Evolved Chiral Hamiltonians in Nuclear Structure: Current Status and Future

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Road Map

Nuclear
Structure & Reaction Observables

Importance-Truncated NCSM

ab initio studies in
the p- & sd-shell

Coupled Cluster Approach

systematic extension
to heavy nuclei

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Similarity Renormalization Group

pre-diagonalization of Hamiltonian by unitary transformation
computational technology for 3N matrix elements

Chiral Effective Field Theory

systematic low-energy effective theory of QCD
consistent & improvable NN, 3N,... interactions

Low-Energy Quantum Chromodynamics

Outline

ab initio nuclear structure with NN+3N interactions
SRG, Talmi-transformation, frequency conversion

SRG for heavy nuclei
emphasis on new challenges

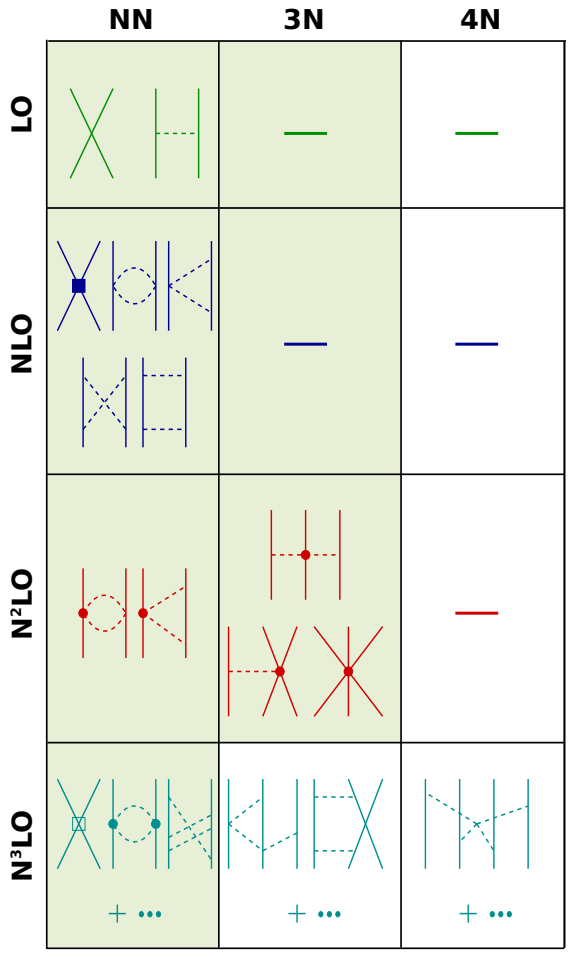
SRG in four-body space
treatment of induced and initial 4N contributions

probe chiral Hamiltonians
spectroscopy with present and next-generation Hamiltonians

Chiral NN+3N Interactions

Weinberg, van Kolck, Machleidt, Entem, Meissner, Epelbaum, Krebs, Bernard,...

- standard interaction:
  - NN @ N^{3}LO: Entem&Machleidt, 500 MeV cutoff
  - 3N @ N^{2}LO: Navrátil, local, 500 MeV cutoff, fitted to Triton and reduced cutoff, fit to Triton and Helium



Similarity Renormalization Group in Three-Body Space

Roth, Langhammer, AC et al. — Phys. Rev. Lett. 107, 072501 (2011)
Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Jurgenson, Navrátil, Furnstahl — Phys. Rev. Lett. 103, 082501 (2009)
Bogner, Furnstahl, Perry — Phys. Rev. C 75 061001(R) (2007)

Similarity Renormalization Group (SRG)

accelerate convergence by **pre-diagonalizing** the Hamiltonian with respect to the many-body basis

- **unitary transformation** leads to **evolution equation**

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\widetilde{\mathrm{H}}_\alpha = [\eta_\alpha, \widetilde{\mathrm{H}}_\alpha] \quad \text{with} \quad \eta_\alpha = (2\mu)^2 [\mathrm{T}_{\mathrm{int}}, \widetilde{\mathrm{H}}_\alpha] = -\eta_\alpha^\dagger$$

advantages of SRG: **flexibility** and **simplicity**

- SRG induces **irreducible** many-body **interactions**

SRG-evolved Hamiltonians

- **NN only**: start with initial NN and evolve in two-body space
- **NN+3N$_{\mathrm{ind}}$**: start initial NN and evolve in three-body space
- **NN+3N$_{\mathrm{full}}$**: start with initial NN+3N and evolve in three-body space

α-variation provides omitted many-body interactions

From Jacobi to $\mathcal{J}$T-Coupled Scheme

transformed interaction in 3B-Jacobi basis

first problem

many-body calculations ($A > 6$) in Jacobi coordinates not feasible

→ advantageous to use ***m*-scheme**

second problem

m-scheme matrix elements become intractable for $N_{\max} > 8$ (p-shell)

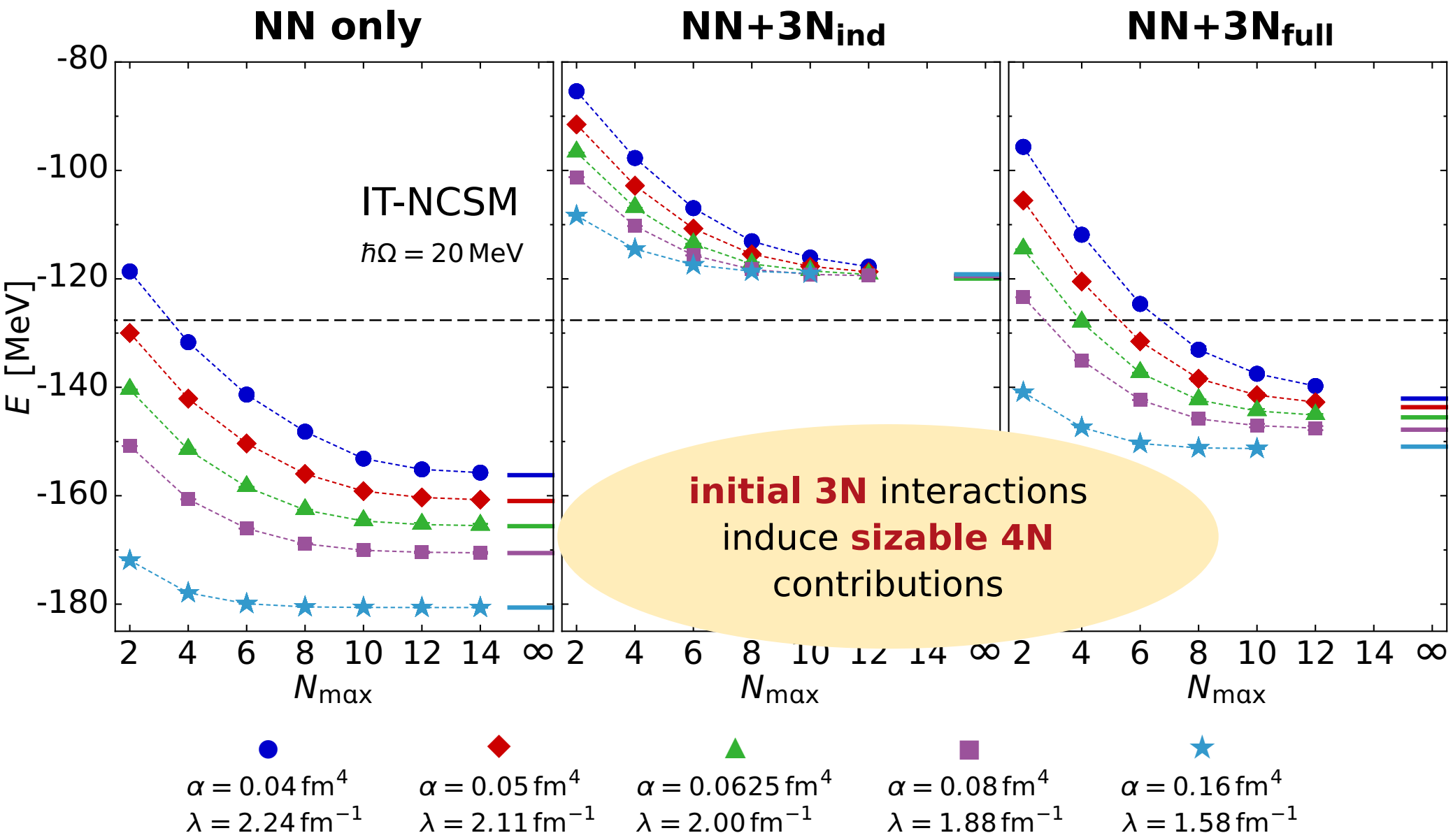
transformation from Jacobi into $\mathcal{J}T$-coupled scheme

