Lattice Methods for Nuclear Physics

Lecture 6: Adiabatic Projection Method

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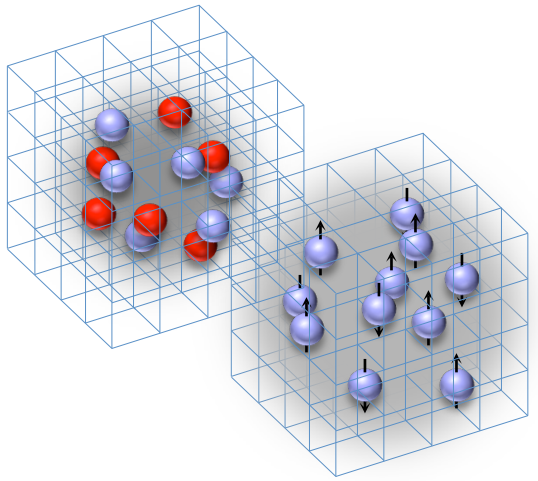
Nuclear Lattice EFT Collaboration



TALENT School
on Nuclear Quantum Monte Carlo Methods
North Carolina State University
July 28, 2016

Hybrid Monte Carlo updates

We start by selecting the initial p_s configuration according to the random Gaussian distribution

$$P[p_s^0(\vec{n}, n_t)] \propto \exp\left\{-\tfrac{1}{2}\left[p_s^0(\vec{n}, n_t)\right]^2\right\}$$

Initial half step for p_s:

$$\tilde{p}_s^0(\vec{n}, n_t) = p_s^0(\vec{n}, n_t) - \frac{\varepsilon_{\text{step}}}{2}\left[\frac{\partial V(s)}{\partial s(\vec{n}, n_t)}\right]_{s=s^0}$$

$$\frac{\partial V}{\partial s(\vec{n}, n_t)} = \frac{\partial S_{ss}(s)}{\partial s(\vec{n}, n_t)} - \frac{\partial \mathrm{Re}[\ln(\det \mathbf{Z})]}{\partial s(\vec{n}, n_t)}$$

$$= \frac{\partial S_{ss}(s)}{\partial s(\vec{n}, n_t)} - \mathrm{Re}\left[\sum_{k,l} \mathbf{Z}^{-1}_{lk} \frac{\partial \mathbf{Z}_{kl}}{\partial s(\vec{n}, n_t)}\right]$$

Full steps for s and p_s:

$$s^{i+1}(\vec{n}, n_t) = s^i(\vec{n}, n_t) + \varepsilon_{\text{step}} \tilde{p}_s^i(\vec{n}, n_t)$$

$$\tilde{p}_s^{i+1}(\vec{n}, n_t) = \tilde{p}_s^i(\vec{n}, n_t) - \varepsilon_{\text{step}} \left[\frac{\partial V(s)}{\partial s(\vec{n}, n_t)} \right]_{s=s^{i+1}}$$

Cut the last step for p_s so it is a half step:

$$p_s^{N_{\text{step}}}(\vec{n}, n_t) = \tilde{p}_s^{N_{\text{step}}}(\vec{n}, n_t) + \frac{\varepsilon_{\text{step}}}{2} \left[\frac{\partial V(s)}{\partial s(\vec{n}, n_t)} \right]_{s=s^0}$$

We accept the new configurations for s and p_s if the uniform random number r between 0 and 1 satisfies

$$r < \exp\left[-H(s^{N_{\text{step}}}, p_s^{N_{\text{step}}}) + H(s^0, p_s^0) \right]$$

Then return back and repeat the steps listed above.

```
!     initial half step for p_sHMC, p_sIHMC, p_pionHMC

CALL getzvecs(s,sI,zvecs,zwave,Lt,0, &
     pion,ztau2x2,n_f)
CALL getzdualvecs(s,sI,zdualvecs,zdualwave, &
     Lt,0,pion,ztau2x2,n_f)
CALL getinvcorr(zvecs,zdualvecs,zldeter, &
     zcorrmatrix,zcorrinv,Lt)
aldeterabs = DBLE(zldeter)
zdeterphase = CDEXP((0.D0,1.D0)*DIMAG(zldeter))
act = bose - aldeterabs
```

⋮

```
DO nt = 0,Lt-1
   DO nz = 0,L-1; DO ny = 0,L-1; DO nx = 0,L-1

      DO npart1 = 0,n_f-1; DO npart2 = 0,n_f-1
         zdcorrmatrix(npart2,npart1) = 0.D0
         DO ni = 0,1; DO ns = 0,1
            zdcorrmatrix(npart2,npart1) = &
                 zdcorrmatrix(npart2,npart1) + &
                 zdualvecs(nx,ny,nz,nt+1,ns,ni,npart2) &
                 *zvecs(nx,ny,nz,nt,ns,ni,npart1) &
                 *CDSQRT(-c0*atovera*(1.D0,0.D0))/L**3
         END DO; END DO
      END DO; END DO

      dVds(nx,ny,nz,nt) = s(nx,ny,nz,nt)
      DO npart1 = 0,n_f-1; DO npart2 = 0,n_f-1
         dVds(nx,ny,nz,nt) = dVds(nx,ny,nz,nt) &
              - DBLE(zdcorrmatrix(npart2,npart1) &
              *zcorrinv(npart1,npart2))
      END DO; END DO

      p_sHMC(nx,ny,nz,nt,0) = &
           p_s(nx,ny,nz,nt) - 0.5D0*eHMC*dVds(nx,ny,nz,nt)


          ⋮
```

```
DO nstep = 0,nHMC-1

   IF (nstep .eq. nHMC-1) THEN
      step = 0.5D0
   ELSE
      step = 1.D0
   END IF

   DO nt = 0,Lt-1
      DO nz = 0,L-1; DO ny = 0,L-1; DO nx = 0,L-1
         sHMC(nx,ny,nz,nt,nstep+1) = sHMC(nx,ny,nz,nt,nstep) &
              + eHMC*p_sHMC(nx,ny,nz,nt,nstep)
      END DO; END DO; END DO
   END DO
```

