

# Ab-initio scattering using Nuclear lattice EFT

Avik Sarkar

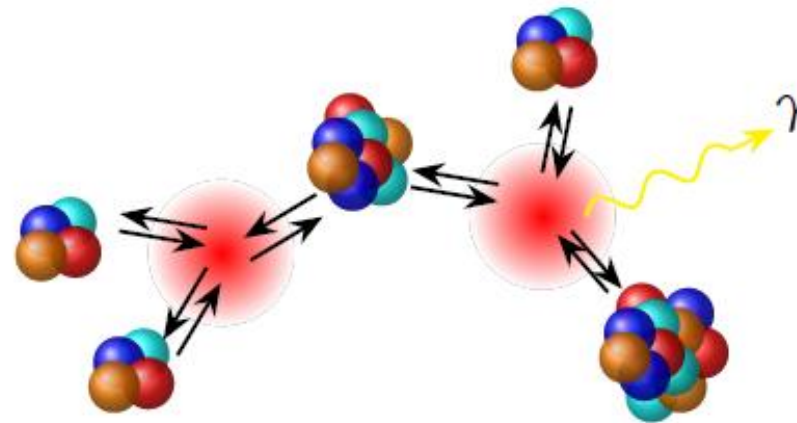
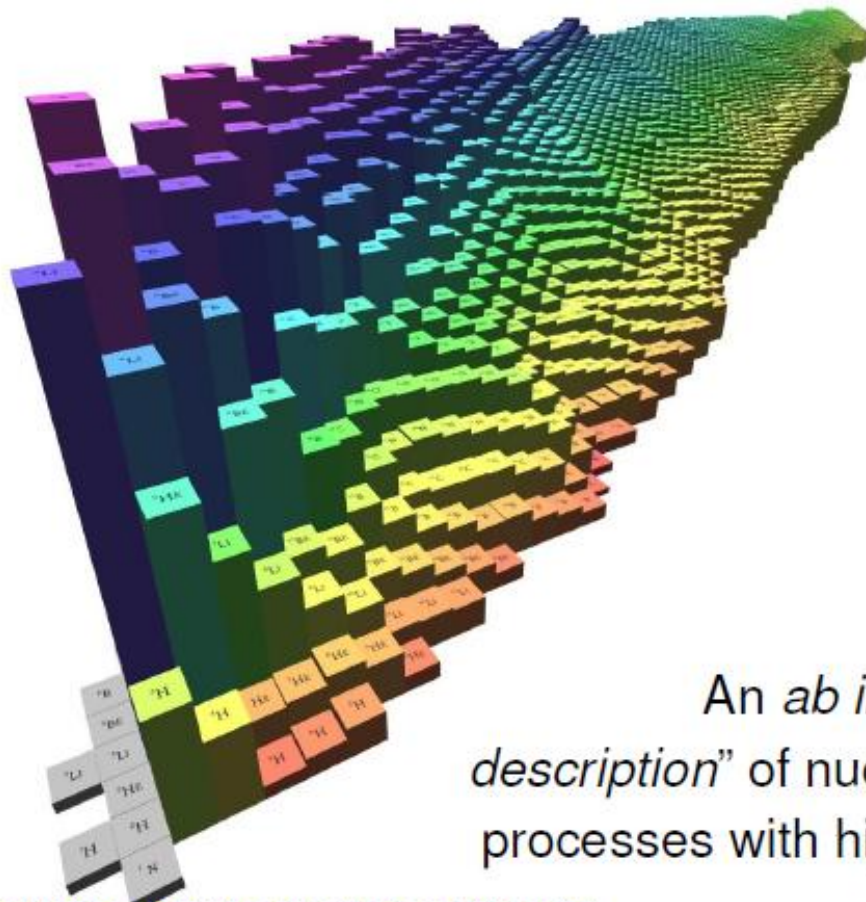
NLEFT Collaboration

# Outline

- Introduction to NLEFT
- Adiabatic Projection Method
- Alpha-alpha scattering
- Summary

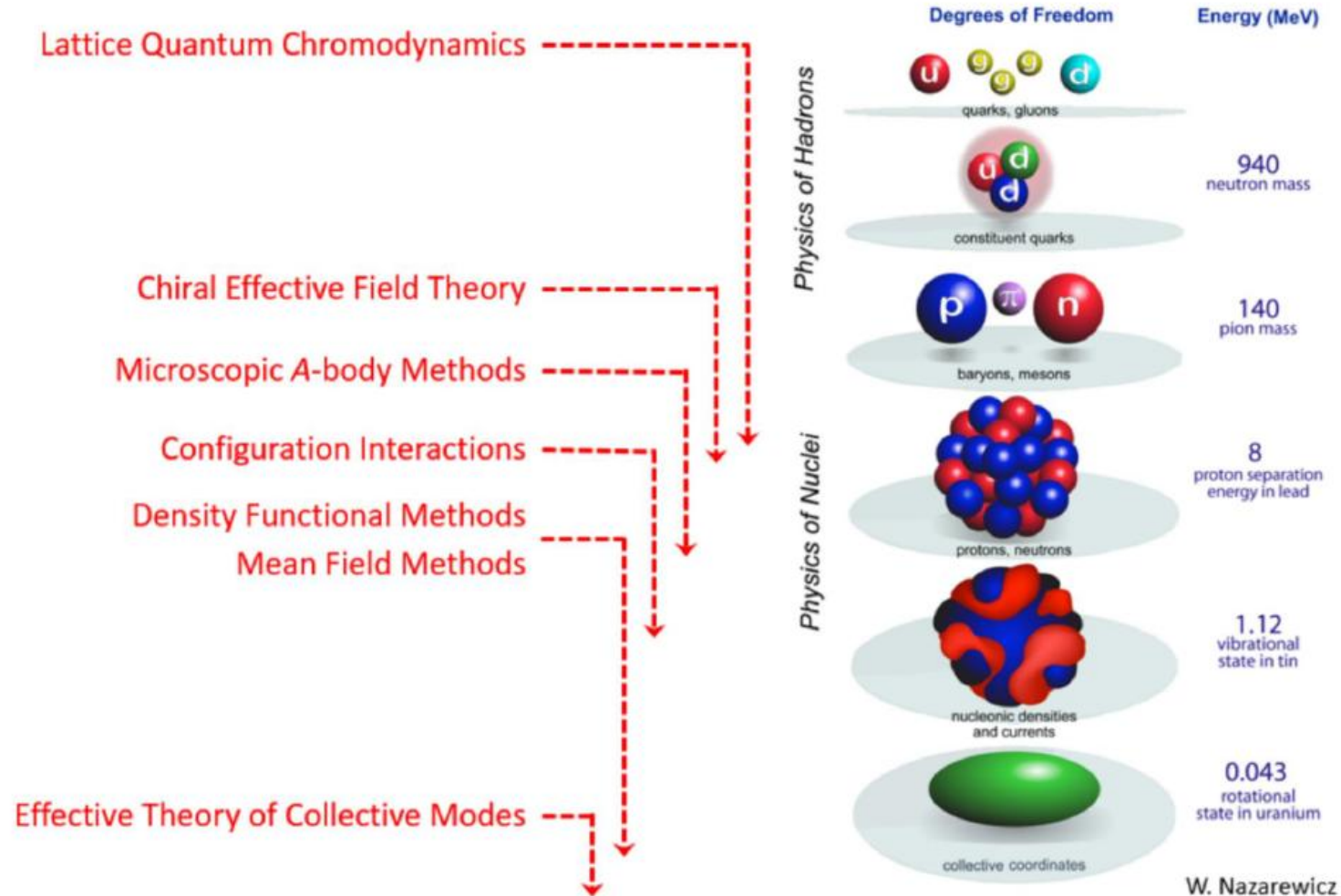
# Ab initio nuclear theory

The aim is to predict the properties of nuclear systems from microscopic nuclear forces



An *ab initio* nuclear theory that has a “*unified description*” of nuclear structure and scattering/reaction processes with high predictive power.

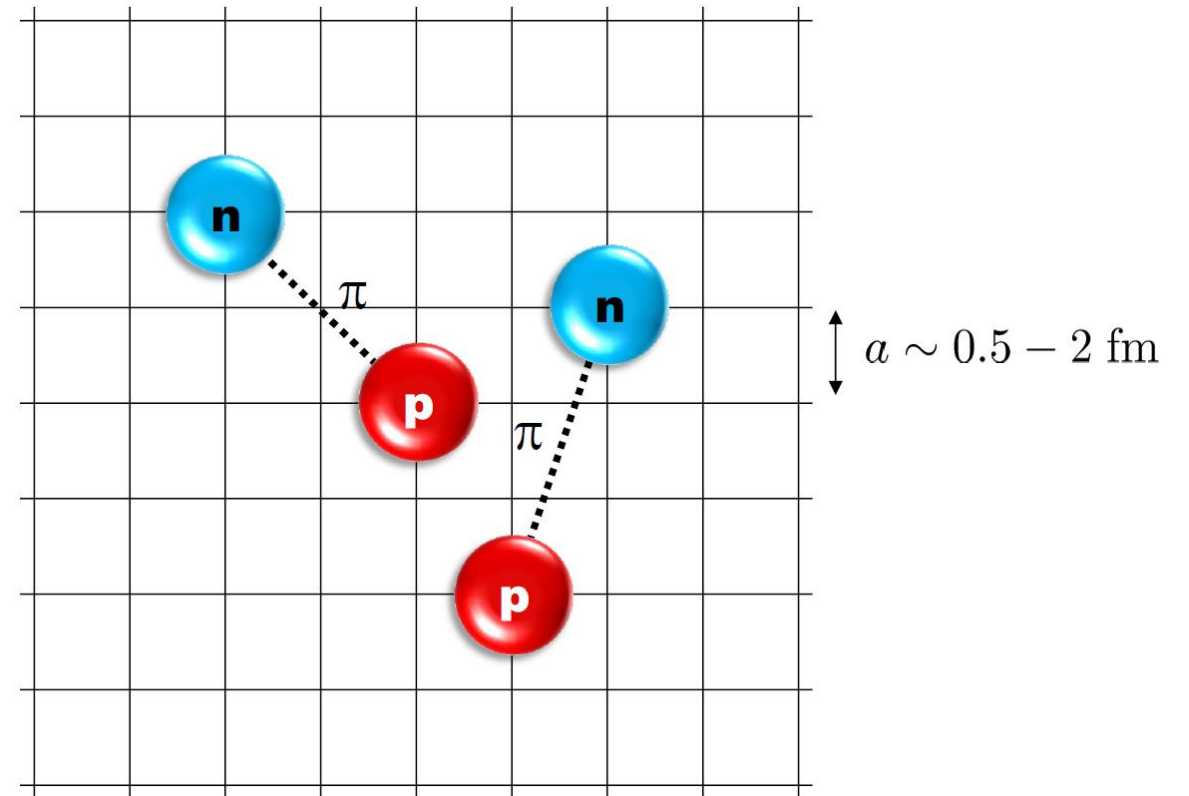
# Hierarchy of Degrees of Freedom



# Nuclear Lattice simulations

Lattice EFT = Chiral EFT + Lattice + Monte Carlo

- Discretized chiral nuclear force
- Lattice spacing  $a \sim 1$  fm
- Protons and neutrons interacting via short-range and long-range pion exchange interactions
- Exact method, polynomial scaling ( $\sim A^2$ )



[D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)]

[Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer]

# Chiral Effective Field Theory

In Chiral EFT, the nuclear forces are systematically constructed order by order.

