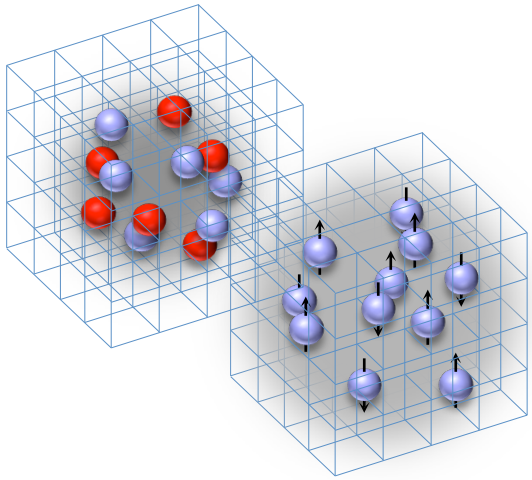
New results in lattice scattering using the adiabatic projection method



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Nuclear Lattice EFT Collaboration

Workshop on Progress in Ab Initio Techniques in Nuclear Physics

TRIUMF, Vancouver
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with special thanks to Serdar for the scattering data analysis

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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

Adiabatic projection method

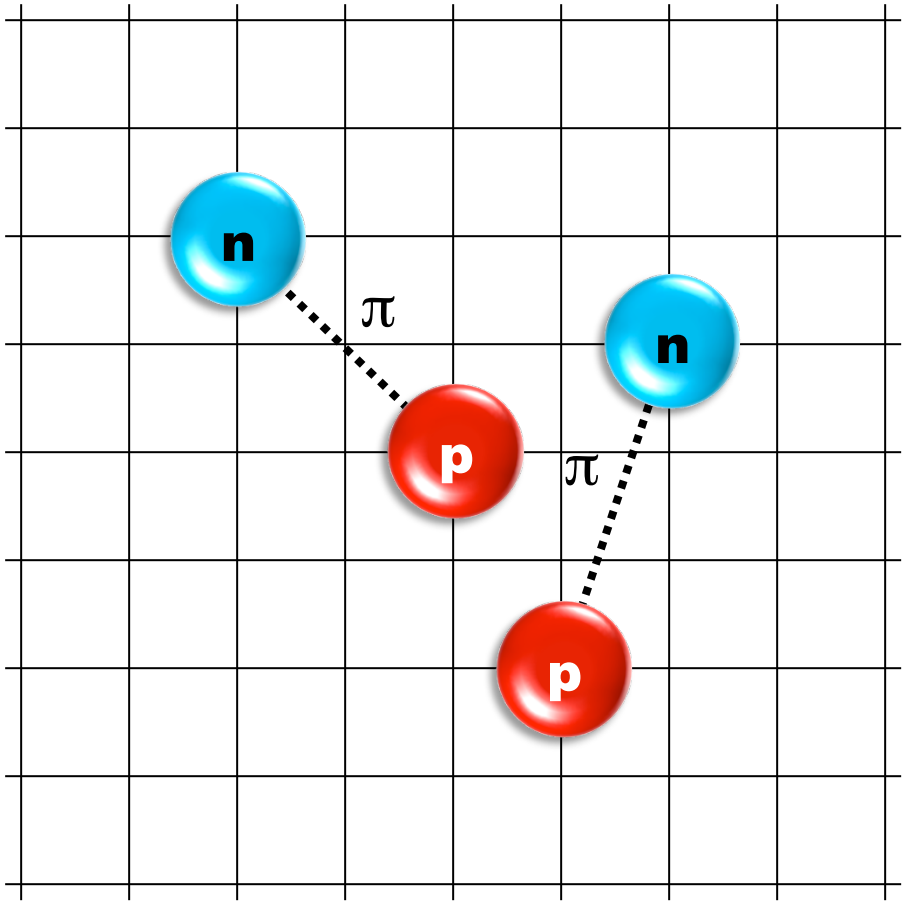
Lüscher's finite-volume method

Asymptotic cluster wave functions

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

Summary and outlook

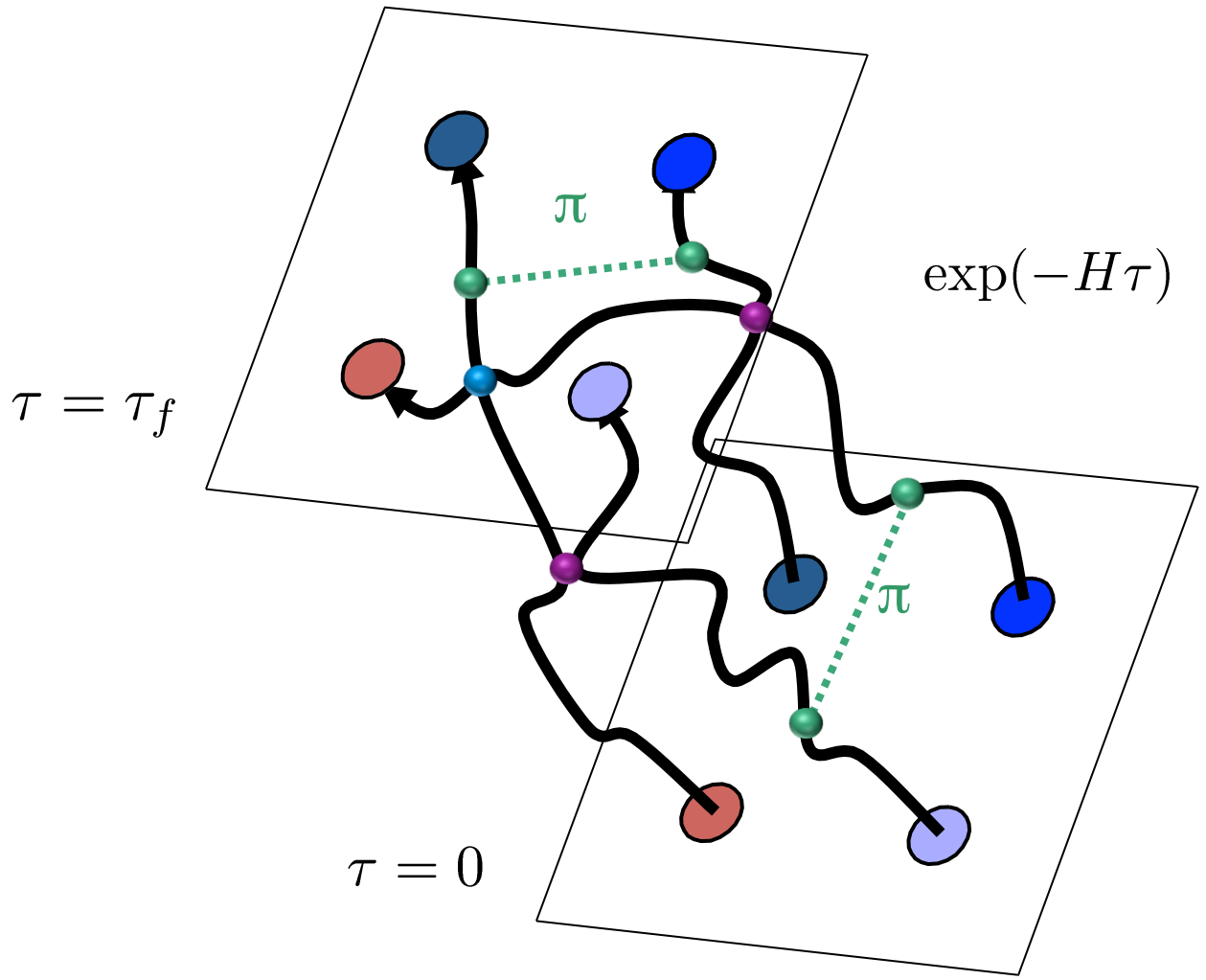
Lattice chiral effective field theory



$a \sim 1 - 2$ fm

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

Euclidean time projection



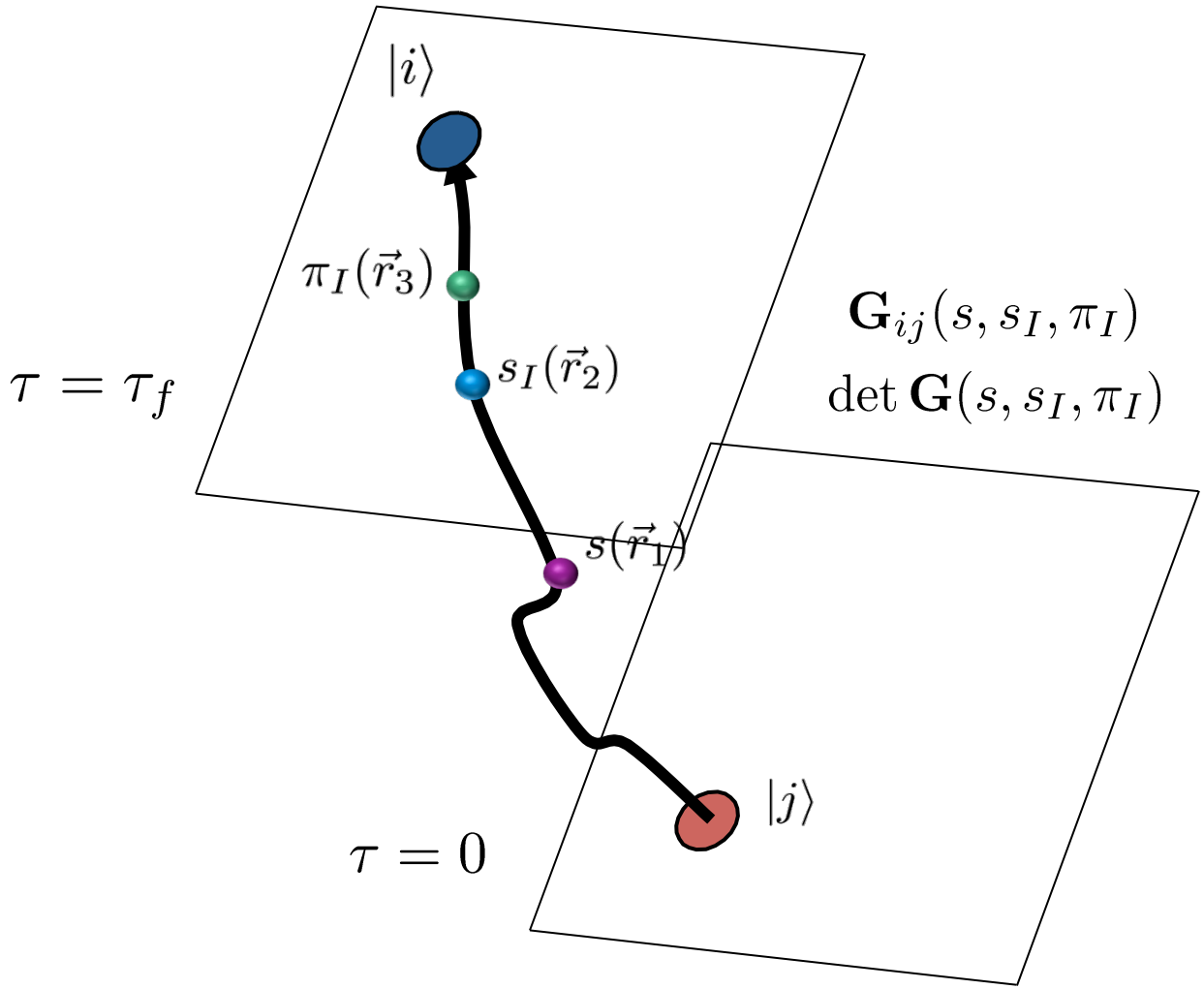
Auxiliary field method

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

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

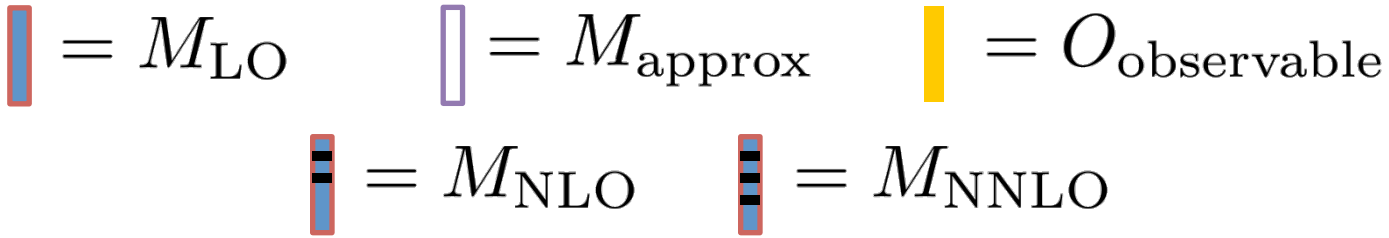
