Medium-Mass

and

Heavy Nuclei

from

Chiral NN+3N Hamiltonians

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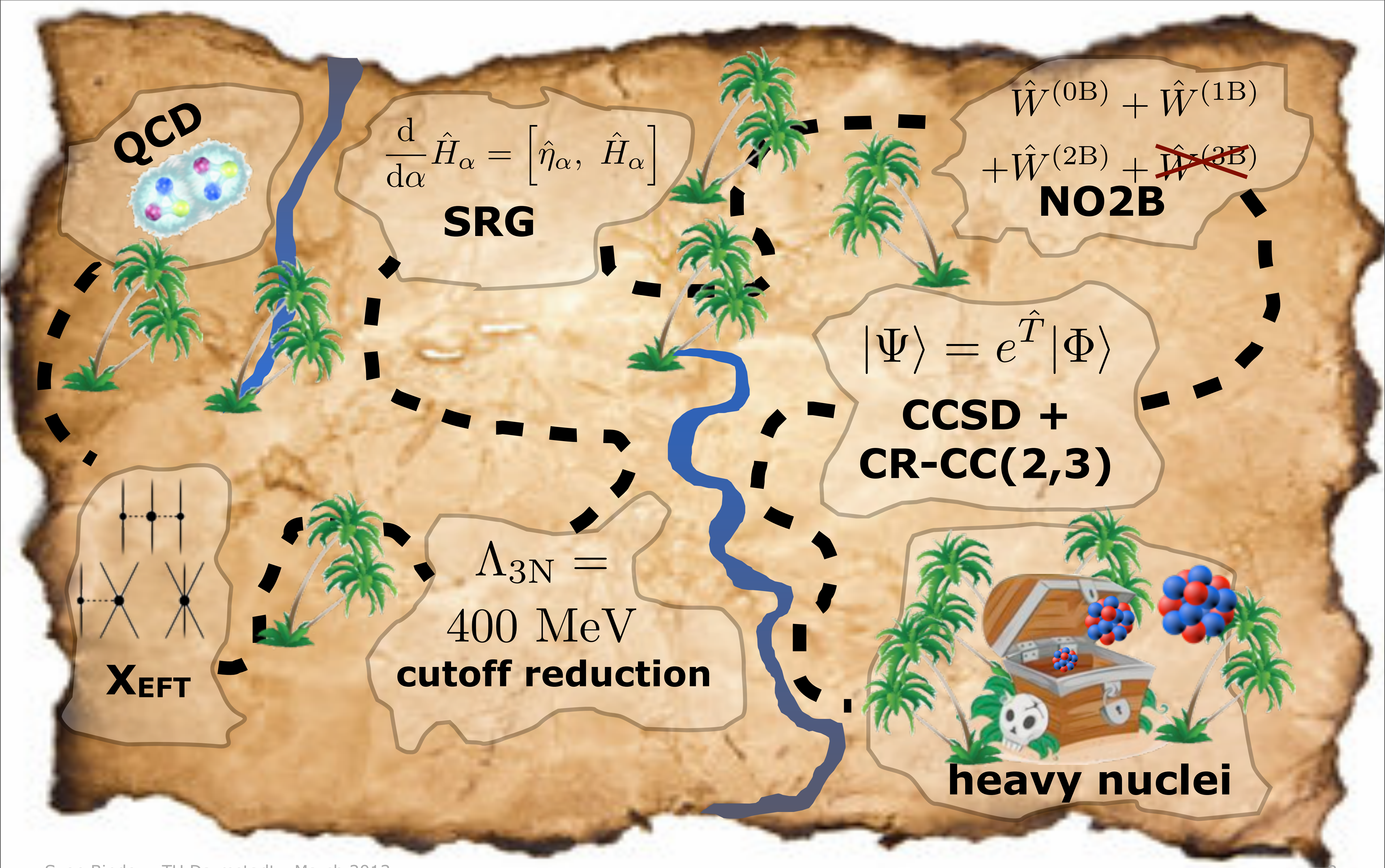
Ab Initio Path to Heavy Nuclei