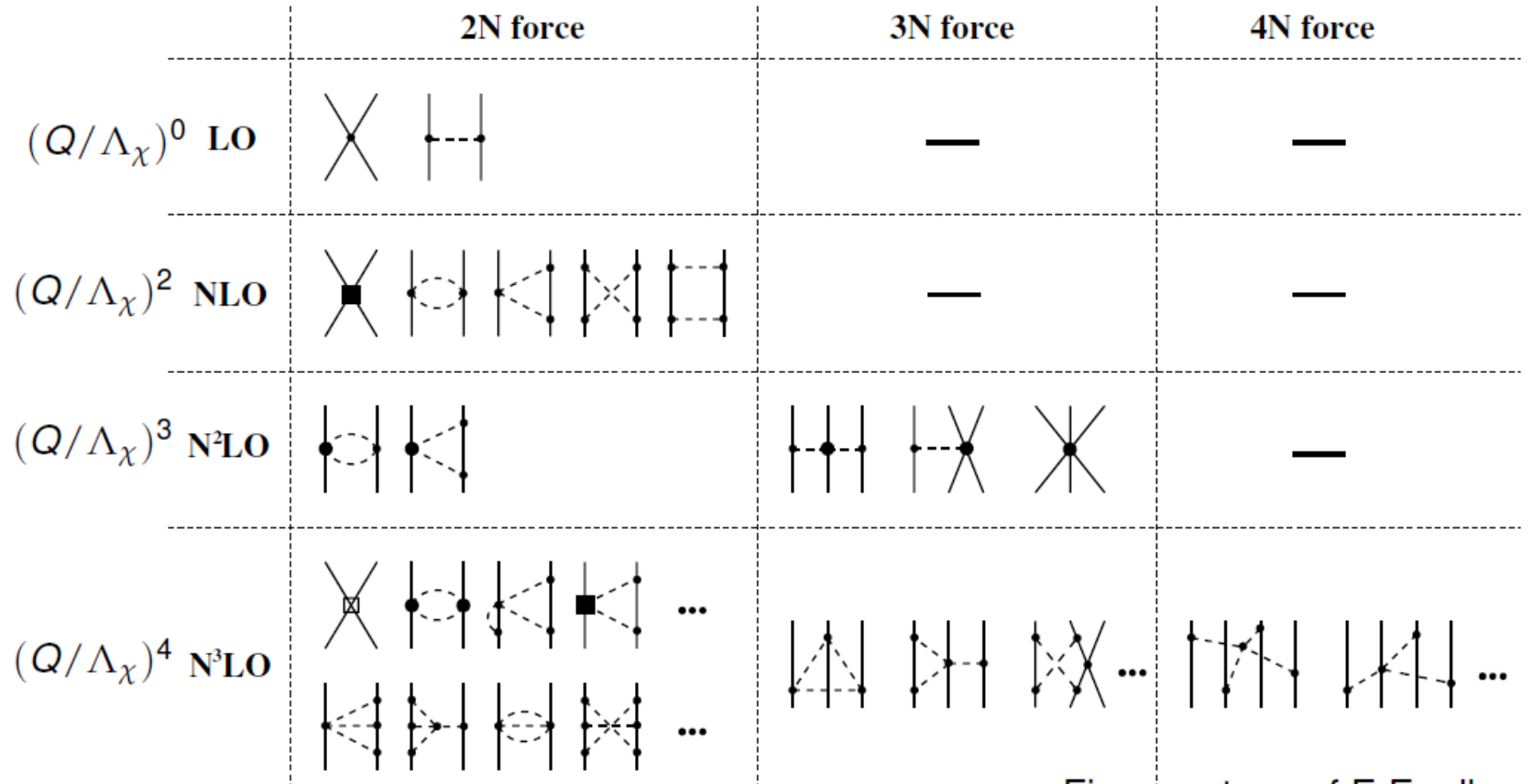


Fig. courtesy of E. Epelbaum

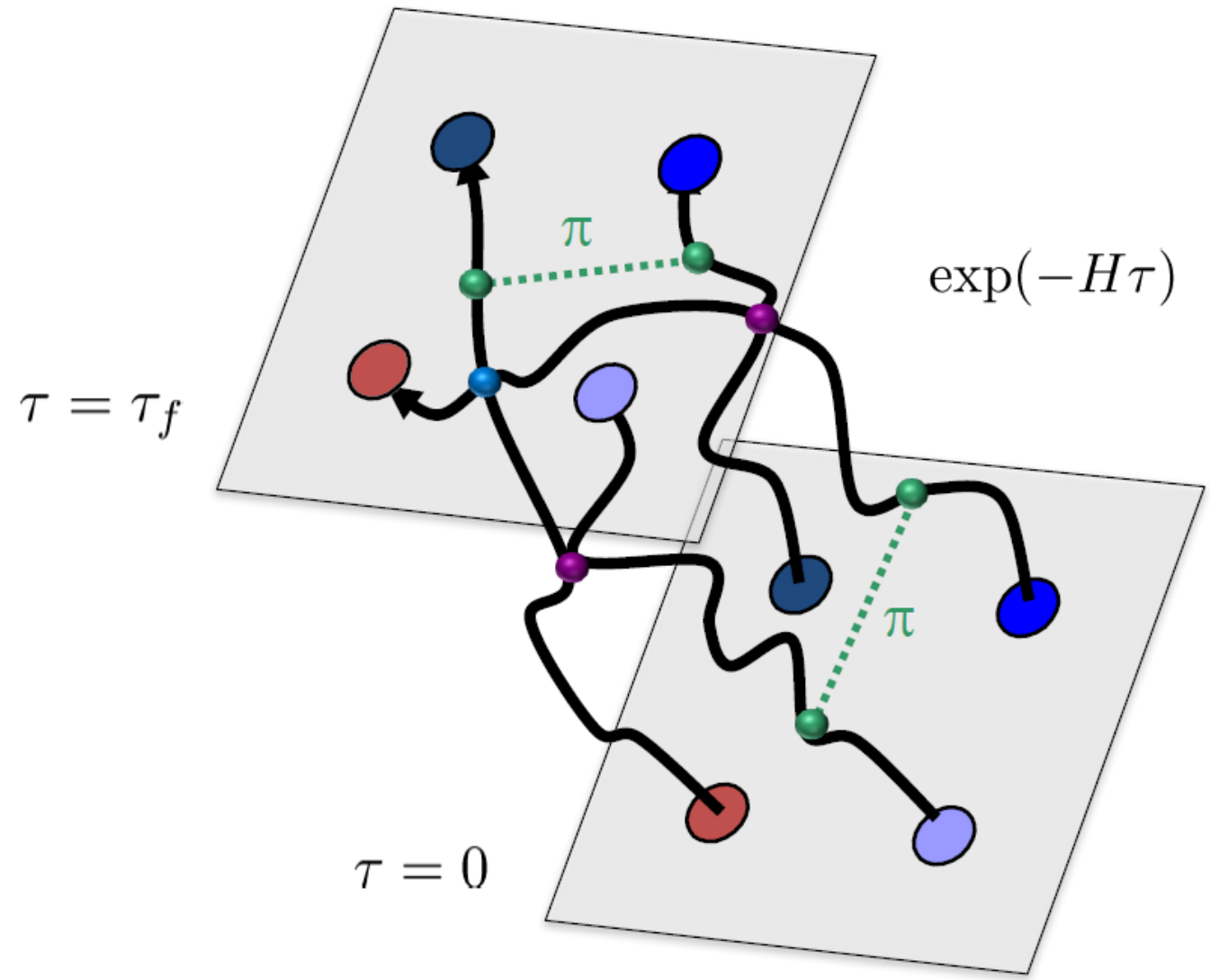
# Euclidean Time Evolution

$$\begin{aligned}\exp[-\tilde{H}t] |\psi\rangle &= \exp[-\tilde{H}t] \sum_i c_i |\psi\rangle_i \\ &= \exp[-H_0 t] c_0 |\psi\rangle_0 + \sum_{i>0} \exp[-H_i t] c_i |\psi\rangle_i \\ &= \exp[-H_0 t] c_0 \left[ |\psi\rangle_0 + \sum_{i>0} \exp[-(H_i - H_0)t] c_i |\psi\rangle_i \right]\end{aligned}$$

$$\lim_{t \rightarrow \infty} \exp[-\tilde{H}t] |\psi\rangle \approx c_0 \exp[-H_0 t] |\psi\rangle_0$$

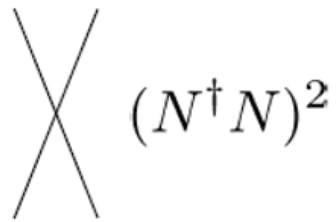
- Low energy filter.
- Excited states can be estimated using multi-channel calculations.

# Euclidean time projection

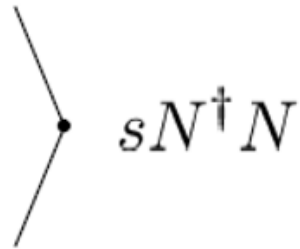


# Auxiliary field method

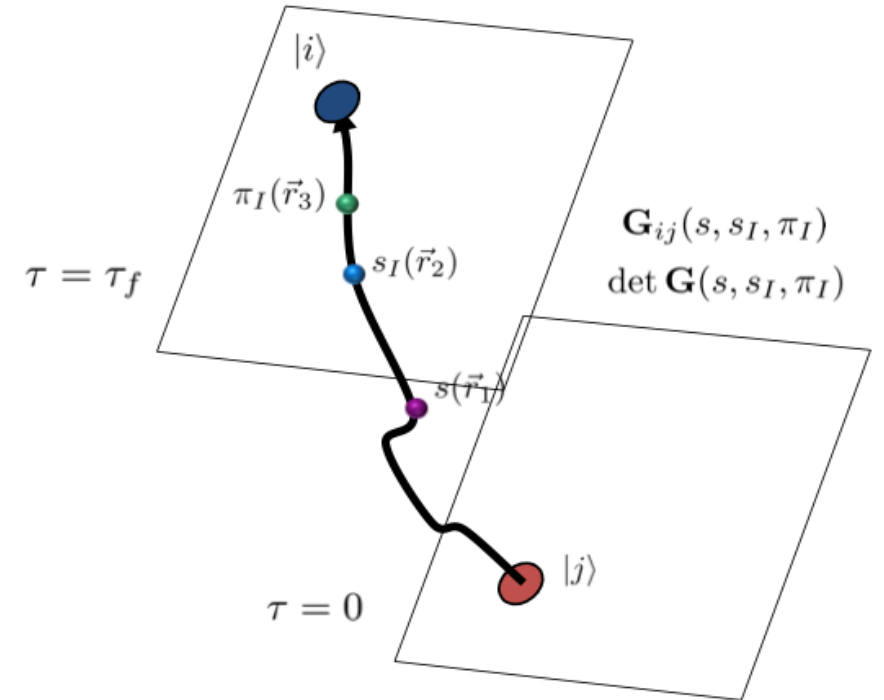
$$\exp\left[-\frac{c}{2}(N^\dagger N)^2\right] = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-c}s(N^\dagger N)\right]$$



Nucleon-nucleon interaction



Nucleon interacting with background field



Many-body amplitude for A-body = Determinant of  $A \times A$  matrix of single nucleon amplitudes

[1] - B. Borasoy, E. Epelbaum, H. Krebs, D. Lee, U.-G Meißner, Eur. Phys. J. A 31, 105 (2007)

[2] - S. Elhatisari, E. Epelbaum, H. Krebs, et al., Phys. Rev. Lett. 119, 222505 (2017)