key to efficient NCSM calculations up to $N_{max} = 14$ for p-shell nuclei

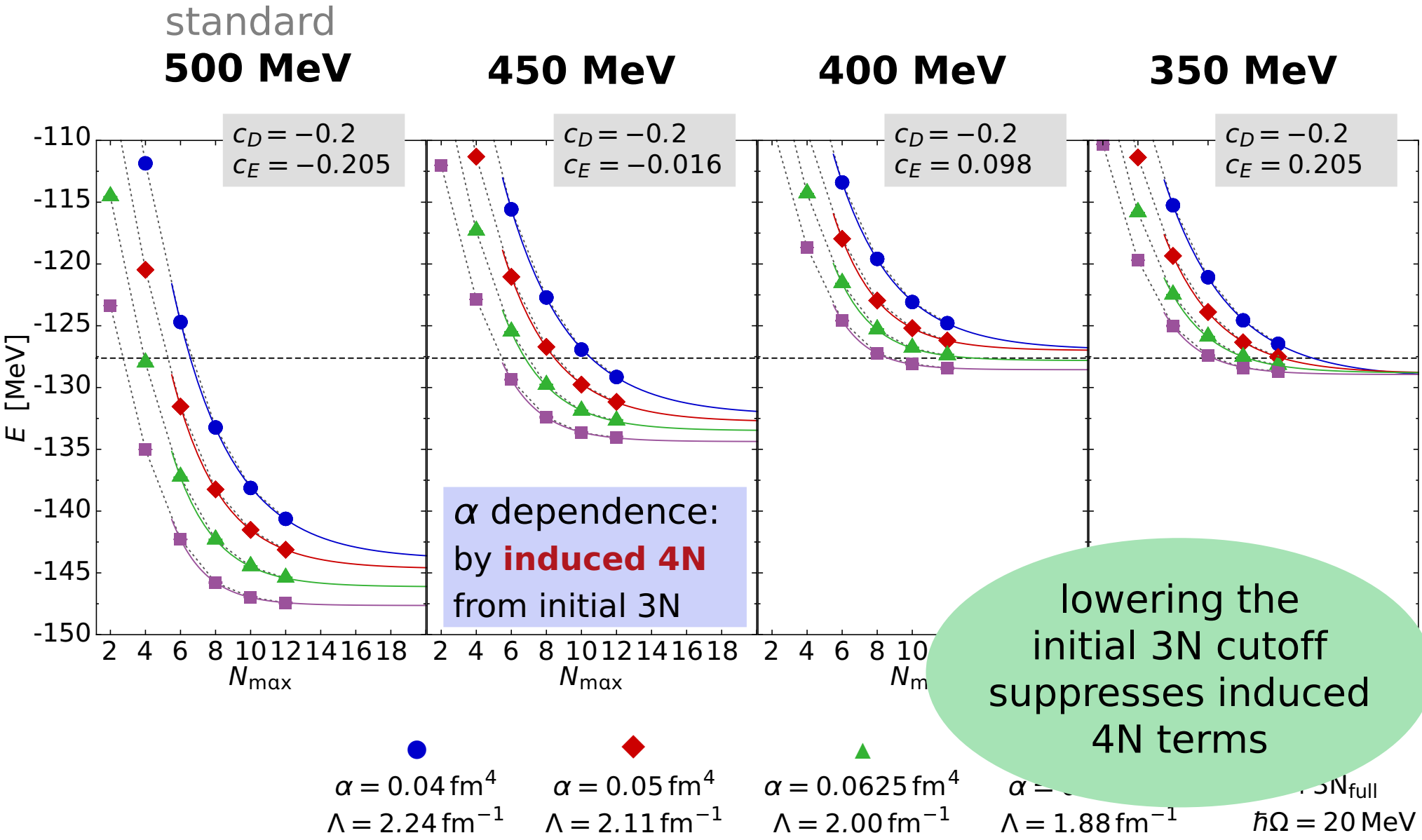
decoupling on the fly

ab-initio many-body calculation

^{16}O: Ground-State Energies



^{16}O: Lowering the Initial 3N Cutoff



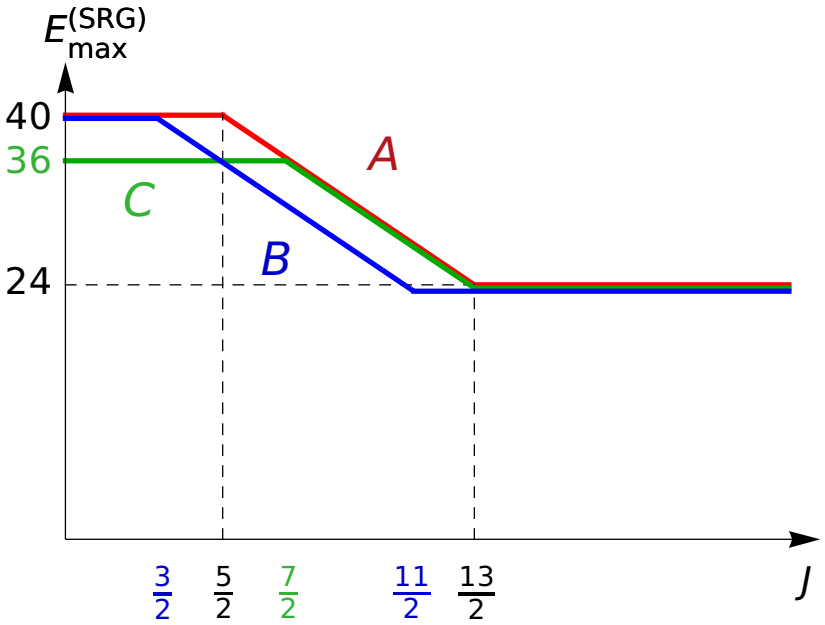
SRG Model Space & Frequency Conversion

Roth, AC, Langhammer, Binder — arXiv:1311.3563

SRG Model Space

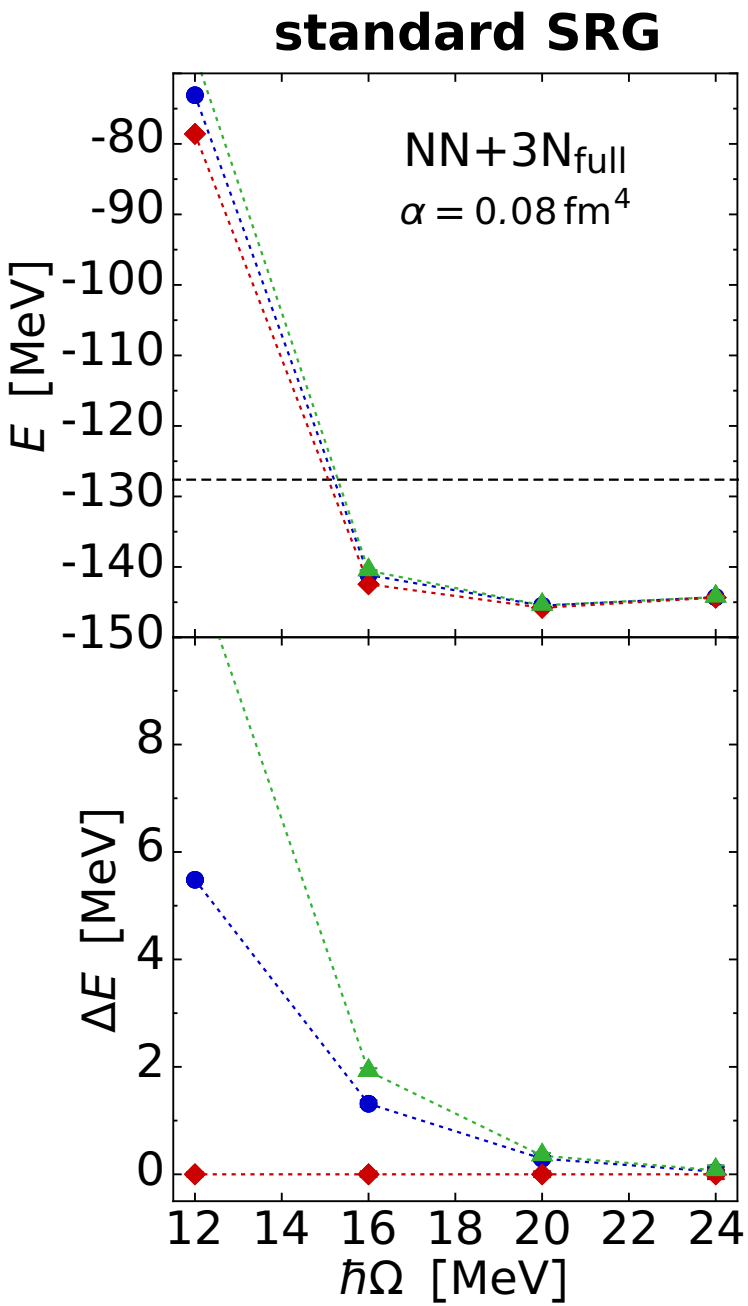
- large angular momenta less important for low-energy properties
  - J-dependent SRG space truncation $E_{\text{max}}^{(\text{SRG})}(J)$

