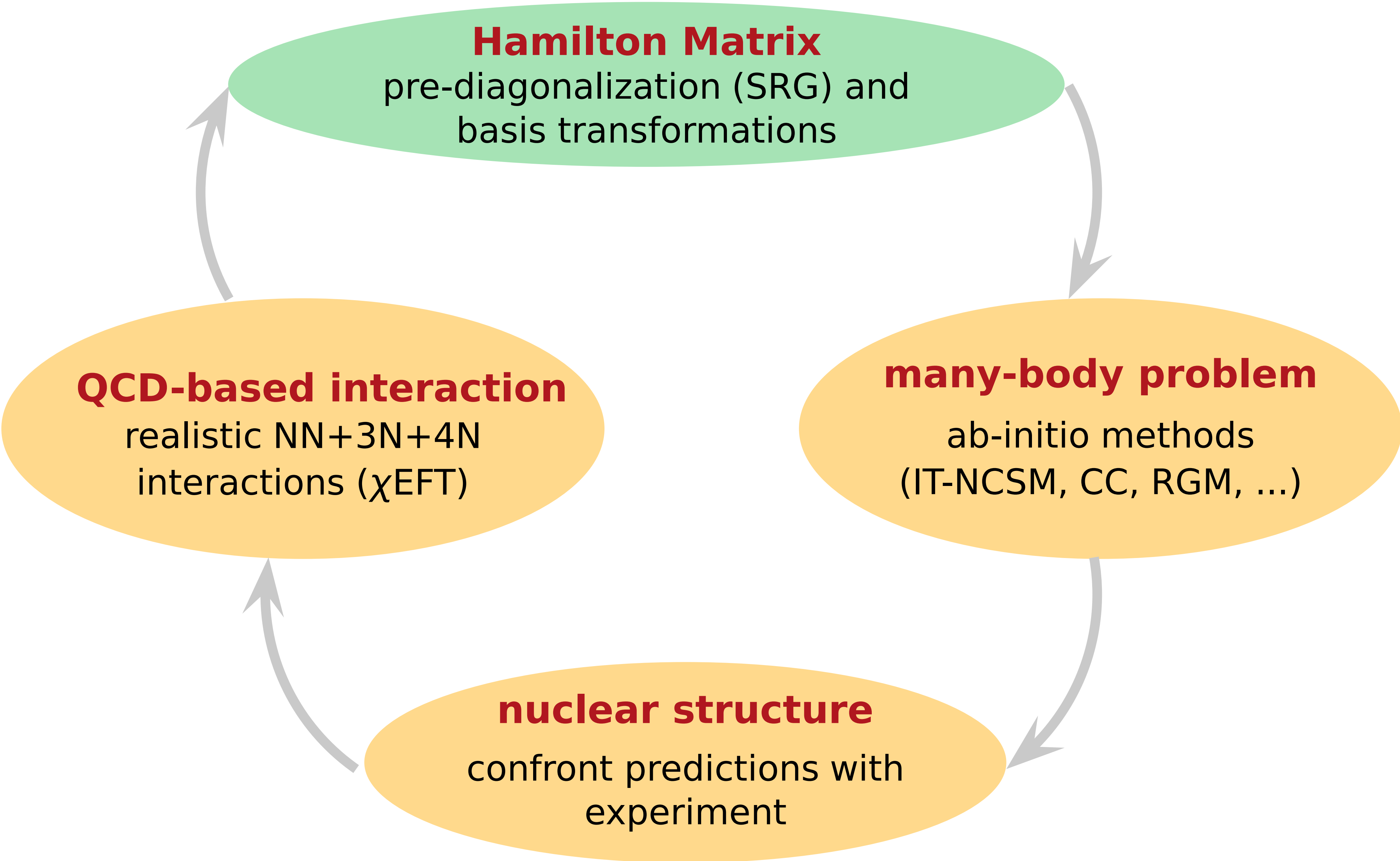
Similarity Renormalization Group and Next Generation Chiral Interactions

Angelo Calci
Institut für Kernphysik

TECHNISCHE UNIVERSITÄT DARMSTADT

Introduction



New Directions

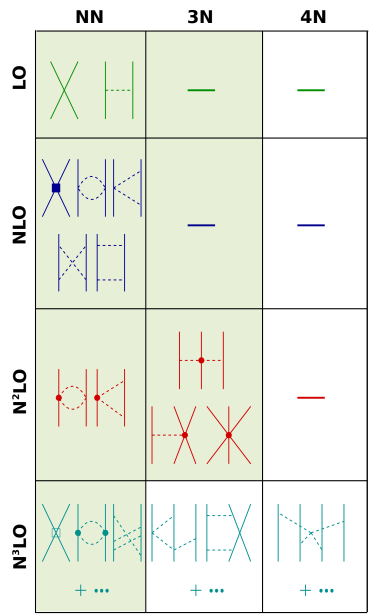
Probe Next-Generation Chiral Potentials
in ab-initio nuclear structure calculations

Frequency Conversion
extends SRG in HO Base to lower HO frequencies

SRG in 4B Space
treatment of induced & 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

Next Generation Interactions

- **consistent N^2LO Interactions:**
  - NN N^2LO: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N N^2LO: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal
- **consistent N^3LO Interactions:**
  - LENPIC-project
  - coming soon. . .
- **optimized N^2LO Interaction:**
  - NN N^2LO: Ekström et al., 500 MeV cutoff, LECs fittet with POUNDerS
  - 3N N^2LO: Navrátil, local, 500MeV cutoff, fitted to Triton

Similarity Renormalization Group in Three-Body Space

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

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**

Three-Body Jacobi Basis

- "**relative coordinates**" for 3-body system

$$\vec{\xi}_0 = \sqrt{\frac{1}{3}}\,[\vec{r}_a + \vec{r}_b + \vec{r}_c] \qquad \vec{\xi}_1 = \sqrt{\frac{1}{2}}\,[\vec{r}_a - \vec{r}_b] \qquad \vec{\xi}_2 = \sqrt{\frac{2}{3}}\left[\frac{1}{2}(\vec{r}_a + \vec{r}_b) - \vec{r}_c\right]$$

- harmonic-oscillator (HO) Jacobi basis
  - antisymmetric under $1 \longleftrightarrow 2$:

$$|\alpha\rangle = |[(N_1L_1, S_1)J_1, (N_2L_2, S_2)J_2]JM_J, (T_1, T_2)TM_T\rangle$$

  - completely antisymmetric:

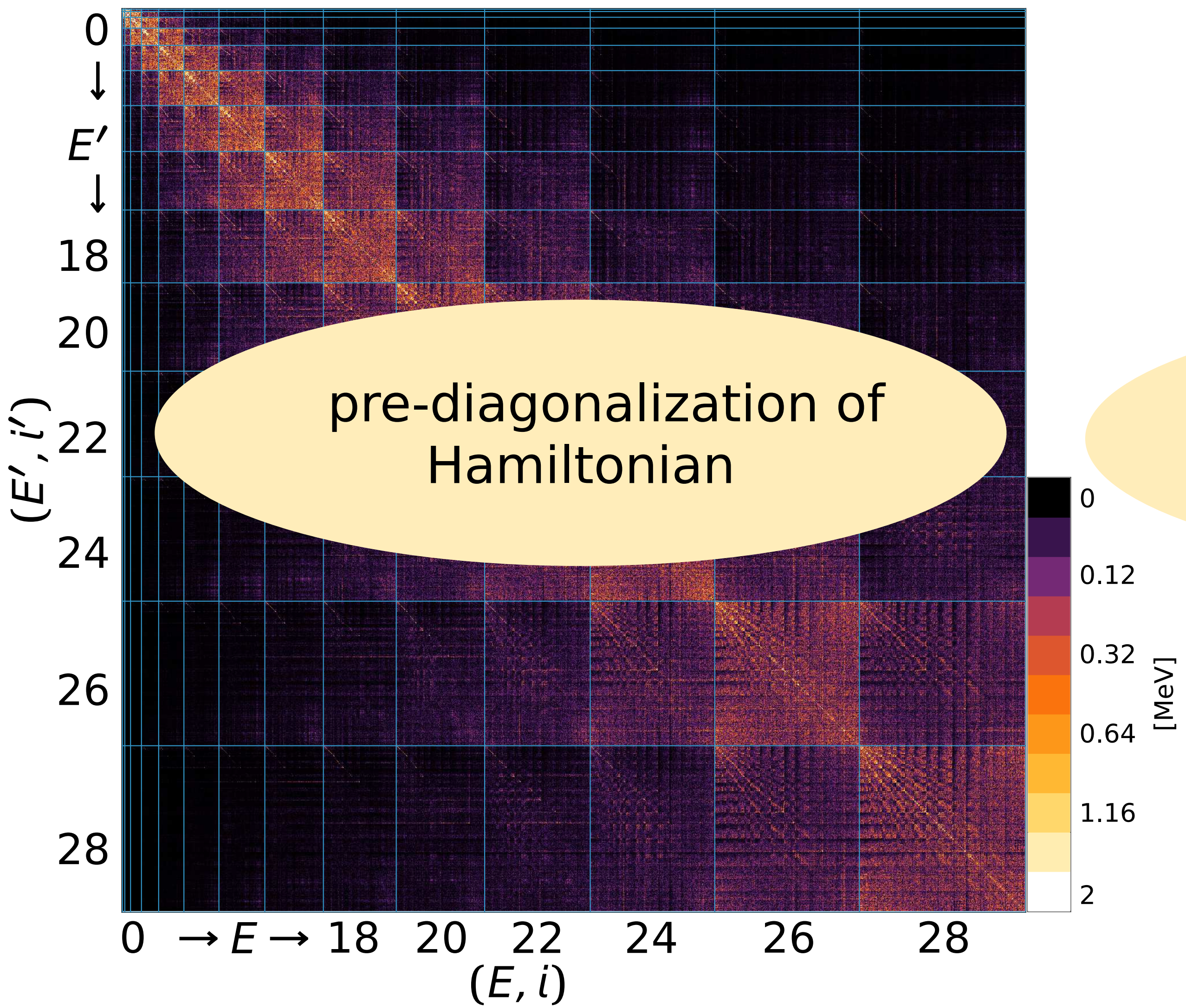
$$|EiJM_JTM_T\rangle = \sum_\alpha c_{\alpha,i}\,|\alpha\rangle$$

$$c_{\alpha,i} = \langle EiJM_JTM_T|\alpha\rangle$$

coefficients of fractional parentage (CFPs) by P. Navrátil

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



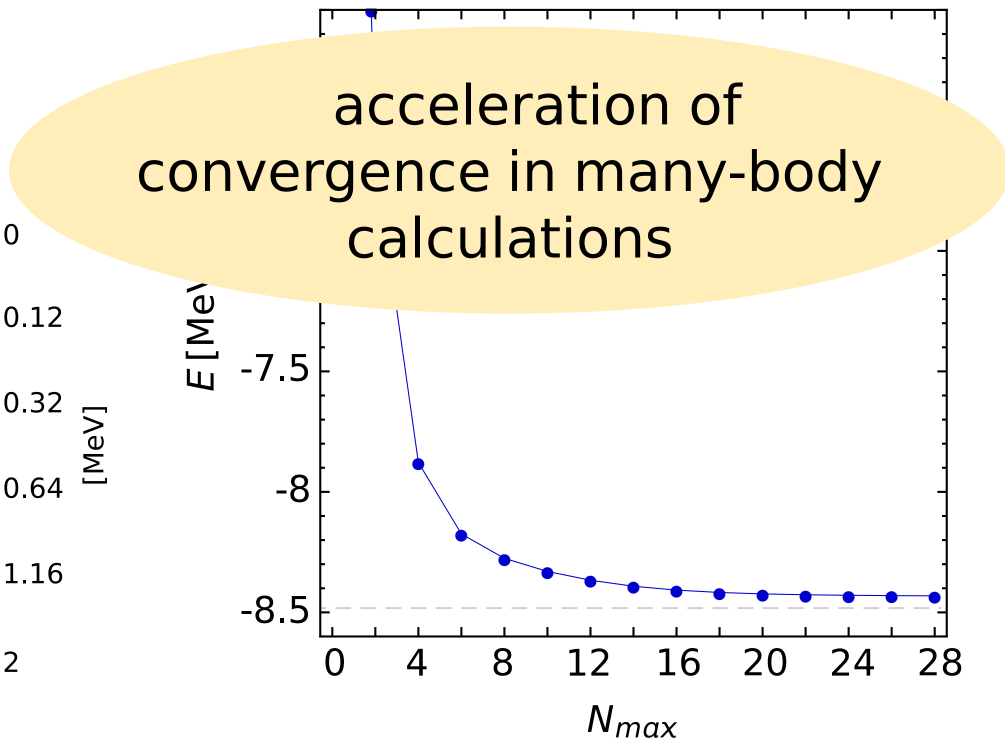
$\alpha = 1.28\,\mathrm{fm}^4$

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

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

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

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-induced**: start with NN initial Hamiltonian and evolve in three-body space
- **NN+3N-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

