Evolved Chiral Hamiltonians at the Three-Body Level and Beyond

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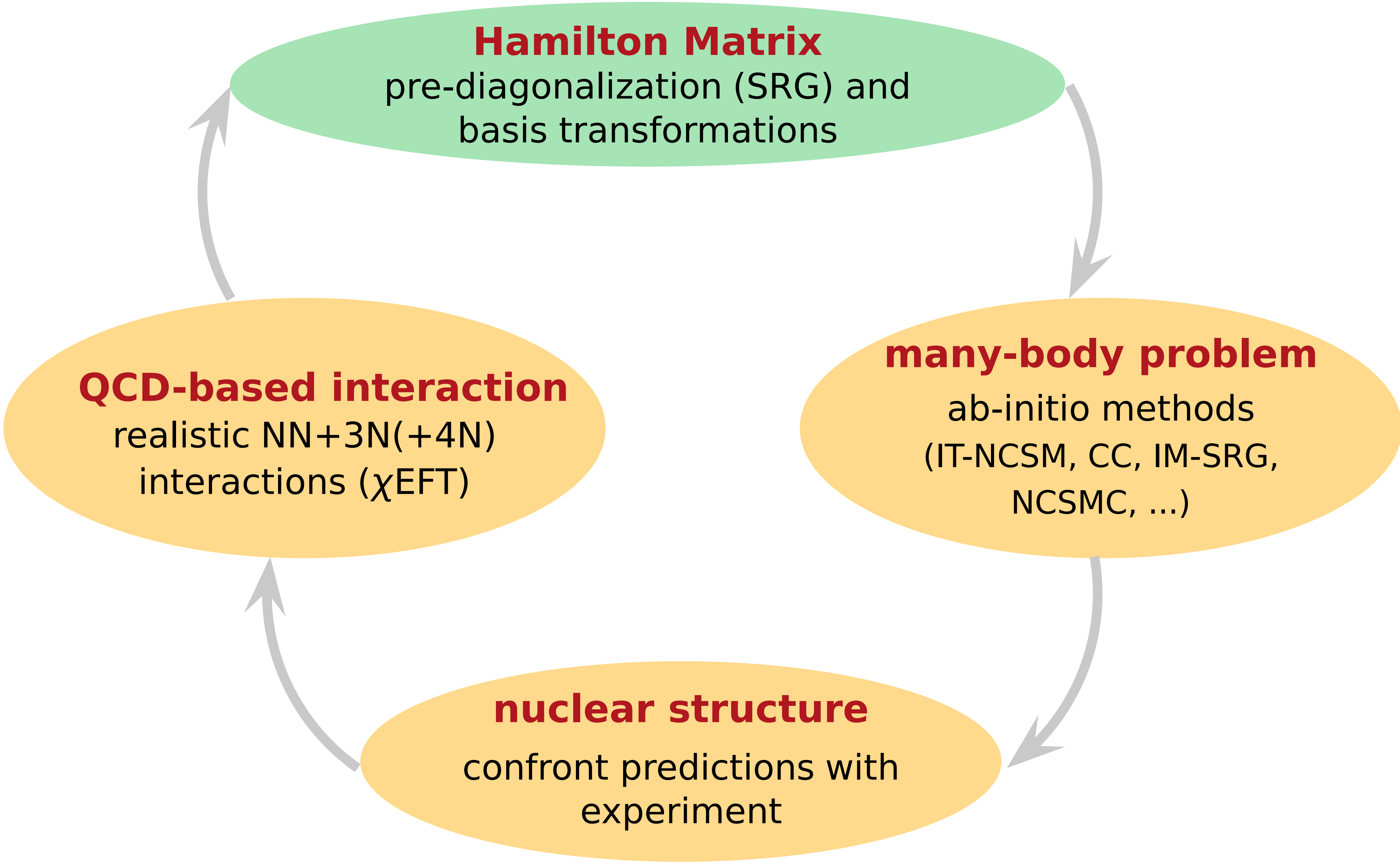
Introduction



Outline

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

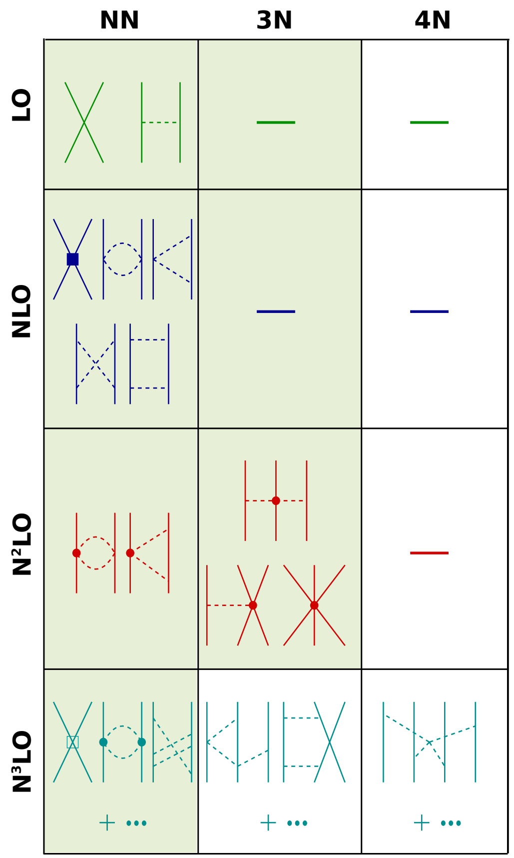
SRG for heavy nuclei
emphasize new challenges

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

Chiral NN+3N Interactions

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

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



next generation interactions

- consistent N^2LO interactions:
  - NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal
- consistent N^3LO interactions: talk by K. Hebeler
  - LENPIC collaboration
  - recently available
- optimized N^2LO interaction: talk by A. Ekström
  - NN: Ekström et al., 500 MeV cutoff, LECs fitted with POUNDerS

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

- continuous **unitary transformation** of the Hamiltonian

$$\widetilde{H}_\alpha = U_\alpha^\dagger H U_\alpha$$

- leads to **evolution equation**

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha] \quad \text{with} \quad \eta_\alpha = -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} = -\eta_\alpha^\dagger$$