SRG model-space ramp



- use A-ramp as standard
- use B- and C-ramp to investigate sensitivity to SRG space truncation

Frequency Conversion: ^{16}O Ground State



A-ramp

B-ramp

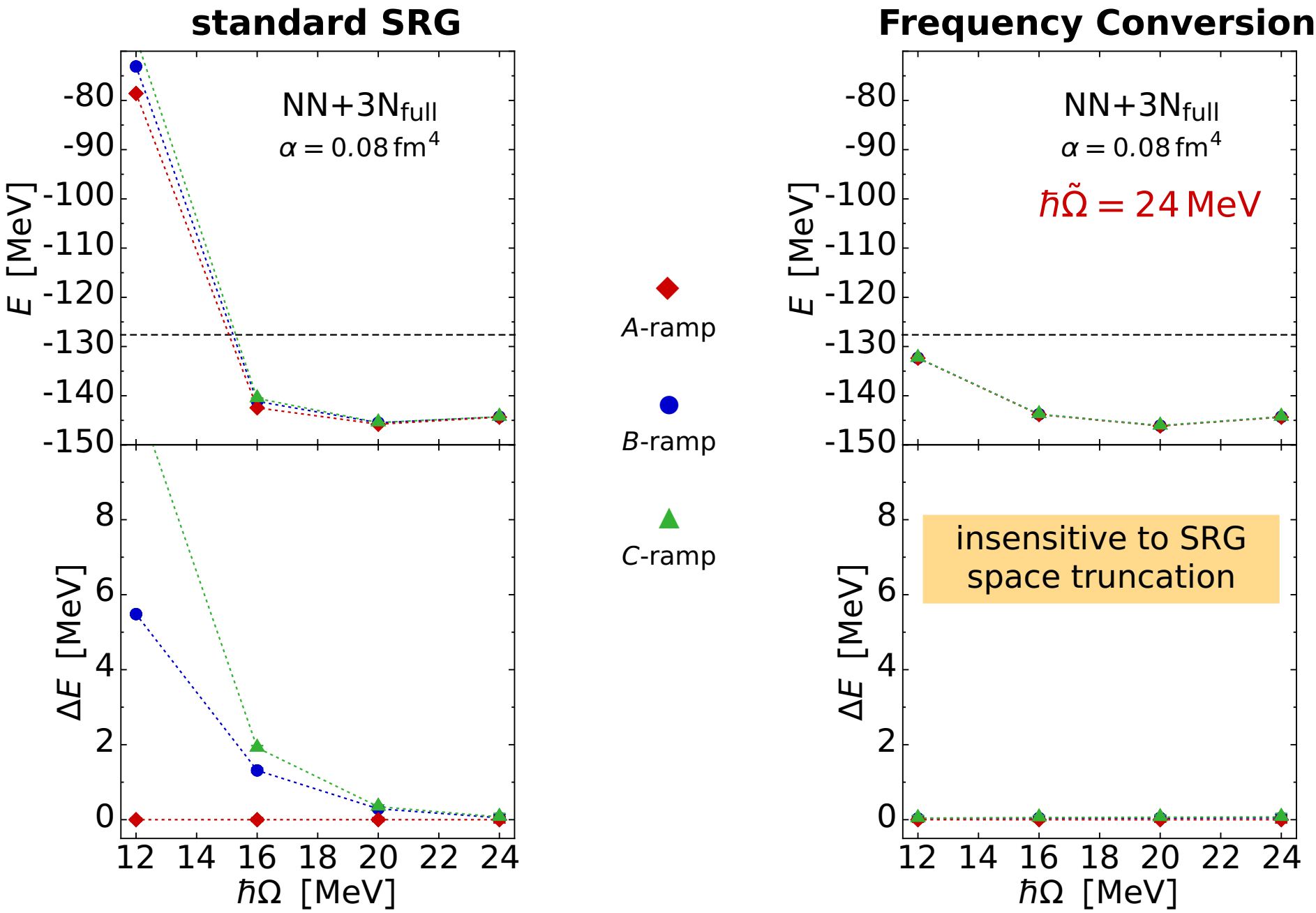
C-ramp

- physical content of SRG space depends on $\hbar\Omega$
- SRG space insufficient for **low $\hbar\Omega$**

Idea:

- **SRG** transformation for adequate $\hbar\tilde{\Omega}$
- convert to $\hbar\Omega$ needed for the **many-body calculations**

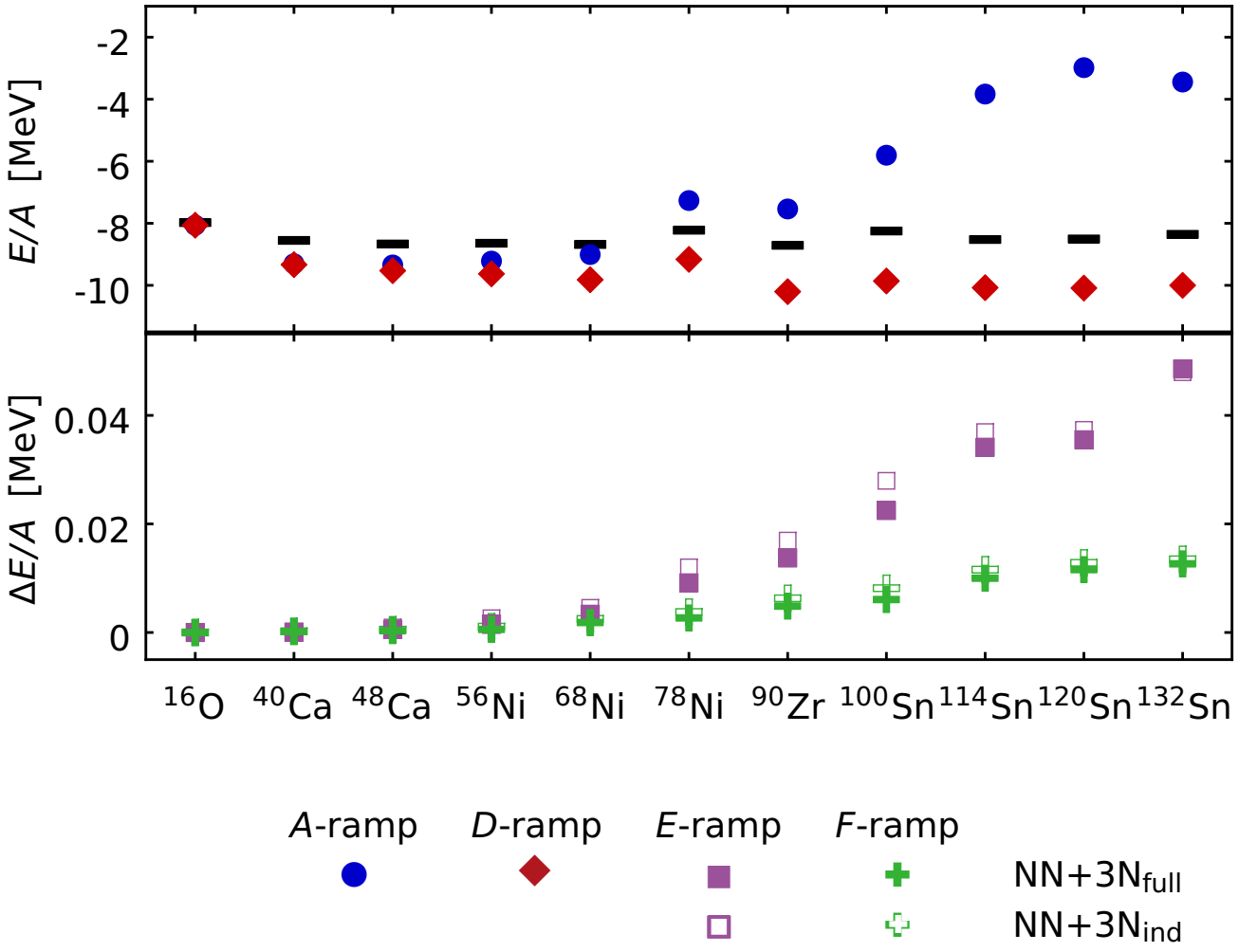
Frequency Conversion: ^{16}O Ground State