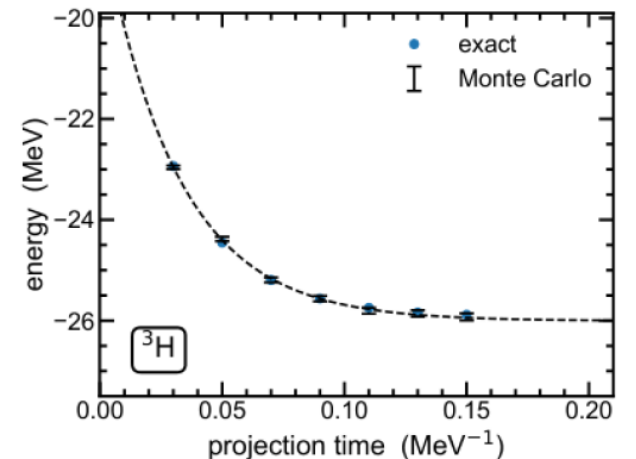
# Quantum Monte Carlo

$$\hat{O}_{Lt} = \frac{\sum \frac{\langle \psi_{init} | e^{-H\delta t} | \dots | \hat{O} | \dots | e^{-H\delta t} | \psi_{init} \rangle}{|\langle \psi_{init} | e^{-H\delta t} | \dots | e^{-H\delta t} | \psi_{init} \rangle|}}{\sum \frac{\langle \psi_{init} | e^{-H\delta t} | \dots | e^{-H\delta t} | \psi_{init} \rangle}{|\langle \psi_{init} | e^{-H\delta t} | \dots | e^{-H\delta t} | \psi_{init} \rangle|}}$$

← Lt steps for Euclidean Time Evolution

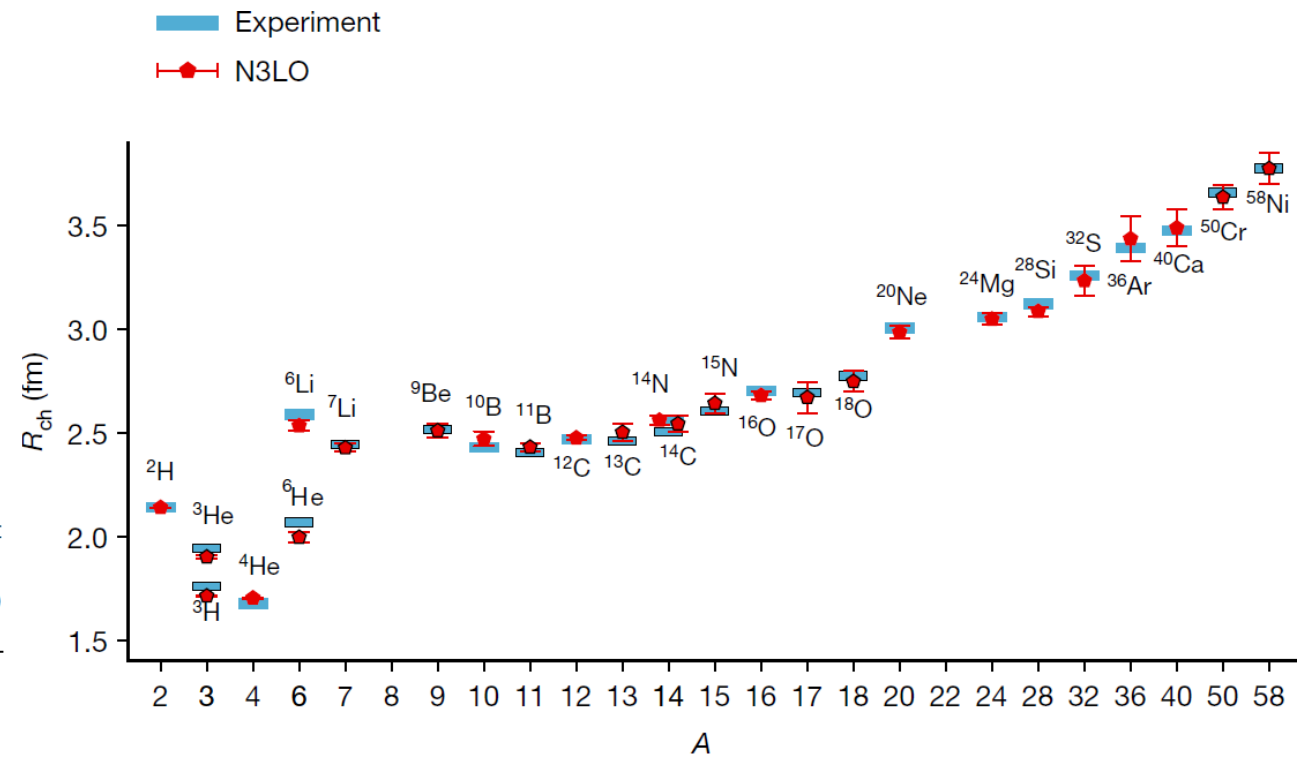
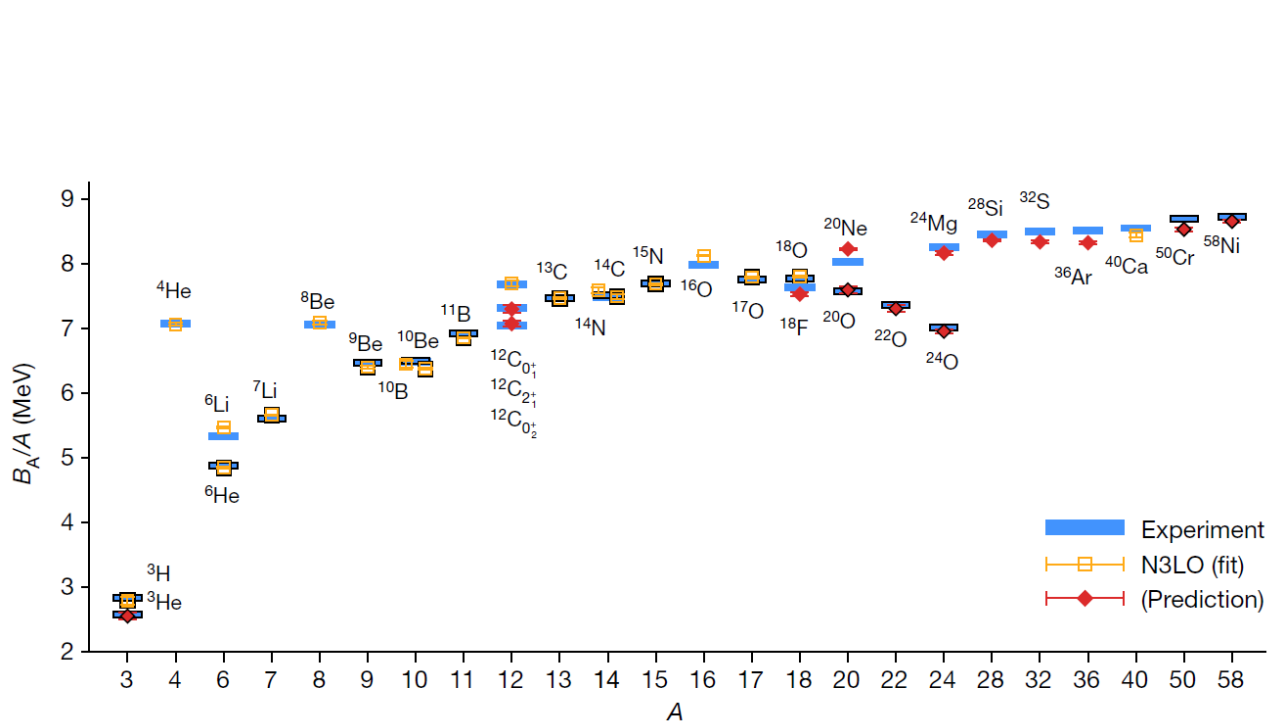
← Importance sampling

$$\bar{O} = \lim_{Lt \rightarrow \infty} \hat{O}_{Lt} \quad \longrightarrow \quad \text{Extrapolated from different Lt data}$$

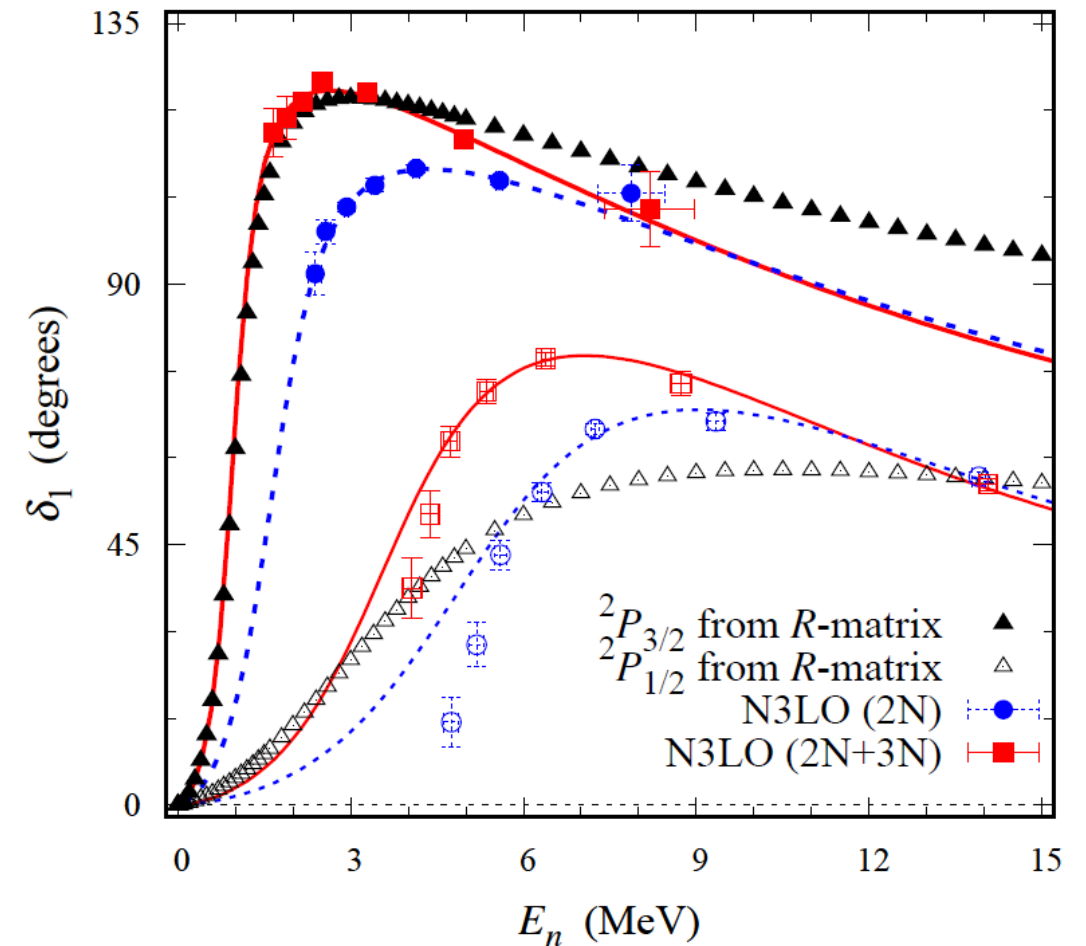
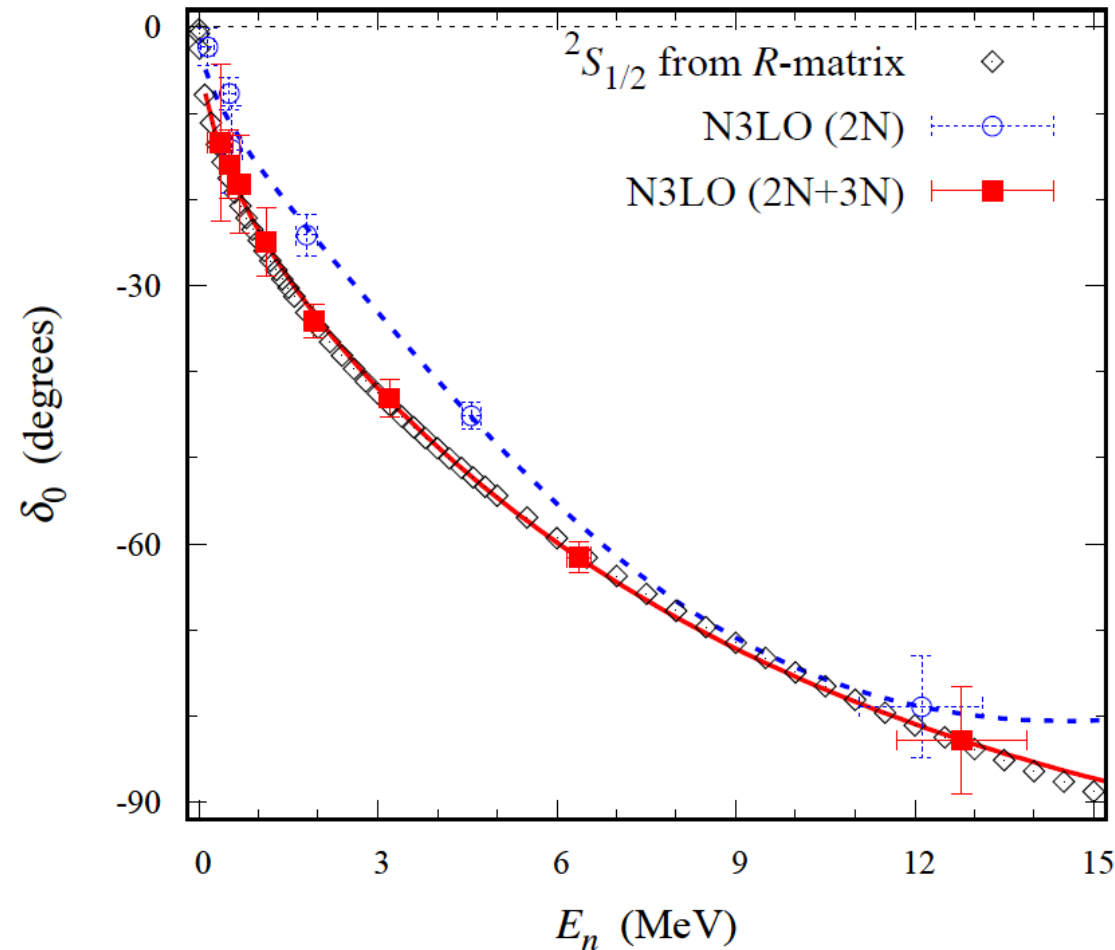