initial value problem with $\widetilde{H}_{\alpha=0} = H$

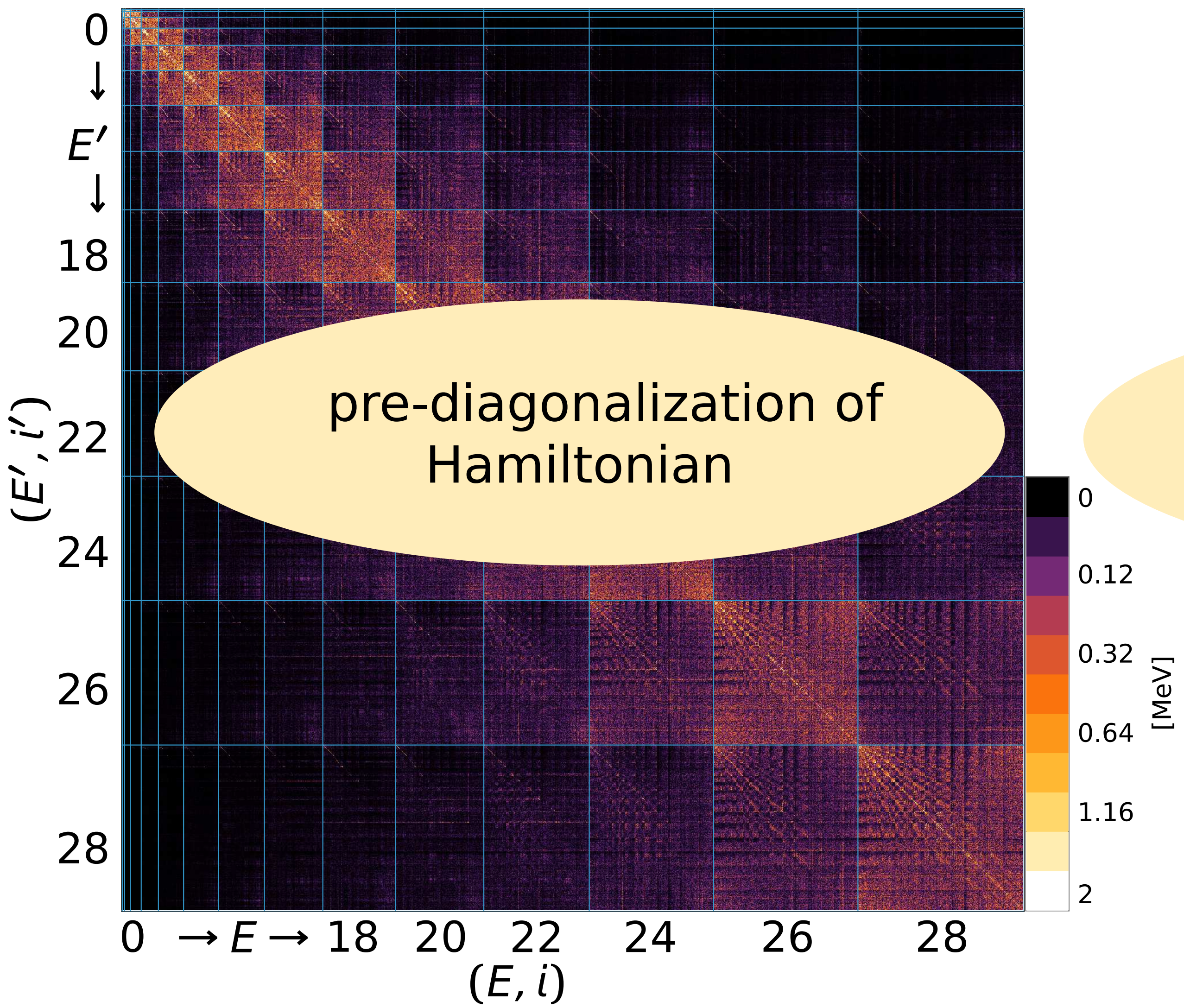
- choose **dynamic generator**

$$\eta_\alpha = (2\mu)^2 [T_{\text{int}}, \widetilde{H}_\alpha]$$

advantages of SRG:
simplicity and **flexibility**

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



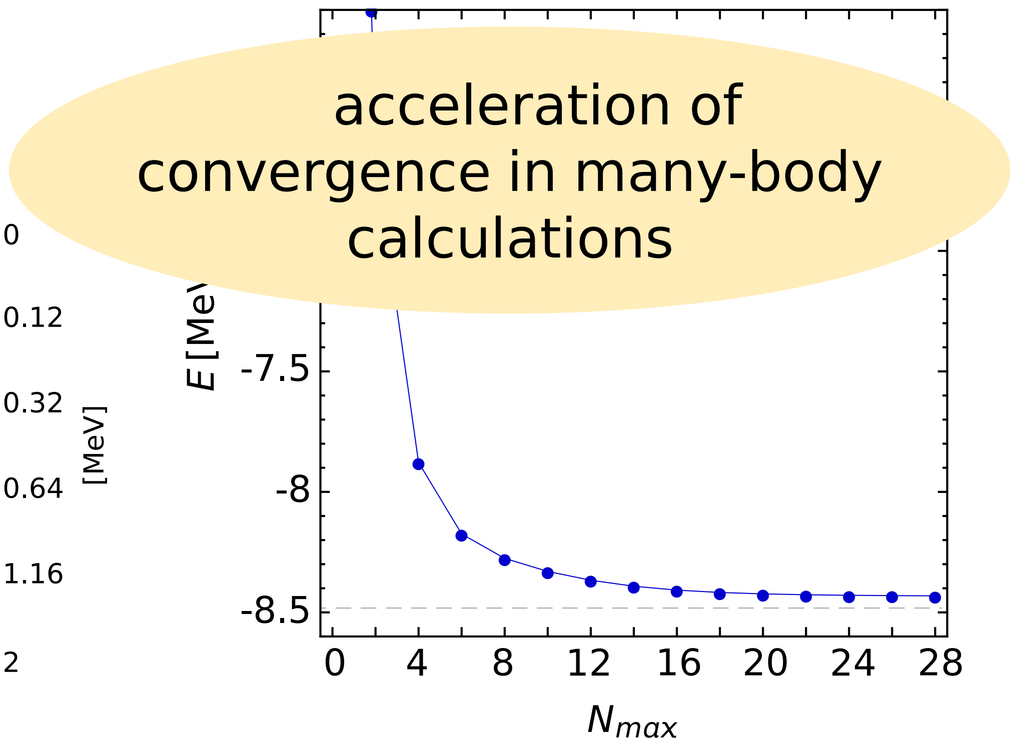
$\alpha = 1.28\,\mathrm{fm}^4$

$\lambda = 0.94\,\mathrm{fm}^{-1}$

$\langle E'i'JT | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | EiJT \rangle$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$

NCSM ground state ^{3}H



SRG Evolution in A-Body Space

- SRG induces **irreducible** many-body **contributions**

$$U_\alpha^\dagger H U_\alpha = \widetilde{H}_\alpha^{[2]} + \widetilde{H}_\alpha^{[3]} + \cdots + \widetilde{H}_\alpha^{[A]}$$

- restricted to SRG evolution in 2B or 3B space

- formal **violation of unitarity**

SRG-evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and evolve in two-body space

- **NN+3N$_{\text{ind}}$**: start with NN initial Hamiltonian and evolve in three-body space

- **NN+3N$_{\text{full}}$**: start with NN+3N initial Hamiltonian and evolve in three-body space

α-variation provides a **diagnostic tool** to assess the contributions of 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

(Importance Truncated) NCSM

No-Core Shell Model (NCSM)

- solve **eigenvalue problem**: $\boldsymbol{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$

- **model space**: spanned by m-scheme states $|\Phi_\nu\rangle$ with unperturbed excitation energy of up to $N_{\max}\hbar\Omega$

- **problem**: tremendous increase of model space with particle number A

Importance Truncated NCSM

- a priori determination of relevant basis states via first-order perturbati

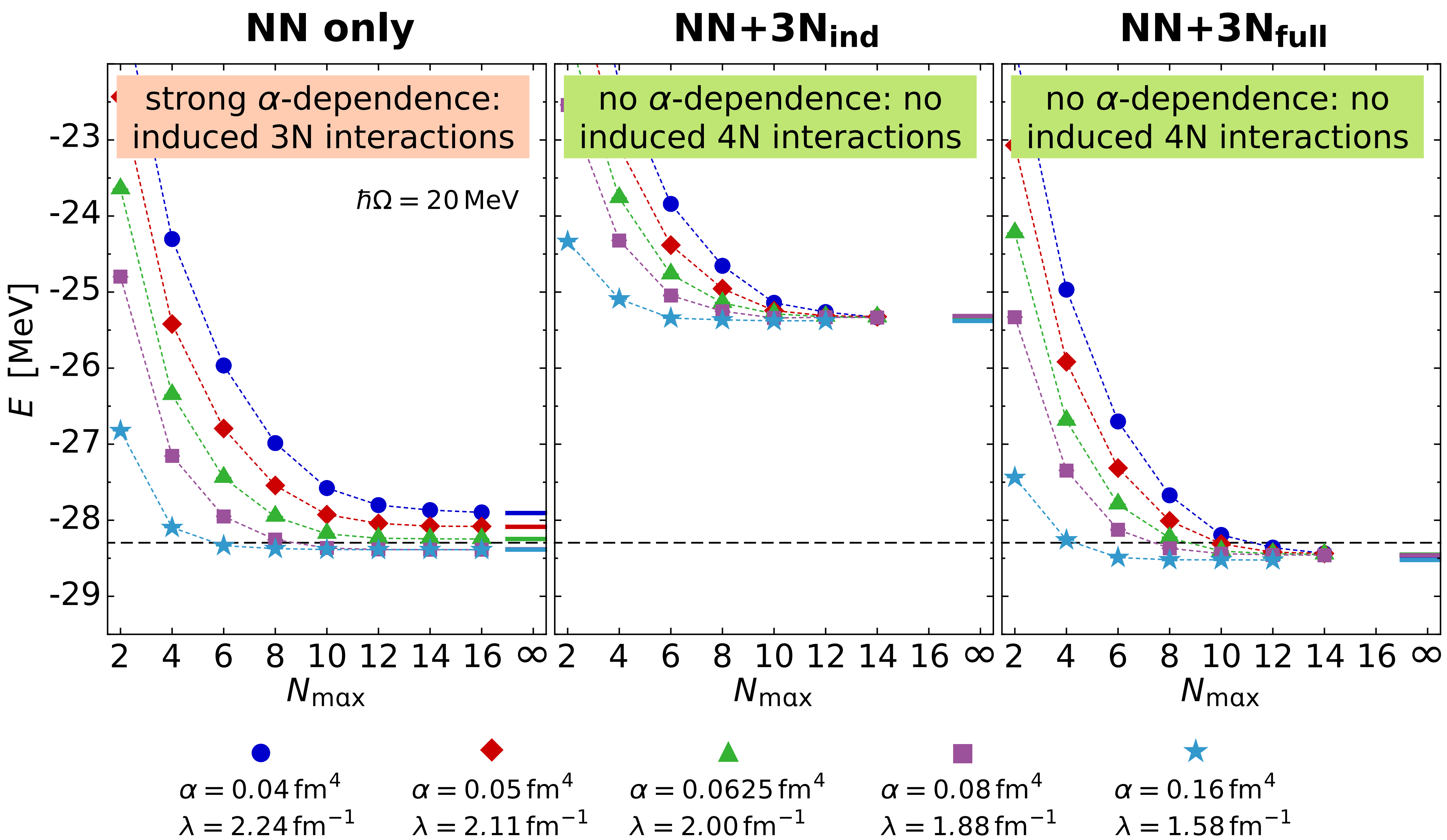
- IT-NCSM provides **same results** as the full NCSM keeping all its advantages