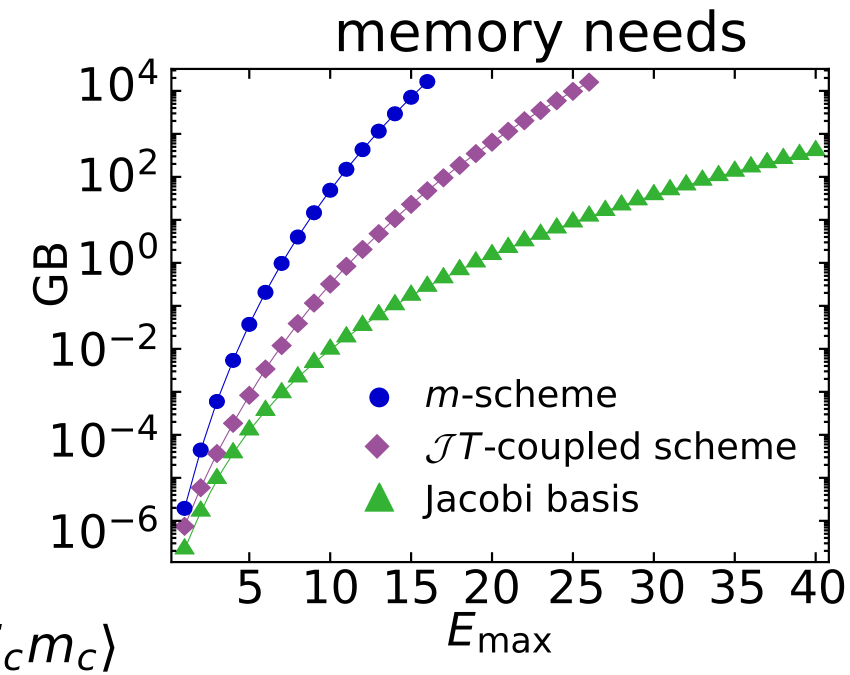
key to efficient NCSM calculations up to $N_{max} = 14$ for p-shell nuclei

decoupling on the fly

ab-initio many-body calculation

HO Basis Sets

- Jacobi basis
  - no center of mass part
  - TJP-channel separate
  - moderate memory needs
  - **ideal basis for SRG**



- *m*-scheme

  $$|(n_a l_a, s_a) j_a m_a, (n_b l_b, s_b) j_b m_b, (n_c l_c, s_c) j_c m_c\rangle$$

  - enormous memory needs
  - **necessary** for ab-initio NCSM calculations

- $\mathcal{J}T$-coupled scheme

  $$|\{[(n_a l_a, s_a) j_a, (n_b l_b, s_b) j_b] j_{ab}, (n_c l_c, s_c) j_c\} \mathcal{J} \mathcal{M}\rangle$$

  - Hamiltonian connects only **equal $\mathcal{J}$ and T** (memory needs decreases)
  - decoupling **on the fly**

(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 of NCSM
enormous increase of model space with particle number A and $N_{\max}$

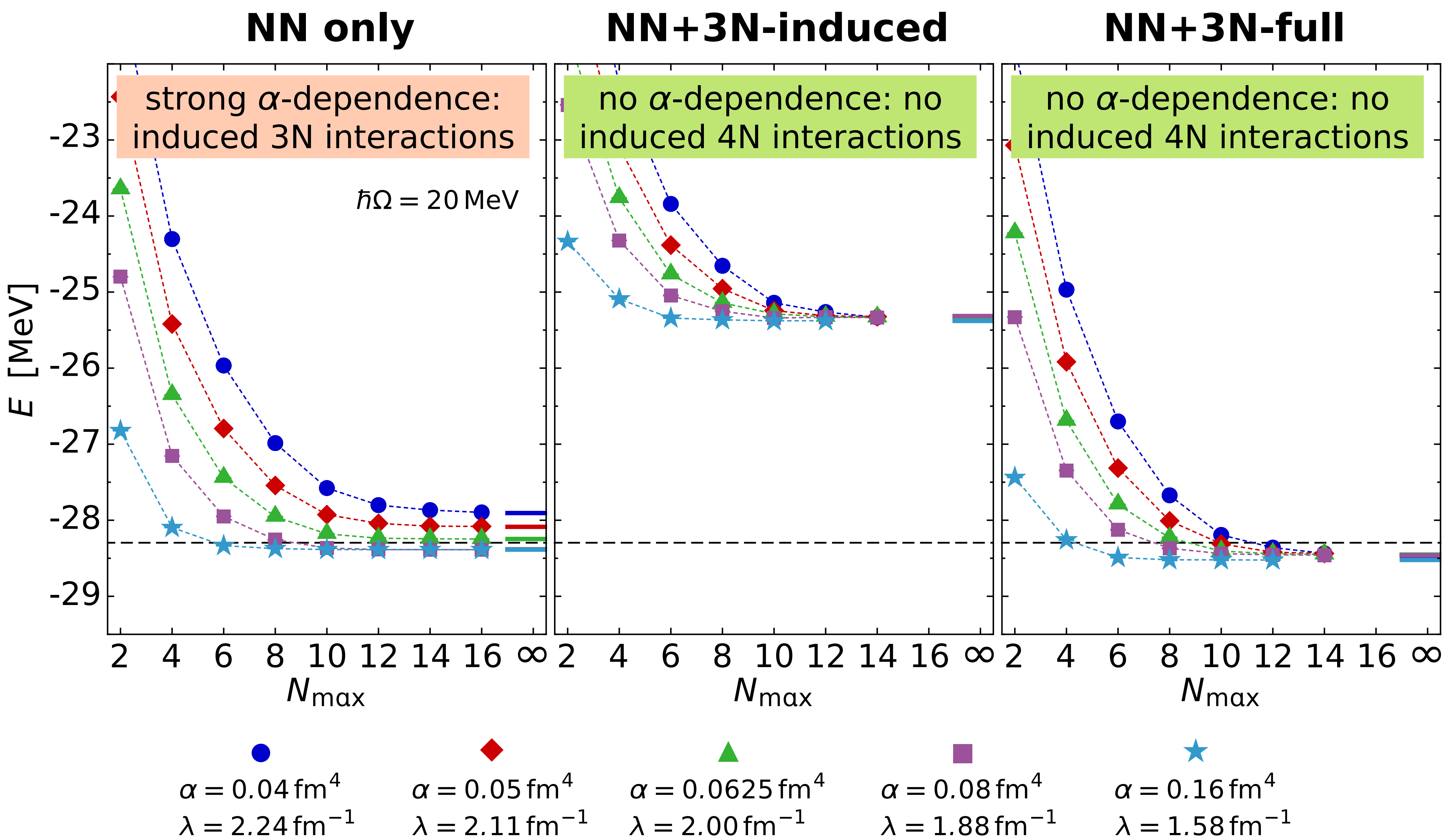
Importance Truncated NCSM

- a priori dete… …ia first-order pert…

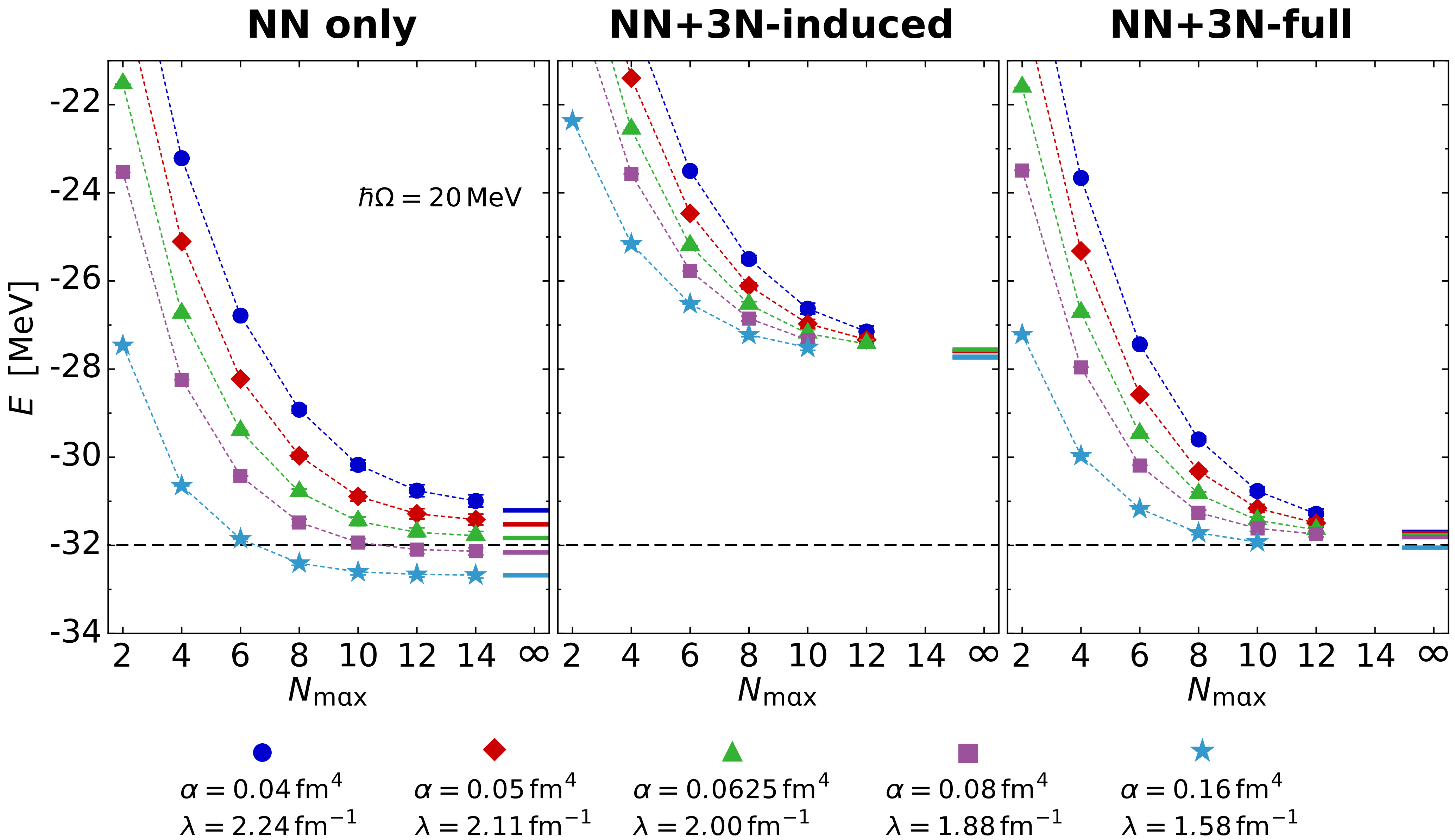
- **impor…** …tes with $|\kappa_\nu| \geq \kappa_{\min}$

- IT-NCSM provides **same results** as the full NCSM keeping all its advantages
- expands **application range** to higher A