- Matrix determinant should not fluctuate strongly in sign or complex phase - Sign problem!

# Binding energies and charge radii



# n-alpha phase shifts from Lüscher formalism



# Adiabatic Projection Method

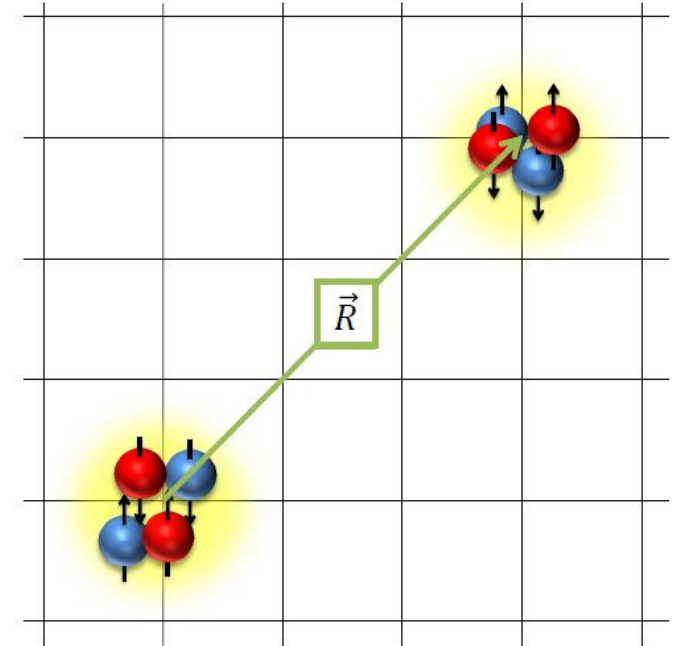
- Initial cluster states with relative separation  $\vec{R}$

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

- Time evolved ‘dressed cluster states’

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

- $H$  is full A-body interacting microscopic Hamiltonian
- $\tau = L_t a_t$
- $\lim_{\tau \rightarrow \infty} \{|\vec{R}\rangle_{\tau}\}$  spans low-energy two-cluster subspace



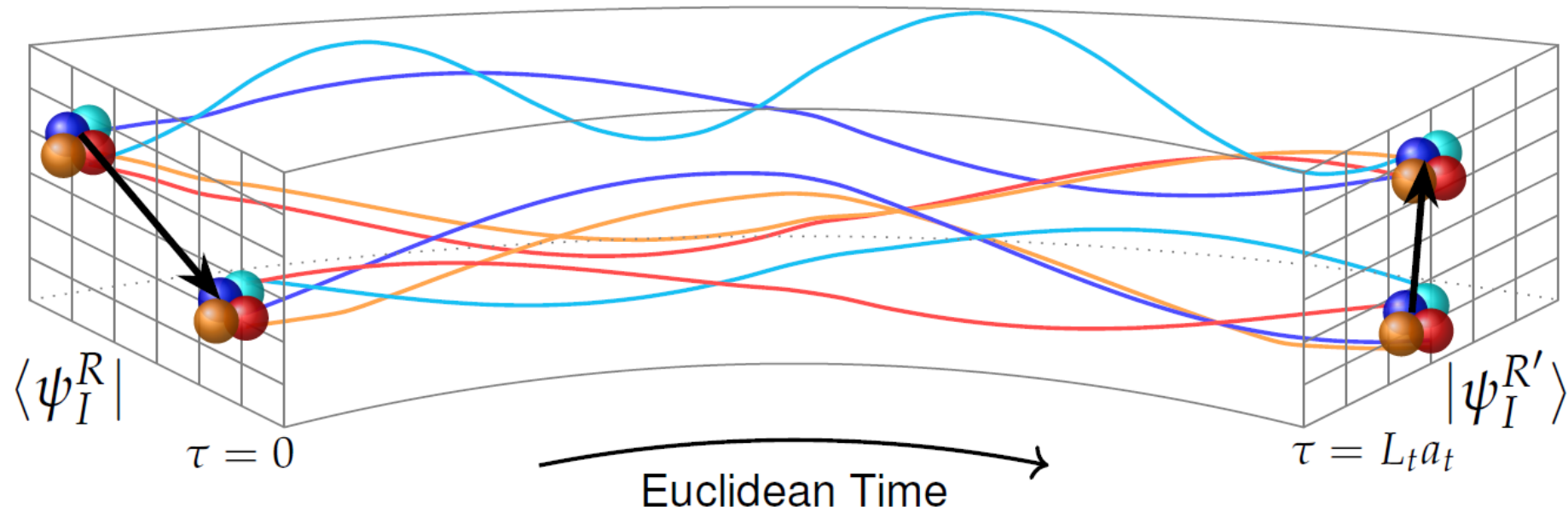
[1] M. Pine, D. Lee, G. Rupak, *Eur. Phys. J. A* 49, 151 (2013)

[2] S. Elhatisari, D. Lee, *Phys. Rev. C* 90, 064001

[3] S. Elhatisari, D. Lee, G. Rupak, E. Epelbaum, H. Krebs, T. Lähde, T. Luu, & U-G. Meißner. *Nature* 528, 111-114 (2015).

[4] S. Elhatisari, D. Lee, U-G. Meißner, G. Rupak, *Eur. Phys. J. A* 52, 174 (2016)

[5] S. Elhatisari, T. Lähde, D. Lee, U-G. Meißner, T. Vonk, *J. High Energ. Phys.* 2022



- Projected Hamiltonian

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

Norm

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

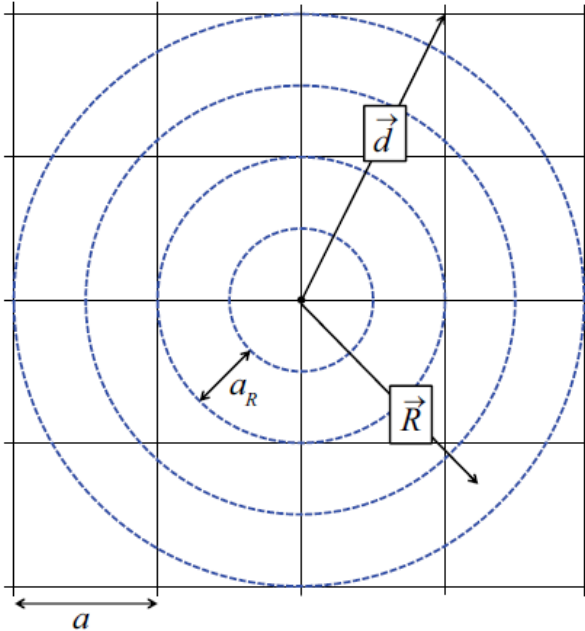
- Adiabatic Hamiltonian

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

# Adiabatic Hamiltonian

- 10x10 matrix  $\rightarrow$  100 elements to be computed  $\rightarrow$  multi-channel calculations.
- Lowest eigenvalue  $\rightarrow$  direct one-channel calculation (after infinite Euclidean time propagation).
- $E_{8Be}(Lt = 20, N3LO) = -57.34 \pm 0.05$   
 $E_{APM}(Lt = 20, N3LO) = -59.34 \pm 0.74$
- Information of the clusters at different distances  $\rightarrow$  can extract phase shifts with spherical wall.
- Adiabatic projection method is better than Lüscher's method for NLEFT

# Radial binning



$L$	$[M_{L_t}^a]_{\vec{d}, \vec{d}'}$	$[M_{L_t}^a]_{d, d'}^{0,0}$	$[M_{L_t}^a]_{R, R'}^{0,0}$	
			$a_R = 0.125 \text{ l.u.}$	$a_R = 0.250 \text{ l.u.}$
10	$10^3 \times 10^3$	$22 \times 22$	$21 \times 21$	$14 \times 14$
20	$20^3 \times 20^3$	$85 \times 85$	$58 \times 58$	$34 \times 34$
30	$30^3 \times 30^3$	$189 \times 189$	$97 \times 97$	$54 \times 54$
40	$40^3 \times 40^3$	$335 \times 335$	$137 \times 137$	$74 \times 74$
50	$50^3 \times 50^3$	$522 \times 522$	$177 \times 177$	$94 \times 94$
60	$60^3 \times 60^3$	$752 \times 752$	$217 \times 217$	$114 \times 114$

- Project initial states on spherical harmonics

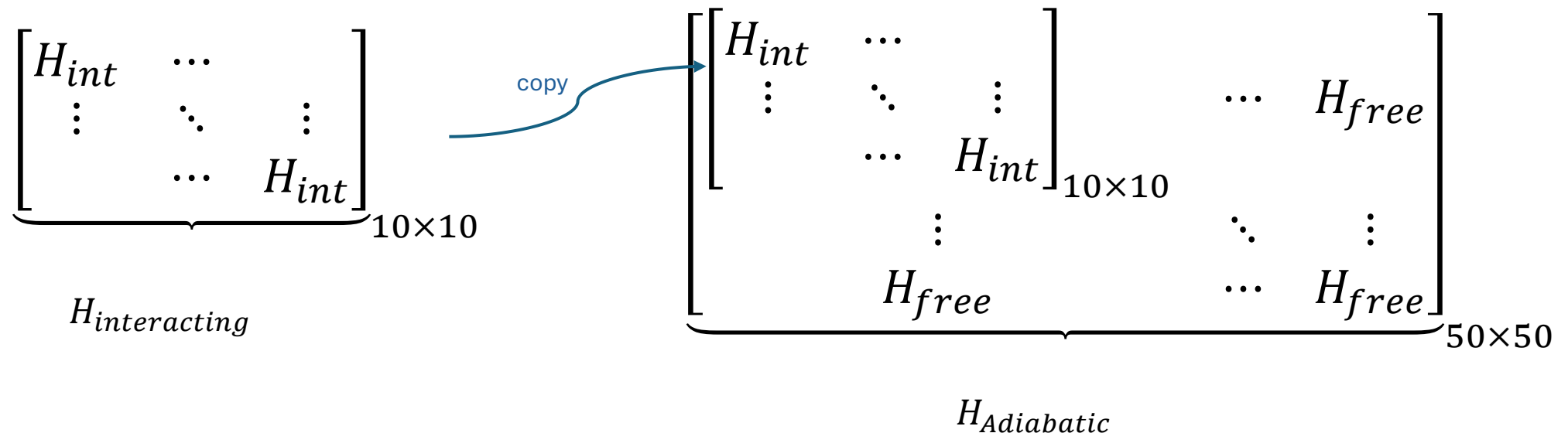
$$|\vec{d}\rangle = \sum_{\vec{n}} |\vec{n} + \vec{d}\rangle_1 \otimes |\vec{n}\rangle_2 \quad \longrightarrow \quad |d\rangle^{\ell, \ell_z} = \sum_{\vec{d}'} Y_{\ell, \ell_z}(\hat{d}') \delta_{d, |\vec{d}'|} |\vec{d}'\rangle$$

