Similarity Renormalization Group with Chiral Hamiltonians: Techniques & New Directions

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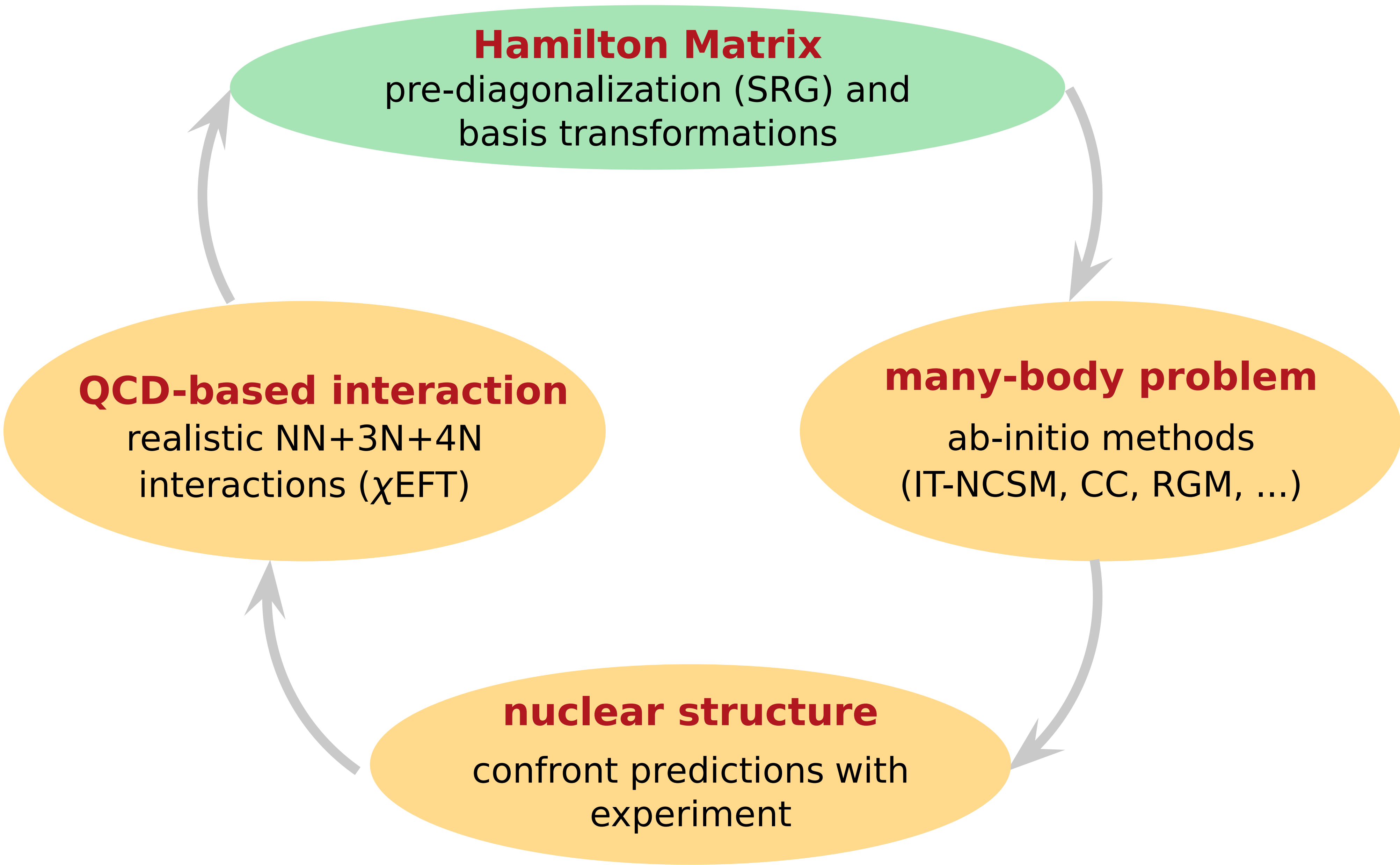
Introduction



New Directions

Applications to Nuclear Spectra
spectroscopy and sensitivity on 3N

Probe Next-Generation Chiral Potentials
with ab-initio nuclear structure

Frequency Conversion
extends SRG in HO Base
to lower HO frequencies

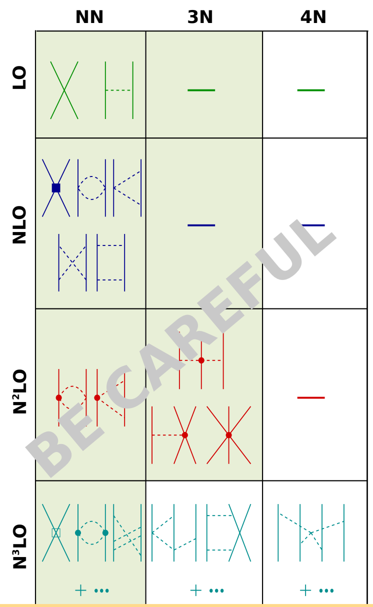
SRG in 4B Space
treatment of induced &
initial 4N contributions

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

- **standard Interaction with modified 3N:**
  - NN N^3LO: Entem&Machleidt, 500 MeV cutoff
  - 3N N^2LO: Navrátil, local, with modified LECs and cutoffs, fitted to ^{4}He



Next Generation Interactions

- **consistent N^2LO Interaction:**
  - NN N^2LO: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N N^2LO: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal

- **consistent N^3LO Interaction:**
  - coming soon. . .

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**

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

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

don't get confused: $\alpha = \frac{1}{\lambda^4}$

- choose **dynamic generator**

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

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 $1 \longleftrightarrow 2$:

$$|\alpha\rangle = |[(N_1 L_1, S_1)J_1, (N_2 L_2, S_2)J_2]J M_J, (T_1, T_2)T M_T\rangle$$

  - completely antisymmetric:

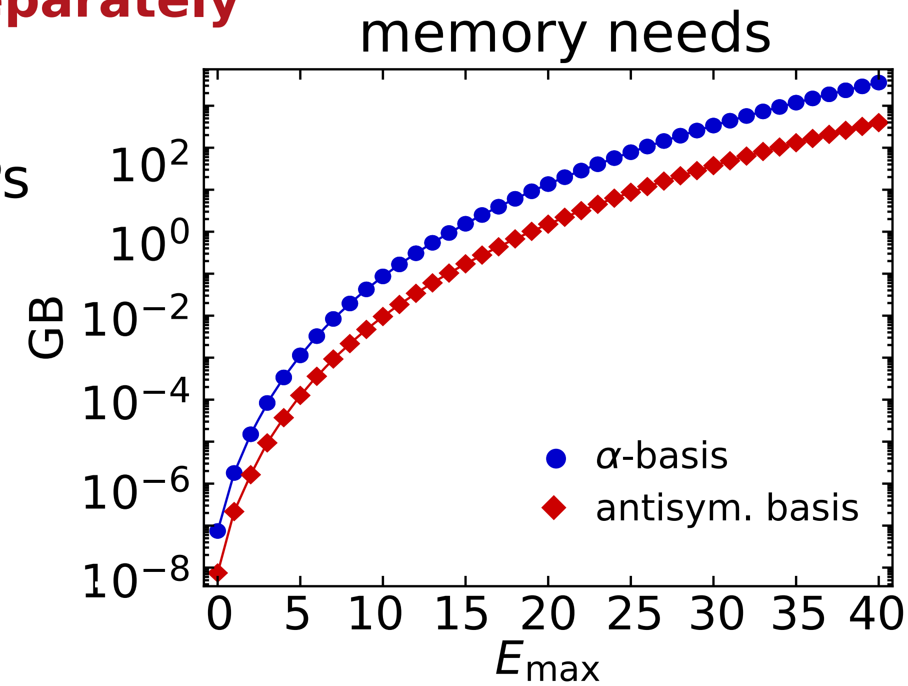
$$|E i J M_J T M_T\rangle = \sum_{\alpha} c_{\alpha,i}\,|\alpha\rangle$$

$$c_{\alpha,i} = \langle E i J M_J T M_T|\alpha\rangle$$

coefficients of fractional parentage (CFPs) by P. Navrátil

SRG in HO Jacobi Basis

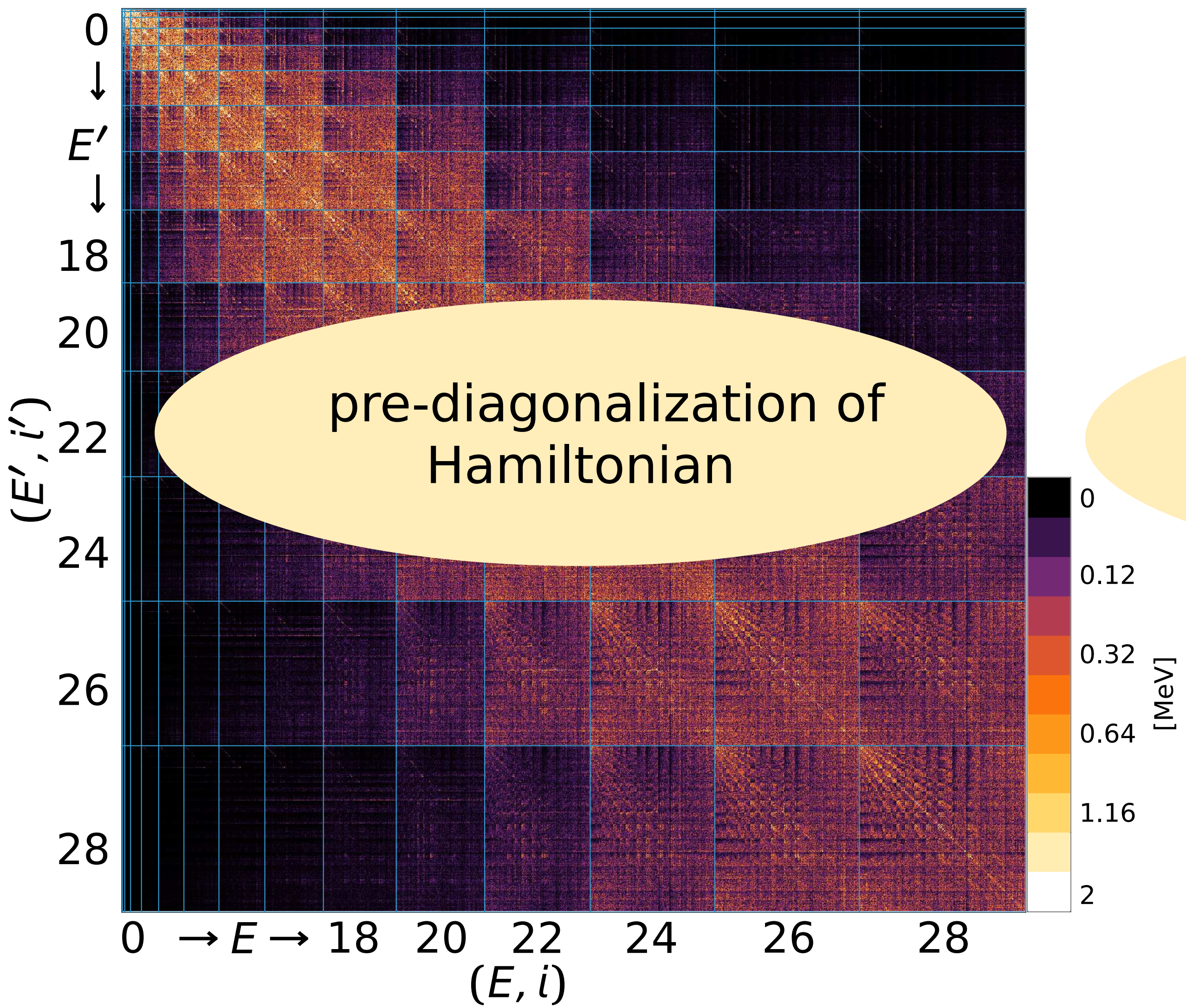
- no center of mass part
  - sizable reduction of model space dimension
- coupling considers properties of interaction
  - can evolve every **TJP-channel separately**
- discrete basis enables use of CFPs
  - antisymmetrization **simple**
  - explicit consideration of the antisymmetry **decreases memory needs**



- **optimized implementation**
  - largest channel ($T = 1/2,\ J^{\pi} = 5/2^{+}$) in **4 hours on a single node**

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



pre-diagonalization of Hamiltonian

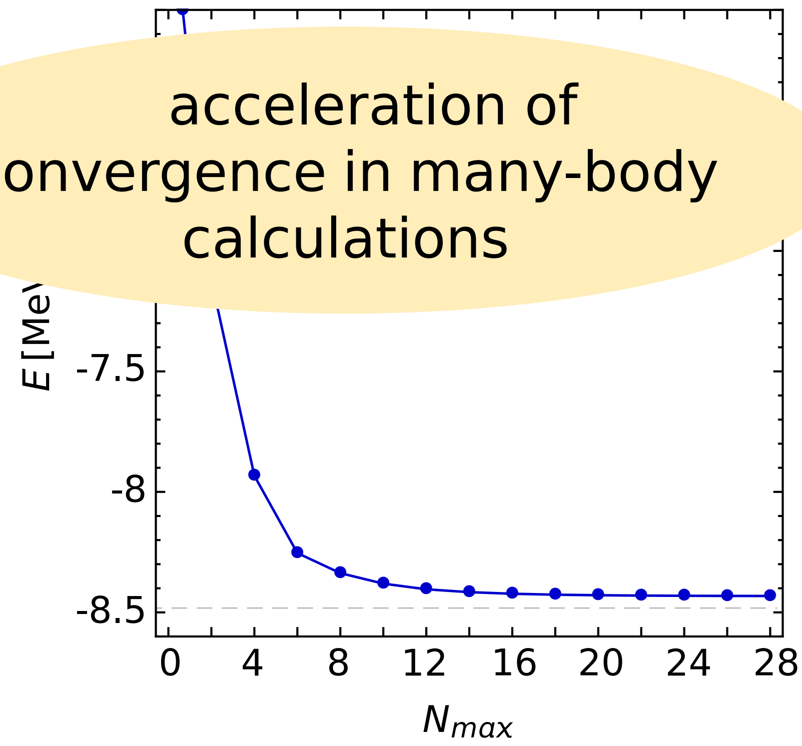
$\alpha = 0.16\,\mathrm{fm}^4$

$\lambda = 1.58\,\mathrm{fm}^{-1}$

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

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

NCSM ground state ^{3}H



acceleration of convergence in many-body calculations

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 a 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 $N_{\text{max}} > 8$ (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