⋮

```
CALL getzvecs(sHMC(0,0,0,0,nstep+1), &
     sIHMC(0,0,0,Ltouter,1,nstep+1), &
     zvecs,zwave,Lt,0, &
     pionHMC(0,0,0,Ltouter,1,nstep+1), &
     ztau2x2,n_f)

CALL getzdualvecs(sHMC(0,0,0,0,nstep+1), &
     sIHMC(0,0,0,Ltouter,1,nstep+1), &
     zdualvecs,zdualwave,Lt,0, &
     pionHMC(0,0,0,Ltouter,1,nstep+1), &
     ztau2x2,n_f)

CALL getinvcorr(zvecs,zdualvecs,zldeter_HMC, &
     zcorrmatrix,zcorrinv,Lt-1)
```

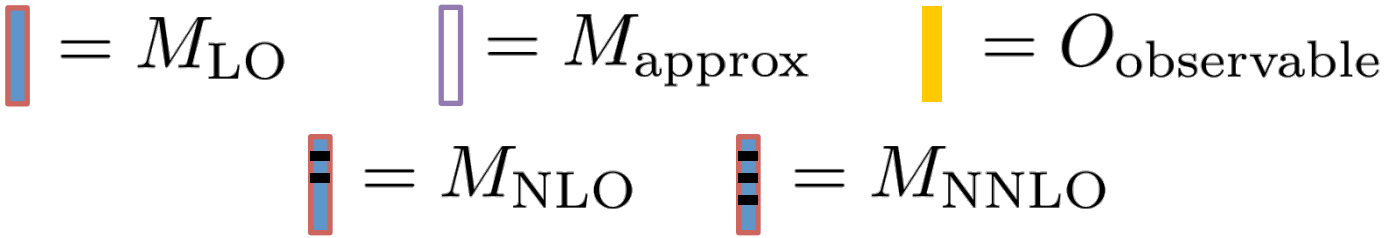
⋮

```
DO nt = 0,Lt-1
   DO nz = 0,L-1; DO ny = 0,L-1; DO nx = 0,L-1

      DO npart1 = 0,n_f-1; DO npart2 = 0,n_f-1
         zdcorrmatrix(npart2,npart1) = 0.D0
         DO ni = 0,1; DO ns = 0,1
            zdcorrmatrix(npart2,npart1) = &
                 zdcorrmatrix(npart2,npart1) &
                 + zdualvecs(nx,ny,nz,nt+1,ns,ni,npart2) &
                 *zvecs(nx,ny,nz,nt,ns,ni,npart1) &
                 *CDSQRT(-c0*atovera*(1.D0,0.D0))/L**3
         END DO; END DO; END DO
      END DO

      dVds(nx,ny,nz,nt) = sHMC(nx,ny,nz,nt,nstep+1)
      DO npart1 = 0,n_f-1; DO npart2 = 0,n_f-1
         dVds(nx,ny,nz,nt) = dVds(nx,ny,nz,nt) &
              - DBLE(zdcorrmatrix(npart2,npart1) &
              *zcorrinv(npart1,npart2))
      END DO; END DO
```

Schematic of lattice Monte Carlo calculations



Hybrid Monte Carlo sampling

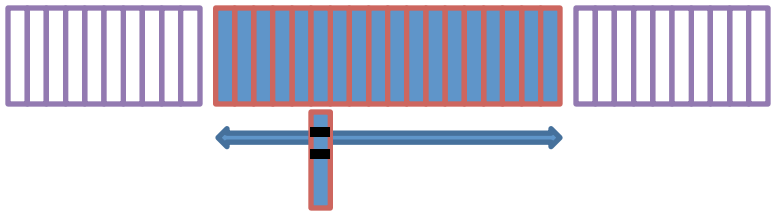
$$Z_{n_t,\mathrm{LO}} = \langle \psi_{\mathrm{init}} | \; \cdots \; | \psi_{\mathrm{init}} \rangle$$

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

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

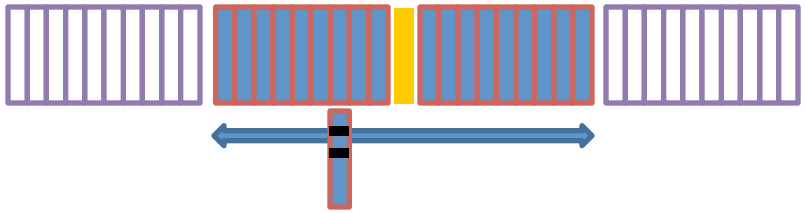
$$\langle O \rangle_{0,\mathrm{LO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

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



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

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



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

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

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.

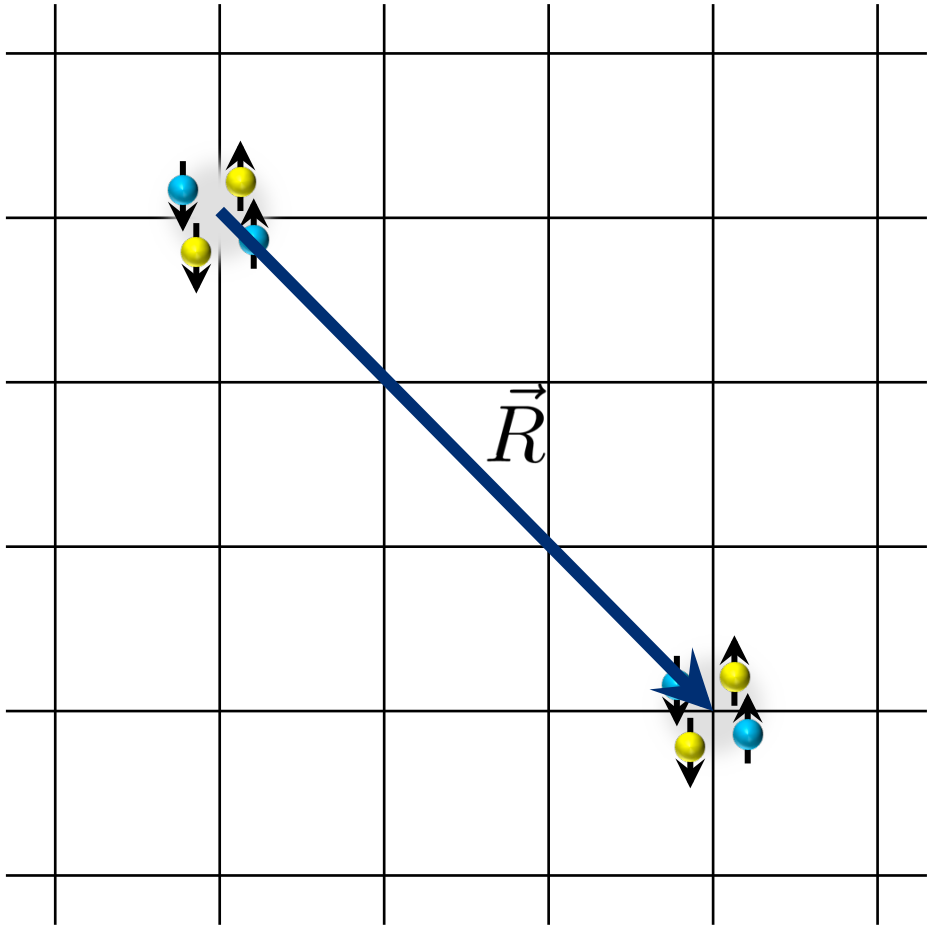
Navratil, Roth, Quaglioni, PRC 82 034609 (2010); Navratil, Quaglioni, PRC 83 044609 (2011); etc.