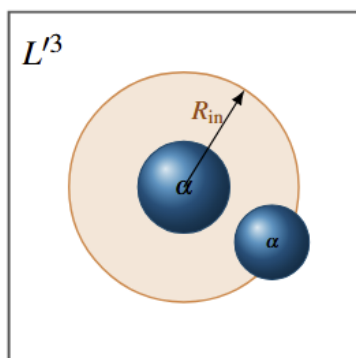
and bin the points together

$$|R\rangle^{\ell, \ell_z} = \sum_{|d-R| < a_R/2} |d\rangle^{\ell, \ell_z}$$

# Constructing large box Adiabatic Hamiltonian

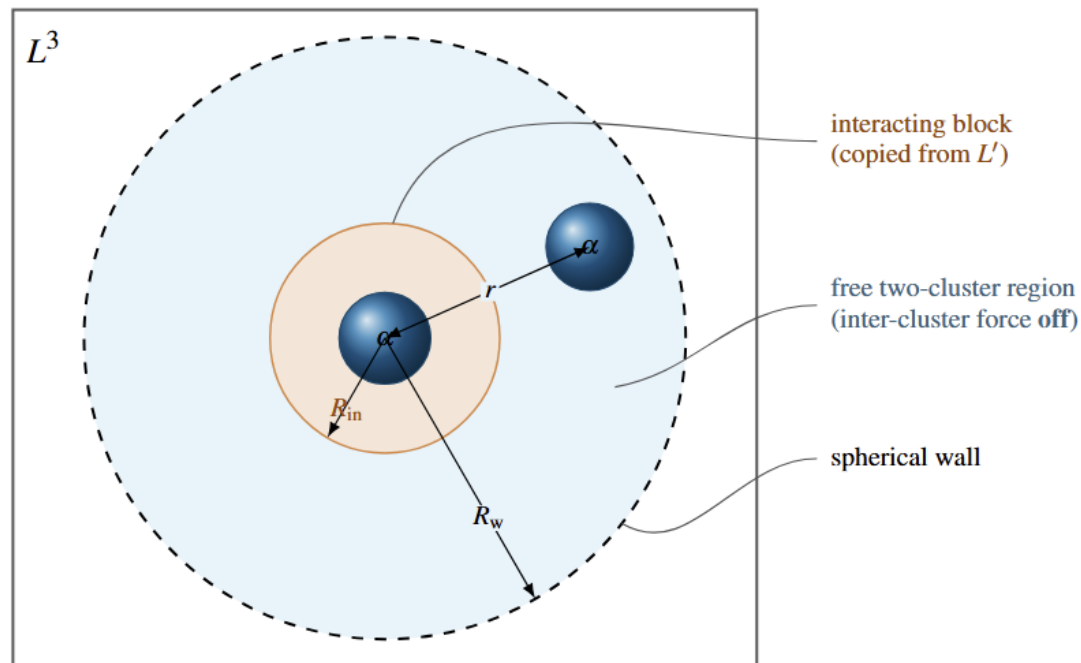
- Low energy phase shifts → large lattice box size → full interacting calculation too expensive
- Two separate calculations – 1. Full interacting microscopic Hamiltonian in small box, 2. Non-interacting Hamiltonian in large box



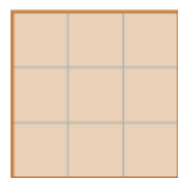


**Step 1.** Full interacting adiabatic Hamiltonian (inter-cluster force on)

copy inner block

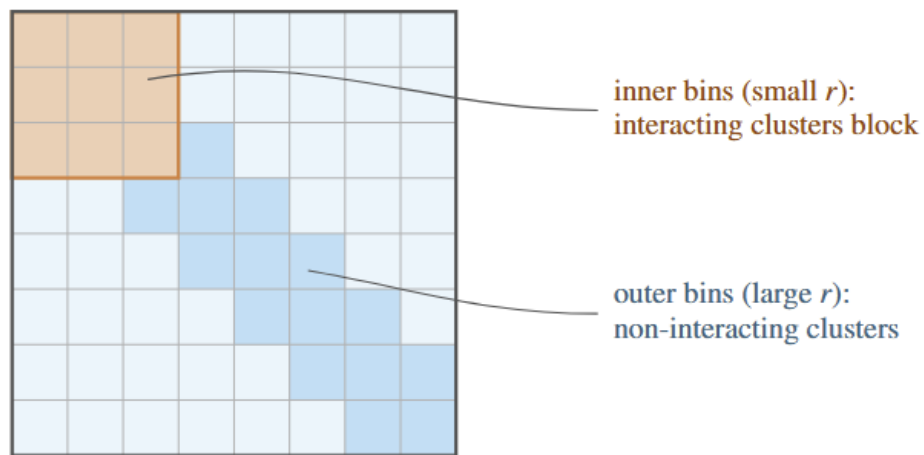
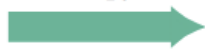


**Step 2.** Free clusters out to the wall, with the interacting block inserted at short range



interacting block, small box  $L'$

copy



full Hamiltonian, large box  $L$

# Phase shift calculation

- Find eigenvector of Adiabatic Hamiltonian and look at asymptotic region

$$R_\ell^{(p)}(r) = N_\ell(p) \times \begin{cases} \cot \delta_\ell(p) j_\ell(pr) - n_\ell(pr), \\ \text{for any finite-range potential,} \\ \cot \delta_\ell(p) F_\ell(pr) + G_\ell(pr), \\ \text{for charged clusters,} \end{cases}$$

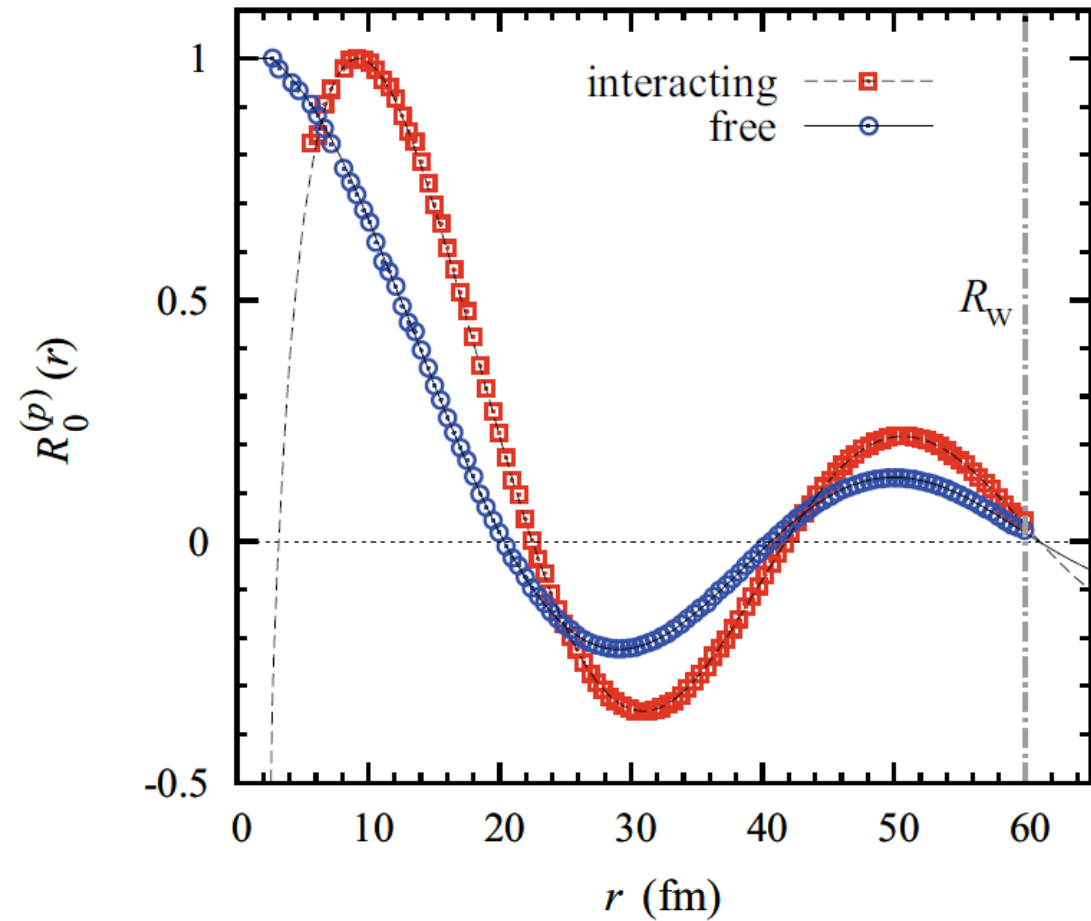
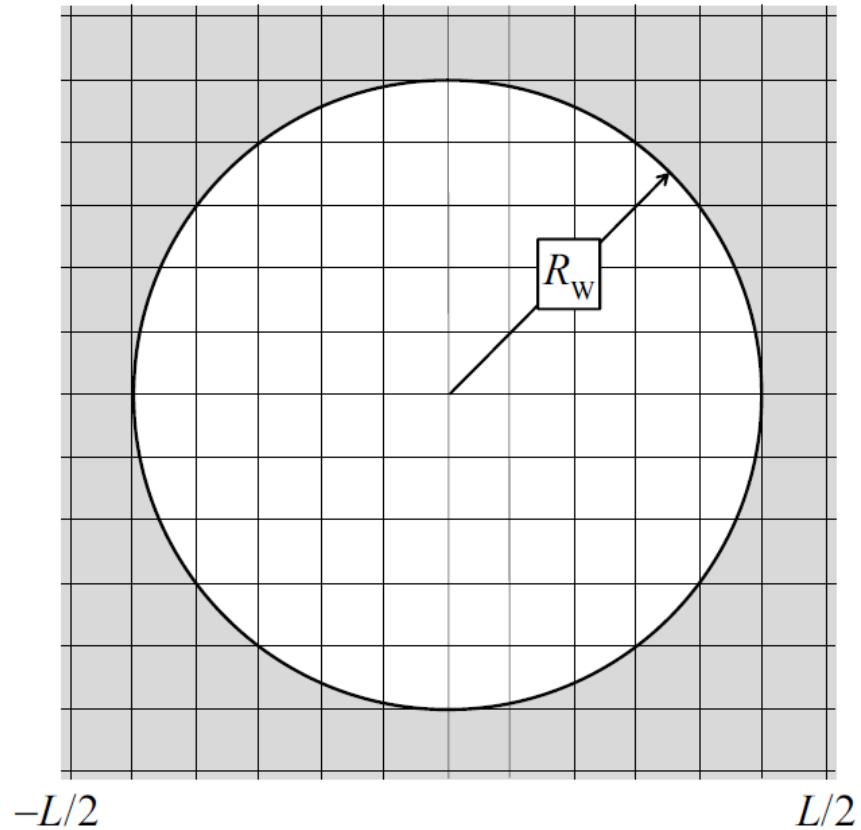
- Impose spherical hard wall and calculate phase shifts

$$\delta_\ell(p) = \begin{cases} \tan^{-1} \left[ \frac{j_\ell(p R'_w)}{n_\ell(p R'_w)} \right], \\ \text{for any finite-range potential,} \\ -\tan^{-1} \left[ \frac{F_\ell(p R'_w)}{G_\ell(p R'_w)} \right], \\ \text{for charged clusters.} \end{cases}$$

[1] J. Carlson, V.R. Pandharipande, R.B. Wiringa, Nucl. Phys. A 424, 47 (1984)

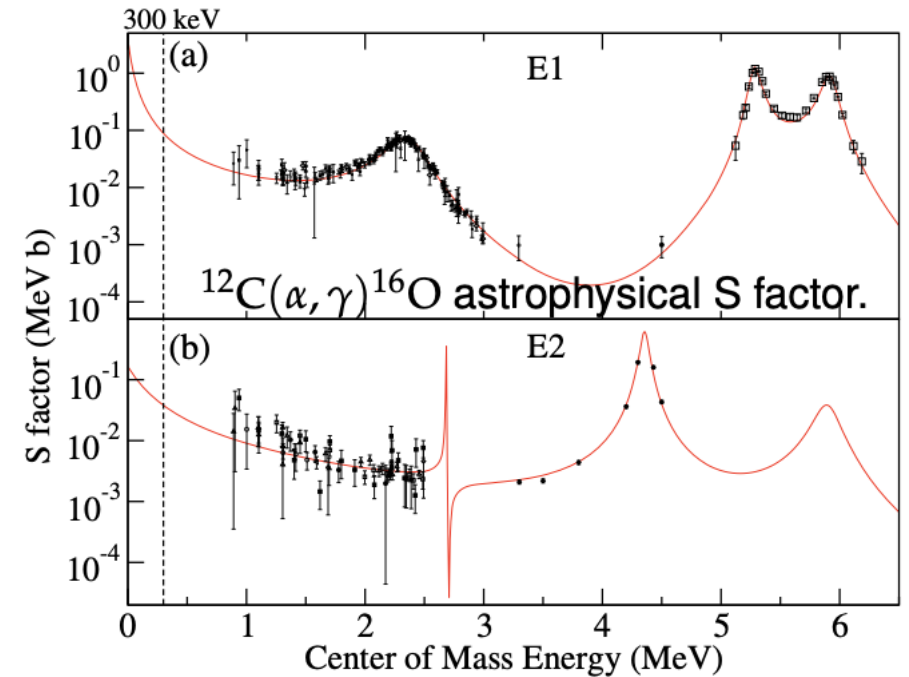
[2] B. Borasoy, E. Epelbaum, H. Krebs, D. Lee, U.-G. Meißner, Eur. Phys. J. A 34, 185 (2007)

# Spherical wall method

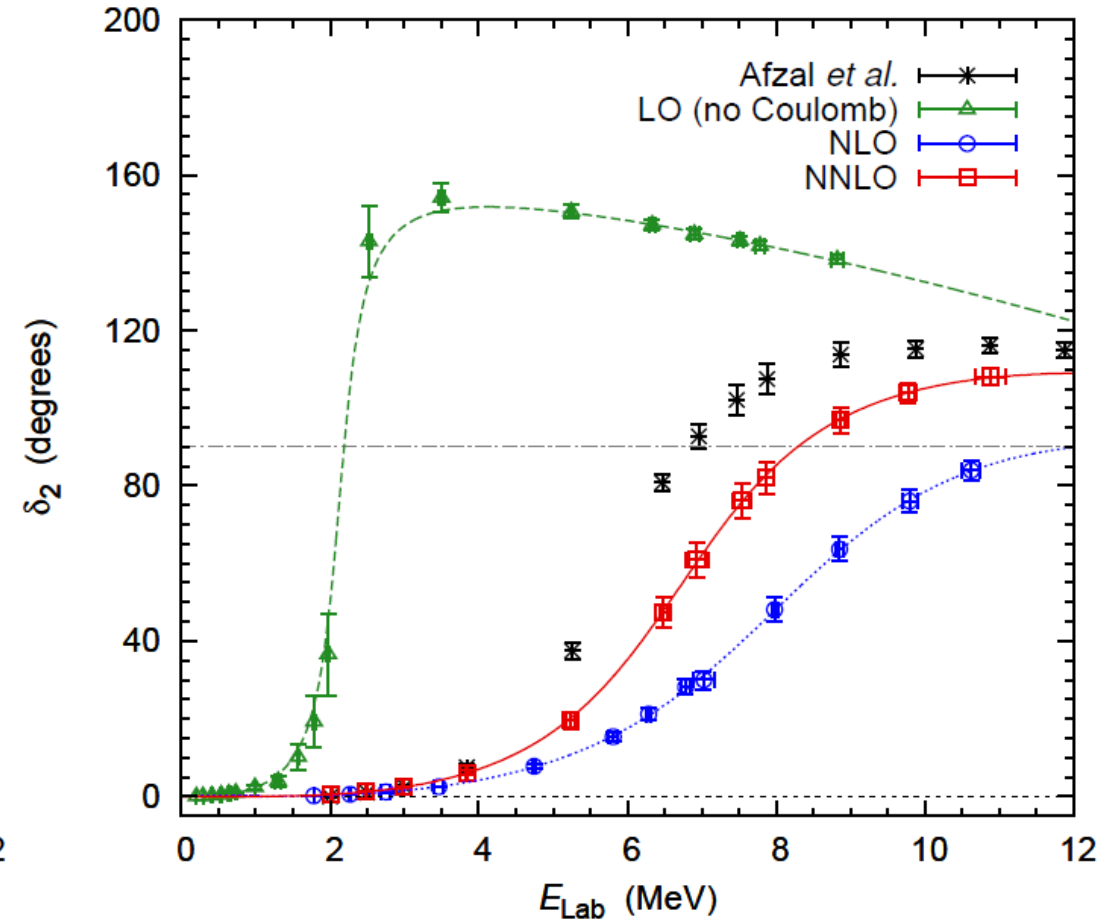
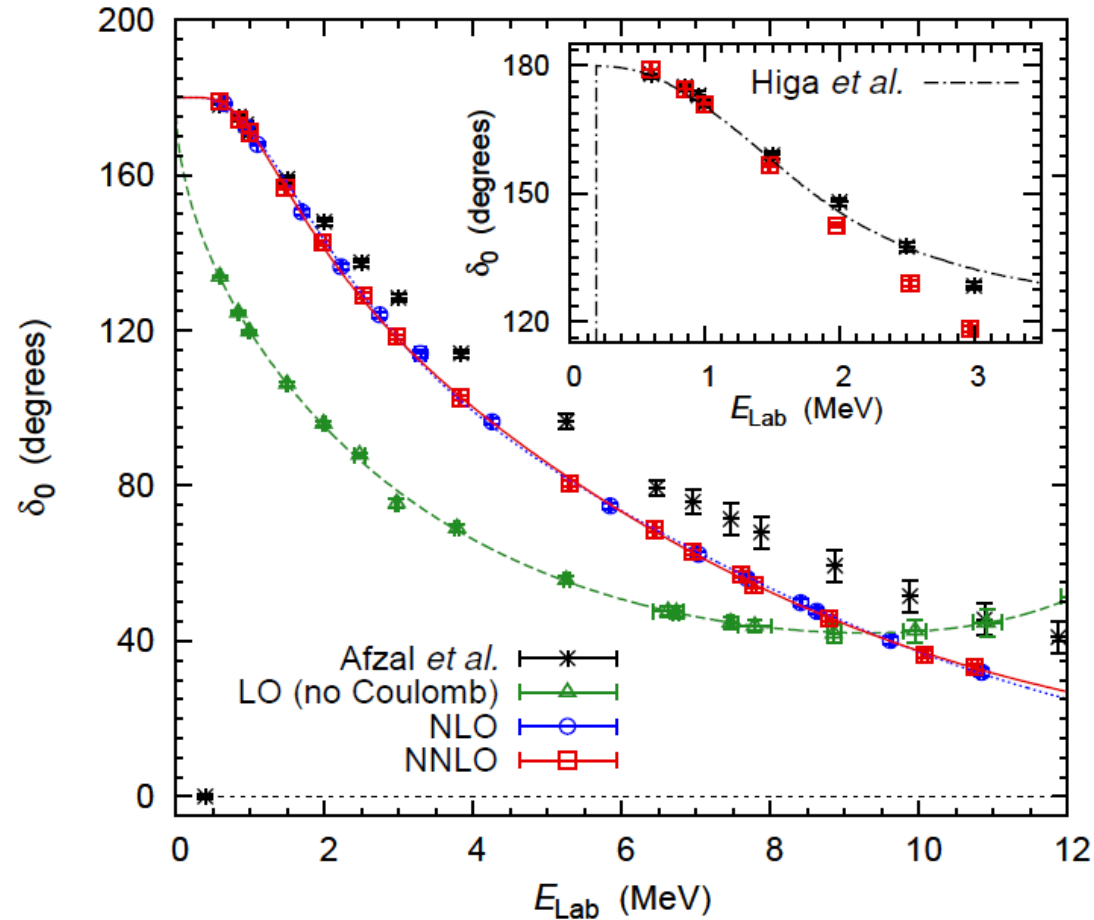


# Alpha-alpha scattering

- One of the most fundamental reactions in nuclear astrophysics.
- Alpha scattering, triple-alpha reaction, alpha capture play major role in stellar nucleosynthesis.
- Direct experimental results at 300 keV is impossible due to Coulomb barrier.
- For accurate reaction rate calculation, we need cross section within energy range 0.15 – 3.4 MeV.
- Study scattering by adiabatic projection method



# Previous alpha-alpha results

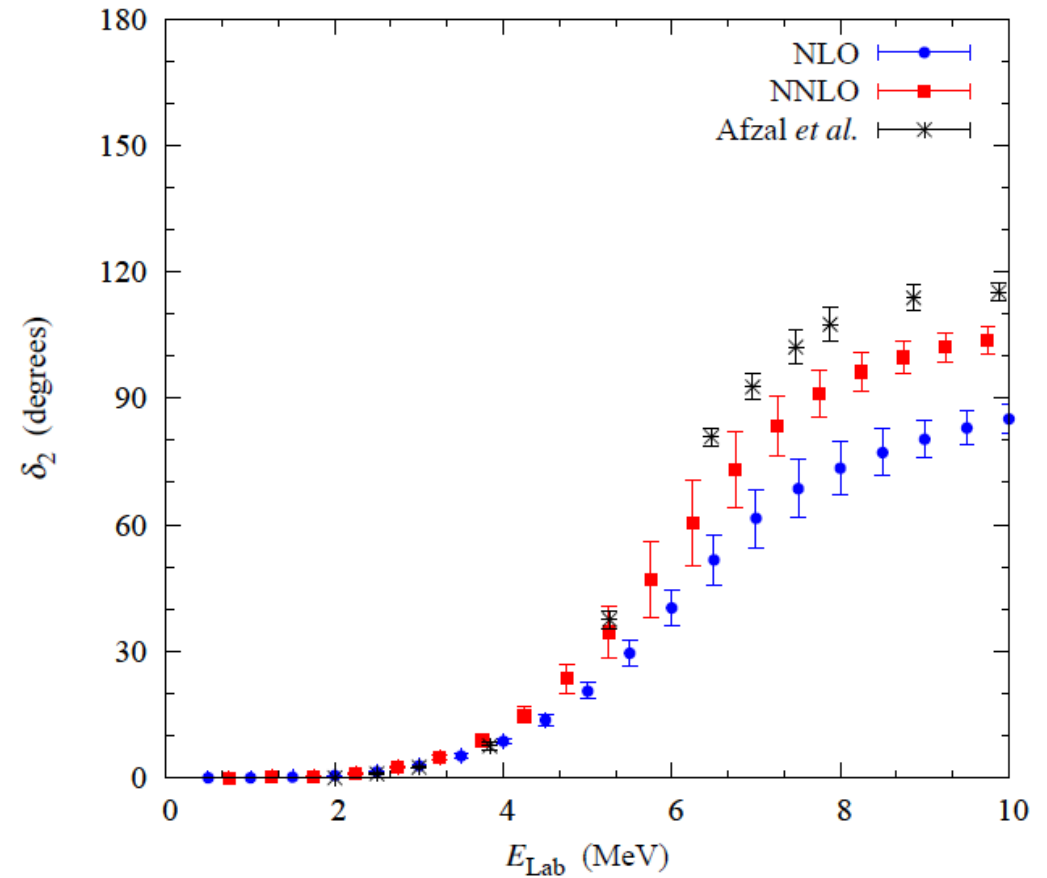
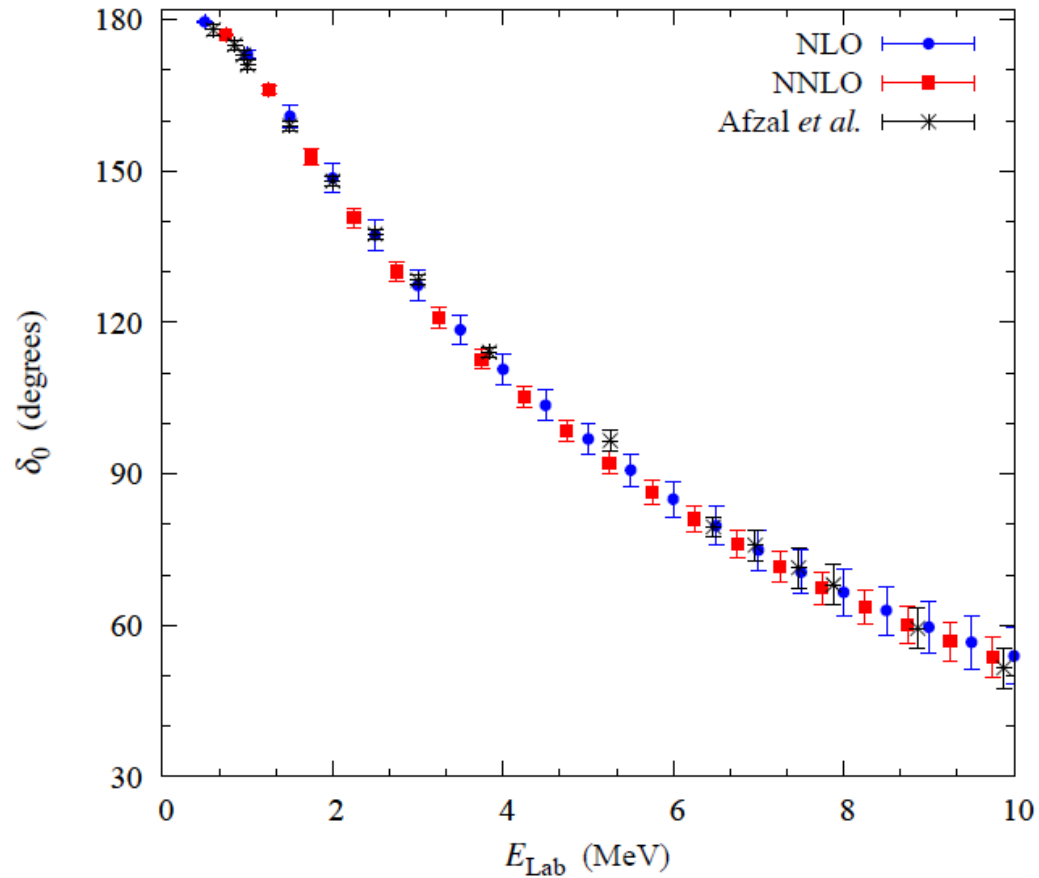


[1] Afzal, Ahmad, Ali, Rev. Mod. Phys. 41, 247, (1969)

[2] Higa, Hammer, van Kolck, Nucl.Phys. A809, 171 (2008), 0802.3426

[3] S. Elhatisari, D. Lee, G. Rupak, E. Epelbaum, H. Krebs, T. Lähde, T. Luu, & U-G. Meißner. Nature 528, 111-114 (2015).

# More recent alpha-alpha results



# What's new?

- Finer discretization – lattice spacing  $a = 1.97 \text{ fm}$  vs  $1.32 \text{ fm}$ ; temporal spacing  $a_t = (150 \text{ MeV})^{-1}$  vs  $(1000 \text{ MeV})^{-1}$ .
- Improved interaction – NNLO vs N3LO with wavefunction matching.

## ***Challenges***

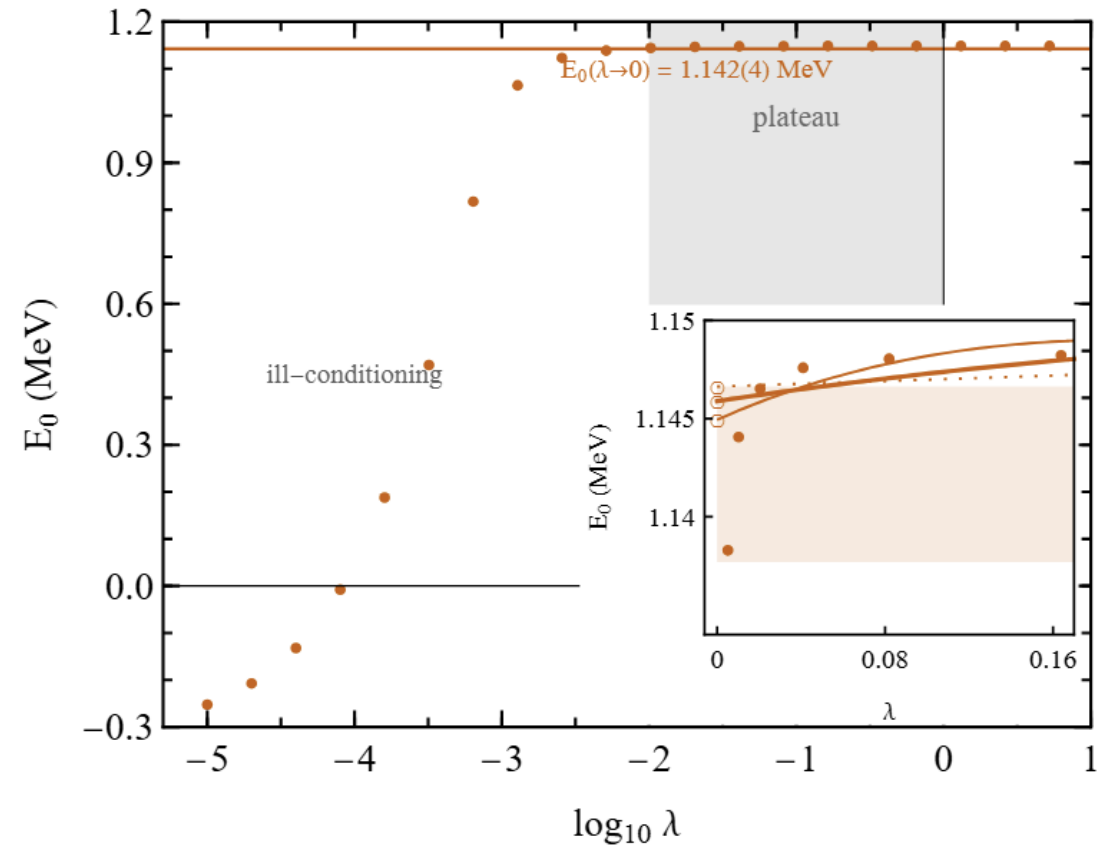
- APM needs to calculate  $N^{-1}$ . At fine lattice spacing, the two-cluster basis is difficult to finely resolve; often  $N$  is ill-conditioned.
- We need absurd amount of Monte Carlo statistics to be get meaningful results from standard APM.

# Tikhonov regularization

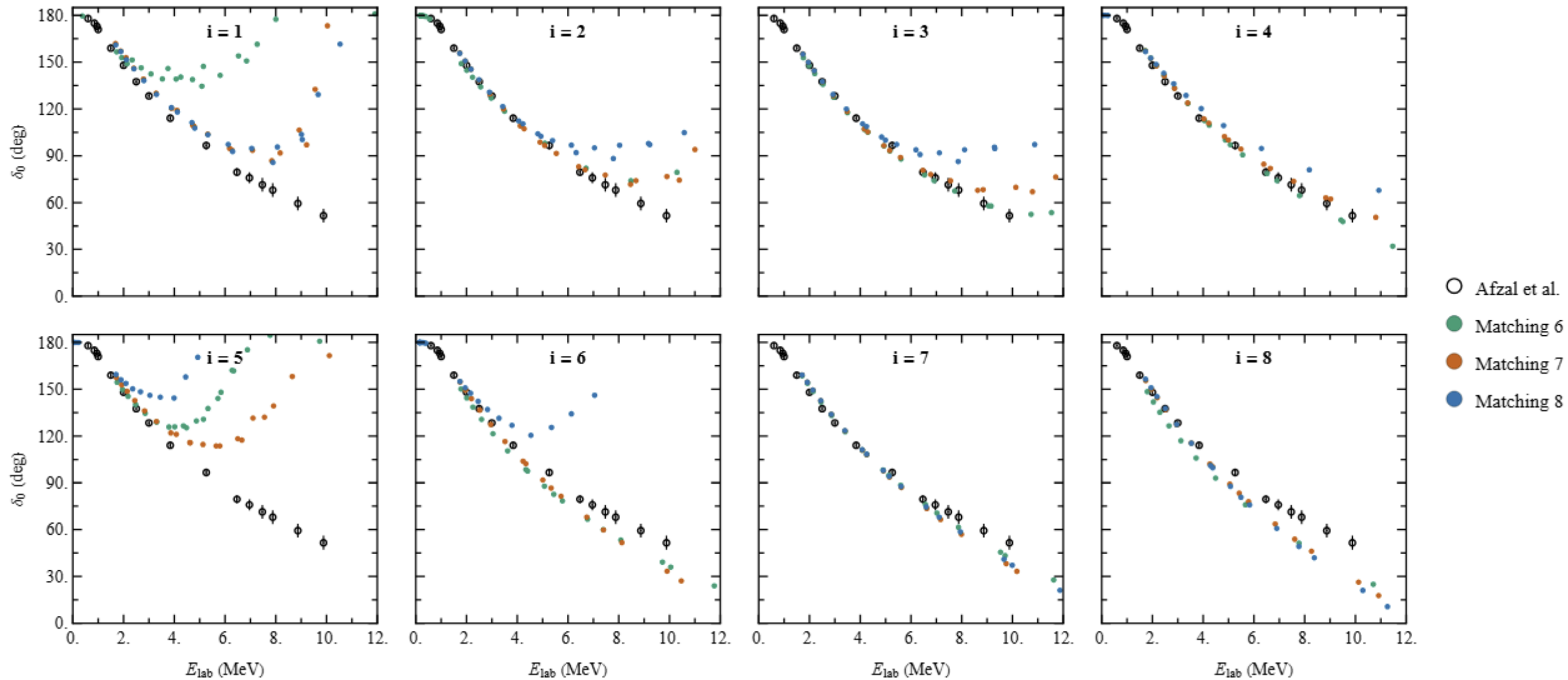
- $N \rightarrow N + \lambda B$ , most common  $B = I$ .
- Extrapolate  $\lambda \rightarrow 0$ .
- Regularize selectively where needed

$$N'(\lambda) = U \begin{pmatrix} \Lambda_i + \lambda I_i & 0 \\ 0 & \Lambda_r \end{pmatrix} U^T$$