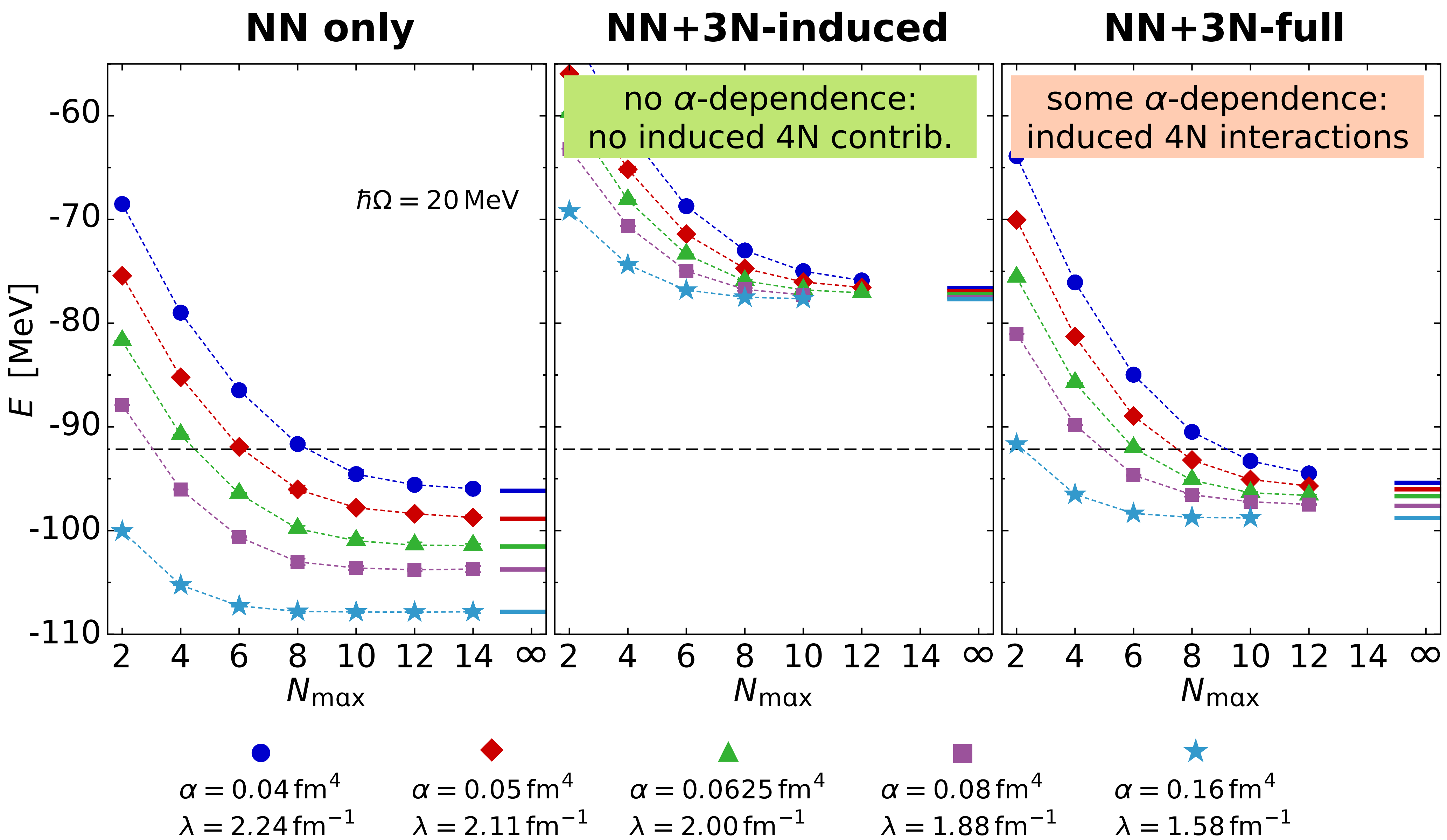
^{4}He: Ground-State Energies



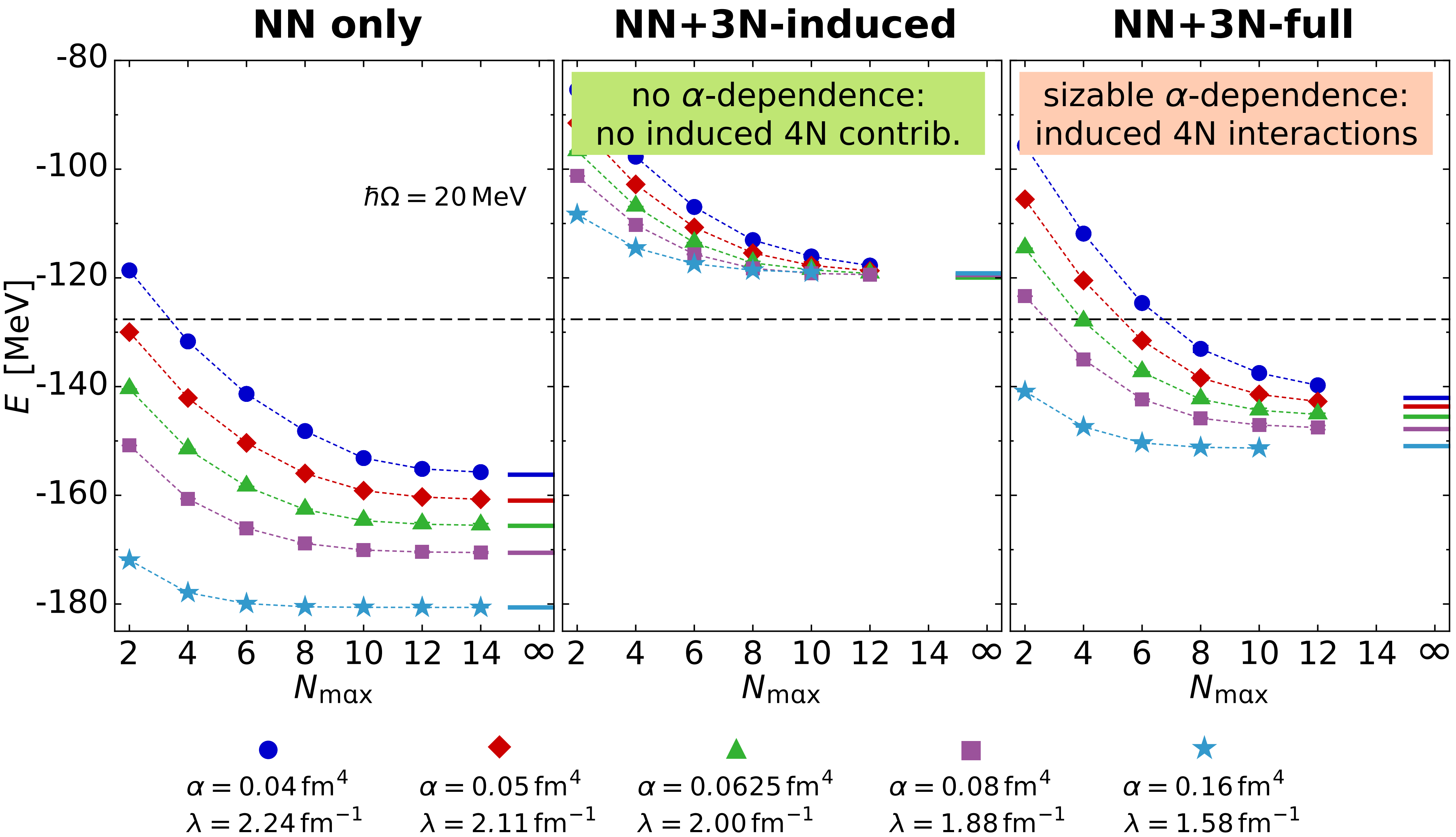
^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies

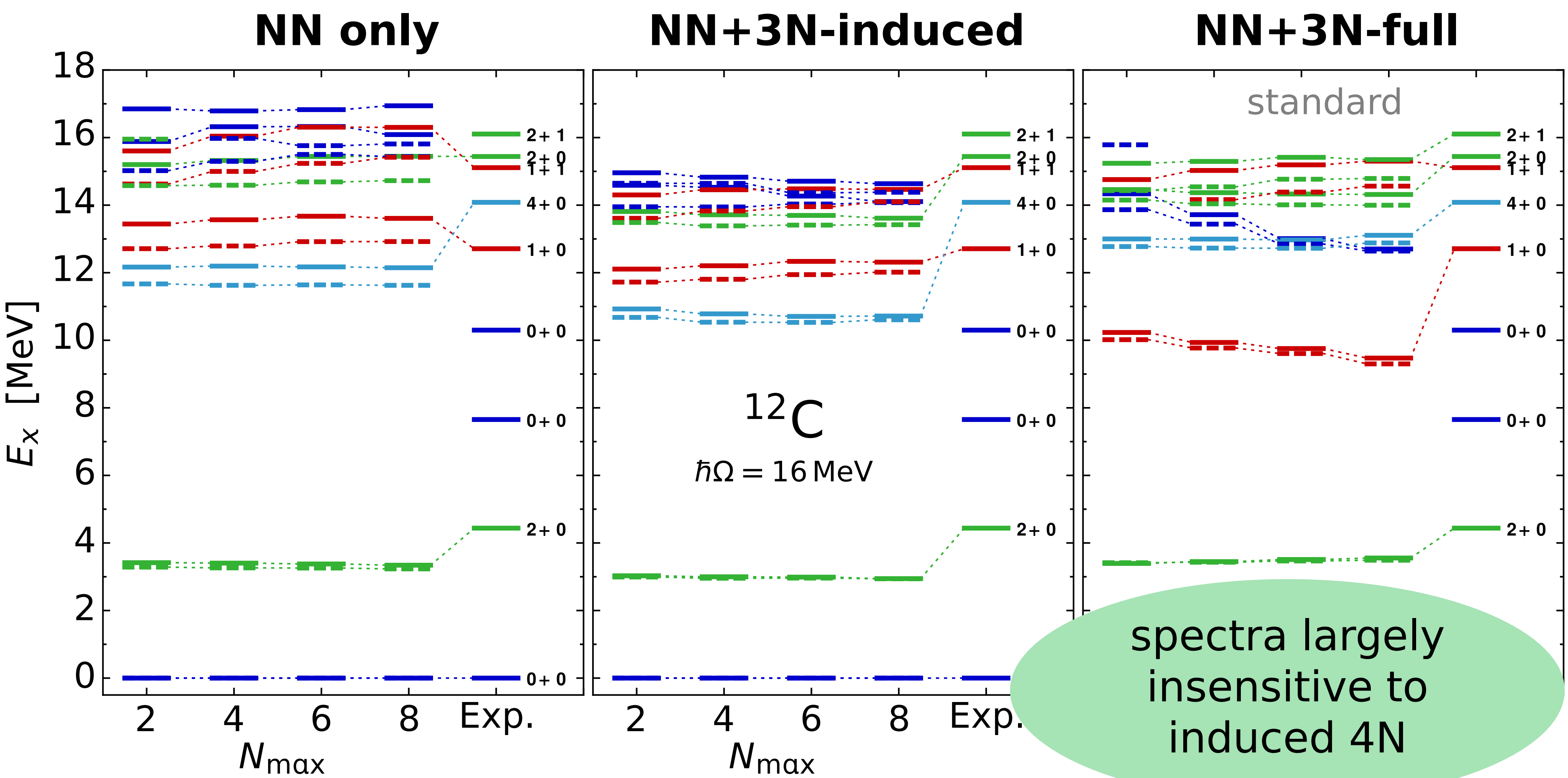


^{16}O: Ground-State Energies



Spectroscopy of ^{12}C

Roth, et al; PRL 107, 072501 (2011)



spectra largely insensitive to induced 4N

$\alpha = 0.04\,fm^4$
$\lambda = 2.24\,fm^{-1}$

$\alpha = 0.08\,fm^4$
$\lambda = 1.88\,fm^{-1}$

SRG Model Space & Frequency Conversion

Roth, AC, Langhammer et al. — in preparation

SRG: Basis Representation

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

- **unitary** transformation driven by

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle E'i'JT|\,\widetilde{\mathrm{H}}_\alpha\,|EiJT\rangle =$$

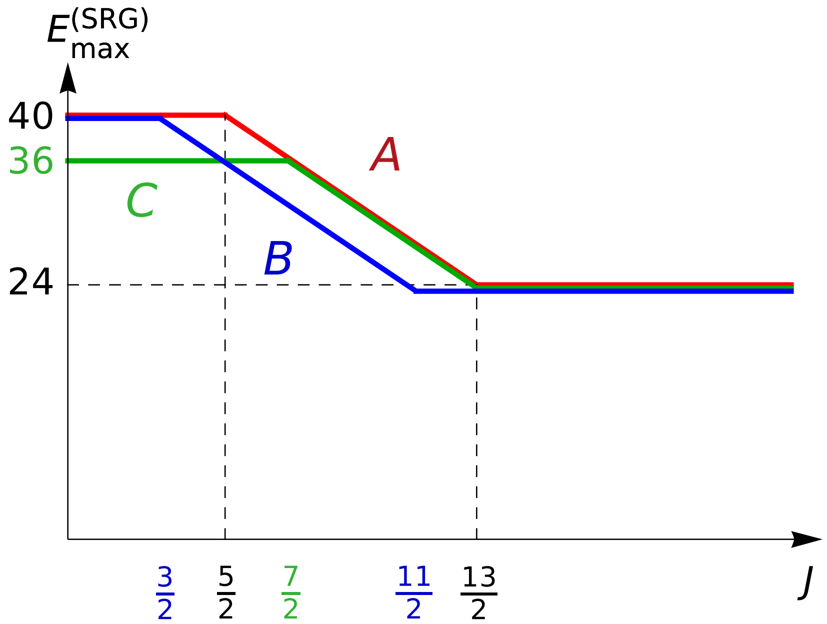
$$(2\mu)^2 \sum_{E'',E'''}^{E_{\max}^{(\mathrm{SRG})}} \sum_{i'',i'''} \langle E'i'JT|\,\mathrm{T}_{\mathrm{int}}\,|E''i''JT\rangle\langle E''i''JT|\,\widetilde{\mathrm{H}}_\alpha\,|E'''i'''JT\rangle\langle E'''i'''JT|\,\widetilde{\mathrm{H}}_\alpha\,|EiJT\rangle$$
$$-2\langle E'i'JT|\,\widetilde{\mathrm{H}}_\alpha\,|E''i''JT\rangle\langle E''i''JT|\,\mathrm{T}_{\mathrm{int}}\,|E'''i'''JT\rangle\langle E'''i'''JT|\,\widetilde{\mathrm{H}}_\alpha\,|EiJT\rangle$$
$$+\langle E'i'JT|\,\widetilde{\mathrm{H}}_\alpha\,|E''i''JT\rangle\langle E''i''JT|\,\widetilde{\mathrm{H}}_\alpha\,|E'''i'''JT\rangle\langle E'''i'''JT|\,\mathrm{T}_{\mathrm{int}}\,|EiJT\rangle$$

SRG model space truncated $E \leq E_{\max}^{(\mathrm{SRG})}$

SRG Model Space

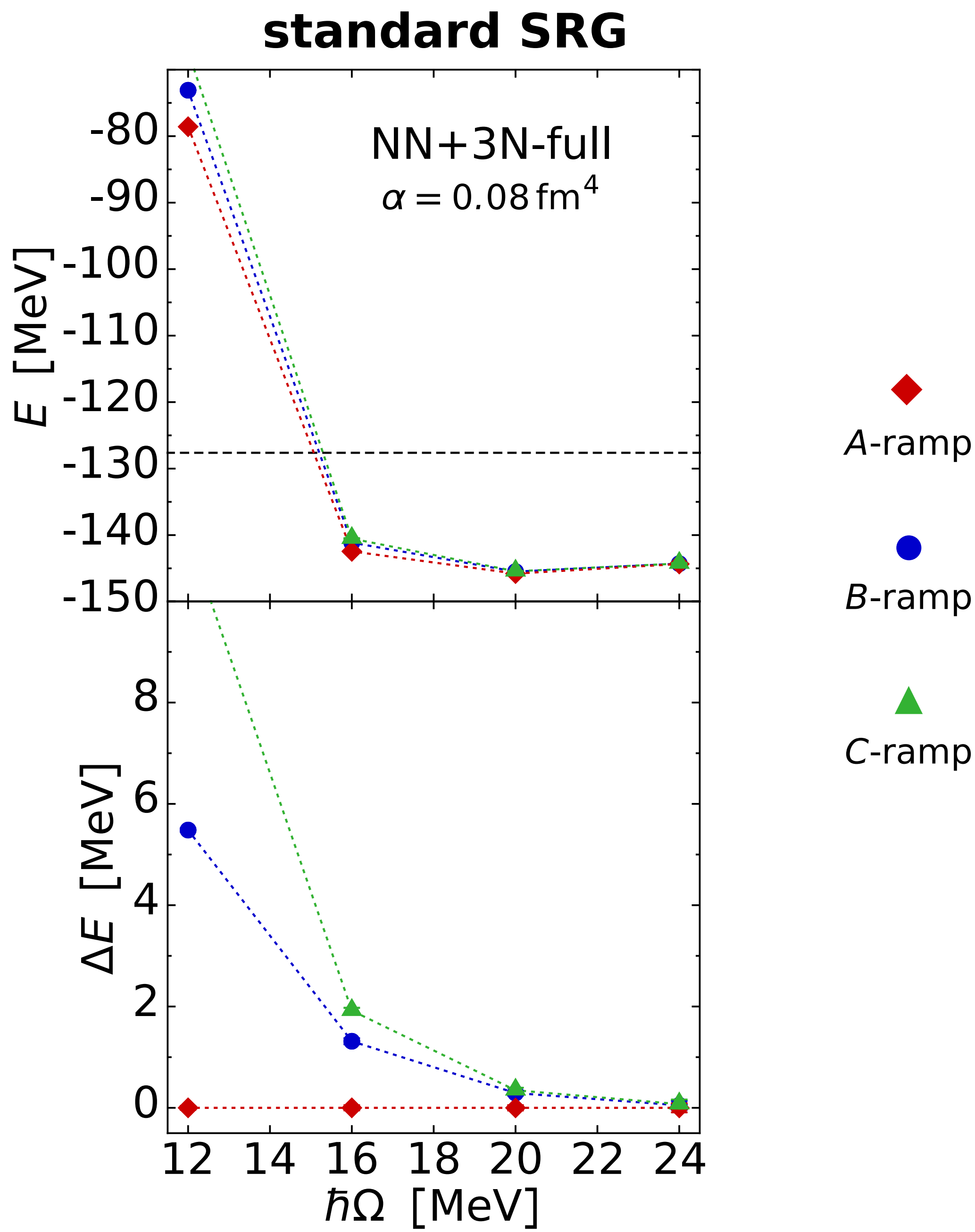
- large angular momenta less important for low-energy properties
  - J-dependent SRG space truncation $E_{\text{max}}^{(\text{SRG})}(J)$

