SRG evolved chiral NN+3N Interactions in ab initio nuclear structure calculations

International Collaborations in Nuclear Theory: Theory for open-shell nuclei near the limits of stability

May 11-29, 2015, Michigan State University and FRIB/NSCL

Angelo Calci | TRIUMF

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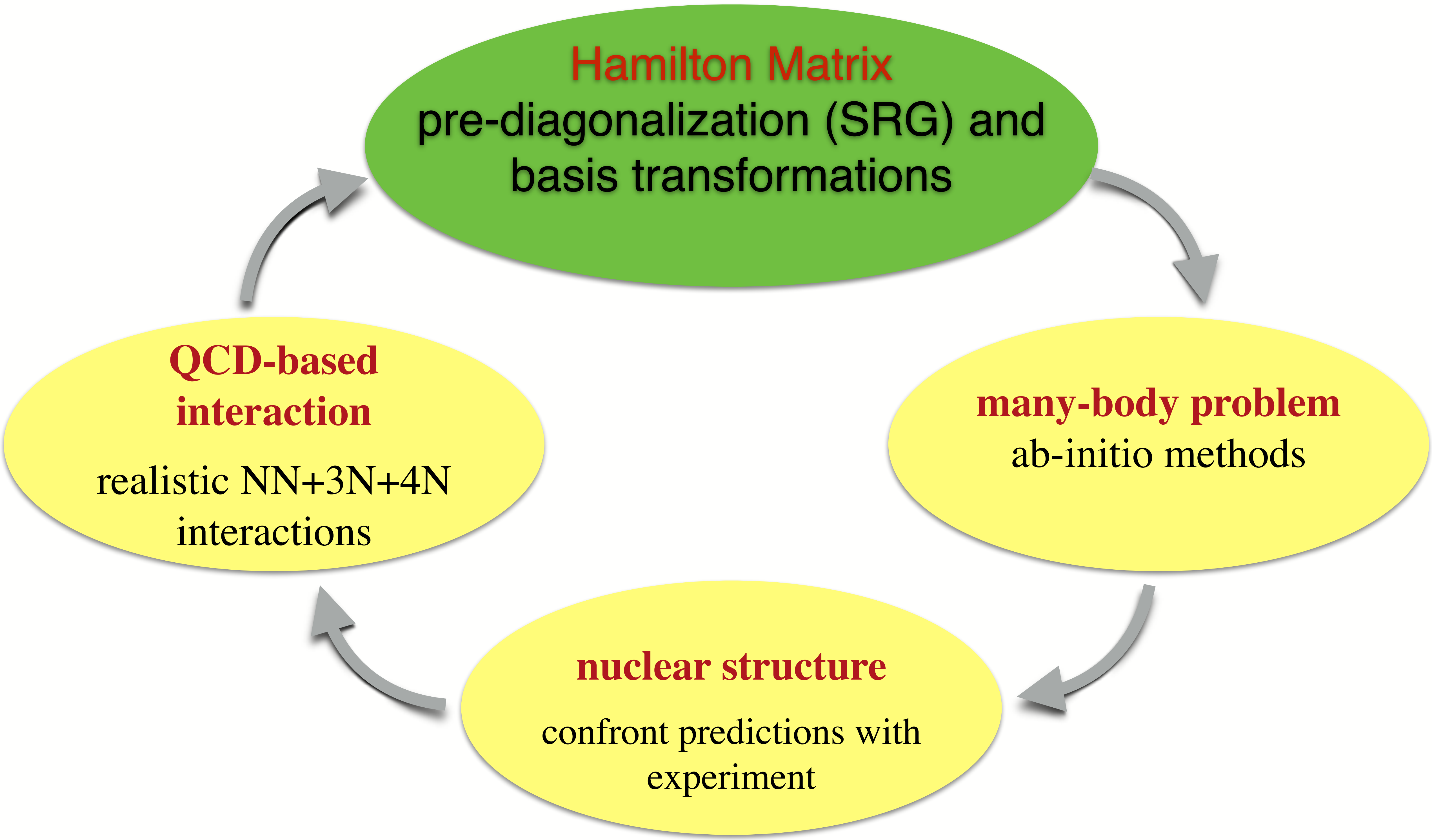
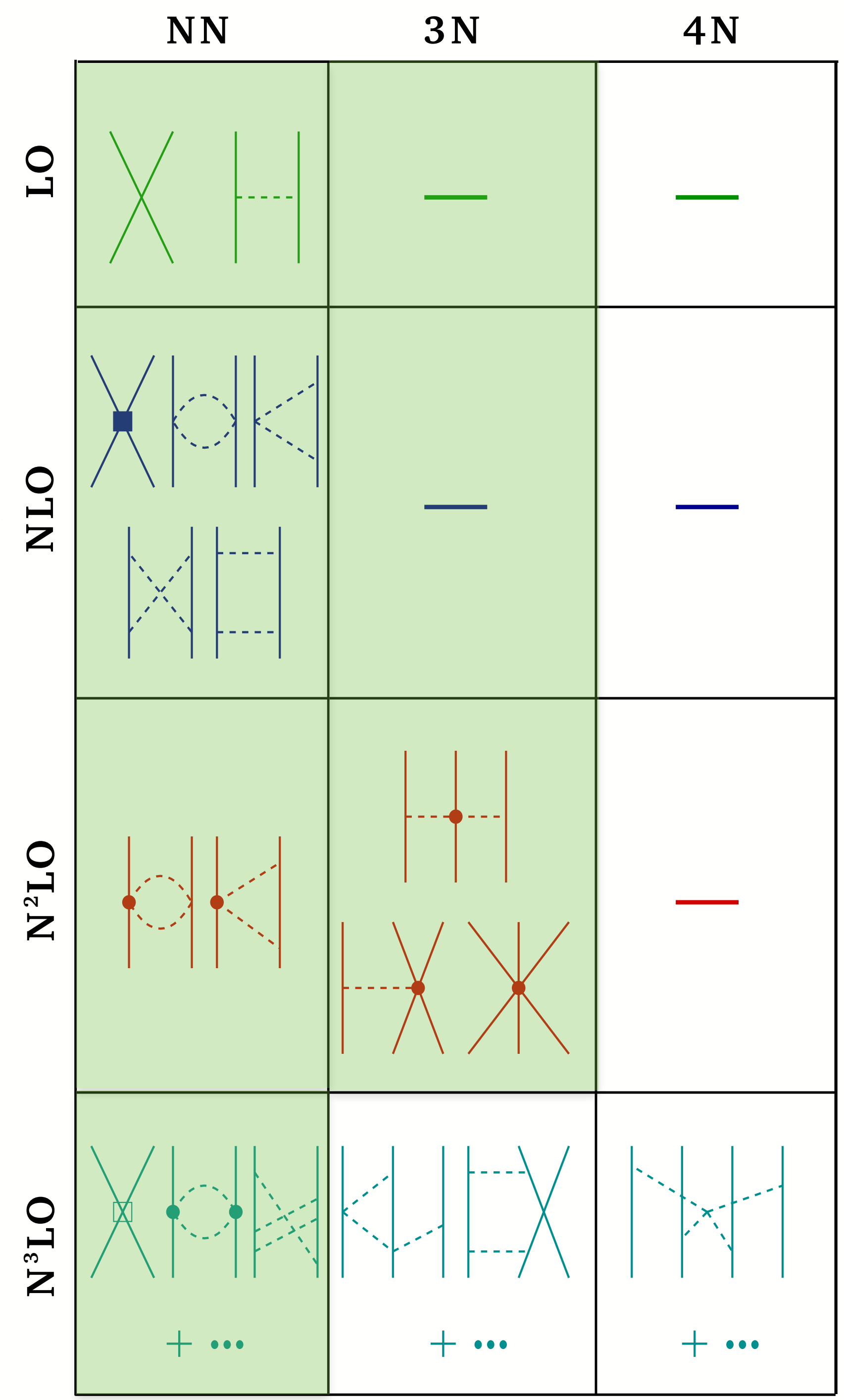
Introduction



Chiral NN+3N Interactions

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

- **standard interaction:**
  - NN @ N3LO: Entem & Machleidt, 500MeV cutoff
  - 3N @ N2LO: Navrátil, local, 400 & 500MeV cutoff, fit to ^{4}He & Triton
- **optimized N^{2}LO interaction:**
  - NN: Ekström et al., 500MeV cutoff, LECs fitted with POUNDerS
  - 3N: Navrátil, local, 500MeV cutoff, fit to ^{4}He & Triton
- **Epelbaum N^{2}LO interaction:**
  - NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal



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Similarity Renormalization Group

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)

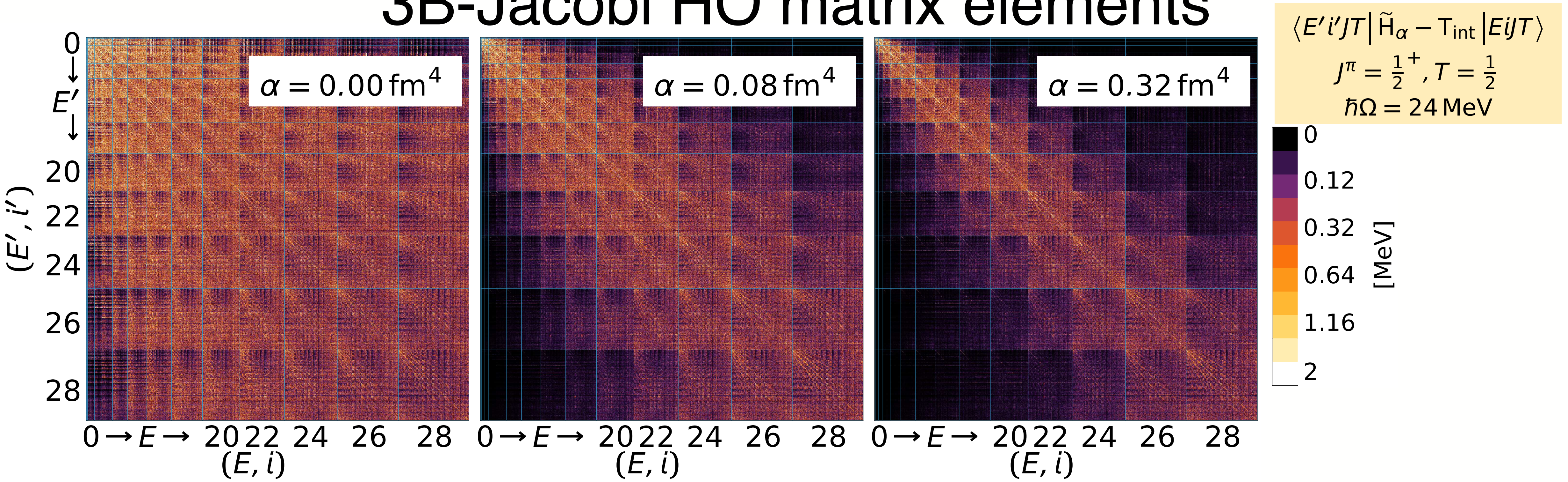
accelerate convergence by **pre-diagonalizing** the Hamiltonian with respect to the many-body basis

- **unitary transformation leads to evolution equation**

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

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

3B-Jacobi HO matrix elements



SRG Evolution in *A*-Body Space

- **cluster decomposition**: decompose evolved Hamiltonian into irreducible *n*-body contributions

$$\widetilde{H}_\alpha = \widetilde{H}_\alpha^{[1]} + \widetilde{H}_\alpha^{[2]} + \widetilde{H}_\alpha^{[3]} + \cdots + \widetilde{H}_\alpha^{[n]} + \cdots$$

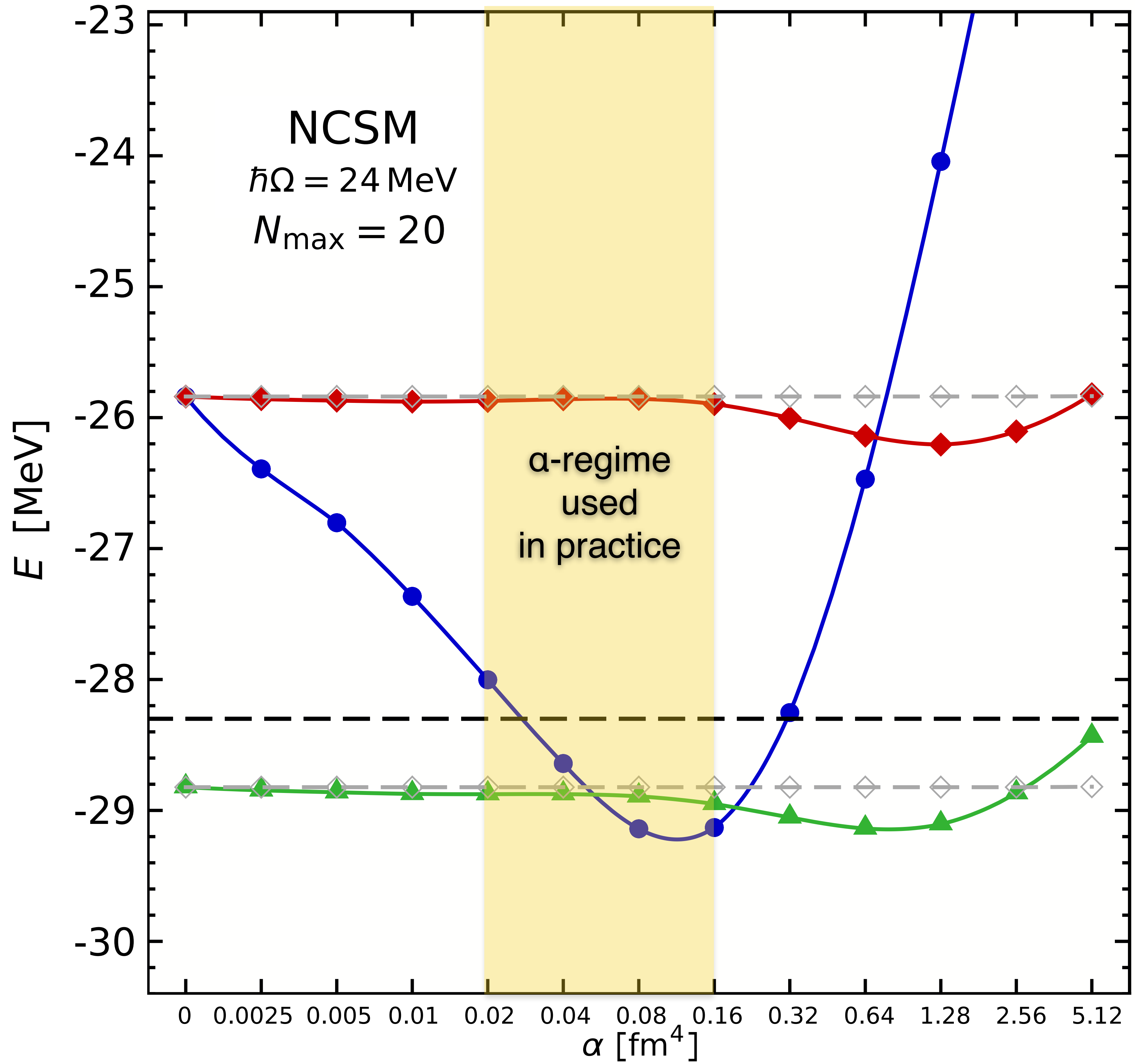
- ***A*-body unitarity**: transformation is unitary only if all terms up to $n = A$ are kept

- **cluster truncation**: evolution in 2B and 3B space generally discard contributions with $n > 3$

- α-dependence of eigenvalues me… …arded many-body contributions

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

^{4}He: Ground-State Energy



initial NN

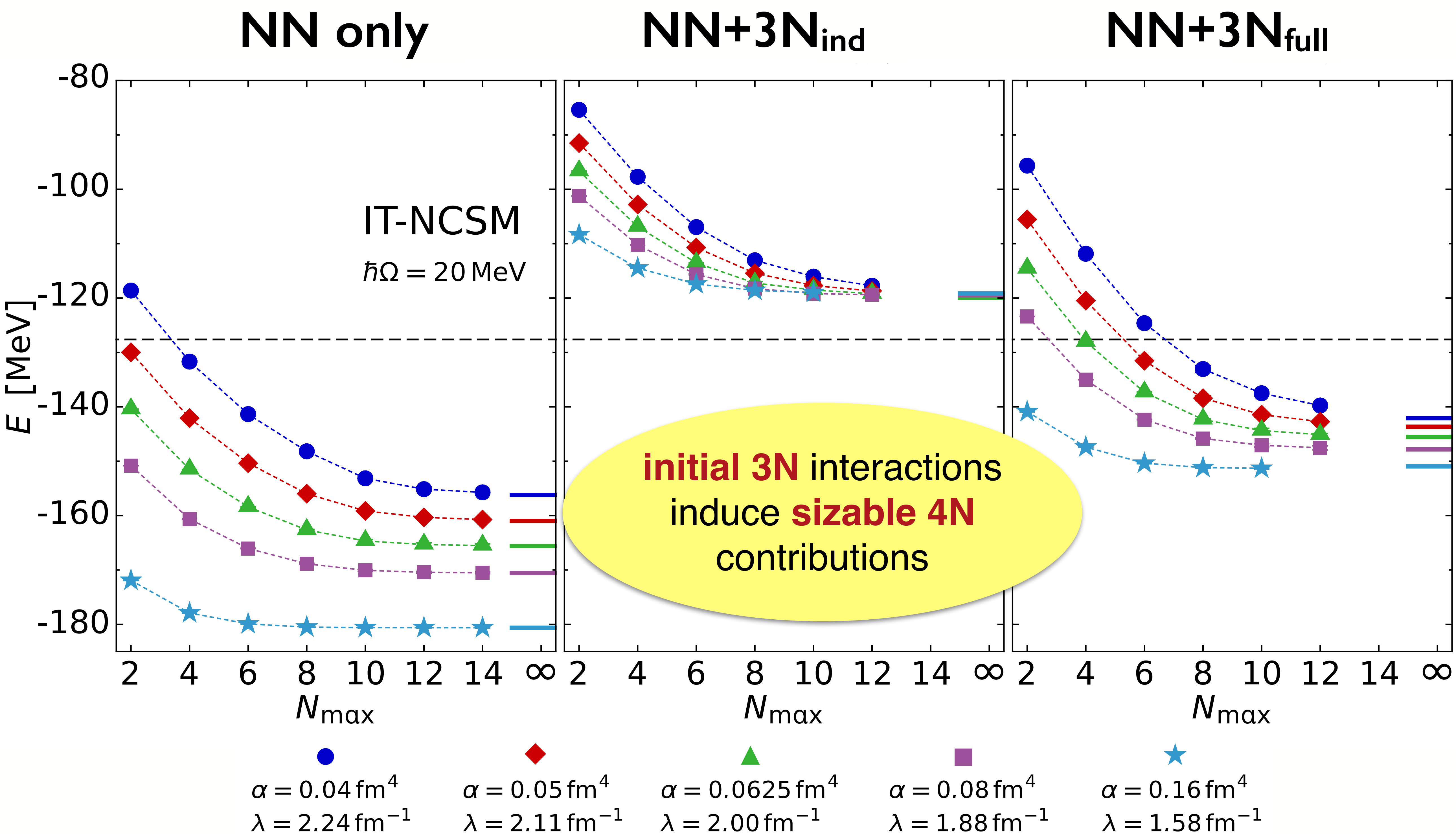
NN_{only} $NN+3N_{ind}$

initial NN+3N

$NN+3N_{full}$

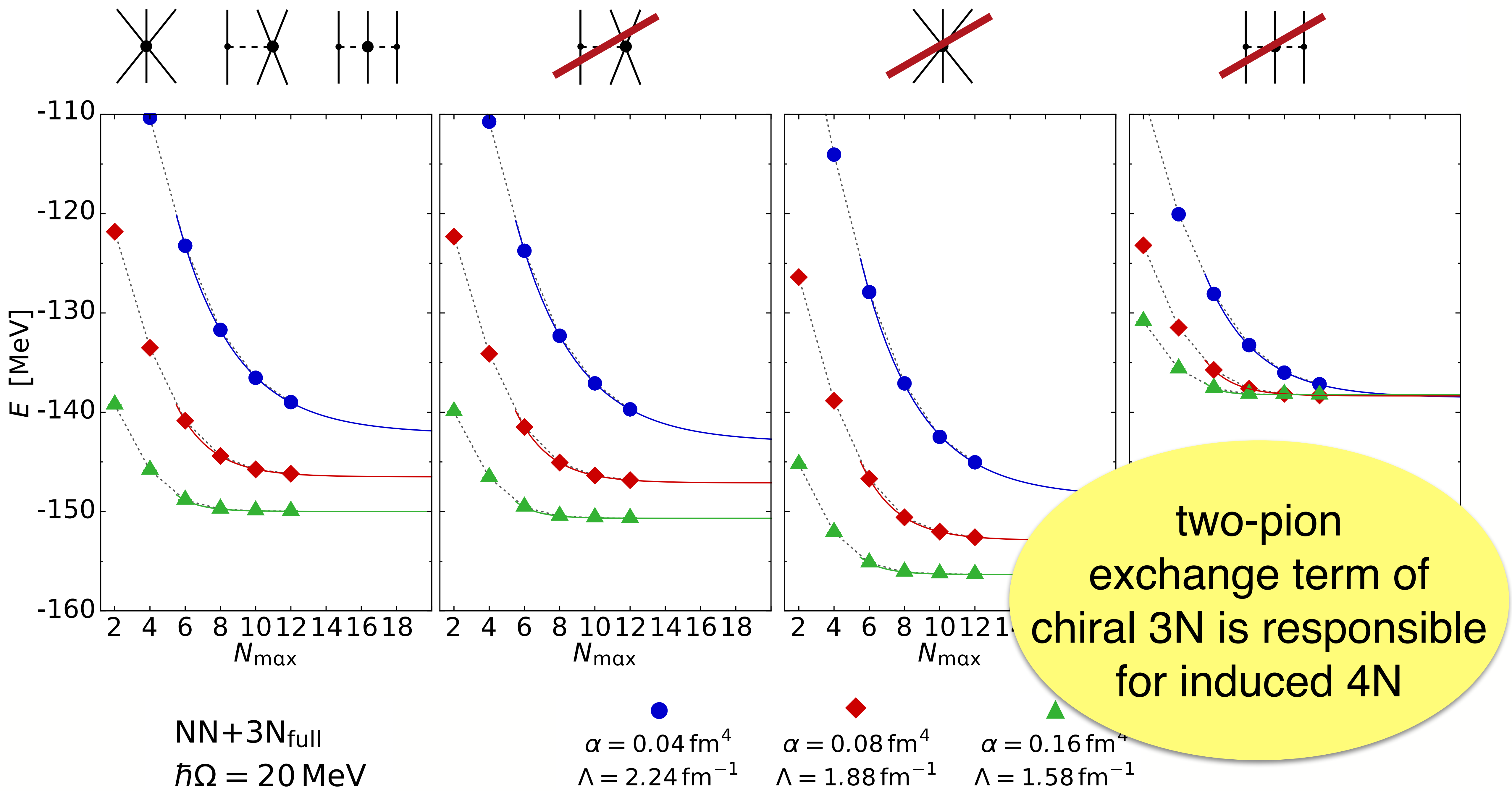
- sizeable induced 3N
- induced **4N negligible** for **large** flow-parameter **range**
- SRG softening has a limit

^{16}O: Ground-State Energy

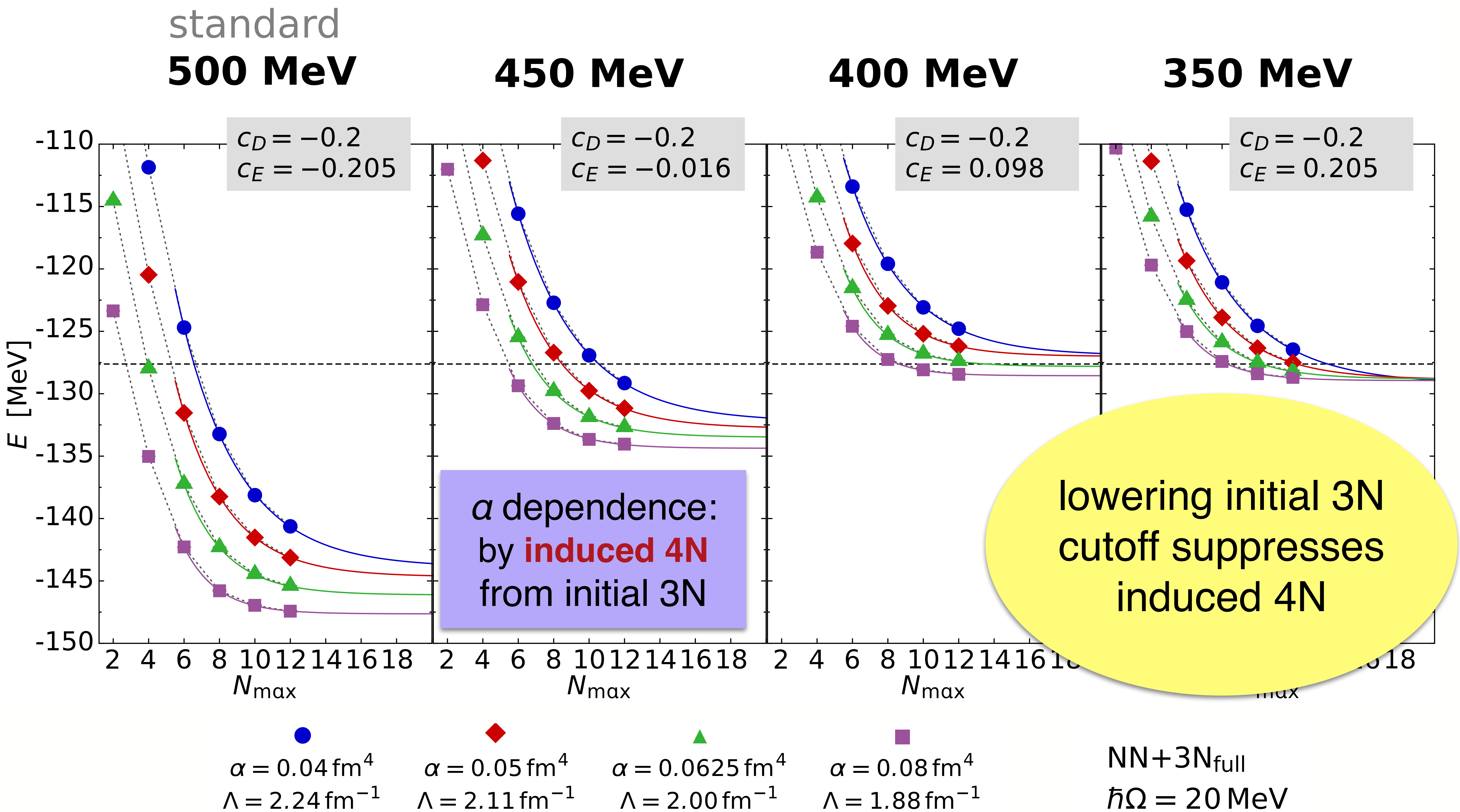


^{16}O: Origin of Induced 4N

switch off individual contributions of the 3N interaction



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



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Towards Heavy Nuclei with NN+3N Interactions

Binder, Langhammer, AC, Roth — Phys. Lett. B 736, 119-123 (2014)

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)

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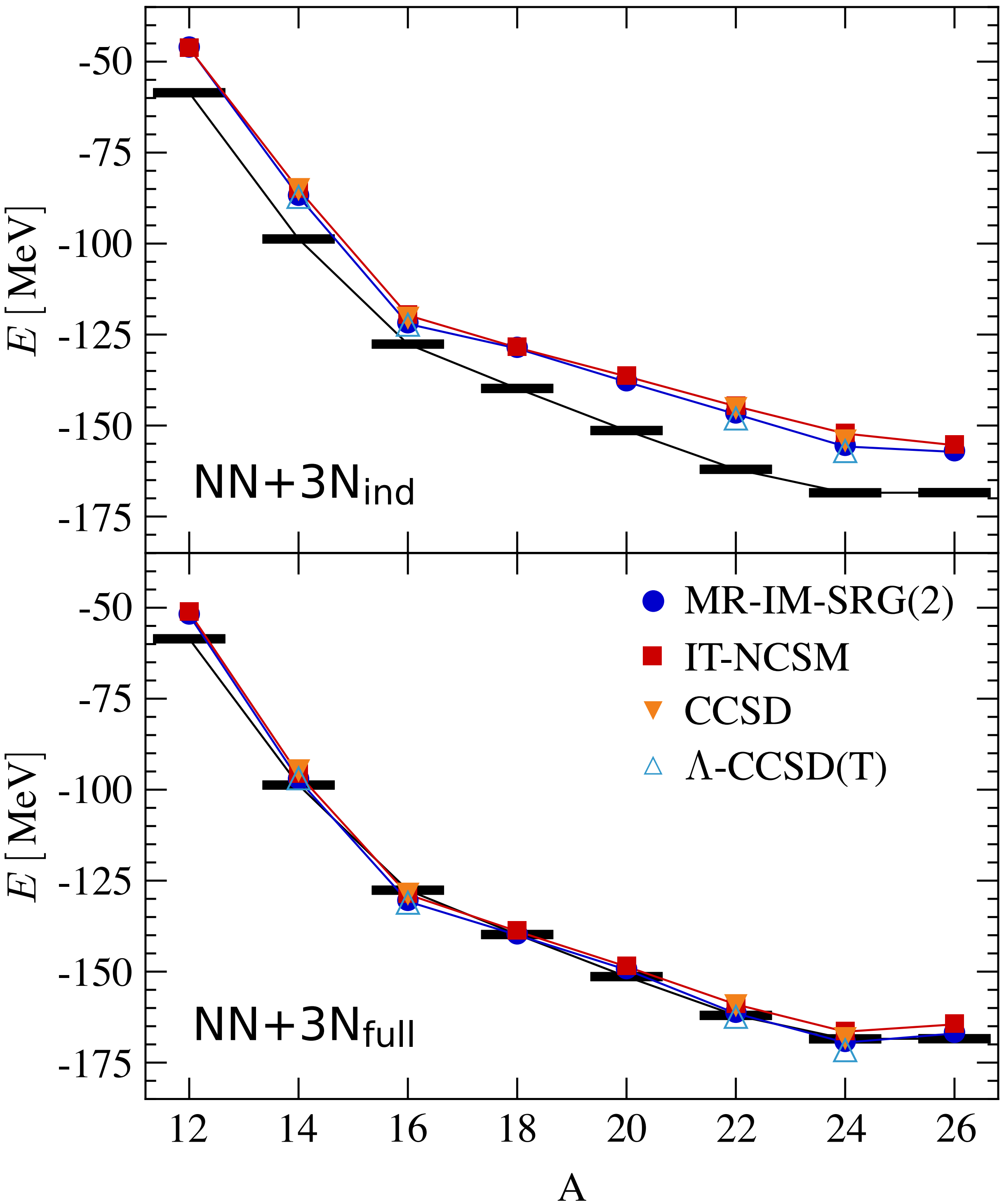
Oxygen Istopes

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

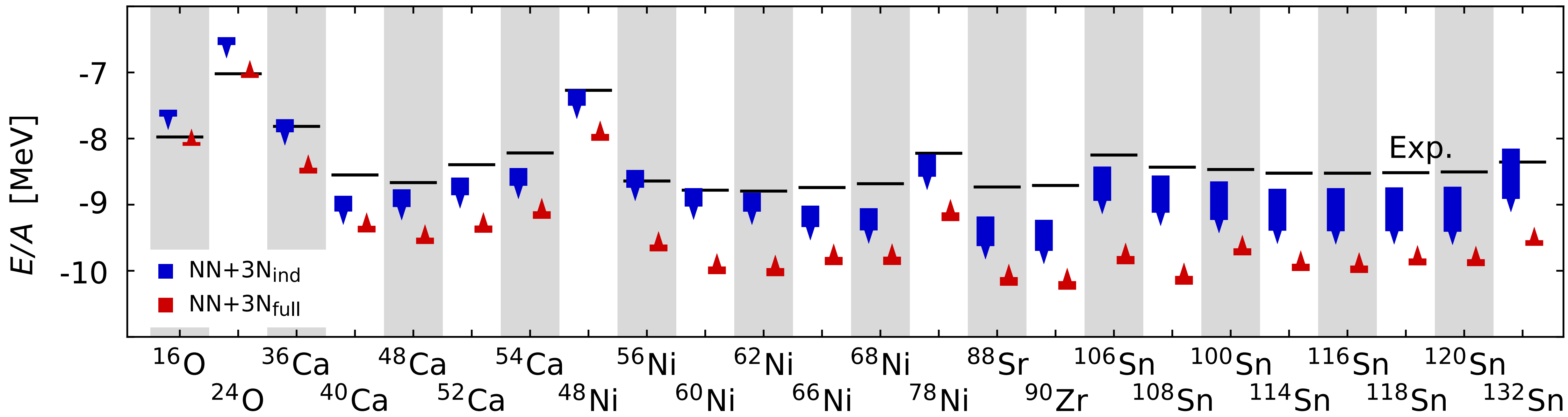


- investigate **effect of 3N** interactions
- **quantify uncertainties** of medium mass approaches
- access nuclei up to **driplines** with ab initio approaches

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

Heavy Nuclei

Binder, Langhammer, AC, Roth *Phys. Lett. B 736 (2014) 119-123*



- many-body method and truncation well under control

➡ **initial NN** interaction **induces sizable 4N** with increasing mass number

- **cancellation between 4N** contributions induced by initial NN (attractive) and 3N (repulsive)

- **mass trend reproduced** throughout nuclear chart

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

Induced Four-Body Contributions

induced 4N constitute **major limitation** for applications of chiral interactions

1. 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)

2. **include 4N contributions**
   - SRG evolution in four-body space
   - extension of all HO developments and IT-NCSM to treat 4N

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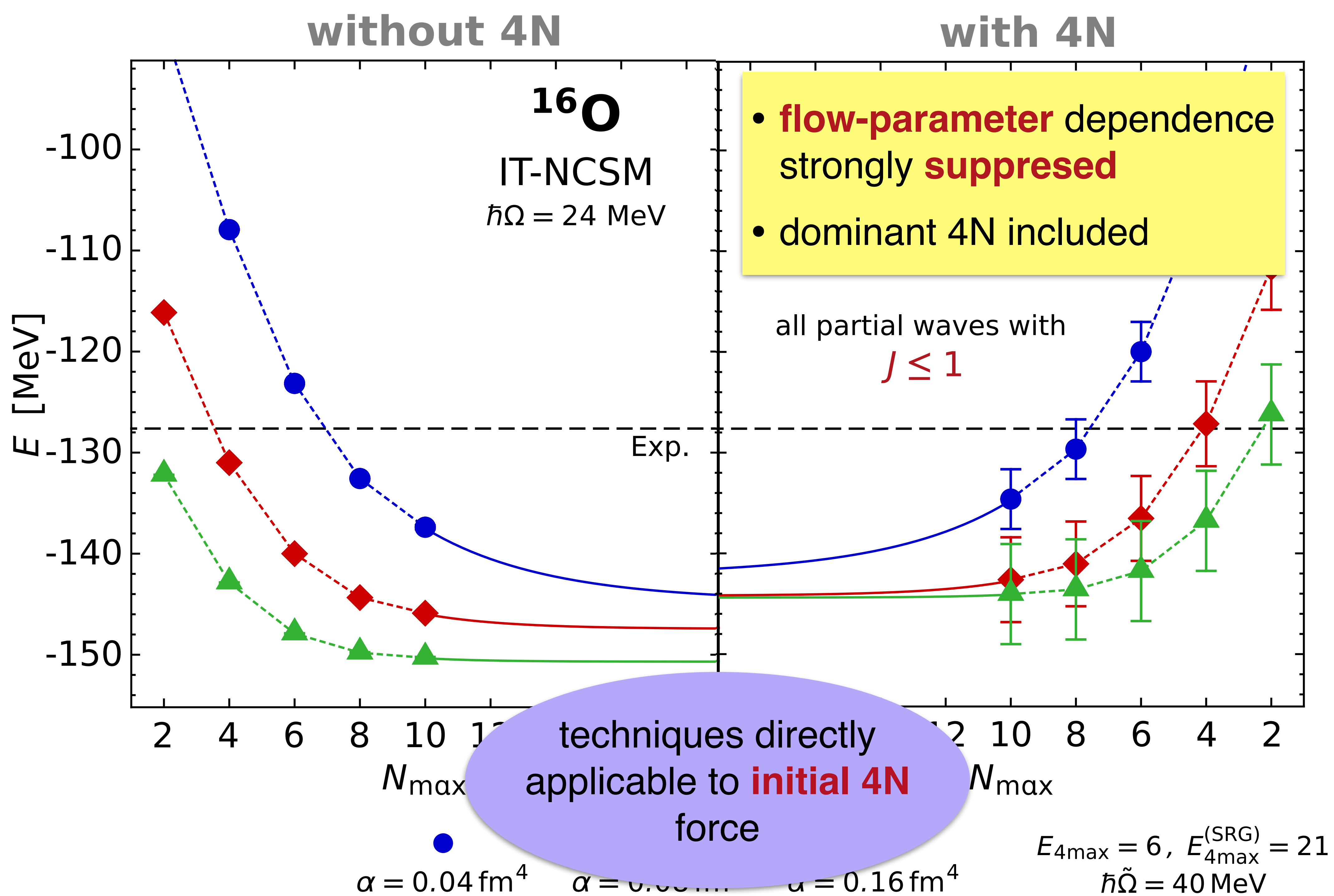
IT-NCSM with Four-Body Contributions



- **flow-parameter** dependence strongly **suppresed**
- dominant 4N included

techniques directly applicable to **initial 4N** force

Induced Four-Body Contributions

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2. include 4N contributions
   - SRG evolution in four-body space
   - extension of all HO developments and IT-NCSM to treat 4N

3. find alternative SRG generator to exclude induced 4N from the outset
   - promising **ideas** for a **better compromise** between induced forces and convergence acceleration
     Dicaire, Omand, Navratil Phys. Rev. C 90, 034302 (2014)

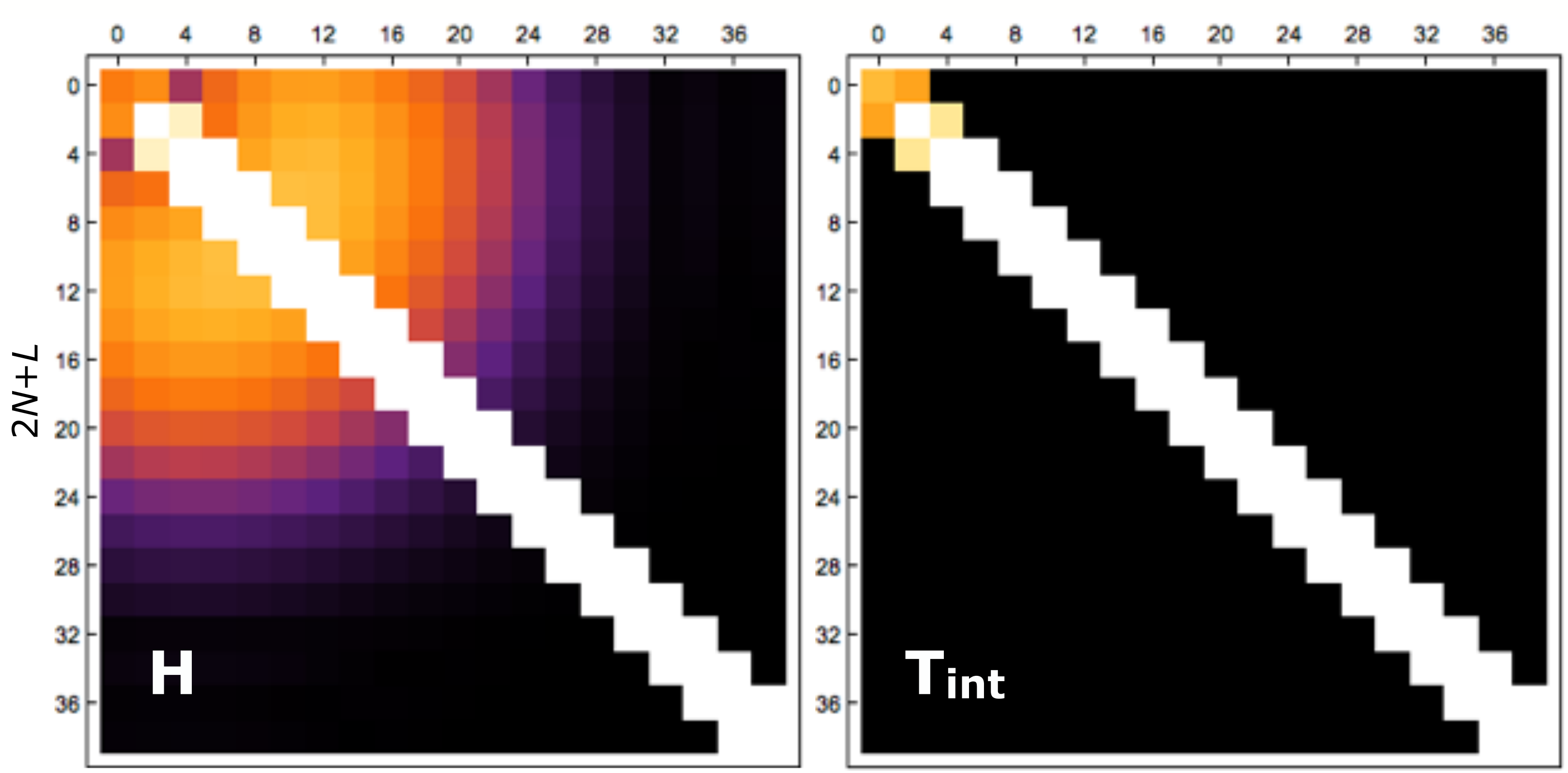
SRG with Block Generators

- SRG flow equation:

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\widetilde{\mathrm{H}}_\alpha = \left[\eta_\alpha, \widetilde{\mathrm{H}}_\alpha\right] \quad \text{with} \quad \eta_\alpha = (2\mu)^2 \left[\mathrm{G}, \widetilde{\mathrm{H}}_\alpha\right]$$

- G determines **trivial fix point** of the flow

$$\mathrm{G} = T_{\mathrm{int}}$$



diagonalizes part of Hamiltonian that can be covered by model space

HO matrix elements, $^1S_0$ channel, $\hbar\Omega$ = 24 MeV

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SRG with Block Generators

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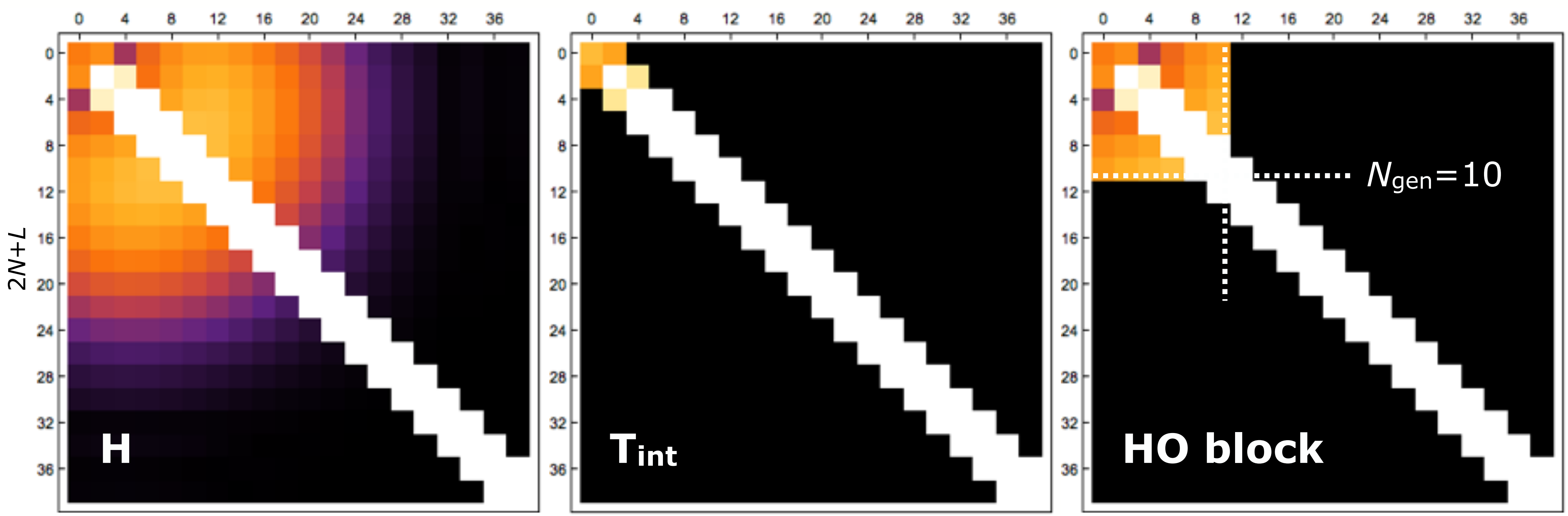
$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha] \quad \text{with} \quad \eta_\alpha = (2\mu)^2 [G, \widetilde{H}_\alpha]$$

- G determines **trivial fix point** of the flow

$$G = T_{\text{int}} + \Pi_{N_{gen}} V \, \Pi_{N_{gen}}$$

with $\Pi_{N_{\text{gen}}}$ projection on HO space defined by $2N + L \leq N_{\text{gen}}$



HO matrix elements, $^1S_0$ channel, $\hbar\Omega$ = 24 MeV

SRG with Block Generators

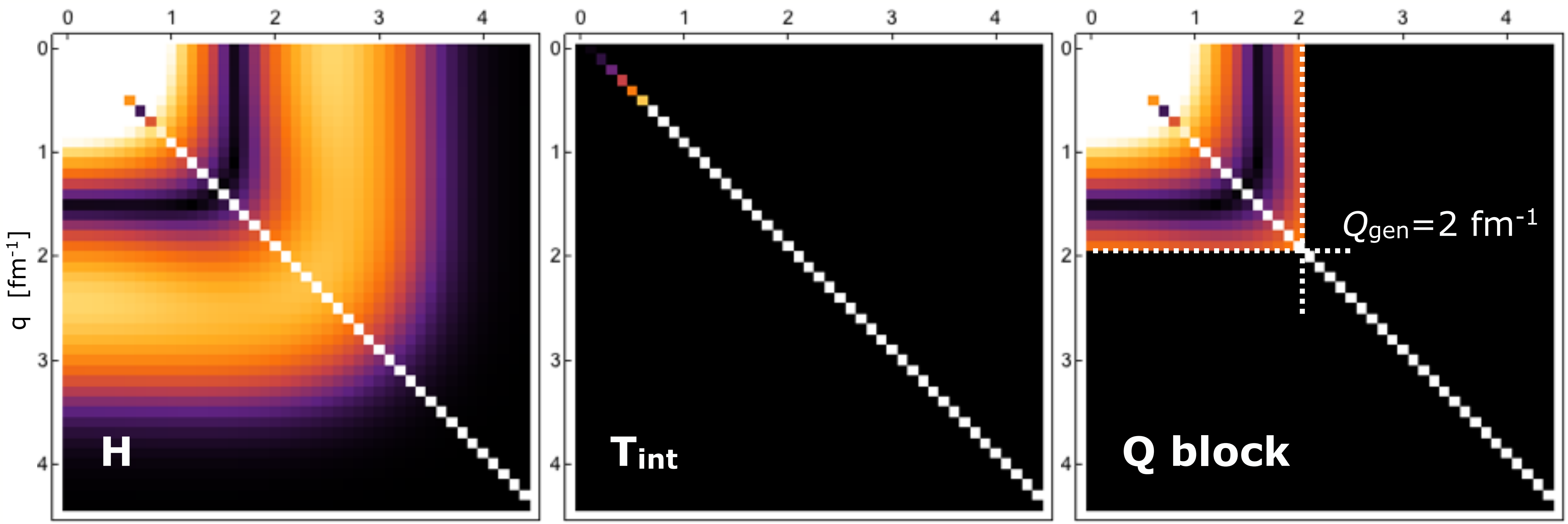
- SRG flow equation:

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha] \quad \text{with} \quad \eta_\alpha = (2\mu)^2 [G, \widetilde{H}_\alpha]$$

- G determines **trivial fix point** of the flow

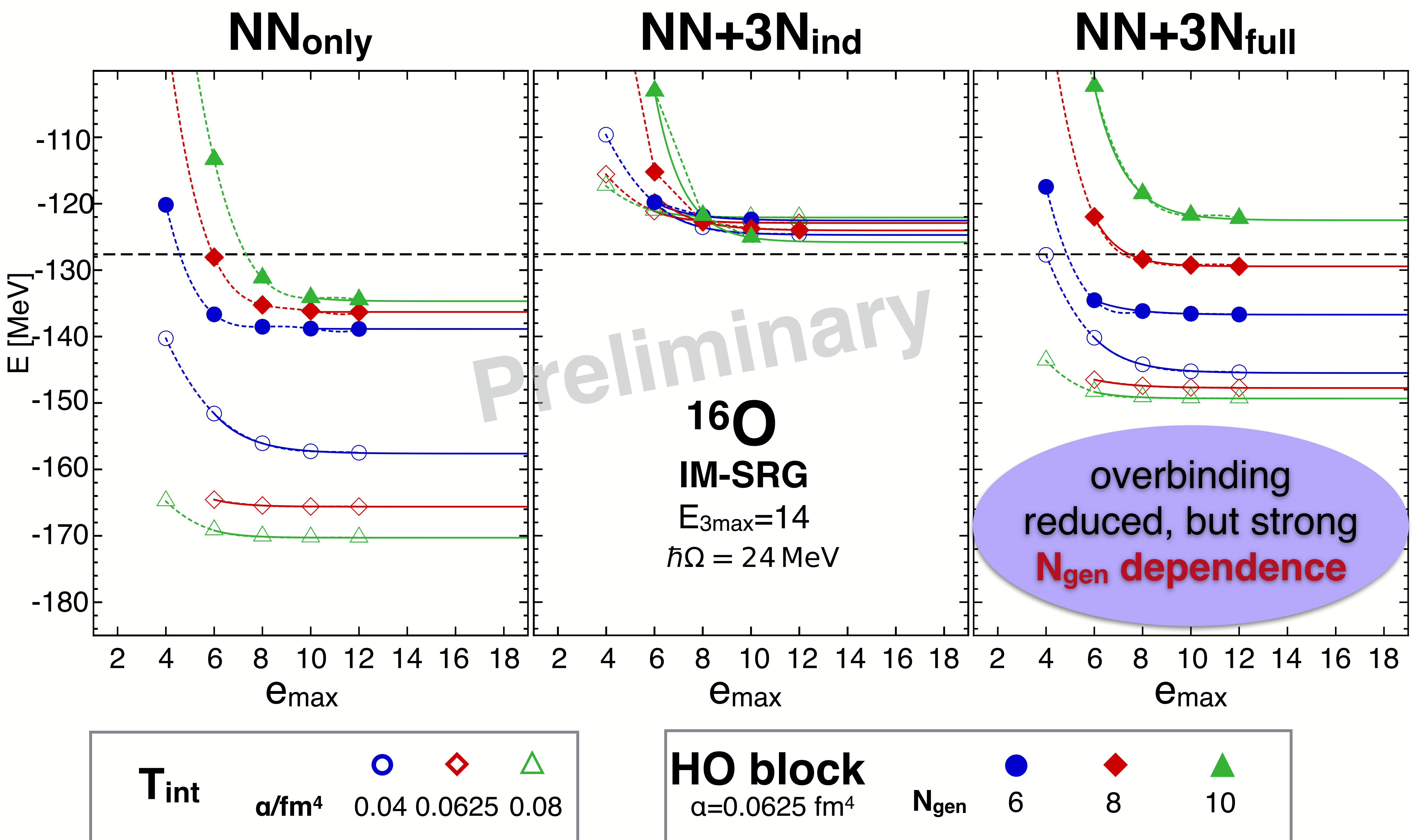
$$G = T_{\text{int}} + \Pi_{Q_{gen}} V \, \Pi_{Q_{gen}}$$

with $\Pi_{Q_{\text{gen}}}$ projection on momentum space defined by $q \leq Q_{\text{gen}}$

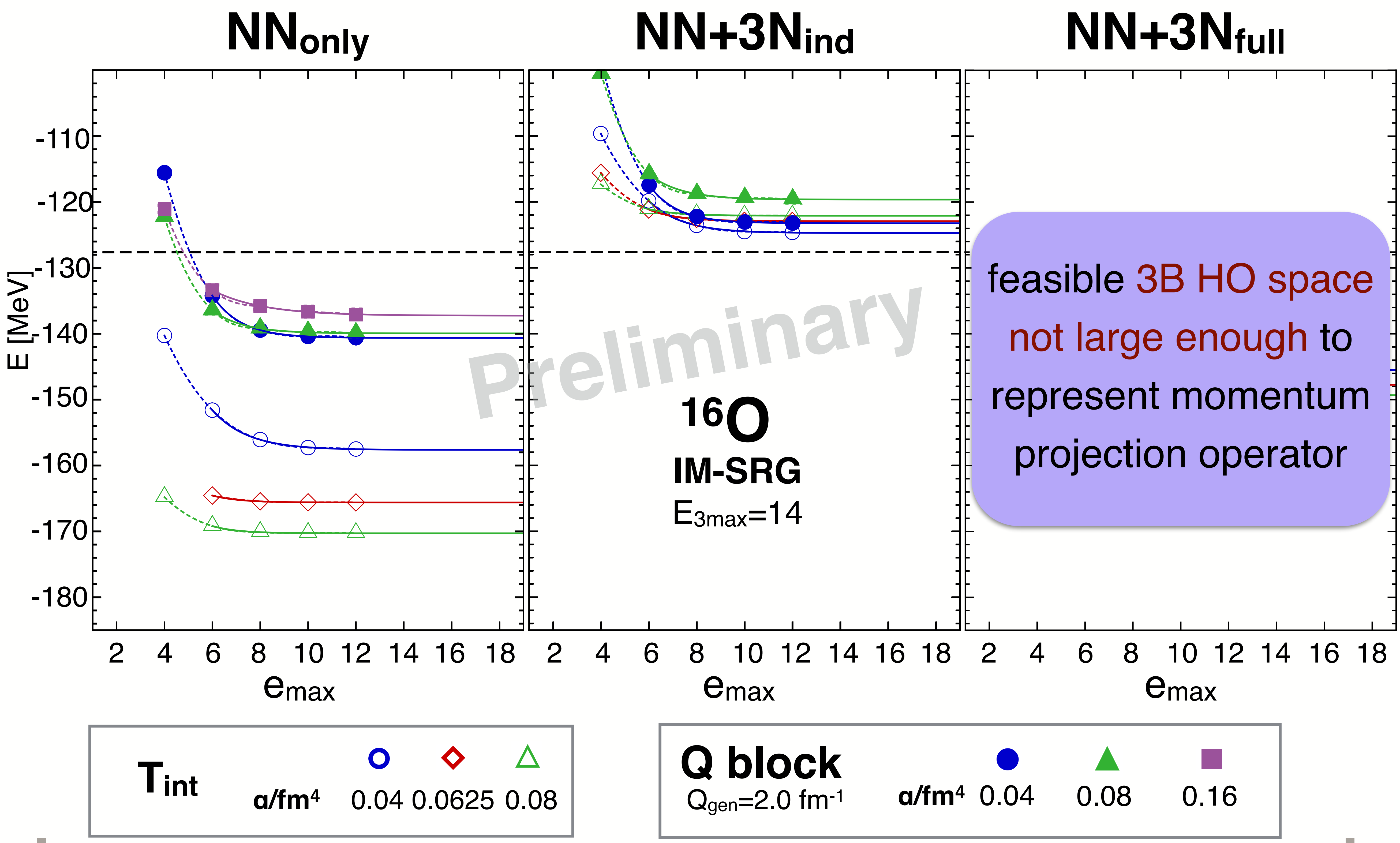


momentum-space matrix elements, $^1S_0$ channel

HO-Block Generator

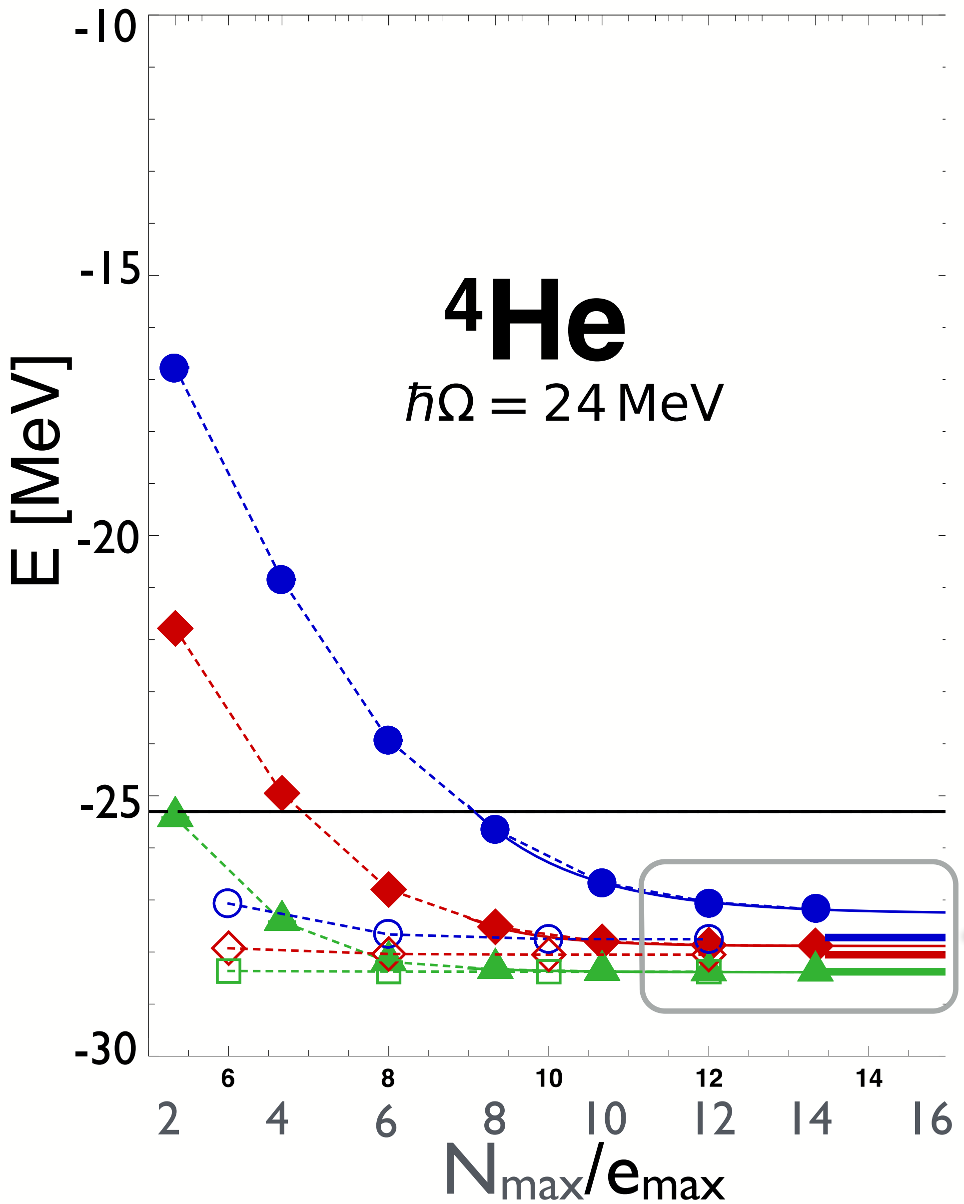


Q-Block Generator



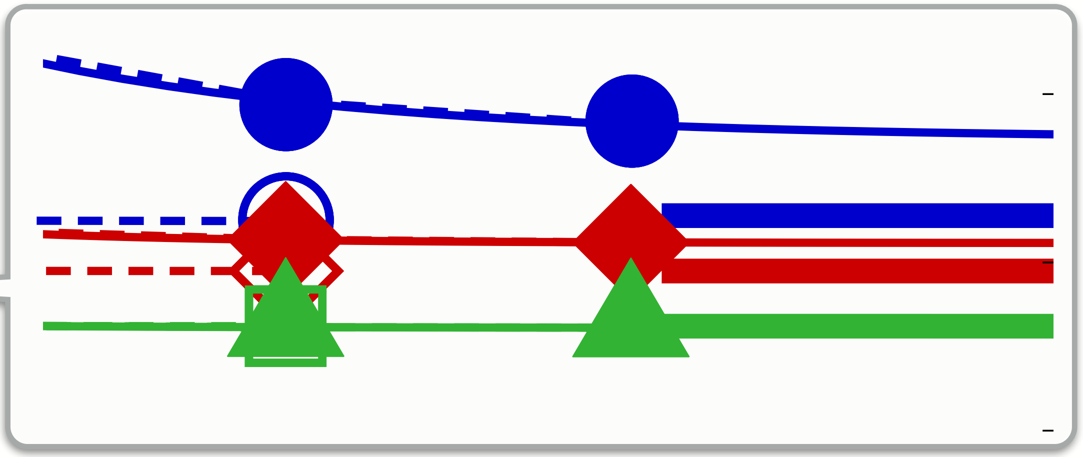
IT-NCSM vs IM-SRG

NN_{only}



T_{int} Generator

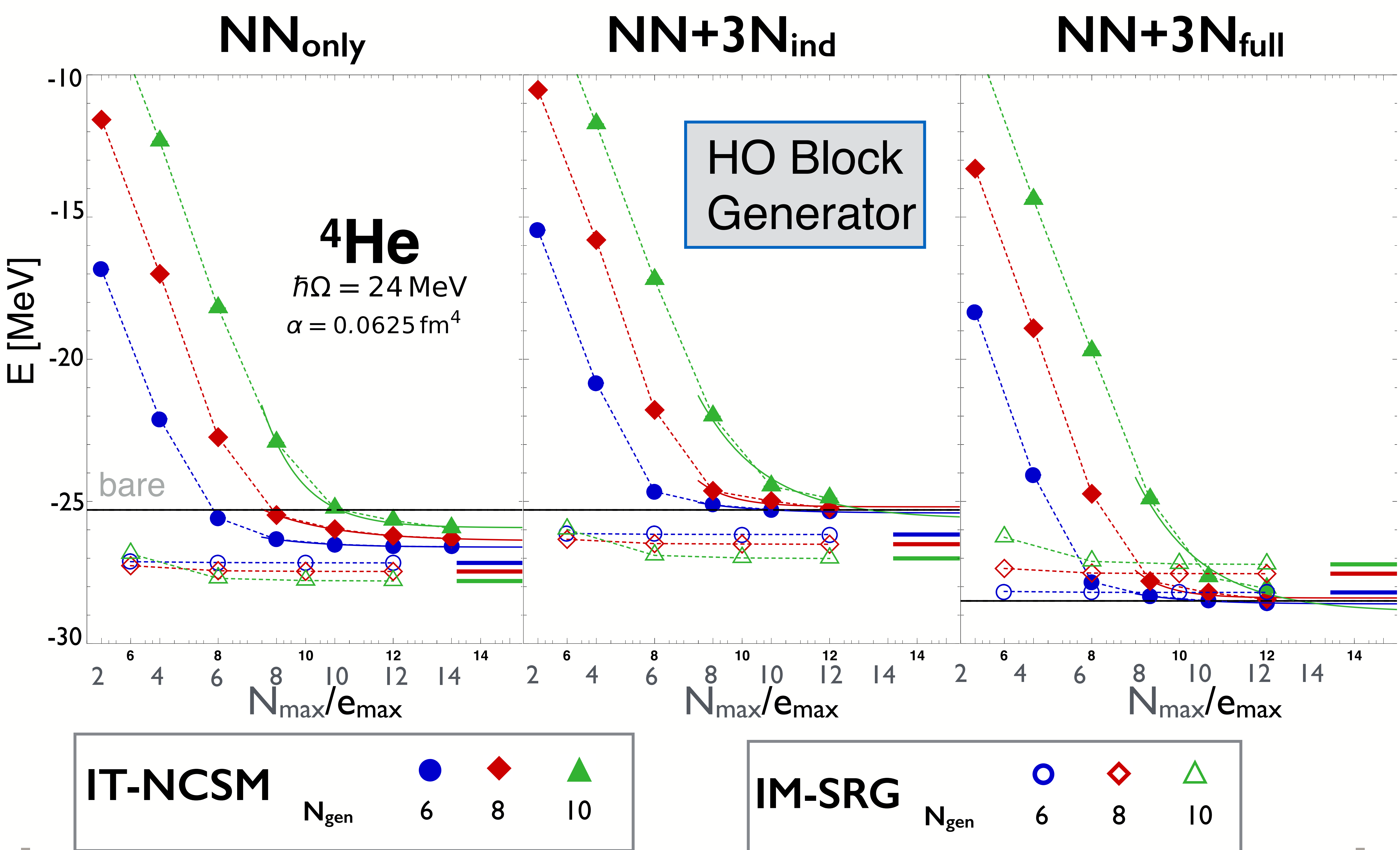
- **discrepancies** between IT-NCSM and IM-SRG for **harder interactions**
- NO2B approximation or IM-SRG?



IT-NCSM α/fm^4 ● 0.02 ◆ 0.04 ▲ 0.08

IM-SRG α/fm^4 ○ 0.02 ◇ 0.04 △ 0.08

HO Block: IT-NCSM vs IM-SRG



Alternative Chiral Hamiltonians & Uncertainty Quantification

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Uncertainties of Chiral Interactions

in the past

- uncertainties **from many-body approach** included
- observables calculated for **single chiral Hamiltonian** (inconsistent chiral order)
- quality of chiral forces assessed by agreement with experiment

present and future

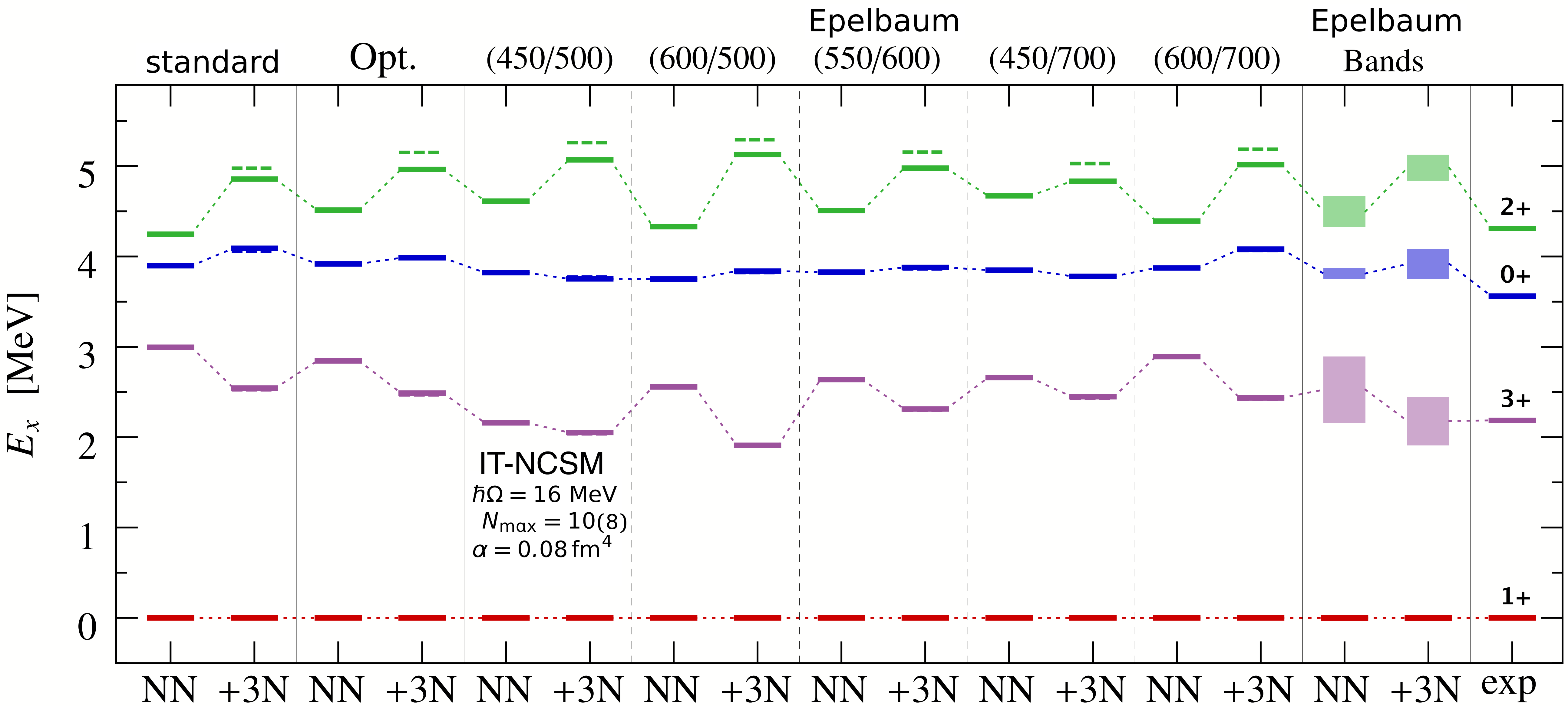
- start with NN+3N force at **consistent** chiral **orders**
- use **sequence of cutoffs** and **different** chiral **orders**

➡ estimate **uncertainties** of chiral EFT and many-body approach

nuclear structure physics approaches new era

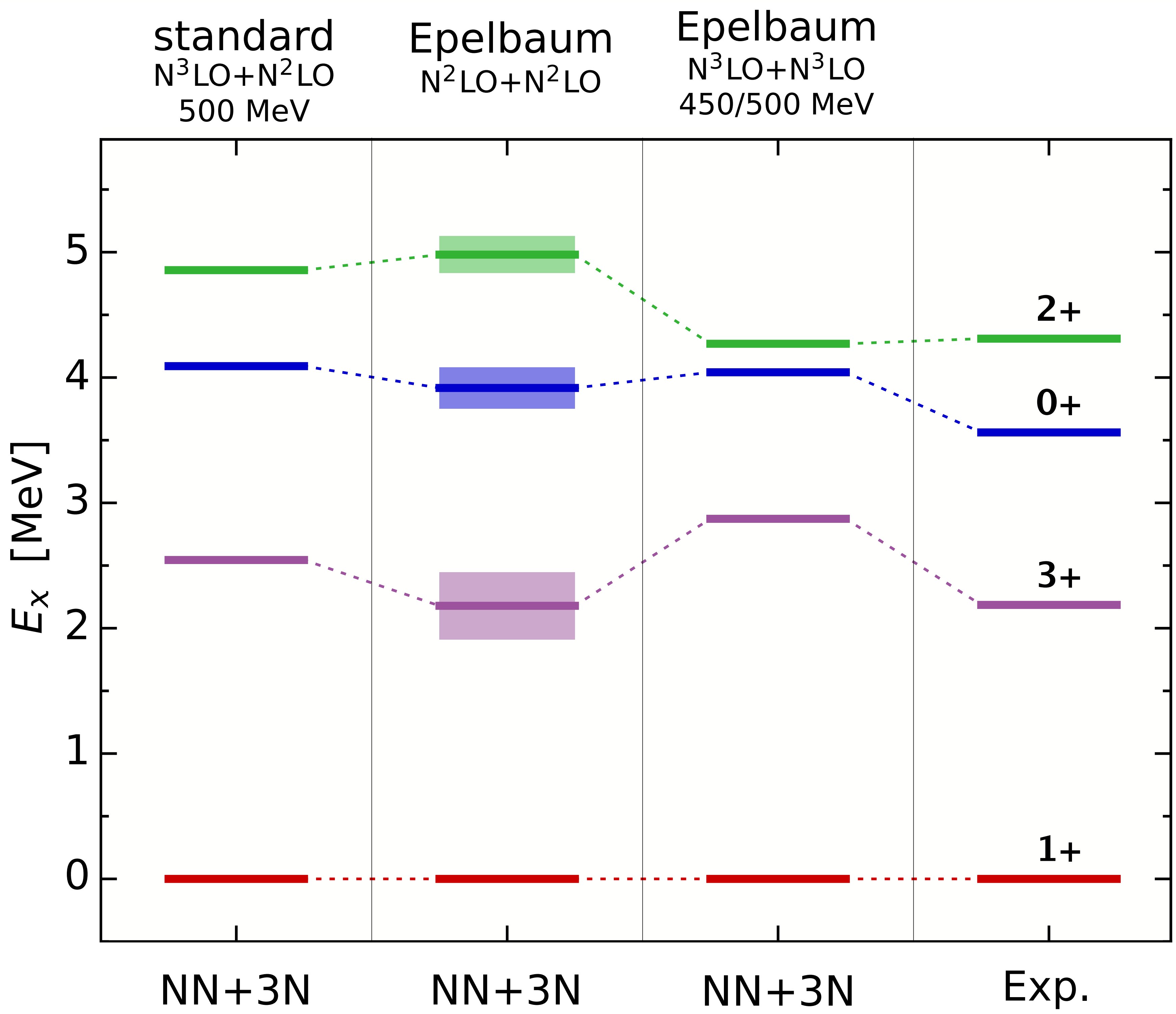
- **ongoing progress** in construction of consistent NN+3N Hamiltonians
  - N^2LO [Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal]
  - N^3LO [Epelbaum et al., 450 MeV cutoff, nonlocal]
- first step towards reliable uncertainty quantification in nuclear spectroscopy

^{6}Li: Cutoff Dependence



- small cutoff dependence
- reasonable predictions

^{6}Li: Chiral Order Dependence



- small cutoff dependence
- reasonable prediction
- further cutoffs required at N^3LO

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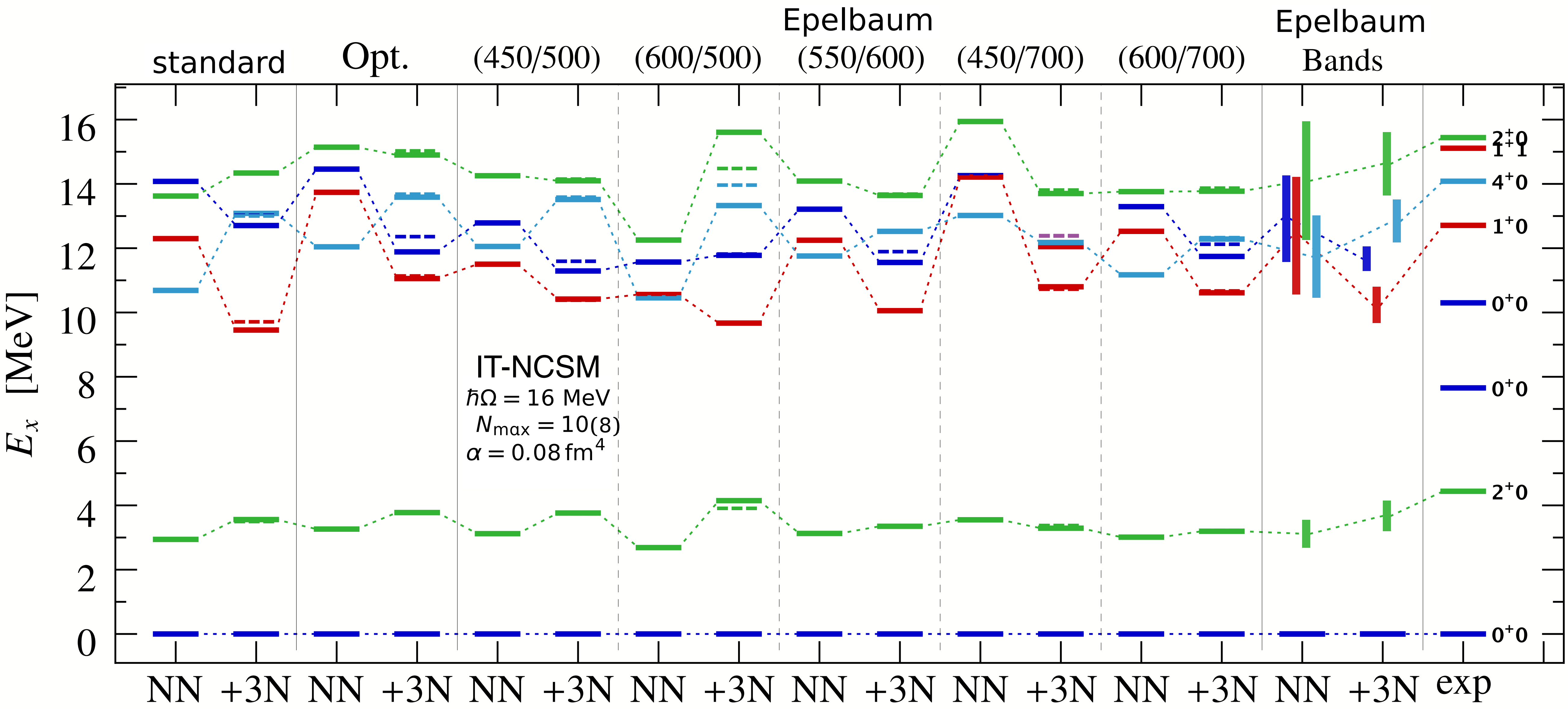
^{12}C: Cutoff Dependence



- small cutoff dependence for NN+3N

Quadrupole Observables

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B(E2) and Quadrupole moment

challenges in calculating quadrupole observables:

- **observables** need to be **SRG evolved**
  - **induced many-body contributions** can become problematic
- generally **slow convergence** in HO space

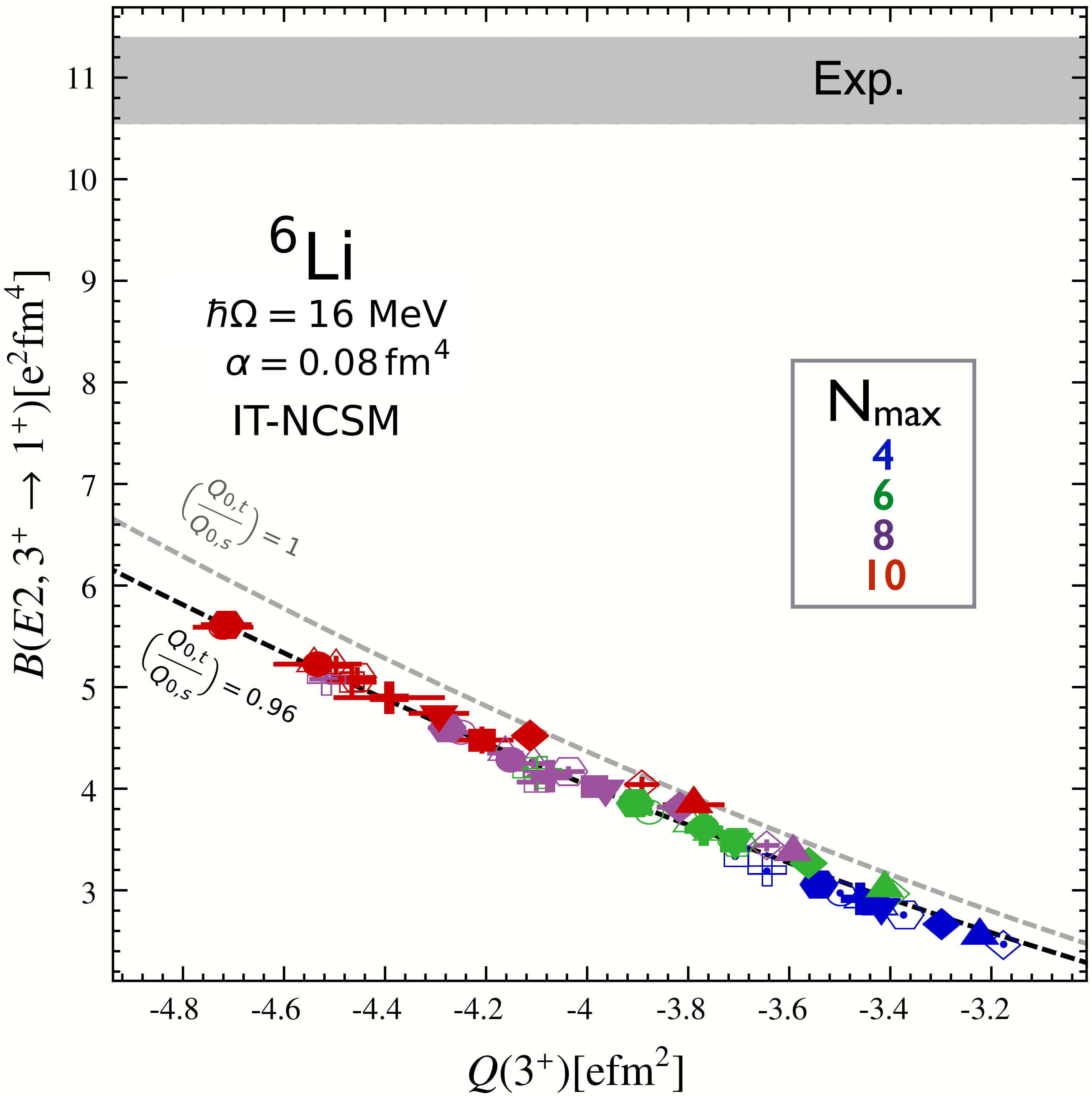
simple rotational model:

- observables connected via intrinsic quadrupole moment Q_0

$$B(E2, J_i \rightarrow J_f) = \frac{5}{16\pi} \frac{((J+1)(2J+3))^2}{(3K^2 - J(J+1))^2} \begin{pmatrix} J_i & 2 & J_f \\ K & 0 & K \end{pmatrix} \left(\frac{Q_{0,t}}{Q_{0,s}}\right)^2$$

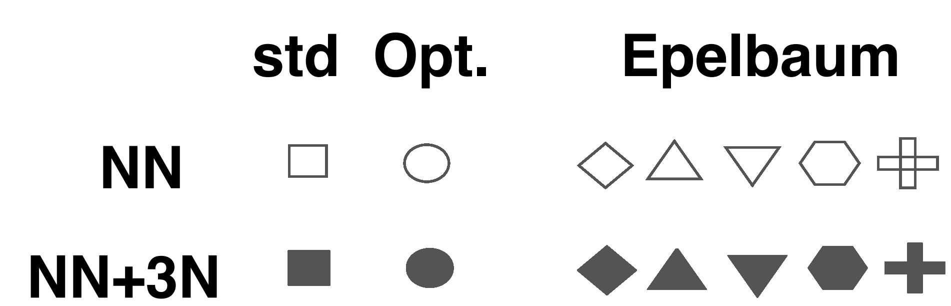
quadratic relation between B(E2) and Quadrupole moment

^{6}Li: Quadrupole Correlation

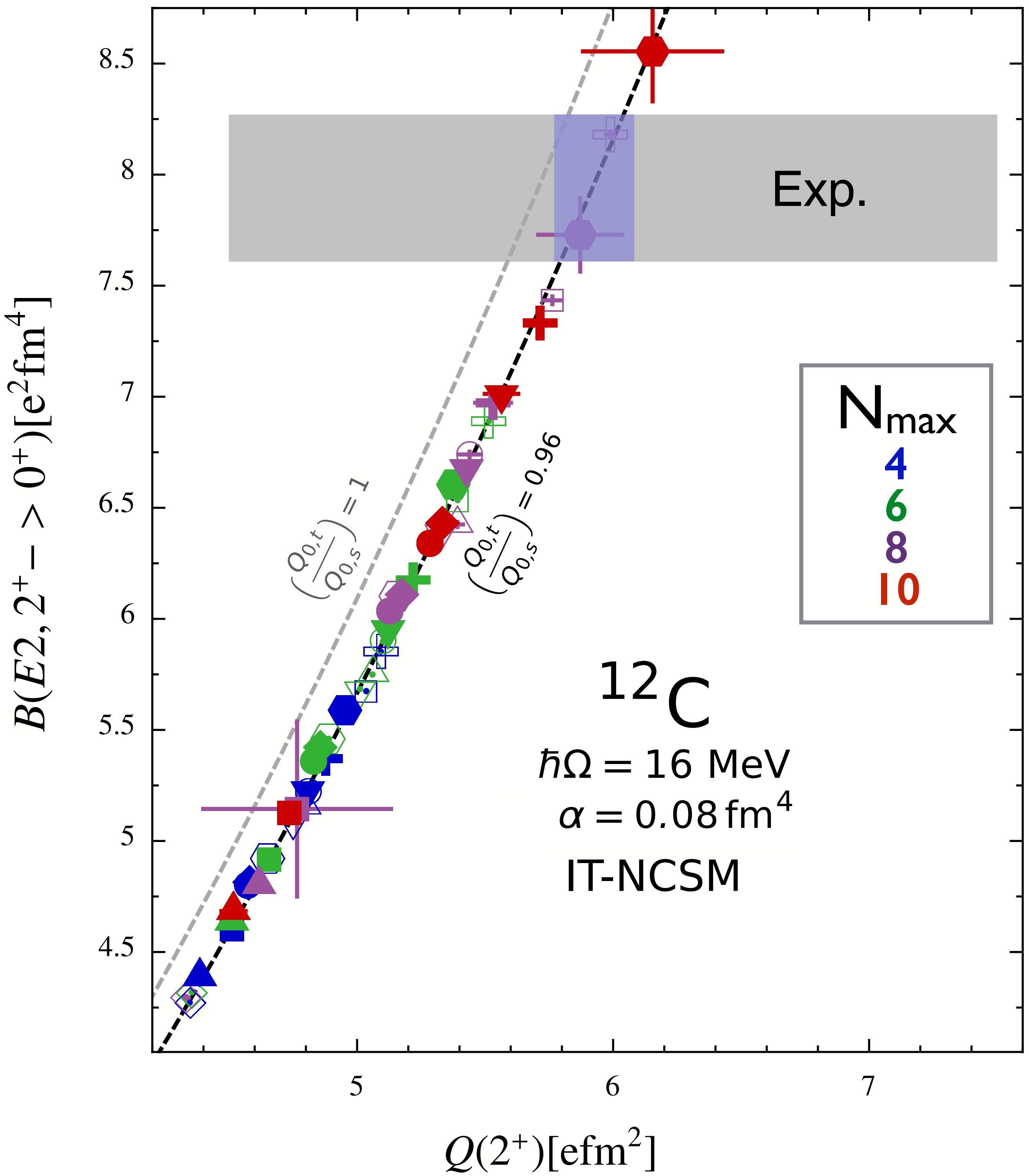


- **robust correlation** between B(E2) and spectroscopic Q value
- independent of:
  - chiral interaction / cutoff
  - model space
  - SRG flow parameter

can combine correlation curve with measured B(E2) to **predict Q** precisely



^{12}C: Quadrupole Correlation

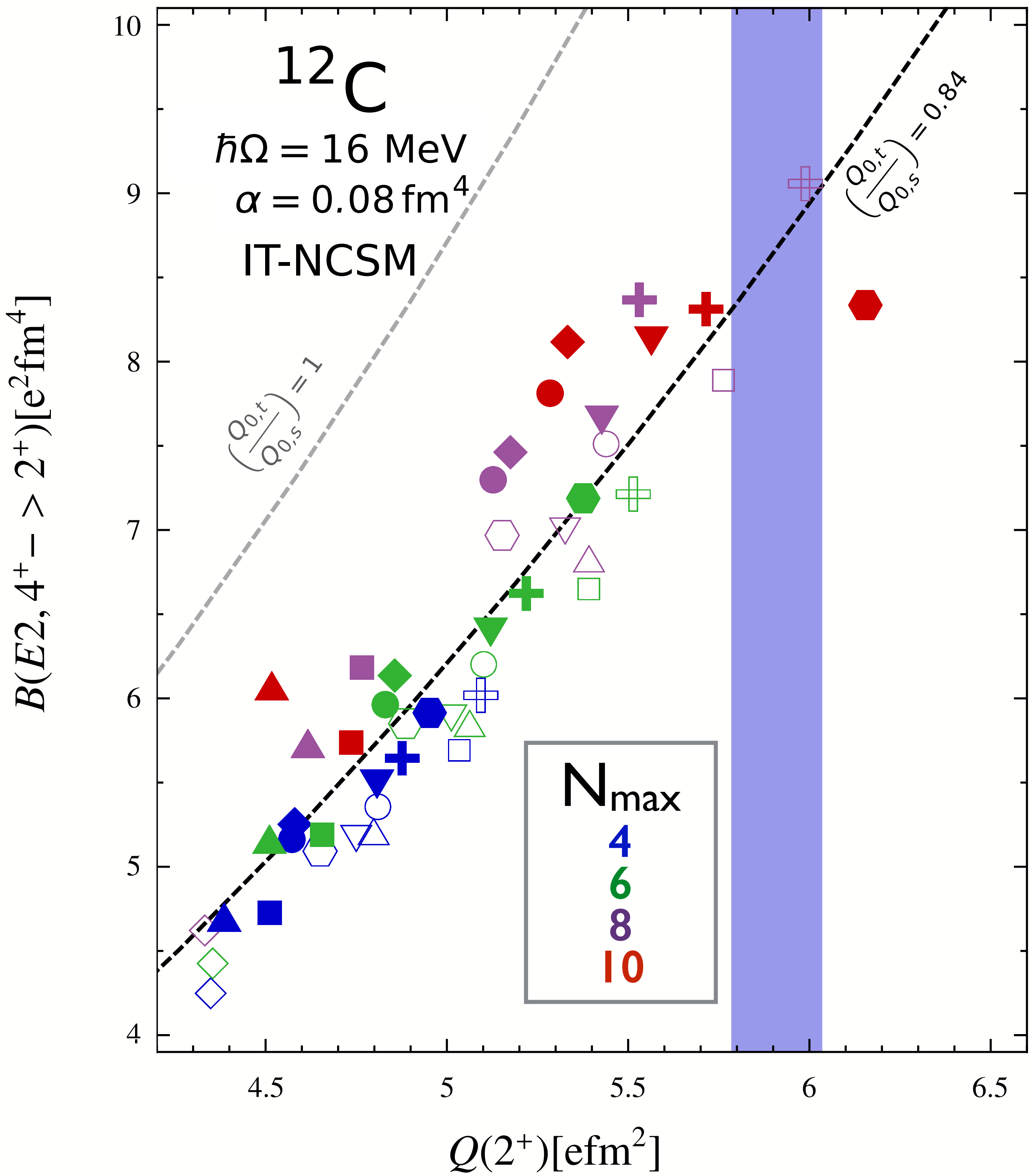


- **robust correlation** between B(E2) and spectroscopic Q value
- independent of:
  - chiral interaction / cutoff
  - model space
  - SRG flow parameter

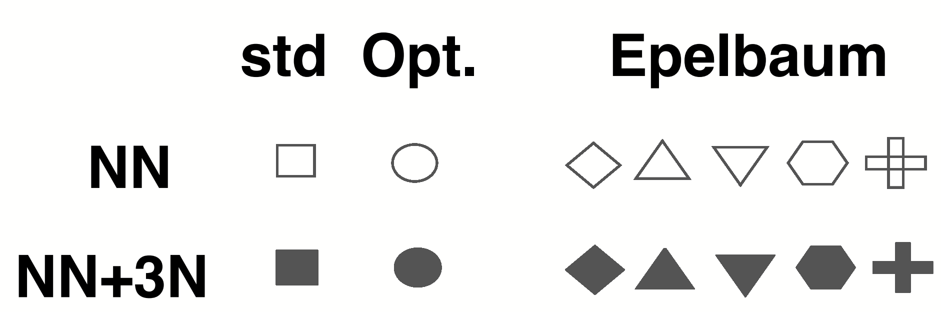
can combine correlation curve with measured B(E2) to **predict Q** precisely

	std	Opt.	Epelbaum
NN	□	○	◇ △ ▽ ⬡ ✚
NN+3N	■	●	◆ ▲ ▼ ⬢ ✚

^{12}C: Quadrupole Correlation



- **less robust correlation** between B(E2) and spectroscopic Q value
- can be used to predict B(E2,$4^+ \rightarrow 2^+$) rather precise



Outlook

- exciting **progress** in construction of **chiral forces**
  - **$N^2LO_{opt/sat/sim/sep}$** different strategies to fit LECs
  - **local interaction** up to N^2LO for quantum Monte Carlo
    Gezerlis, Tews, Epelbaum et al. Phys. Rev. C 90, 054323 (2014)
  - **minimally n**... ...lude Δ in TPE
    comp...
    Pia...

self-contained framework to employ **present and future chiral NN+3N +4N interactions** in a variety of many-body methods

- improved NN up to N...
  Epelbaum et al. arXiv:1412.0142; arXiv:1412.4623
- **3N** up to N^3LO
  - allow to vary cutoff and chiral order to quantify uncertainty

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Thank you! Merci!

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  - H. Feldmeier
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COMPUTING TIME