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.

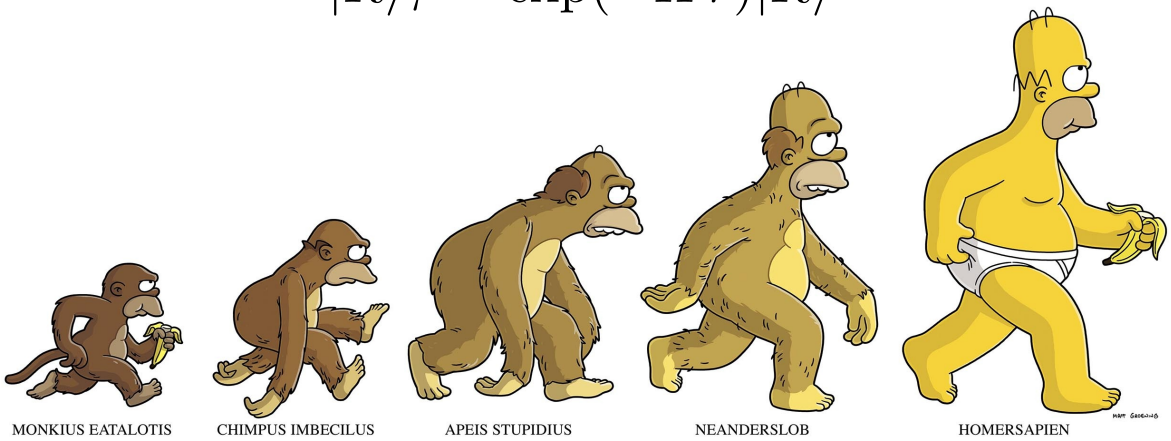
Start with localized cluster states for all possible separation vectors $\vec{R}$

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



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

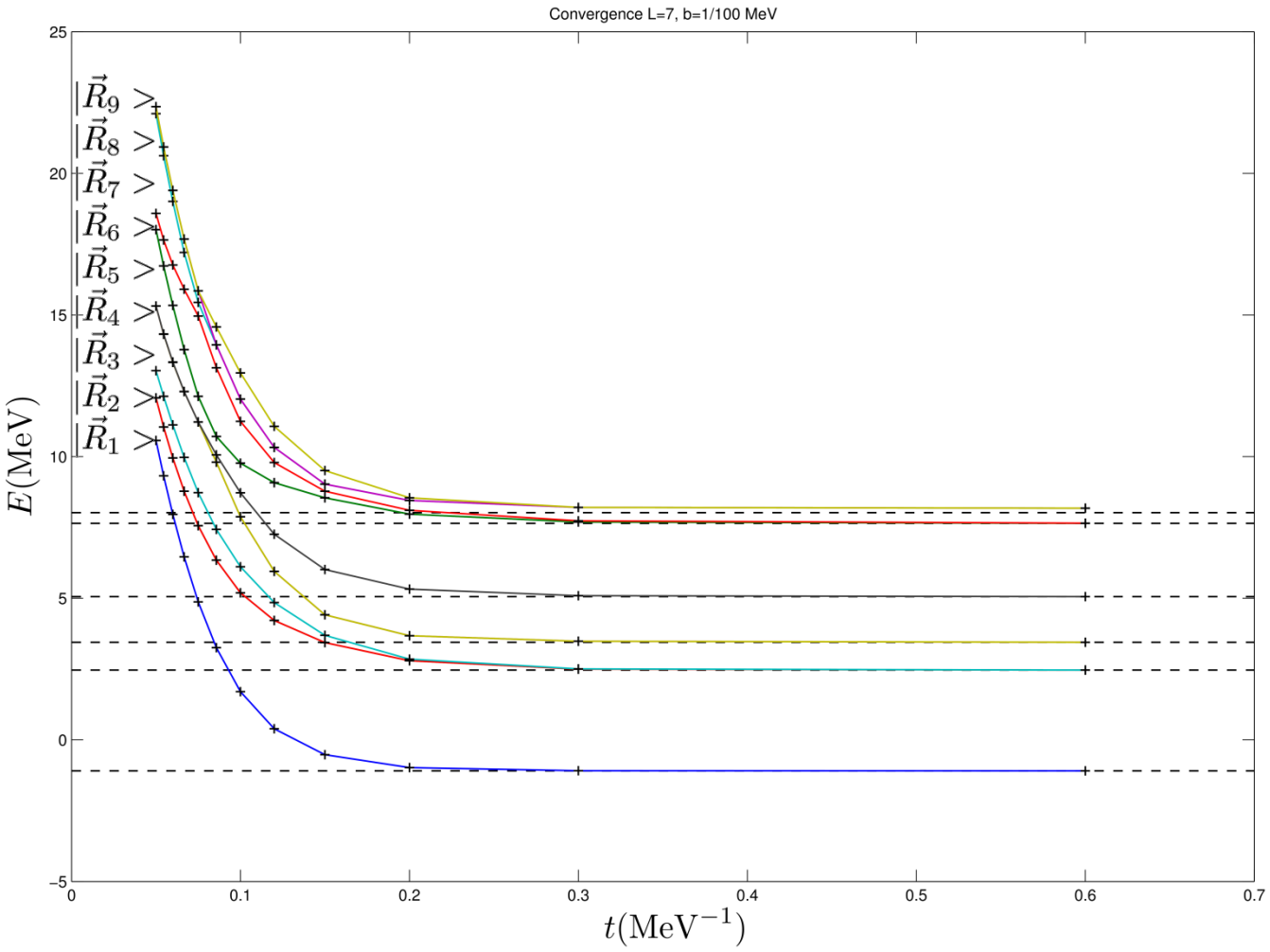
$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

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.