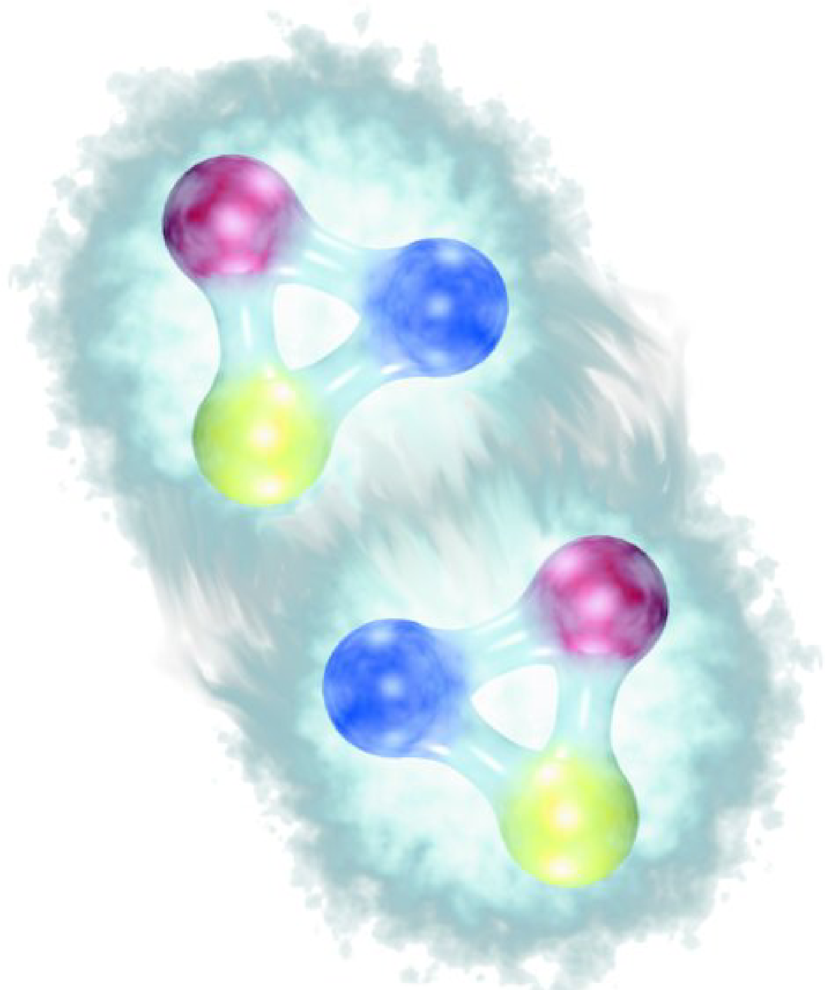
Nuclear Interactions from Chiral EFT

- Nuclear interaction is **not fundamental**

- QCD **non-perturbative** at low energies

- Low-energy **effective field theory** for relevant degrees of freedom (π,N) based on symmetries of QCD

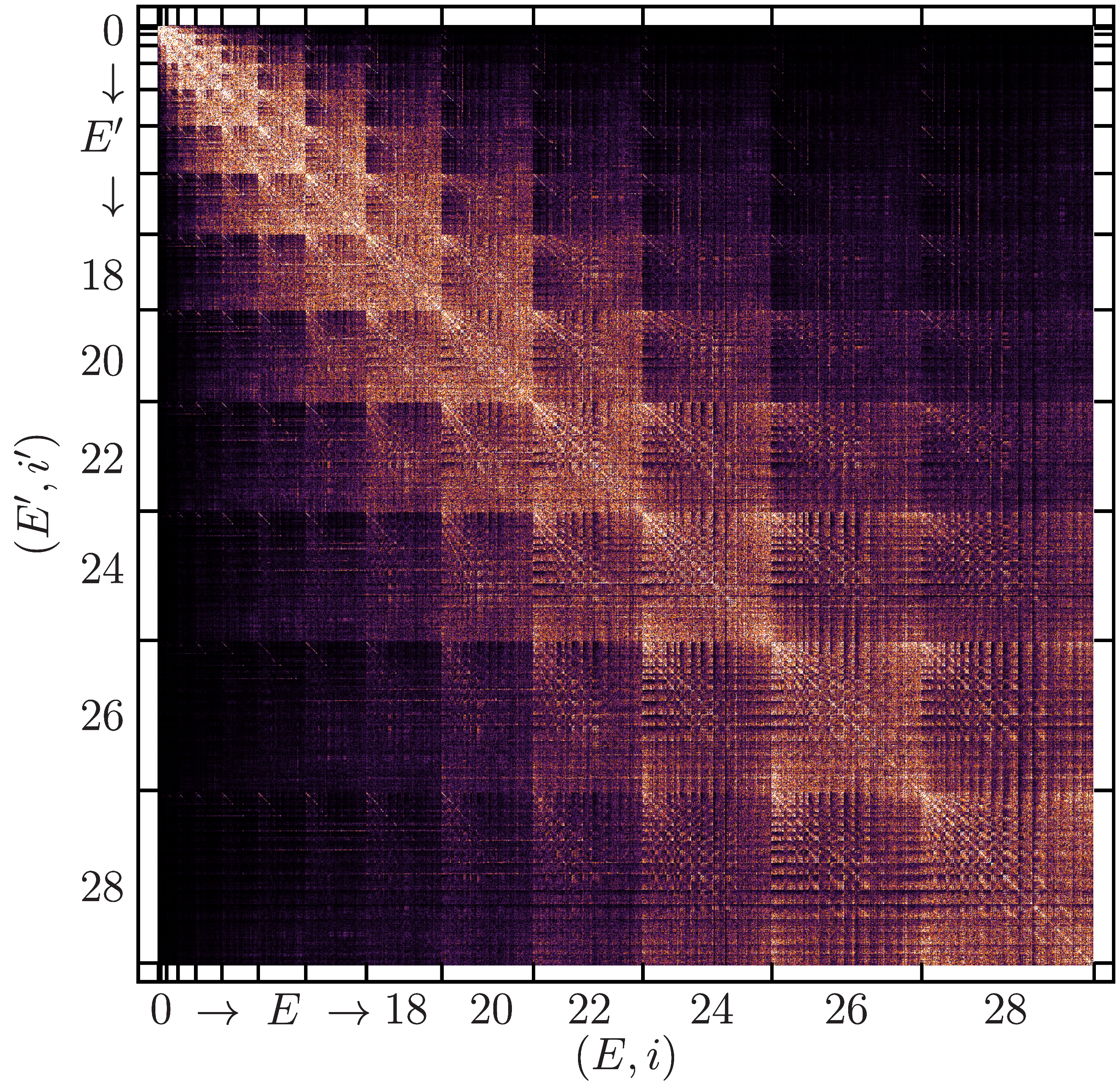
- Hierarchy of **consistent NN, 3N, ... interactions** (plus currents)