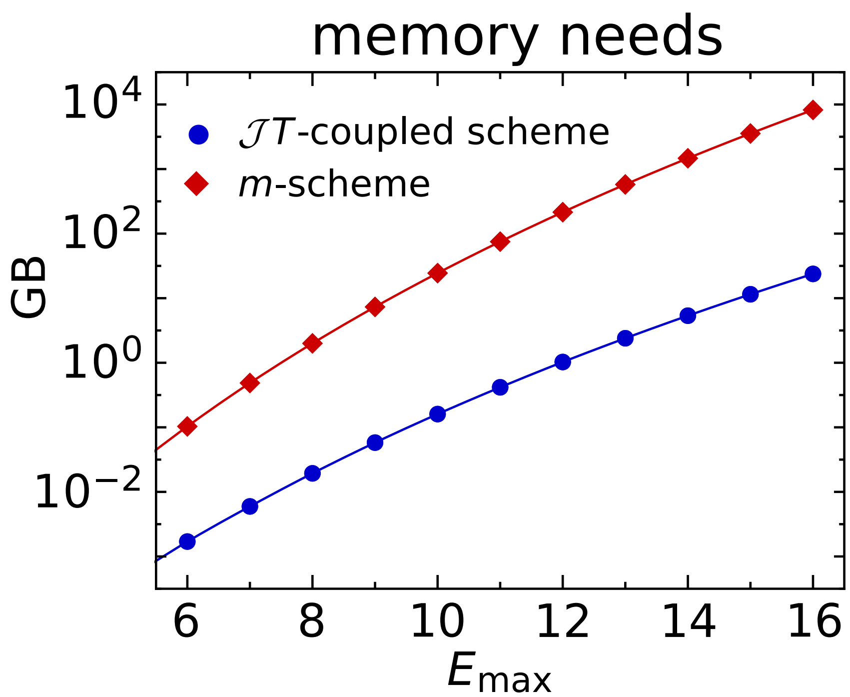
$\mathcal{J}T$-Coupled Scheme vs. m-Scheme

- m-scheme

$$|(n_a l_a, s_a) j_a m_a, (n_b l_b, s_b) j_b m_b, (n_c l_c, s_c) j_c m_c; t_a m_{t_a}, t_b m_{t_b}, t_c m_{t_c}\rangle$$

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

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



- explicit consideration of interaction properties in $\mathcal{J}T$-coupled scheme
  - Hamiltonian connects only **equal $\mathcal{J}$ and T**
  - **memory needs decreases** by two orders of magnitude

No-Core Shell Model (NCSM)

- **solve eigenvalue problem**: $\boldsymbol{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$
- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

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

- **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

- 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

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

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

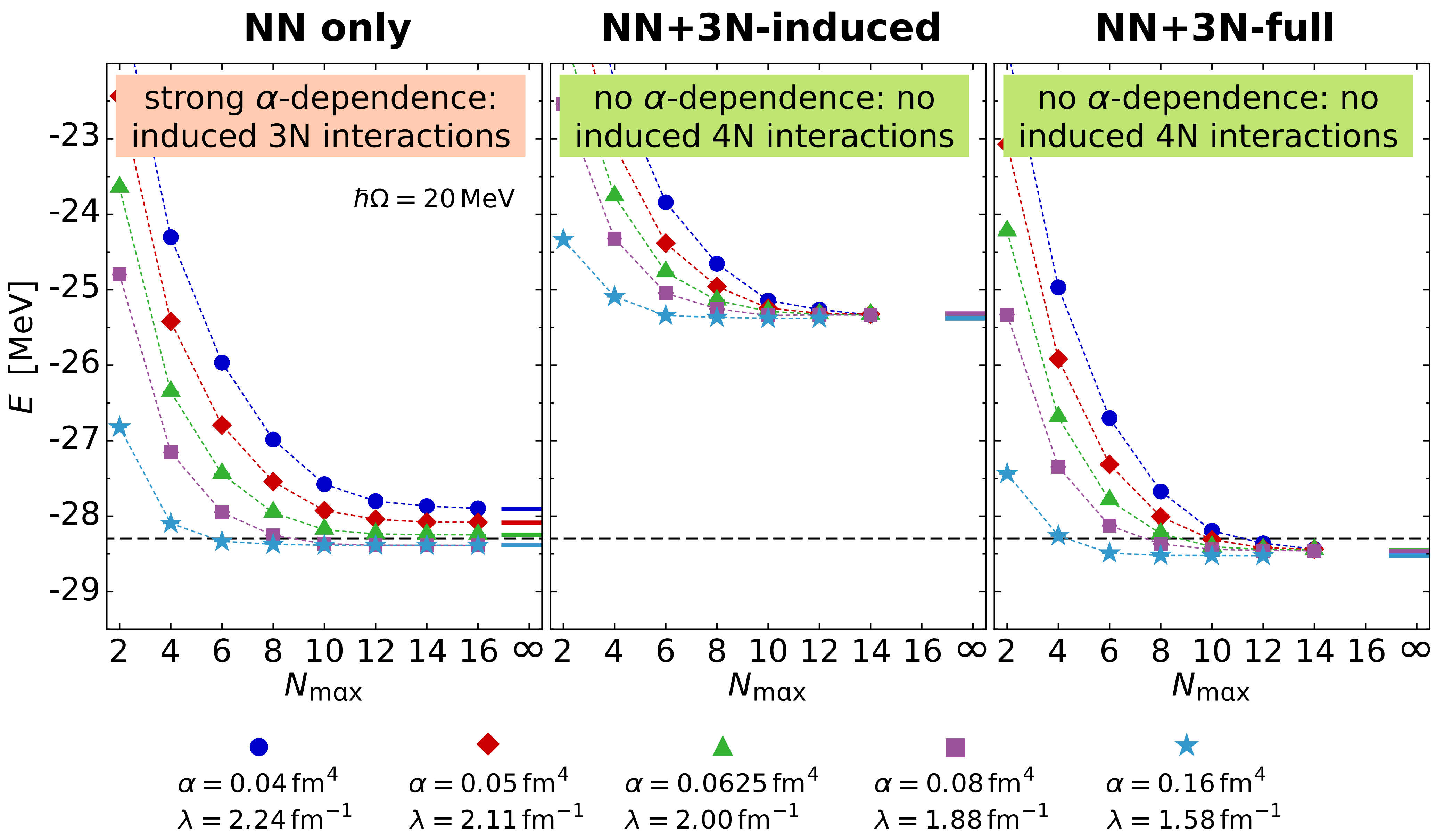
- **solving eigenvalue problem** in $\mathcal{M}(\kappa_{\mathrm{min}})$ provides improved approximation for target state

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

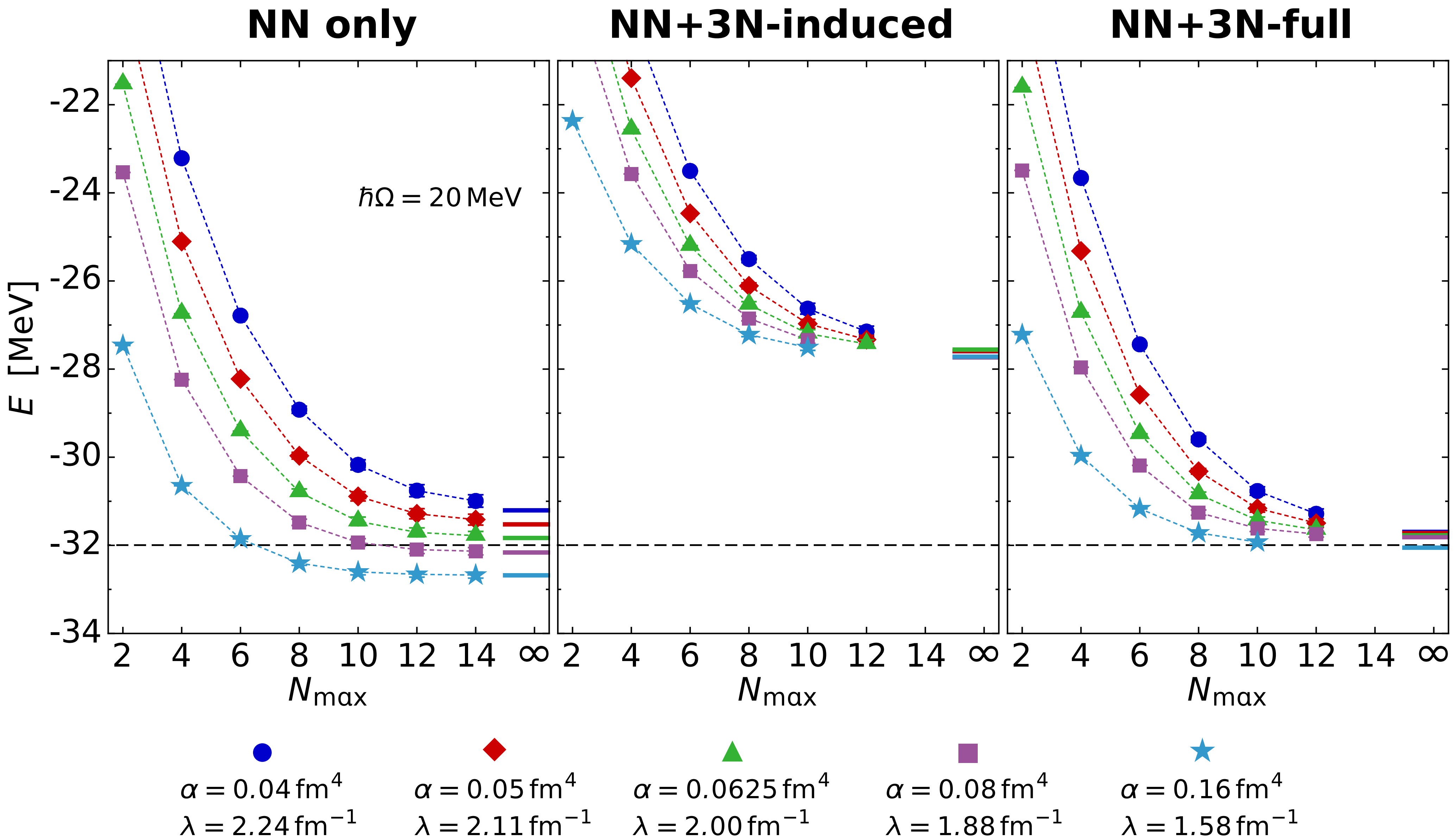
- provides **same results** as the full NCSM keeping all its advantages