- expands **application range** to higher A

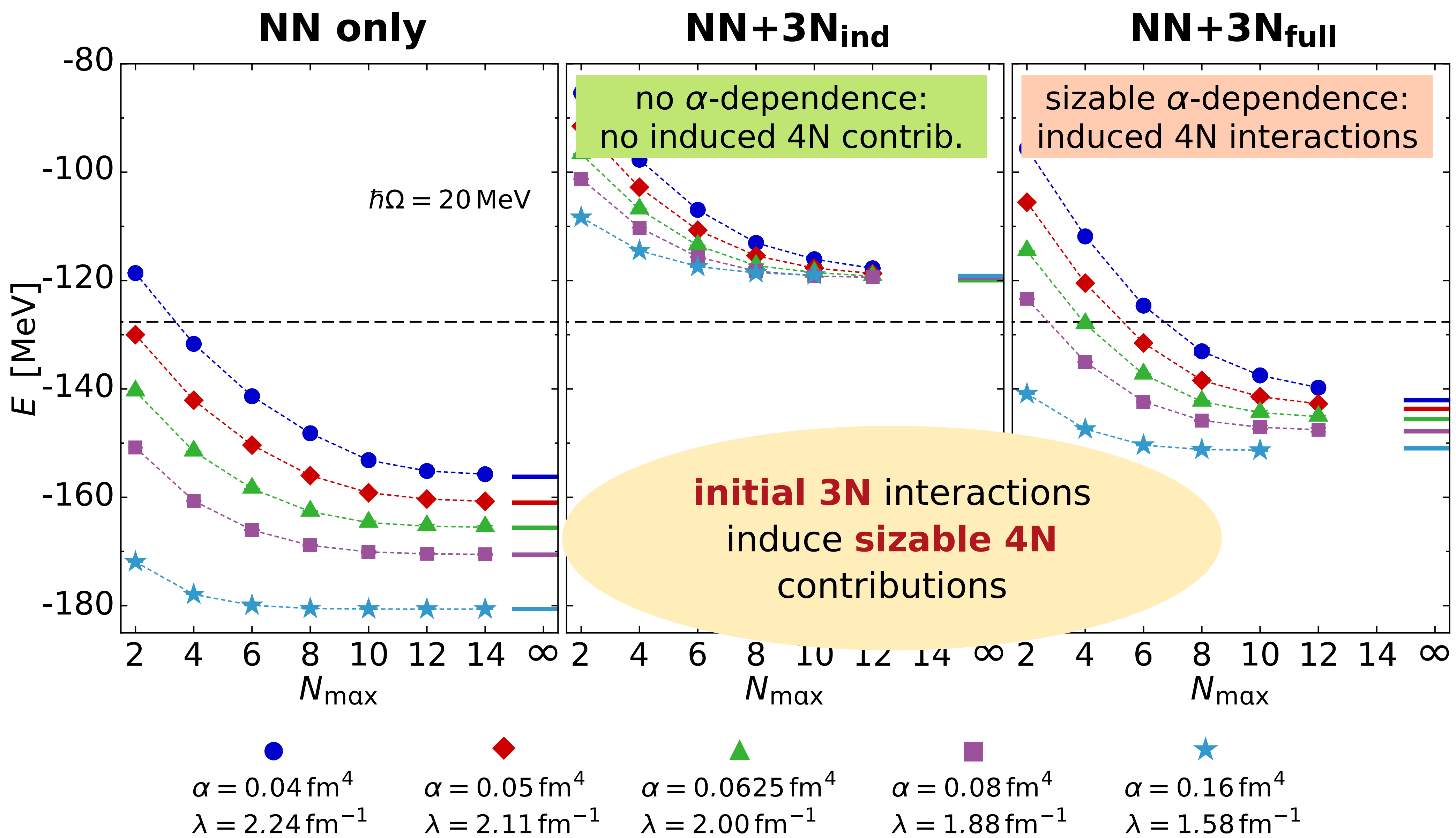
- **im** $_\nu| \geq \kappa_{\min}$

- **extrapolatio** configurations

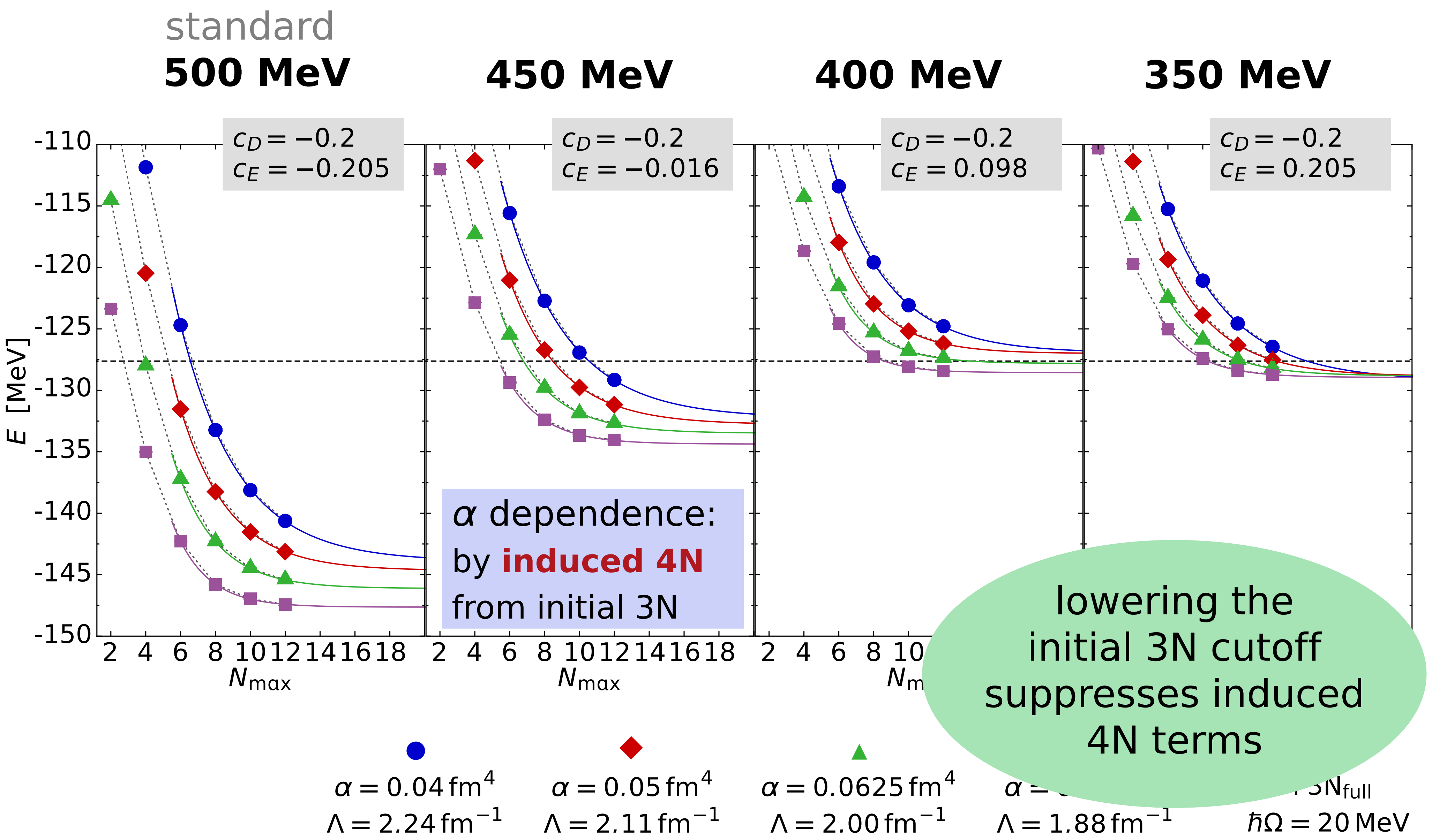
^{4}He: Ground-State Energies



^{16}O: Ground-State Energies



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



α dependence:
by **induced 4N**
from initial 3N

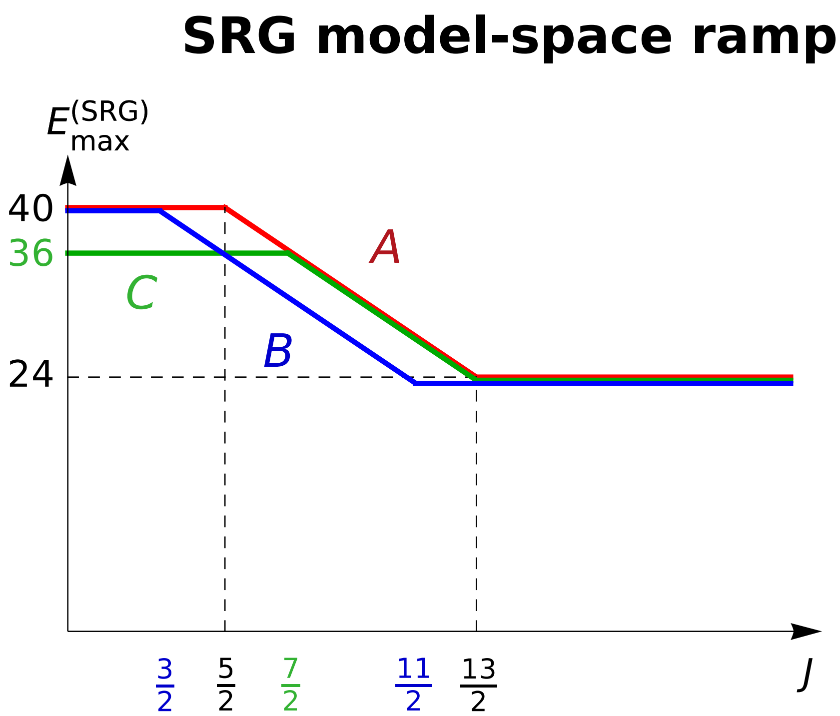
lowering the
initial 3N cutoff
suppresses induced
4N terms