Similarity Renormalization Group

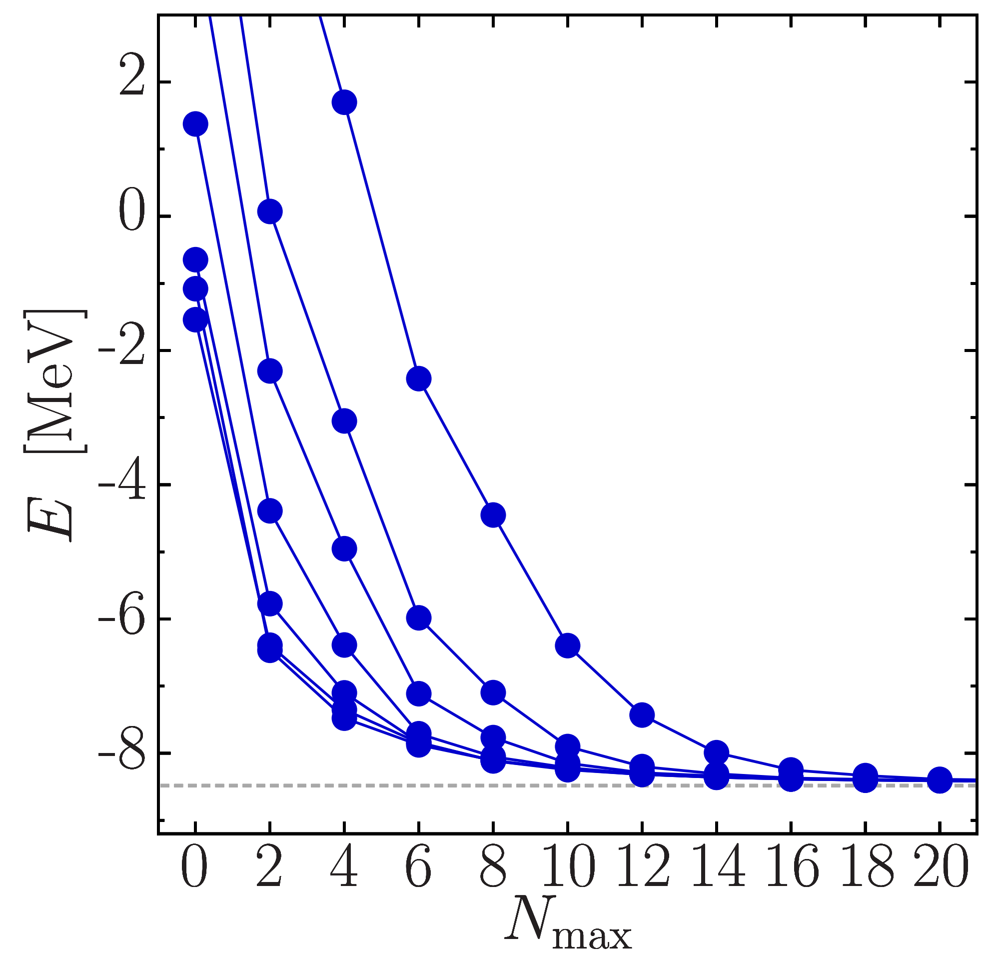
SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



α = 0.320 fm^4

NCSM ground state ^{3}H



Coupled-Cluster Method

G. Hagen, T. Papenbrock, M. Hjorth-Jensen, D.J. Dean --- arXiv:1312.7872 [nucl-th] (2013)

G. Hagen, T. Papenbrock, D.J. Dean, M. Hjorth-Jensen --- Phys. Rev. C 82, 034330 (2010)

G. Hagen, T. Papenbrock, D.J. Dean et al. --- Phys. Rev. C 76, 034302 (2007)

Coupled-Cluster Approach

- **exponential Ansatz** for wave operator

$$|\Psi\rangle = \hat{\Omega}|\Phi_0\rangle = e^{\hat{T}_1+\hat{T}_2+\cdots+\hat{T}_A}|\Phi_0\rangle$$