- expands **application range** to higher A

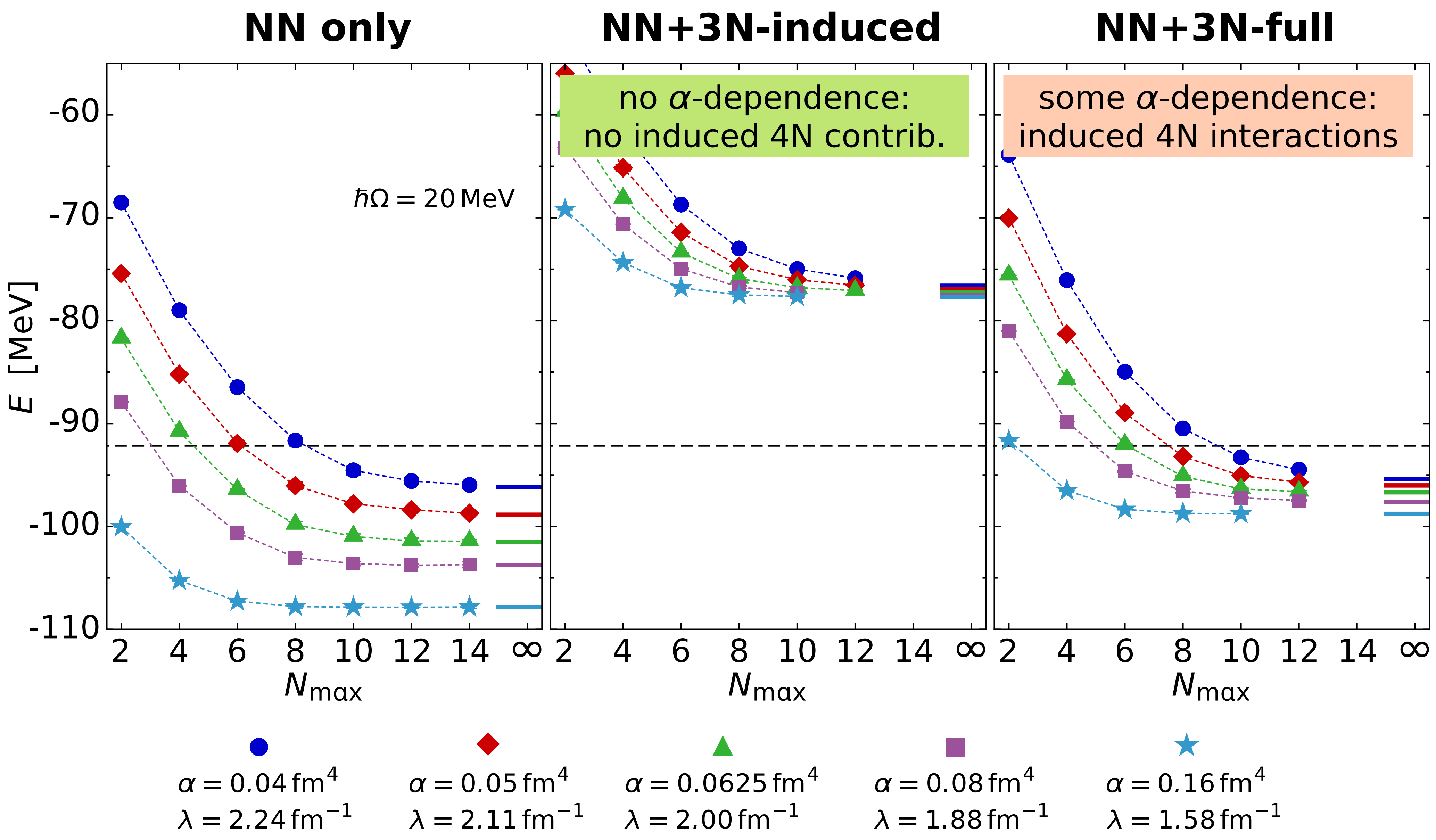
^{4}He: Ground-State Energies



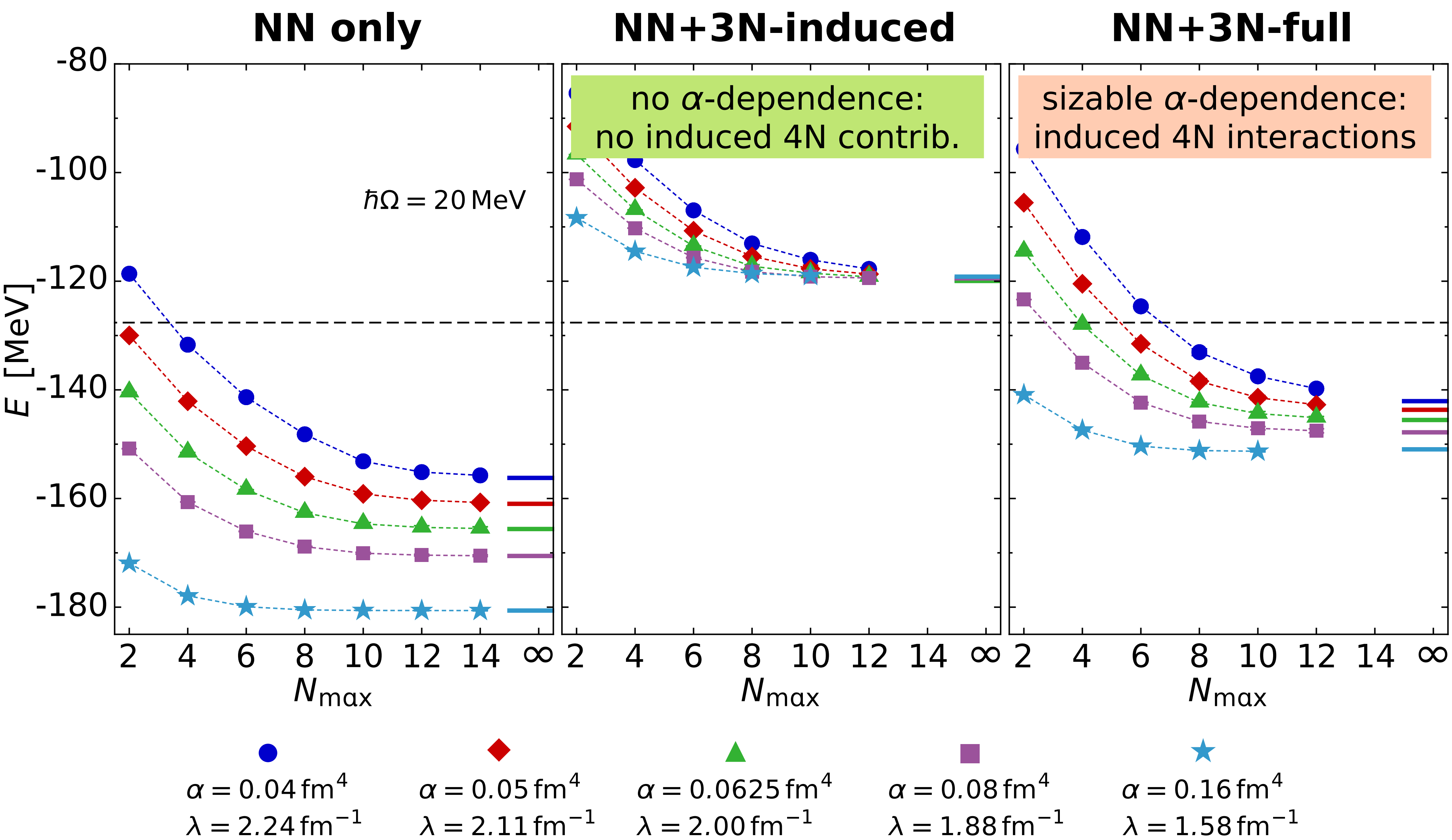
^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies

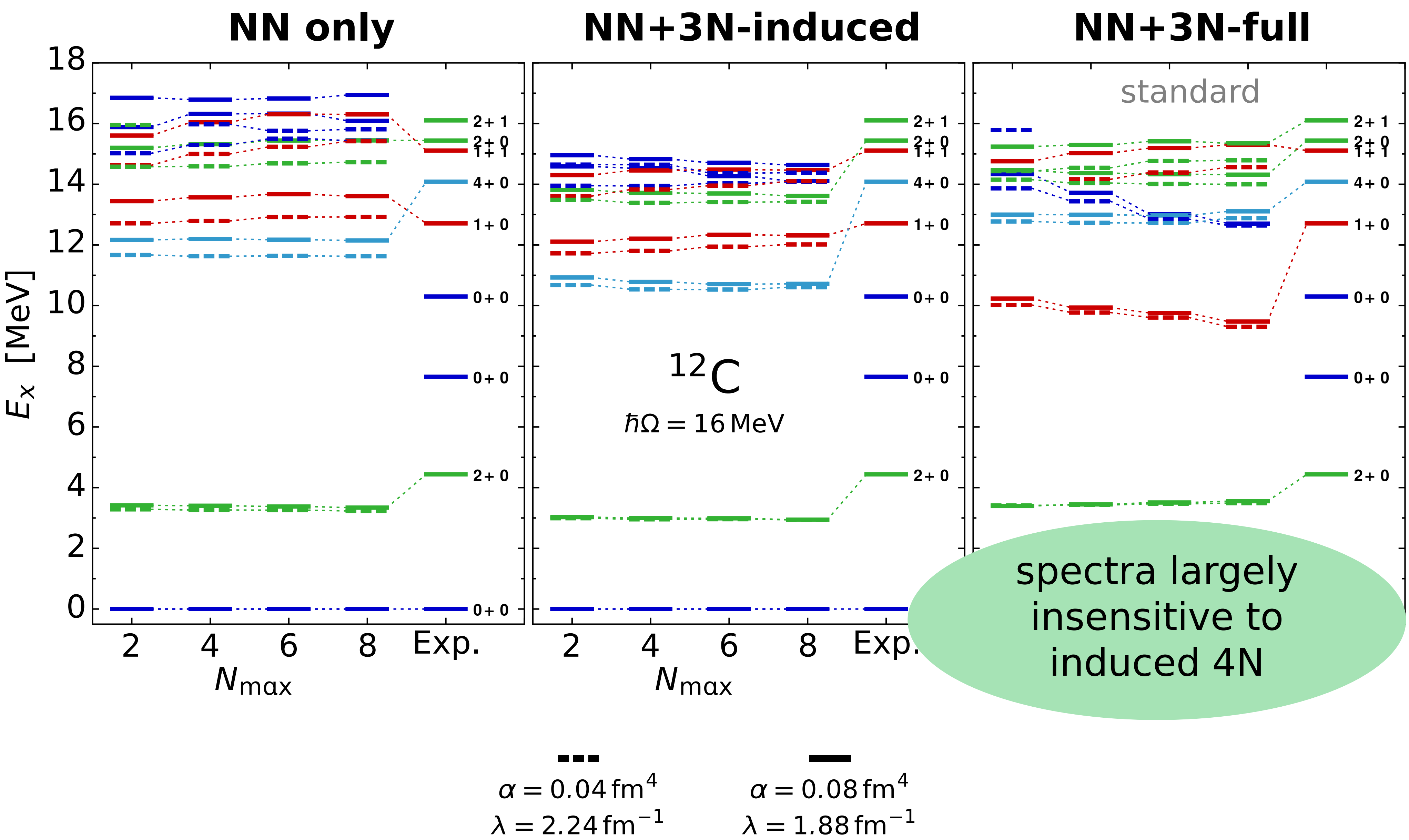


^{16}O: Ground-State Energies



Spectroscopy of ^{12}C

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



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

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

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

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

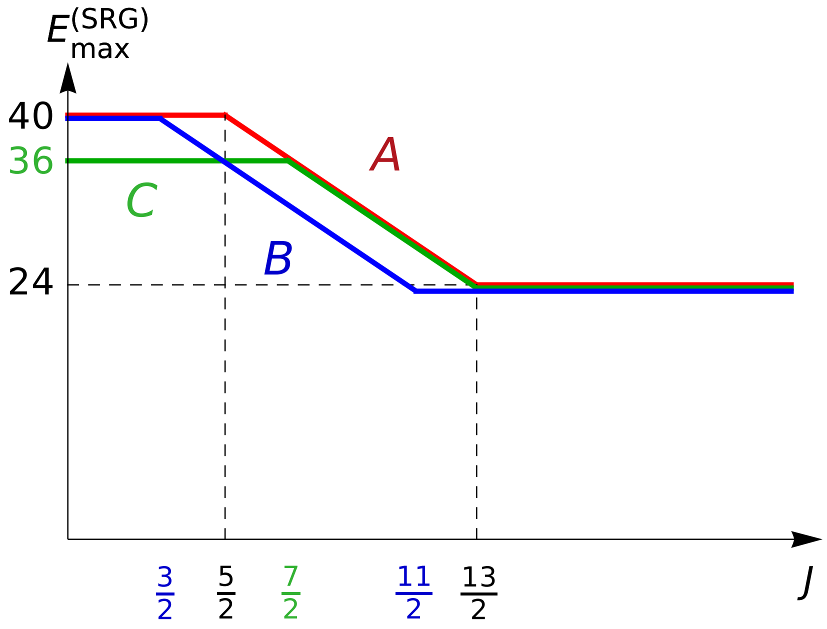
$$+\langle E'i'JT|\,\widetilde{\mathrm{H}}_\alpha\,|E''i''JT\rangle\langle E''i''JT|\,\widetilde{\mathrm{H}}_\alpha\,|E'''i'''JT\rangle\langle E'''i'''JT|\,\mathrm{T}_{\mathrm{int}}\,|EiJT\rangle$$

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

SRG Model Space

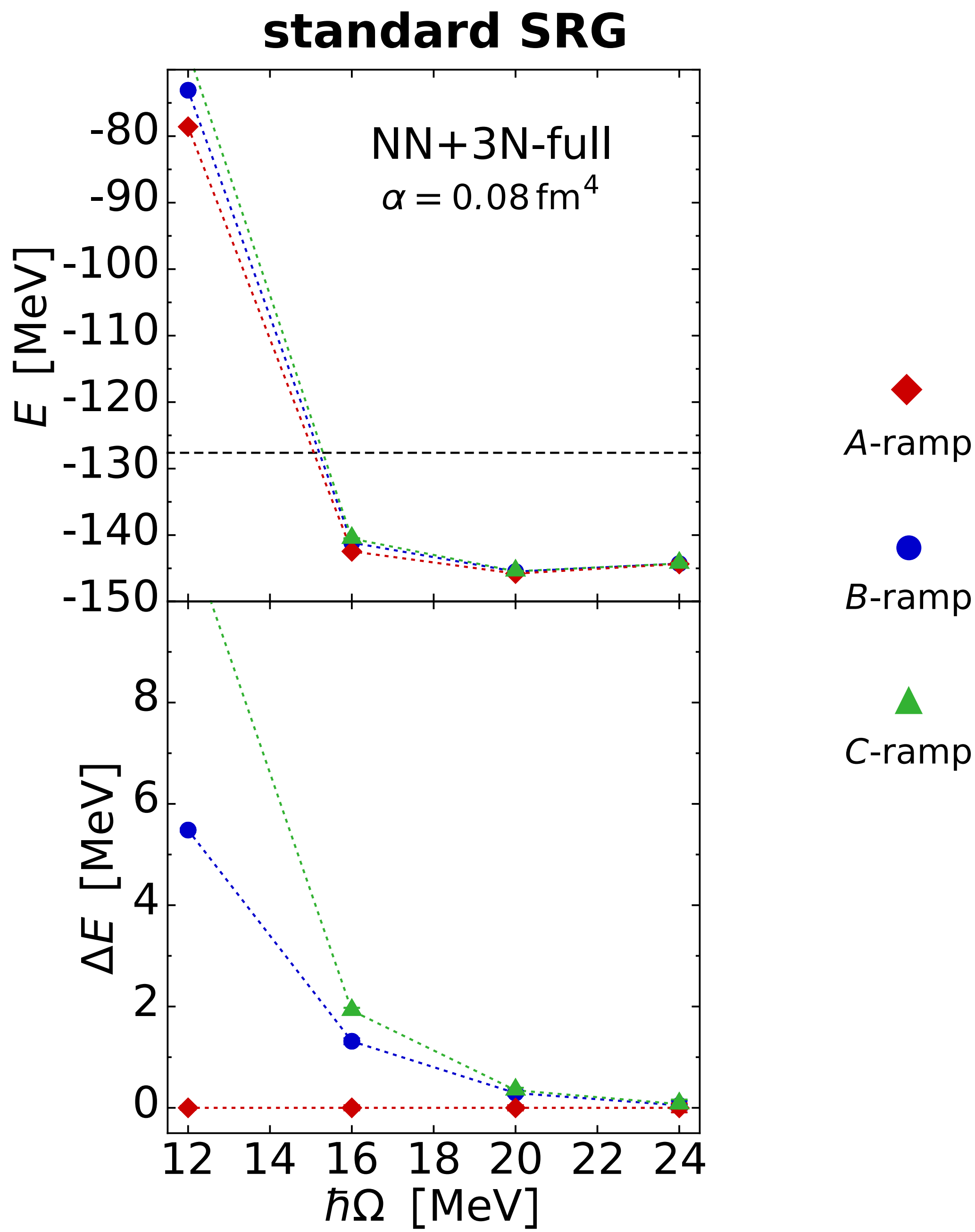
- large angular momenta less important for low-energy properties
  - J-dependent model space truncation $E_{\max}^{(\mathrm{SRG})}(J)$

SRG model-space ramp



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

Frequency Conversion: ^{16}O Ground State

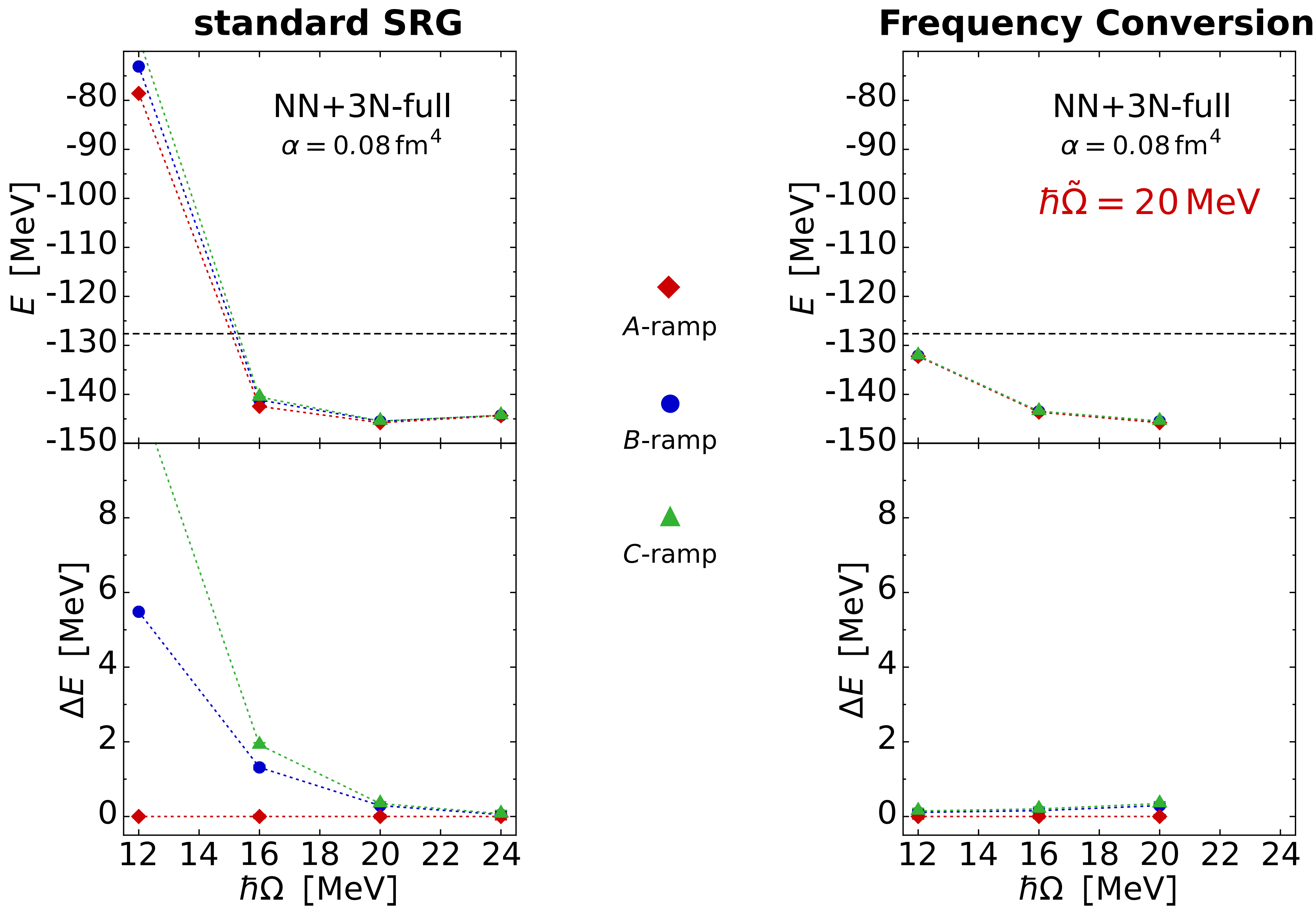


- physical content of SRG model space depends on $\hbar\Omega$
- SRG model space insufficient for **low $\hbar\Omega$**
  - especially for increasing mass number

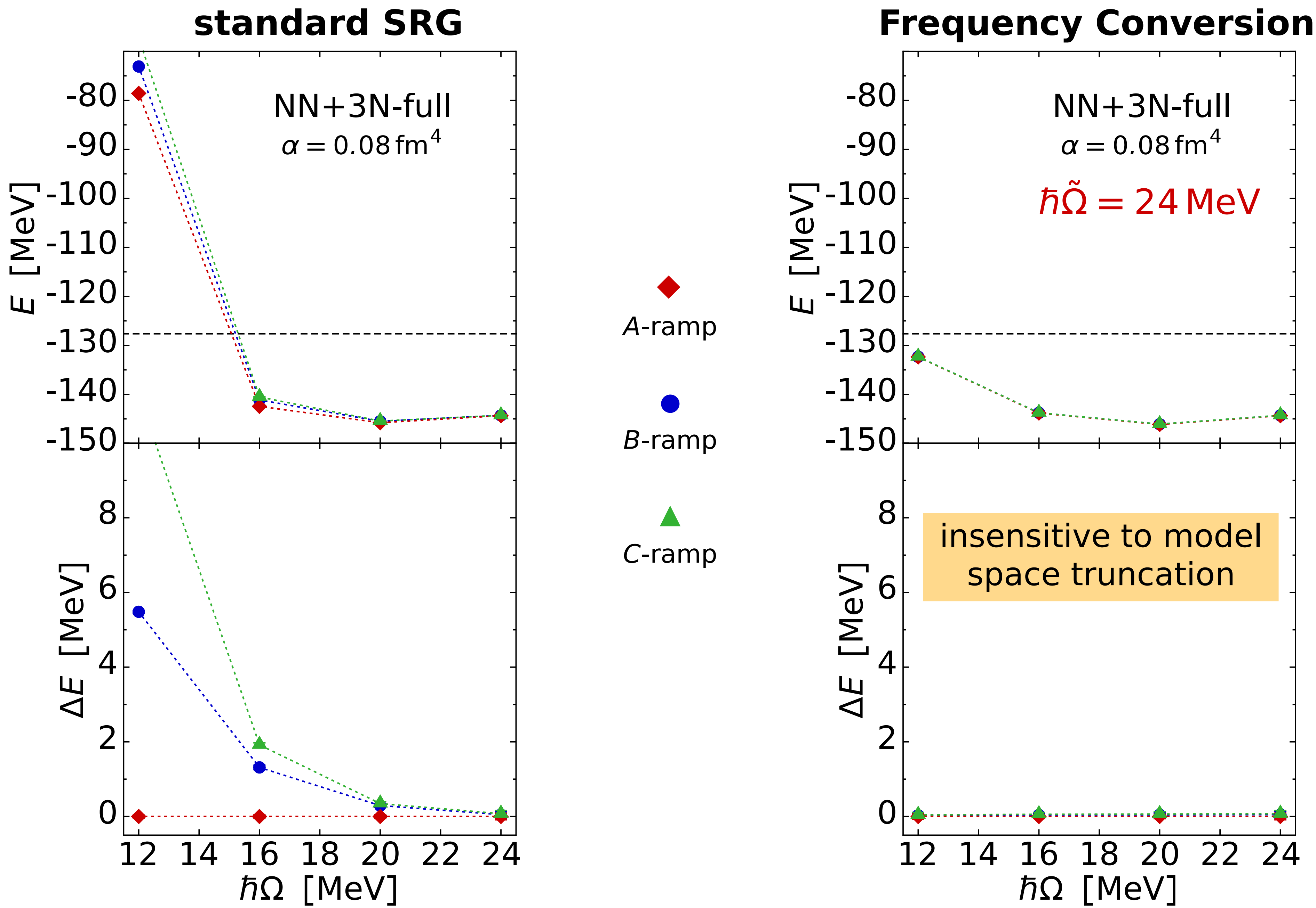
Idea:

- **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



Sensitivity of Nuclear Spectra on Chiral 3N Interactions

Roth, Langhammer, AC et al. — in preparation

Sensitivity on Chiral 3N Interactions

- analyze the sensitivity of spectra on **low-energy constants** (c_i, c_D, c_E) and **cutoff** (Λ) of the chiral 3N interaction at N^2LO

- why this is interesting:
  - **impact of N^3LO contributions**: some N^3LO diagrams can be absorbed into the N^2LO structure by shifting the c_i constants

$$\bar{c}_1 = c_1 - \frac{g_A^2 M_\pi}{64\pi F_\pi^2}\,, \quad \bar{c}_3 = c_3 + \frac{g_A^4 M_\pi}{16\pi F_\pi^2}\,, \quad \bar{c}_4 = c_4 - \frac{g_A^4 M_\pi}{16\pi F_\pi^2}$$

(Bernard et al., Ishikawa, Robilotta)

  - **uncertainty propagation**: sizable variati... of the c_i from different extractions (also affects N...

$$c_1 = -1.23 \ldots -0.76\,, \quad c_3 = -5.\ldots$$

  - **cutoff dependence**: does t... ...ti-on affect nuclear structure obser...

provide **constraints** for the development of chiral Hamiltonians and **quantify theoretical uncertainties**

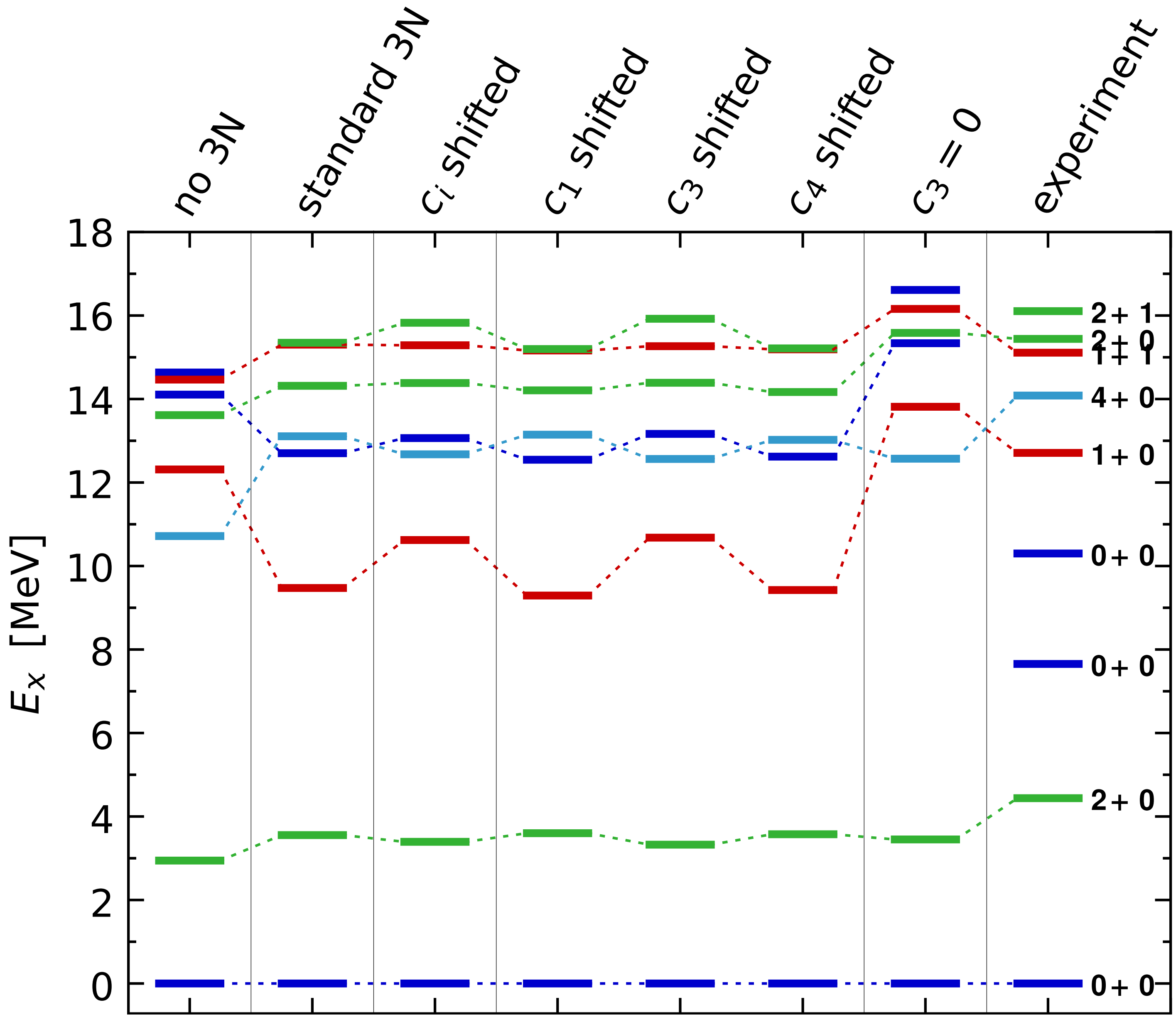
Sensitivity of Spectra on 3N Interactions

- analyze the sensitivity of spectra on **low-energy constants** (c_i, c_D, c_E) and **cutoff** (Λ) of the chiral 3N interaction at N^2LO

	c_1 [GeV^{-1}]	c_3 [GeV^{-1}]	c_4 [GeV^{-1}]	c_D	c_E
standard 3N	−0.81	−3.2	+5.4	−0.2	−0.205
c_i shifted	−0.94	−2.3	+4.5	−0.2	−0.085
c_1 shifted	−0.94	−3.2	+5.4	−0.2	−0.247
c_3 shifted	−0.81	−2.3	+5.4	−0.2	−0.200
c_4 shifted	−0.81	−3.2	+4.5	−0.2	−0.130
$c_D = -1$	−0.81	−3.2	+5.4	−1.0	−0.386
$c_D = +1$	−0.81	−3.2	+5.4	+1.0	−0.038
$\Lambda = 400$ MeV	−0.81	−3.2	+5.4	−0.2	+0.098
$\Lambda = 450$ MeV	−0.81	−3.2	+5.4	−0.2	−0.016

- refit c_E parameter to reproduce ^{4}He ground-state energy

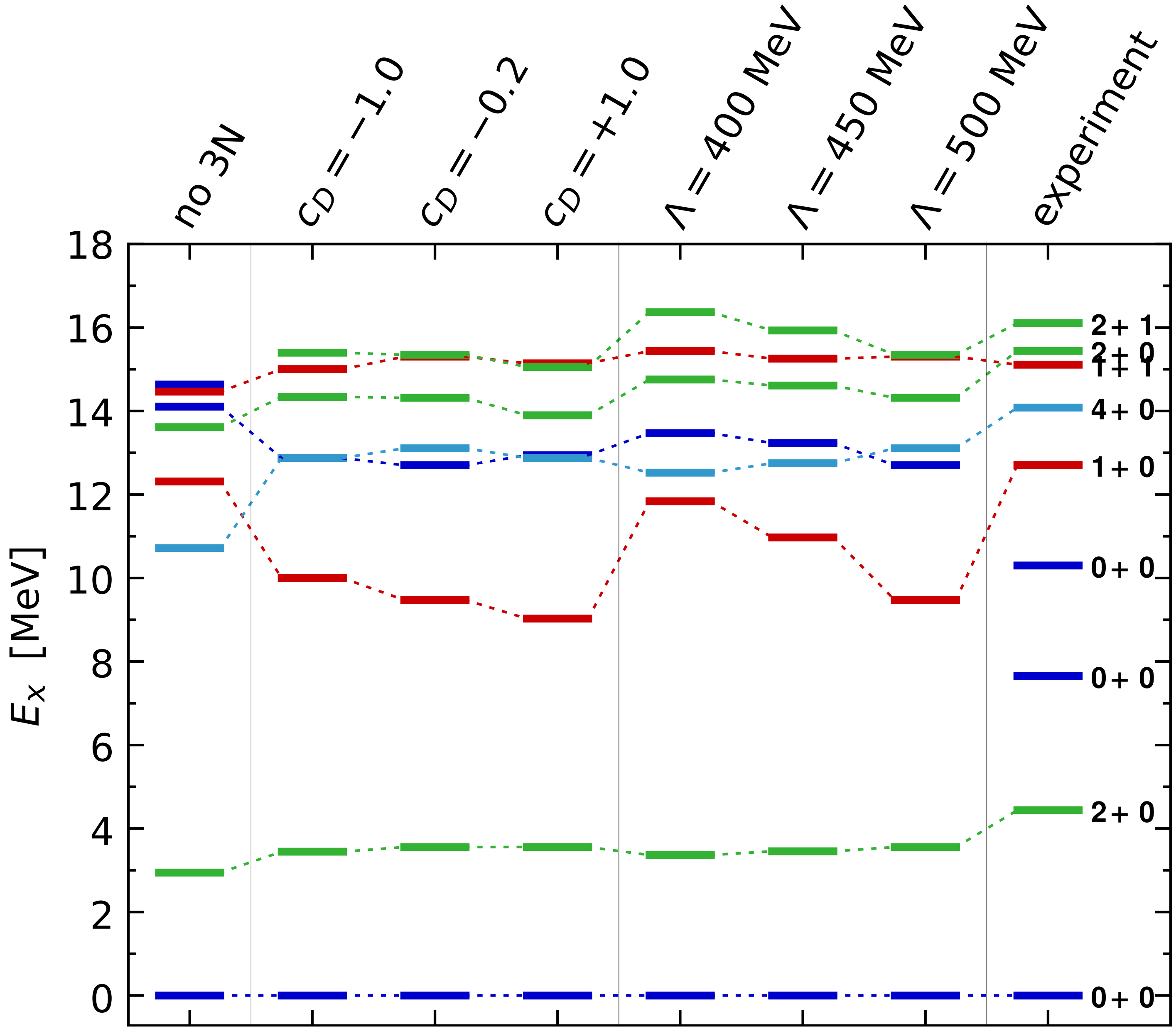
^{12}C : Sensitivity on c_i



- many states are rather c_i-insensitive
- first 1^+ state shows strong c_3-sensitivity

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

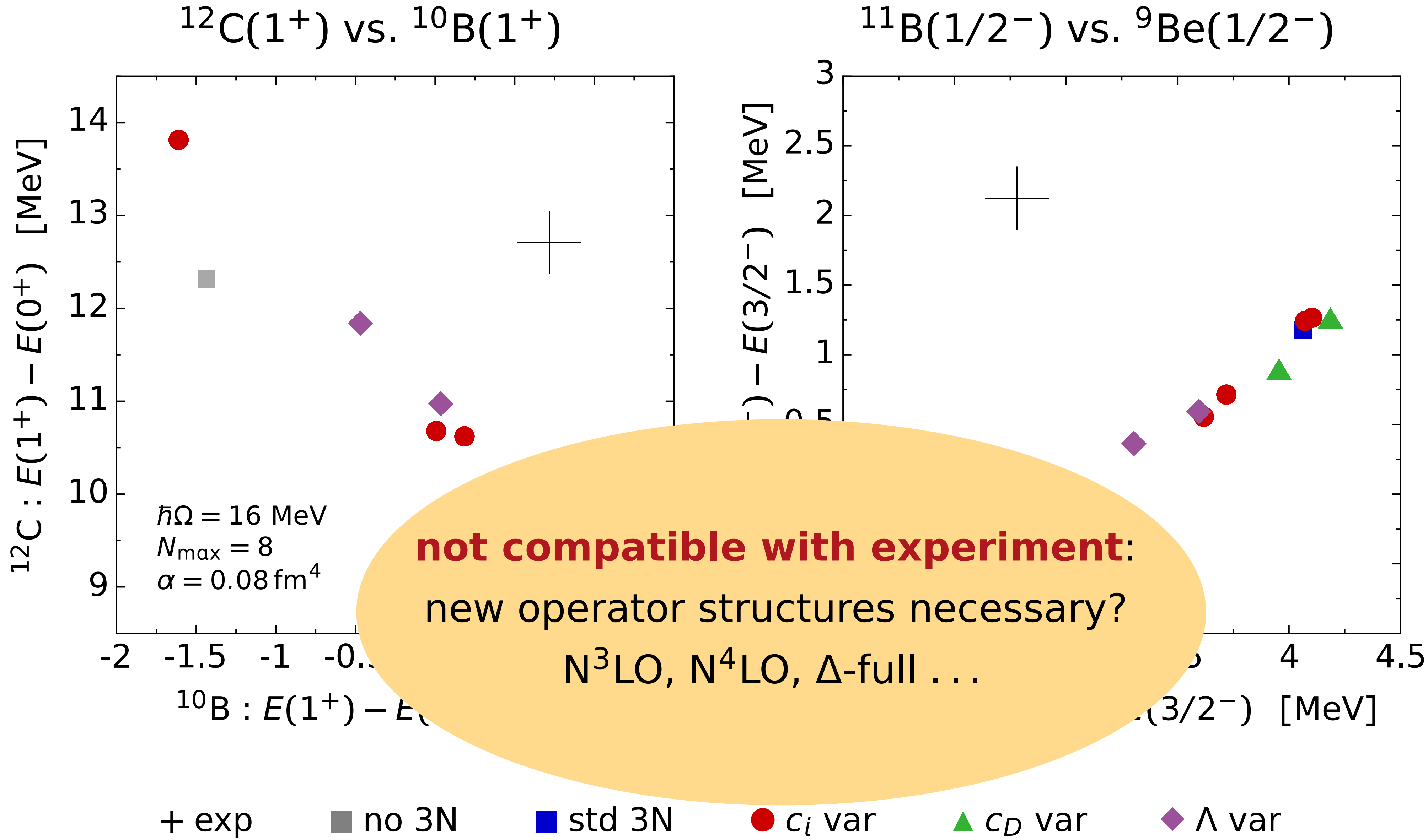
^{12}C : Sensitivity on c_D & Cutoff



- weak dependence on c_D, stronger dependence on Λ
- again first 1^+ state is most sensitive

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

Correlation Analysis



not compatible with experiment:

new operator structures necessary?

N^3LO, N^4LO, Δ-full . . .

Towards Next-Generation Chiral Hamiltonians

Technical Aspects

- **starting point**: numerical 3N matrix elements in partial-wave Jacobi-momentum basis (antisym. under $1 \longleftrightarrow 2$)

$$\langle p_1' p_2' \beta' | V_3 (1+P) | p_1 p_2 \beta \rangle \quad \text{or} \quad \langle p_1' p_2' \beta' | (1+P) V_3 (1+P) | p_1 p_2 \beta \rangle$$

$$|p_1 p_2 \beta\rangle = |p_1 p_2 \{(L_1, S_1) J_1, (L_2, S_2) J_2\} J M_J; (T_1, T_2) T M_T\rangle$$

  - numerical partial-wave decomposition of Skibinski et al.
  - ongoing collaborative effort to produce N^2LO/N^3LO matrix elements (Cracow, Bochum, Bonn, Ohio SU, Iowa SU, Darmstadt)

- **need** transformation to **HO basis** for nuclear structure calculations!
  - SRG in momentum space then transformation to HO basis (Kai Hebeler)
  - direct transformation to HO basis

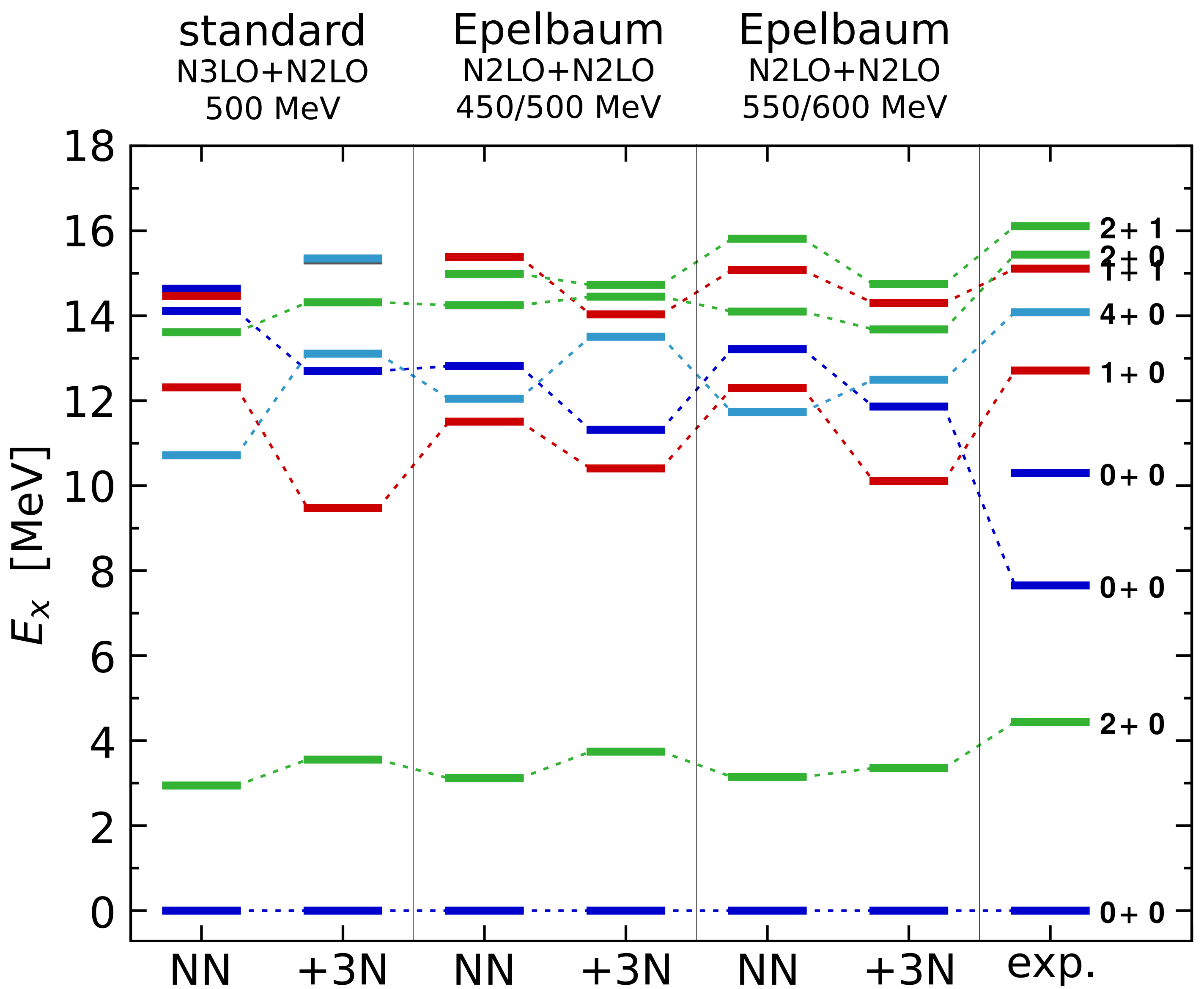
Machinery 3-Body Momentum Basis

Our Strategy:

- transform initial interaction to antisym. HO Jacobi basis
- use HO machinery afterwards (SRG; $\mathcal{J}, T$-coupled scheme;...)
  - SRG in HO basis very efficient (discrete, consider antisymmetry)
  - new developments in HO basis applicable for all chiral interactions

- **first application**: consistent NN+3N Hamiltonian at N^2LO
  - NN at N^2LO: Epelbaum et al., cutoffs 450,...,600 MeV, phase-shift fit χ^2/dat ~ 10 (~ 1) up to 300 MeV (100 MeV)
  - 3N at N^2LO: Epelbaum et al., cutoffs 450,...,600 MeV, nonlocal, fit to $\alpha(nd)$ and $E(^3H)$, included up to J=7/2

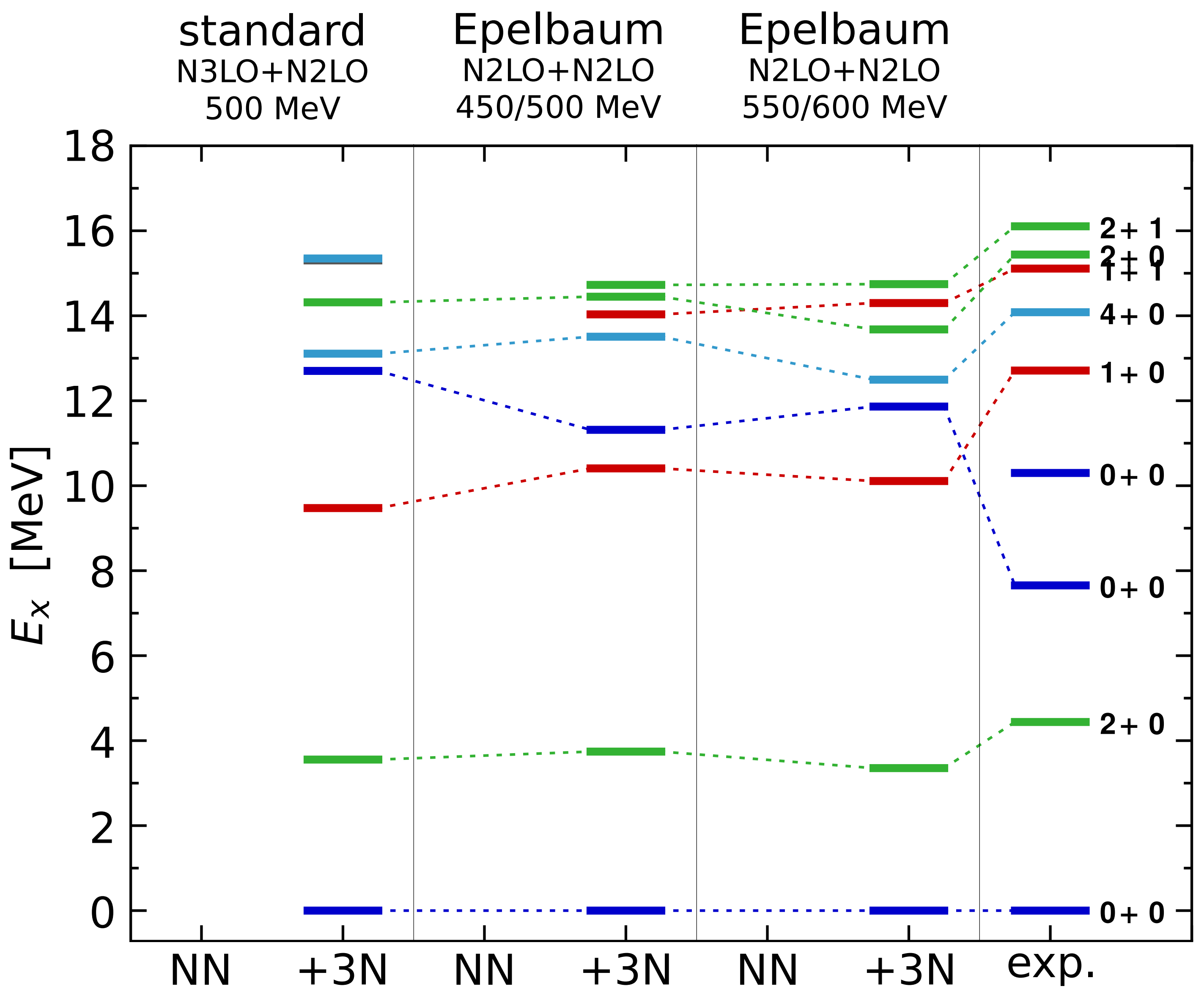
^{12}C : Consistent N^{2}LO Hamiltonians



- rather consistent description with different NN+3N Hamiltonians

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

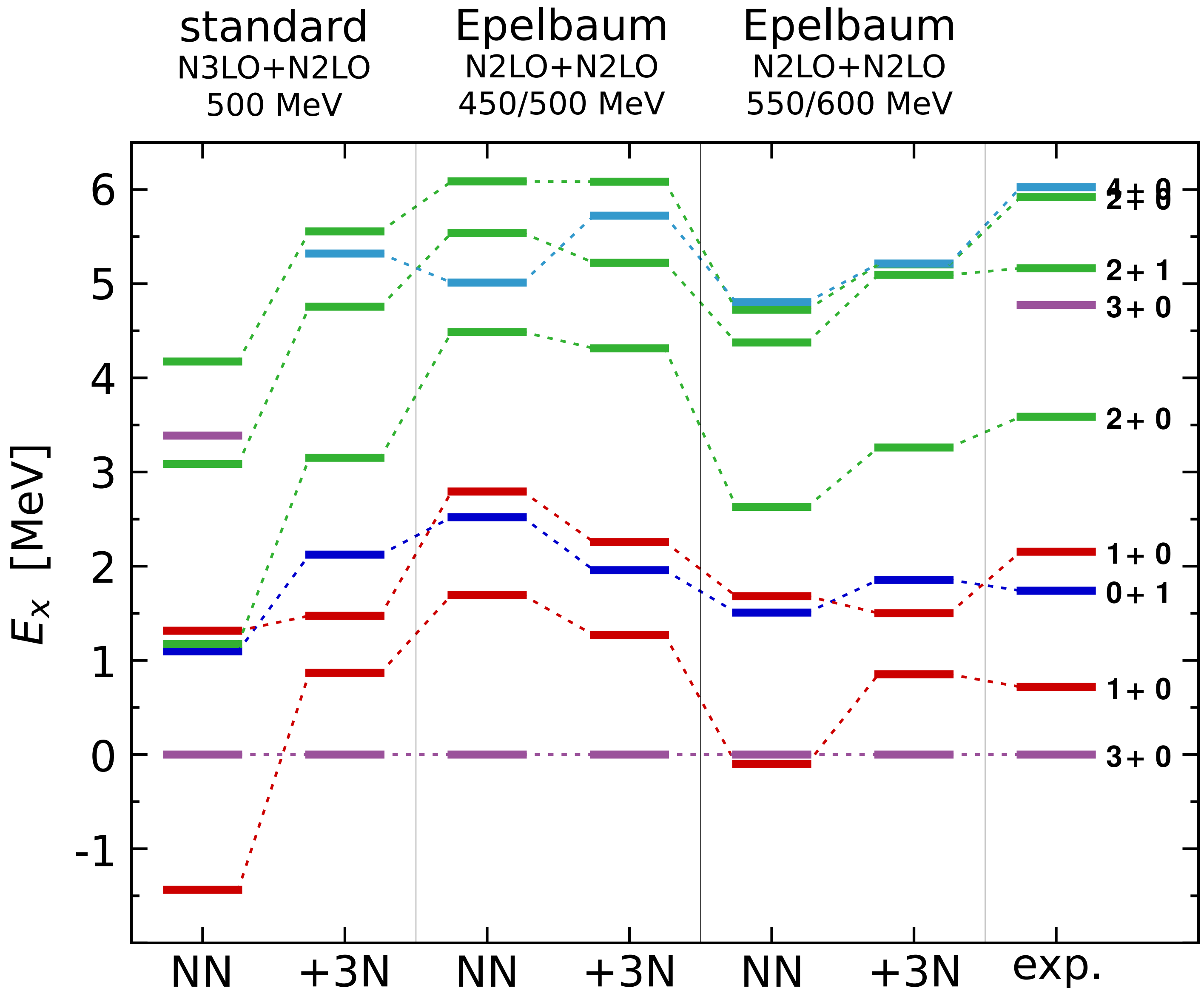
^{12}C : Consistent N^{2}LO Hamiltonians



- rather consistent description with different NN+3N Hamiltonians

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

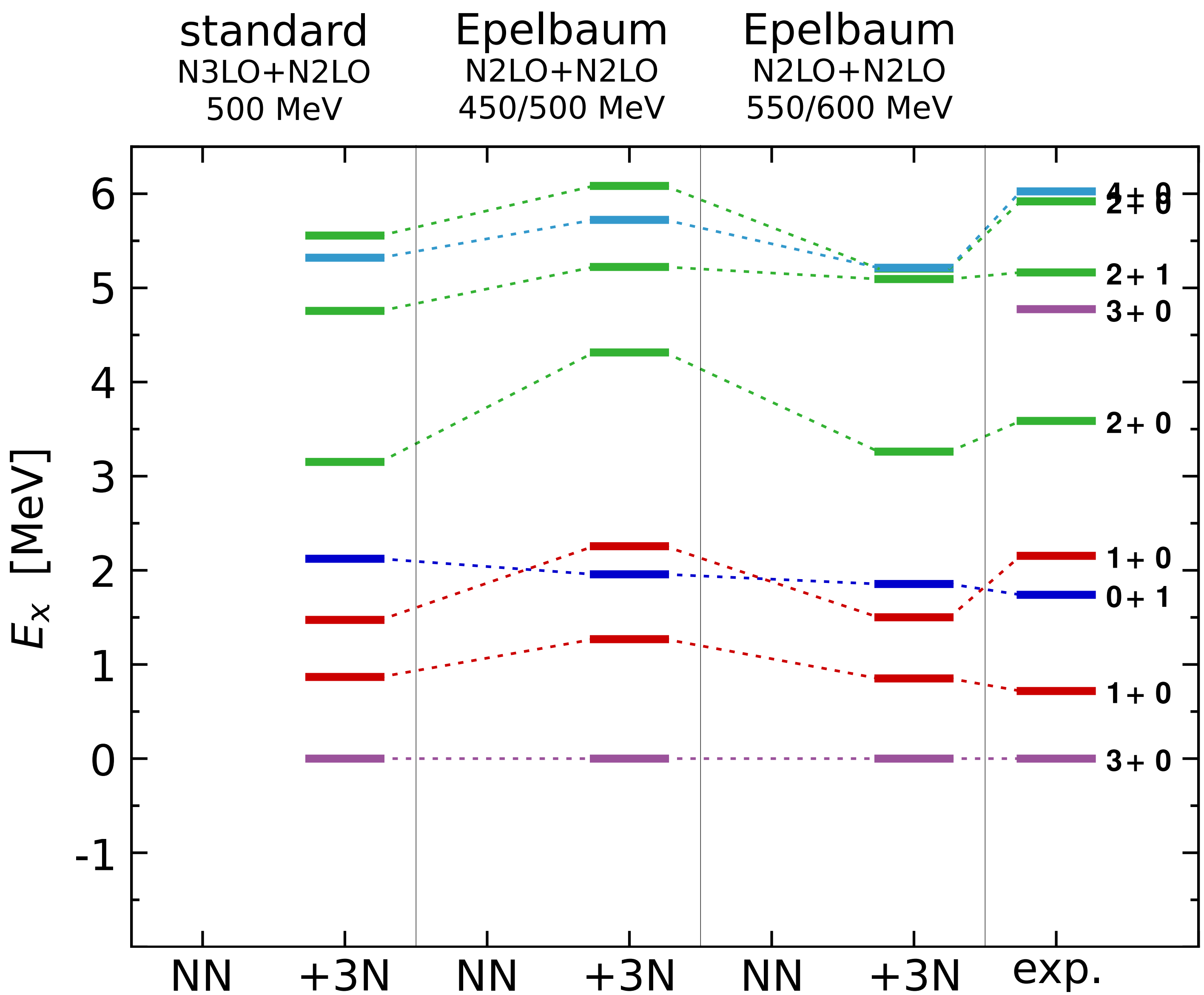
^{10}B : Consistent N^{2}LO Hamiltonians



- large variations at NN level
- more consistent description with NN+3N

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

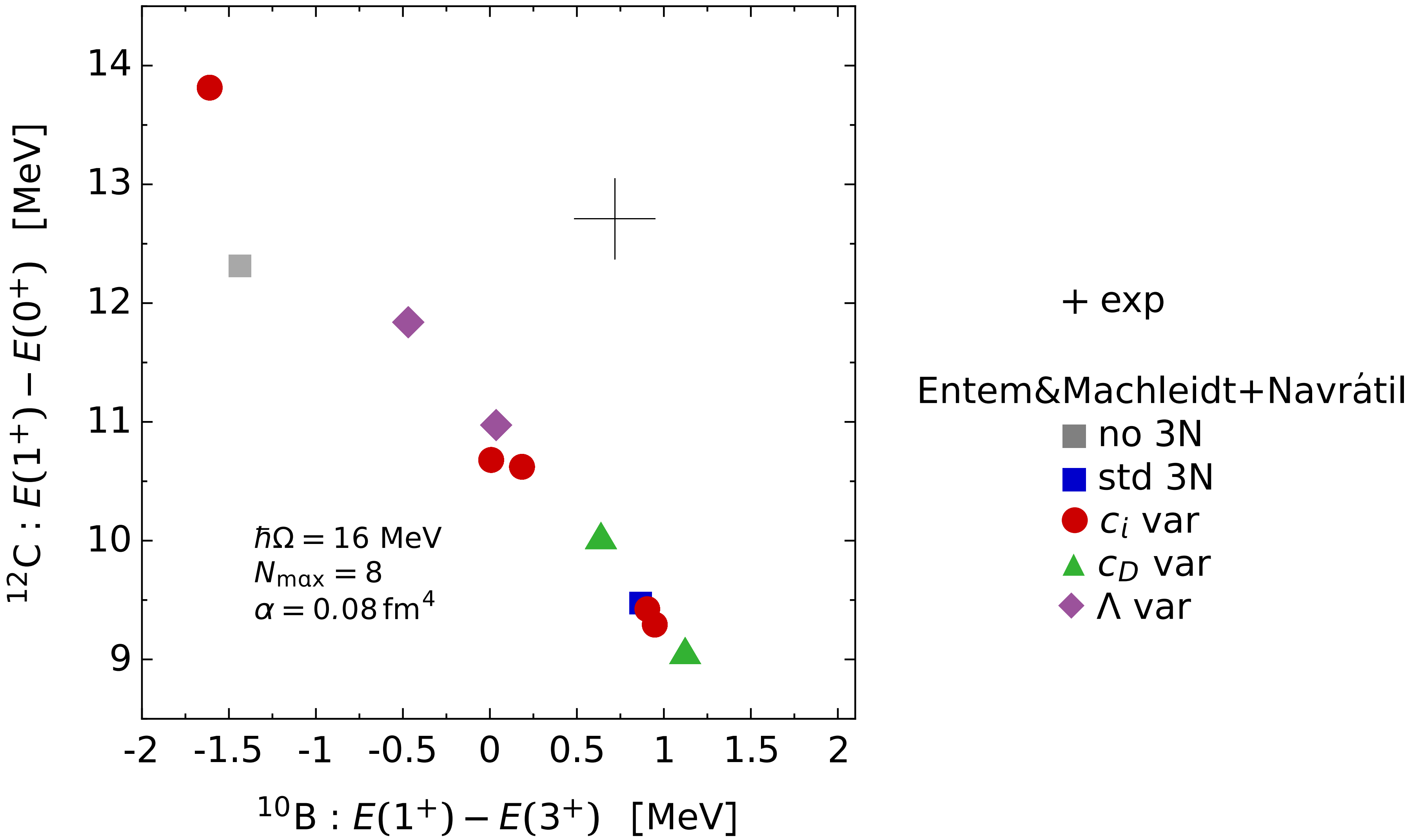
^{10}B : Consistent N^{2}LO Hamiltonians



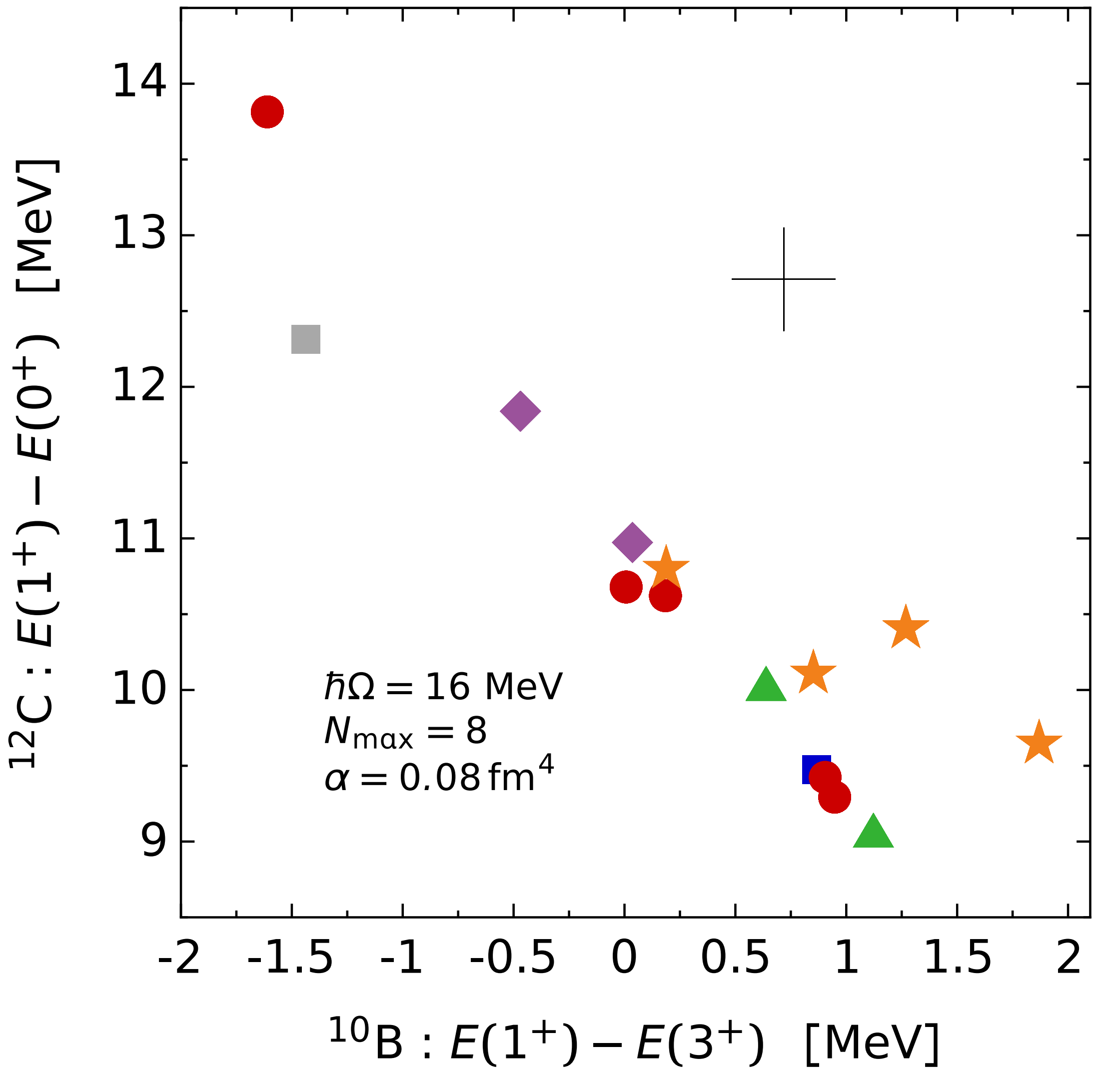
- large variations at NN level
- more consistent description with NN+3N

$\hbar\Omega = 16$ MeV
$N_{\max} = 8$
$\alpha = 0.08\,\mathrm{fm}^4$

Correlation Analysis: $^{12}C(1^+)$ vs. $^{10}B(1^+)$



Correlation Analysis: ^{12}C(1^+) vs. ^{10}B(1^+)



- interesting **deviation** from E&M+N systematics
- **NN** possible reason

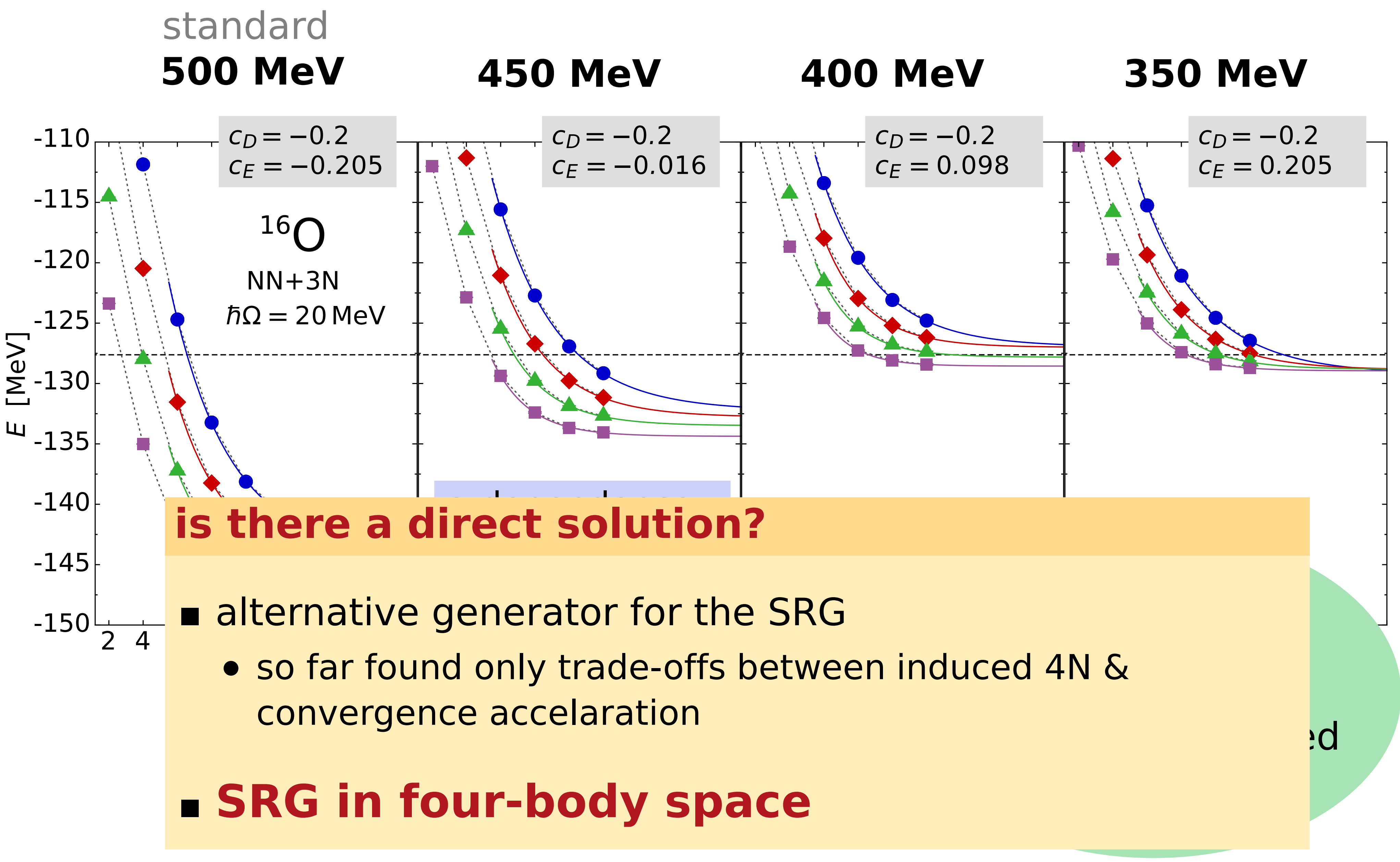
+ exp

Entem&Machleidt+Navrátil
- no 3N
- std 3N
- c_i var
- c_D var
- Λ var

Epelbaum @ N^2LO
- NN+3N

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)

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

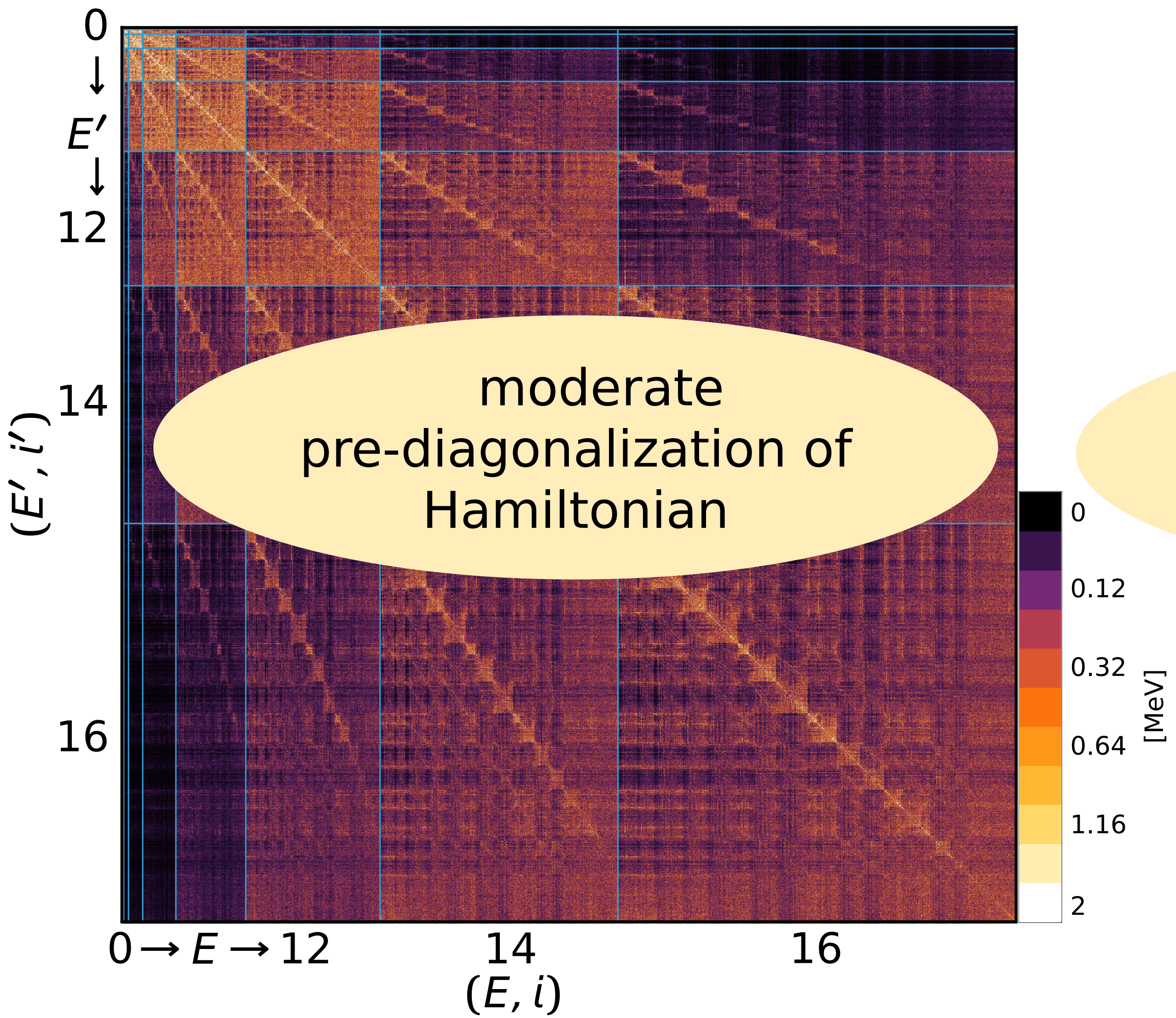
- antisym. Jacobi state

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

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

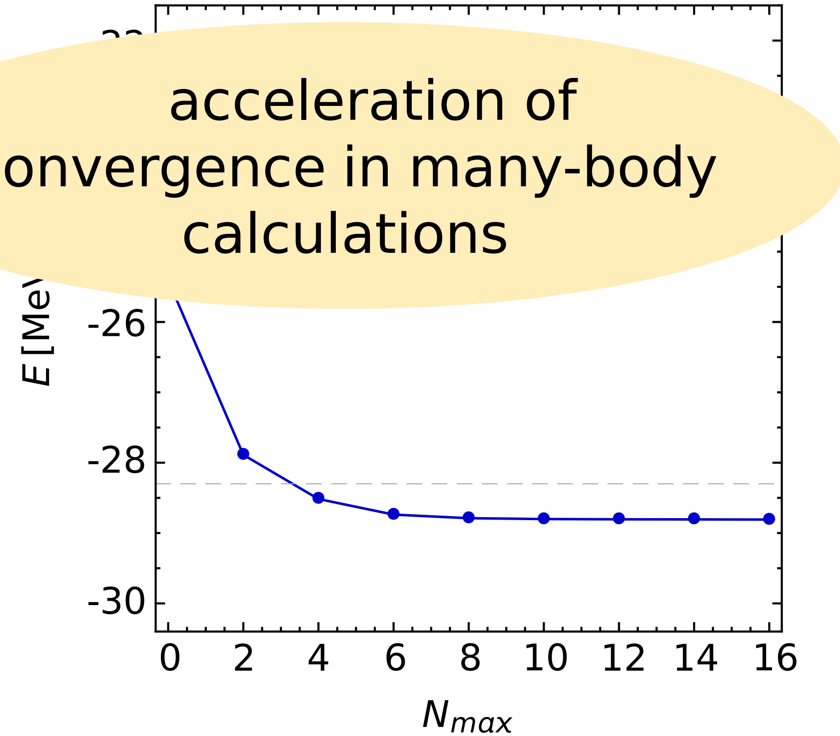
$$\alpha = 0.16\,\mathrm{fm}^4$$

$\lambda = 1.58\,\mathrm{fm}^{-1}$

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

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

NCSM ground state ^{4}He



acceleration of
convergence in many-body
calculations

First Shot: Sum over Fourth Particle

- transformation to **four-body *m*-scheme** basis and additional **normal-ordering** approximation in progress

- meanwhile:
  create **effective three-body interaction** in Jacobi basis

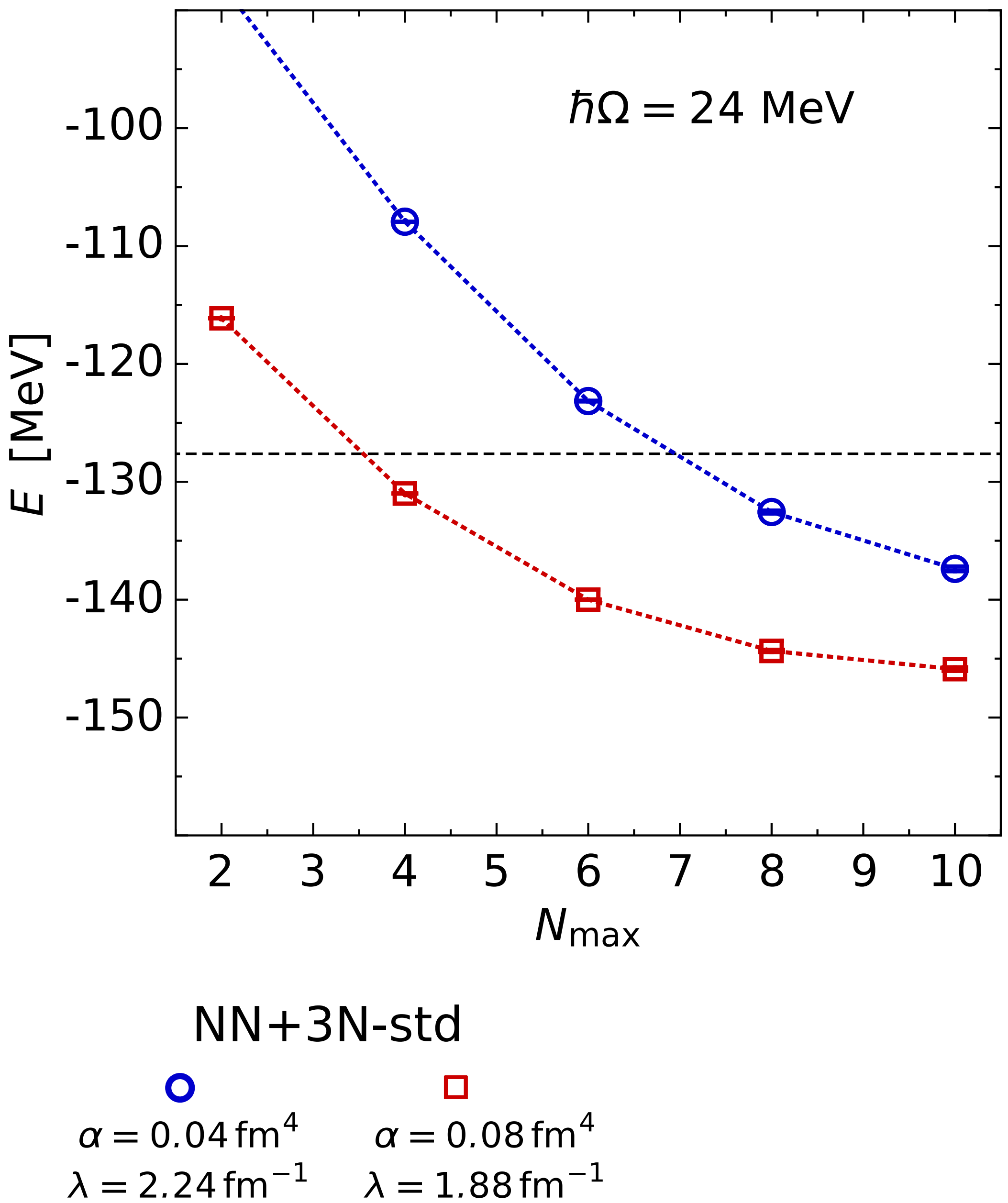
  - sum over fourth particle (unperturbed m-scheme state)
  - only consider equal J_{12}, T_{12} in Bra and Ket and average over projections
  - set three-body center of mass motion to ground-state

$$\langle E'_{12} i'_{12} J_{12} T_{12} | \hat{V}^{\text{eff}}_{3N} | E_{12} i_{12} J_{12} T_{12} \rangle$$

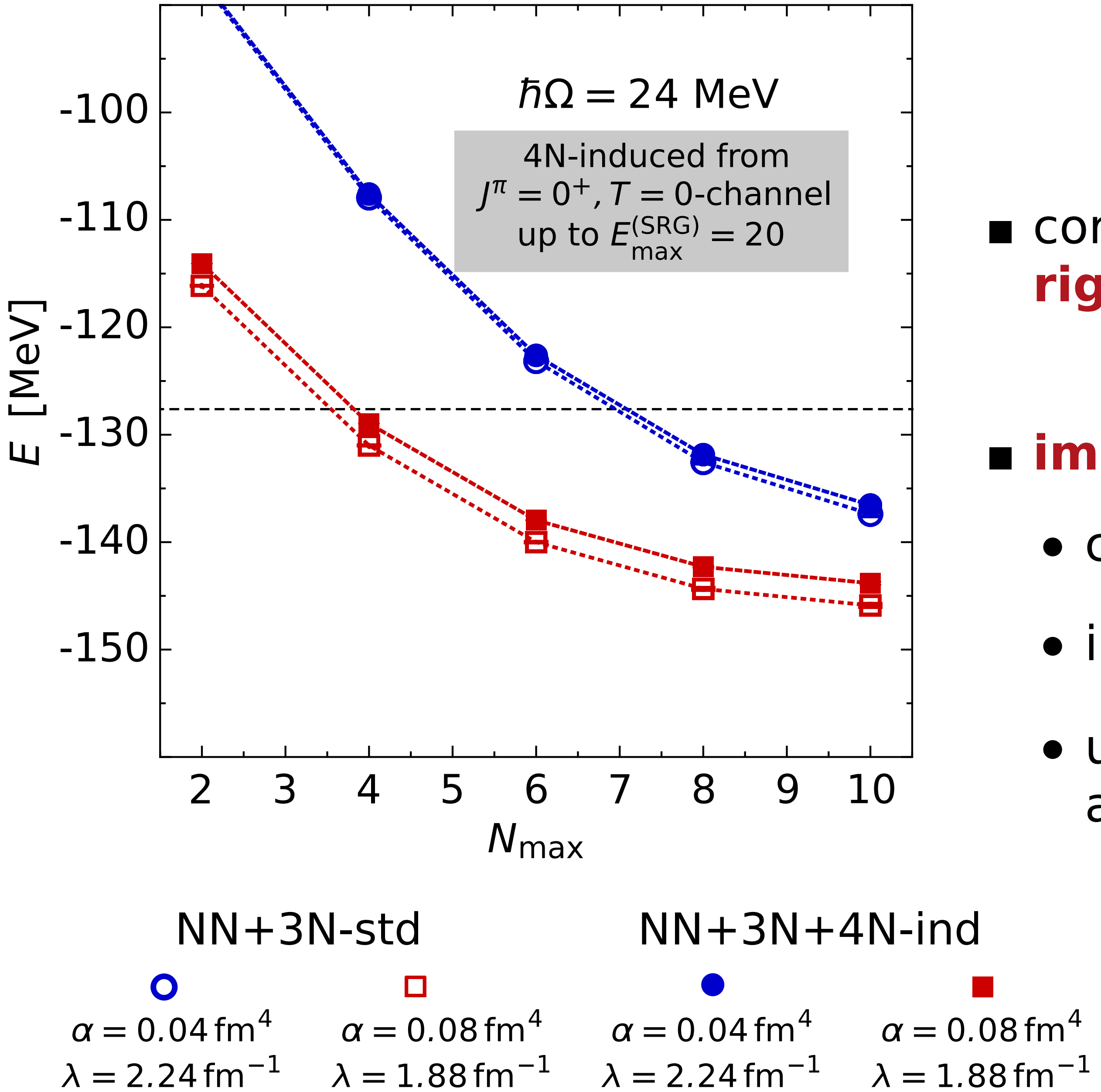
$$\times \left\{ |000\rangle \otimes |E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}}\rangle \otimes |n_d (l_d s_d) j_d m_{j_d}; t_d m_{t_d}\rangle \right\}$$

Motivation:
reproduces ground-state energy for closed shell nuclei in $\boldsymbol{N_{\max} = 0}$ space

First Shot: ^{16}O Ground State



First Shot: ^{16}O Ground State



- correction by induced 4N in **right direction**, but **too small**
- **improvements**:
  - consider further 4N channels
  - increase $E_{max}^{(SRG)}$
  - use normal-ordering approximation

Conclusions

Conclusions

- **SRG** evolution in **HO basis** efficient and **improvable**
  - frequency conversion & model space increase
- **consistent four-body** SRG evolution
  (for induced and initial contributions)
  - inclusion via **effective three-body** interaction
  - next step: use normal-ordering approximation
- **p-shell spectra** provide powerful testbed for chiral potentials
- machinery ready to use **3N @ N^3LO** in momentum Jacobi basis
  - directly applicable in IT-NCSM, CC, IM-SRG, RGM ...

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, E. Gebrerufael, P. Isserstedt, H. Krutsch, **J. Langhammer**, S. Reinhardt, **R. Roth**, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, R. Wirth
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    LLNL Livermor
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    Michigan State University, USA
  - H. Hergert, K. Hebeler
    Ohio State University, USA
  - P. Papakonstantinou
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  - umeier, T. Neff
    GSI Helmholtzzentrum

LENPIC

Low-Energy Nuclear Physics International Collaboration

Deutsche Forschungsgemeinschaft

Helmholtz International Center

Exzellente Forschung für Hessens Zukunft

Bundesministerium für Bildung und Forschung

JUROPA | LOEWE-CSC | HOPPER

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