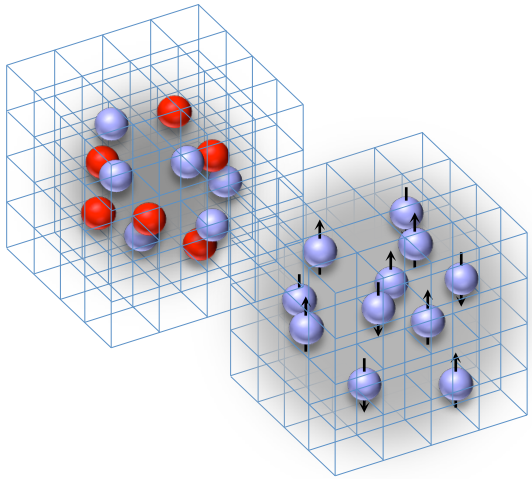
New Results in Lattice Scattering Using the Adiabatic Projection Method



Dean Lee

North Carolina State University

Nuclear Lattice EFT Collaboration

12th International Conference on Nucleus-Nucleus Collisions

University of Catania

Catania, Italy

June 22, 2015

Collaborators

Serdar Elhatisari - Bonn

Evgeny Epelbaum - Bochum

Hermann Krebs - Bochum

Timo Lähde - Jülich

Bingnan Lu - Jülich

Thomas Luu - Jülich

Ulf-G. Meißner - Bonn/Jülich

Michelle Pine - NC State

Alexander Rokash - Bochum

Gautam Rupak - MS State

with special thanks to Serdar for the scattering data analysis

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/cluster EFT calculations?