SRG Model Space & Frequency Conversion

Roth, AC, Langhammer, Binder — arXiv:1311.3563

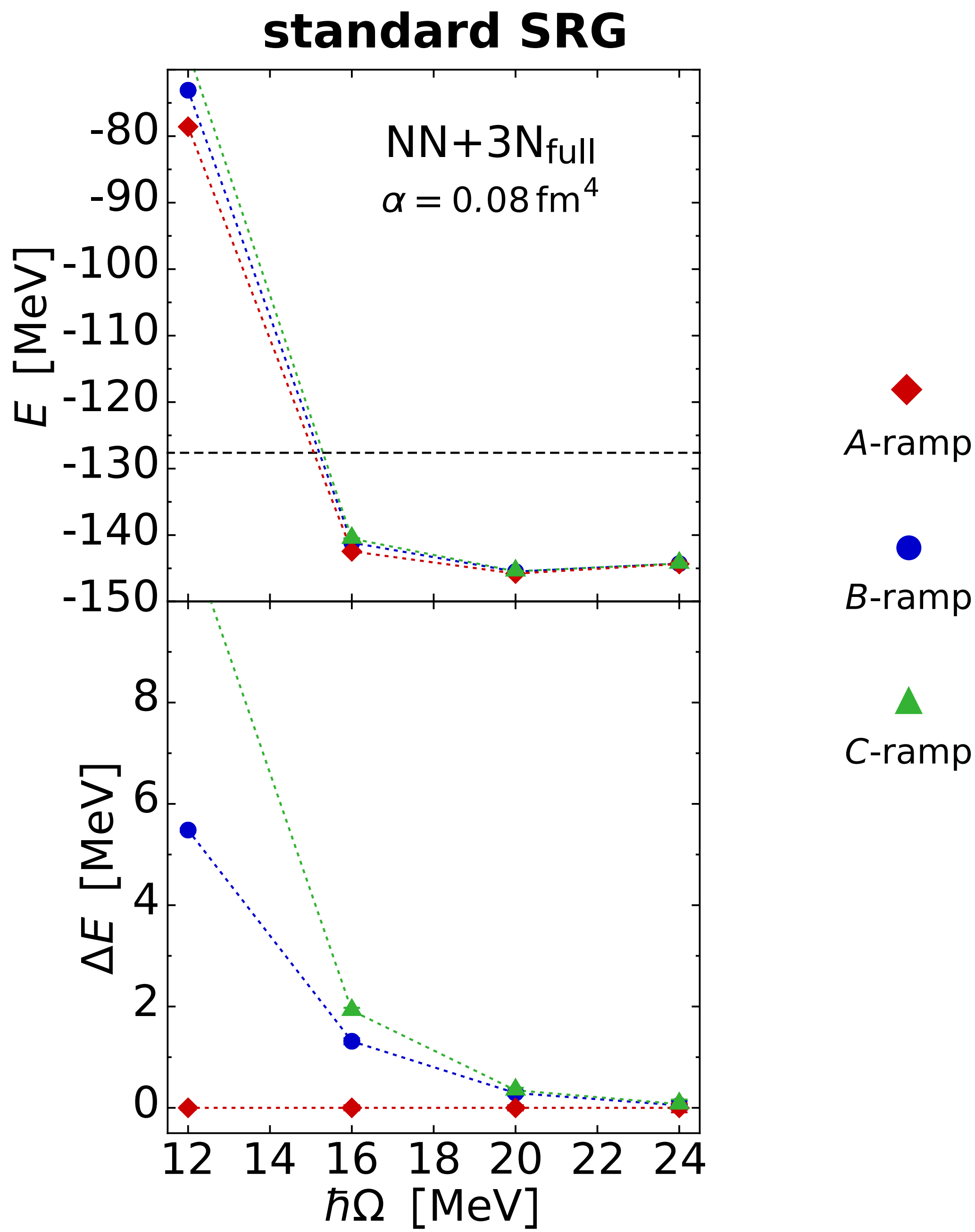
SRG Model Space

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



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

Frequency Conversion: ^{16}O Ground State

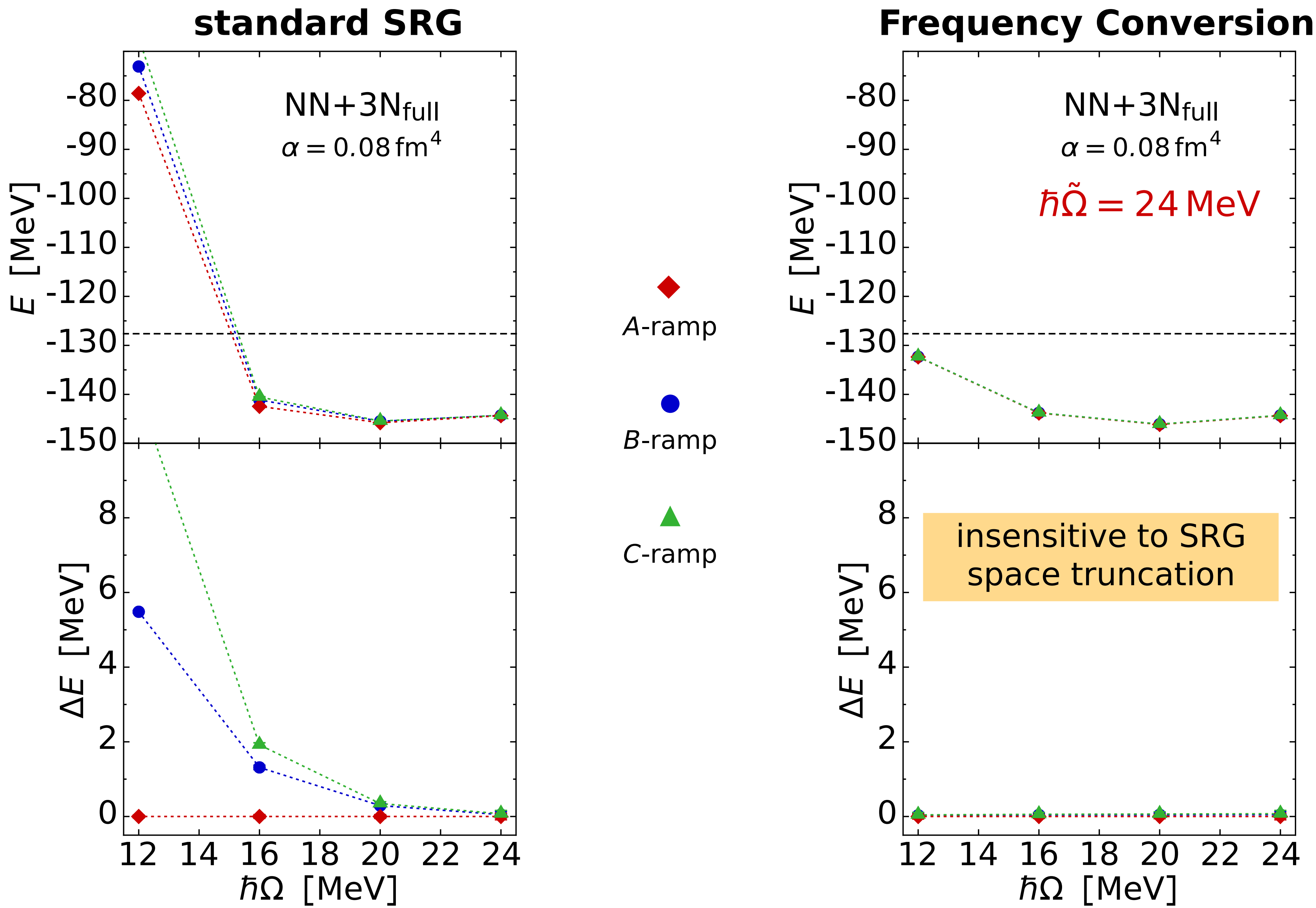


- physical content of SRG space depends on $\hbar\Omega$
- SRG space insufficient for **low $\hbar\Omega$**
  - in particular for increasing mass number

Idea:

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

Frequency Conversion: ^{16}O Ground State



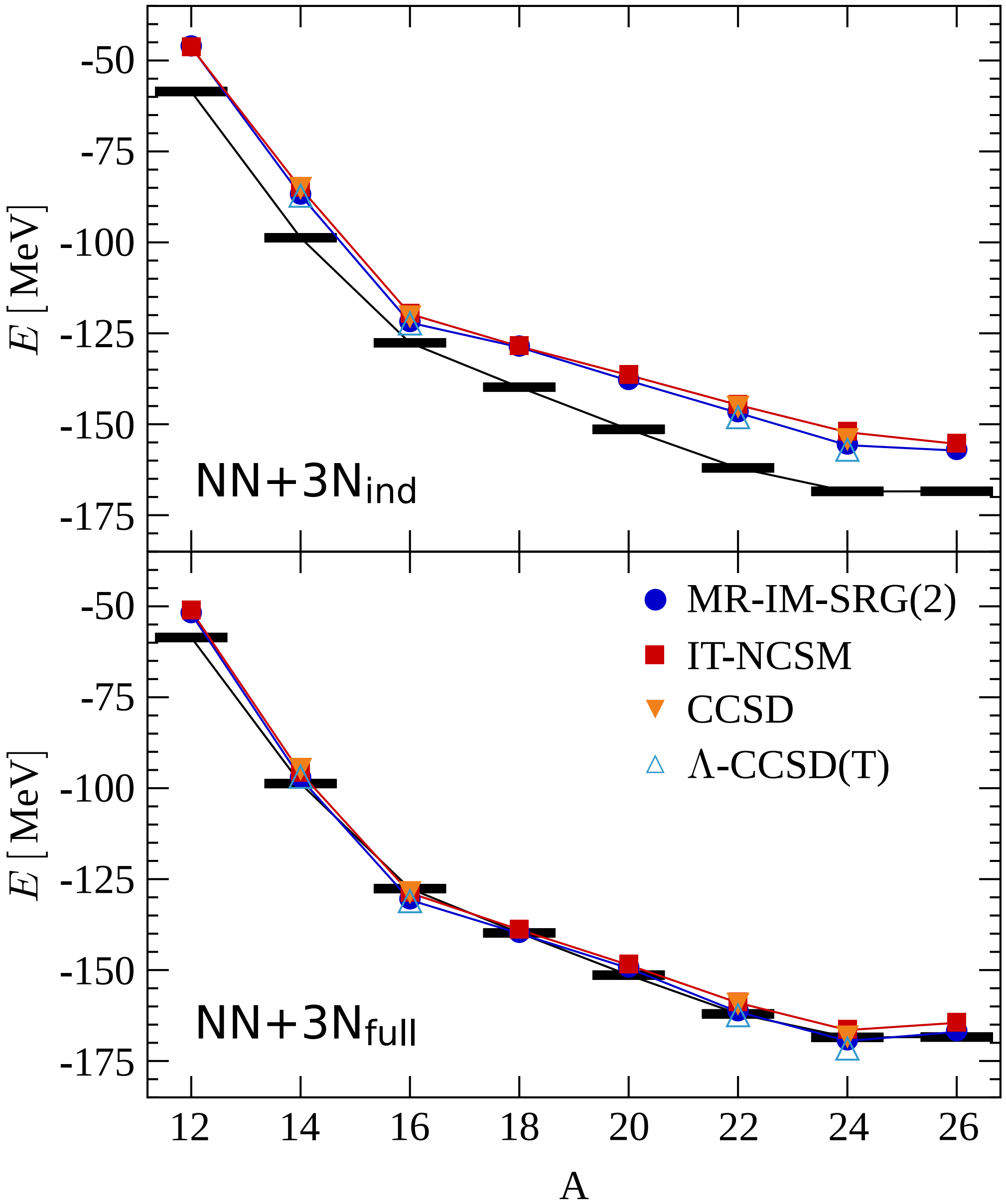
Medium-Mass and Heavy Nuclei with NN+3N Interactions

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)

Hergert, Binder, AC, Langhammer, Roth — Phys. Rev. Lett. 110, 242501 (2013)
Tsukiyama, Bogner, Schwenk — Phys. Rev. Lett. 106, 222502 (2011)

Oxygen Istopes

H. Hergert, S. Binder, AC, J. Langhammer, R. Roth   Phys. Rev. Lett. 110, 242501 (2013)

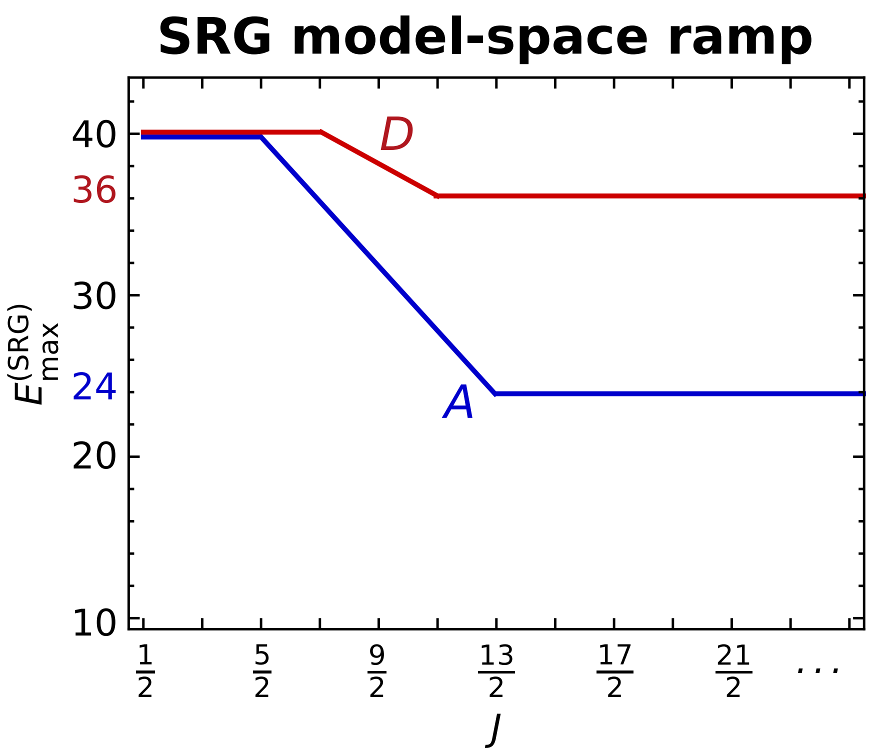


- investigate **effect of 3N** interactions
- **quantify uncertainties** of medium mass approaches
- access nuclei up to **driplines** with ab initio approaches