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

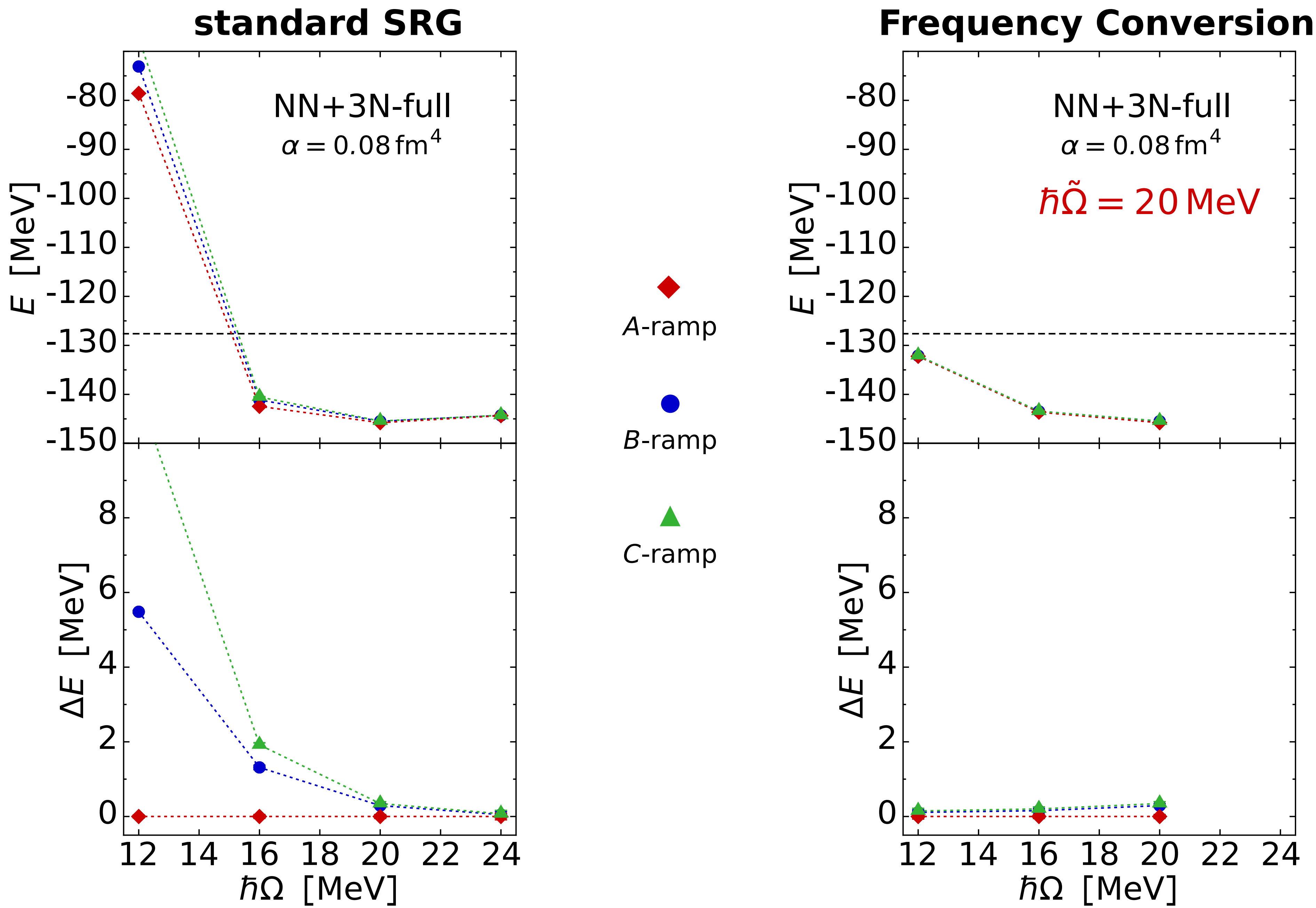


- physical content of SRG space depends on $\hbar\Omega$
- SRG space insufficient for **low $\hbar\Omega$**
  - especially for increasing mass number

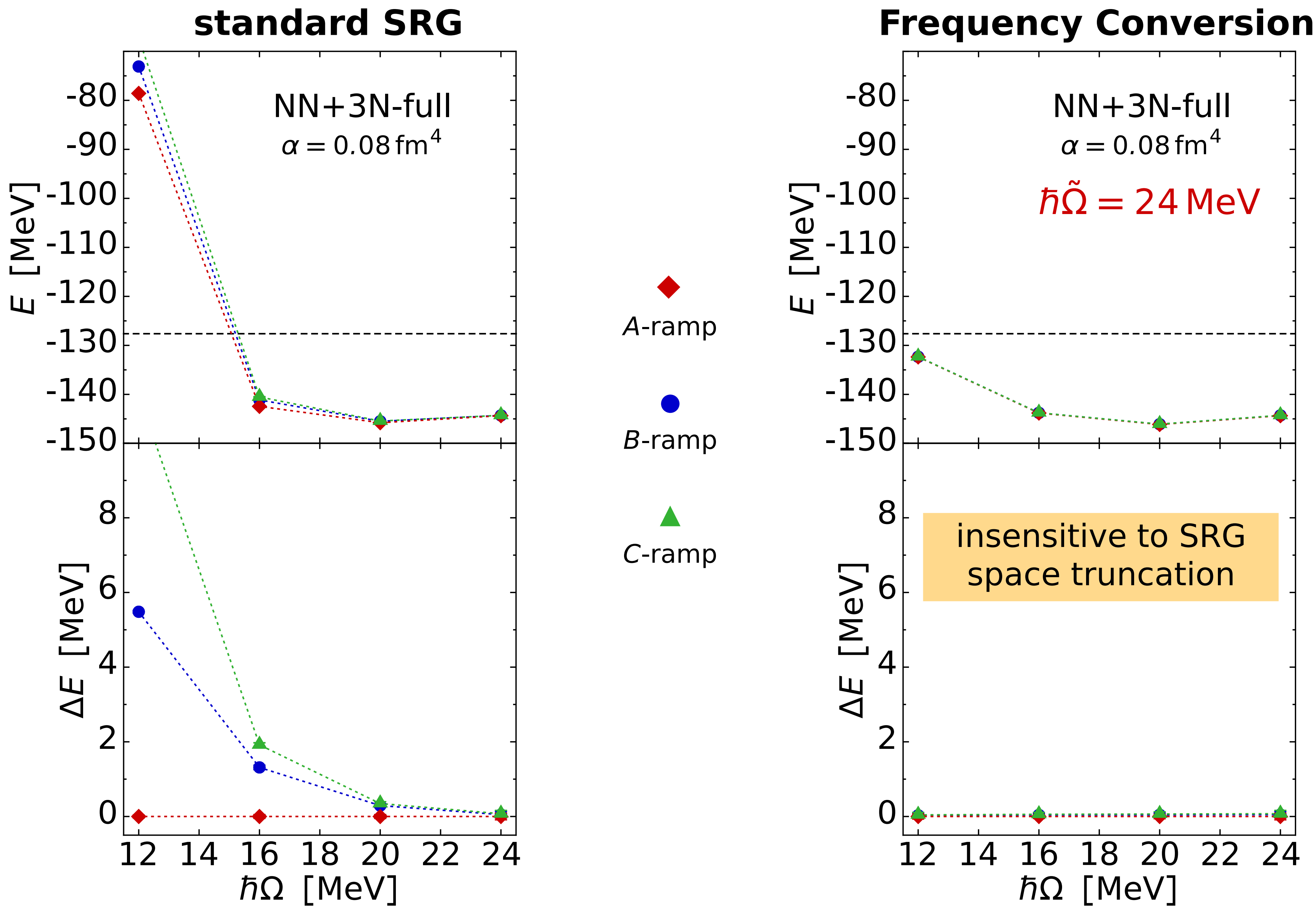
Idea:

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

Frequency Conversion: ^{16}O Ground State



Frequency Conversion: ^{16}O Ground State



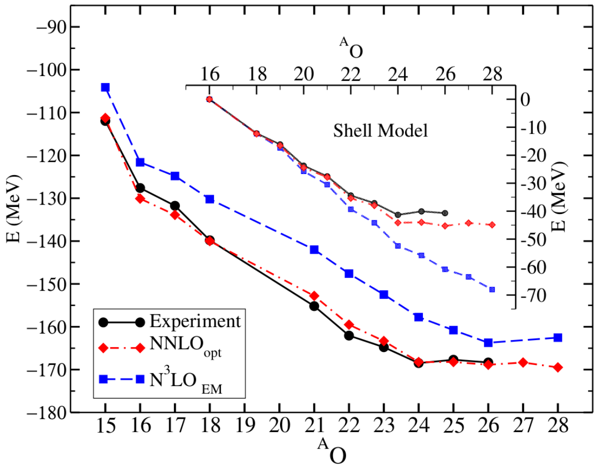
Towards Next-Generation Chiral Hamiltonians

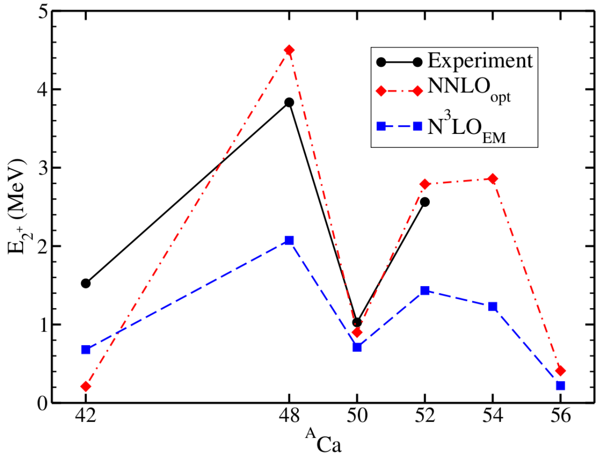
Consistent N^{2}LO Hamiltonians

- **starting point**: numerical 3N matrix elements in partial-wave Jacobi-momentum basis (antisym. under $1 \longleftrightarrow 2$)
  - numerical partial-wave decomposition of Skibinski et al.
  - ongoing collaborative effort to produce N^{2}LO/N^{3}LO matrix elements (LENPIC)
- **direct** transformation to **HO basis** for nuclear structure calculations
  - use HO machinery afterwards (SRG, $\mathcal{J}T$-coupled scheme,...)
- **first application**: consistent NN+3N Hamiltonian at N^{2}LO
  - NN at N^{2}LO: Epelbaum et al., cutoffs 450,...,600 MeV, phase-shift fit χ^2/dat ~ 10 (~ 1) up to 300 MeV (100 MeV)
  - 3N at N^{2}LO: Epelbaum et al., cutoffs 450,...,600 MeV, nonlocal, fit to $a(nd)$ and $E(^3\text{H})$, included up to J=7/2

Optimized N^2LO Hamiltonian

- NN interaction at N^2LO
  - LECs refittet using state-of-the-art optimization algorithm (**POUNDerS**)
  - more **accurate description** of NN data
    (comparable to previous N^3LO interactions)