$$= \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s(N^\dagger N)\right] \qquad \rangle \bullet \; sN^\dagger N$$

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

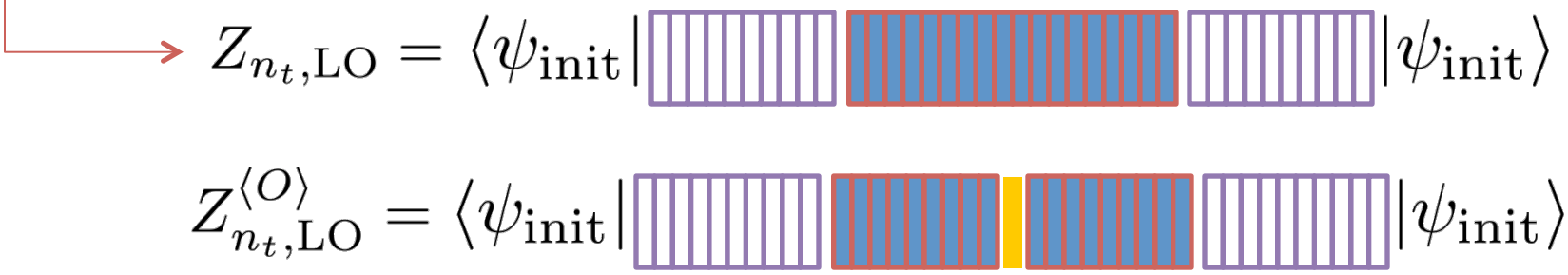


Sign oscillations in determinant suppressed by approximate Wigner SU(4) symmetry

Schematic of lattice Monte Carlo calculation



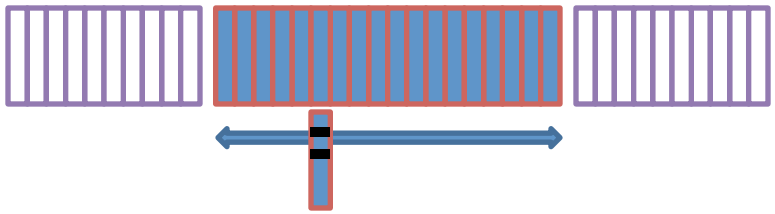
Hybrid Monte Carlo sampling



$$e^{-E_{0,\mathrm{LO}} a_t} = \lim_{n_t \to \infty} Z_{n_t+1,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

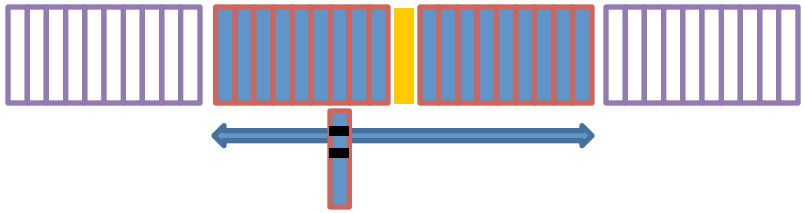
$$\langle O \rangle_{0,\mathrm{LO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

$$Z_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$$



$$| \psi_{\mathrm{init}} \rangle$$

$$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$$



$$| \psi_{\mathrm{init}} \rangle$$

$$\langle O \rangle_{0,\mathrm{NLO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} / Z_{n_t,\mathrm{NLO}}$$

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.

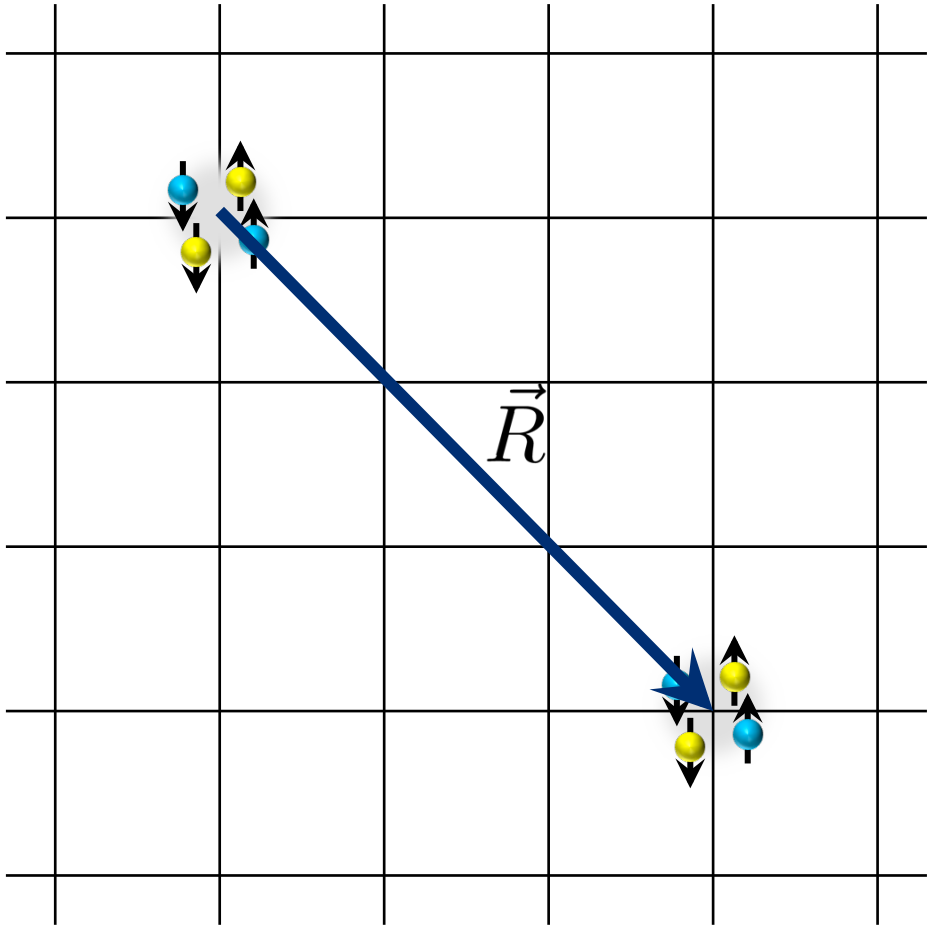
Navratil, Roth, Quaglioni, PRC 82 034609 (2010); Navratil, Quaglioni, PRC 83 044609 (2011); etc.

