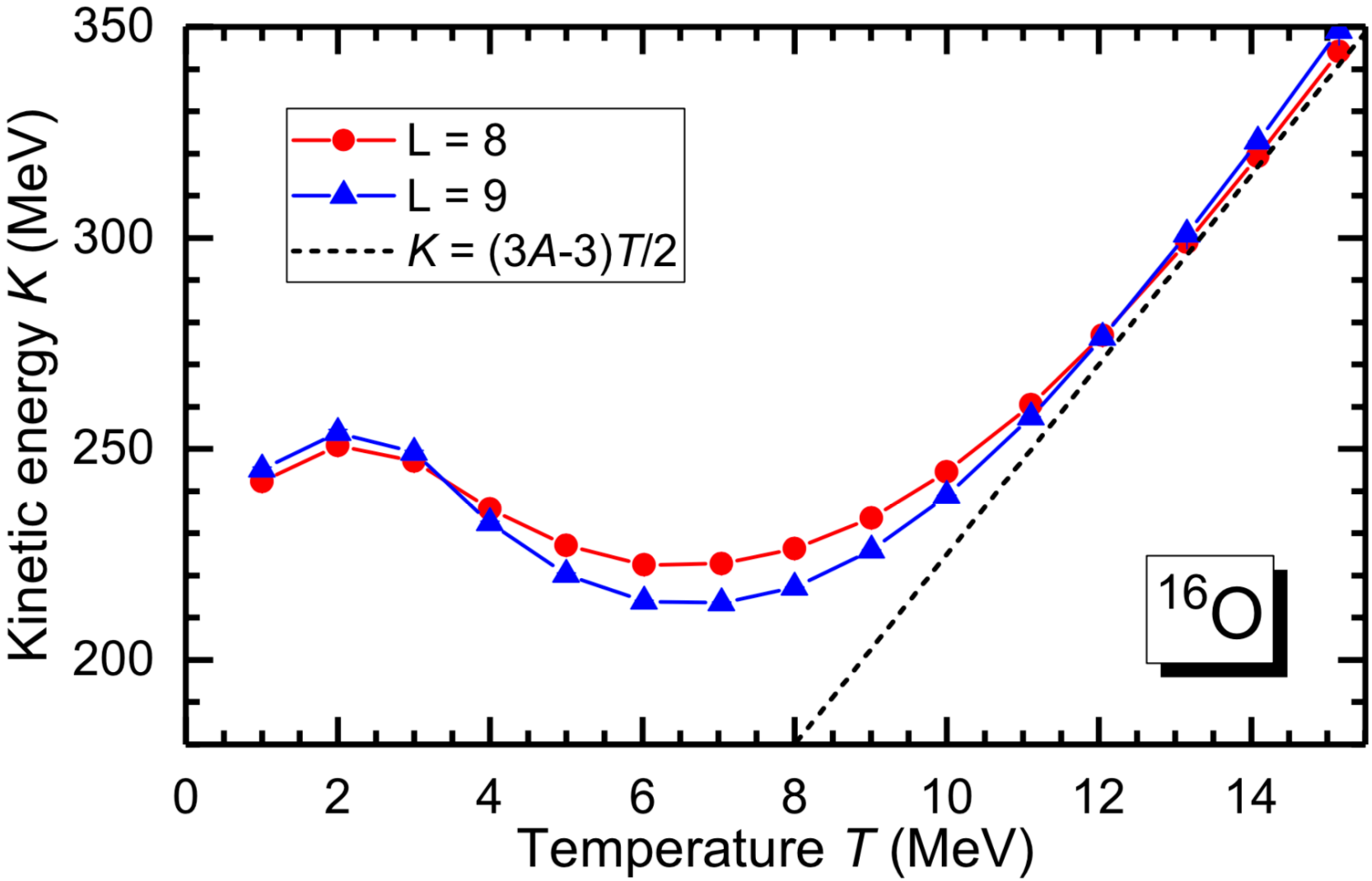
Metropolis updates of pinholes