- $\hat{T}_n$: ***npnh* excitation** (cluster) operators

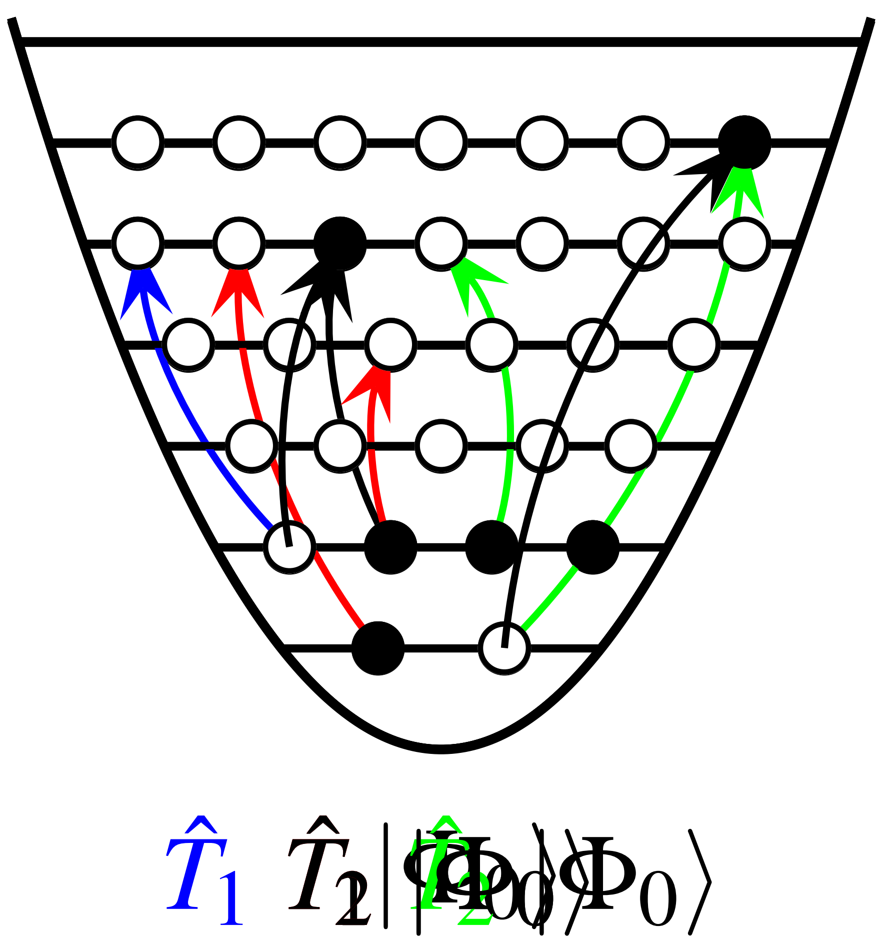
$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{ijk\ldots \\ abc\ldots}} t_{ijk\ldots}^{abc\ldots}\{\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \ldots \hat{a}_k \hat{a}_j \hat{a}_i\}$$

- **similarity-transformed** Schroedinger equation

$$\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle \ , \quad \hat{\mathcal{H}} = e^{-\hat{T}} \ \hat{H}_N \ e^{\hat{T}}$$

Singles and Doubles Excitations: CCSD

- **CCSD**: truncate $\hat{T}$ at the **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$



- $e^{\hat{T}}$- Ansatz: **higher** excitations from **products** of lower excitation operators

- CCSD equations

$$\Delta E^{(\mathrm{CCSD})} = \langle \Phi_0 | \hat{\mathcal{H}} | \Phi_0 \rangle$$

$$0 = \langle \Phi_i^a | \hat{\mathcal{H}} | \Phi_0 \rangle \ , \ \forall \ a, i$$

$$0 = \langle \Phi_{ij}^{ab} | \hat{\mathcal{H}} | \Phi_0 \rangle \ , \ \forall \ a, b, i, j$$

- Coupled system of **nonlinear equations**

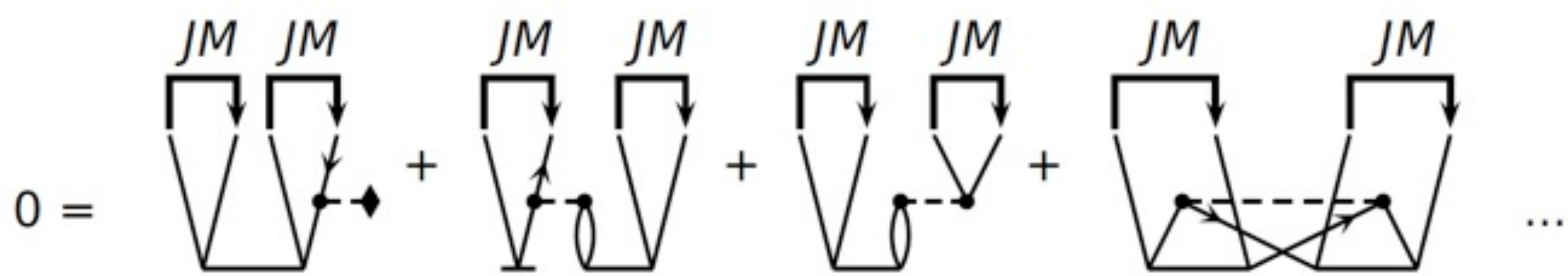
Coupled Cluster – Spherical Scheme

- exploit **spherical symmetry** for closed-shell nuclei, use spherical tensor operator formulation

$$\hat{T}_1 = \sum_{ai} t_i^a \left\{ \hat{a}_a^\dagger \otimes \hat{\tilde{a}}_i \right\}_0^{(0)}$$

$$\hat{T}_2 = \sum_{abij} \sum_{J} t_{ij}^{ab}(J) \left\{ \left\{ \hat{a}_a^\dagger \otimes \hat{a}_b^\dagger \right\}^{(J)} \otimes \left\{ \hat{\tilde{a}}_j \otimes \hat{\tilde{a}}_i \right\}^{(J)} \right\}_0^{(0)}$$