Quartet neutron-deuteron scattering (pionless EFT)



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

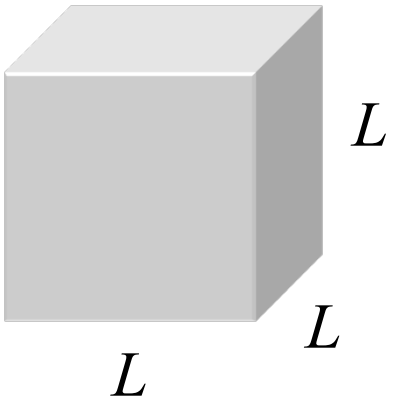
Lüscher's finite-volume formula

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

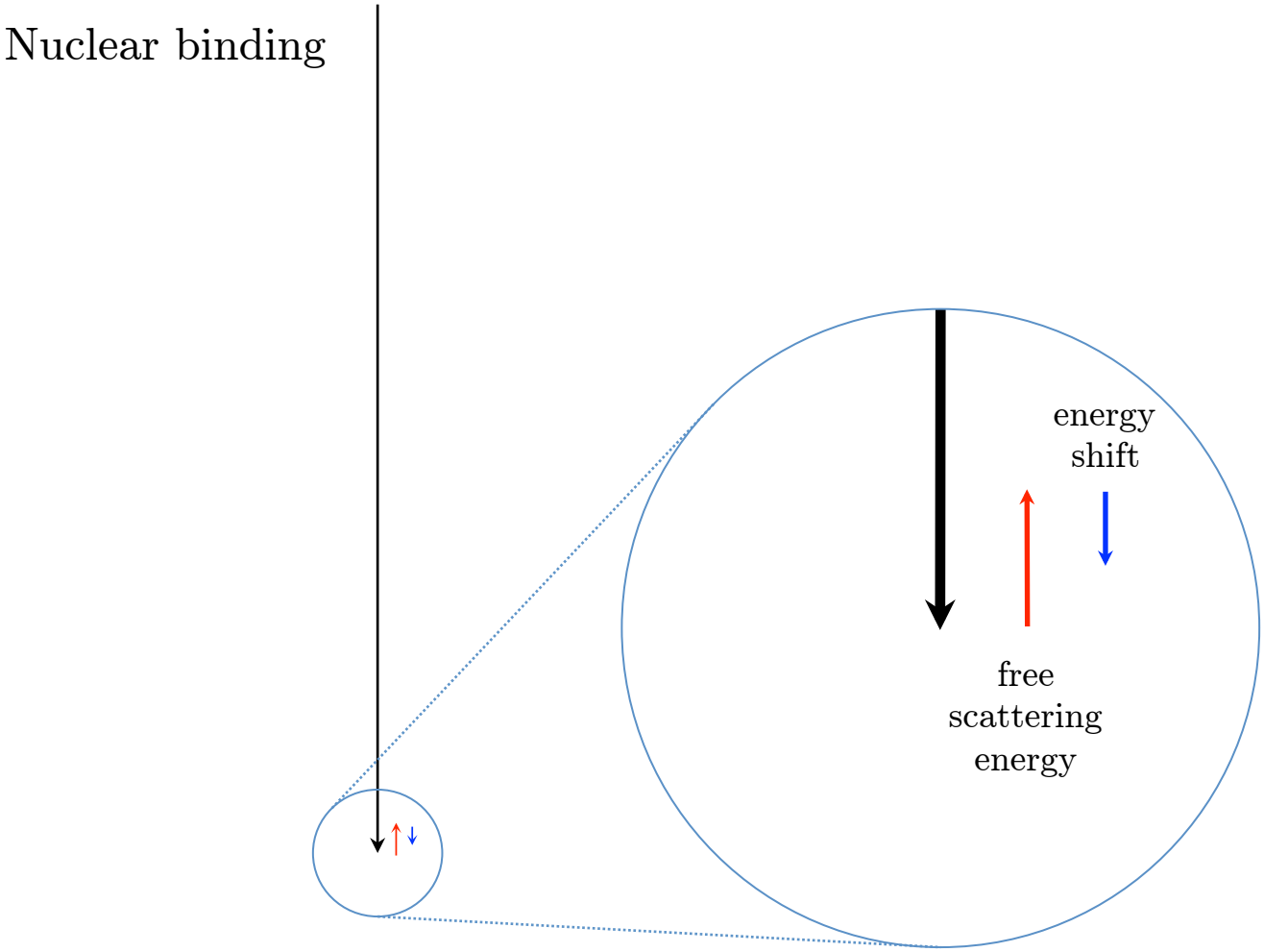
Two-particle energy levels near threshold in a periodic cube are related to the elastic phase shifts

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

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



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^{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, 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

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

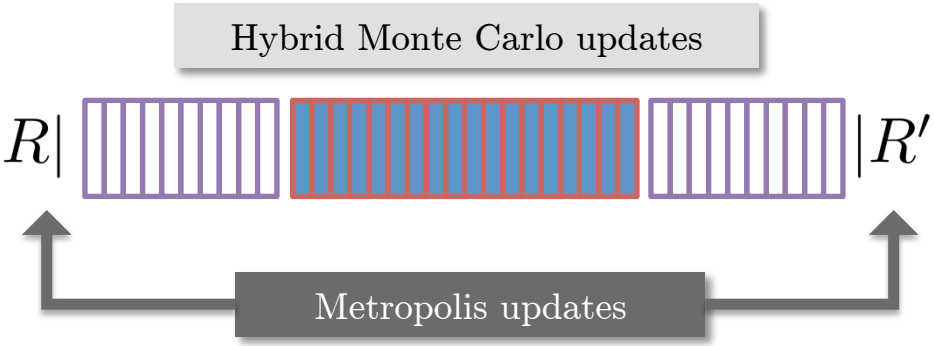
In the asymptotic region, we are inverting the diffusion process when computing the adiabatic Hamiltonian and are left with an effective cluster Hamiltonian in position space basis.

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

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

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

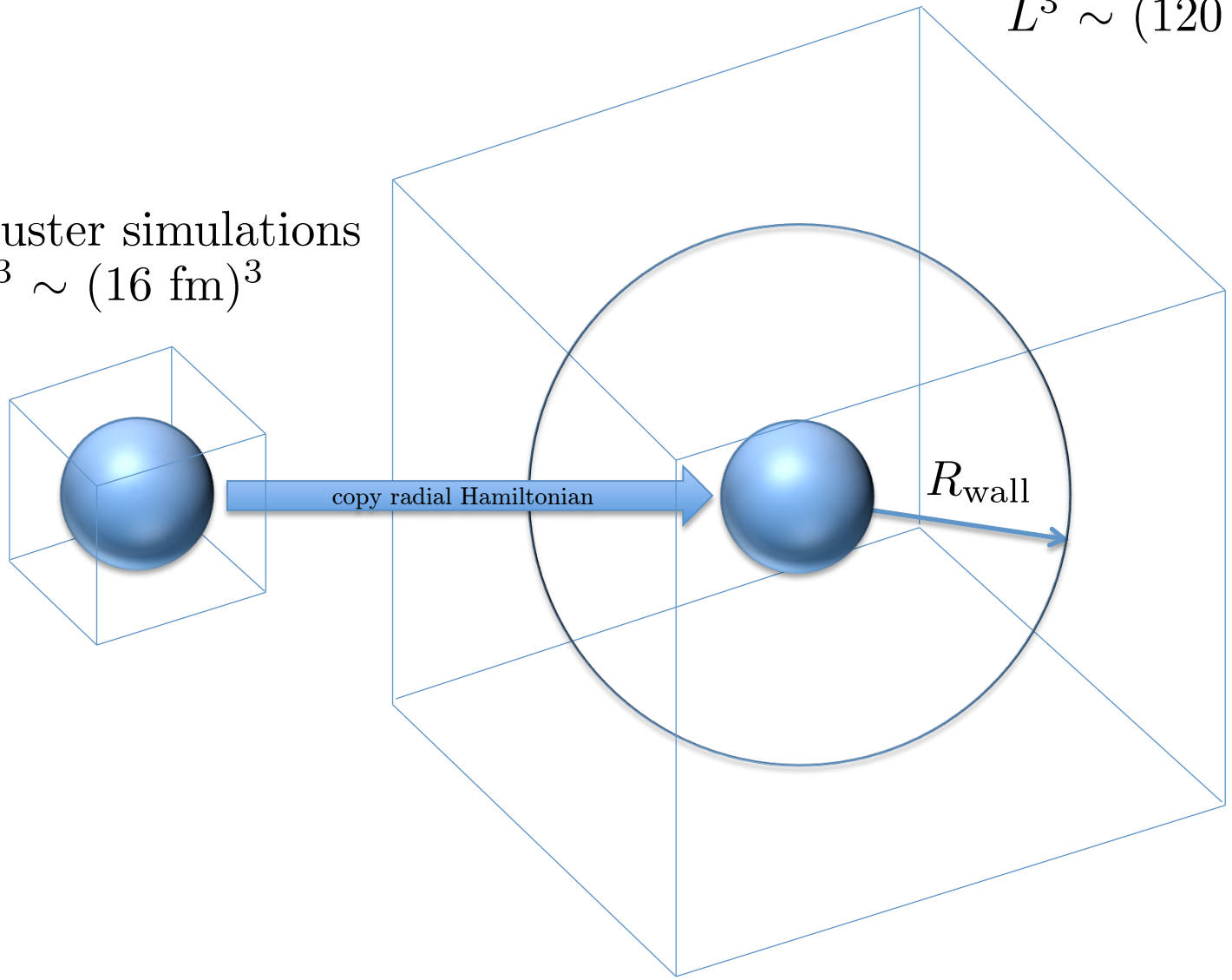
$$[Z_{n_t,\mathrm{LO}}]^{L,L_z}_{R,R'} = {}^{L,L_z}\langle R|$$



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

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

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

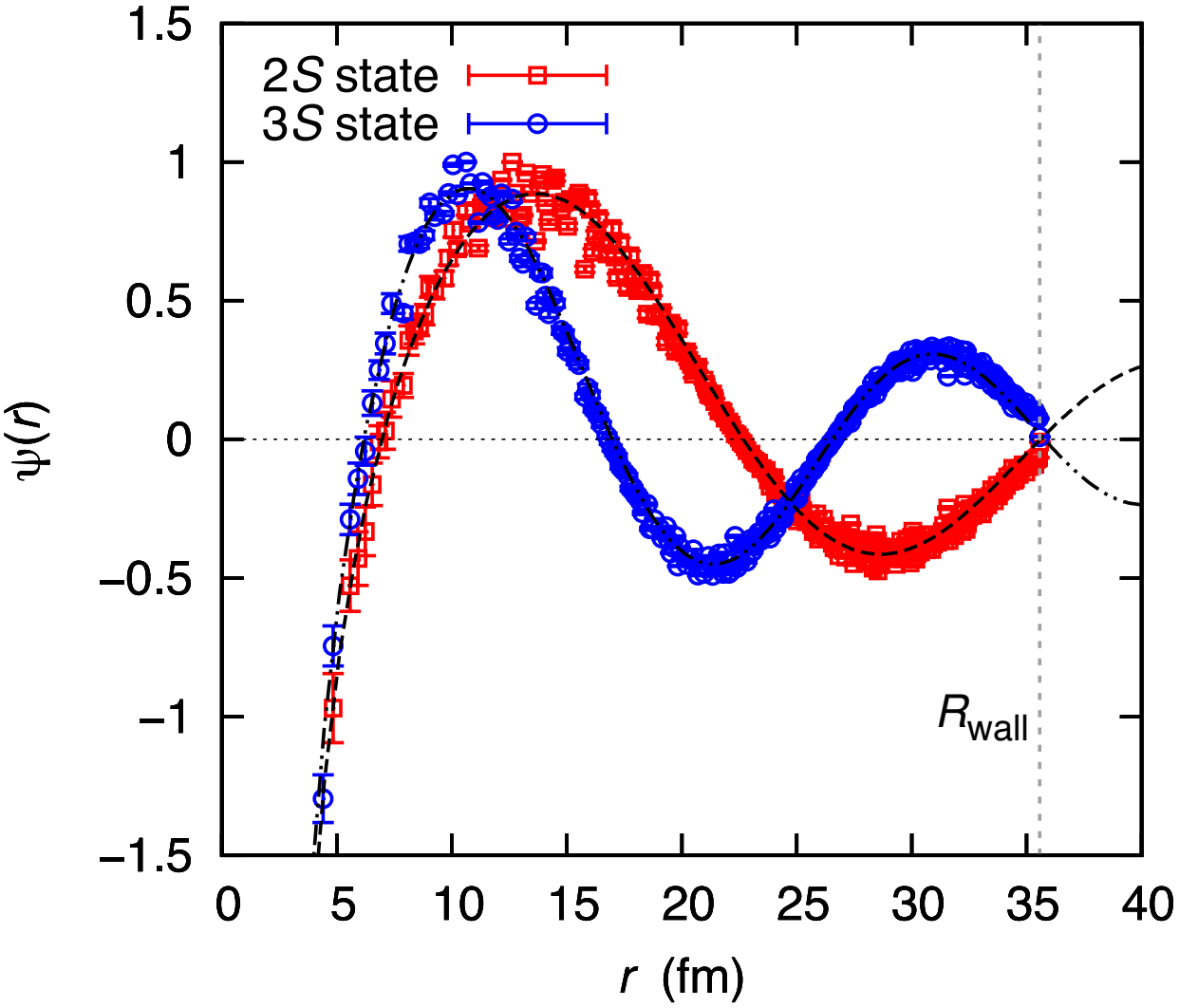


$^4\mathrm{He} + {}^4\mathrm{He} \to {}^4\mathrm{He} + {}^4\mathrm{He}$

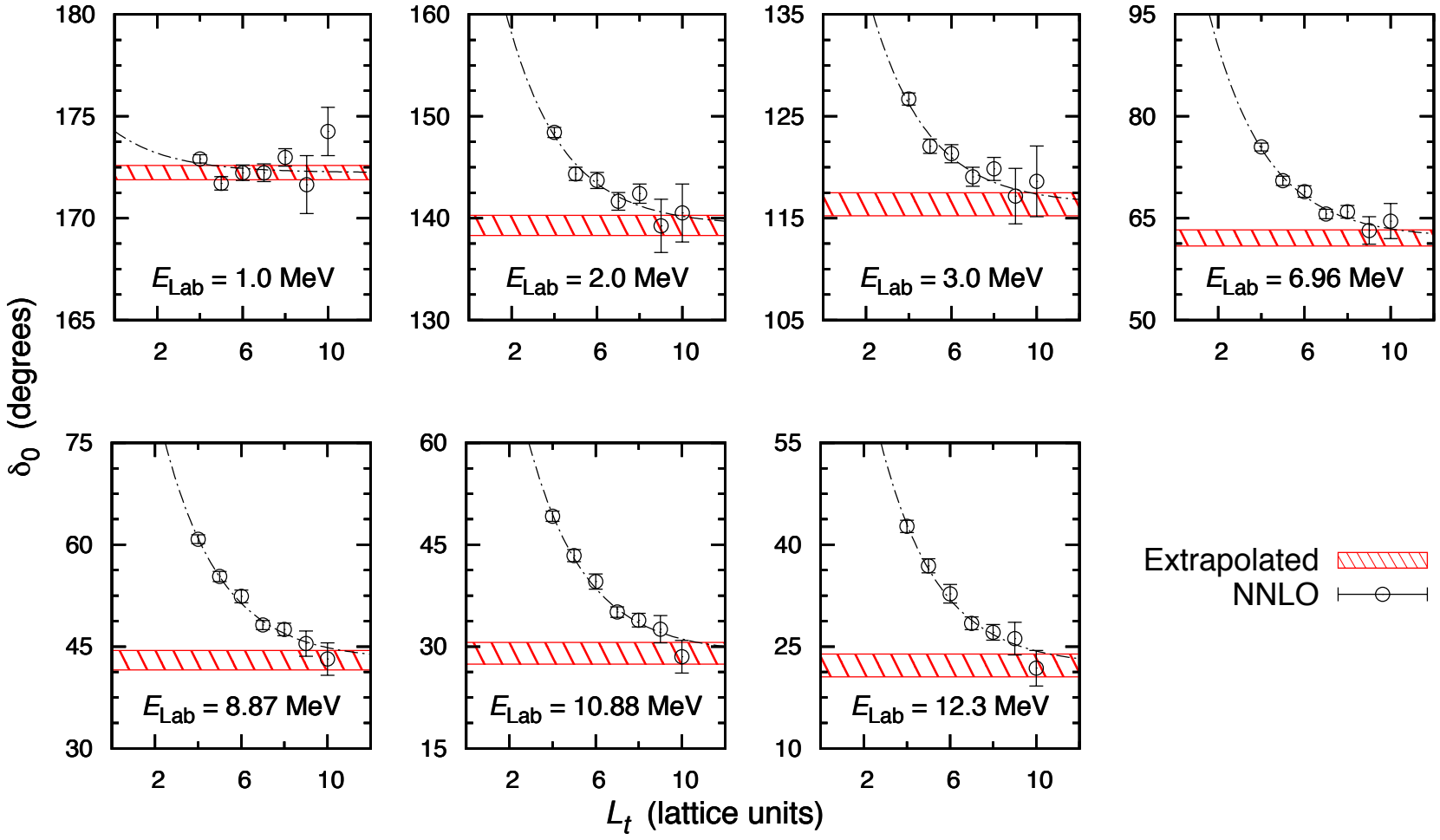
We now present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