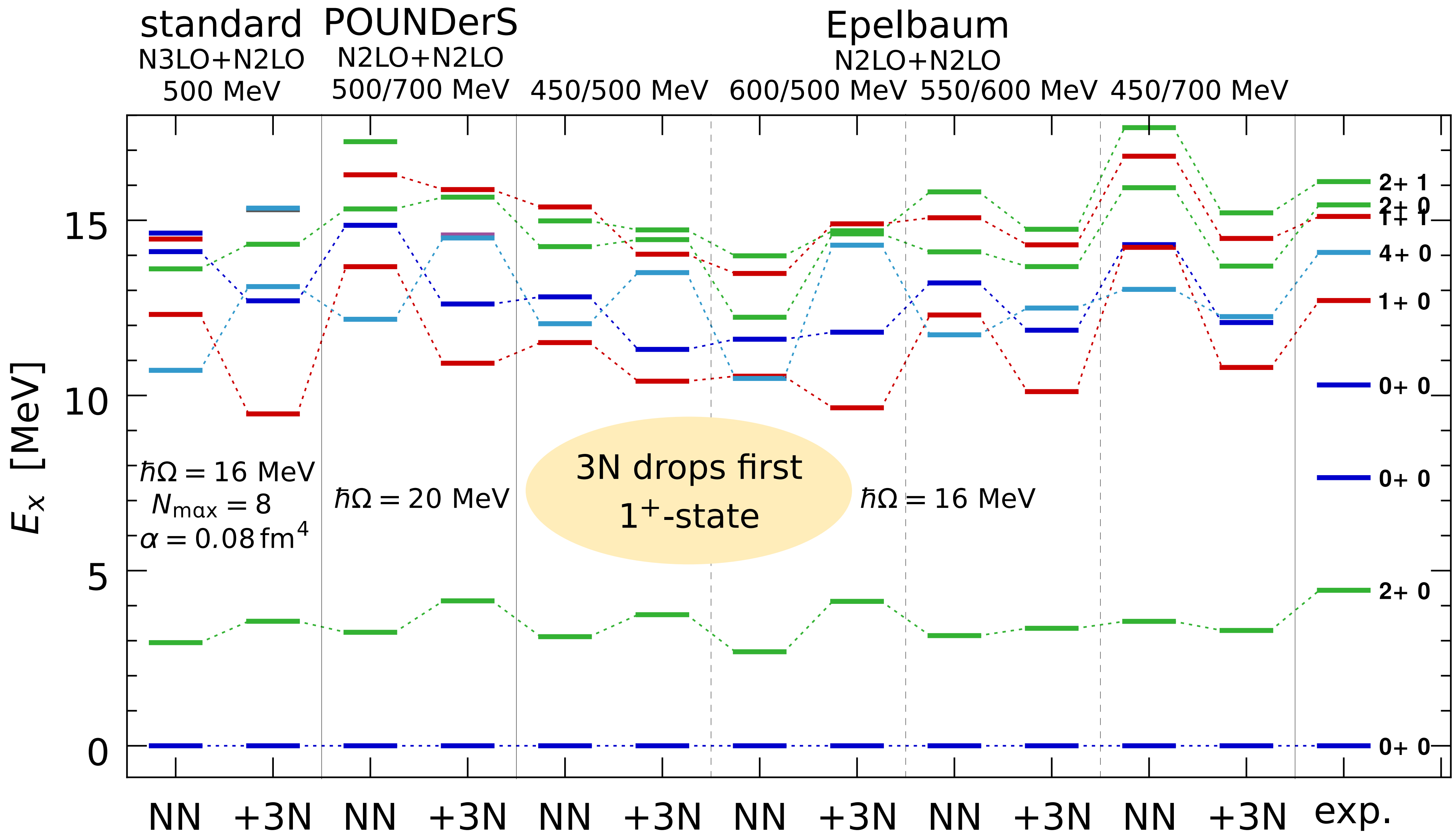
Ekström, et al; PRL 110, 192502 (2013)

more in Talk of G. Hagen

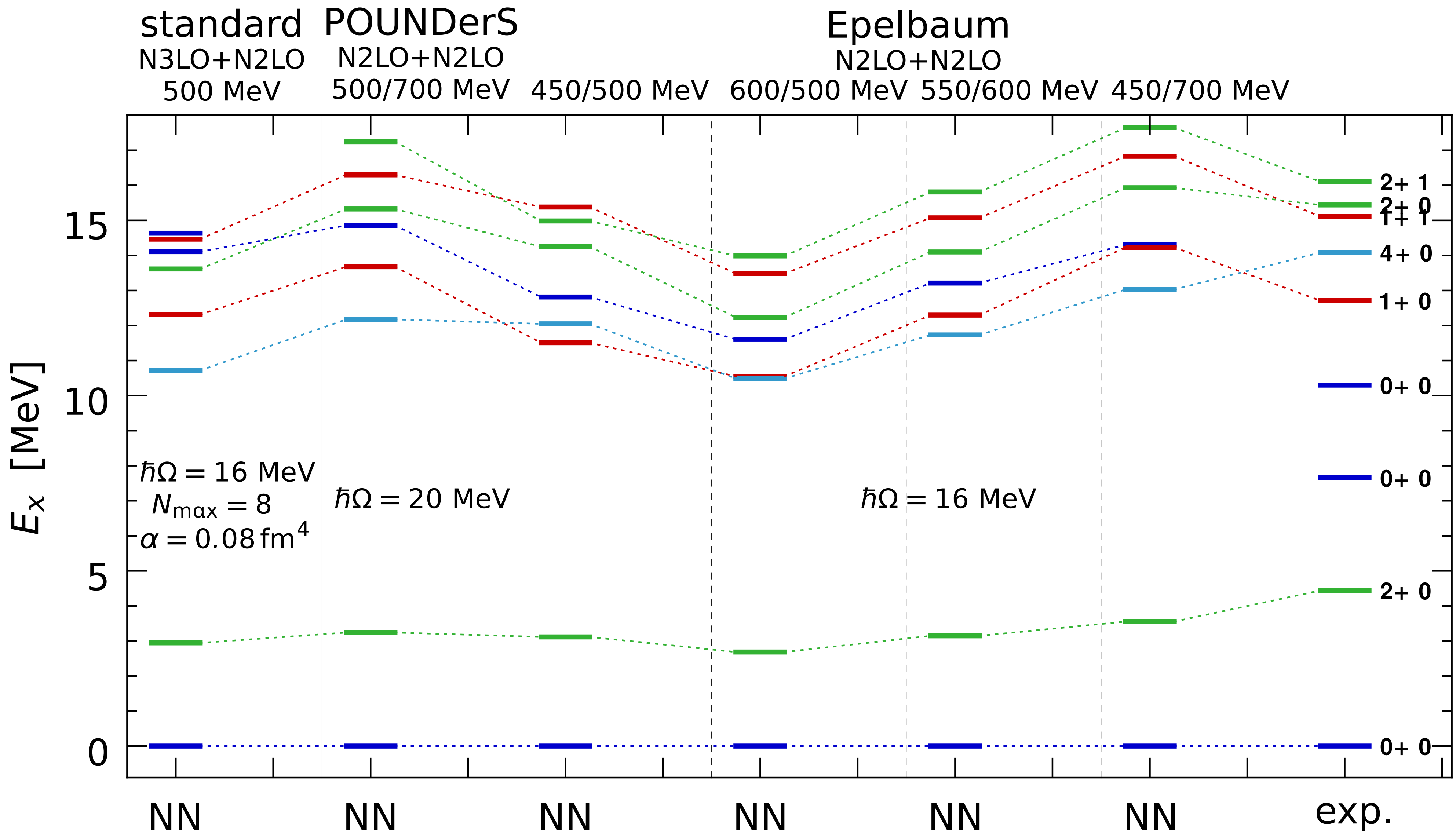
  - **impressive** results in Oxygen- and Calcium-chain even **without 3N**

- **3N interaction** at N^2LO
  - std. 3N ($\Lambda = 500\,\text{MeV}$) with *cD* and *cE* fittet to Triton by Navrátil & Quaglioni

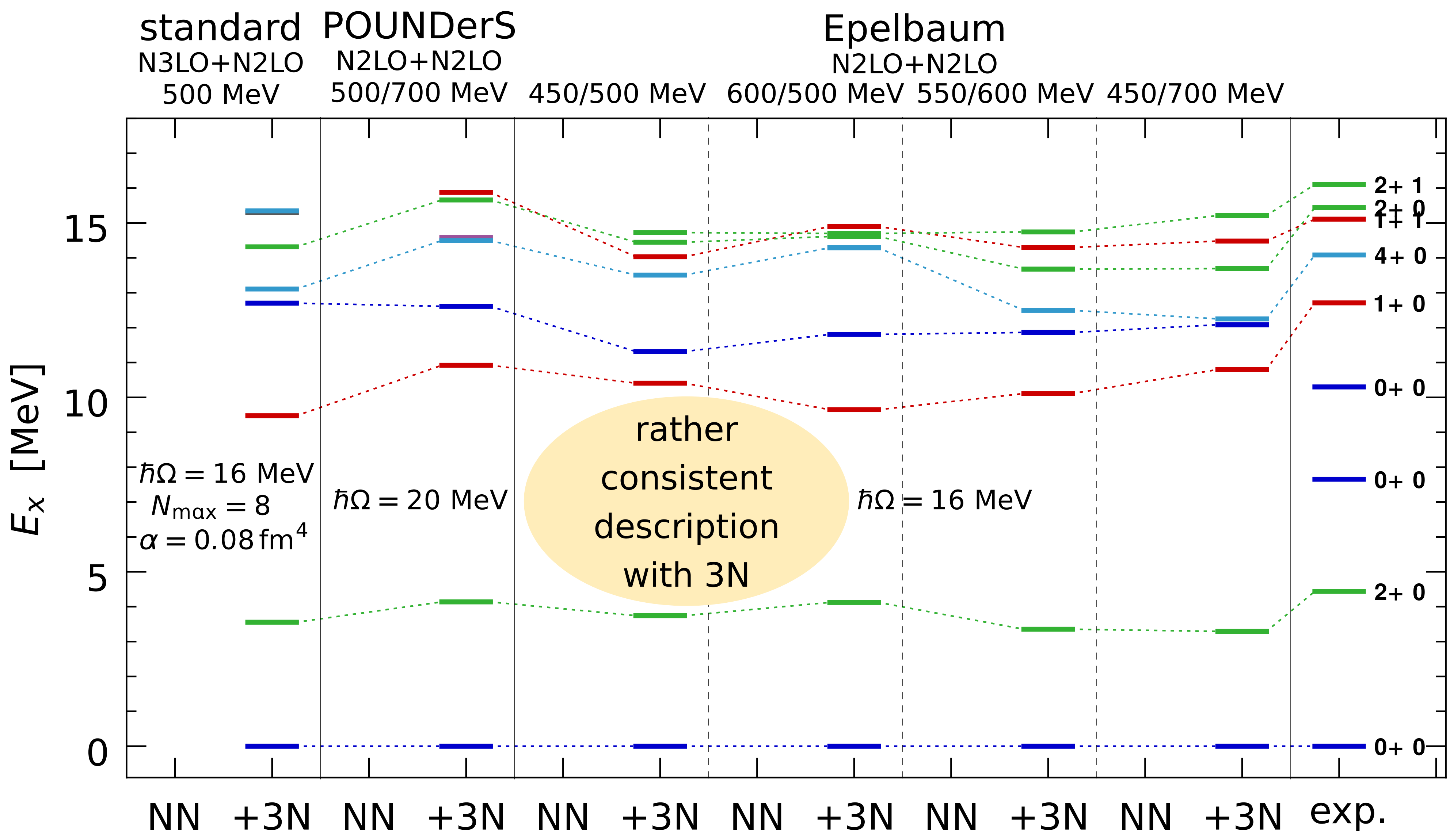
^{12}C: Compare Next Generation Interactions



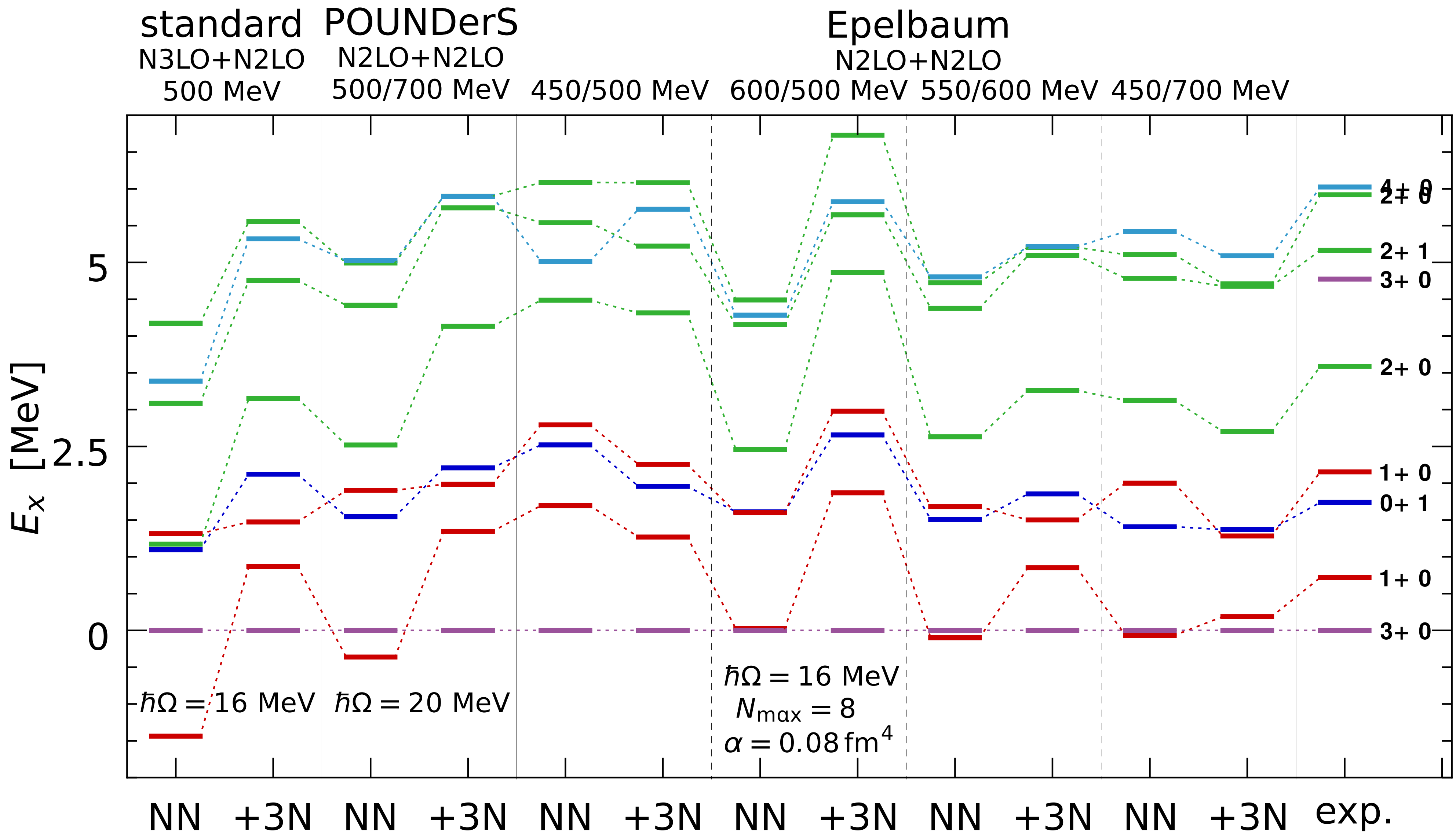
^{12}C: Compare Next Generation Interactions