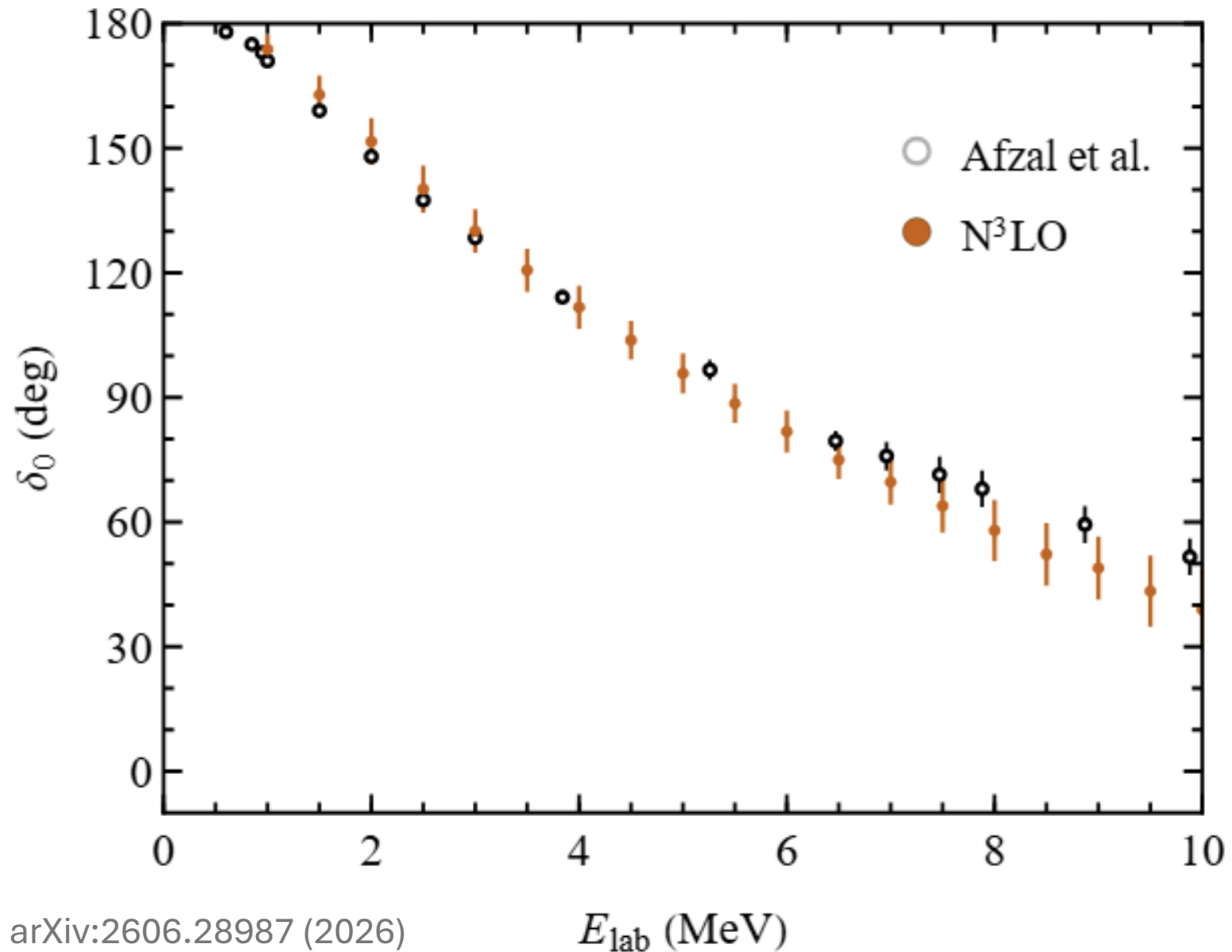
- Cross-verified with TSVD approach



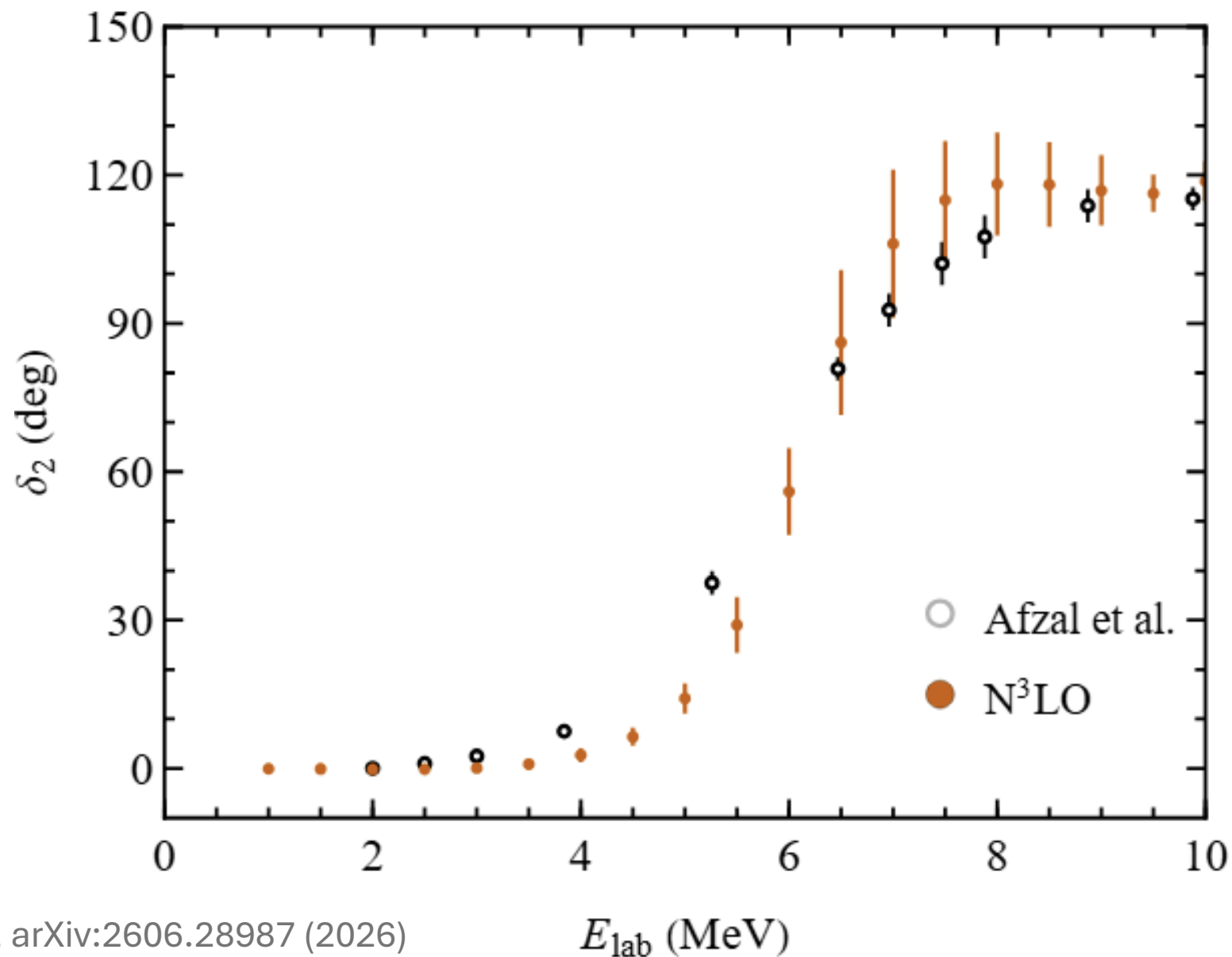
# Tikhonov regularization dimension



# S-wave phase shifts



# D-wave phase shifts



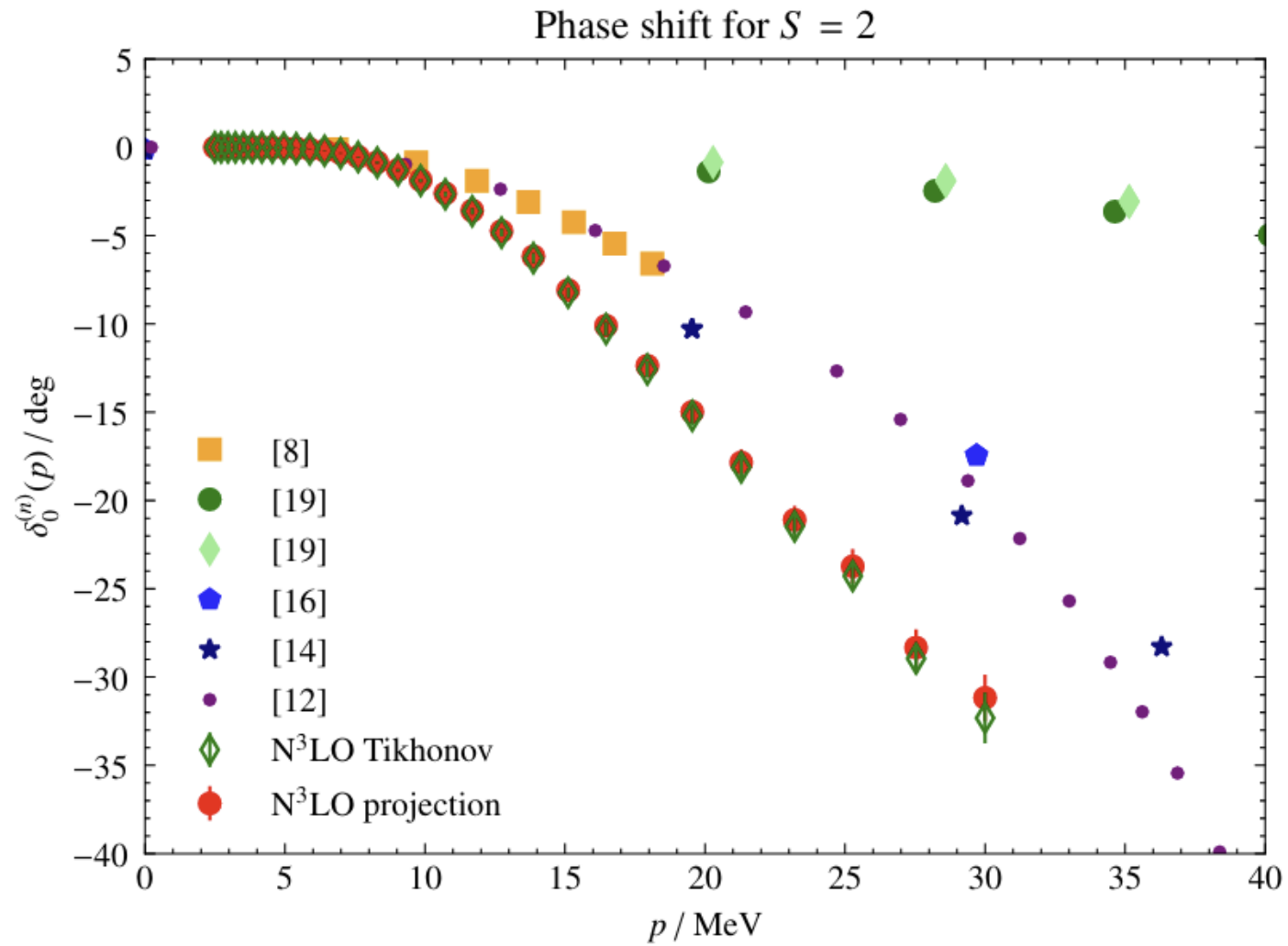
ERE fit:  
 $E_0 = 3.25 \pm 0.25 \text{ MeV}$   
 $\Gamma = 0.75 \pm 0.25 \text{ MeV}$

Emperical:  
 $E_0 = 2.92 \pm 0.18 \text{ MeV}$   
 $\Gamma = 1.34 \pm 0.50 \text{ MeV}$

# Summary and Outlook

- Ab-initio phase shifts with NLEFT and APM.
- Expensive calculations and regularization of norm matrix is needed.
- Phase shifts not perfect – need to tune interaction further.
- Alpha-capture and d-d scattering (arXiv: 2607.00681) in progress.
- We can only study two-clusters with APM. We are working to construct a formalism to study resonances and break-up cross sections with two or more clusters in NLEFT – persistent state method (in preparation).

# d-d scattering



Thank you