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

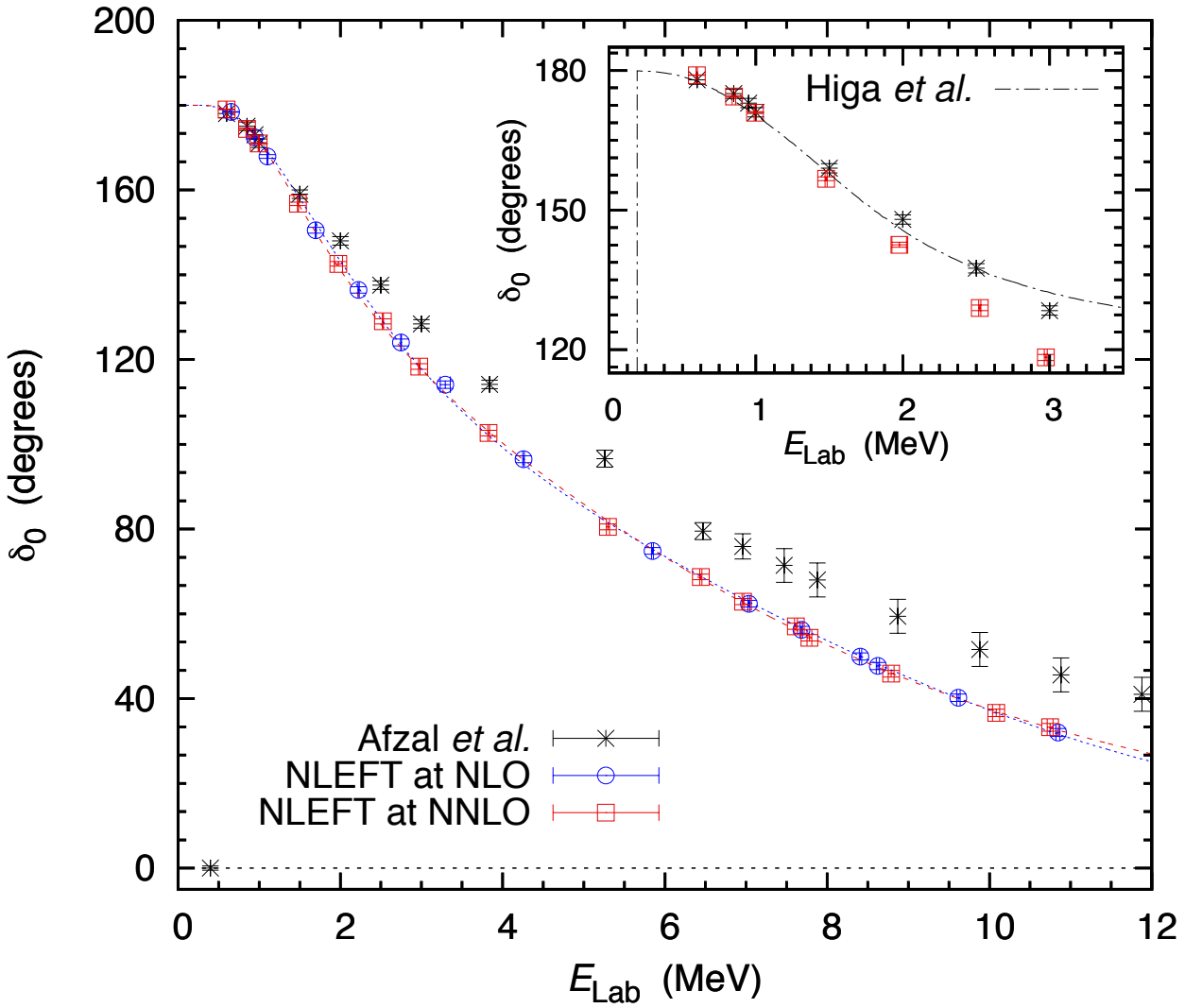
Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)


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



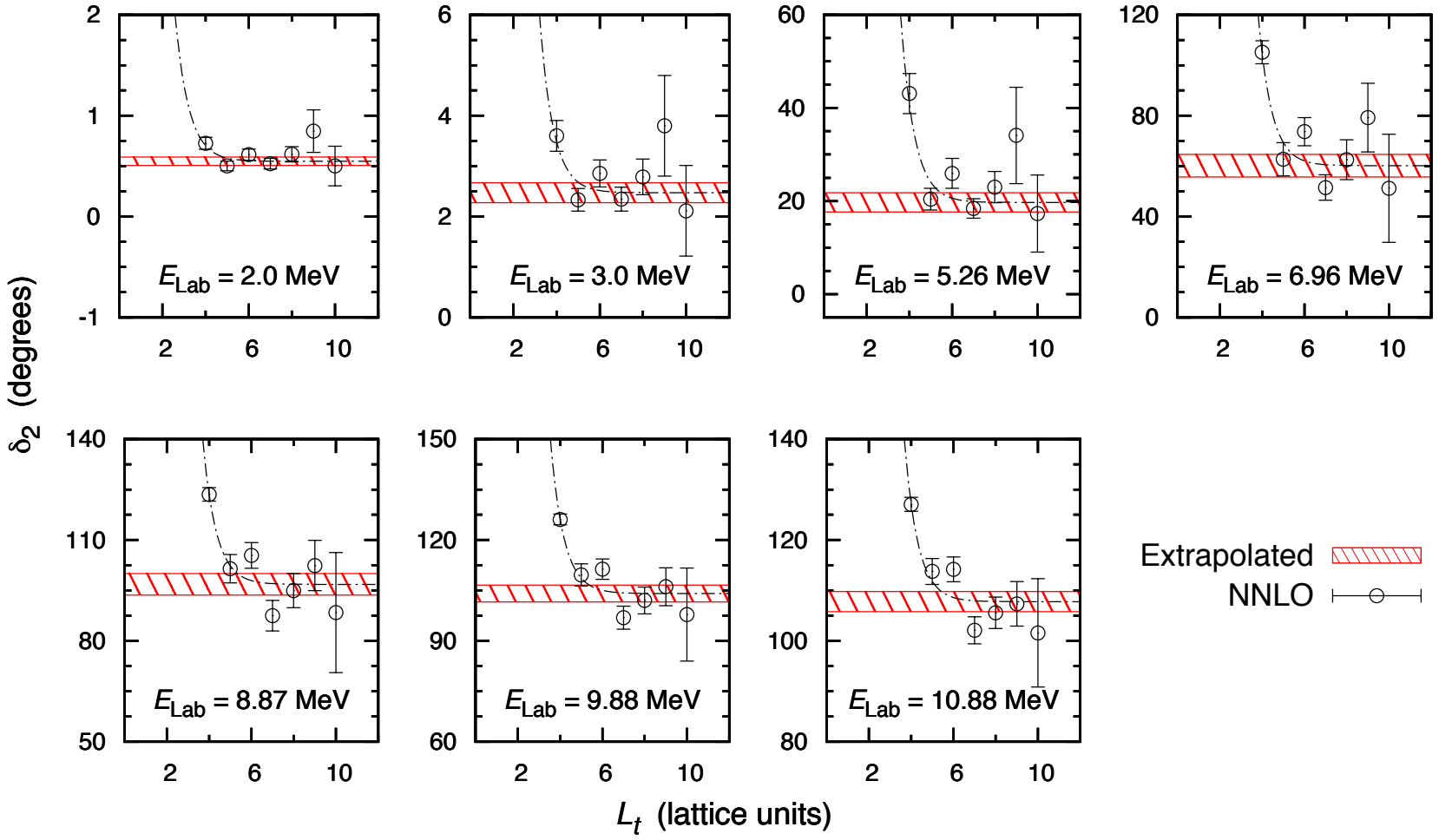
S-wave scattering



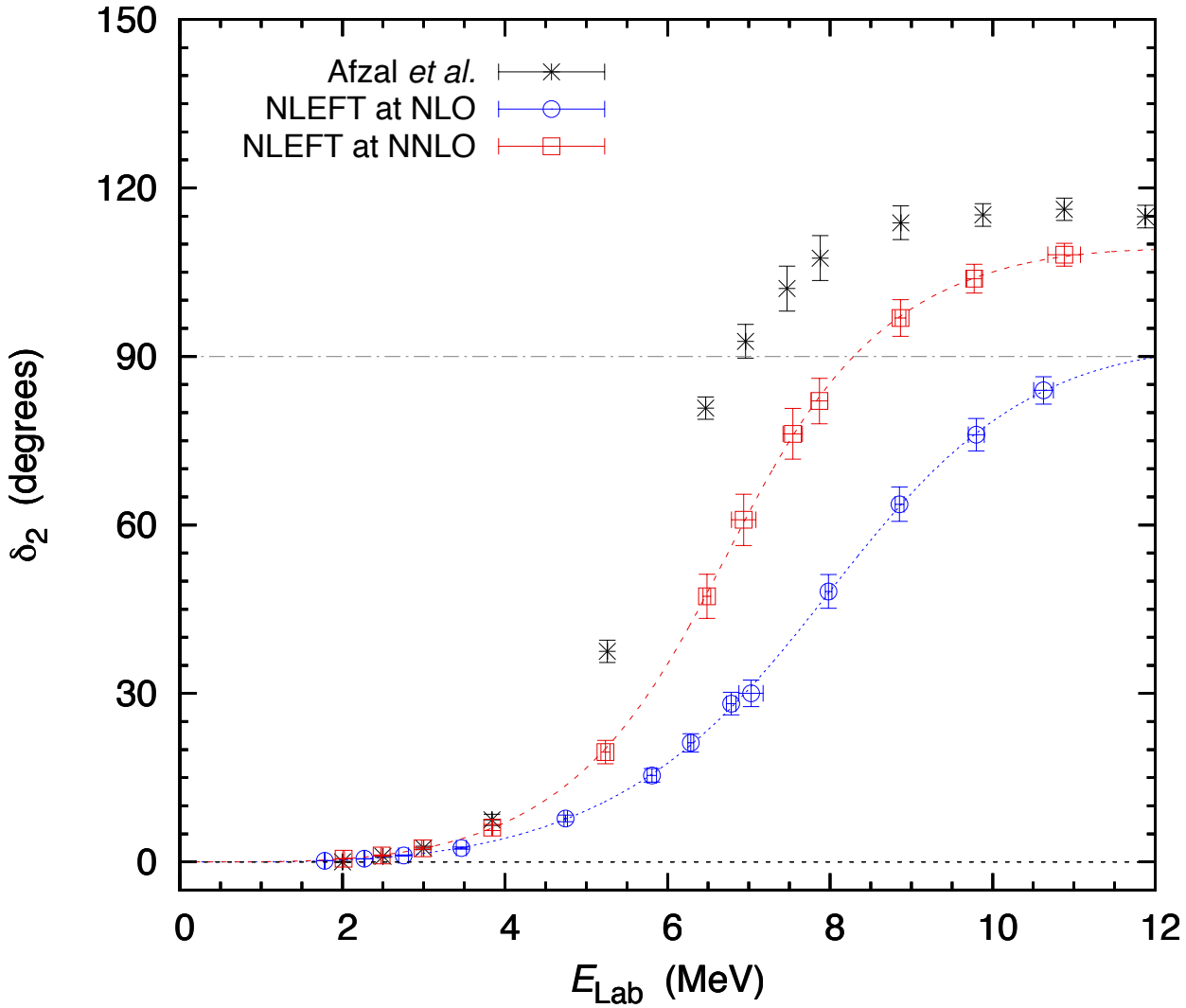
Afzal, Ahmad, Ali, RMP 41 247 (1969)

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

D-wave scattering



D-wave scattering



Summary

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 $(A_1 + A_2)^2$.

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 fruitful to explore connections with halo/cluster EFT calculations. Adiabatic projection calculations can be used as input for halo/cluster EFT calculations.

Would be exciting for these methods to be applied to lattice QCD calculations of hadronic scattering and reactions. All of the algorithms used here have direct analogues in lattice QCD simulations.