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 $\vec{R}$

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



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

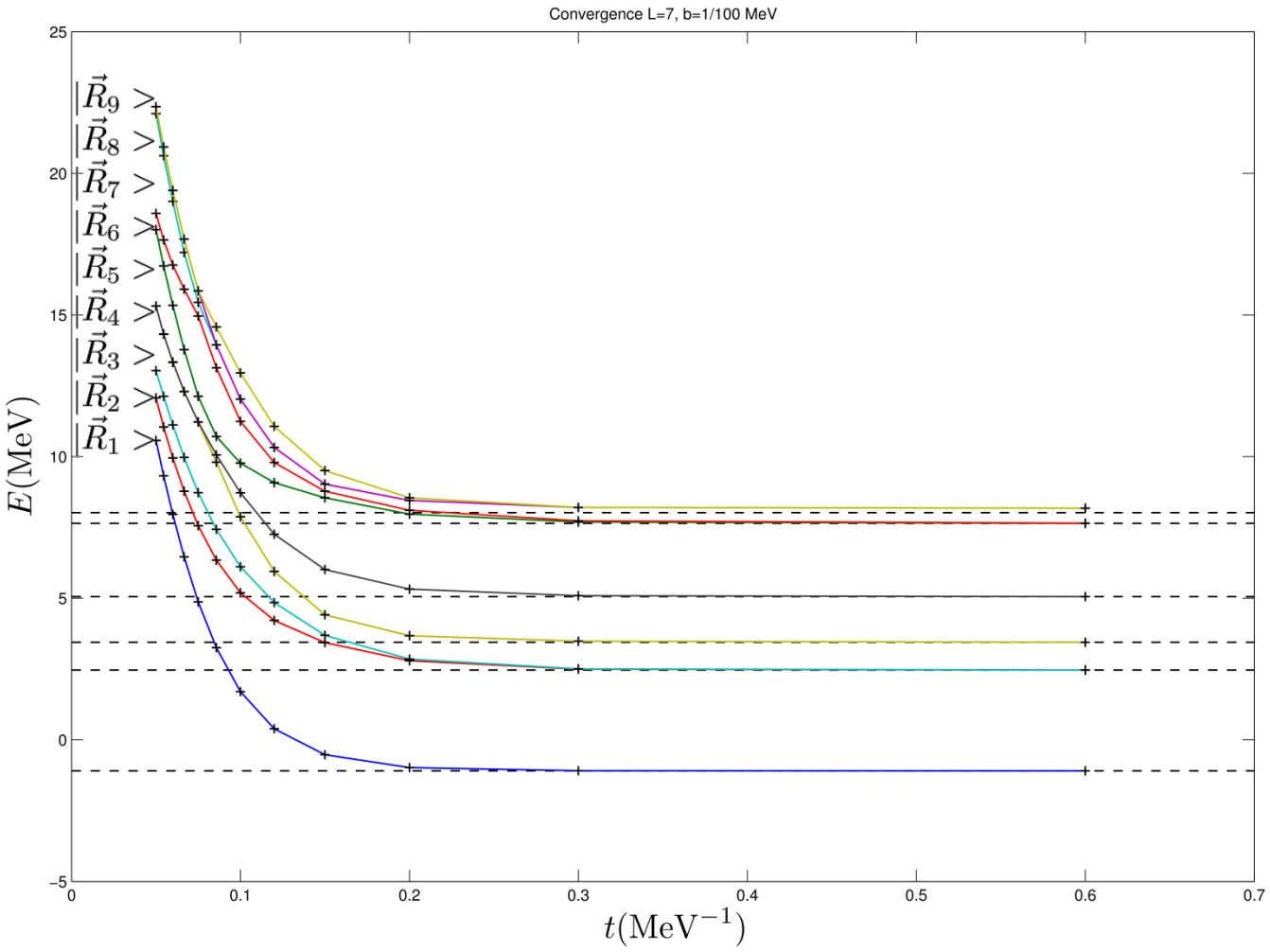
$$[H^a_\tau]_{\vec{R},\vec{R}'} = \sum_{\vec{R}'',\vec{R}'''} \left[N_\tau^{-1/2}\right]_{\vec{R},\vec{R}''} [H_\tau]_{\vec{R}'',\vec{R}'''} \left[N_\tau^{-1/2}\right]_{\vec{R}''',\vec{R}'}$$

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)

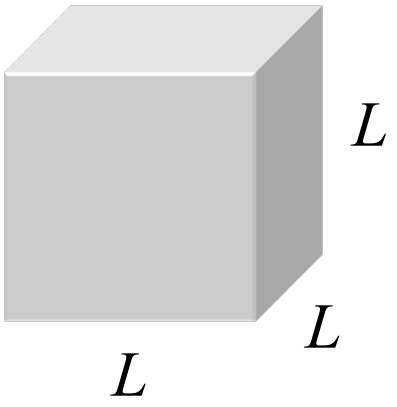
Lüscher's finite-volume formula

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

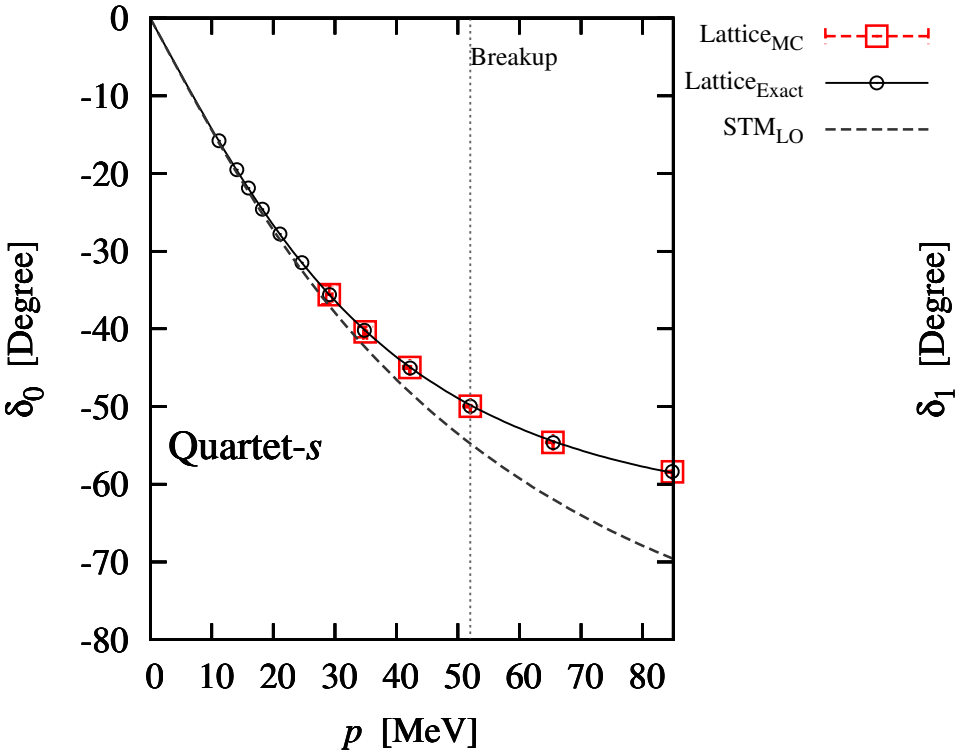
Two-particle energy levels near threshold in a periodic cube are related to the elastic phase shifts

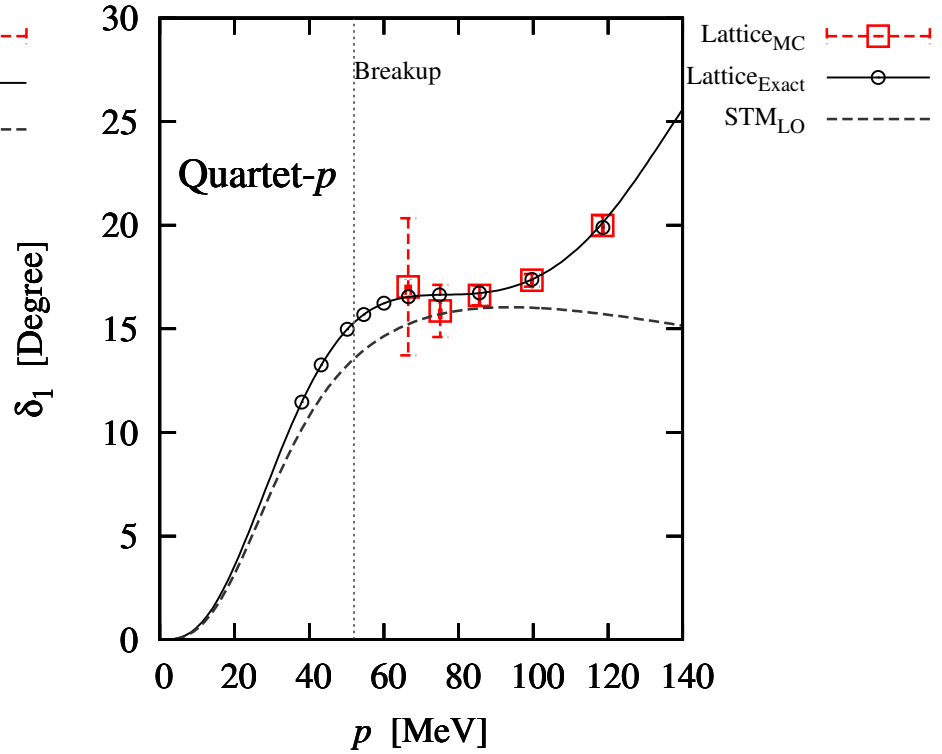
$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta), \qquad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

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

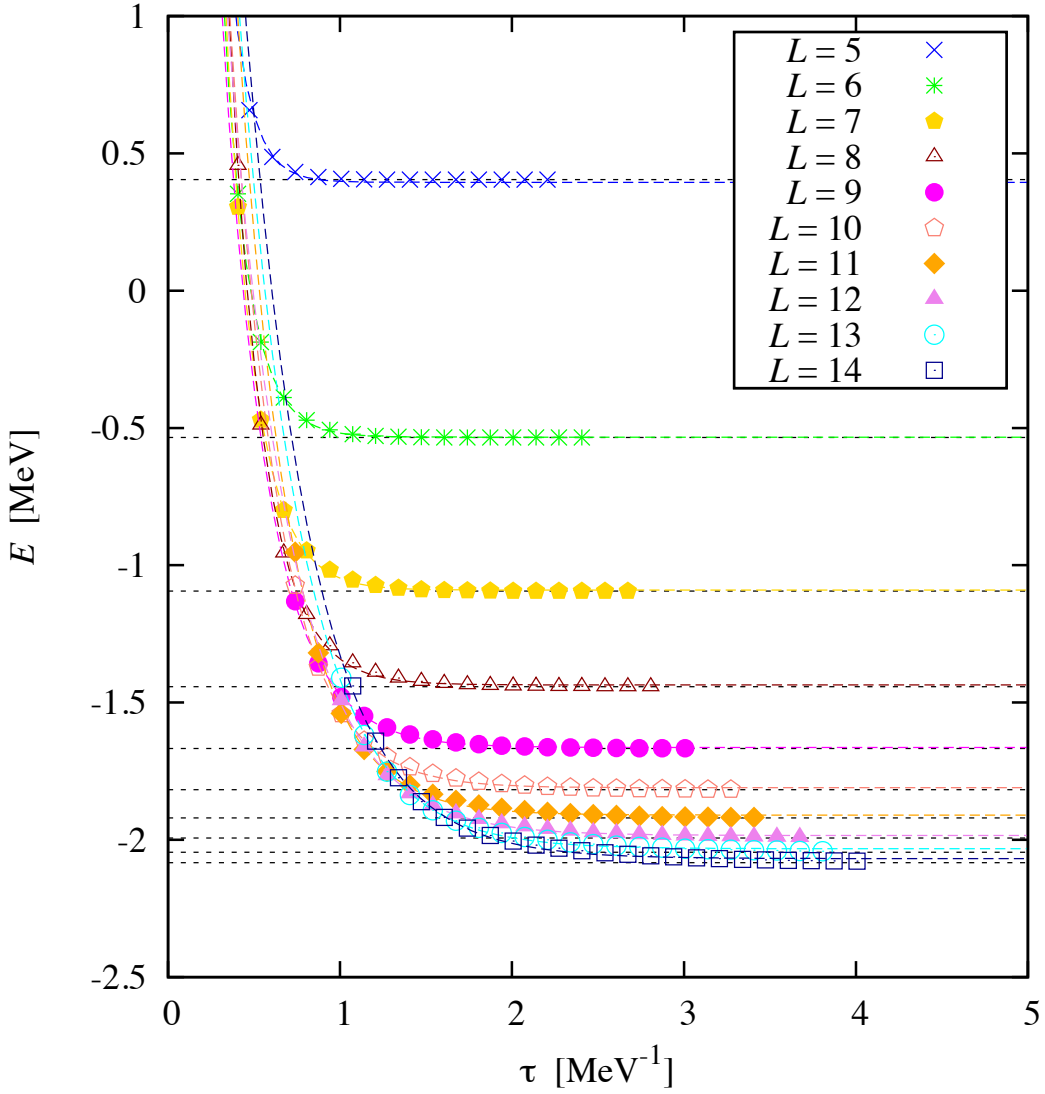


Quartet neutron-deuteron scattering (pionless EFT)



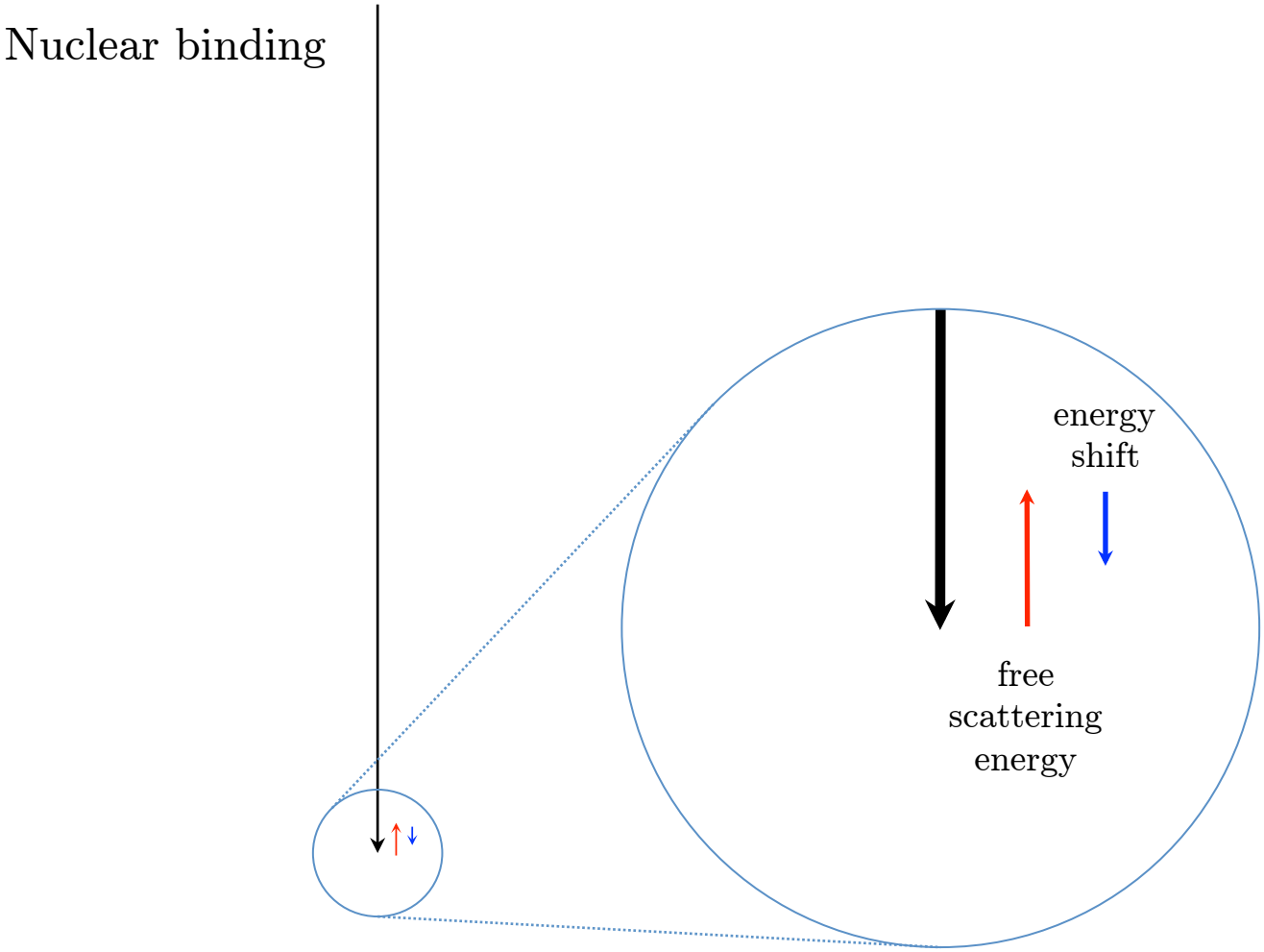


Elhatisari, D.L., PRC 90 064001 (2014)



Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, in progress

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



Asymptotic cluster scattering wave functions

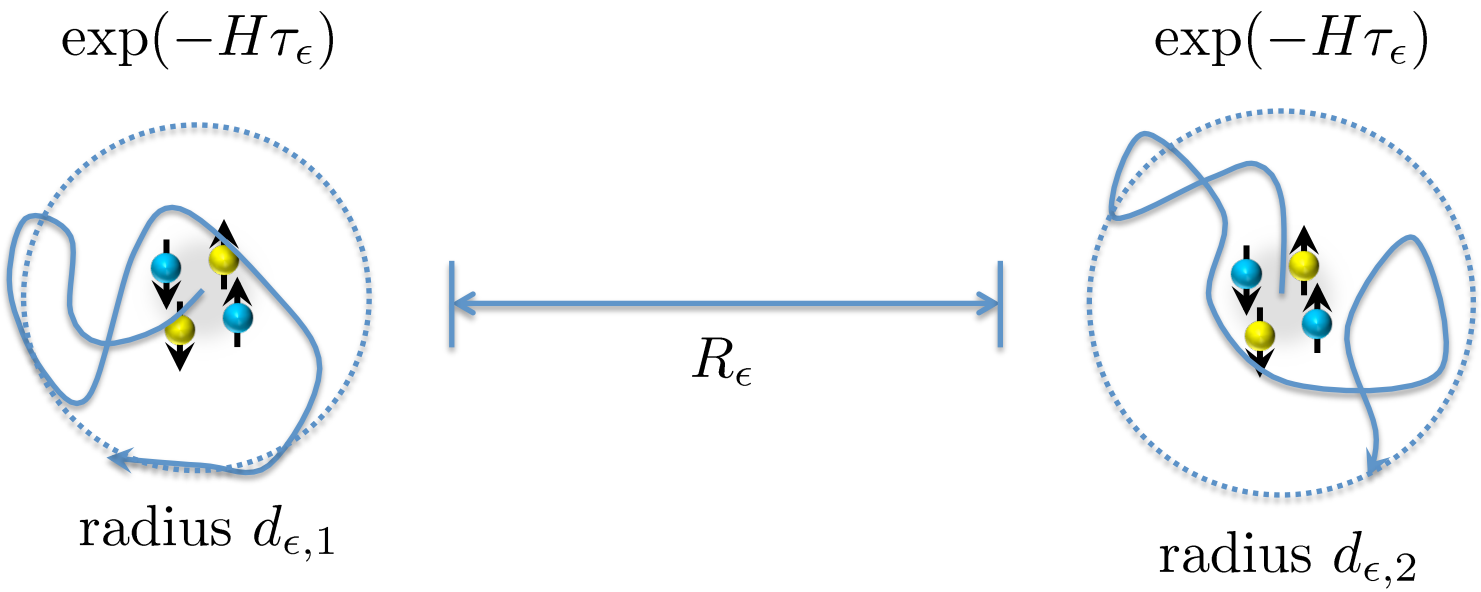
In order to explain the various time and length scales it is useful to define a relative error tolerance, ϵ.

As we project to large Euclidean time, the dressed cluster states for very widely separated clusters are simply two non-overlapping wave packets with less and less contamination from excited cluster states.

We define τ_ϵ as the time at which the relative contamination due to excited cluster states is less than ϵ.

During the Euclidean time interval τ_ϵ, each cluster will undergo spatial diffusion by a distance proportional to $\sqrt{\tau_\epsilon/M}$, where M is the mass of the cluster. Let $d_{\epsilon,1}$ be the diffusion length for the first cluster, and $d_{\epsilon,2}$ be the diffusion length for the second cluster.

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, in progress



We take our periodic box length, L to be much larger than $d_{\epsilon,1}$ and $d_{\epsilon,2}$. When $|\vec{R}| \gg d_{\epsilon,1}, d_{\epsilon,2}$ the dressed cluster state $|\vec{R}\rangle_{\tau_\epsilon}$ consists of non-overlapping clusters. We now define an asymptotic radius R_ϵ as the radius such that for $|\vec{R}| > R_\epsilon$ the amount of overlap between the cluster wave packets is less than ϵ.

In the asymptotic region $|\vec{R}| > R_\epsilon$, our dressed clusters are widely separated and 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, in progress

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.

With no loss of precision we have found it very efficient to work with a radial adiabatic Hamiltonian on the lattice by projection onto spherical harmonics defined on sets of lattice points with the same distance from the origin.

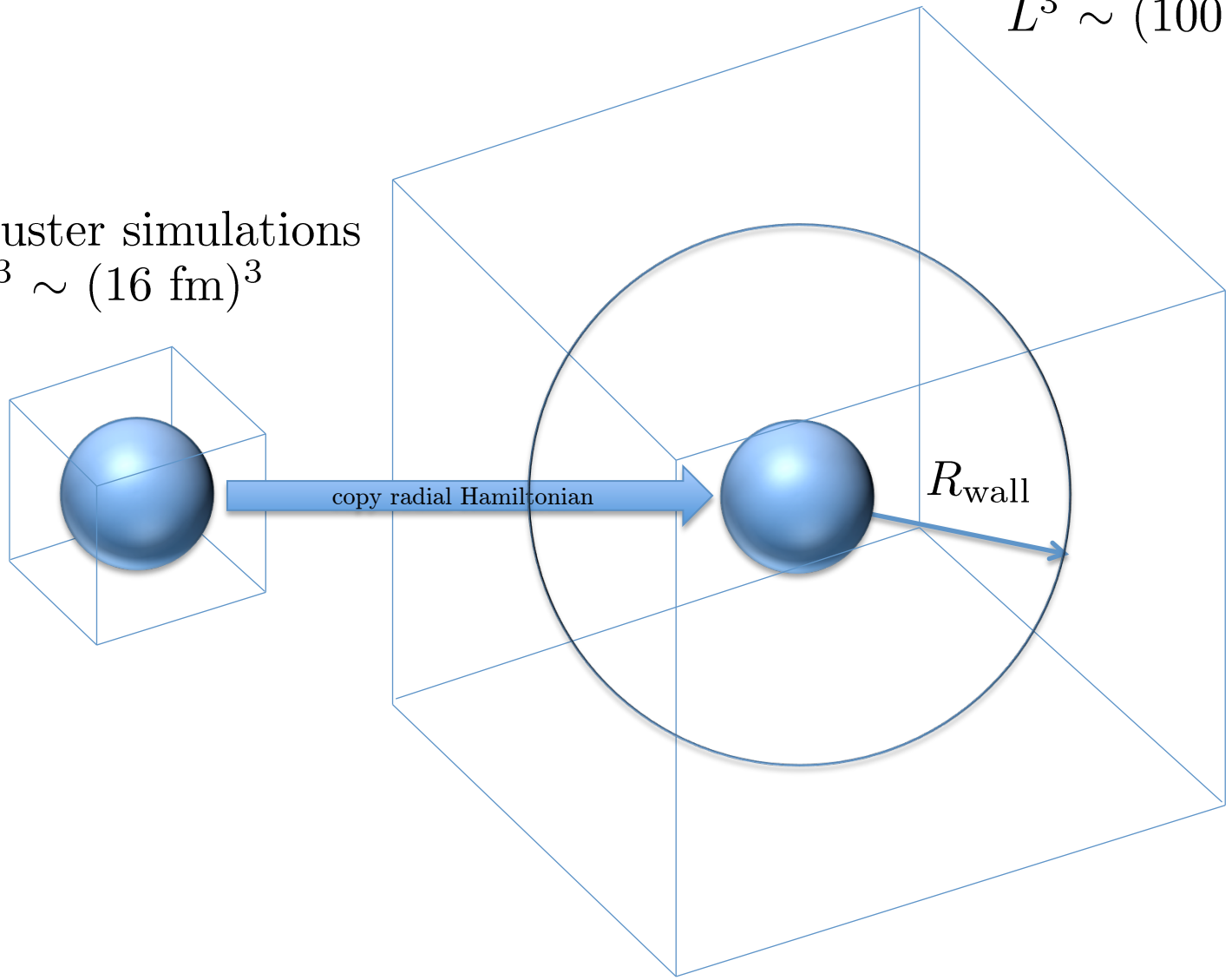
Moinard, Elhatisari, D.L. work in progress

$$[H^a_\tau]_{\vec{R},\vec{R}'} \to [H^a_\tau]^{L,L_z}_{R,R'}$$

We compute the radial adiabatic Hamiltonian for a lattice of length about 16 fm. We also compute the radial adiabatic Hamiltonian for a much larger system of length about 100 fm. The large-system radial Hamiltonian is computed from single cluster simulations and includes only infinite-range interactions such as Coulomb between the clusters. We then do surgery and transplant the full interactions into the large system and impose hard spherical wall boundary conditions at radius $R_{\rm wall}$.

single cluster simulations
$L^3 \sim (100 \text{ fm})^3$

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

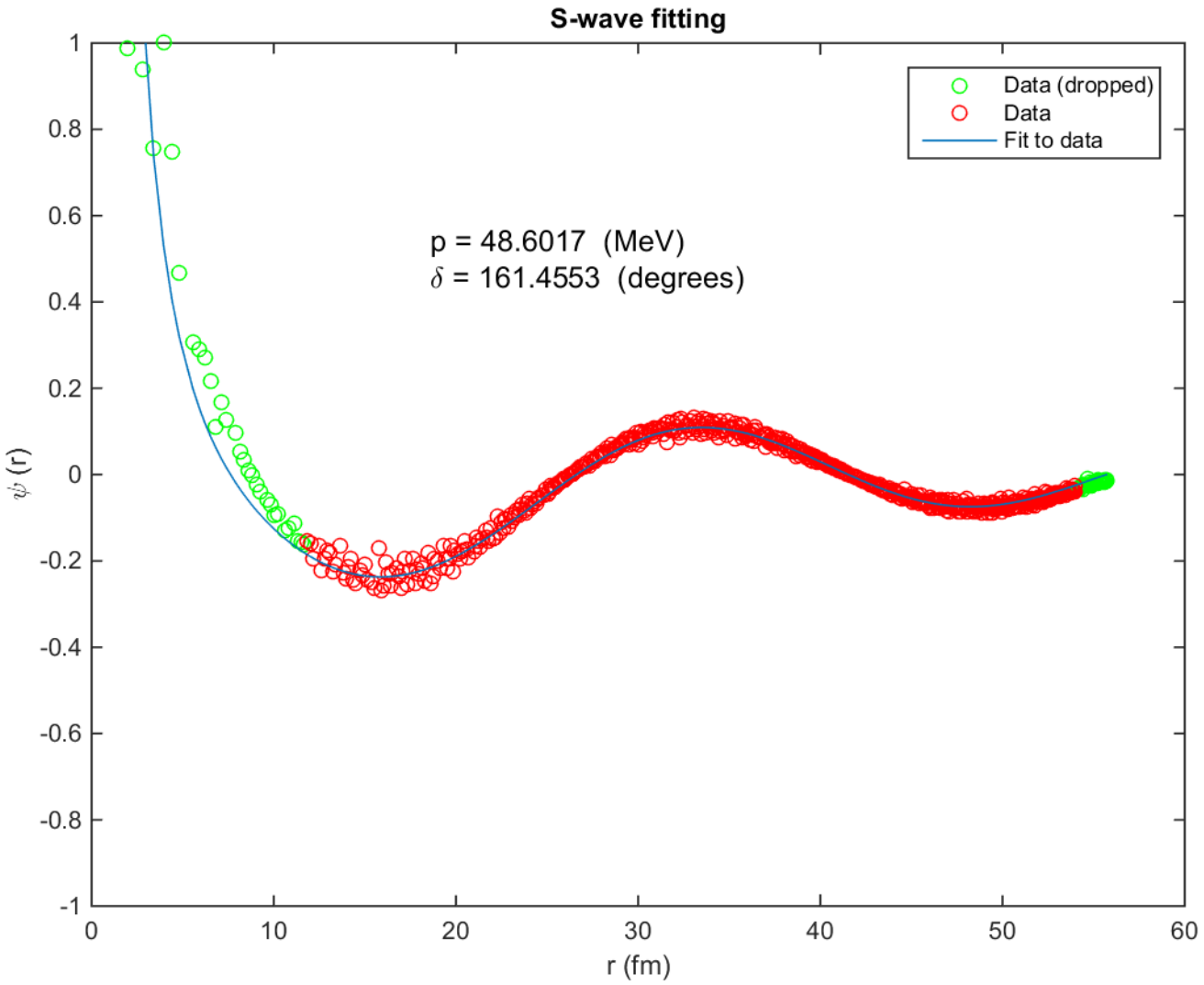


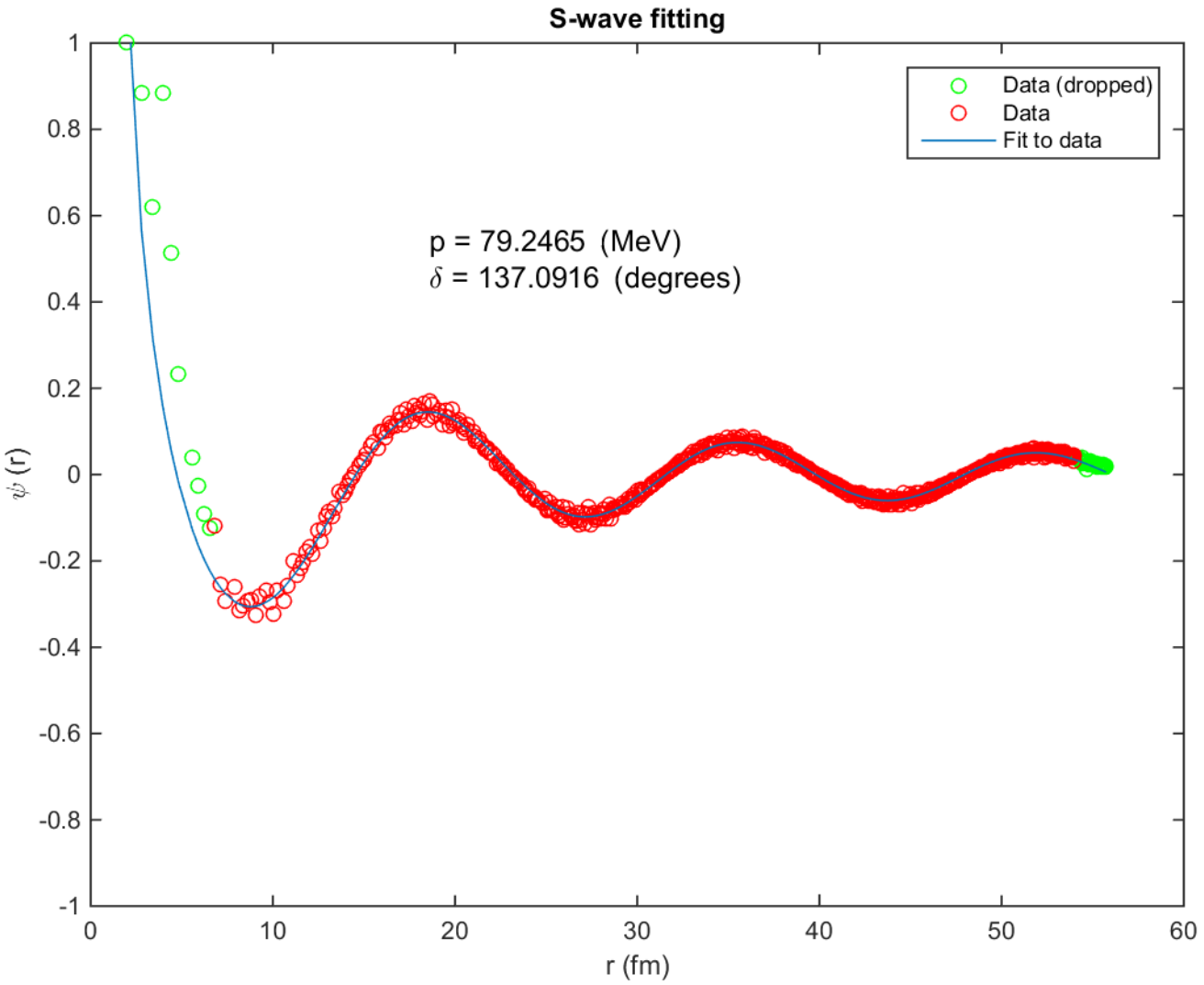
$^4\mathrm{He} + {}^4\mathrm{He} \to {}^4\mathrm{He} + {}^4\mathrm{He}$

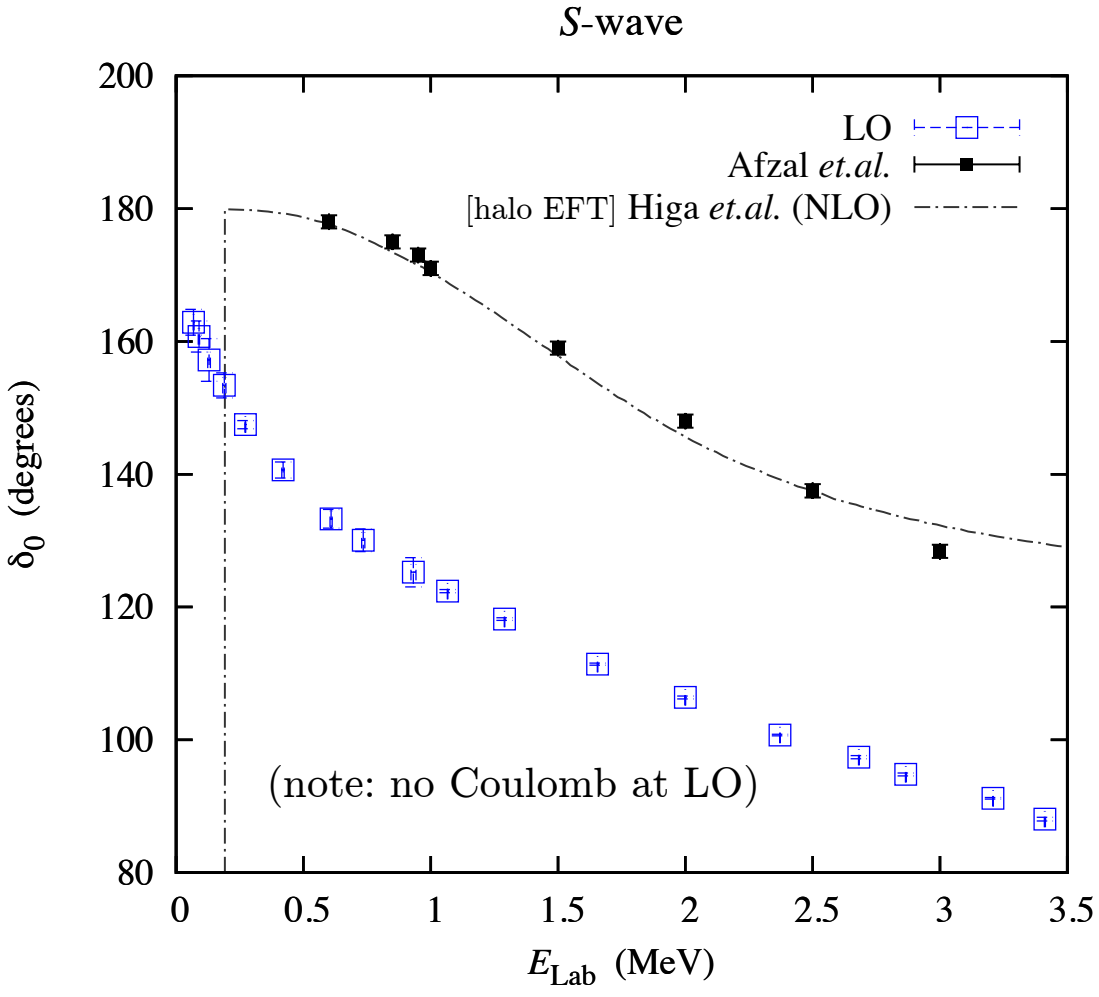
We now present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm. The results are preliminary.

Elhatisari, Epelbaum, Krebs, Lähde, Lee, Luu, Meißner, work in progress

Developed completely new lattice algorithm to allow for an arbitrary number of independent channels where the auxiliary fields are updated by the hybrid Monte Carlo algorithm but the initial and final channels are updated according to the Metropolis algorithm. For the fully interacting $A = 8$ system, we used 16 radial coordinate points and computed 256 matrix elements. We did calculations for the S-wave and $L = 2$, $L_z = 0$ D-wave projections.

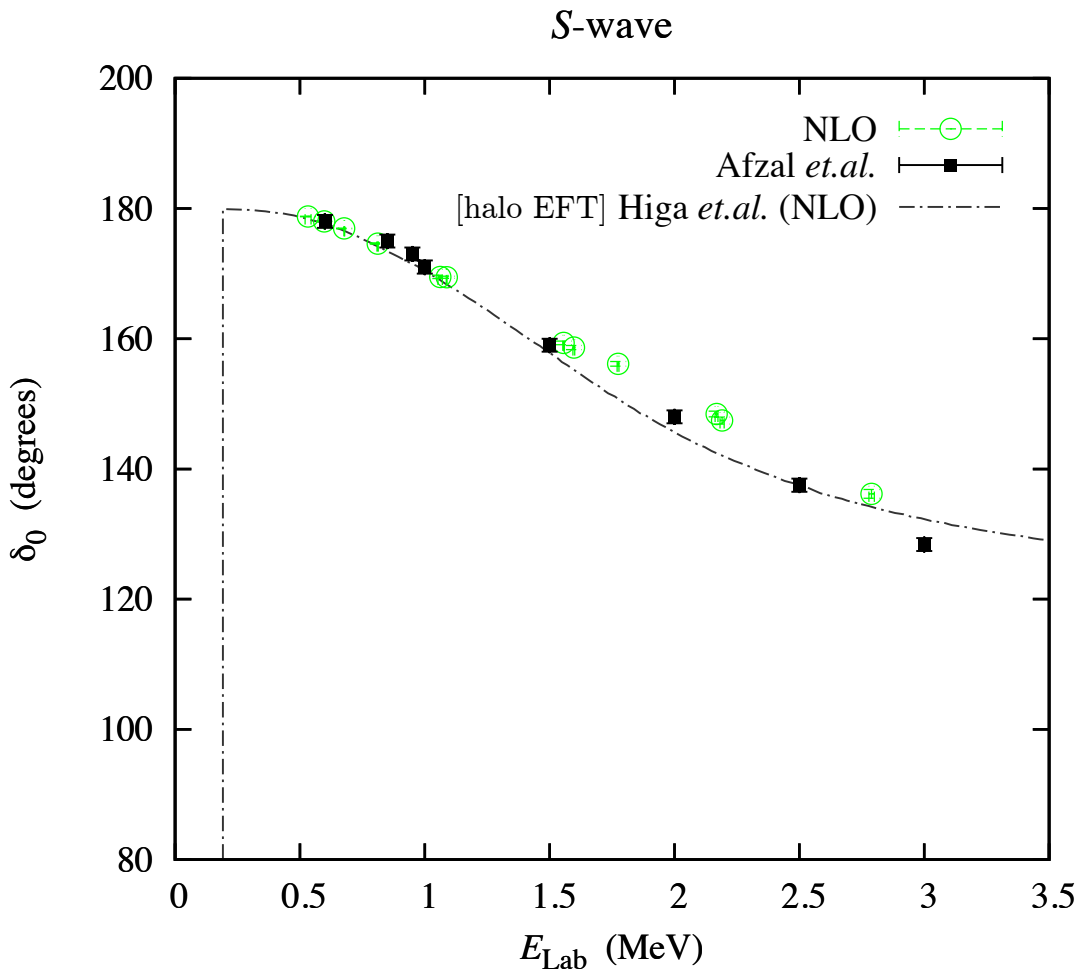

S-wave fitting
Data (dropped)
Data
Fit to data
p = 48.6017 (MeV)
δ = 161.4553 (degrees)
ψ (r)
r (fm)
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
10
20
30
40
50
60

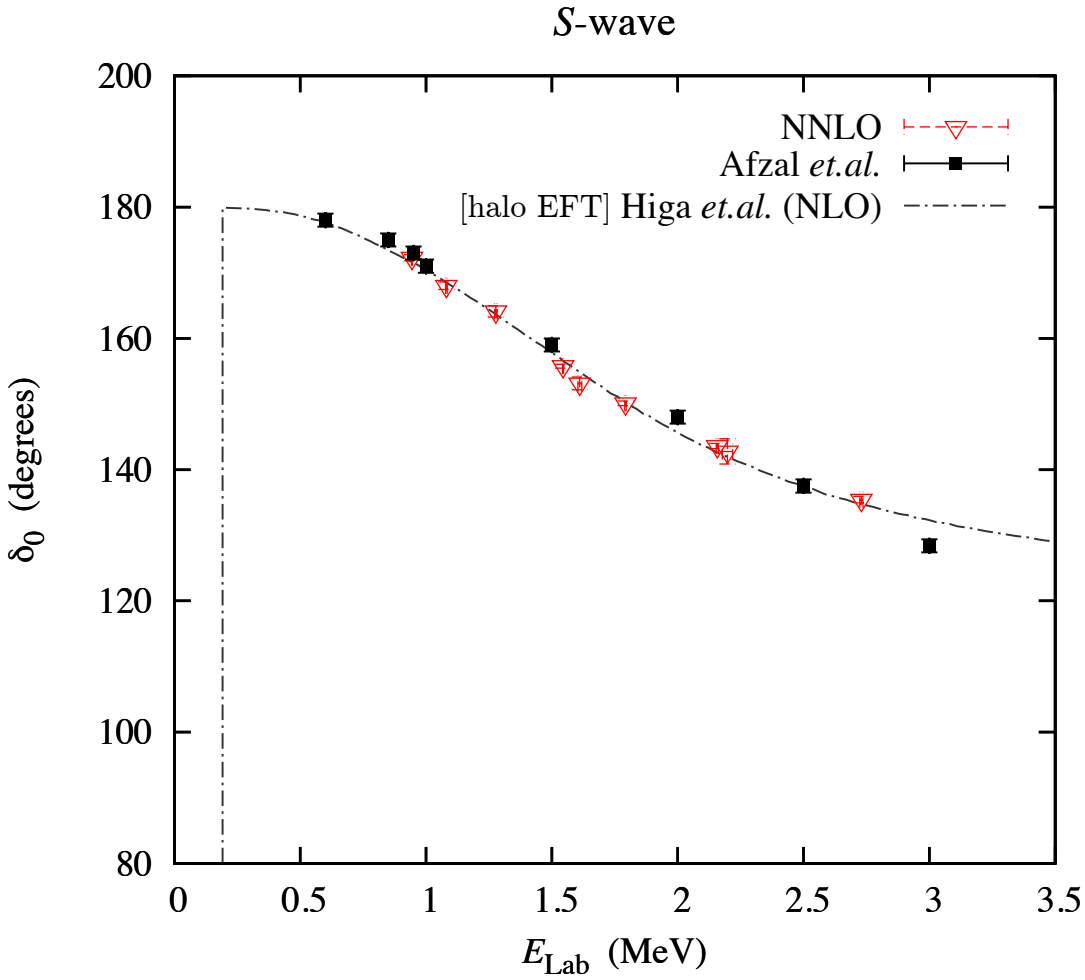

S-wave fitting
Data (dropped)
Data
Fit to data
p = 79.2465 (MeV)
δ = 137.0916 (degrees)
ψ (r)
r (fm)
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
10
20
30
40
50
60