$\Lambda = 400\,\mathrm{MeV}$
optimal $\hbar\Omega$
$e_{max} = 14$
$E_{3\,max} = 14$

SRG Model Space for Heavy Nuclei

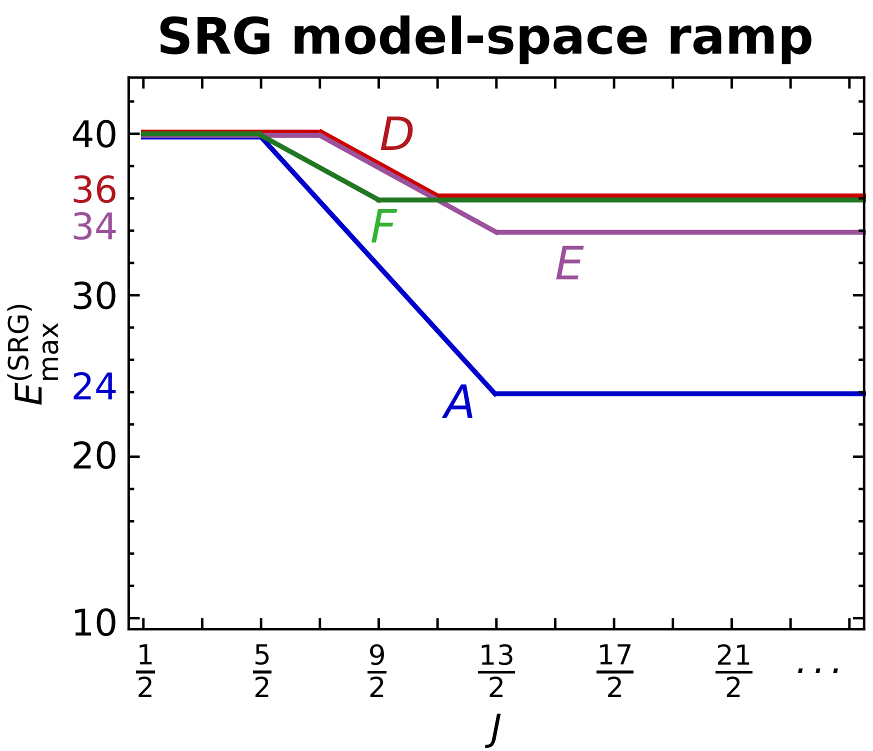
- studied **SRG space dependence** with several SRG ramps
  ⇒ **insufficient** model space for partial waves with $J > \frac{5}{2}$
- introduce extended SRG space D as **standard for heavy nuclei**



SRG space D much larger than model spaces in previous works

SRG Model Space for Heavy Nuclei

- studied **SRG space dependence** with several SRG ramps
  ⇒ **insufficient** model space for partial waves with $J > \frac{5}{2}$
- introduce extended SRG space D as **standard for heavy nuclei**
  - ramps E and F probe vital parts with large angular momenta



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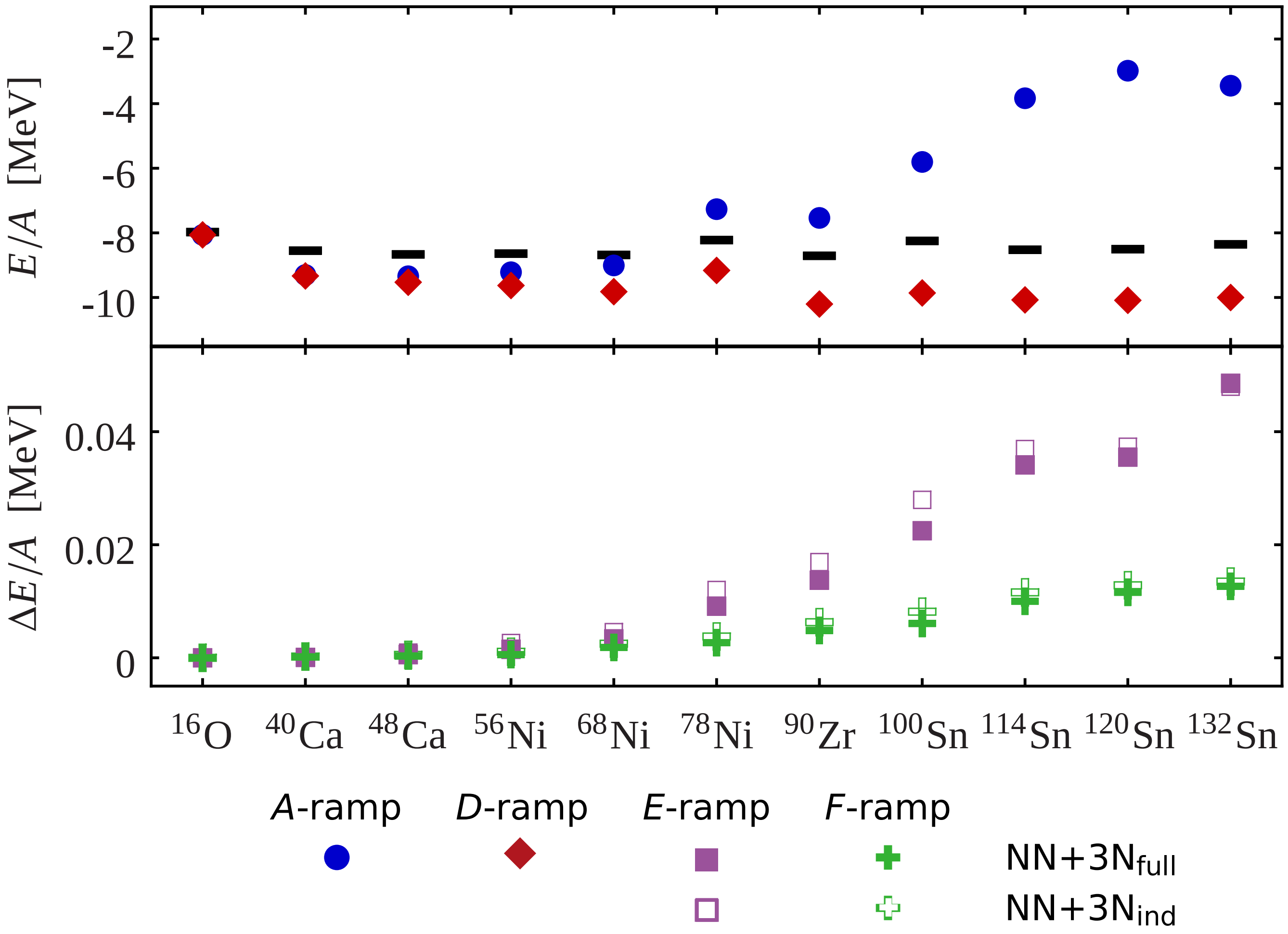
SRG Model Space for Heavy Nuclei



large angular momenta important for heavy mass nuclei

initial 3N have minor effect on SRG space dependence

CCSD

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

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

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

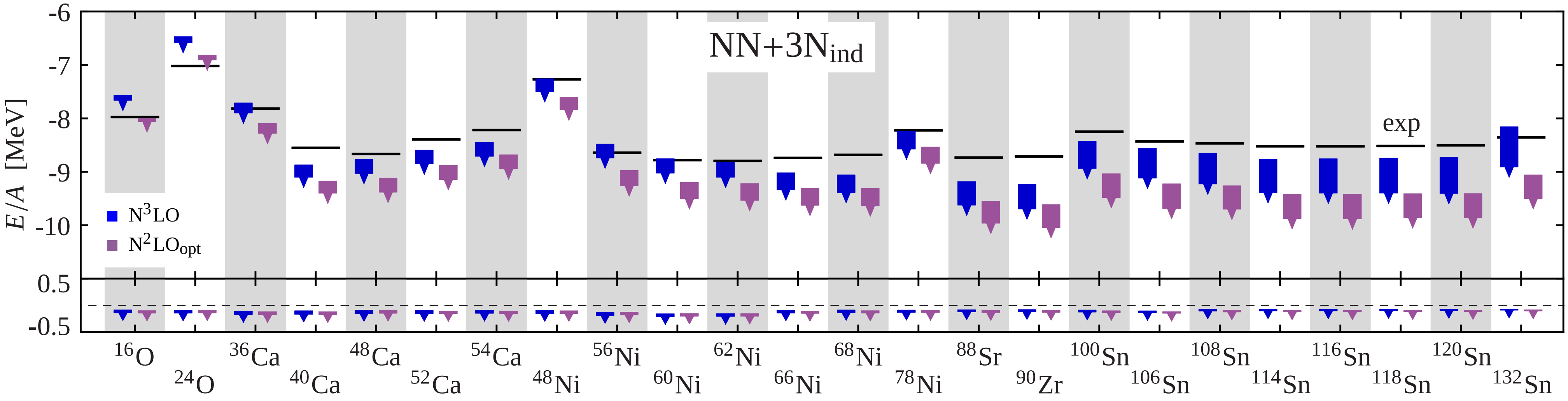
$\Lambda_{3N} = 400\,\mathrm{MeV}$

$E_{3max} = 14$

$e_{max}{=}12$

Heavy Mass 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)
$\hbar\tilde{\Omega} = 36\,\text{MeV}$
$\hbar\Omega = 24\,\text{MeV}$
$\alpha = 0.04 - 0.08\,\text{fm}^4$
$E_{3\text{max}} = 18$
$e_{\text{max}}=12$

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

initial 4N might be relevant as well

SRG in Four-Body Space

Induced Four-Body Contributions

observation
induced 4N of initial 3N become sizable during the 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