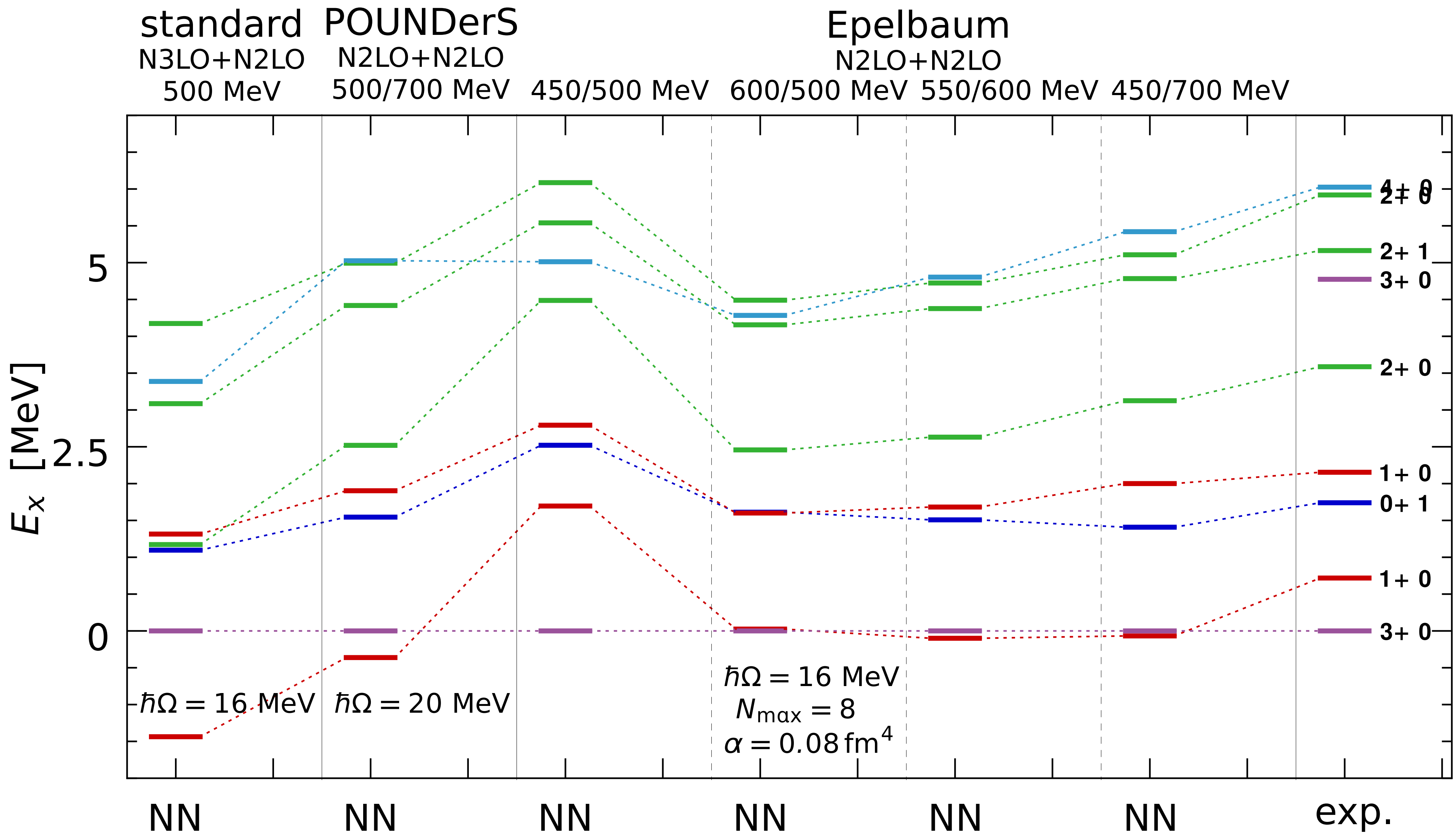
^{12}C: Compare Next Generation Interactions



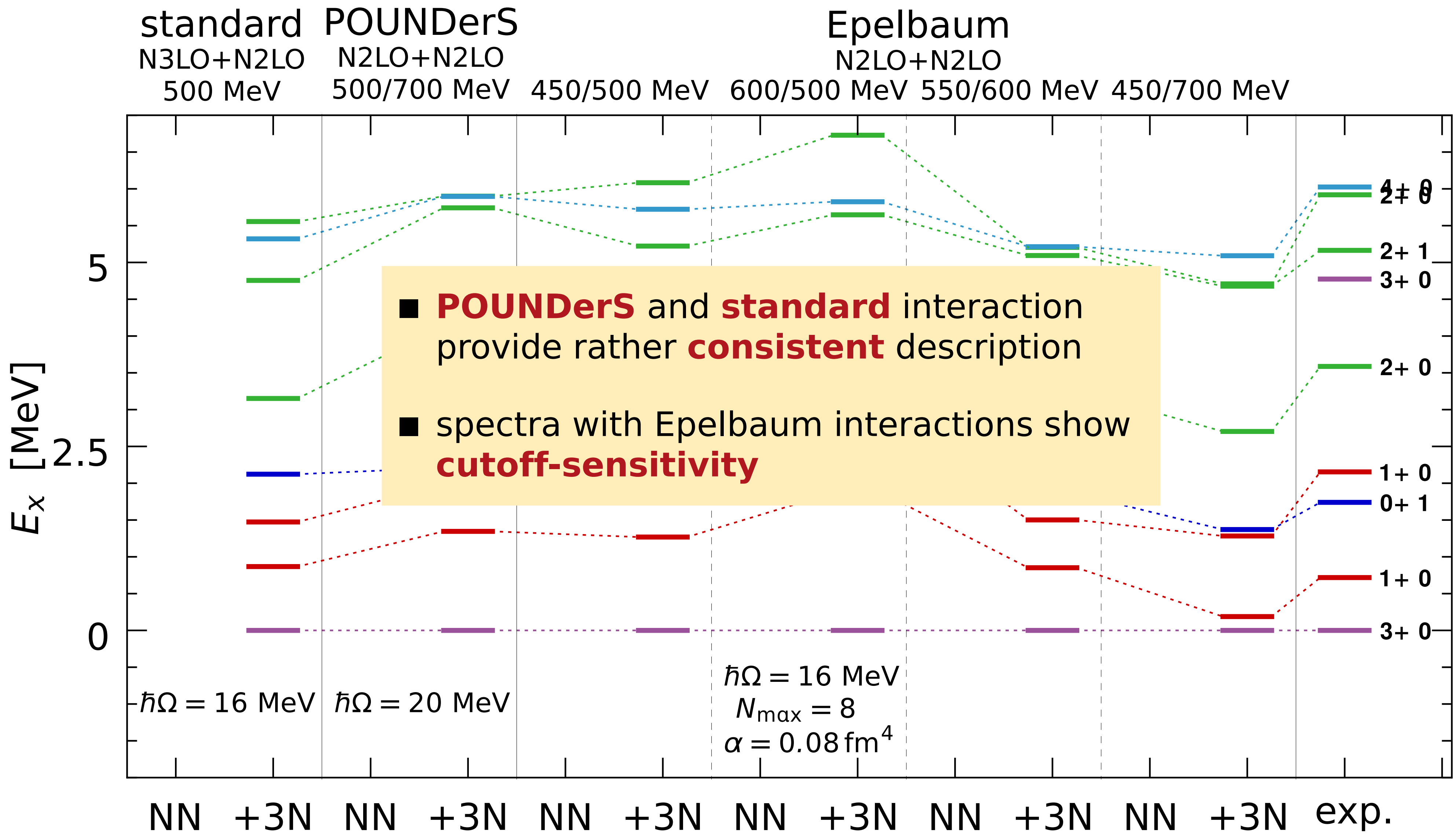
^{10}B: Compare Next Generation Interactions