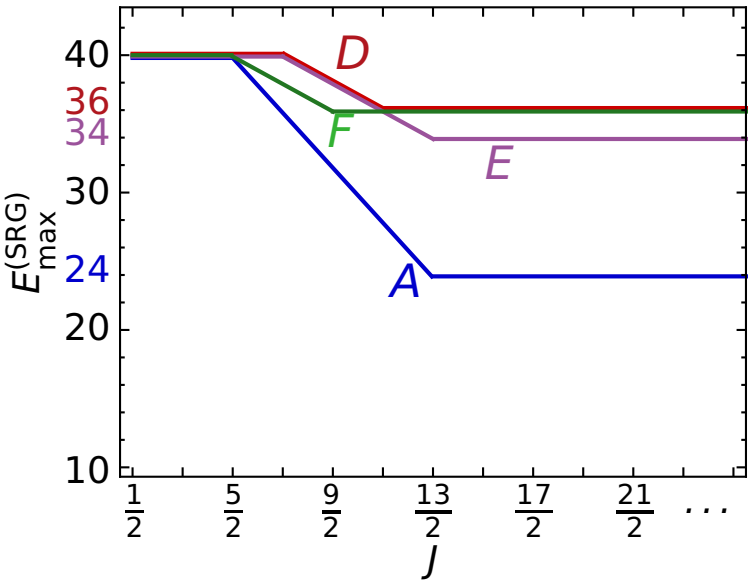
Towards Heavy Nuclei with NN+3N Interactions

Binder, Langhammer, AC, Roth	—	arXiv:1312.5685
Binder, Piecuch, AC, Langhammer, Navrátil, Roth	—	Phys. Rev. C 88, 054319 (2013)
Hagen, Papenbrock, Dean, Hjorth-Jensen	—	Phys. Rev. C 82, 034330 (2010)
Taube, Bartlett	—	J. Chem. Phys. 128, 044111 (2008)

SRG Model Space for Heavy Nuclei



SRG model-space ramp



CCSD

$\hbar\tilde{\Omega} = 36\,\mathrm{MeV}$

$\hbar\Omega = 24\,\mathrm{MeV}$

$\alpha = 0.08\,\mathrm{fm}^4$

$\Lambda_{3N} = 400\,\mathrm{MeV}$

$E_{3\mathrm{max}} = 14$

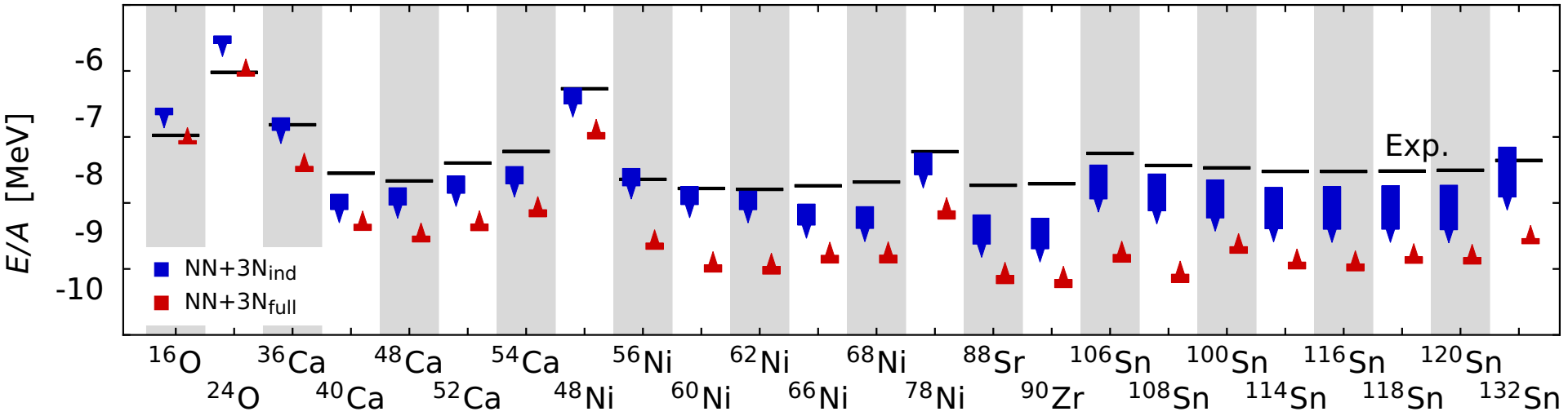
$e_{\mathrm{max}} = 12$

large angular momenta important for heavy mass nuclei

initial 3N have minor effect on SRG space dependence

Heavy Nuclei

Binder, Langhammer, AC, Roth arXiv:1312.5685



- many-body method and truncation well under control

talk by S. Binder

⇒ flow-parameter dependence caused by induced 4N contributions

CR-CC(2,3)
$\hbar\tilde{\Omega} = 36\,\mathrm{MeV}$
$\hbar\Omega = 24\,\mathrm{MeV}$
$\alpha = 0.04 - 0.08\,\mathrm{fm}^4$
$E_{3\mathrm{max}} = 18$
$e_{\mathrm{max}} = 12$

- **cancell**
  ir
  - strong

initial NN interaction requires **large SRG spaces** and **induces sizable 4N** with increasing mass number

SRG in Four-Body Space

Induced Four-Body Contributions

observation
induced 4N of initial 3N become sizable in mid-p shell

❶ suppress induced 4N contributions by reducing the cutoff Λ_{3N}

- **circumvention**: restriction to 3N interactions with lower cutoffs
- might not work for all interactions or system (heavy masses)

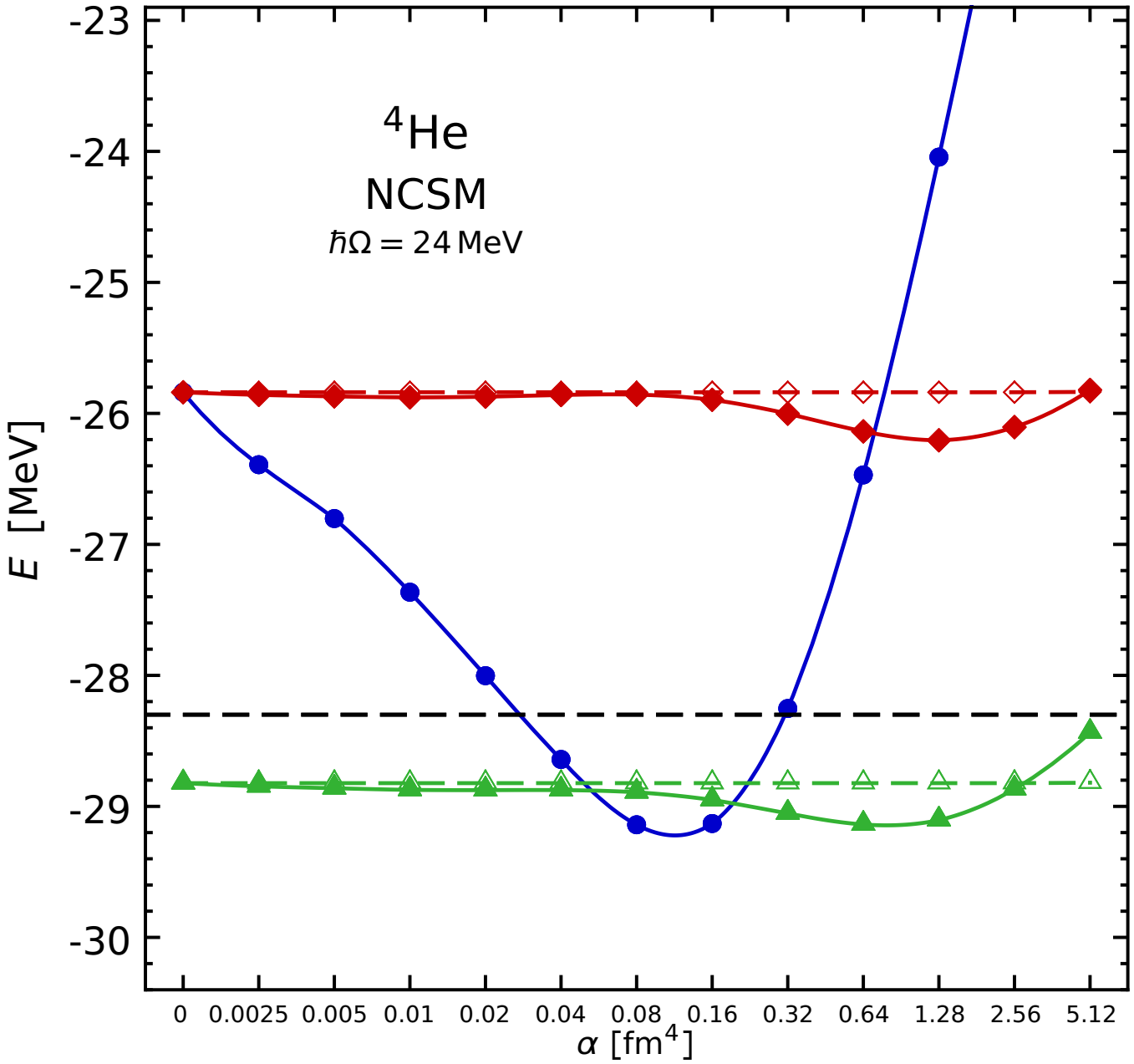
❷ find alternative SRG generator to exclude induced 4N from the outset

- so far **no better compromise** between induced 4N and convergence acceleration than with canonical generator

❸ include 4N contributions

- SRG evolution in four-body space
- apply induced (or initial) 4N to many-body methods explicitly or via approximative approaches

SRG Evolution in Four-Body Space



initial NN

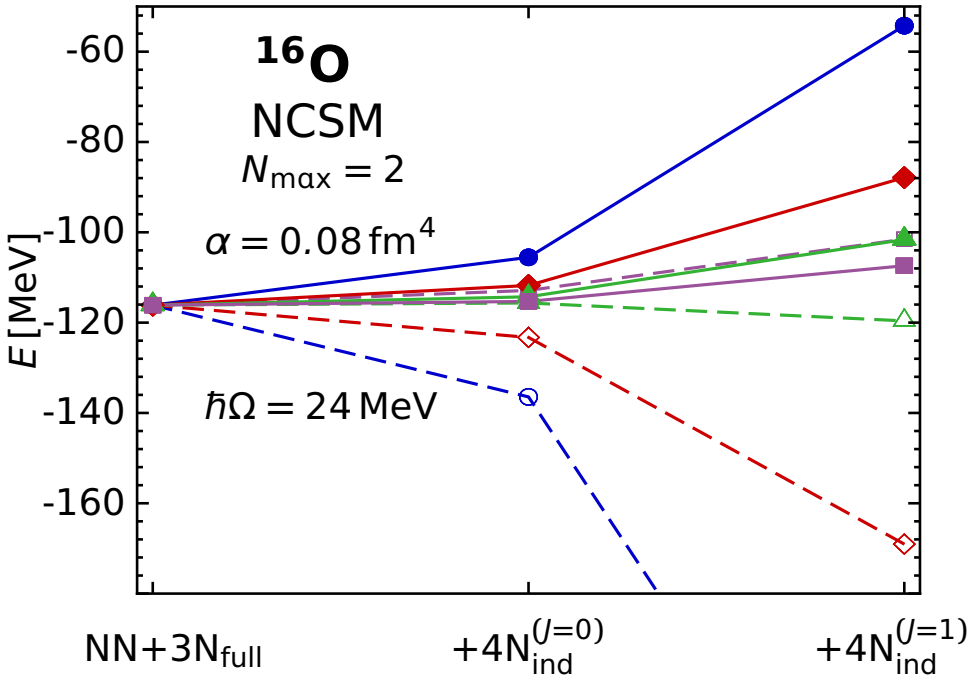
NN $+3N_{ind}$ $+4N_{ind}$

initial NN + 3N

$NN+3N_{full}$ $+4N_{ind}$

- sizable 4N effects at large flow parameters
- successful inclusion during SRG

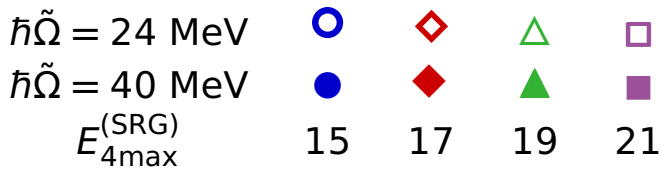
Four-Body SRG Model Space



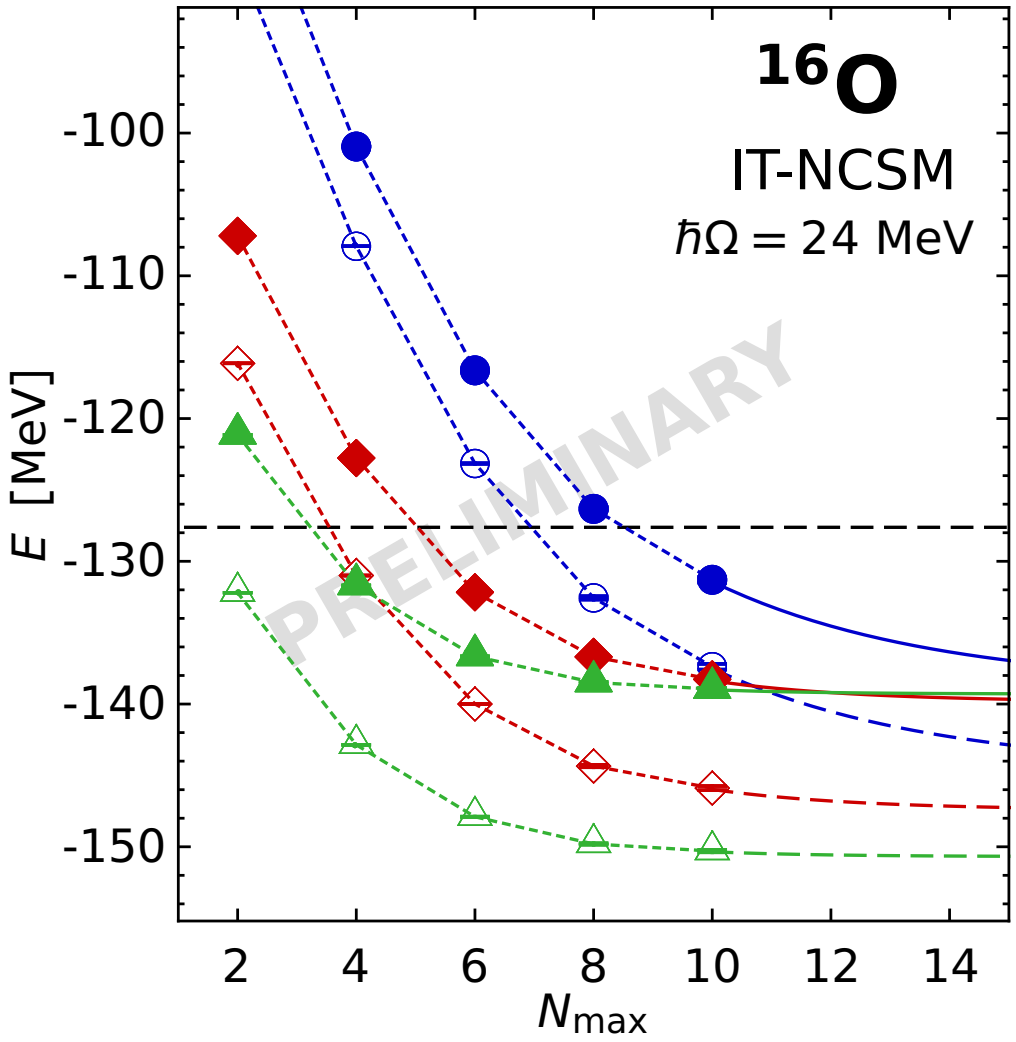
- $J = 0$: well under control
- $J = 1$: significantly **depend on SRG space**
- $J = 2$: not even close to convergence

- include induced 4N:
  - **Talmi-transformation** from Jacobi to $\mathcal{J}T$-coupled scheme
  - **extend IT-NCSM** to include explicit 4N interactions

Frequency Conversion improves convergence w.r.t. SRG space



IT-NCSM with Four-Body Contributions



- **flow-parameter** dependence strongly **suppresed**
- $J = 1$ channels **not fully converged** w.r.t. SRG space
- $J \geq 2$ channels are missing

induced 4N

all partial waves with $J = 0, 1$

$E_{4\max} = 6$, $E_{4\max}^{(\mathrm{SRG})} = 21$
$\hbar\tilde{\Omega} = 40$ MeV

$\mathrm{NN+3N_{full}}$ ○ ◇ △

$\mathrm{NN+3N_{full}+4N_{ind}}$ ● ◆ ▲

$\alpha = 0.04\,\mathrm{fm}^4$	$\alpha = 0.08\,\mathrm{fm}^4$	$\alpha = 0.16\,\mathrm{fm}^4$
$\lambda = 2.24\,\mathrm{fm}^{-1}$	$\lambda = 1.88\,\mathrm{fm}^{-1}$	$\lambda = 1.58\,\mathrm{fm}^{-1}$

Towards Next-Generation Chiral Hamiltonians

Chiral NN+3N Interactions

Weinberg, van Kolck, Machleidt, Entem, Meissner, Epelbaum, Krebs, Bernard,...

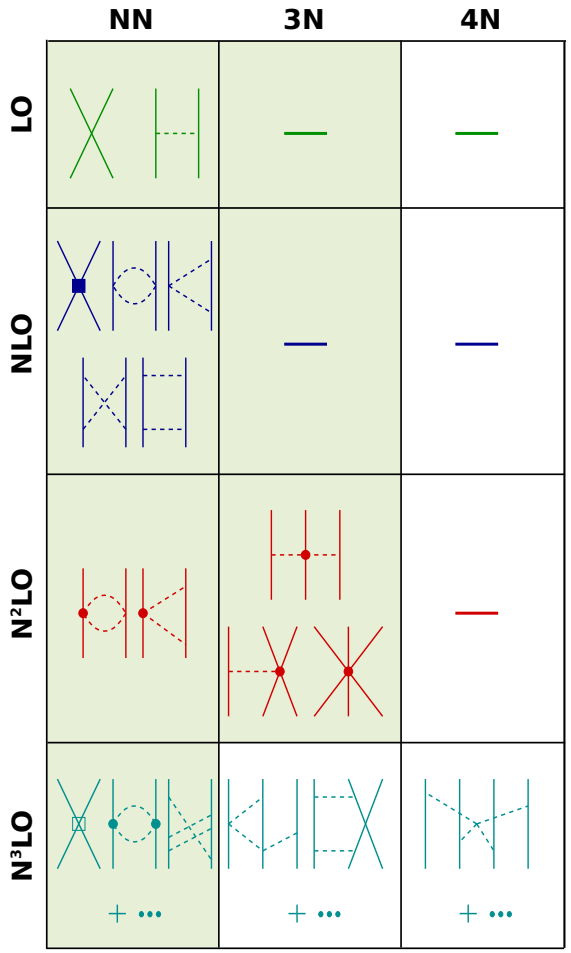
- standard interaction:
  - NN @ N^{3}LO: Entem&Machleidt, 500 MeV cutoff
  - 3N @ N^{2}LO: Navrátil, local, 500 MeV cutoff, fitted to Triton and reduced cutoff, fit to Triton and Helium

alternatives

- optimized N^{2}LO interaction:
  - NN: Ekström et al., 500 MeV cutoff, POUNDerS fit
  - 3N @ N^{2}LO: Navrátil, local, 500 MeV cutoff, fitted to Triton
- consistent N^{2}LO interactions:
  - NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal

next-generation interactions

- consistent N^{3}LO interactions:
  - LENPIC collaboration
  - first test: NN+3N @ N^{3}LO: 450 MeV cutoff, nonlocal



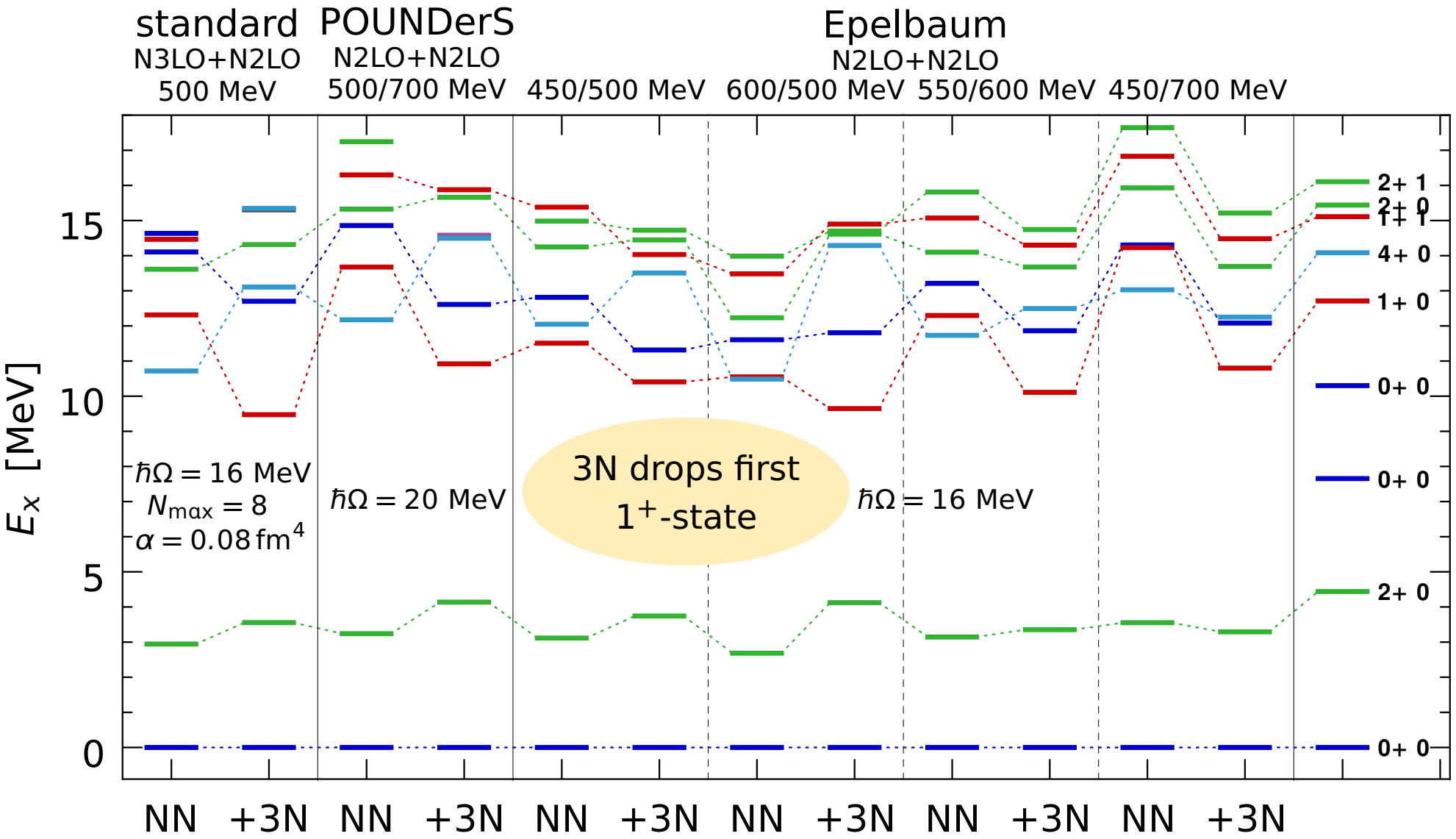
Technical Aspects

- **starting point**: numerical 3N matrix elements in partial-wave Jacobi-momentum basis (antisym. under $1 \leftrightarrow 2$)
  - numerical partial-wave decomposition of Skibinski et al.
  - recent improvements by Hebeler, Krebs et al.
  - ongoing collaborative effort to produce N^2LO/N^3LO matrix elements (LENPIC)

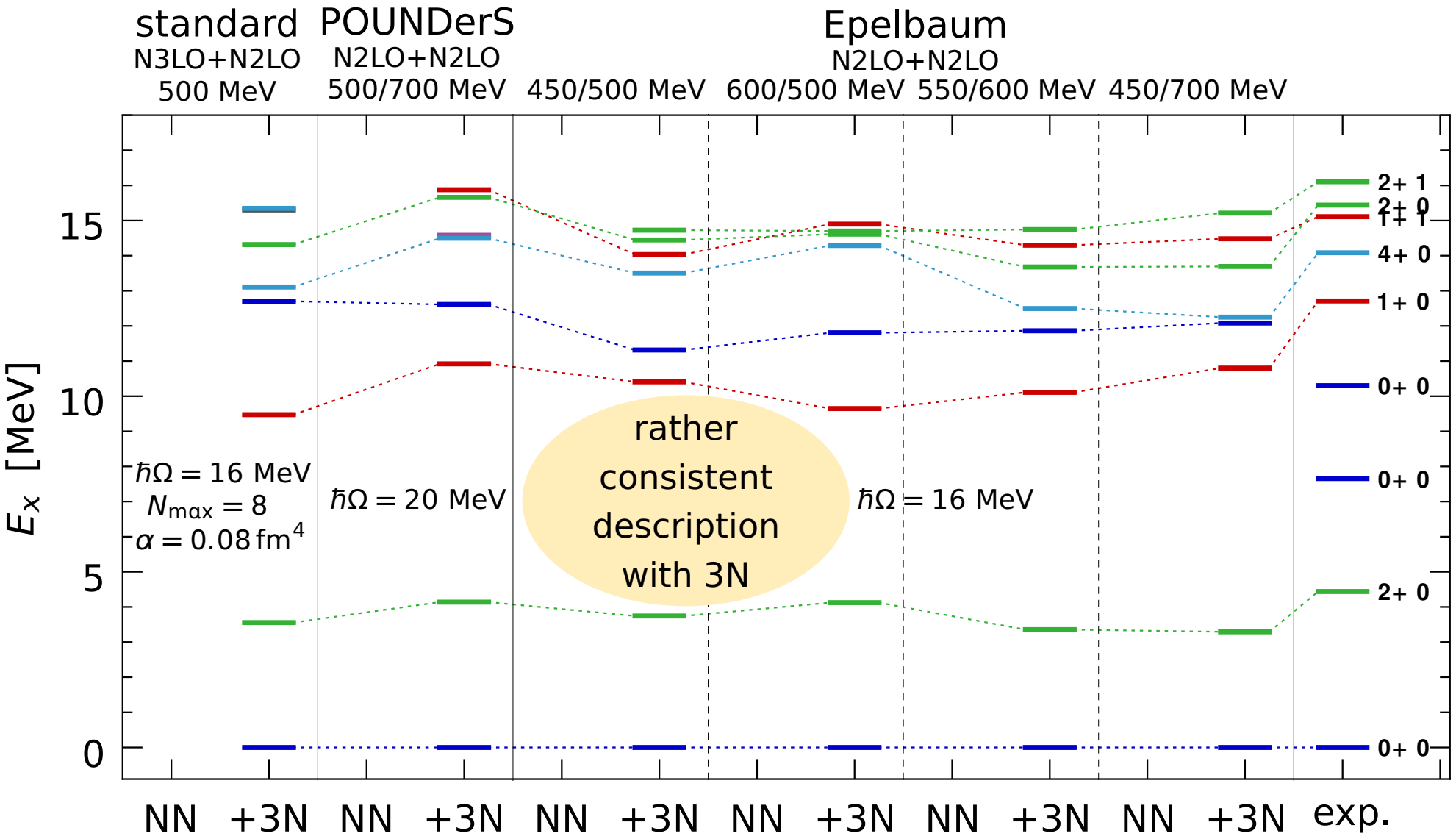
- regularization, antisymmetrization, and transformation to **HO basis**
  - use HO machinery afterwards (SRG, $\mathcal{J}T$-coupled scheme,...)

- **first applications in nuclear spectroscopy** with consistent NN+3N Hamiltonians
  - at N^2LO
  - at N^3LO

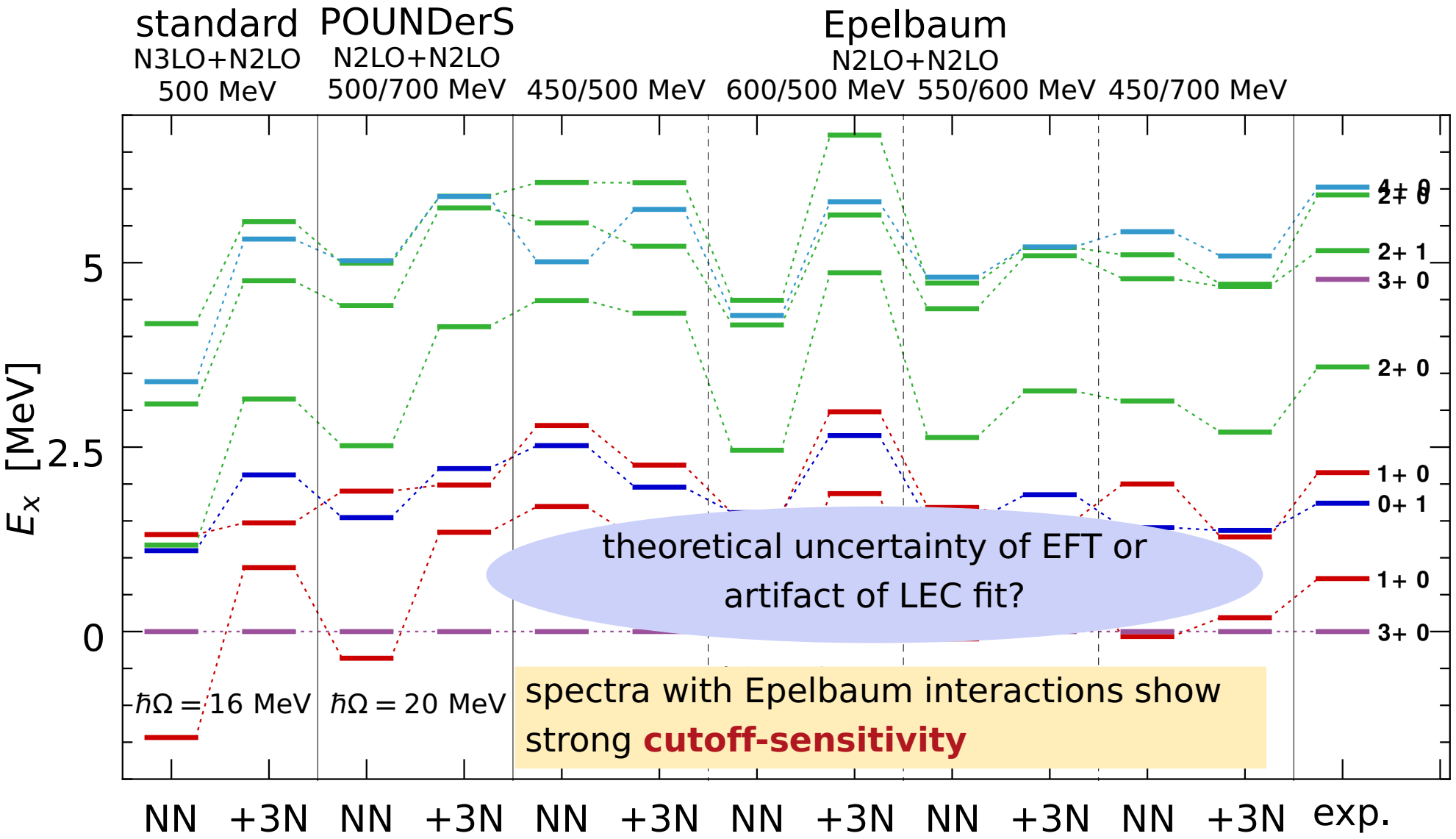
^{12}C: Compare Alternative Interactions



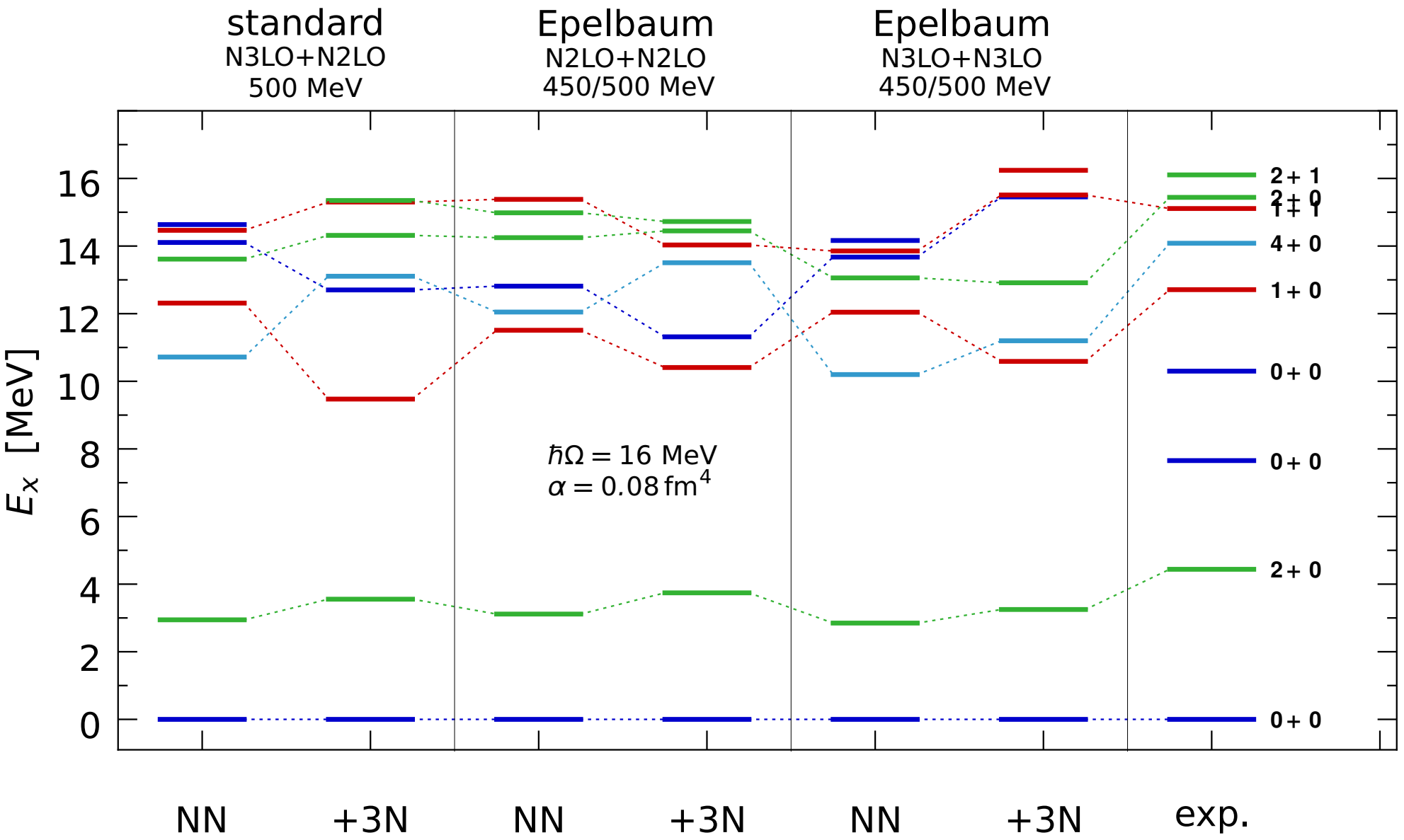
^{12}C: Compare Alternative Interactions



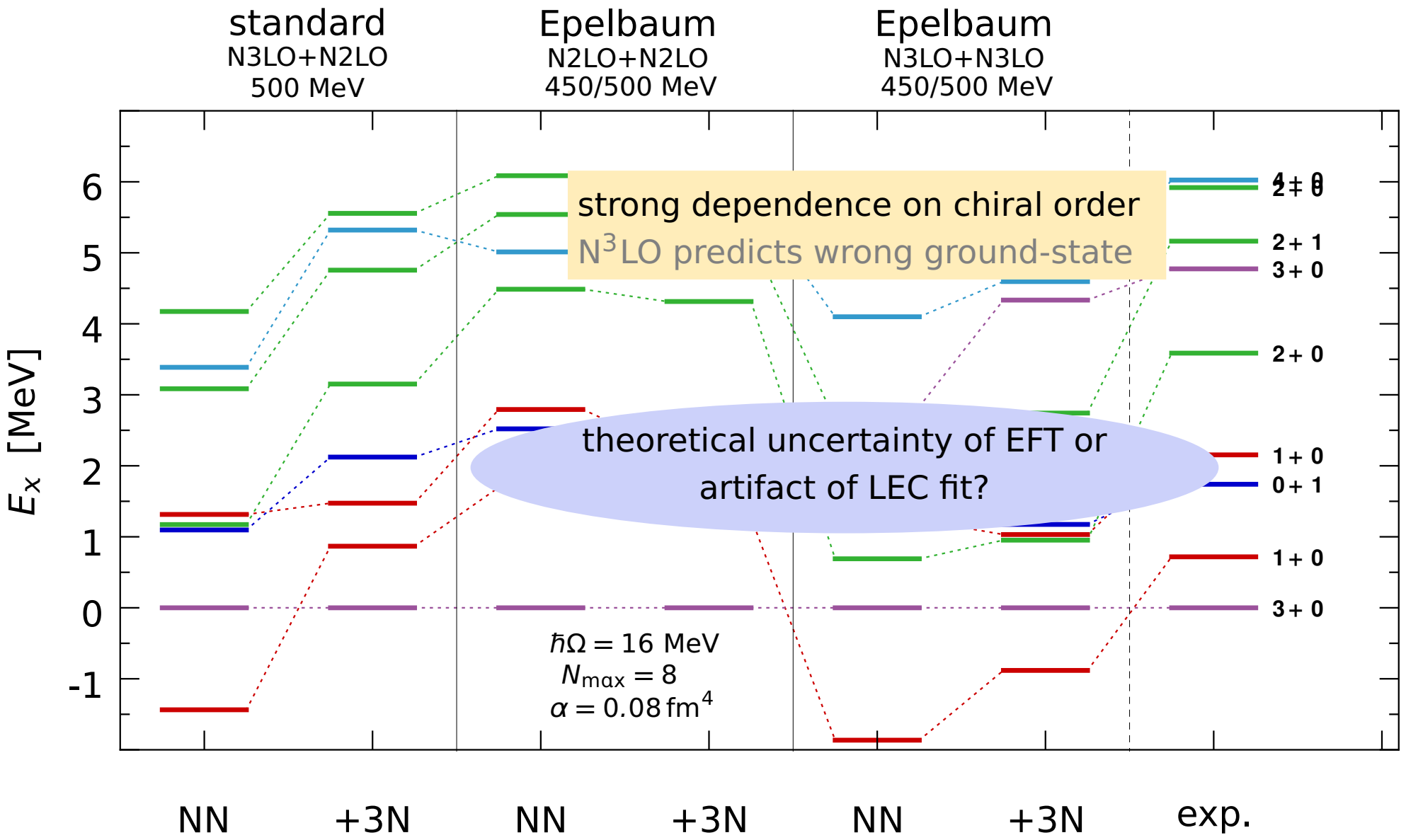
^{10}B: Compare Alternative Interactions



^{12}C: Next-Generation Interactions



^{10}B: Next-Generation Interactions



Status & Needs

Status

- we have established the **complete 3N toolchain**
  - starting from Jacobi-HO or momentum-space matrix elements
  - through consistent **SRG evolution**
  - through **Talmi transformation** to JT-coupled scheme
  - into NCSM, CC, IM-SRG, NCSMC,. . .
  - with optional normal-ordering approximation
- we are happy to collaborate

Requirements

- aim: study of **cutoff-dependence** & dependence on **chiral order** (convergence)
- revisit NN: need **precise NN** interactions at N^2LO & N^3LO for **range of cutoffs**
- adjust 3N: corresponding **fits of 3N** at N^2LO & N^3LO
- short-term: keep **Entem & Machleidt NN** at N^3LO
  - combine **with nonlocal 3N** at N^2LO & N^3LO
  - study dependence on 3N regularization-scheme & chiral order

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, K. Böhnke, J. Braun, E. Gebrerufael, K. Hebeler, H. Krutsch, **J. Langhammer**, S. Reinhardt, **R. Roth**, M. Schmidt, **S. Schulz**, C. Stumpf, A. Tichai, R. Trippel, K. Vobig, R. Wirth
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LENPIC
Low-Energy Nuclear Physics International Collaboration

JUROPA
JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC
Center for Scientific Computing Frankfurt

HOPPER
NERSC

COMPUTING TIME

SFB 634
Deutsche Forschungsgemeinschaft
DFG

HIC for FAIR
Helmholtz International Center

LOEWE
Exzellente Forschung für Hessens Zukunft

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