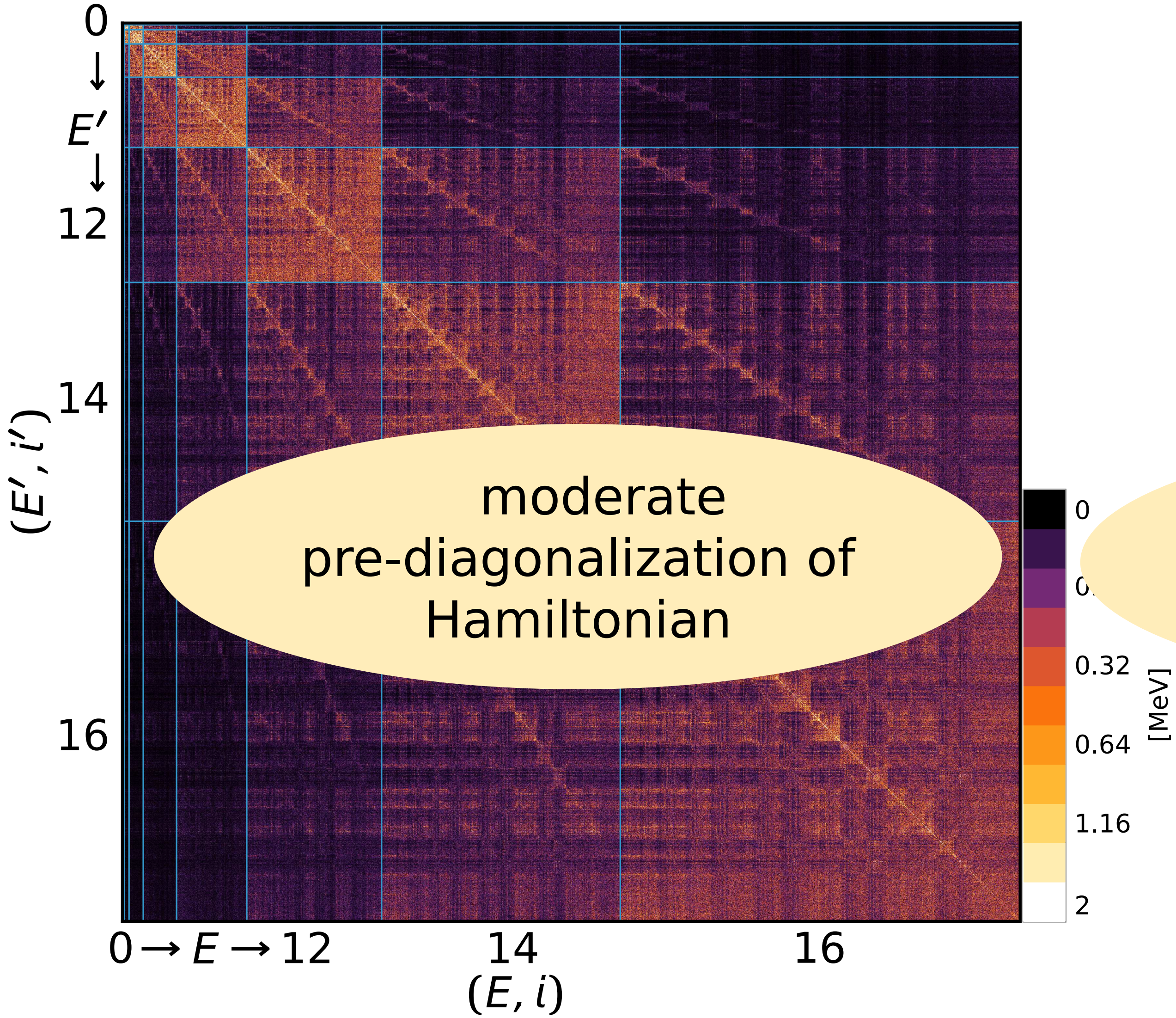
- so far **no better compromise** between induced 4N and convergence acceleration than with canonical generator

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

4B-Jacobi HO matrix elements



moderate pre-diagonalization of Hamiltonian

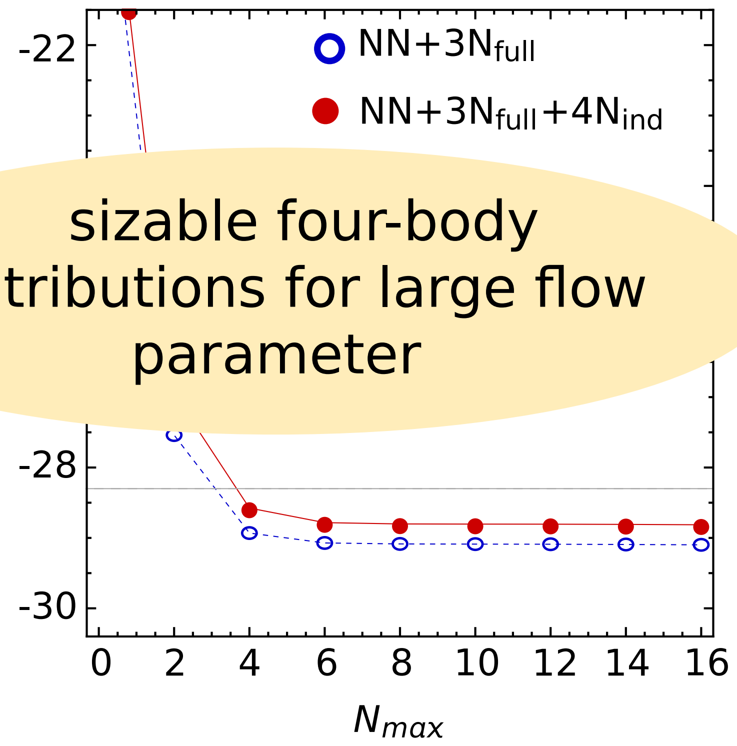
$\alpha = 1.28\,\mathrm{fm}^4$

$\lambda = 0.94\,\mathrm{fm}^{-1}$

$\langle E' i' J T | \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | E i J T \rangle$

$J^\pi = 0^+, T = 0, \hbar\Omega = 24\,\mathrm{MeV}$

NCSM ground state ^{4}He

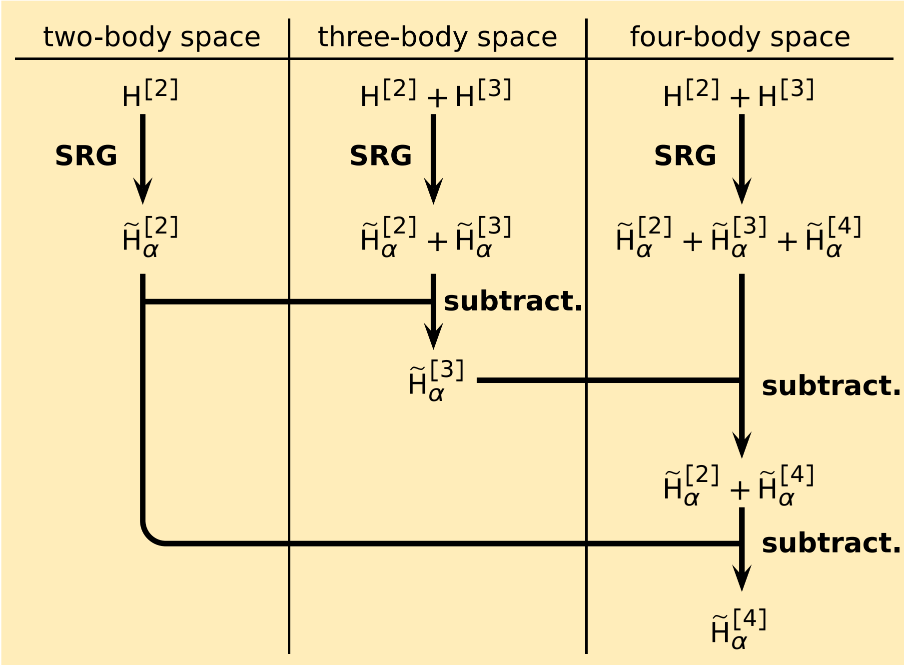


sizable four-body contributions for large flow parameter

SRG Model Space & Subtraction Schemes

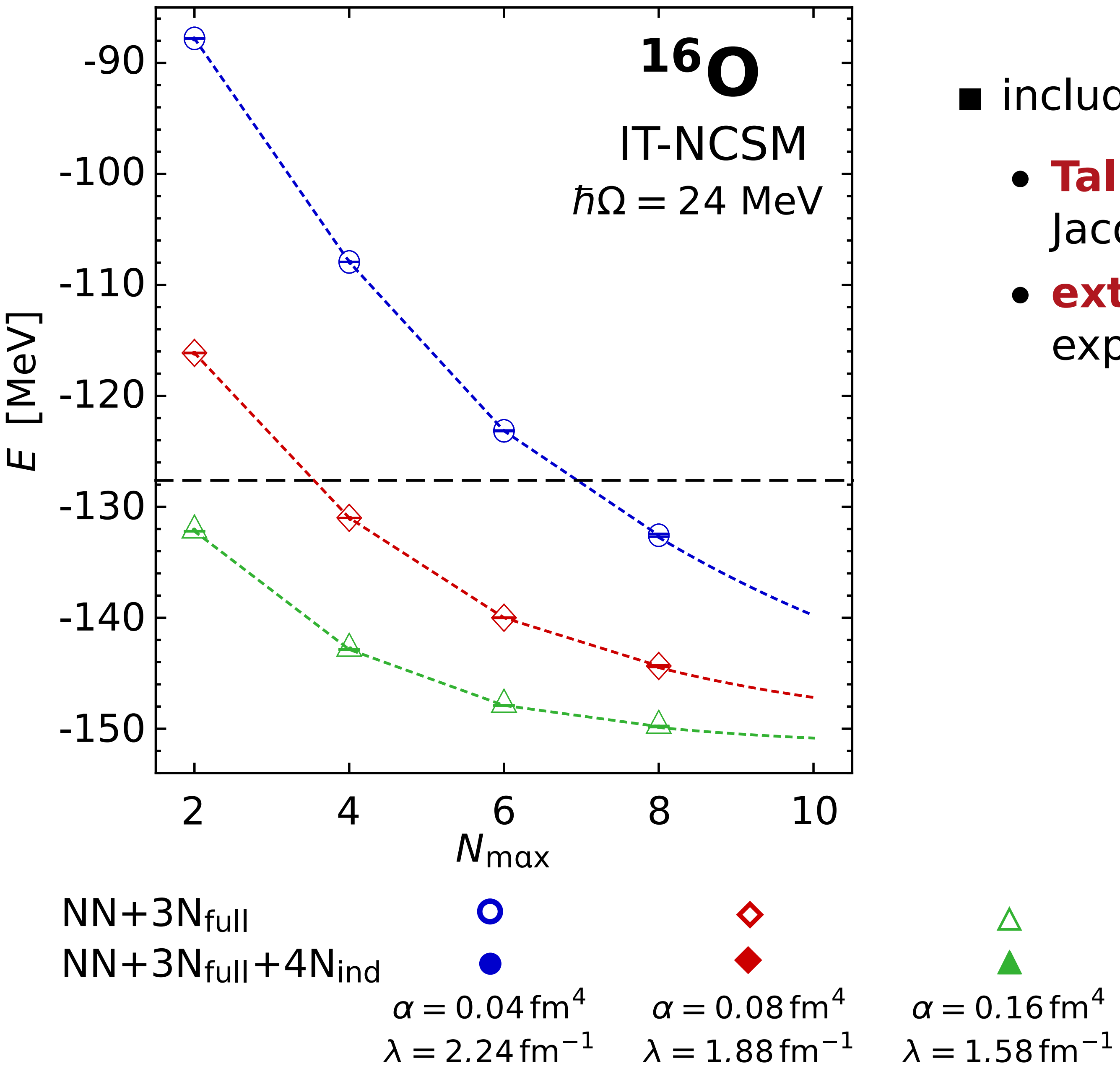
SRG for *A*-body calculations

- **require** irreducible **2N, 3N, and 4N** contributions **separately**
- subtract irreducible contributions
  - must be evolved consistently
- SRG model space truncated by $E_{max}^{(SRG)}$
  - **truncation different** for two-, three-, or four-body space
  - **no unique subtraction** scheme



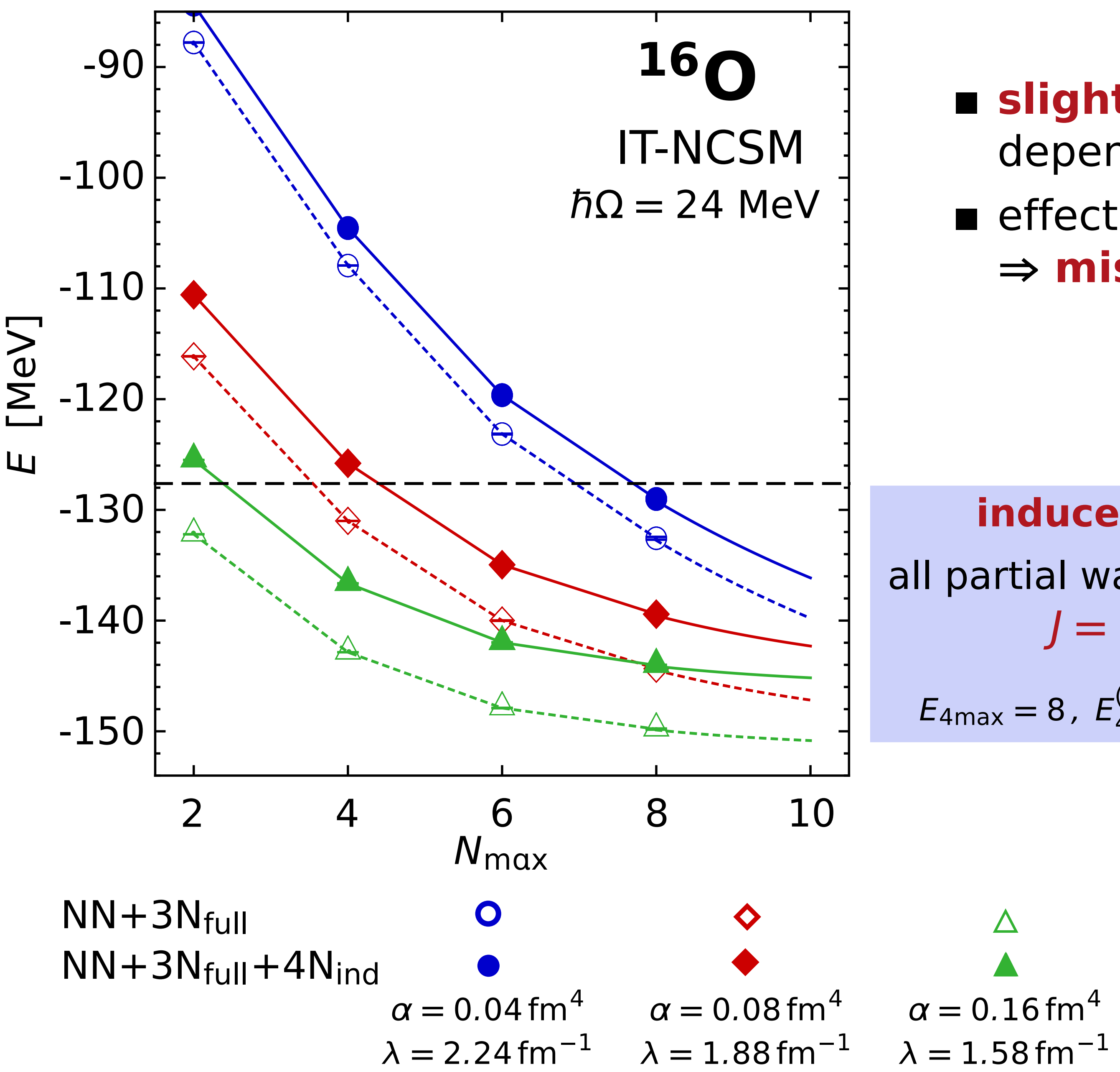
for $E_{max}^{(SRG)} \to \infty$ subtraction schemes are **equivalent**

IT-NCSM with Four-Body Contributions



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

IT-NCSM with Four-Body Contributions



- **slightly reduced** flow-parameter dependence
- effect to small
  ⇒ **missing 4N** contributions

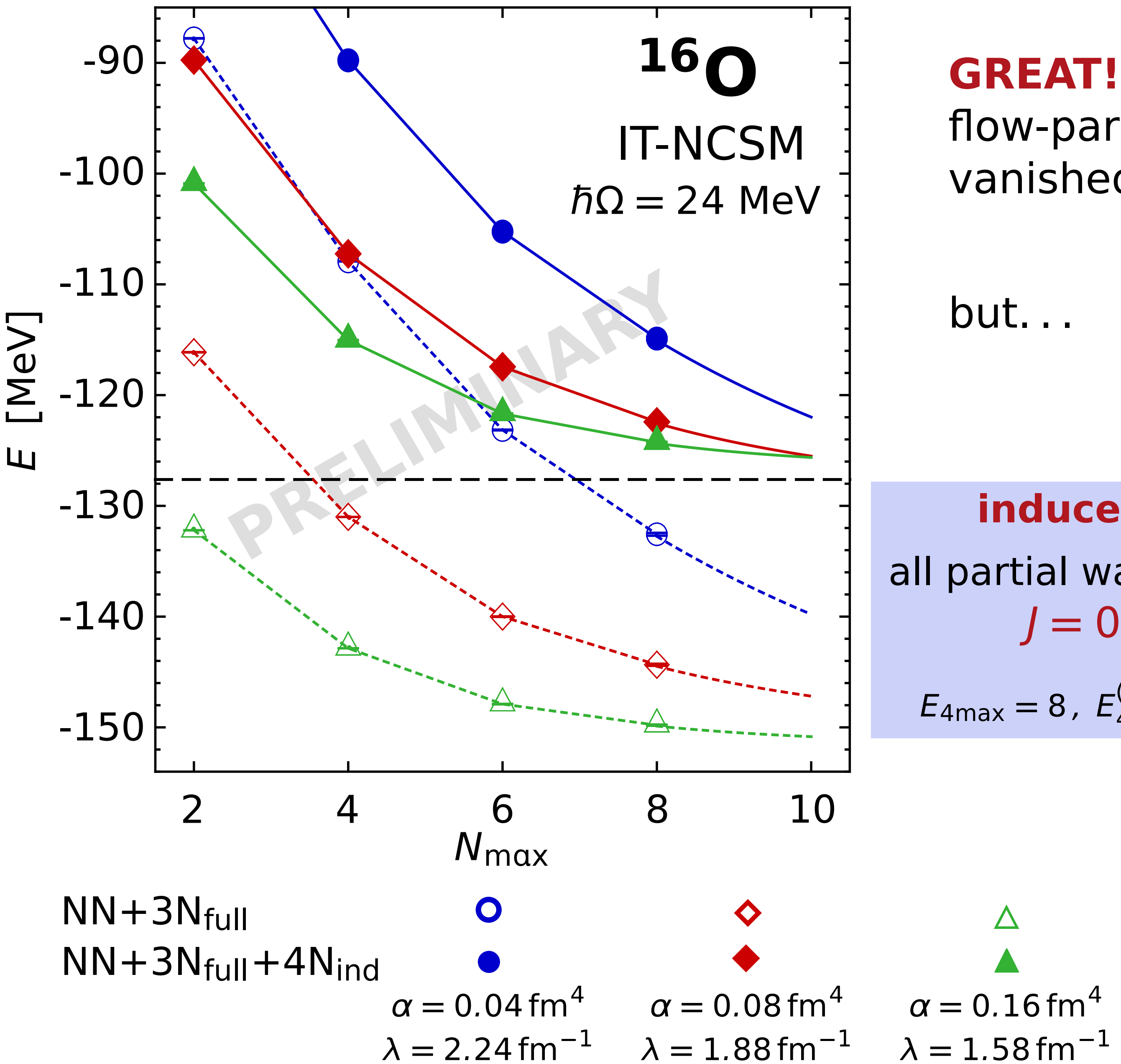
induced 4N

all partial waves with

$J = 0$

$E_{4max} = 8\,,\; E_{4max}^{(SRG)} = 19$

IT-NCSM with Four-Body Contributions



GREAT!
flow-parameter dependence almost vanished

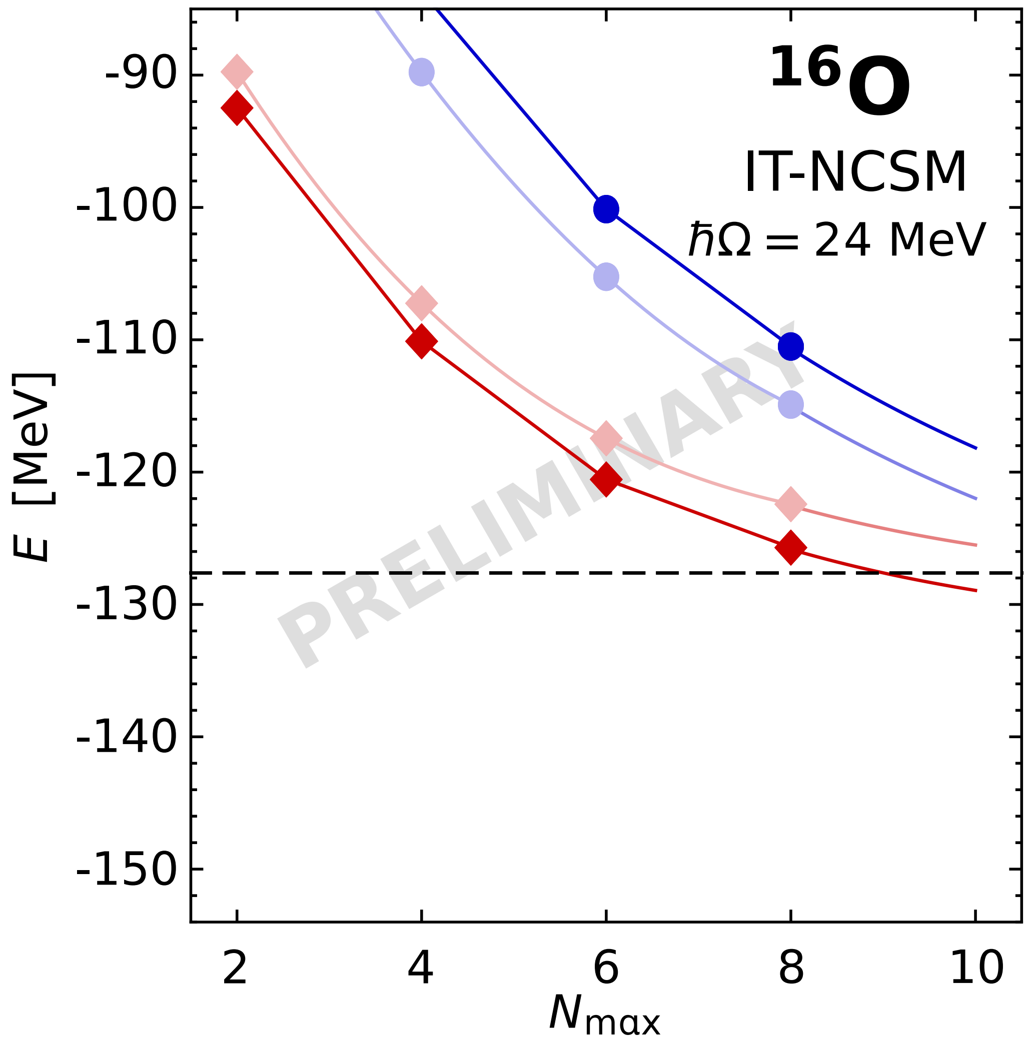
but. . .

induced 4N

all partial waves with $J = 0, 1$

$E_{4\mathrm{max}} = 8\,,\; E^{(\mathrm{SRG})}_{4\mathrm{max}} = 19$

IT-NCSM with Four-Body Contributions



- 4N channels with $J = 1$ require huge SRG spaces
- not yet converged

induced 4N

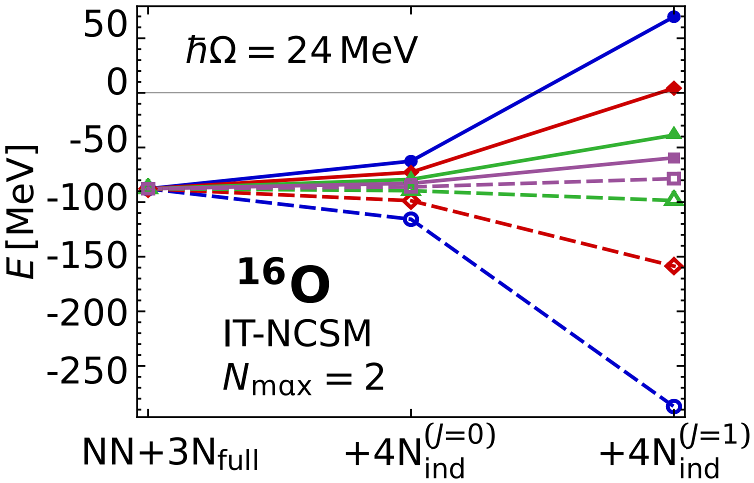
all partial waves with

$J = 0, 1$

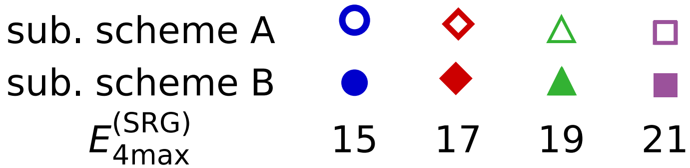
$E_{4max} = 8\,,\ E_{4max}^{(SRG)} = \mathbf{21}$

NN+3N$_{full}$	○	◇	△
NN+3N$_{full}$+4N$_{ind}$	●	◆	▲
	$\alpha = 0.04\,\text{fm}^4$ $\lambda = 2.24\,\text{fm}^{-1}$	$\alpha = 0.08\,\text{fm}^4$ $\lambda = 1.88\,\text{fm}^{-1}$	$\alpha = 0.16\,\text{fm}^4$ $\lambda = 1.58\,\text{fm}^{-1}$

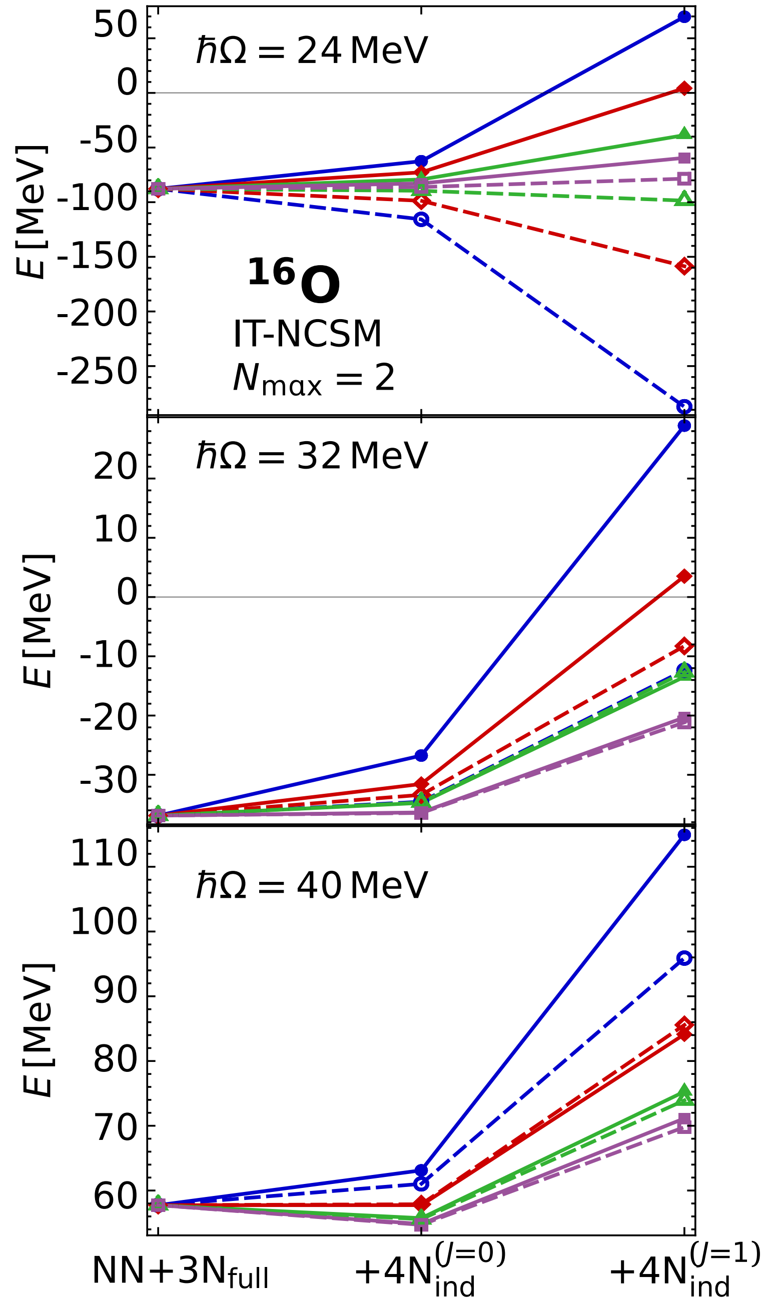
SRG Model Space & Subtraction Schemes



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



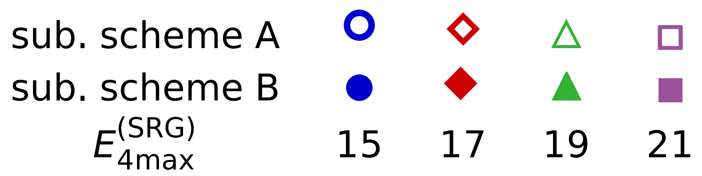
SRG Model Space & Subtraction Schemes



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

- improved convergence for large frequencies

in progress:
frequency conversion to evolve $J = 1$ contributions accurately



Conclusions

Conclusions

- **SRG** evolution in **HO basis** efficient and **improvable**
  - increased SRG space and frequency conversion
- **heavy mass nuclei** provides **challenges** for SRG
  - large angular momenta and induced 4N contributions important
  - improvements necessary already for initial NN
- **consistent four-body** SRG evolution
  - inclusion of induced and initial 4N contributions
  - $J = 1$ contributions crucial and require huge SRG spaces
- machinery ready to use **3N @ N^3LO** in momentum Jacobi basis
  - directly applicable in IT-NCSM, CC, IM-SRG, NCSMC,...

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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Low-Energy Nuclear Physics International Collaboration

SFB 634

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COMPUTING TIME