- **angular-momentum coupling** of external lines



- express CC equations in terms of

$$\langle \overset{J0}{p\;q} \| \overset{J0}{r\;s} \rangle, \quad \langle \overset{J0}{a\;b} | t | \overset{J0}{i\;j} \rangle, \quad \langle \overset{00}{\tilde{a} | t | i} \rangle, \; etc.$$

Coupled-Cluster Triples Corrections

- **CCSDT**, $\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3$, **too expensive**

- Coupled-Cluster **energy functional**

$$\mathcal{E} = \langle \Phi_0 | (1 + \hat{\Lambda}) \hat{\mathcal{H}} | \Phi_0 \rangle_C$$

perturbation theory

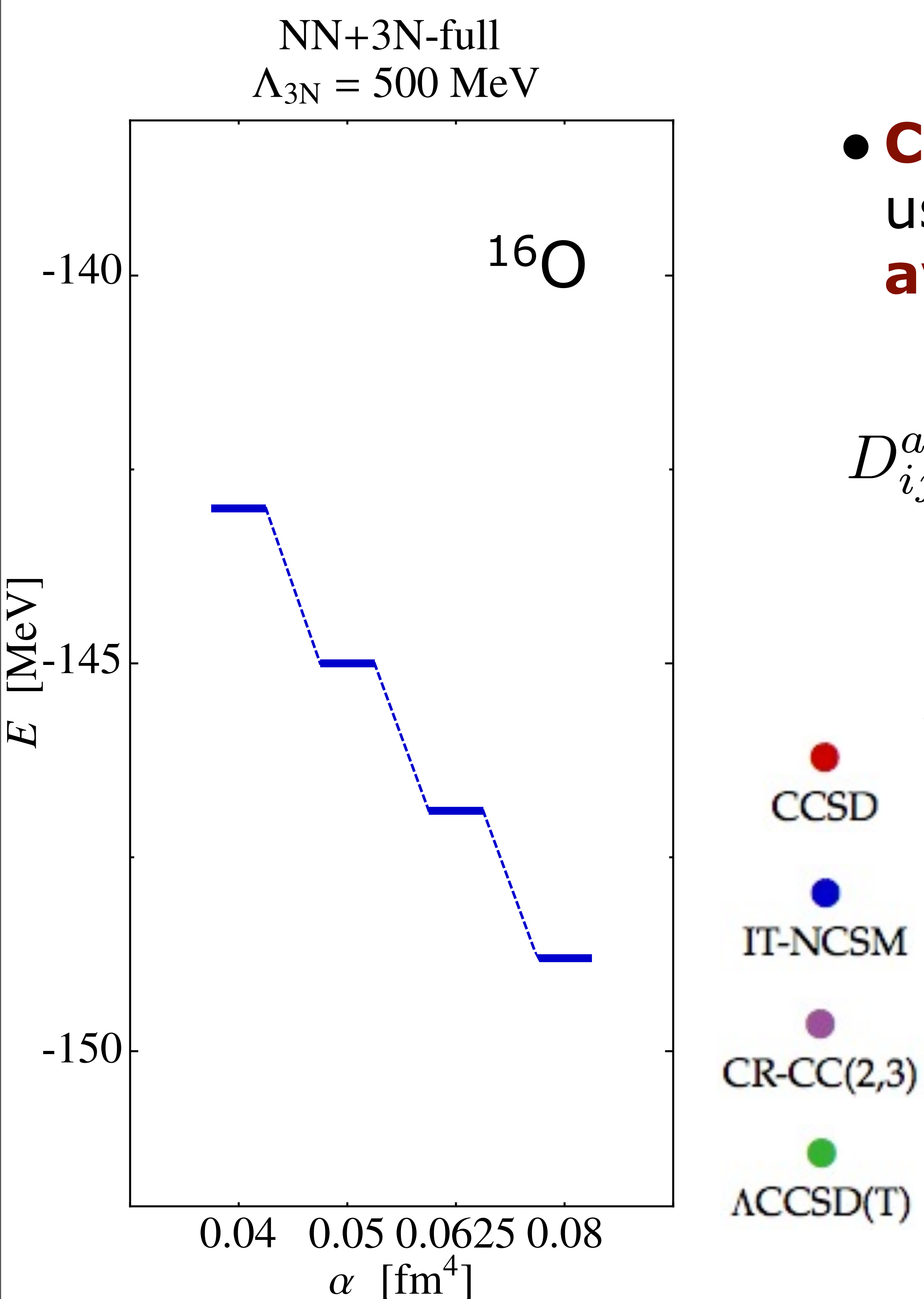
method of moments

$$\Lambda\mathrm{CCSD(T)} \qquad\qquad \mathrm{CR-CC}(2,3)$$

- Non-iterative **triples corrections**

$$\delta E^{(\mathrm{T})} = \frac{1}{(3!)^2} \sum_{\substack{abc \\ ijk}} \mathfrak{L}^{ijk}_{abc} \, \frac{1}{D^{abc}_{ijk}} \, \mathfrak{R}^{abc}_{ijk}$$

CR–CC(2,3) vs. ΛCCSD(T) and IT–NCSM



- **CR-CC(2,3)**:
  using **angular-momentum projection averaged** denominator

$$
\begin{aligned}
D^{abc}_{ijk} &\approx \overline{D}^{abc}_{ijk} \\
&= \mathcal{H}^{i}_{i} + \dots + \overline{\mathcal{H}}^{ij}_{ij} + \dots + \overline{\mathcal{H}}^{ijk}_{ijk} + \dots
\end{aligned}
$$

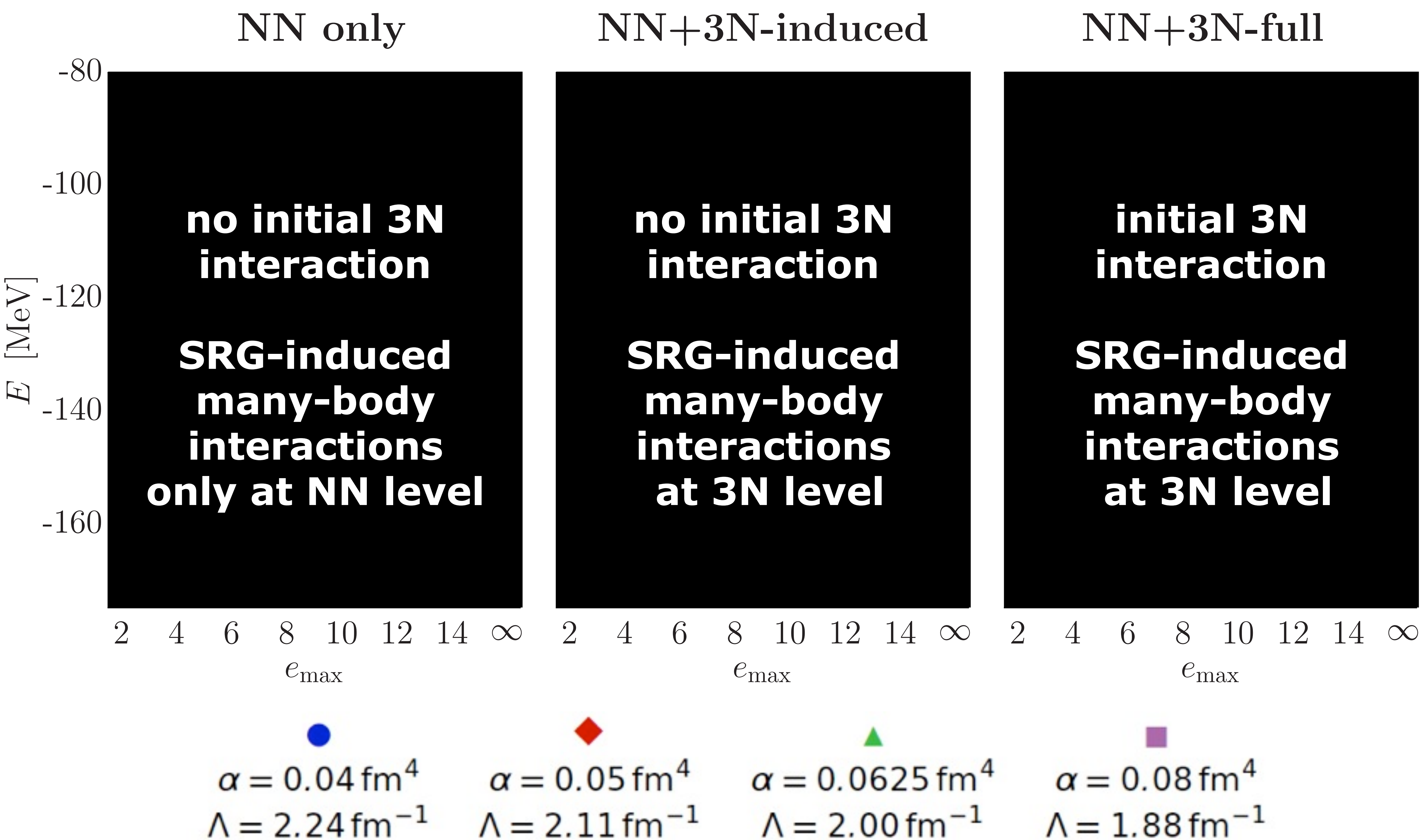
$$
\overline{\mathcal{H}}^{p\dots q}_{p\dots q} = \frac{1}{(2j_p+1)\dots(2j_q+1)} \sum_{m_p\dots m_q} \mathcal{H}^{p\dots q}_{p\dots q}
$$

Reduced-Cutoff 3N Interaction

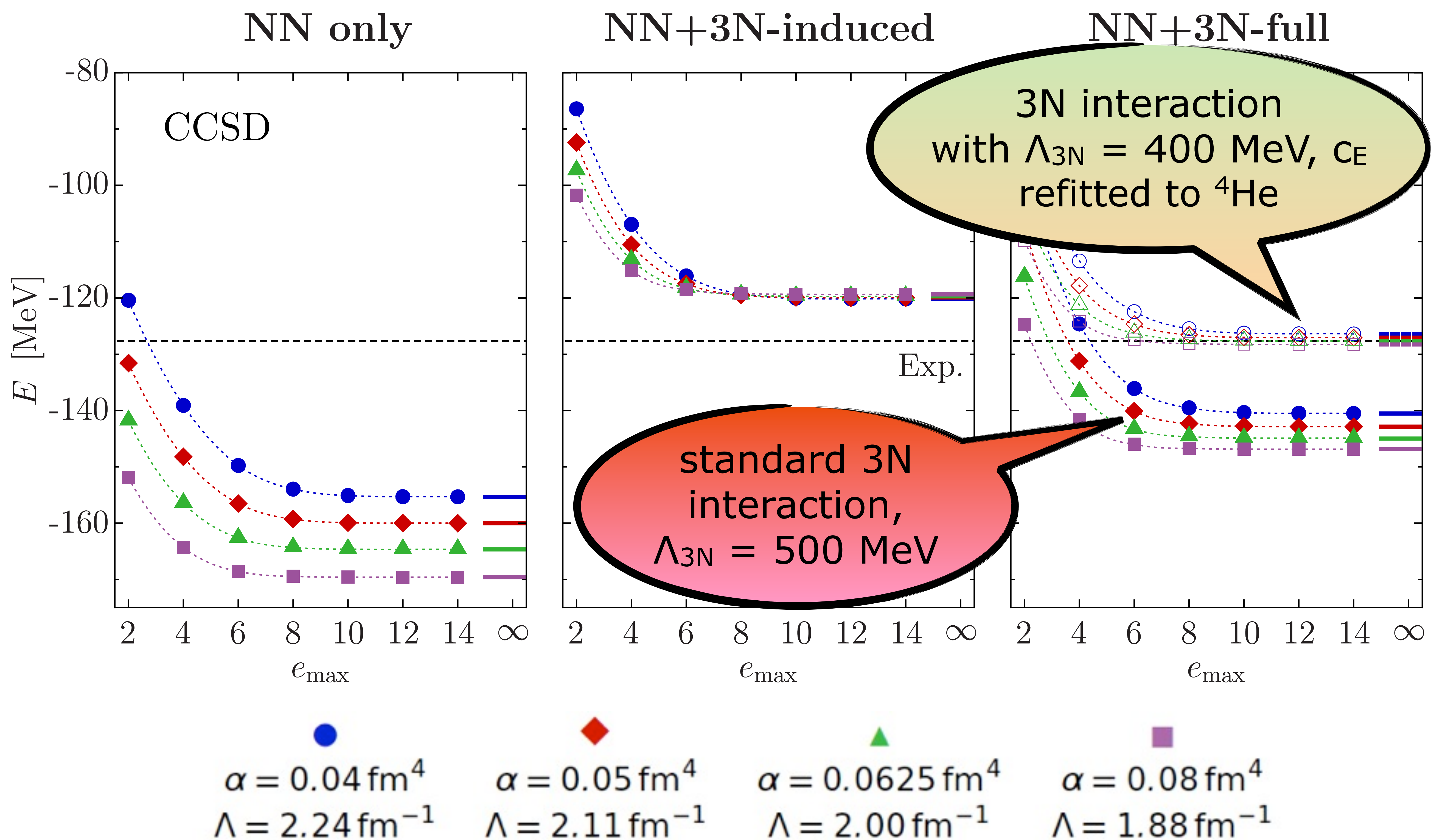
R. Roth, S. Binder, K. Vobig, A. Calci, J. Langhammer, P. Navrátil --- PRL 109, 052501 (2012)

R. Roth, A. Calci, J. Langhammer, S. Binder --- arXiv:1311.3563

^{16}O: Reduced–Cutoff 3N Interaction



^{16}O: Reduced-Cutoff 3N Interaction



Normal-Ordering Two-Body Approximation

G. Hagen, T. Papenbrock, D.J. Dean et al. --- Phys. Rev. C 76, 034302 (2007)

R. Roth, S. Binder, K. Vobig et al. --- Phys. Rev. Lett. 109, 052501(R) (2012)

S. Binder, J. Langhammer, A. Calci et al. --- Phys. Rev. C 82, 021303 (2013)

Normal-Ordered 3N Interaction

Avoid technical challenge of including explicit 3N interactions in many-body calculation

- **Idea**: write 3N interaction in normal-ordered form with respect to an A-body reference Slater determinant ($0\hbar\Omega$ state)

$$\hat{V}_{3\mathrm{N}} = \sum V^{3\mathrm{N}}_{\circ\circ\circ\circ\circ\circ}\ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

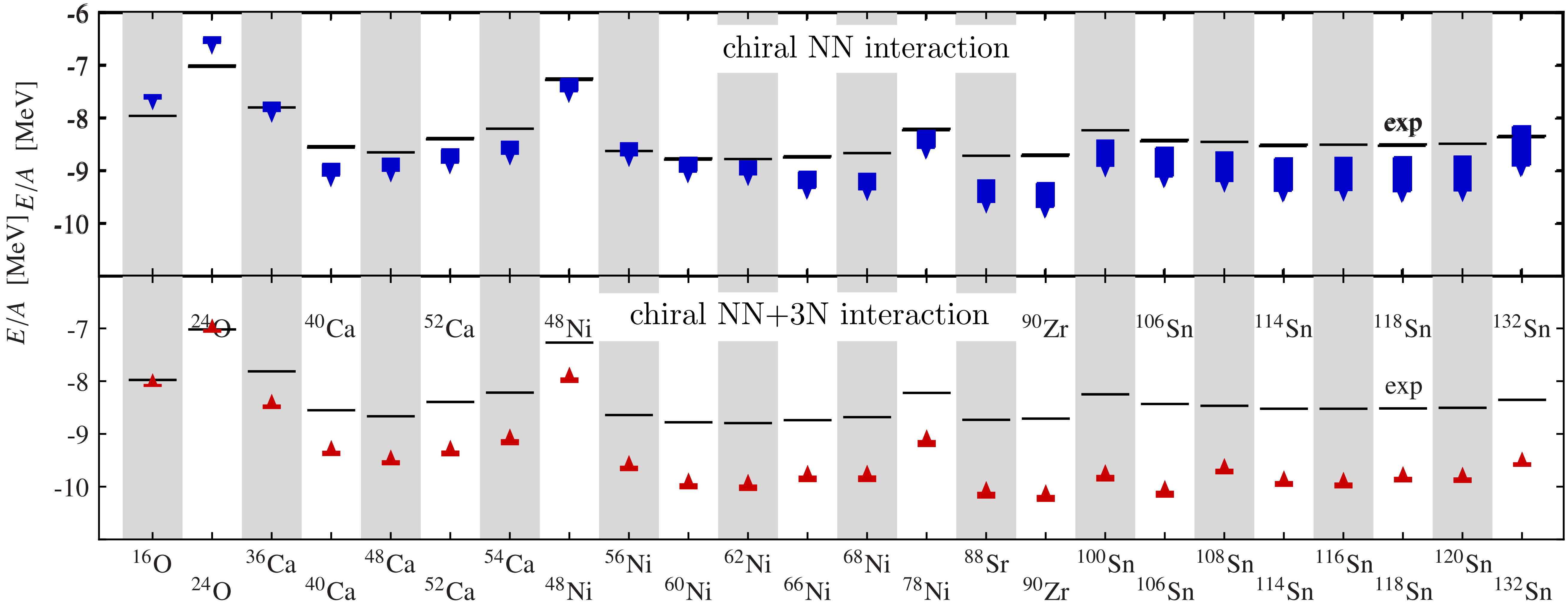
$$\hat{V}_{3\mathrm{N}} = W^{0\mathrm{B}} + \sum W^{1\mathrm{B}}_{\circ\circ}\ \hat{a}^\dagger_\circ \hat{a}_\circ + \sum W^{2\mathrm{B}}_{\circ\circ\circ\circ}\ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ$$

$$\cancel{+ \sum W^{3\mathrm{B}}_{\circ\circ\circ\circ\circ\circ}\ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ}$$

Heavy Nuclei

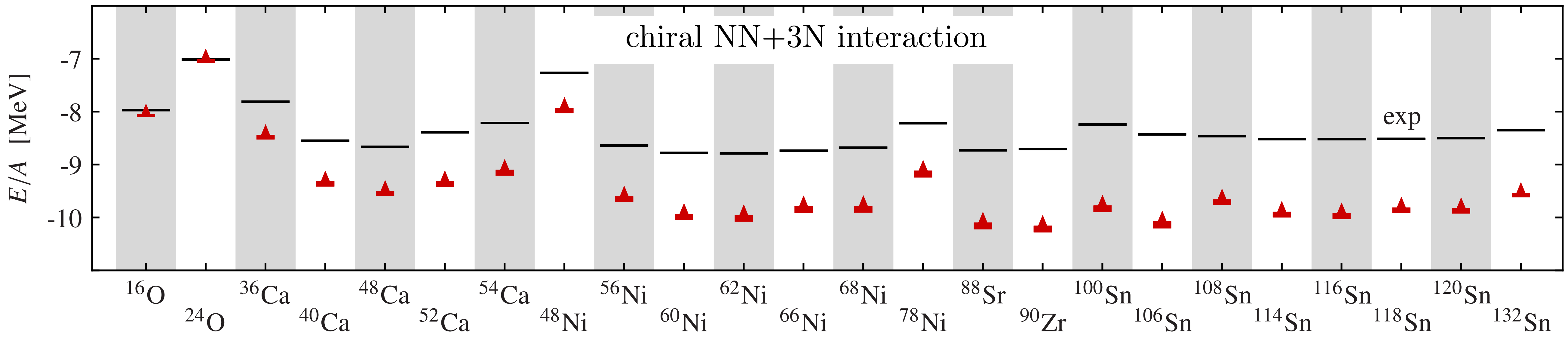
S. Binder, J. Langhammer, A. Calci, R. Roth, arXiv:1312.5685

Heavy Nuclei from Chiral Interactions



- NN interaction: **strong** SRG-induced **4N**, ... interactions
- NN+3N interaction: **cancellation** of SRG-induced **4N**, ... interactions

Heavy Nuclei from Chiral Interactions



- Hamiltonians fixed in **A≤4** systems

- **current** chiral Hamiltonians capable of describing the **experimental trend** of binding energies

- systematic overbinding ⇒ still **deficiencies**
  - **consistent 3N** interaction at N^{3}LO, and **4N** interaction
  - SRG-induced **4N, ...** interactions

Epilogue

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Thanks for your attention!

Computing Time

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HIC for FAIR Helmholtz International Center

LOEWE Exzellente Forschung für Hessens Zukunft

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