^{10}B: Compare Next Generation Interactions

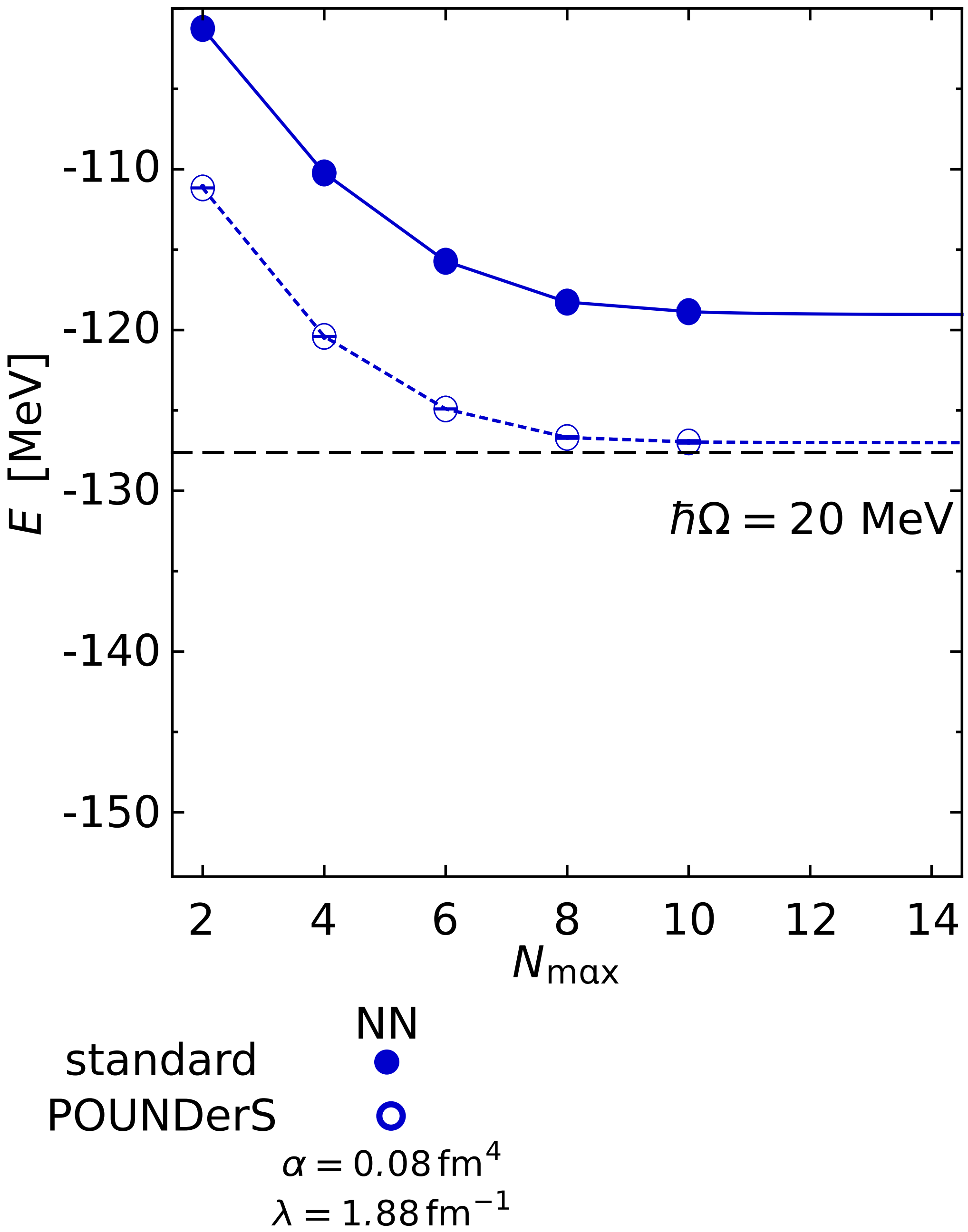


^{10}B: Compare Next Generation Interactions



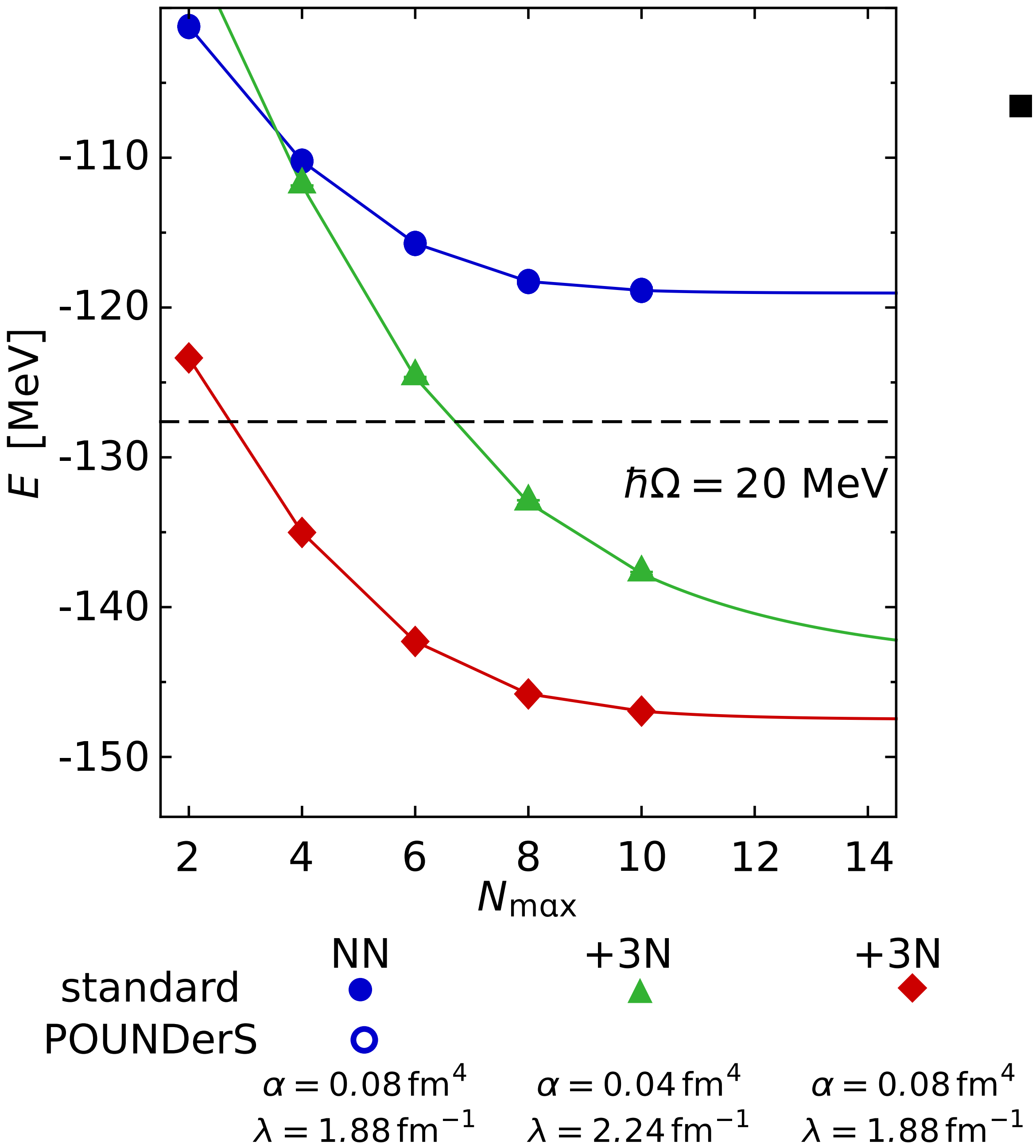
- **POUNDerS** and **standard** interaction provide rather **consistent** description
- spectra with Epelbaum interactions show **cutoff-sensitivity**

^{16}O: Optimized Interaction (POUNDerS)



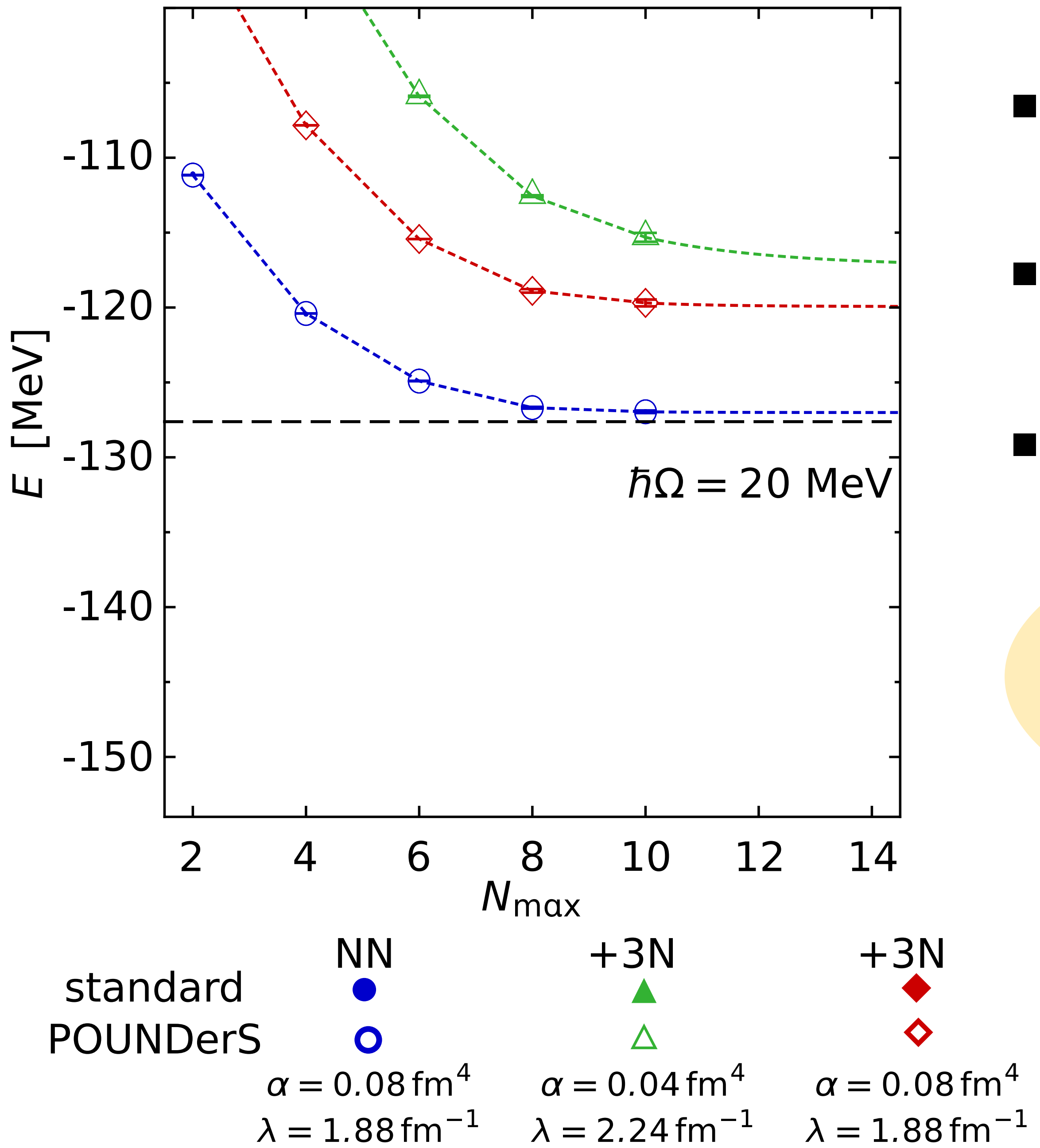
- POUNDerS **NN** interaction already **describes experiment**

^{16}O: Optimized Interaction (POUNDerS)



- POUNDerS **NN** interaction already **describes experiment**

^{16}O: Optimized Interaction (POUNDerS)

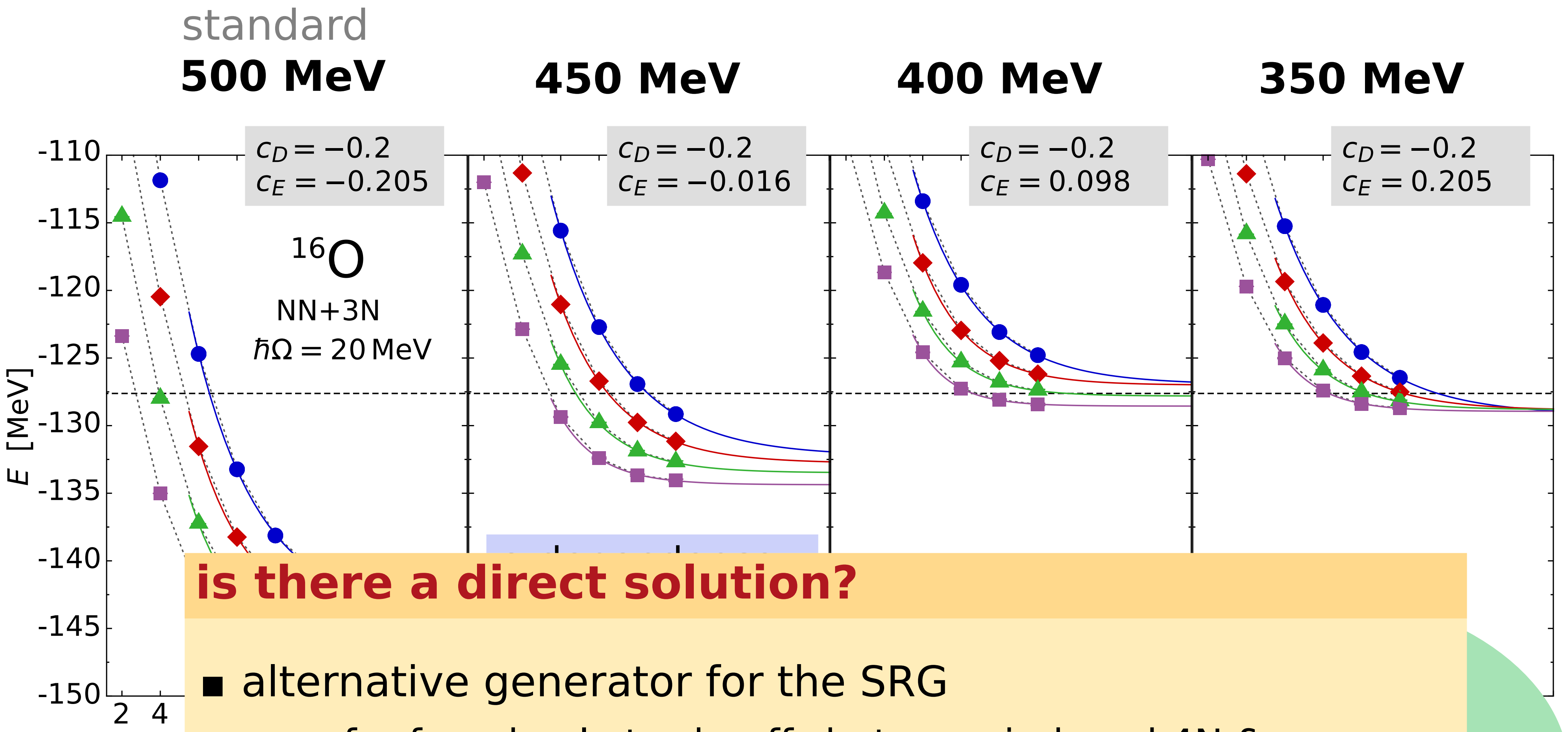


- POUNDerS **NN** interaction already **describes experiment**
- **3N** becomes **repulsive** for POUNDerS interaction
- induced 4N are repulsive as well

POUNDerS NN+3N underbounds ^{16}O ground-state by more than 10 MeV

SRG in Four-Body Space

Induced Four-Body Contributions



is there a direct solution?

- alternative generator for the SRG
  - so far found only trade-offs between induced 4N & convergence accelaration
- **SRG in four-body space**

Four-Body Jacobi Basis

Navrátil, Barrett, Glöckle   Phys. Rev. C 59 611 (1999)

- Jacobi coordinate: $\vec{\xi}_3 = \sqrt{\frac{3}{4}}[\frac{1}{2}(\vec{r}_a + \vec{r}_b + \vec{r}_c) - \vec{r}_d]$

- Jacobi state antisym. under $1 \longleftrightarrow 2 \longleftrightarrow 3$
  (extension of antisym. three-body Jacobi state)

$$|E_{12}E_3 i_{12}; \alpha\rangle = |E_{12}E_3 i_{12}[J_{12},(L_3,S_3)J_3]JM_J;(T_{12}T_3)TM_T\rangle$$