Outline

Lattice effective field theory

Cluster stuctures in ^{12}C and ^{16}O

Adiabatic projection method

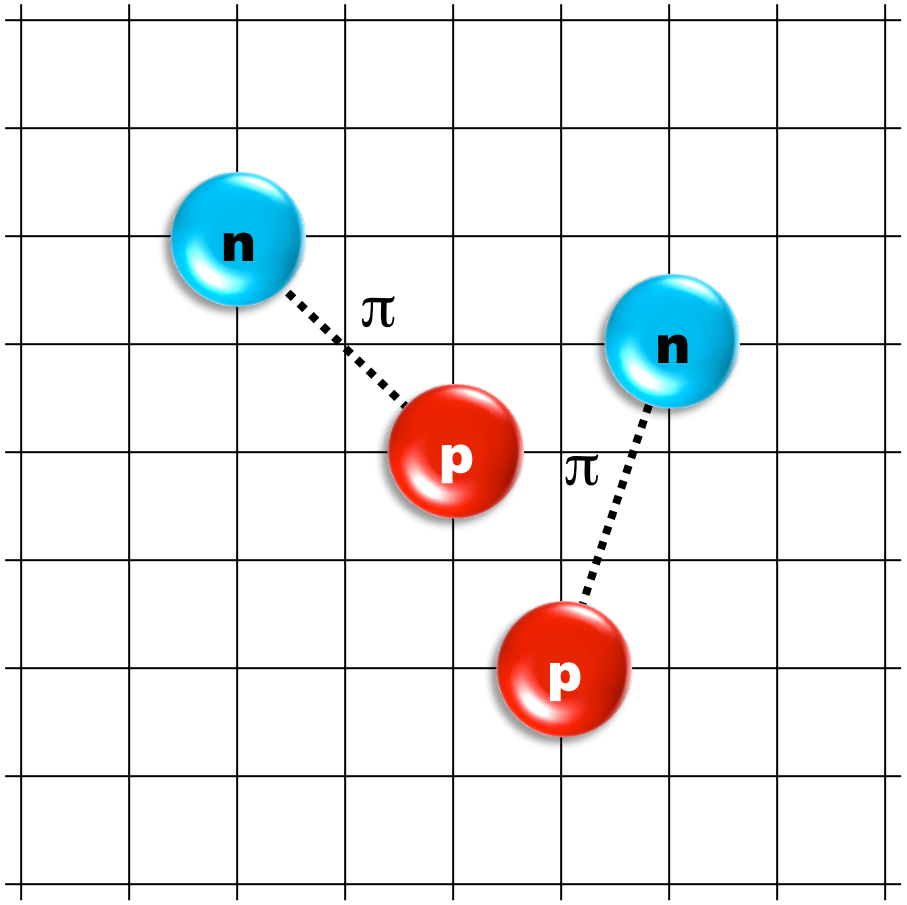
Lüscher's finite-volume method

Asymptotic cluster wave functions

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

Summary and outlook

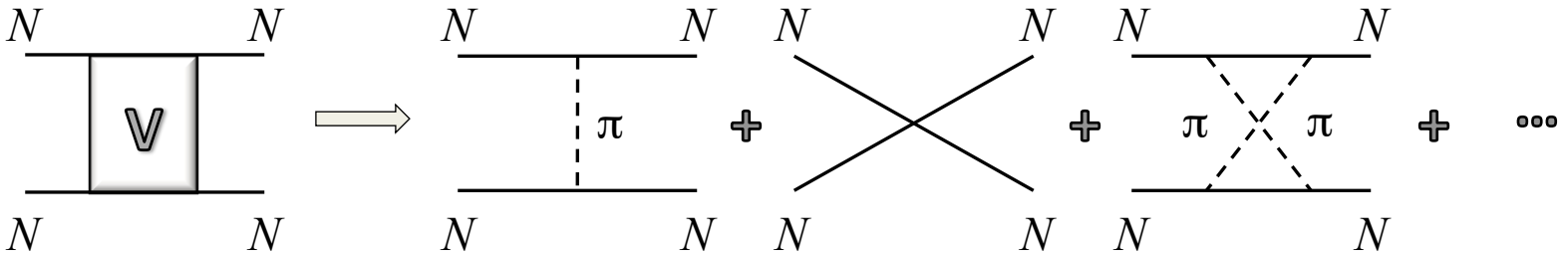
Lattice chiral effective field theory



Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

Chiral effective field theory

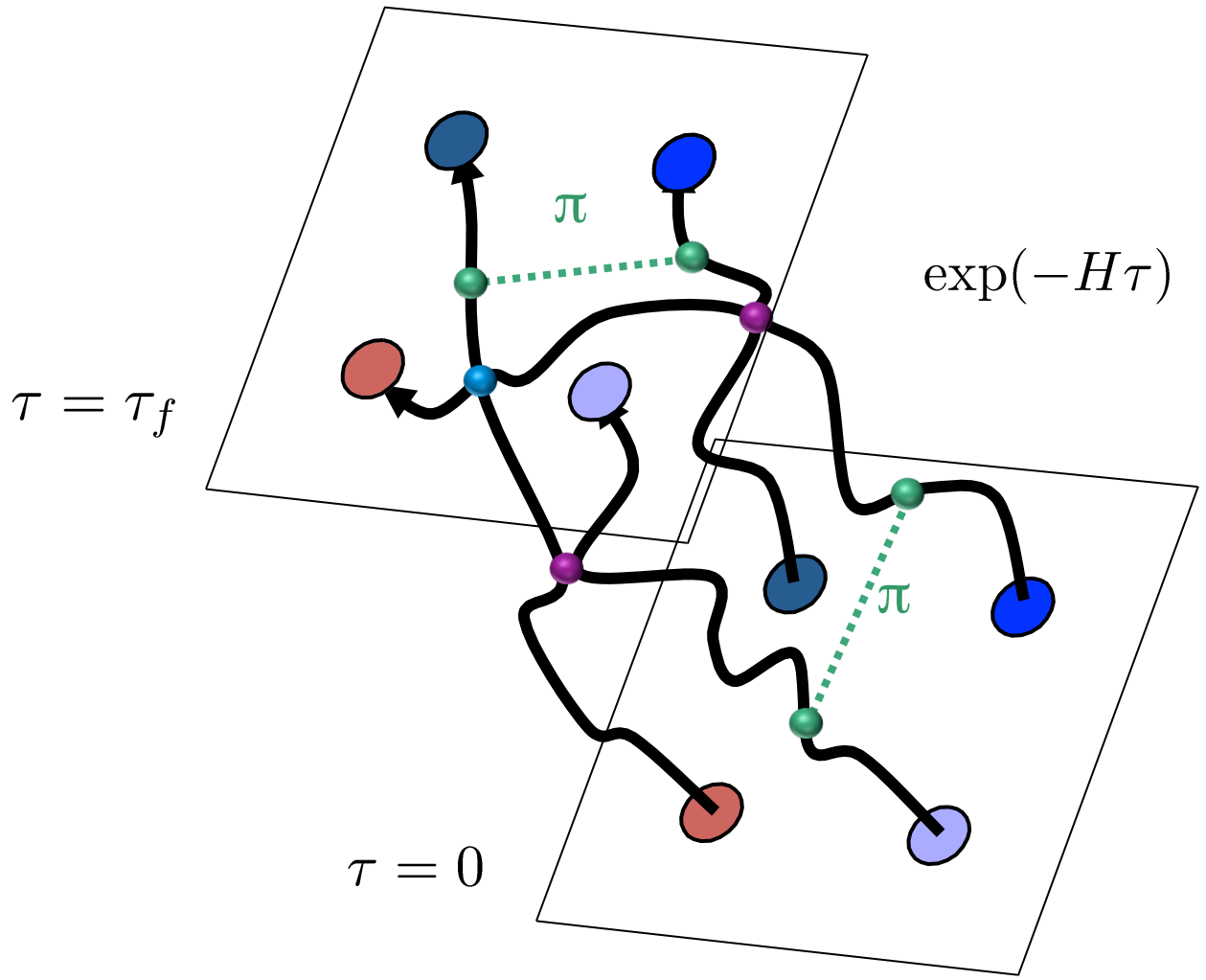
Construct the effective potential order by order



V^{OPEP} Contact interactions V^{TPEP}

Leading order (LO) Next-to-leading order (NLO)

Euclidean time projection



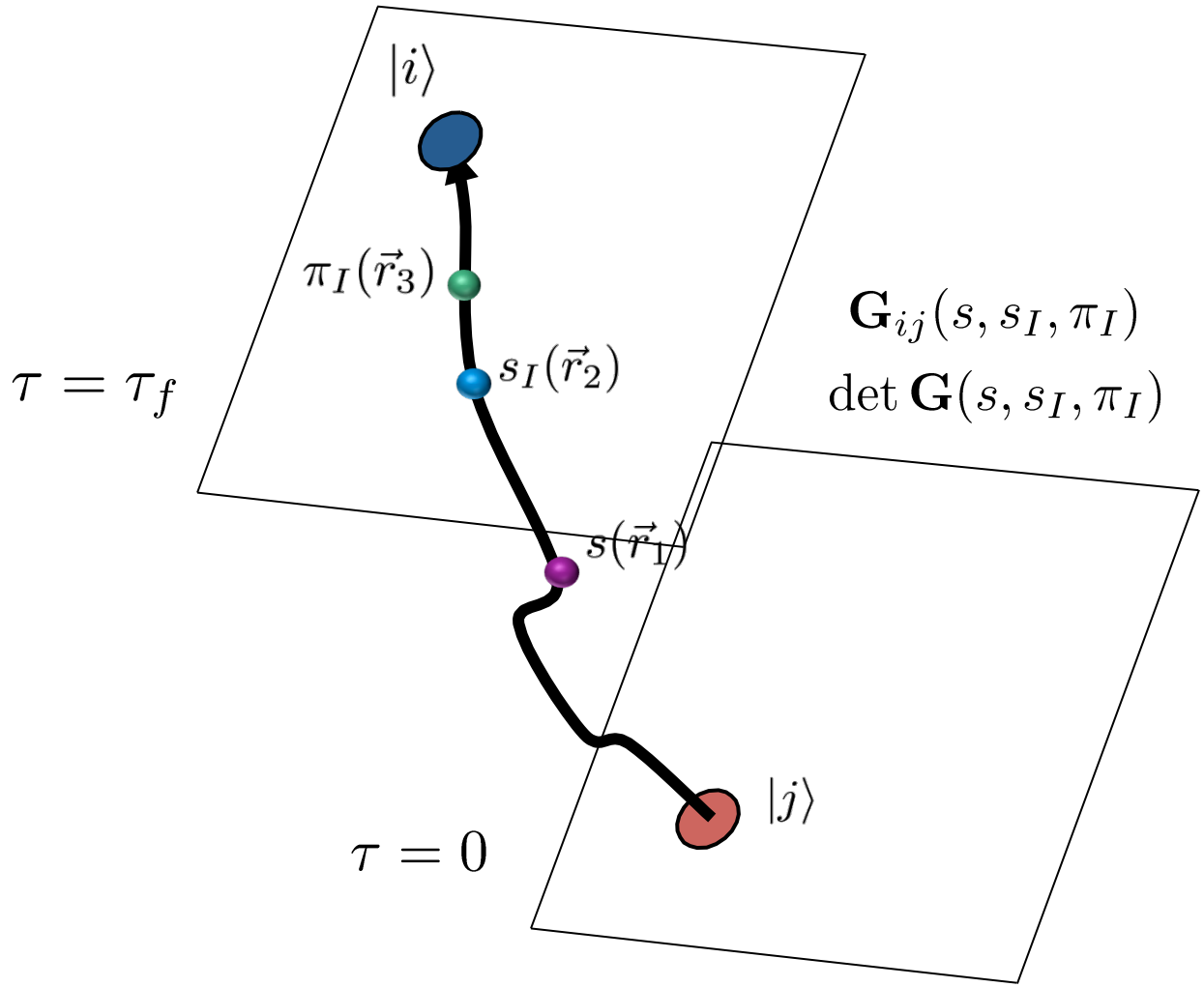
Auxiliary field method

We can write exponentials of the interaction using a Gaussian integral identity

$$\exp\left[-\frac{C}{2}(N^\dagger N)^2\right] \qquad \times \quad (N^\dagger N)^2$$

$$= \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s(N^\dagger N)\right] \qquad \rangle \bullet \; sN^\dagger N$$

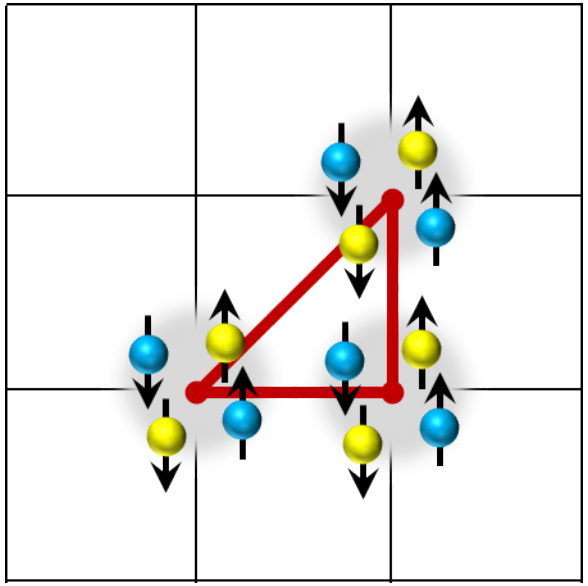
We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.