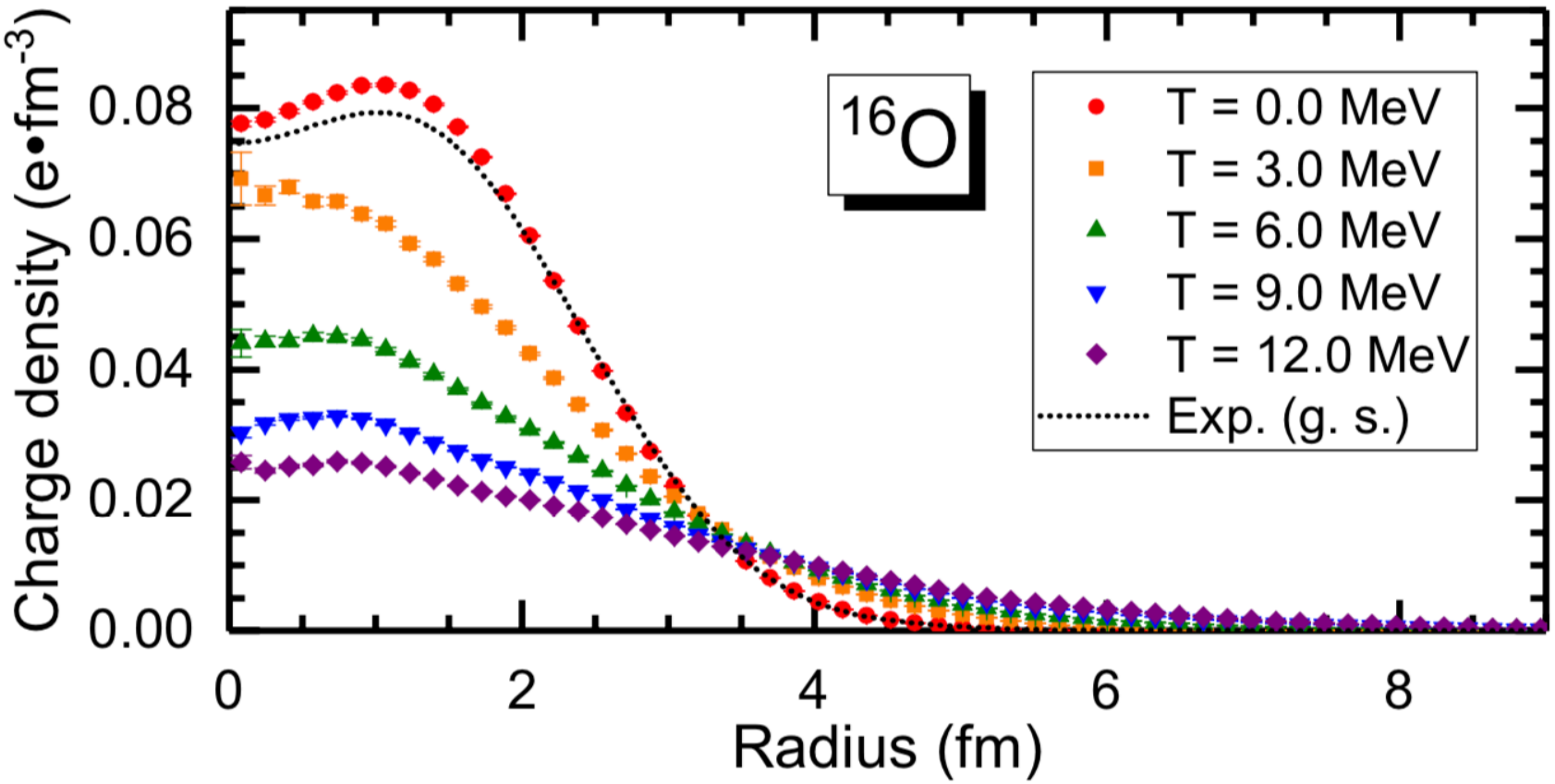


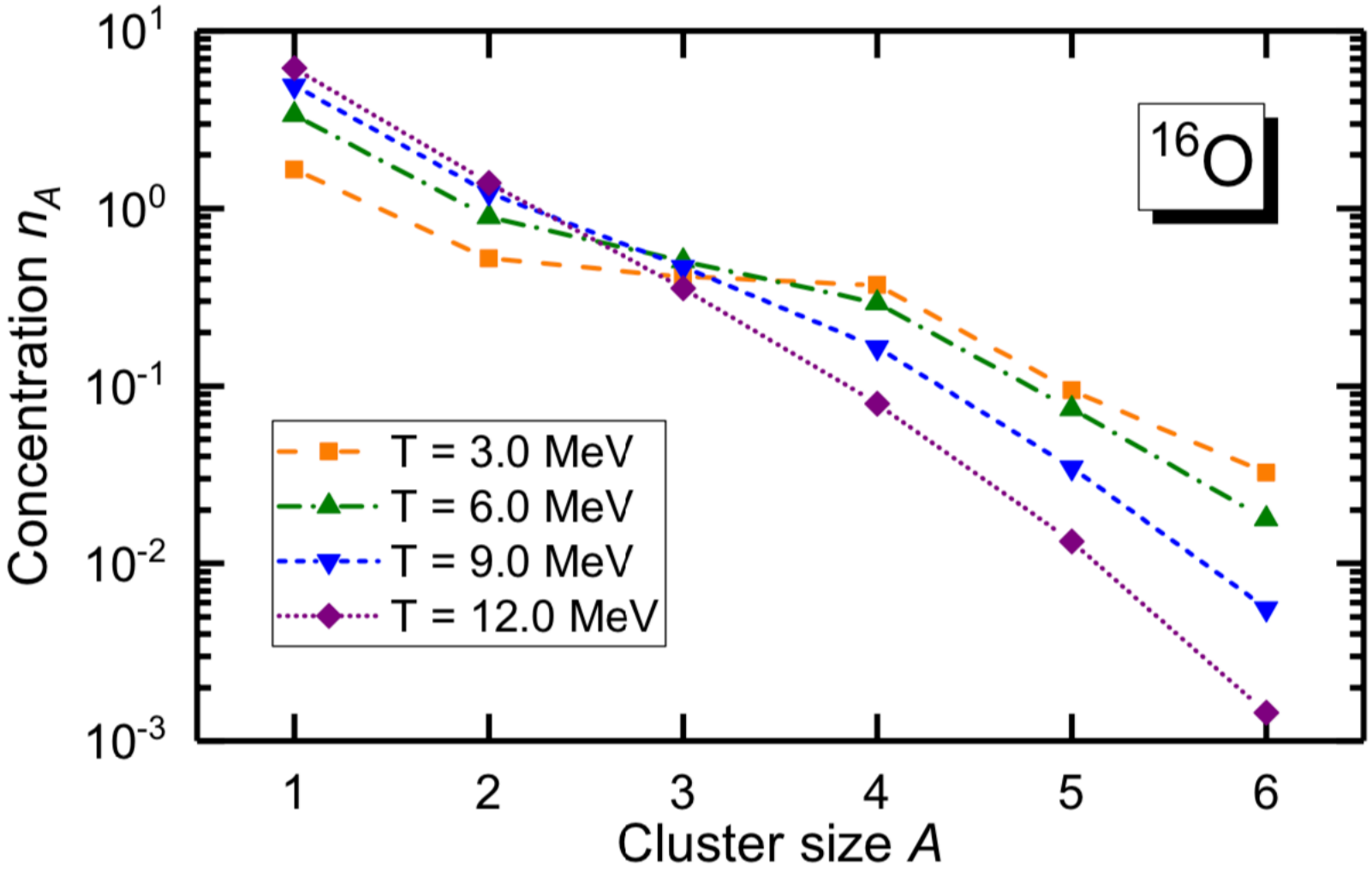
hybrid Monte Carlo
updates of auxiliary/pion fields

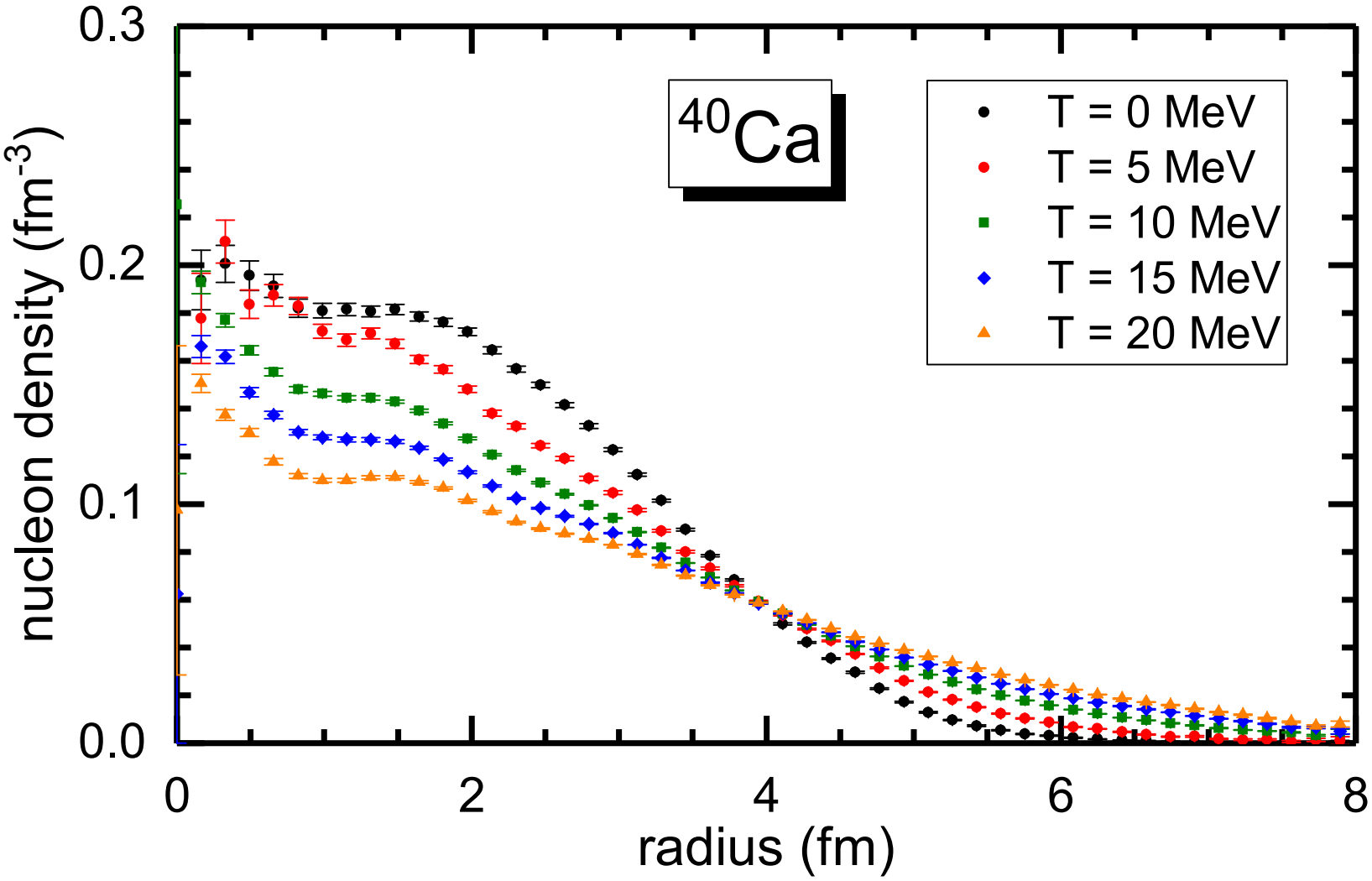


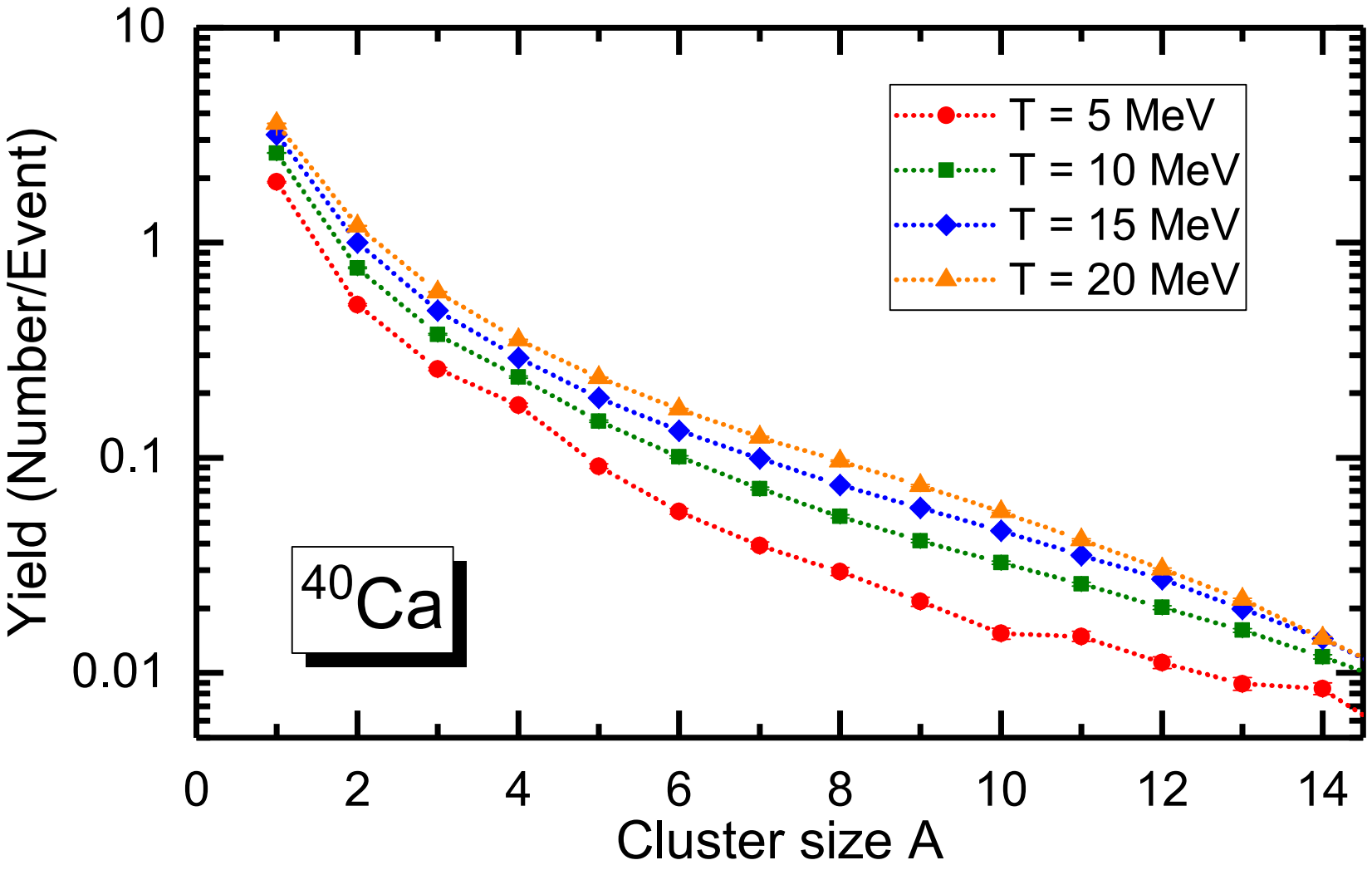
Figures by Bing-Nan Lu


350
300
250
200
Kinetic energy K (MeV)
L = 8
L = 9
$K = (3A\text{-}3)T/2$
^{16}O
0
2
4
6
8
10
12
14
Temperature T (MeV)


Charge density (e•fm^{-3})
0.00
0.02
0.04
0.06
0.08
0
2
4
6
8
Radius (fm)
^{16}O
T = 0.0 MeV
T = 3.0 MeV
T = 6.0 MeV
T = 9.0 MeV
T = 12.0 MeV
Exp. (g. s.)


Concentration n_A
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
1
2
3
4
5
6
Cluster size A
^{16}O
T = 3.0 MeV
T = 6.0 MeV
T = 9.0 MeV
T = 12.0 MeV


^{40}Ca
T = 0 MeV
T = 5 MeV
T = 10 MeV
T = 15 MeV
T = 20 MeV
nucleon density (fm^{-3})
radius (fm)
0.0
0.1
0.2
0.3
0
2
4
6
8


10
1
0.1
0.01
Yield (Number/Event)
0
2
4
6
8
10
12
14
Cluster size A
T = 5 MeV
T = 10 MeV
T = 15 MeV
T = 20 MeV
40Ca