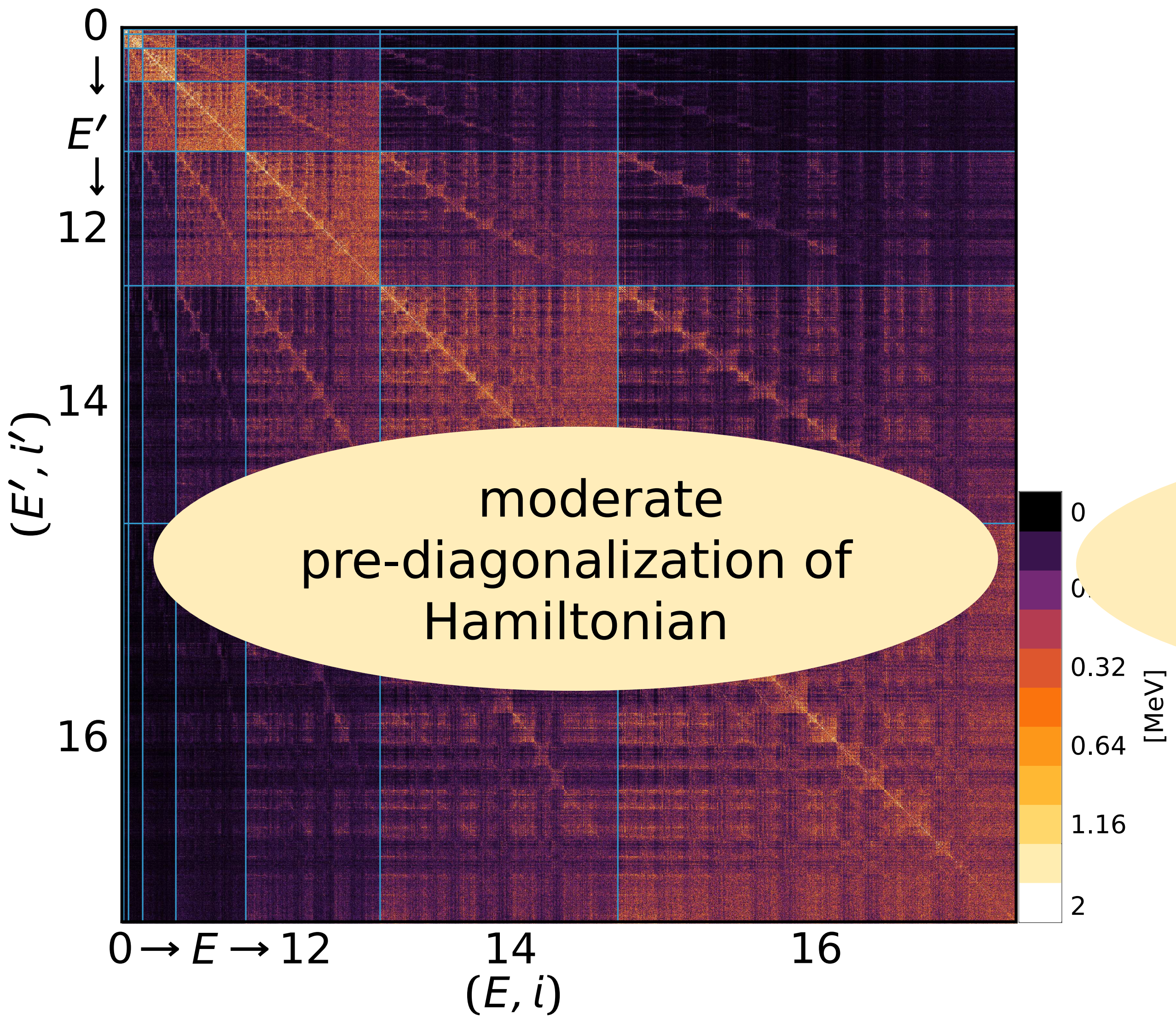
- antisym. Jacobi state

$$|EiJM_J TM_T\rangle = \sum_{i_{12},\beta} \tilde{c}^{\alpha,i}_{E_{12},E_3,i_{12}} |E_{12}E_3 i_{12}; \alpha\rangle \qquad \text{with} \quad E = E_{12} + E_3$$

introduce **four-body CFPs**: $\tilde{c}^{\alpha,i}_{E_{12},E_3,i_{12}}$

SRG Evolution in Four-Body Space

4B-Jacobi HO matrix elements



moderate pre-diagonalization of Hamiltonian

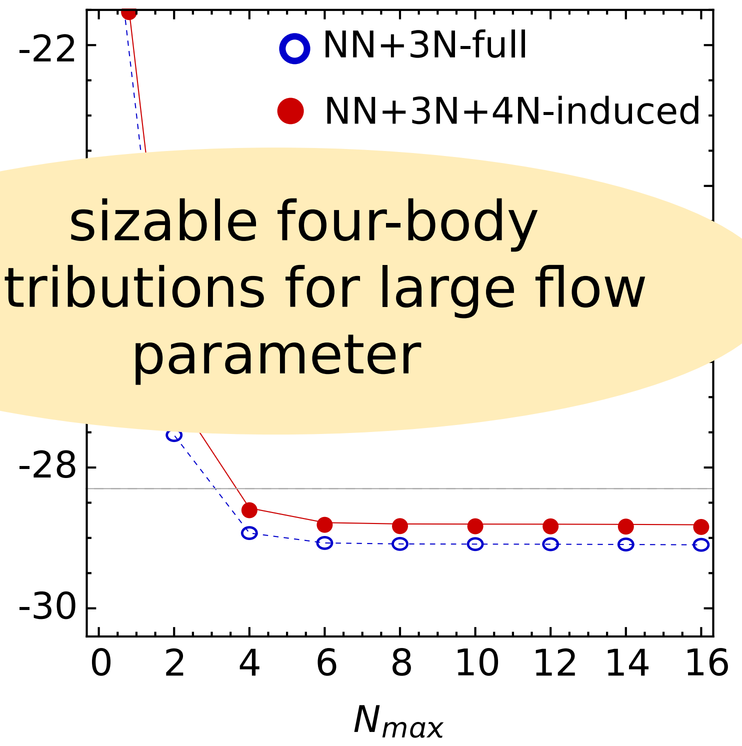
$\alpha = 1.28\,\mathrm{fm}^4$

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

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

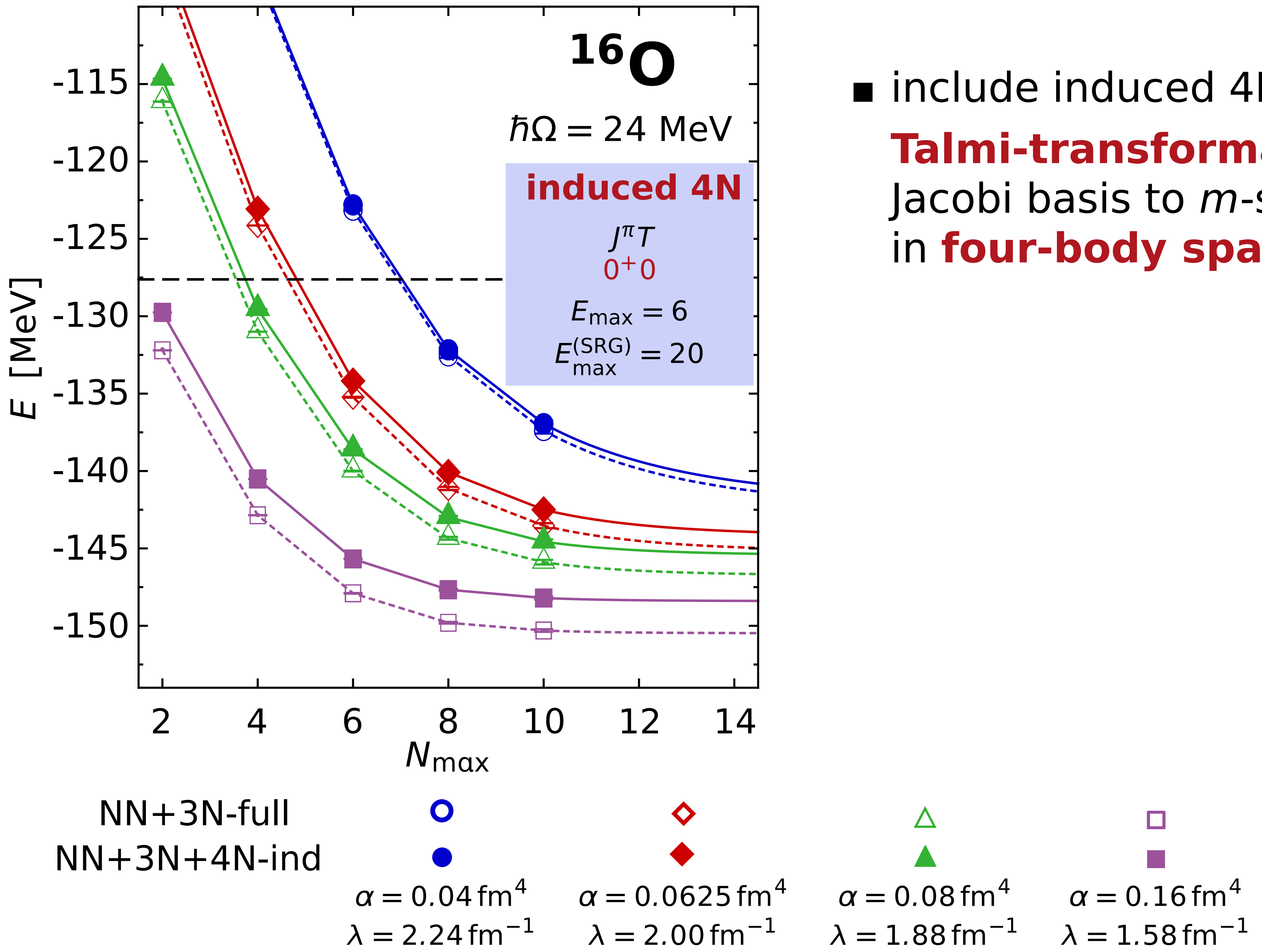
$J^\pi = 0^+, T = 0, \hbar\Omega = 24\,\mathrm{MeV}$

NCSM ground state ^{4}He



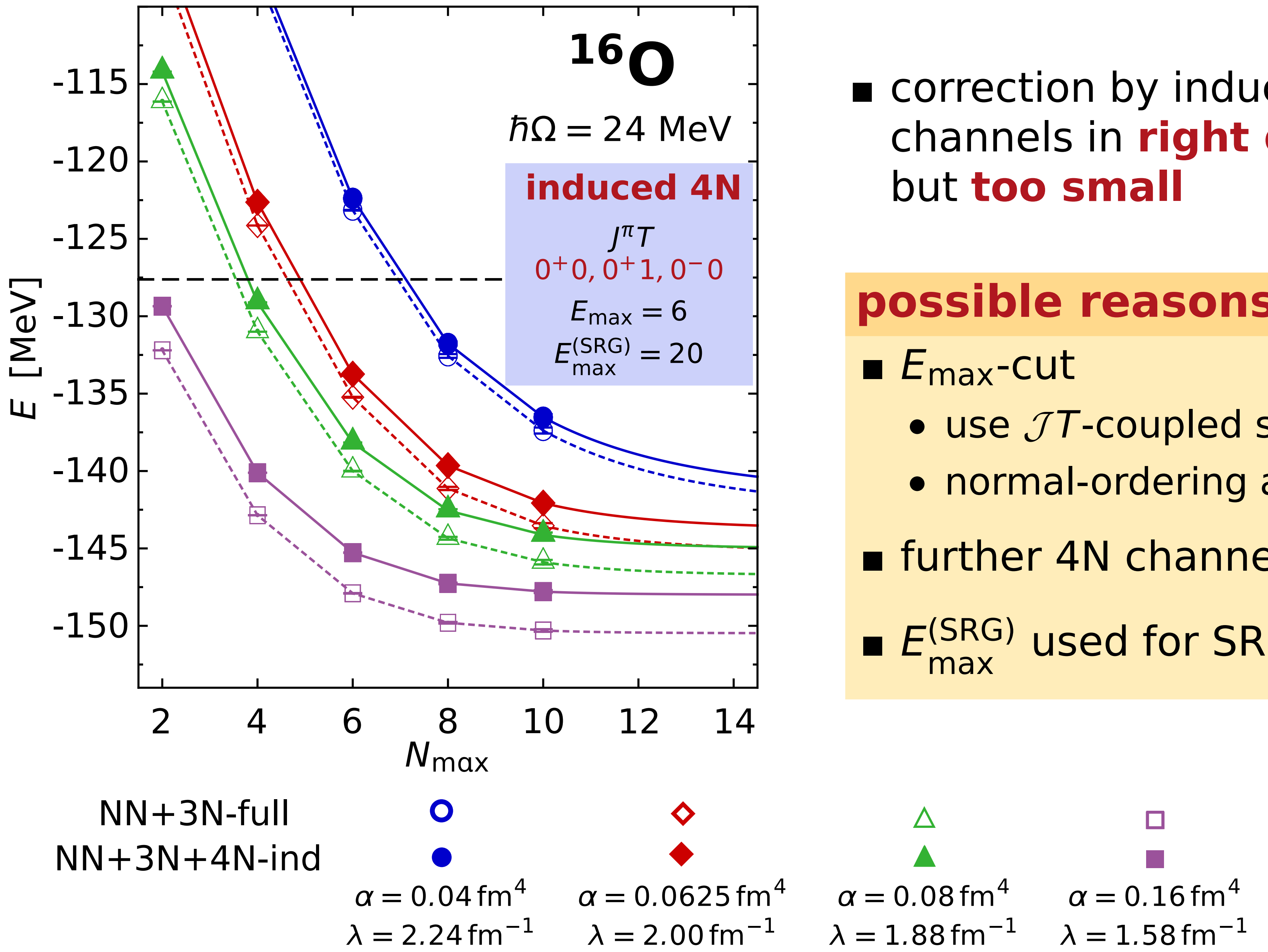
sizable four-body contributions for large flow parameter

IT-NCSM with Four-Body Contributions



- include induced 4N:
  Talmi-transformation from Jacobi basis to *m*-scheme in **four-body space**

IT-NCSM with Four-Body Contributions



- correction by induced 4N channels in **right direction**, but **too small**

possible reasons

- E_{max}-cut
  - use $\mathcal{J}T$-coupled scheme
  - normal-ordering approximation
- further 4N channels
- $E^{(SRG)}_{max}$ used for SRG

Conclusions

Conclusions

- **SRG** evolution in **HO basis** efficient and **improvable**
  - frequency conversion & SRG space increase
- **consistent four-body** SRG evolution
  (for induced and initial contributions)
  - in progress: $\mathcal{J}T$-coupling and normal-ordering approximation
- **p-shell** provide powerful testbed for upcoming chiral potentials
  - cutoff-sensitivity in ^{10}B spectrum
  - ^{16}O ground state underbound by POUNDerS NN+3N interaction
- machinery ready to use **3N @ N^{3}LO** in momentum Jacobi basis
  - directly applicable in IT-NCSM, CC, IM-SRG, RGM ...

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, E. Gebrerufael, K. Hebeler, H. Krutsch, **J. Langhammer**, S. Reinhardt, **R. Roth**, M. Schmidt, **S. Schulz**, C. Stumpf, A. Tichai, R. Trippel, R. Wirth
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  - J. Vary, P. Maris
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  - P. Piecuch
    Michigan State University, USA
  - H. Hergert
    Ohio State University, USA
  - P. Papakonstantinou
    say, F
  - iversity, Sweden
  - meier, T. Neff
    GSI Helmholtzzentrum

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

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung