Effective Nuclear Hamiltonians for ab initio Nuclear Structure Calculations

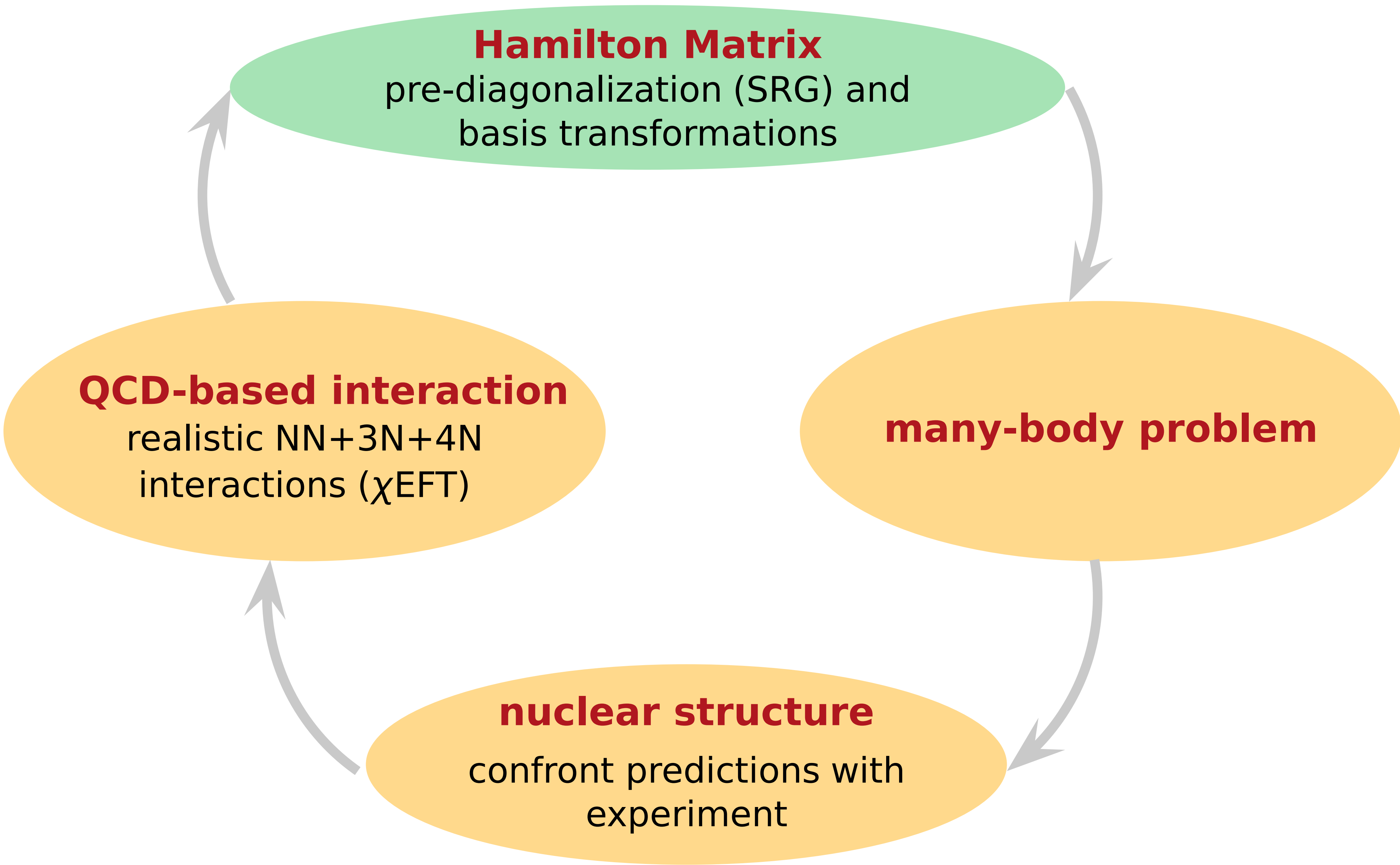
Angelo Calci

TRIUMF

Hirschegg 2015

Nuclear Structure and Reactions: Weak, Strange and Exotic

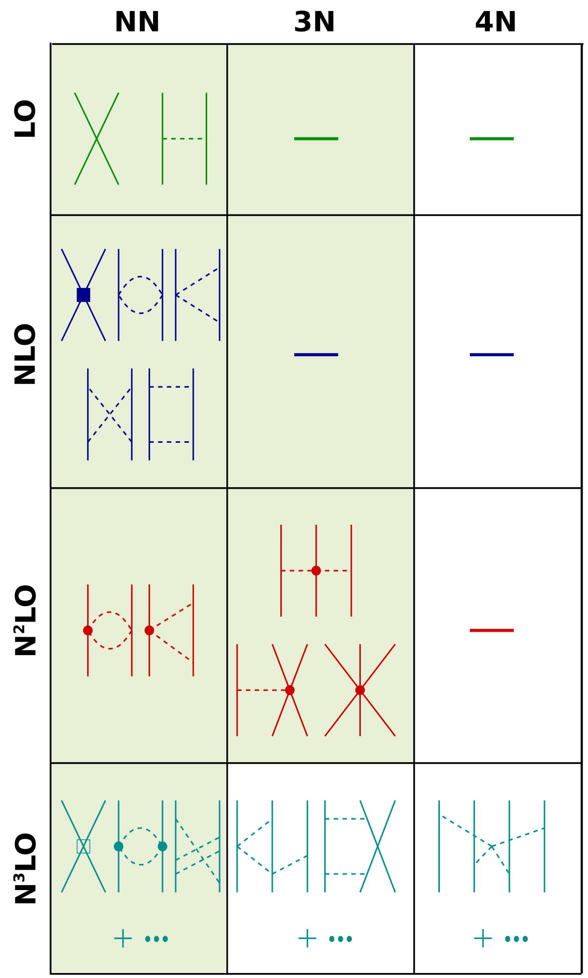
Introduction



Chiral NN+3N Interactions

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

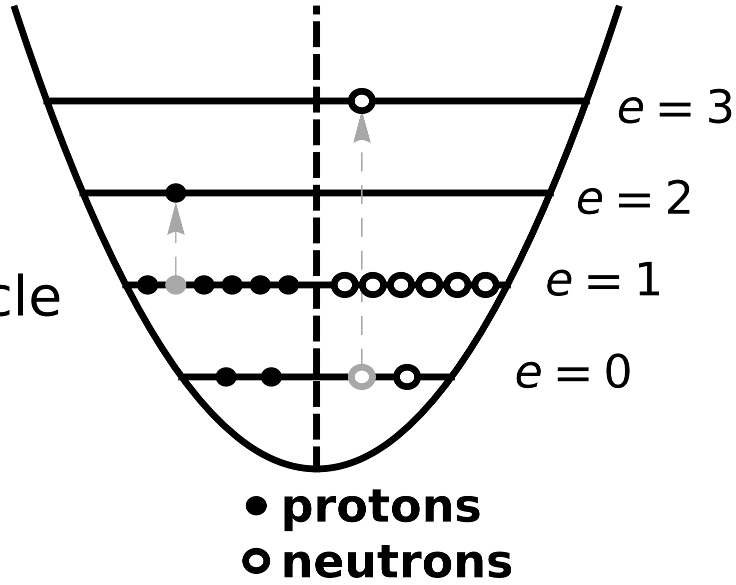
- **standard interaction:**
  - NN @ N^3LO: Entem & Machleidt, 500 MeV cutoff
  - 3N @ N^2LO: Navrátil, local, 500 MeV cutoff, fit to Triton
- **standard interaction with modified 3N:**
  - NN @ N^3LO: Entem & Machleidt, 500 MeV cutoff
  - 3N @ N^2LO: Navrátil, local, with modified LECs and cutoffs, fit to ^{4}He
- **consistent N^2LO interaction:**
  - NN: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal
- **consistent N^3LO interaction:**
  - 3N recently obtained by the LENPIC Collaboration



No-Core Shell Model (NCSM)

- **solving the eigenvalue problem**

$$\mathrm{H_{int}}|\Psi_n\rangle = E_n|\Psi_n\rangle$$



- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states (m-scheme)

$$|\Psi_n\rangle = \sum_\nu C_\nu^n |\Phi_\nu\rangle$$

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

problem

enormous increase of model space with particle number A

$\Rightarrow$ converged calculation limited to small A

Importance-Truncated NCSM

- start with **reference state** $|\Psi_{ref}\rangle$ as approximation of target state $|\Psi_n\rangle$ from limited reference space $\mathcal{M}_{ref}$

- a priori determination of relevant basis states $|\phi_\nu\rangle \notin \mathcal{M}_{ref}$ via first-order perturbation theory

$$\kappa_\nu = -\frac{\langle \Phi_\nu | \mathrm{H}_{\mathrm{int}} | \Psi_{\mathrm{ref}} \rangle}{\epsilon_\nu - \epsilon_{\mathrm{ref}}}$$

- **importance truncated space** $\mathcal{M}(\kappa_{\min})$ spanned by basis states with $|\kappa_\nu| \geq \kappa_{\min}$

- **solving eigenvalue problem** in $\mathcal{M}(\kappa_{\min})$ provides improved approximation for target state

- **extrapolation** of $\kappa_{\min} \to 0$ recovers effect of omitted contributions

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

- expands **application range** to higher A and $N_{\max}$

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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)

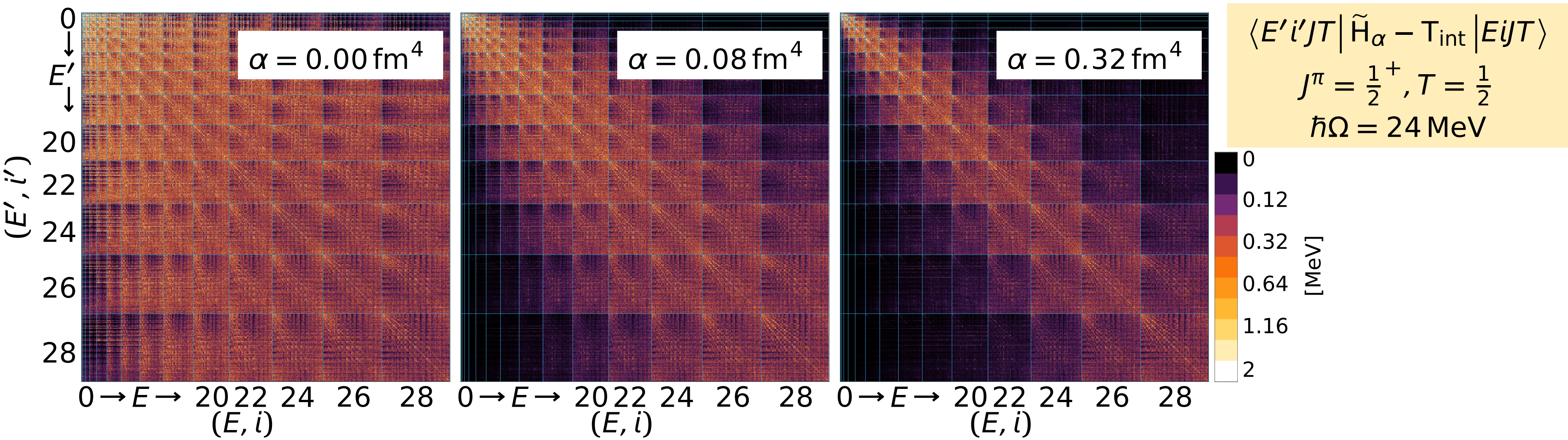
accelerate convergence by **pre-diagonalizing** the Hamiltonian with respect to the many-body basis

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

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

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

3B-Jacobi HO matrix elements



SRG Evolution in A-Body Space

- assume **initial Hamiltonian** and intrinsic kinetic energy are two-body operators written in second quantization

$$\widetilde{H}_0 = \sum \ldots a^\dagger a^\dagger a a\,, \qquad T_{\text{int}} = T - T_{\text{cm}} = \sum \ldots a^\dagger a^\dagger a a$$

- perform **single evolution step** $\Delta\alpha$ in Fock-space representation

$$\widetilde{H}_{\Delta\alpha} = \widetilde{H}_0 + \Delta\alpha \left[\left[T_{\text{int}}, \widetilde{H}_0 \right], \widetilde{H}_0 \right]$$

$$= \sum \ldots a^\dagger a^\dagger a a$$

$$+ \Delta\alpha \left(\sum \ldots a^\dagger a^\dagger a a \right) \left(\sum \ldots a^\dagger a^\dagger a a \right) \left(\sum \ldots a^\dagger a^\dagger a a \right) + \ldots$$

- unitary transformation **induces many-body contributions** in the Hamiltonian

Hamiltonian in *A*-Body Space

- **cluster decomposition**: decompose evolved Hamiltonian into irreducible n-body contributions $\widetilde{\mathrm{H}}_\alpha^{[n]}$

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

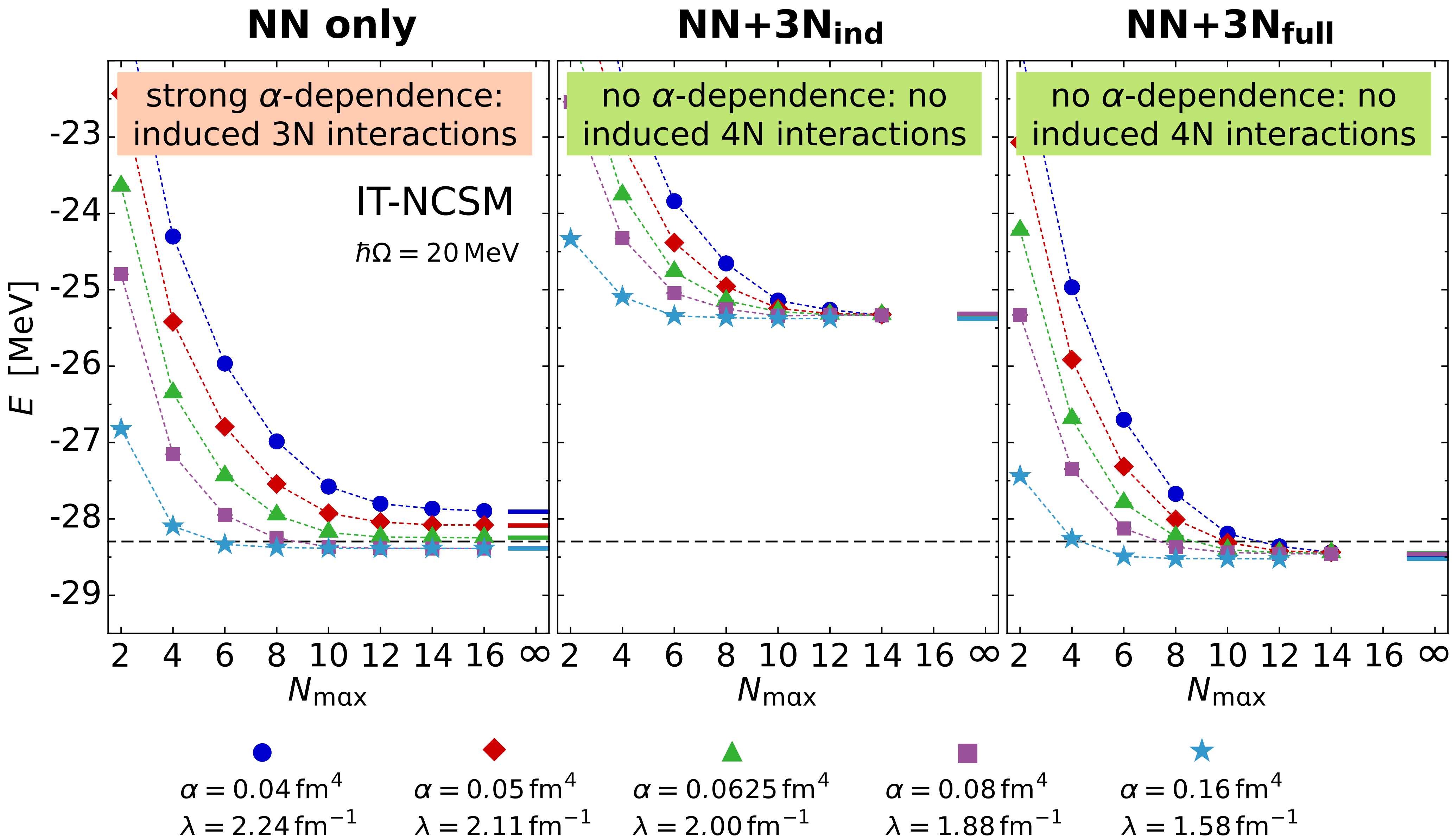
- ***A*-body unitarity**: transformation is unitary only if all terms up to $n = A$ are kept, then all eigenvalues are independent of α

- **cluster truncation**: can construct contributions up to $n = 3$ from evolution in 2B and 3B space, but have to discard $n > 3$

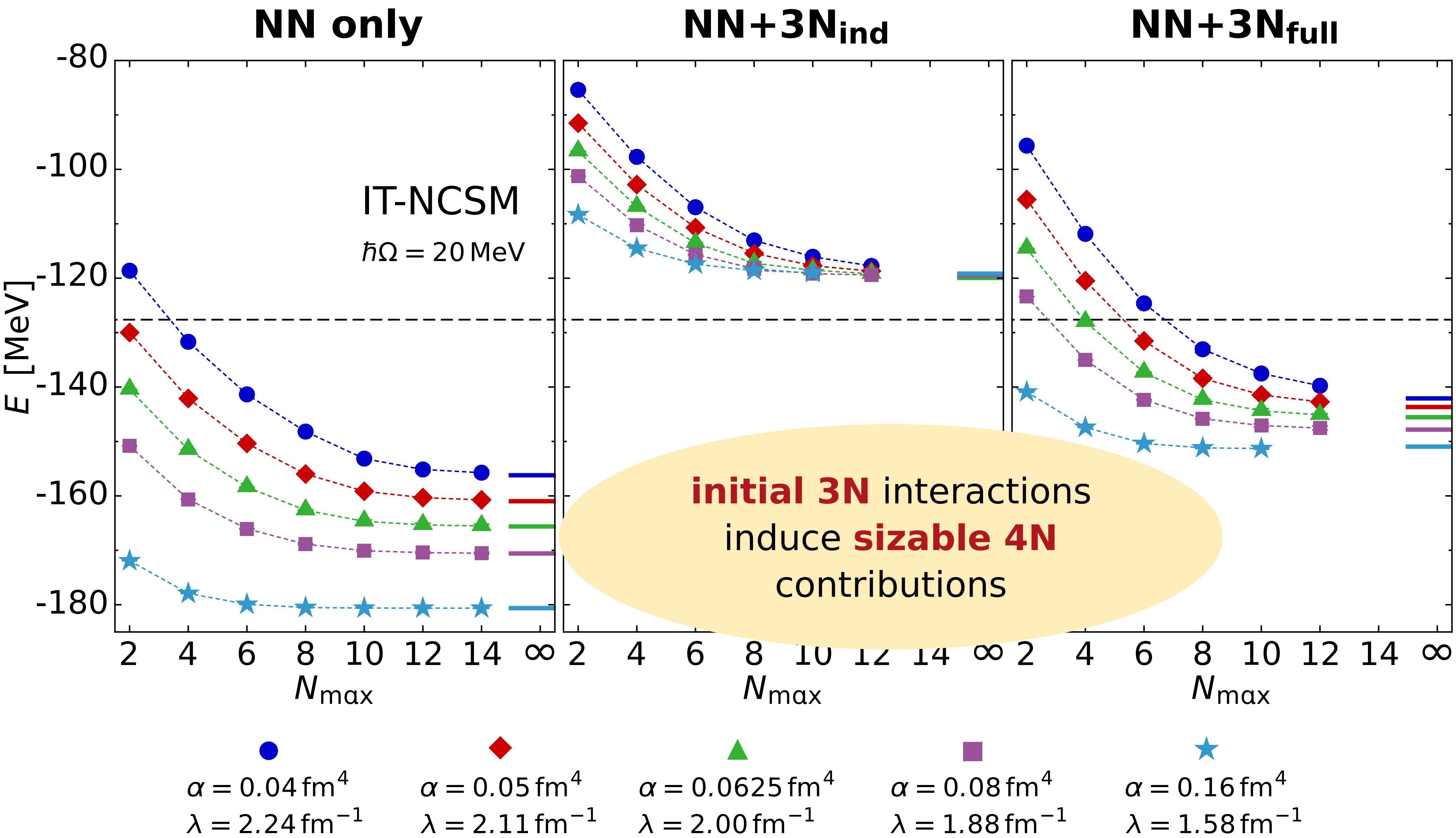
- α-dependence of eigenvalu… **…nian** measures impact of discar…

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

^{4}He: Ground-State Energies

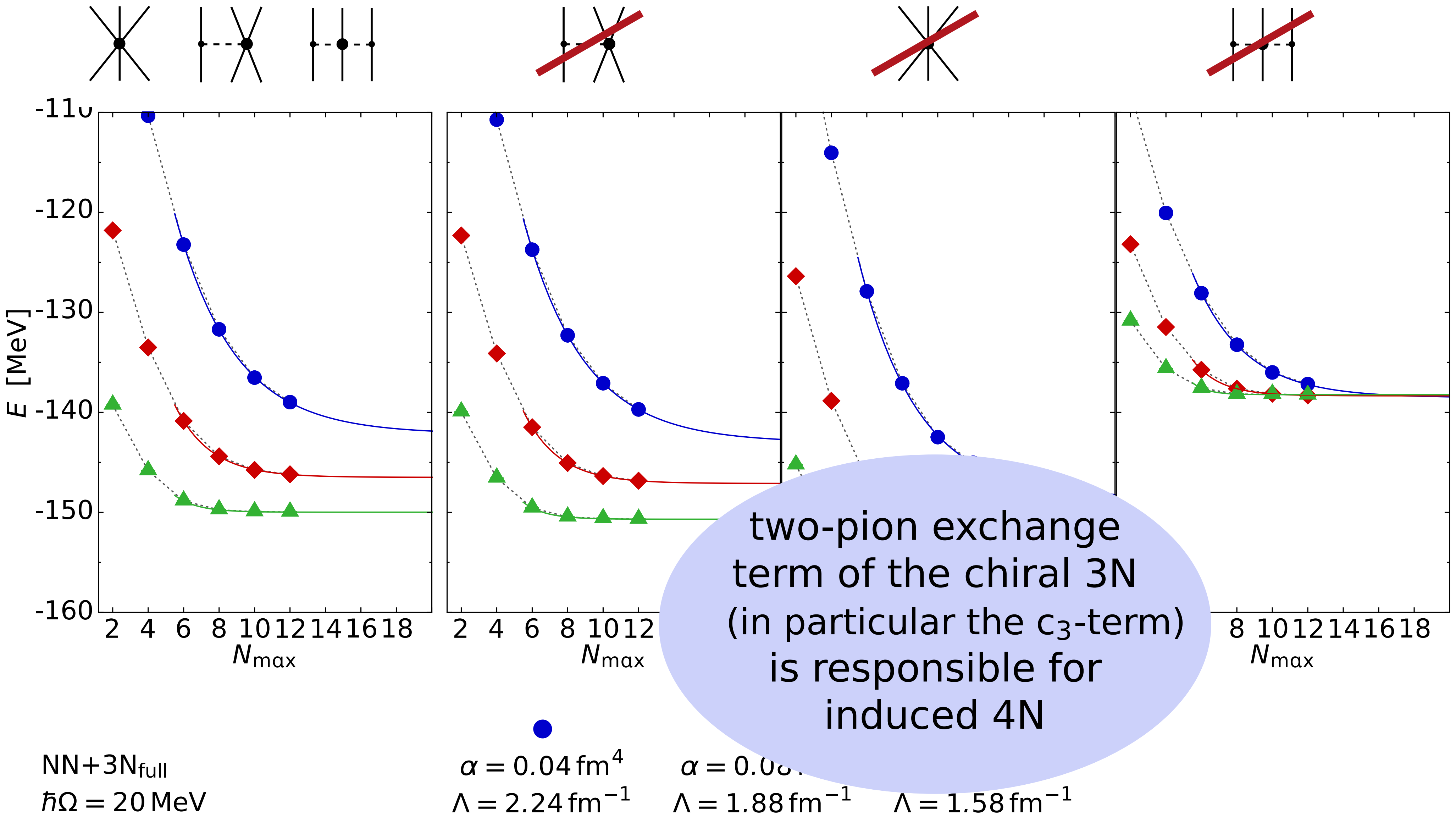


^{16}O: Ground-State Energies



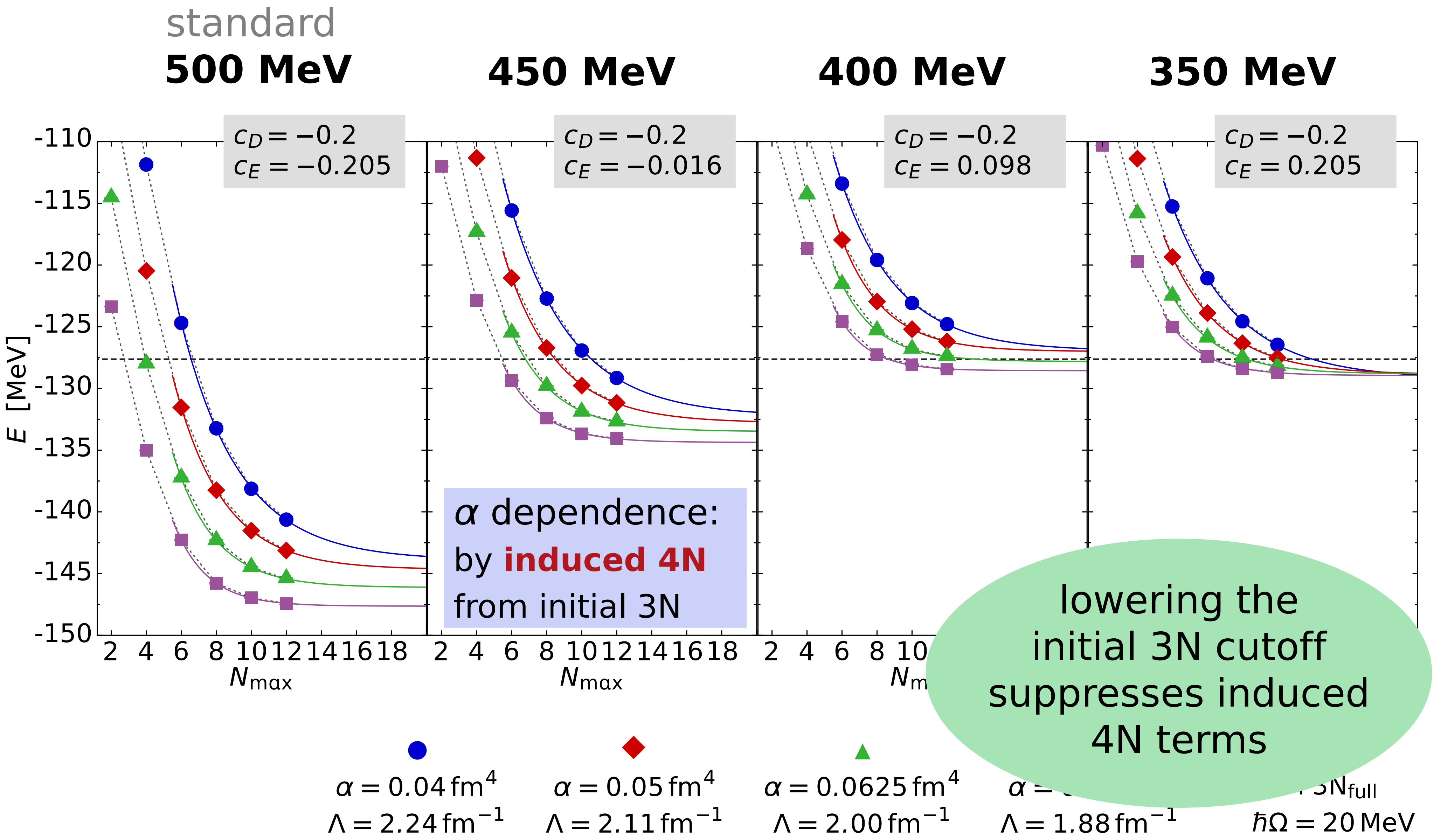
^{16}O: Origin of Induced 4N

switch off individual contributions of the 3N interaction



two-pion exchange term of the chiral 3N (in particular the c_3-term) is responsible for induced 4N

^{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)

Coupled-Cluster Approach

- **exponential Ansatz** to solve Eigenvalue problem

$$\left|\Psi\right\rangle = e^{\mathrm{T}}\left|\Phi_{\mathrm{ref}}\right\rangle = e^{\mathrm{T}_1+\mathrm{T}_2+\mathrm{T}_3+\cdots+\mathrm{T}_A}\left|\Phi_{\mathrm{ref}}\right\rangle$$

- T_n: npnh **excitation (cluster) operator**

$$\mathrm{T}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{\nu_1\ldots\nu_n\\ \mu_1\ldots\mu_n}} t^{\mu_1\ldots\mu_n}_{\nu_1\ldots\nu_n} a^\dagger_{\mu_1}\cdots a^\dagger_{\mu_n} a_{\nu_n}\cdots a_{\nu_1}$$

- **similarity-transformed** Eigenvalue problem

$$\overline{\mathrm{H}_N}\left|\Phi_{\mathrm{ref}}\right\rangle = \Delta E\left|\Phi_{\mathrm{ref}}\right\rangle \qquad \text{with} \qquad \overline{\mathrm{H}_N} = e^{-\mathrm{T}}\mathrm{H}_N\, e^{\mathrm{T}}$$

- **CC equations**: coupled system of non-linear equations

$$\left\langle\Phi_{\mathrm{ref}}\right|\overline{\mathrm{H}_N}\left|\Phi_{\mathrm{ref}}\right\rangle = \Delta E$$

$$\left\langle\Phi^{\mu_1..\mu_n}_{\nu_1..\nu_n}\right|\overline{\mathrm{H}_N}\left|\Phi_{\mathrm{ref}}\right\rangle = 0\,, \qquad \forall \quad \nu_1\ldots\nu_n\,,\ \mu_1\ldots\mu_n$$

Cluster Truncation

- **exponential Ansatz** to solve Eigenvalue problem

$$\left|\Psi\right\rangle = e^{T}\left|\Phi_{ref}\right\rangle = e^{T_1+T_2+T_3+\cdots+T_A}\left|\Phi_{ref}\right\rangle$$

- **CCSD**: singles and doubles excitations, $T = T_1 + T_2$
  - exponential Ansatz: **excitation beyond 2p2h** included by products of excitation operators

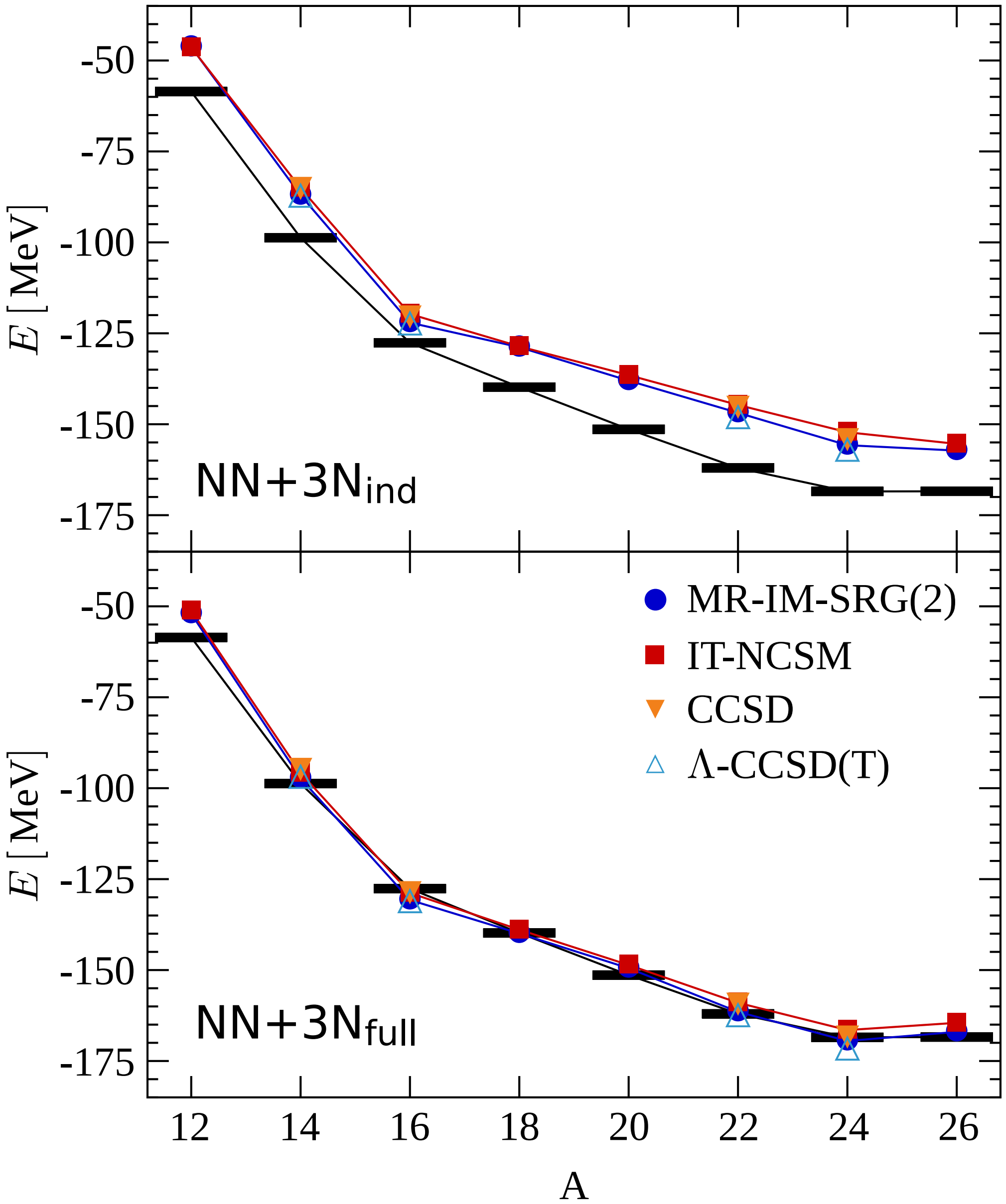
- **CCSDT**: include triples excitations, $T = T_1 + T_2 + T_3$
  - explicit inclusion to expensive
  - use approximations to **estimate triples effects**
    Λ-CCSD(T) and CR-CC(2,3)

Ab Initio Coupled Cluster:

- applicable far beyond the sd shell
- typically restricted to ground states of closed-shell nuclei

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

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

SRG: Basis Representation

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

- **unitary** transformation driven by

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

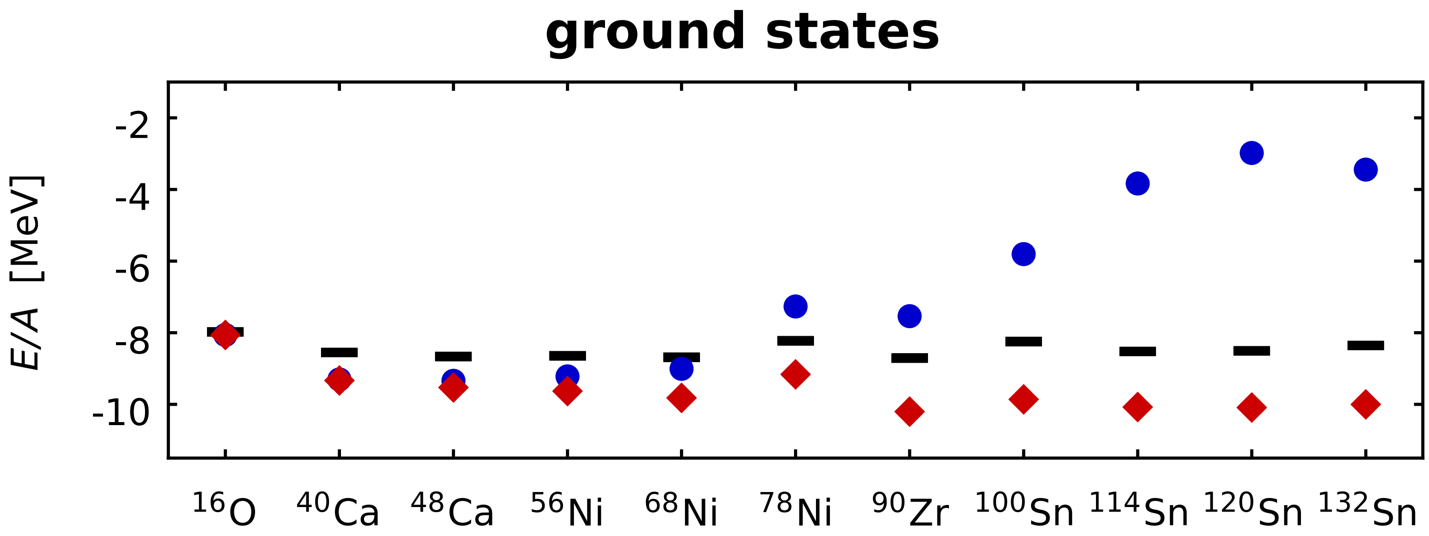
$$(2\mu)^2 \sum_{E'',E'''}^{E_{\max}^{(\mathrm{SRG})}} \sum_{i'',i'''} \langle E'i'JT|\,\mathrm{T}_{\mathrm{int}}\,|E''i''JT\rangle\langle E''i''JT|\,\widetilde{\mathrm{H}}_\alpha\,|E'''i'''JT\rangle\langle E'''i'''JT|\,\widetilde{\mathrm{H}}_\alpha\,|EiJT\rangle$$

$$-2\langle E'i'JT|\,\widetilde{\mathrm{H}}_\alpha\,|E''i''JT\rangle\langle E''i''JT|\,\mathrm{T}_{\mathrm{int}}\,|E'''i'''JT\rangle\langle E'''i'''JT|\,\widetilde{\mathrm{H}}_\alpha\,|EiJT\rangle$$

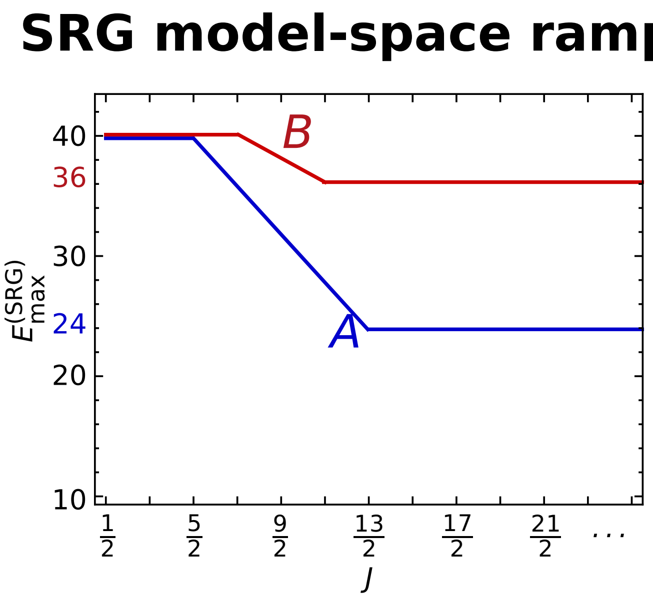
$$+\langle E'i'JT|\,\widetilde{\mathrm{H}}_\alpha\,|E''i''JT\rangle\langle E''i''JT|\,\widetilde{\mathrm{H}}_\alpha\,|E'''i'''JT\rangle\langle E'''i'''JT|\,\mathrm{T}_{\mathrm{int}}\,|EiJT\rangle$$

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

SRG Model Space for Heavy Nuclei



CCSD
$\hbar\tilde{\Omega} = 36\,\text{MeV}$
$\hbar\Omega = 24\,\text{MeV}$
$\alpha = 0.08\,\text{fm}^4$
$\Lambda_{3N} = 400\,\text{MeV}$
HF basis
$E_{3max} = 14$
e_{max}=12



- introduce extended SRG space as standard for heavy mass nuclei
- SRG space *B* much larger then model spaces in previous works

large angular momenta important for heavy mass nuclei

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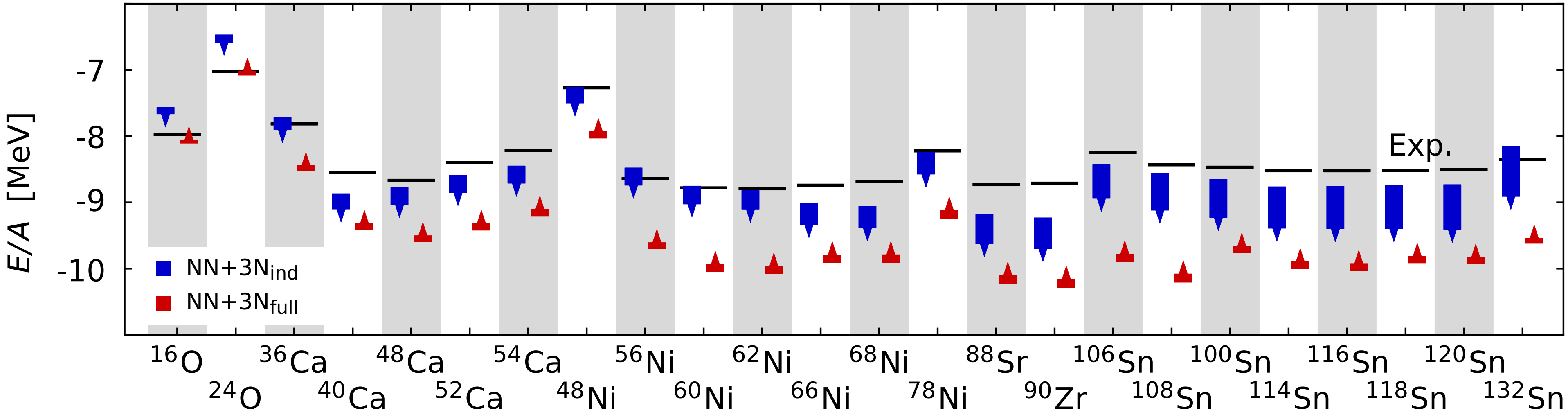
Heavy Nuclei

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)
  - strongly reduced flow-parameter dependence
- **mass trend reproduced** throughout nuclear chart

CR-CC(2,3)

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

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

$\alpha = 0.04 - 0.08\,\mathrm{fm}^4$

$E_{3\max} = 18$

$e_{\max}=12$

SRG in Four-Body Space

Induced Four-Body Contributions

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

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

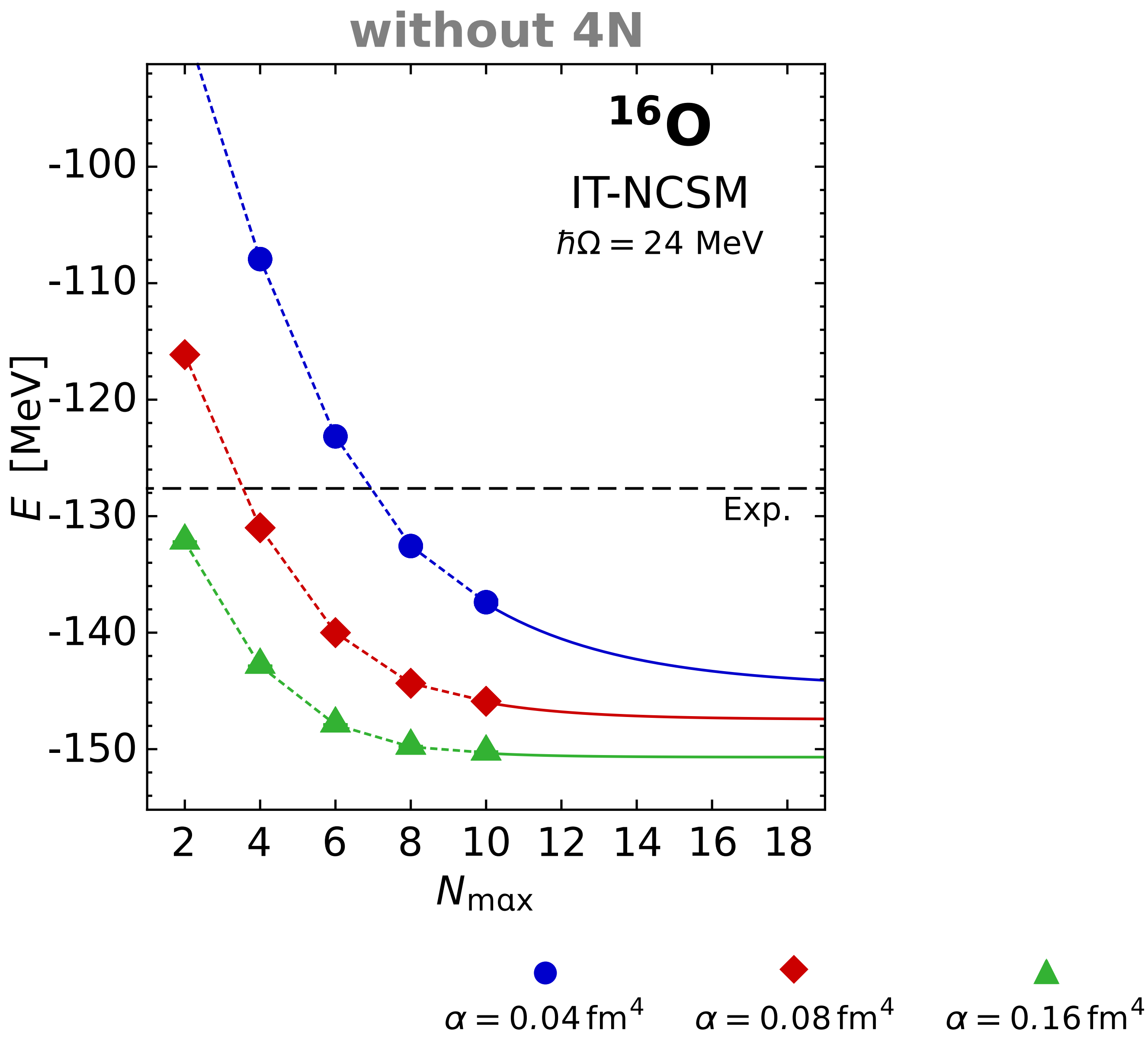
- promising **ideas** for a **better compromise** between induced forces and convergence acceleration

  Dicaire, Omand, Navratil   Phys. Rev. C 90, 034302 (2014)

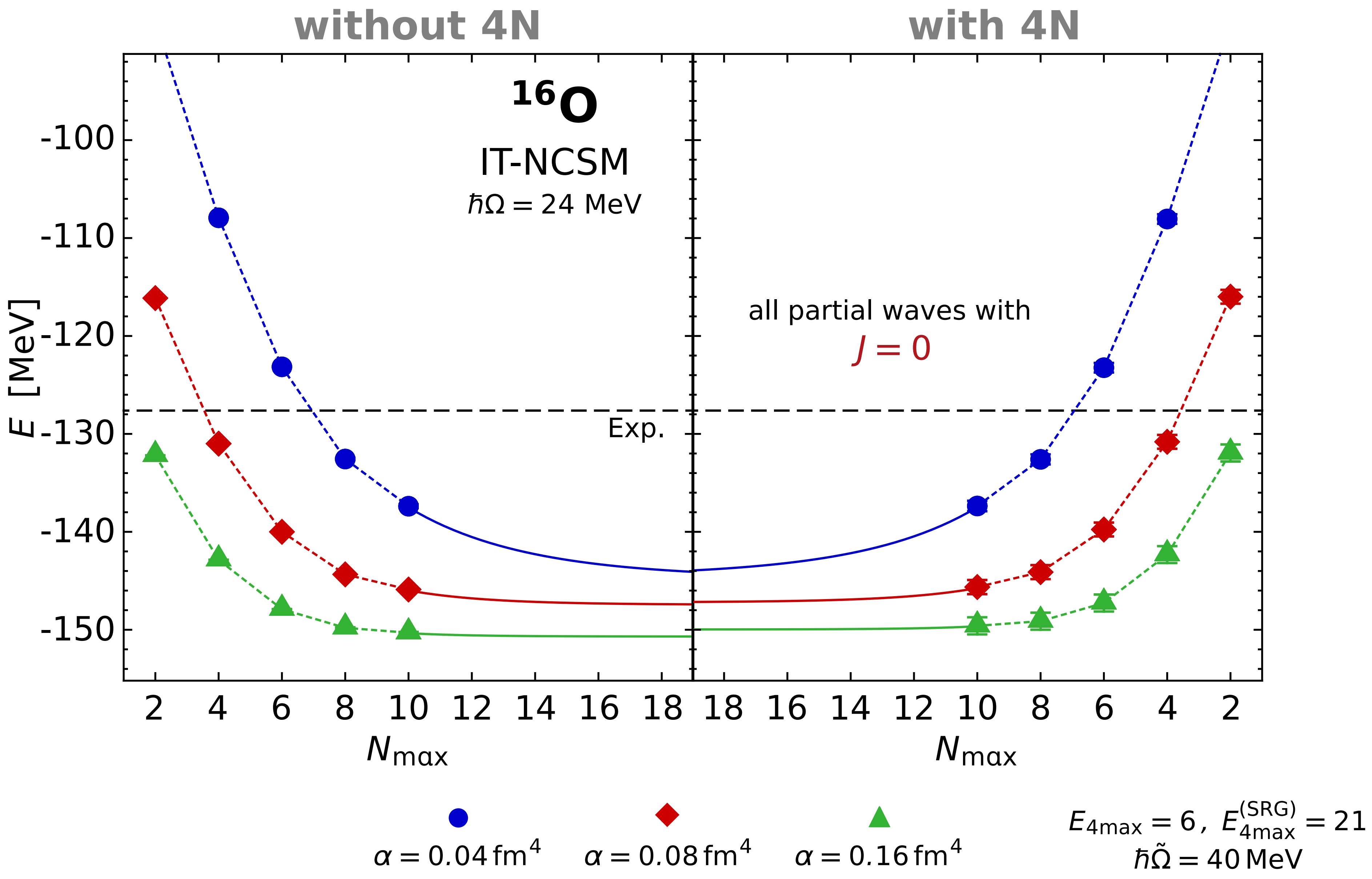
❸ **include 4N contributions**

- SRG evolution in four-body space
- extension of all HO developments and IT-NCSM to treat 4N interactions

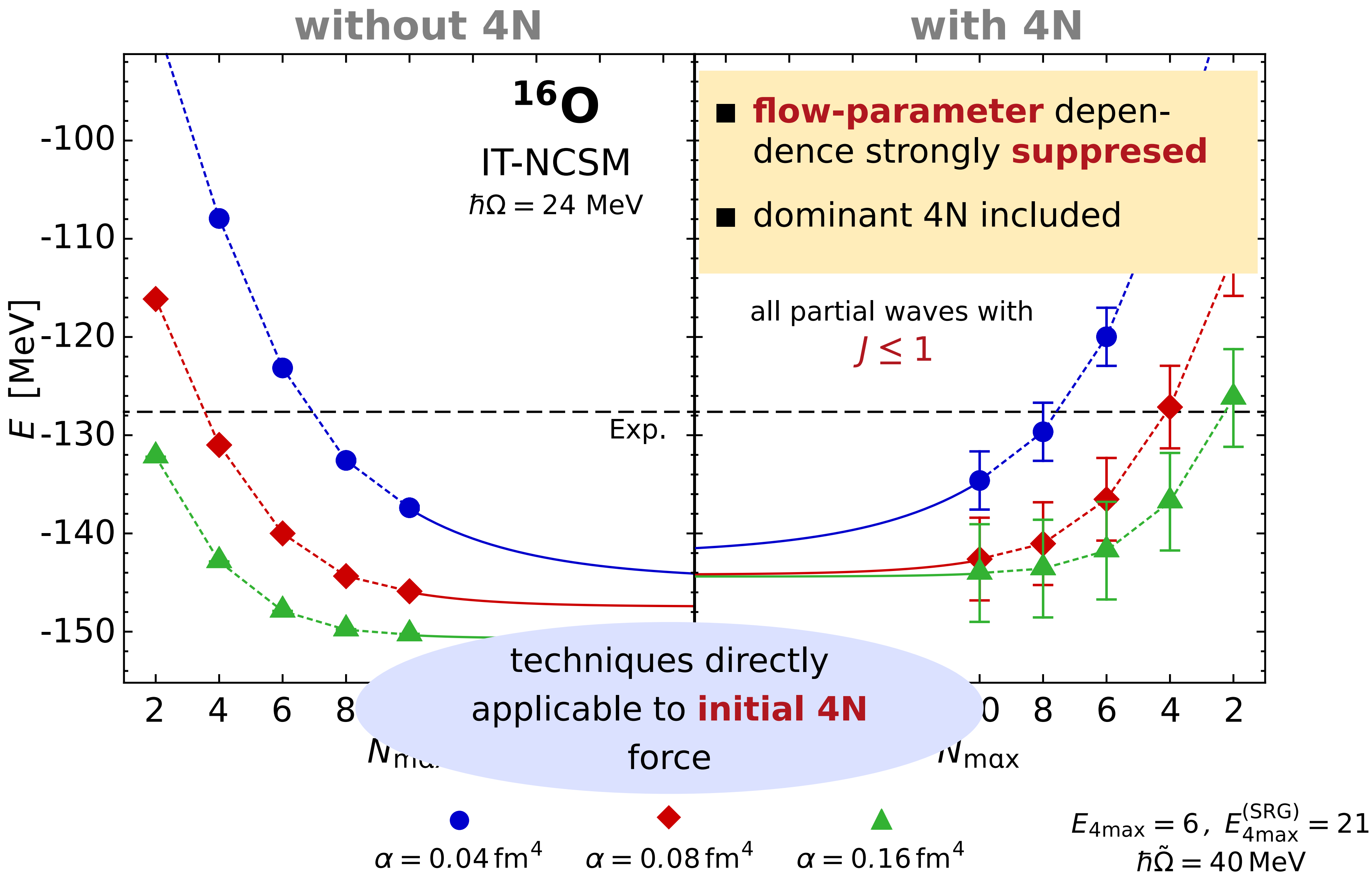
IT-NCSM with Four-Body Contributions



IT-NCSM with Four-Body Contributions



IT-NCSM with Four-Body Contributions



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

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

Alternative Chiral Hamiltonians & Uncertainty Quantification

Uncertainties of Chiral Interactions

ideal

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

  ⇒ estimate uncertainties

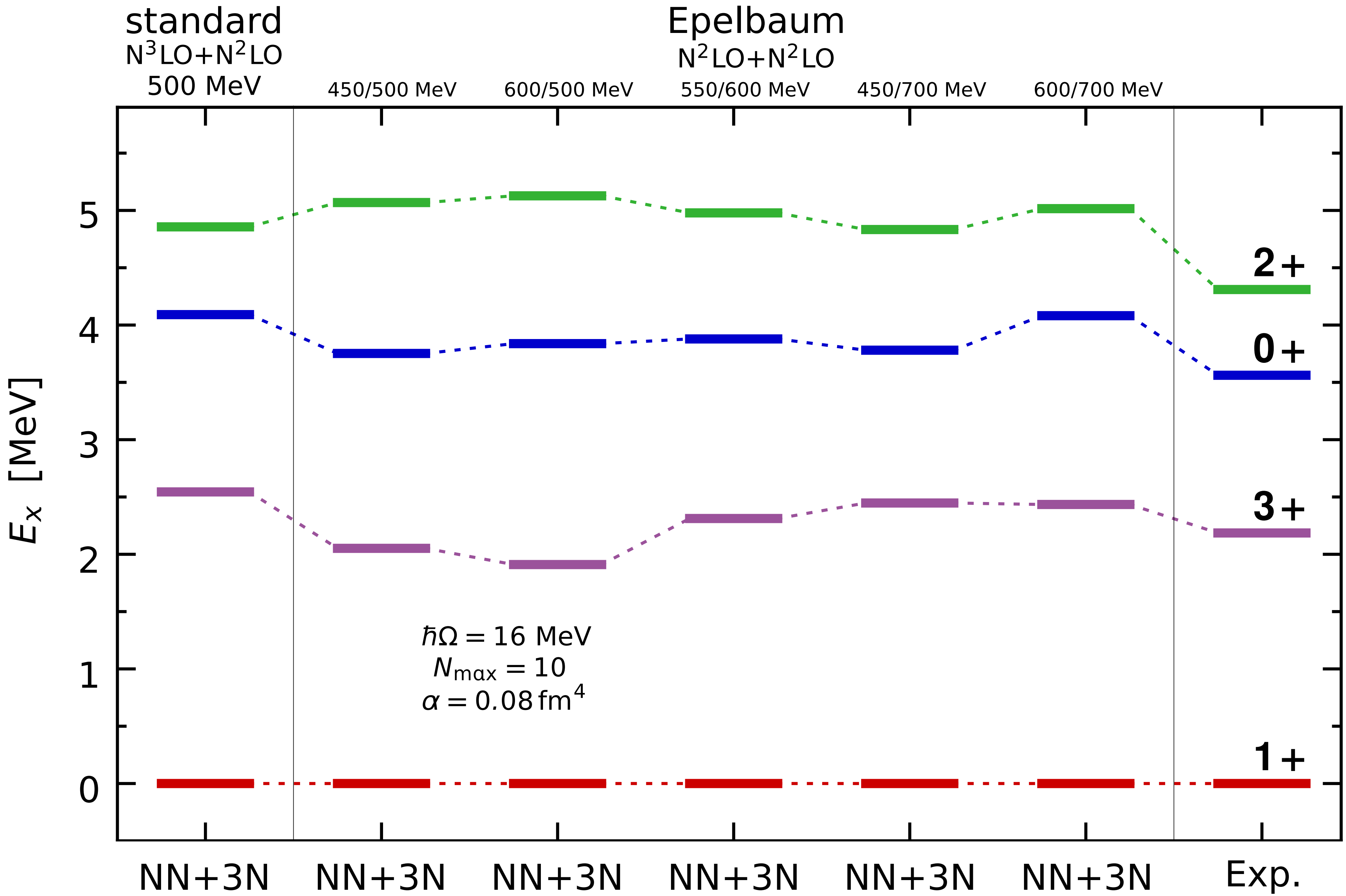
practice

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

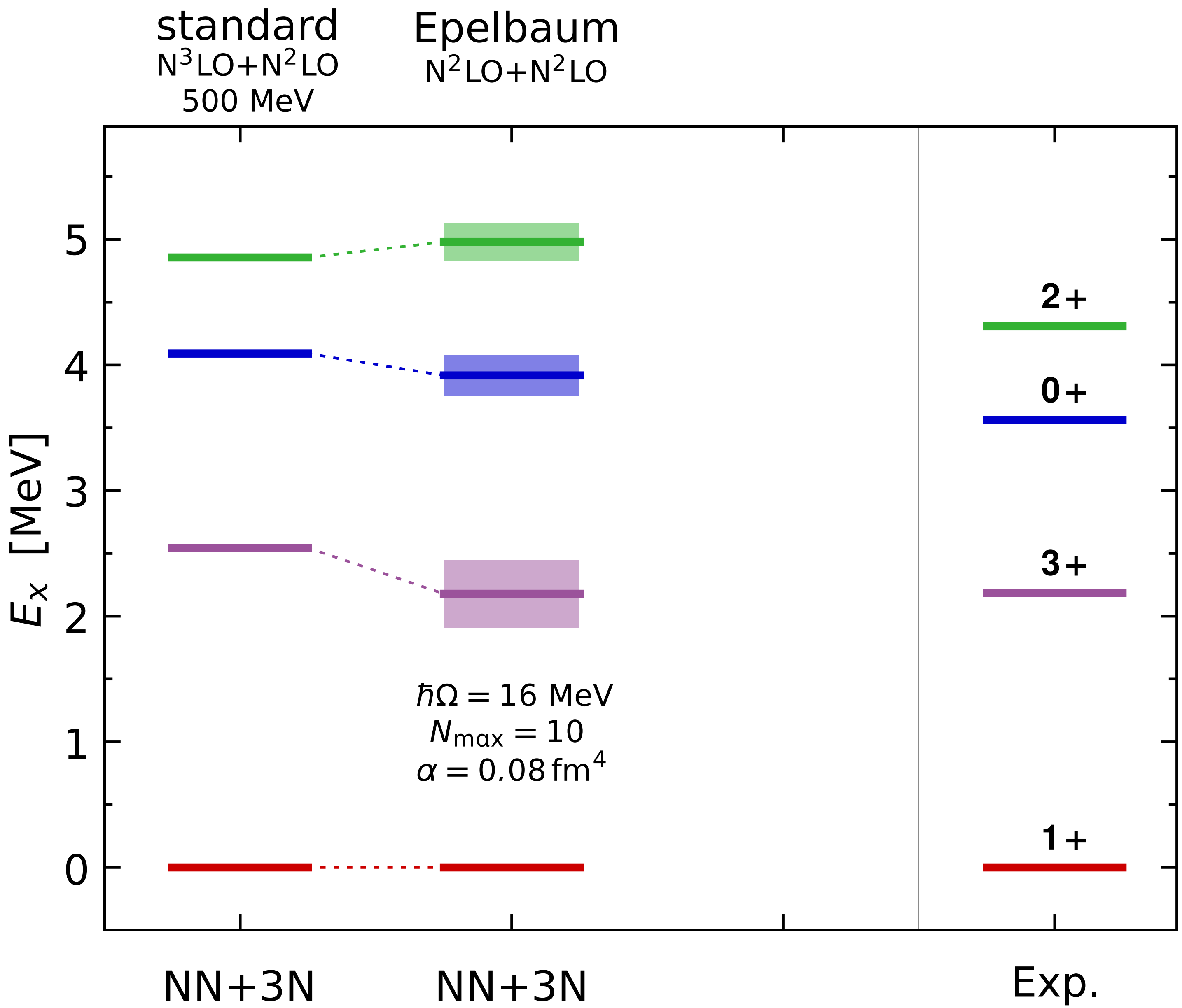
nuclear structure physics approaches new era

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

^{6}Li: Alternative Interactions

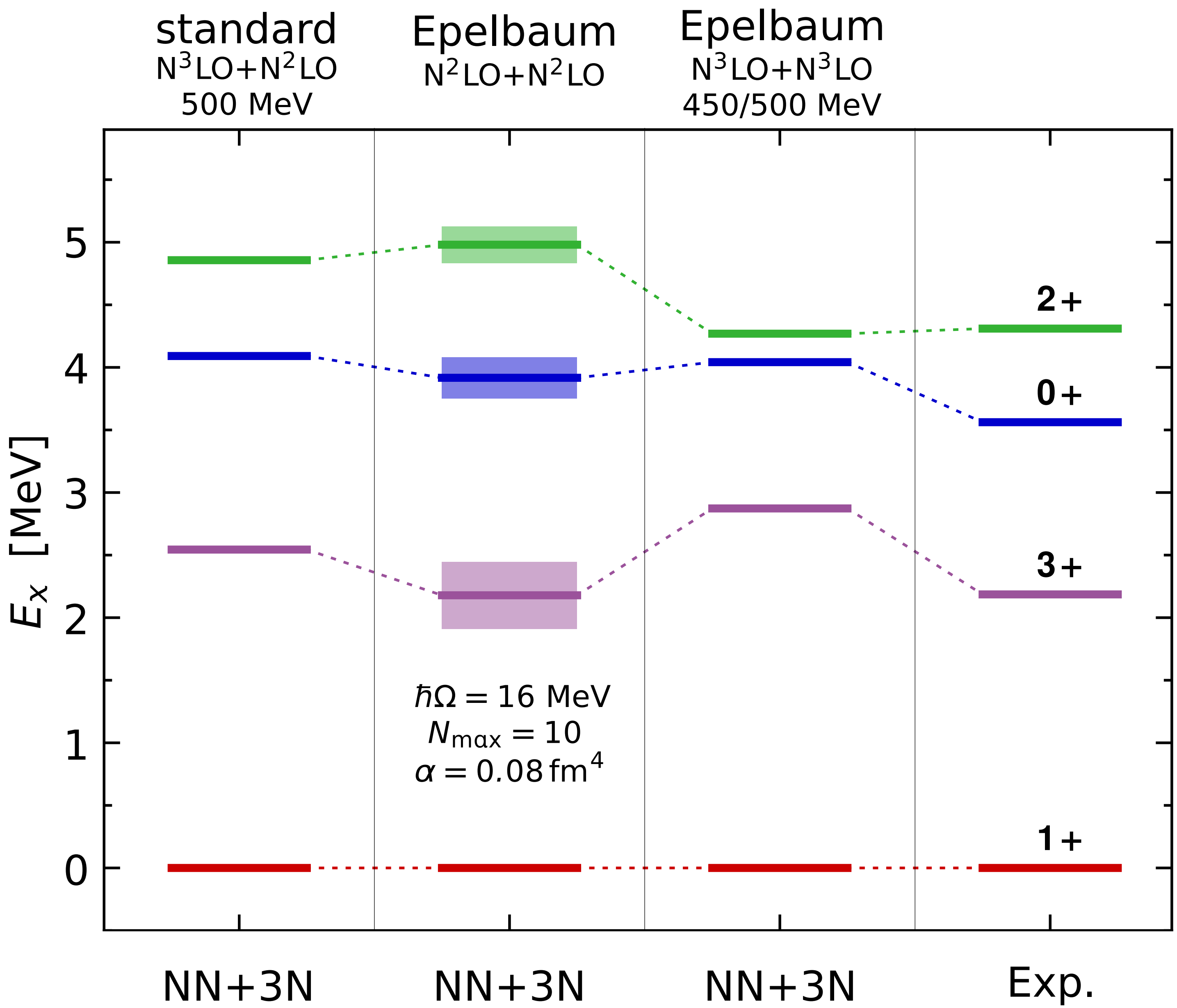


^{6}Li: Dependence on Chiral Order



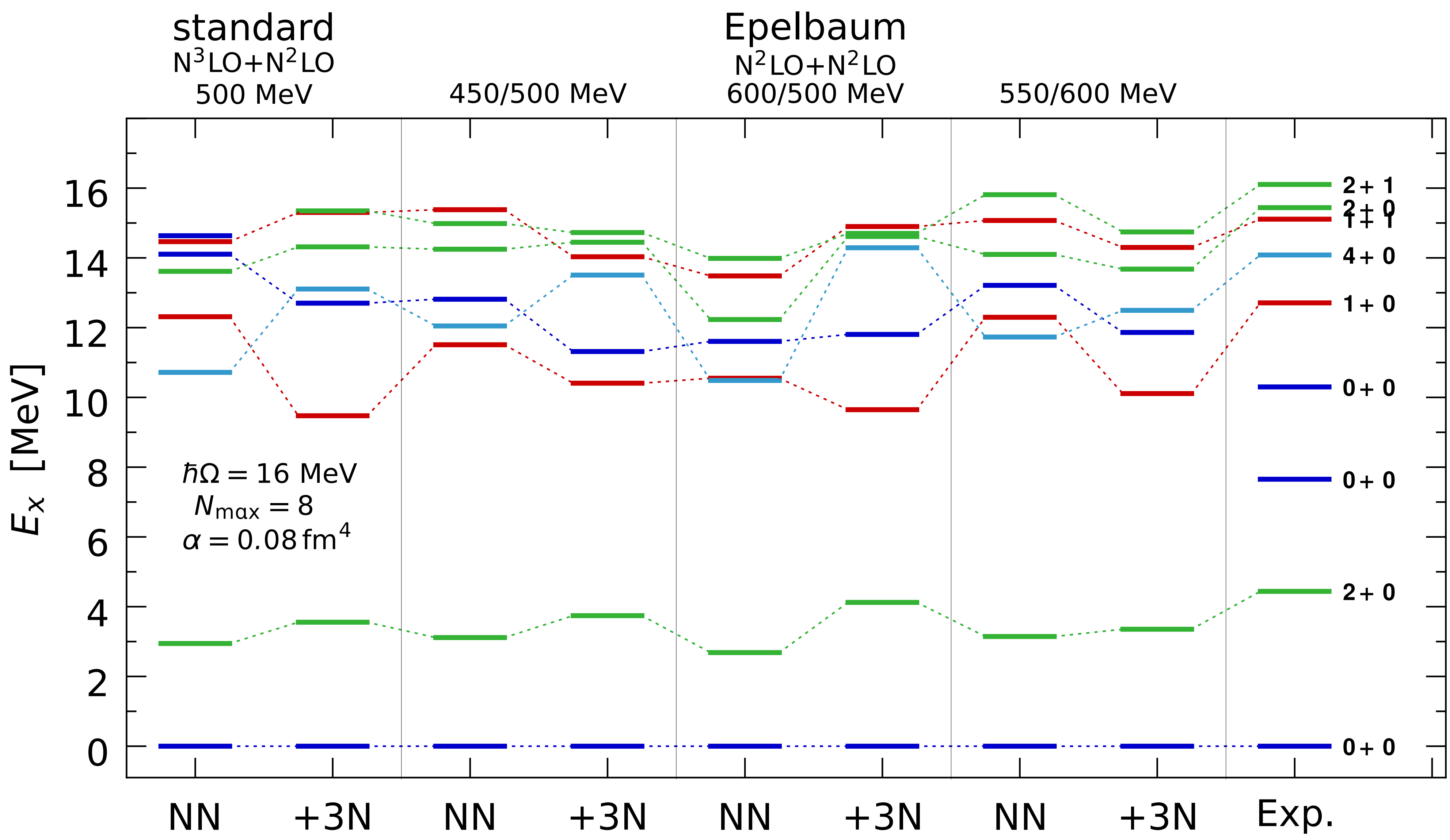
- small cutoff dependence
- reasonable predictions

^{6}Li: Dependence on Chiral Order

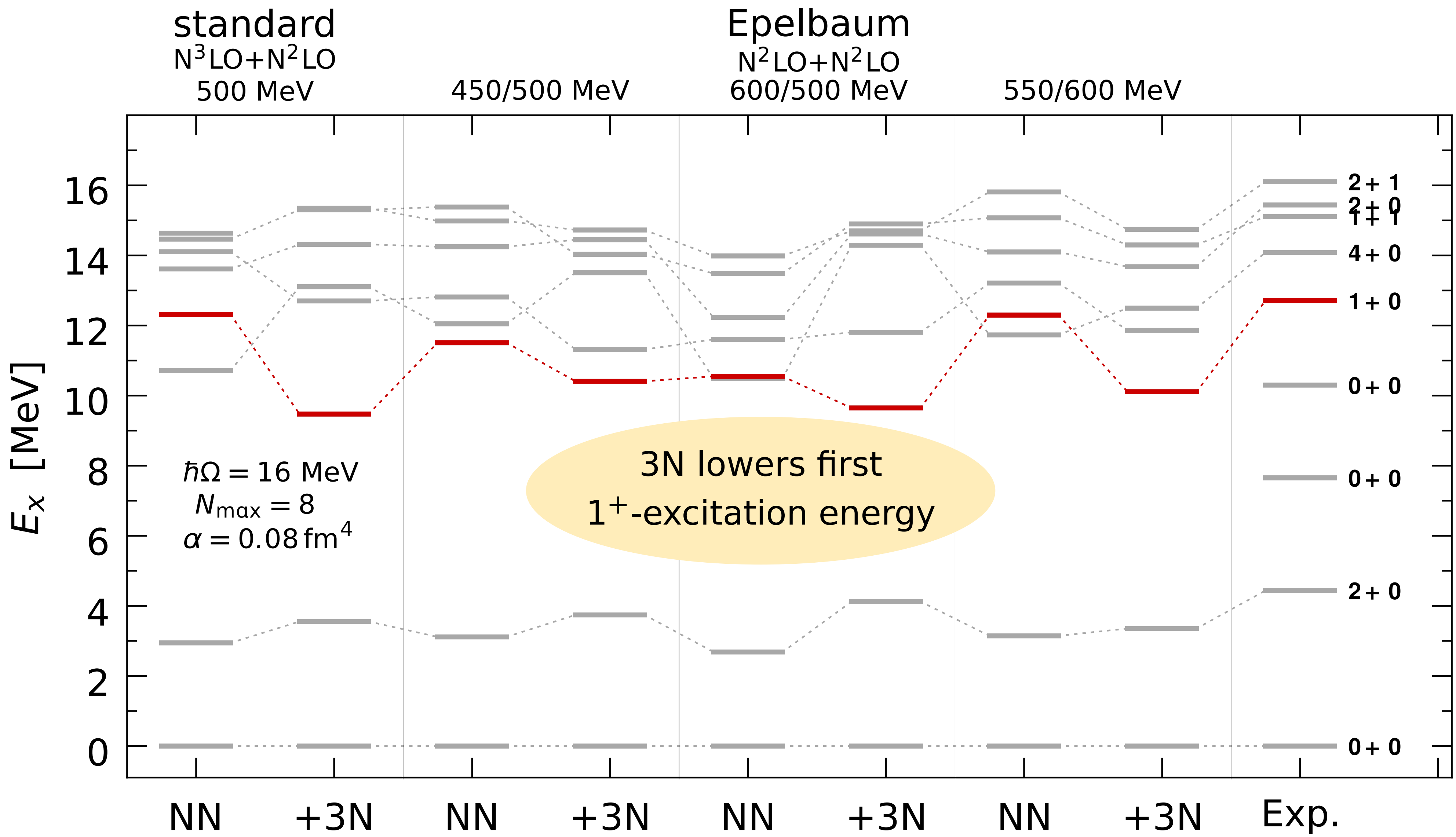


- small cutoff dependence
- reasonable predictions
- further cutoffs and orders re- quired

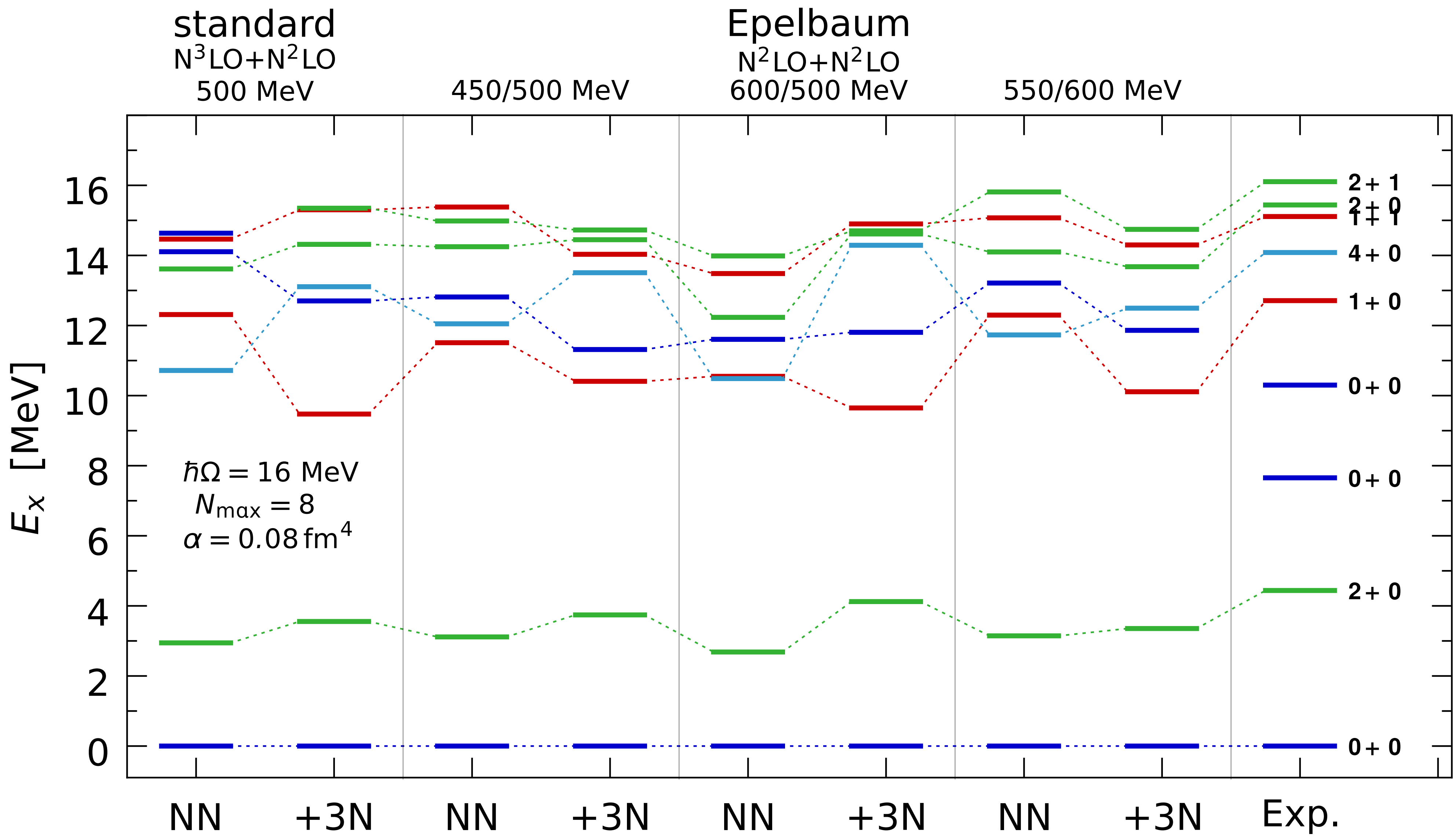
^{12}C: Alternative Interactions



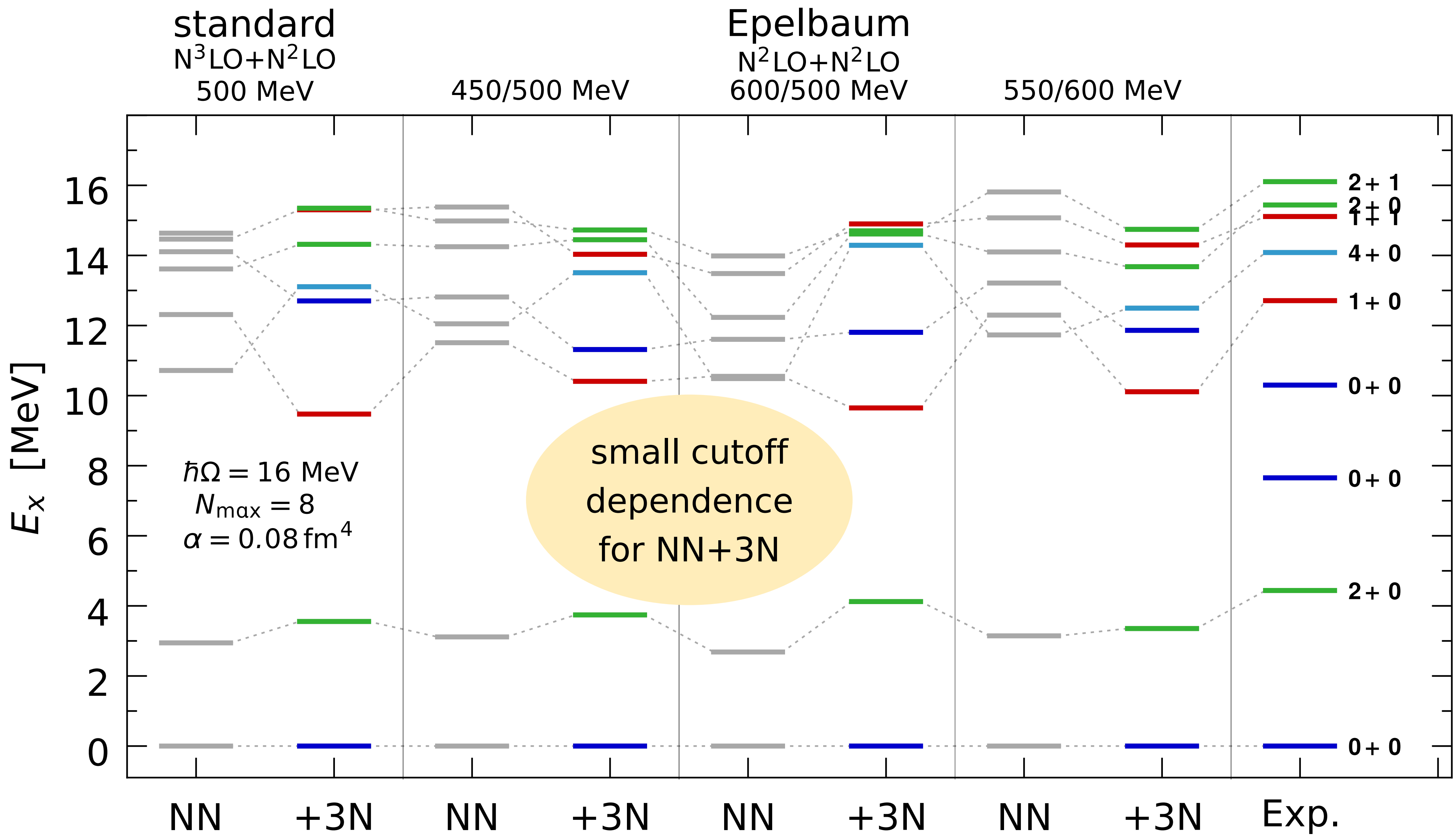
^{12}C: Alternative Interactions



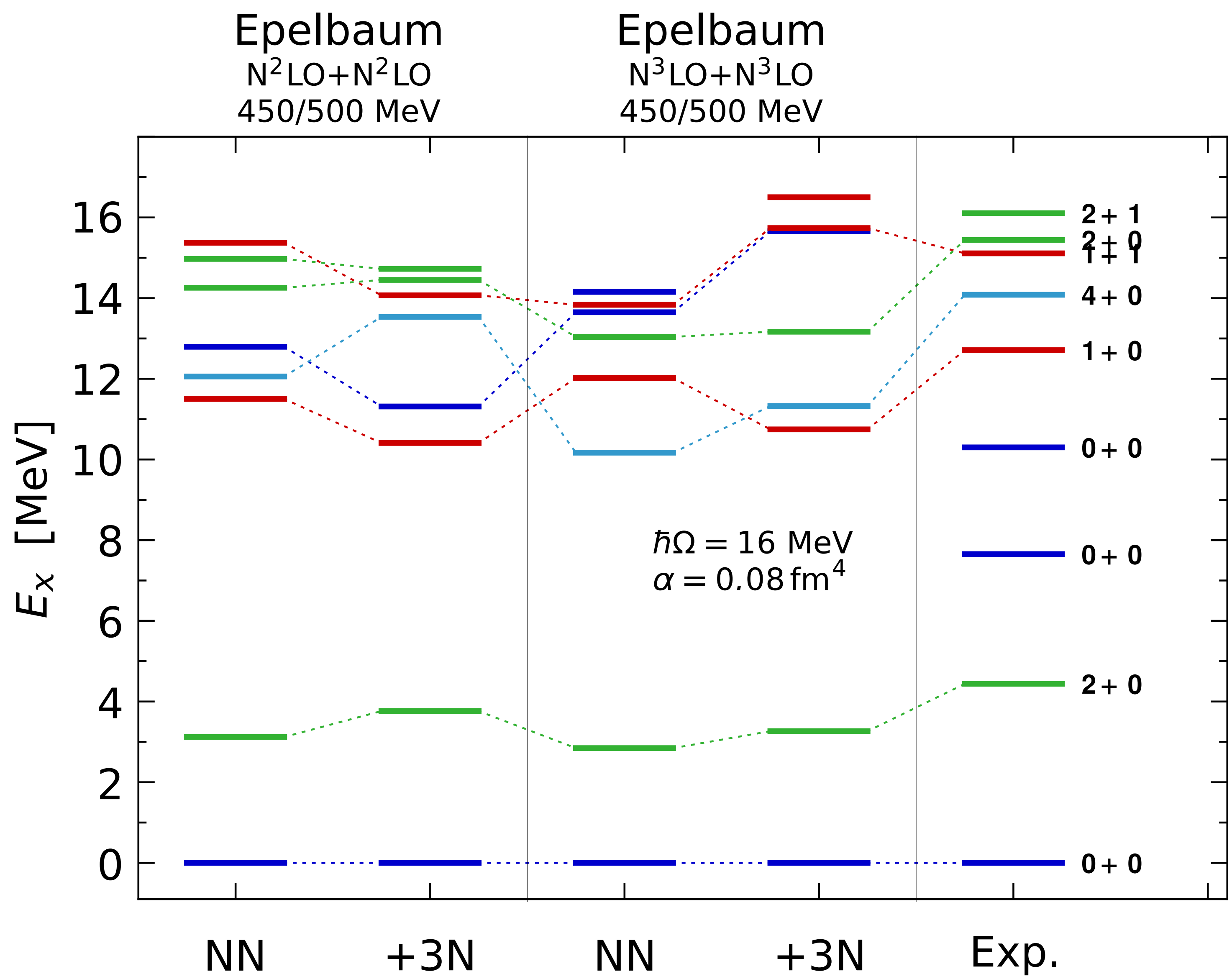
^{12}C: Alternative Interactions



^{12}C: Alternative Interactions



^{12}C: Dependence on Chiral Order



- first results with NN+3N force at N^{3}LO
- reasonable predictions
- cutoff dependence need to be studied

Conclusions

- **consistent three- and four-body** SRG evolution
  - successful application of chiral 3N forces
  - promising ideas for **alternative generators**
- **heavy nuclei** accessable with ab initio approaches
  - mass systematics can be reproduced
- **p-shell spectra** provide powerful testbed for chiral potentials
  - **first** nuclear structure application of **3N force at N^3LO**
  - constraints for interactions

Outlook

- exciting **progress** in construction of **chiral forces**
  - **N^2LO_{sat}** NN+3N: fit LECs to many-body observables

    Ekström, Machleidt et al.
  - **l**
  - **m** ...mponent

    Piarulli, Girlanda, ...

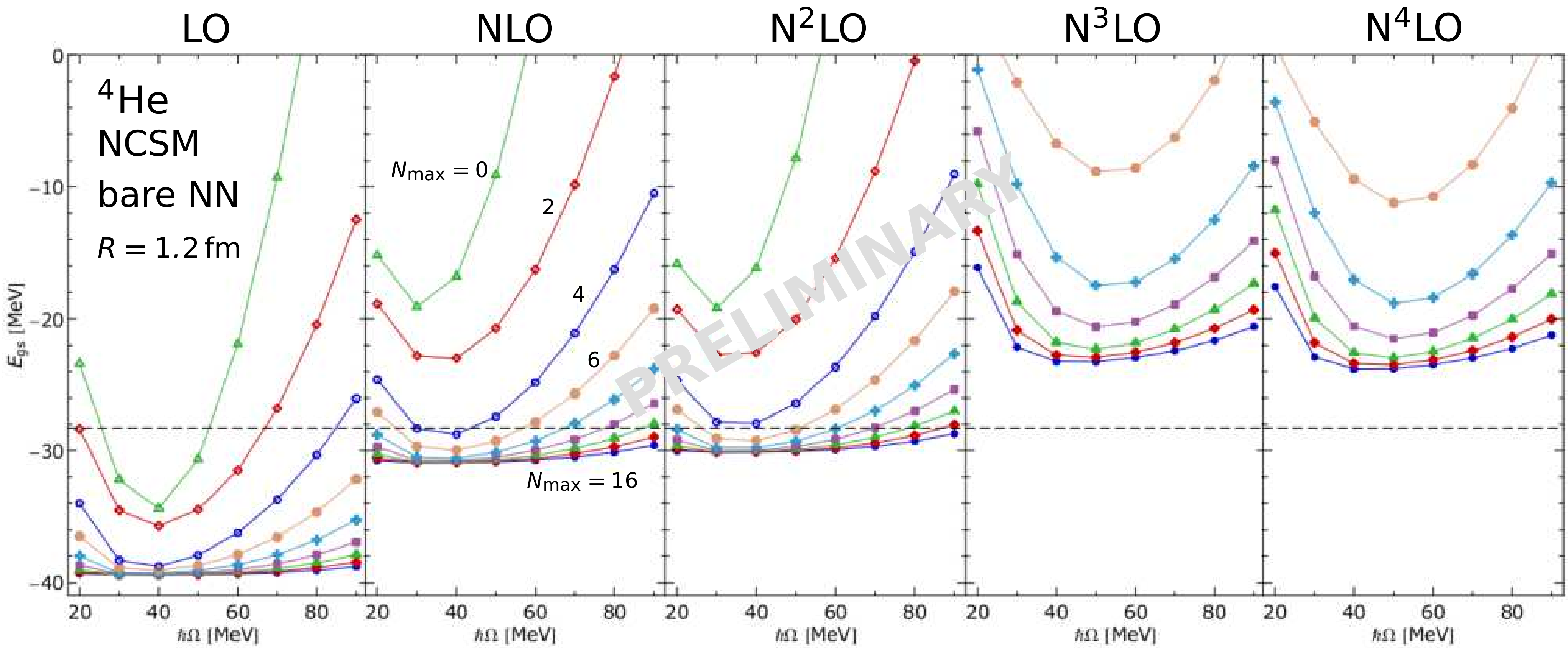
self-contained framework to employ **present and future chiral NN+3N+4N interactions** in a variety of many-body methods

LENPIC Collaboration

- **improved NN** up to N^4LO

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

Outlook: Improved NN



- sequence of cutoffs and chiral orders can be studied
- 3N forces in progress

Epilogue

- **thanks to my collaborators**
  - **S. Binder**, **J. Langhammer**, K. Hebeler, **R. Roth**, **S. Schulz**
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    GSI Helmholtzzentrum

LENPIC
Low-Energy Nuclear Physics International Collaboration

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NSERC CRSNG

SFB 634

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COMPUTING TIME