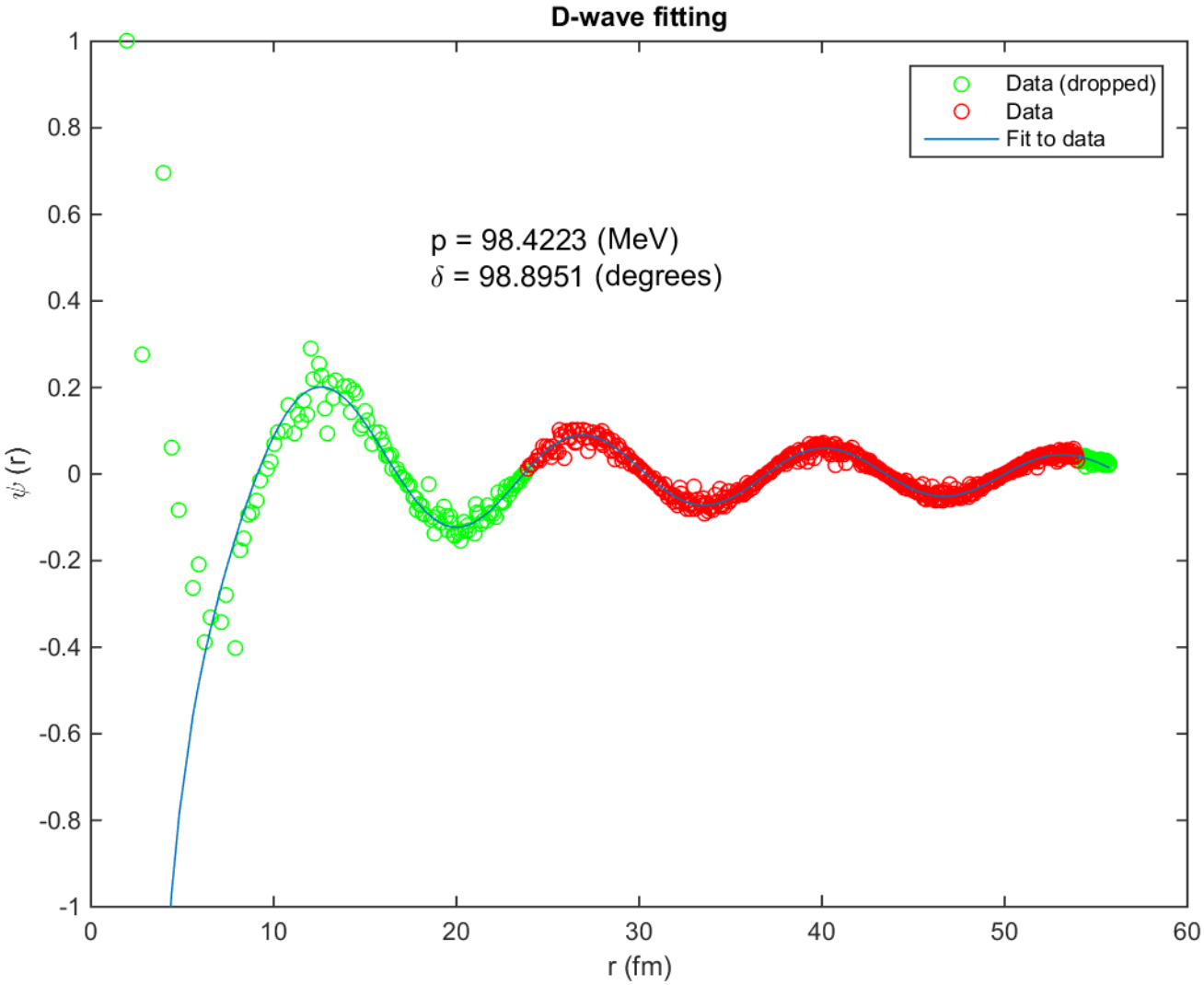


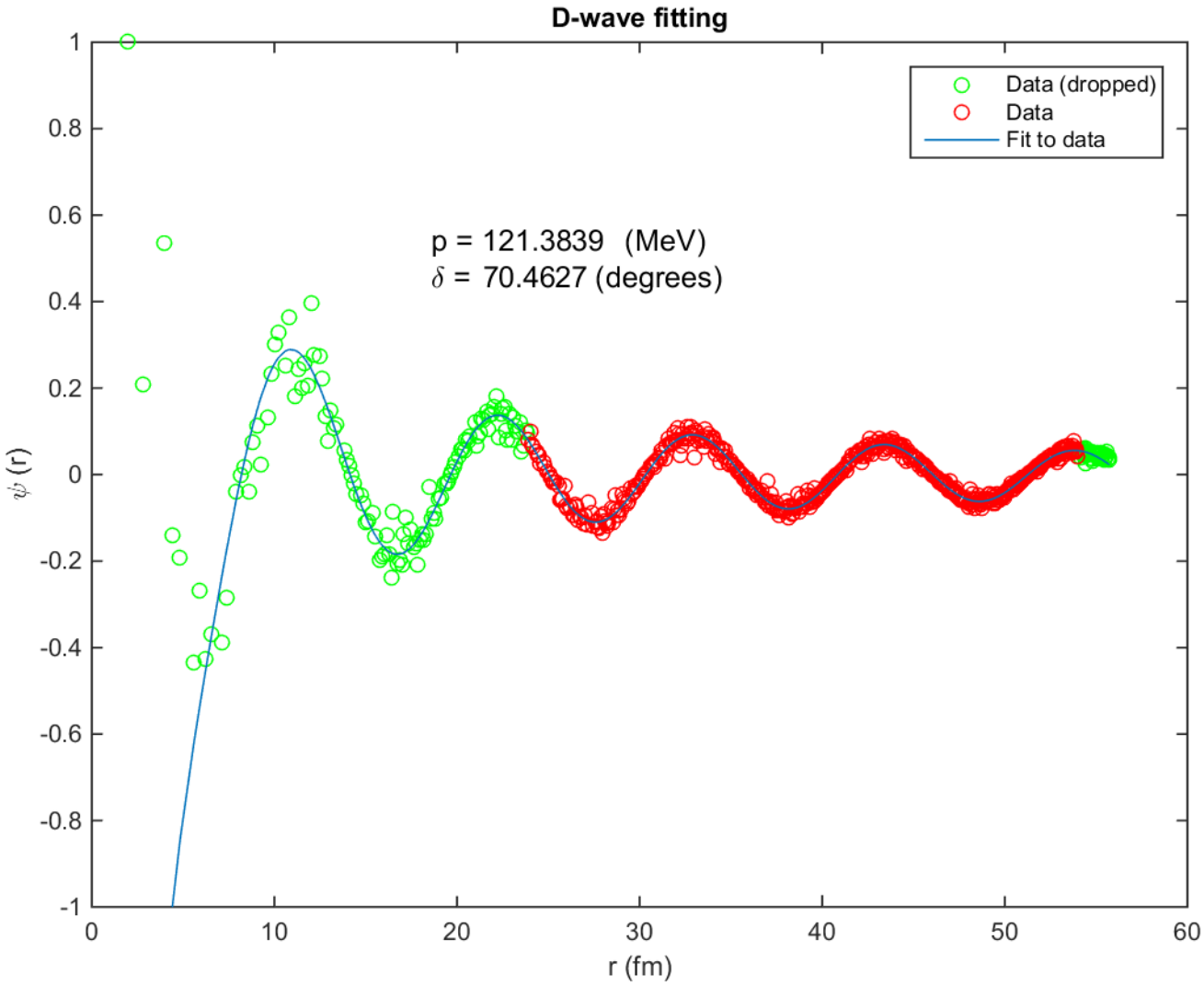
Higa, Hammer, van Kolck, NPA 809 171(2008)

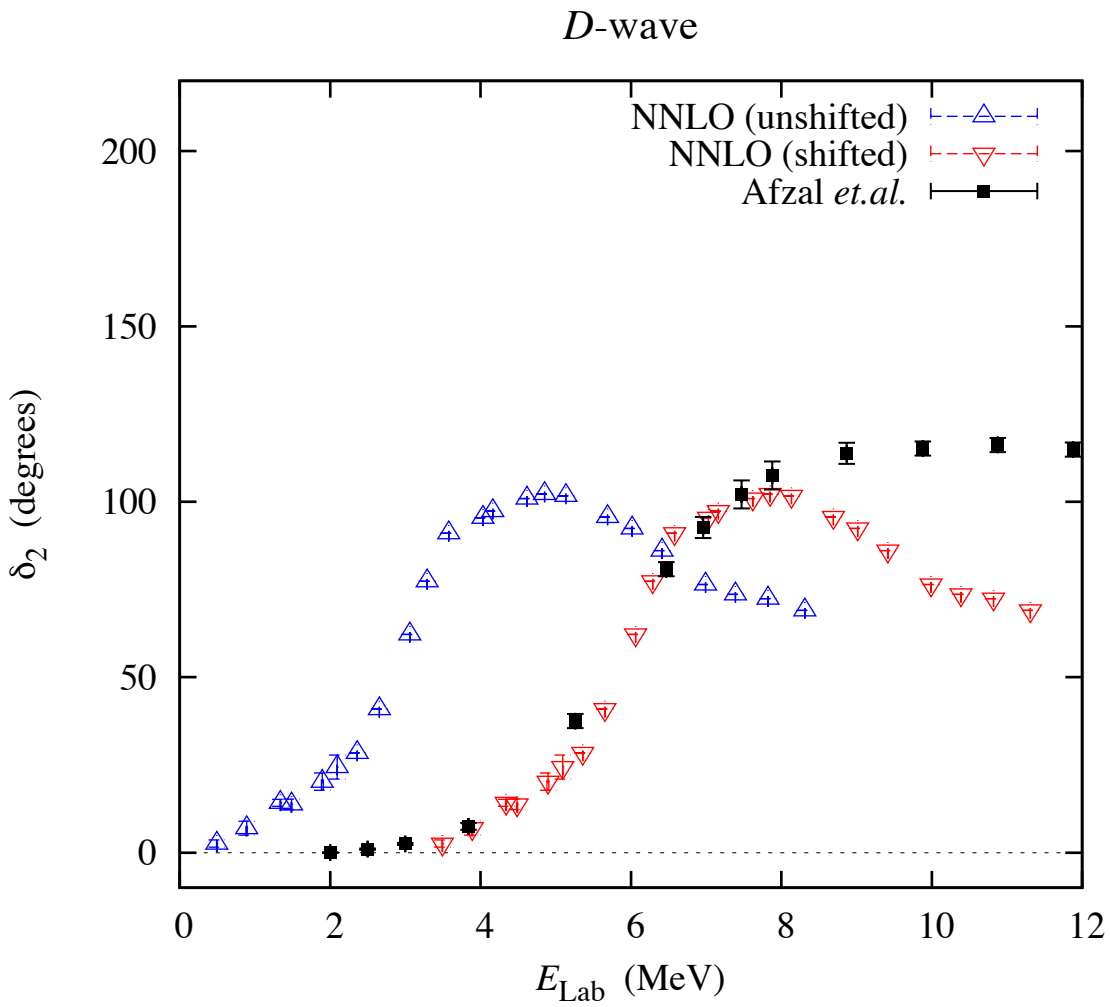
Afzal, Ahmad, Ali, RMP 41 247 (1969)


S-wave
NLO
Afzal et.al.
[halo EFT] Higa et.al. (NLO)
δ0 (degrees)
ELab (MeV)
200
180
160
140
120
100
80
0
0.5
1
1.5
2
2.5
3
3.5


S-wave
NNLO
Afzal et.al.
[halo EFT] Higa et.al. (NLO)
δ0 (degrees)
ELab (MeV)
200
180
160
140
120
100
80
0
0.5
1
1.5
2
2.5
3
3.5


D-wave fitting
Data (dropped)
Data
Fit to data
p = 98.4223 (MeV)
δ = 98.8951 (degrees)
ψ (r)
r (fm)
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
10
20
30
40
50
60


D-wave fitting
Data (dropped)
Data
Fit to data
p = 121.3839 (MeV)
δ = 70.4627 (degrees)
ψ (r)
r (fm)
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
10
20
30
40
50
60



At NNLO 2^+ resonance at 1.7 MeV. Physical value is 3.1 MeV.

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)

Providing *ab initio* input for halo/cluster EFT calculations could be a useful and fun theoretical space to explore. In cases where the separation of scales is good, the radial adiabatic Hamiltonian should reproduce halo/cluster EFT calculations. In cases where the separation of scales is not large, the halo/cluster EFT calculations could use the radial adiabatic Hamiltonian to test convergence.