Sign oscillations in determinant suppressed by approximate Wigner SU(4) symmetry

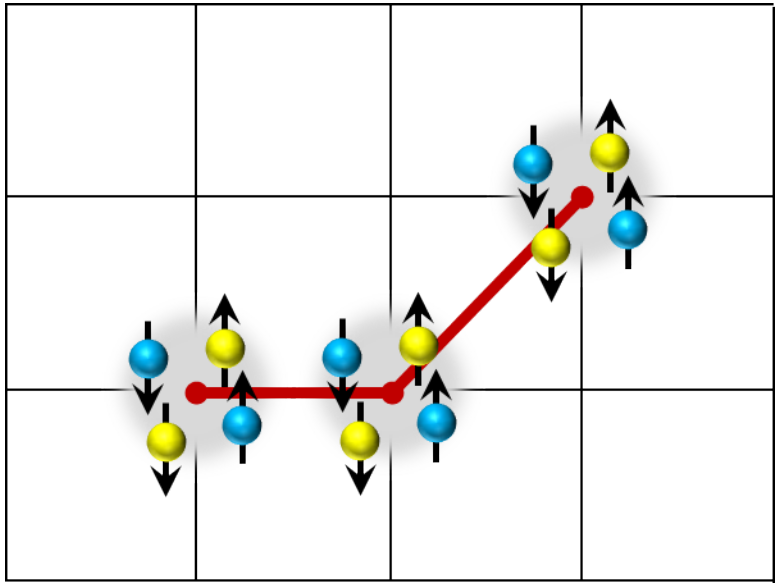
Carbon-12

0_1^+, 2_1^+



Compact triangular

0_2^+, 2_2^+



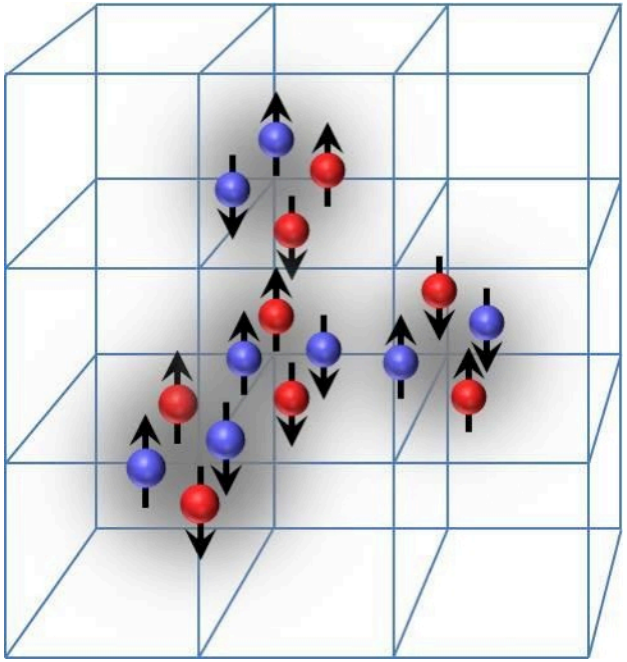
Bent-arm structure

$a = 1.97$ fm

PRL 106, 192501, 2011; PRL 109, 252501, 2012

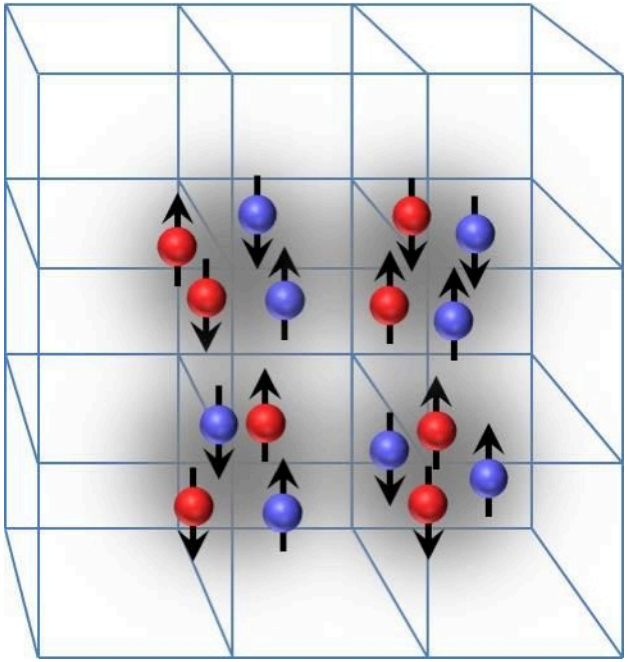
Oxygen-16

0_1^+



Tetrahedral structure

$0_2^+,\ 2_1^+$



Square-like structure

$a = 1.97$ fm

PRL 112, 102501, 2014

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.

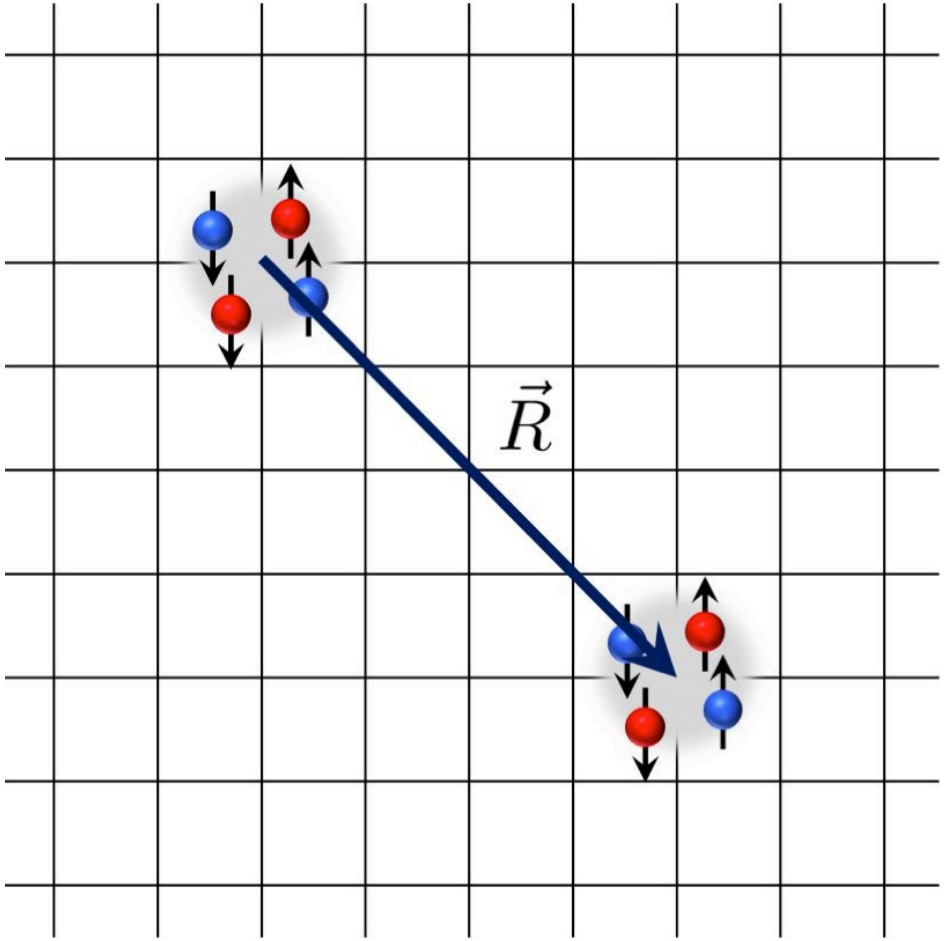
Navratil, Roth, Quaglioni, PRC 82 034609 (2010); Navratil, Quaglioni, PRC 83 044609 (2011); etc.

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.

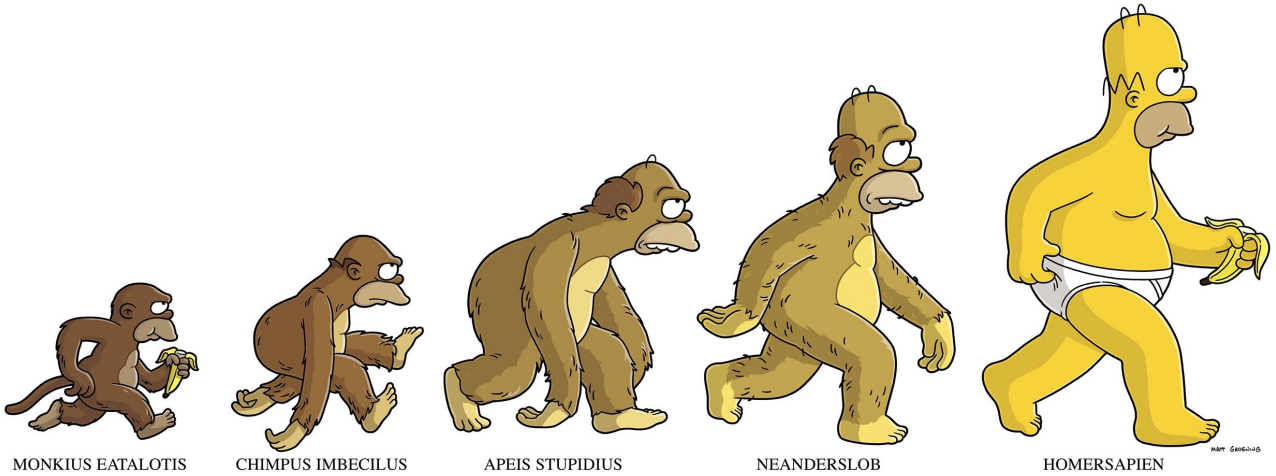
Start with localized cluster states for all possible separation vectors $\vec{R}$

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



Cluster evolution with Euclidean time

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



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

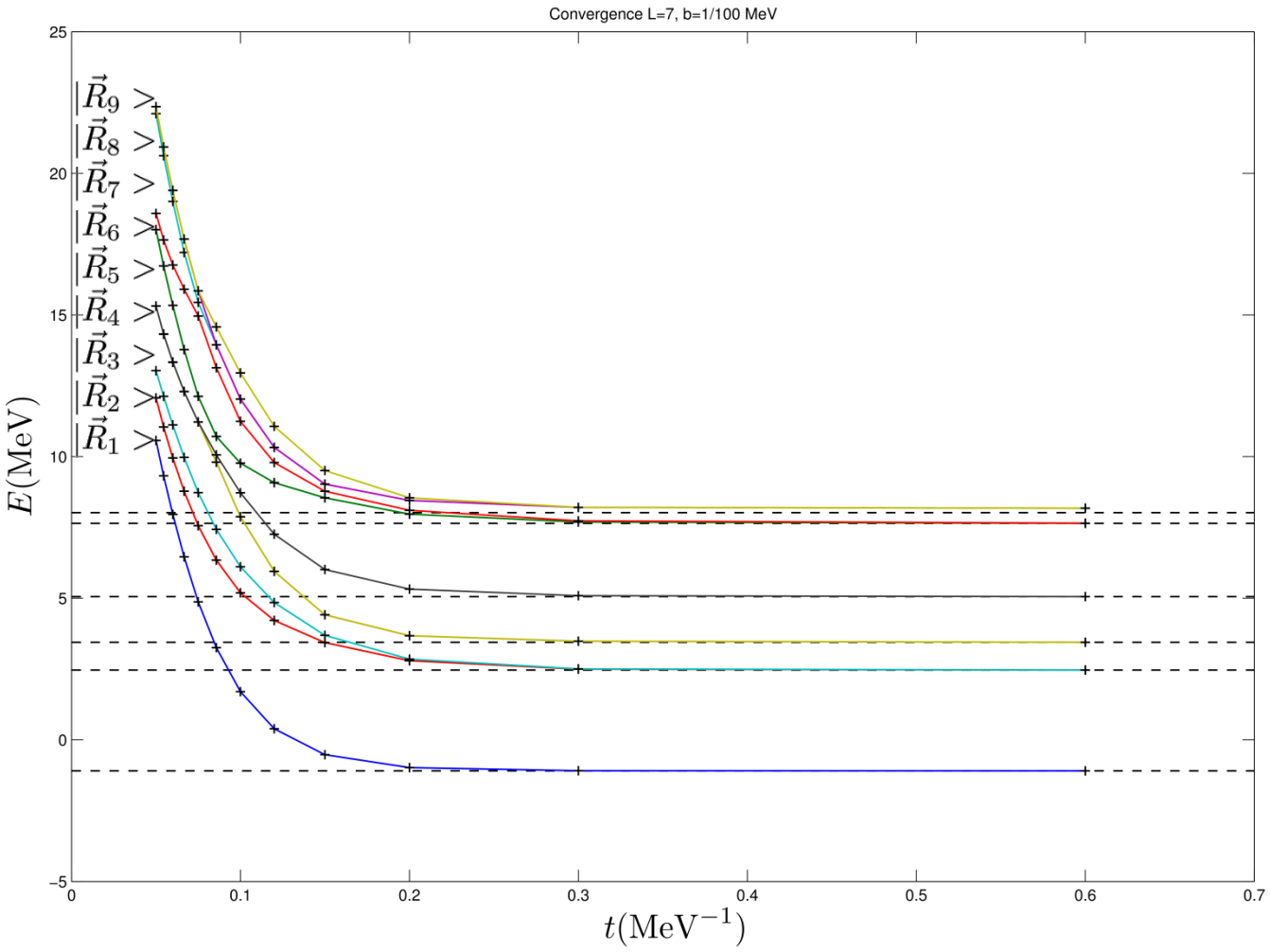
$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

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.

Quartet neutron-deuteron scattering (pionless EFT)



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

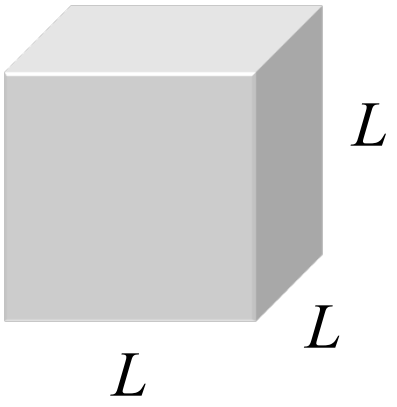
Lüscher's finite-volume formula

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

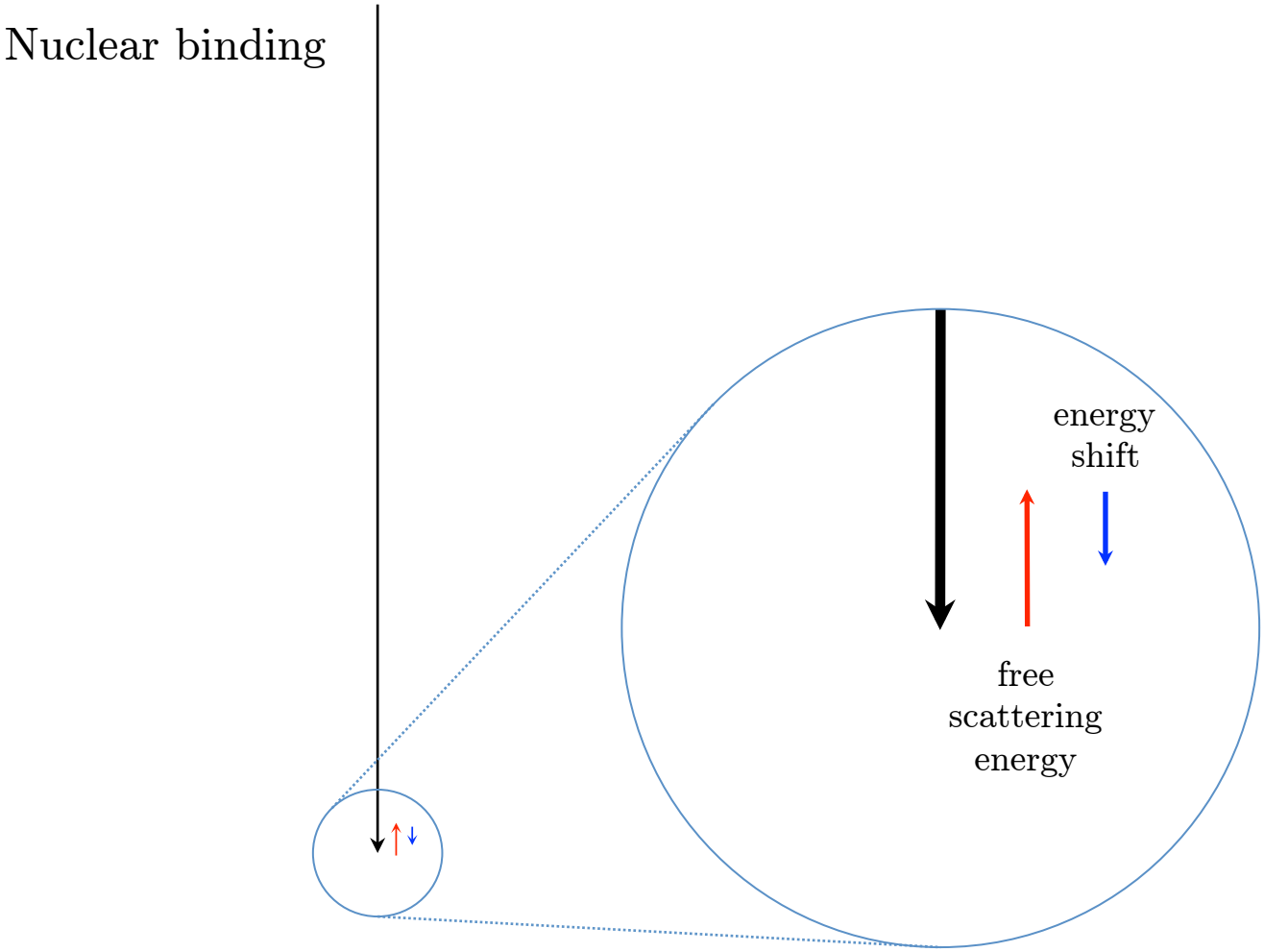
Two-particle energy levels near threshold in a periodic cube are related to the elastic phase shifts

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

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



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 $H^{\rm eff}$ 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

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

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

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, arXiv:1505.02967

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

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

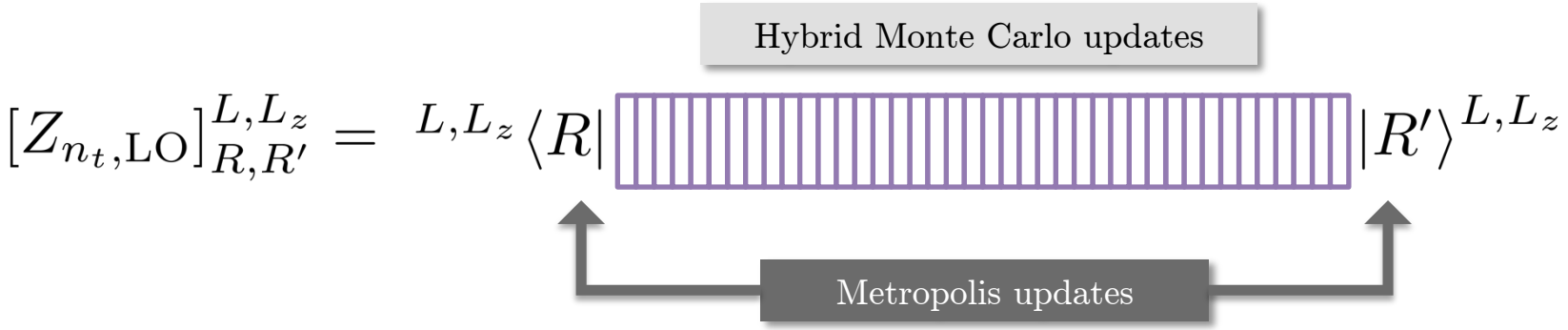
In the asymptotic region, we are inverting the diffusion process when computing the adiabatic Hamiltonian and are left with an effective cluster Hamiltonian in position space basis.

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

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

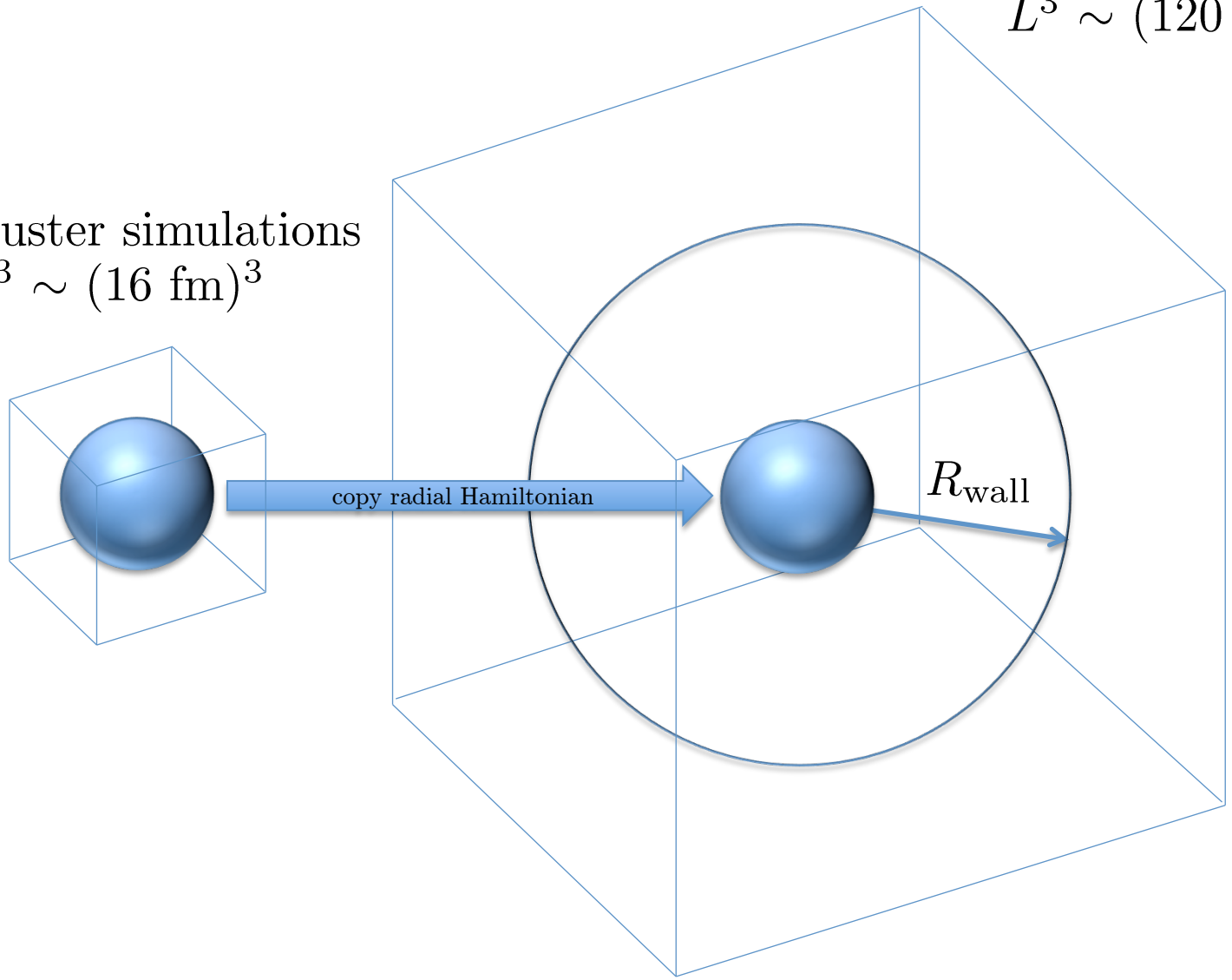
Lu, Lähde, Lee, Meißner, arXiv:1506.05652

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



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

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

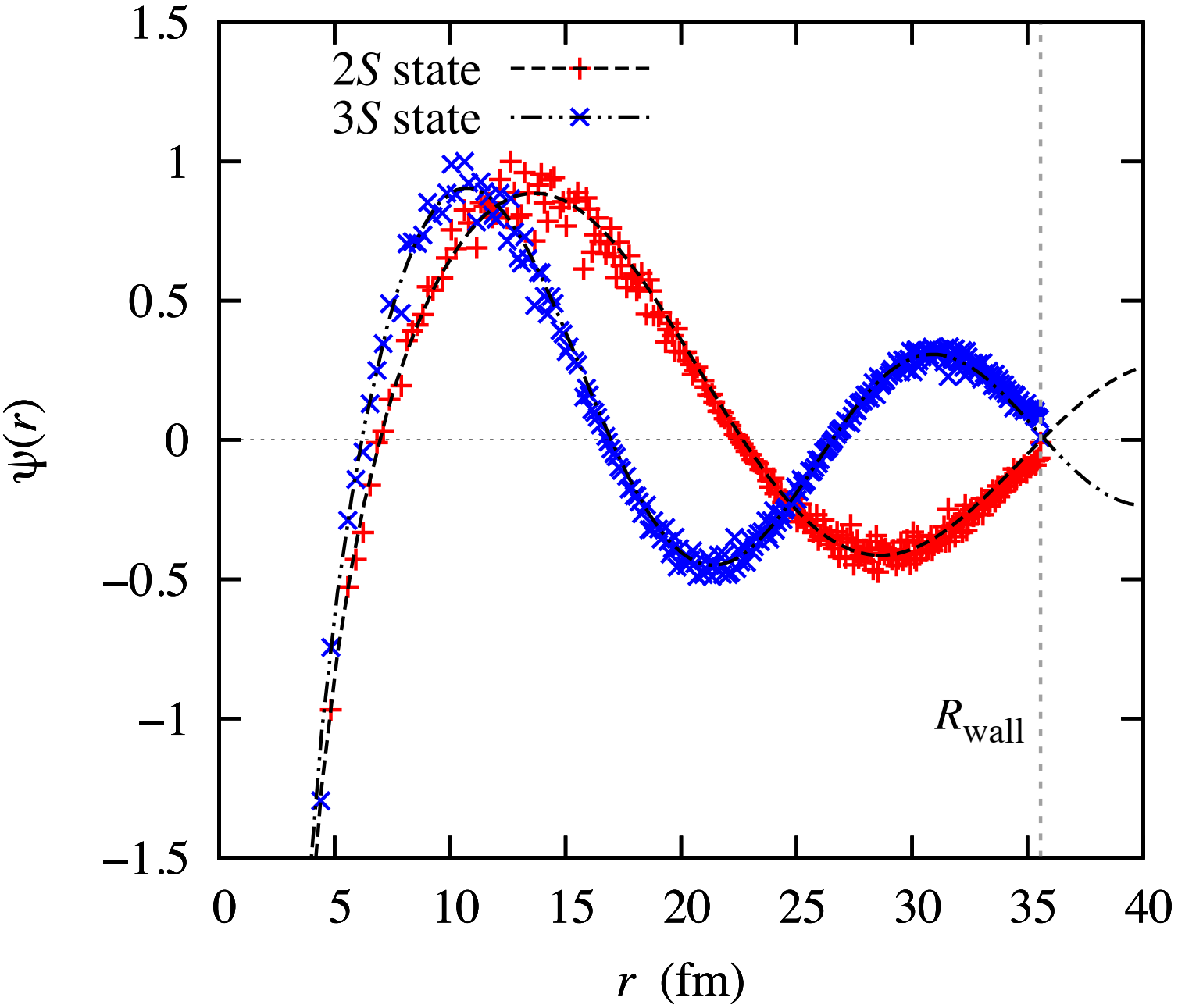


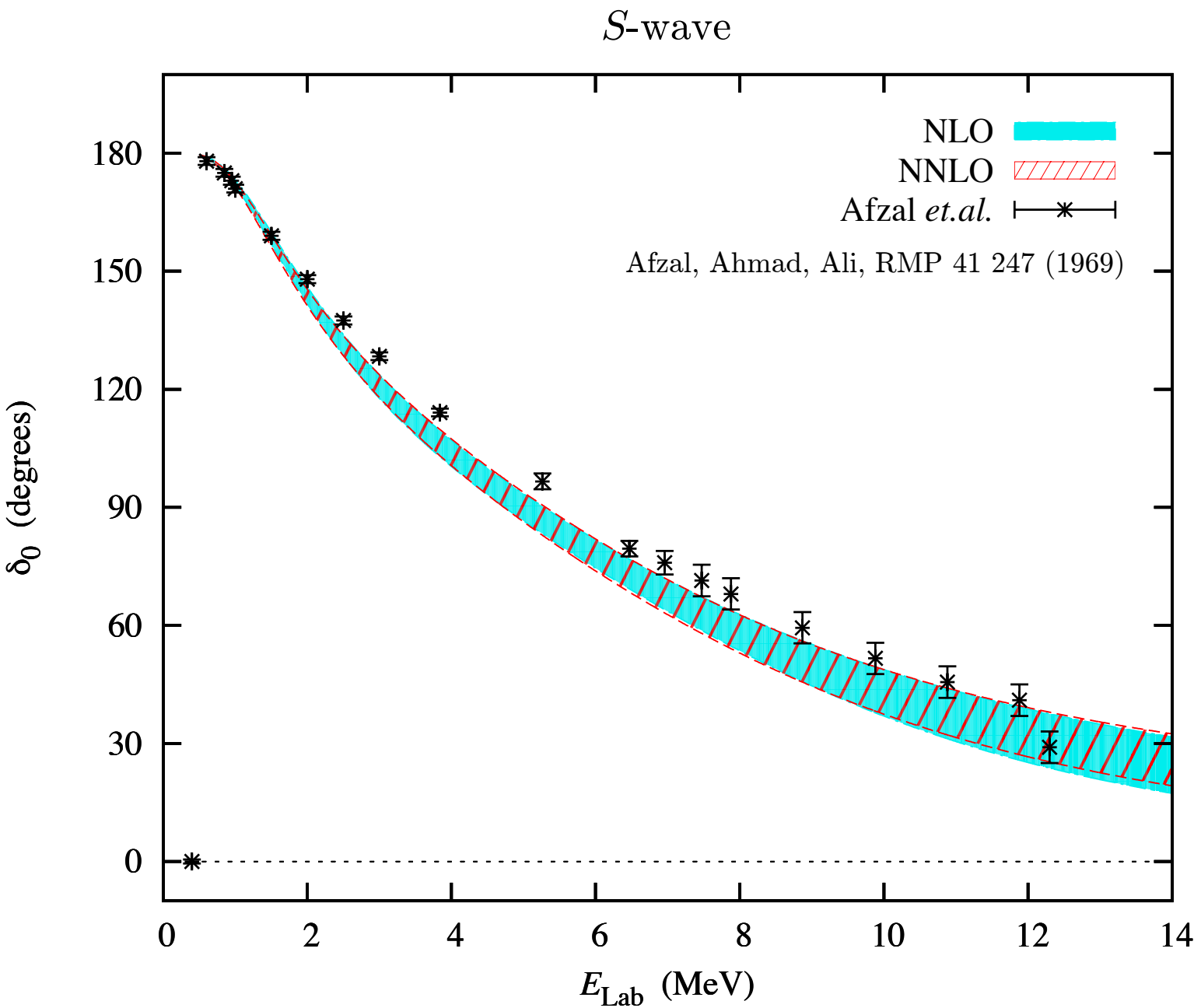
$^4\mathrm{He} + {}^4\mathrm{He} \to {}^4\mathrm{He} + {}^4\mathrm{He}$

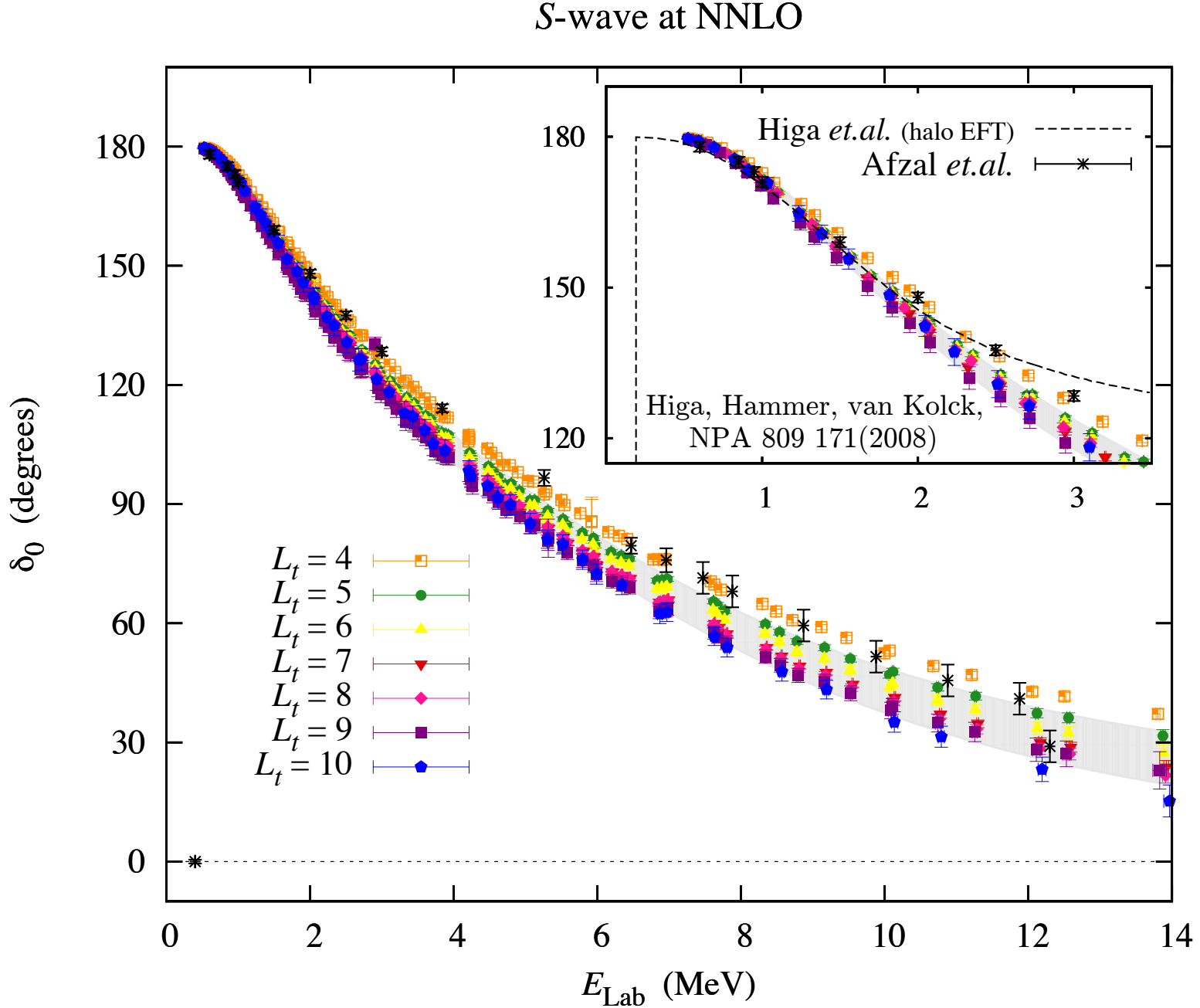
We now present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

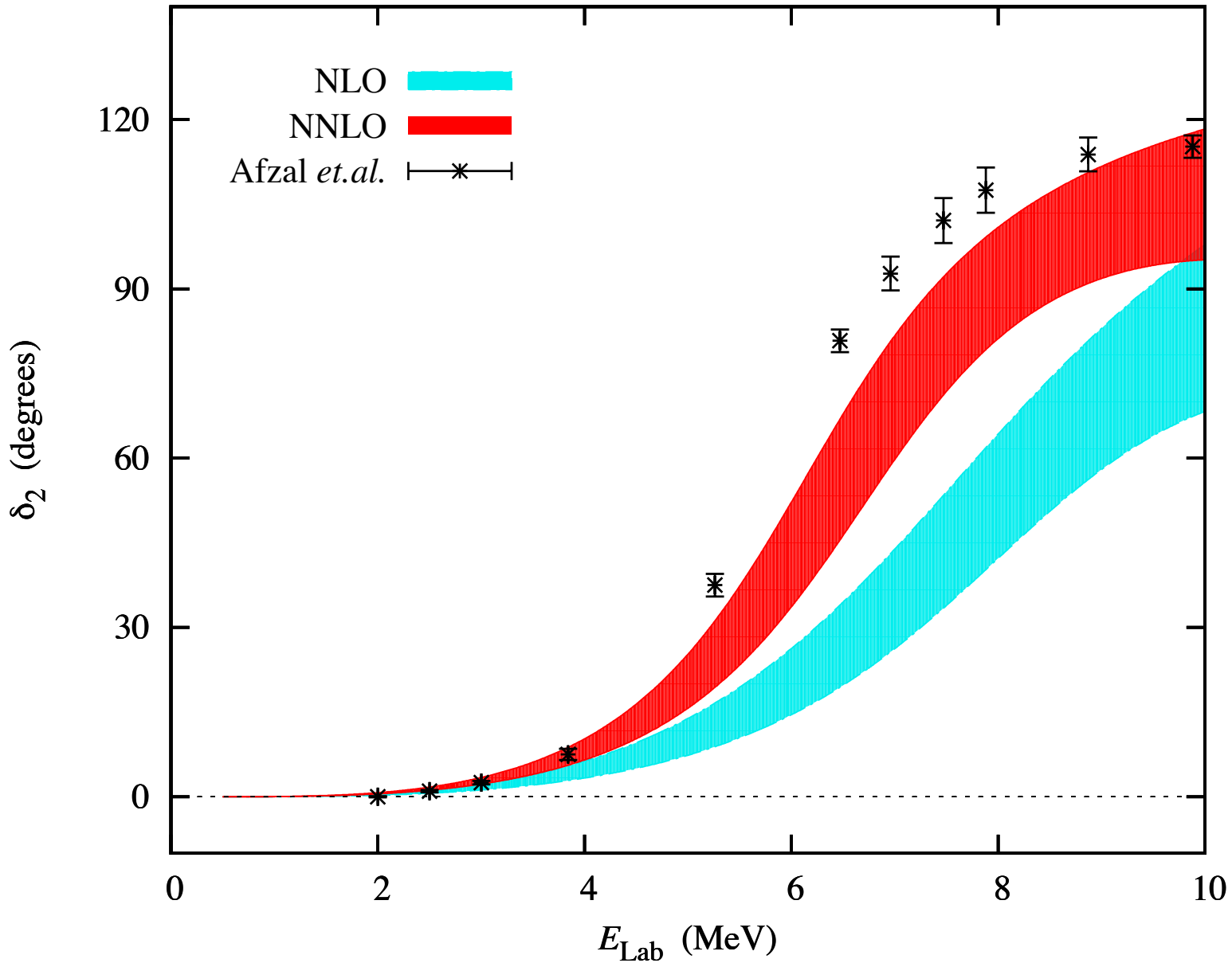
Elhatisari, Epelbaum, Krebs, Lähde, Lee, Luu, Meißner, Rupak, arXiv:1506.03513

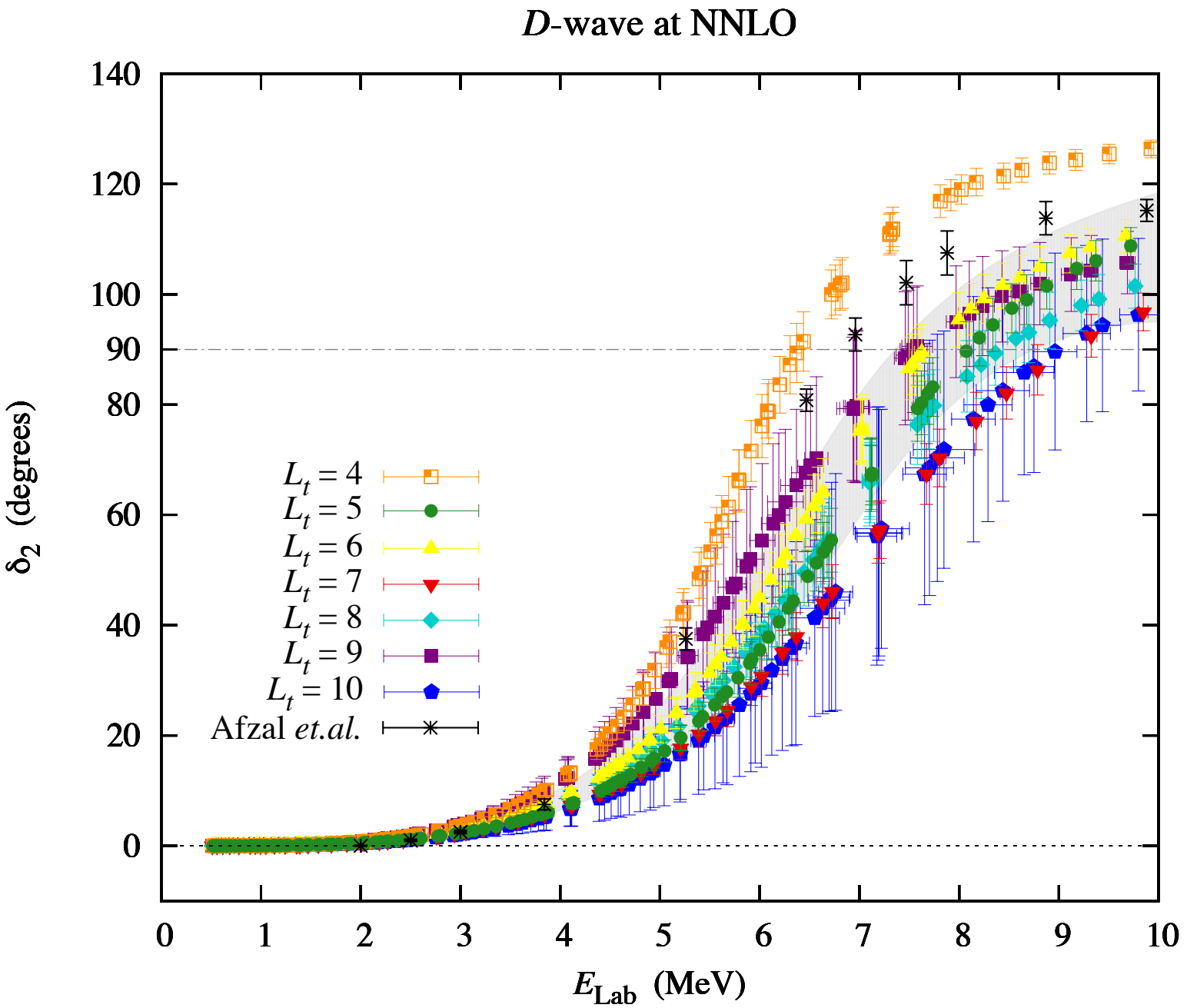
We did calculations for the S-wave and for the $L = 2$, $L_z = 0$ D-wave projections.


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


S-wave
NLO
NNLO
Afzal et.al.
Afzal, Ahmad, Ali, RMP 41 247 (1969)
δ0 (degrees)
180
150
120
90
60
30
0
0
2
4
6
8
10
12
14
ELab (MeV)


S-wave at NNLO
δ0 (degrees)
ELab (MeV)
Lt = 4
Lt = 5
Lt = 6
Lt = 7
Lt = 8
Lt = 9
Lt = 10
Higa et.al. (halo EFT)
Afzal et.al.
Higa, Hammer, van Kolck,
NPA 809 171(2008)


NLO
NNLO
Afzal et.al.
120
90
60
30
0
δ_2 (degrees)
0
2
4
6
8
10
E_{Lab} (MeV)


D-wave at NNLO
δ2 (degrees)
E_Lab (MeV)
L_t = 4
L_t = 5
L_t = 6
L_t = 7
L_t = 8
L_t = 9
L_t = 10
Afzal et.al.
0
20
40
60
80
90
100
120
140
0
1
2
3
4
5
6
7
8
9
10

Summary and outlook

More work needs to be done. But alpha processes now appear to be in reach of *ab initio* methods. Since the sign oscillations are mild for alpha nuclei, the scaling is very favorable.

For an A_1-body + A_2-body scattering or reaction process the computational scaling is typically $\sim (A_1 + A_2)^2$.

For mass and charge transfer processes, we do the same steps but consider coupled channel scattering. For capture reactions, we include one-photon matrix elements and compute overlaps between bound states and scattering states.

Rupak, D.L., PRL 111 032502 (2013)

Could be useful and interesting to explore connections with halo/cluster EFT calculations. In cases where the separation of scales is good, halo/cluster EFT calculations should agree with adiabatic projection method. In cases where the separation of scales is not large, the halo/cluster EFT calculations can use the adiabatic projection method as guidance.

Would be interesting to see if some of these methods can be used for calculations in relativistic field theories, in particular lattice QCD.