Chiral Hamiltonians & Similarity Renormalization Group: New Directions

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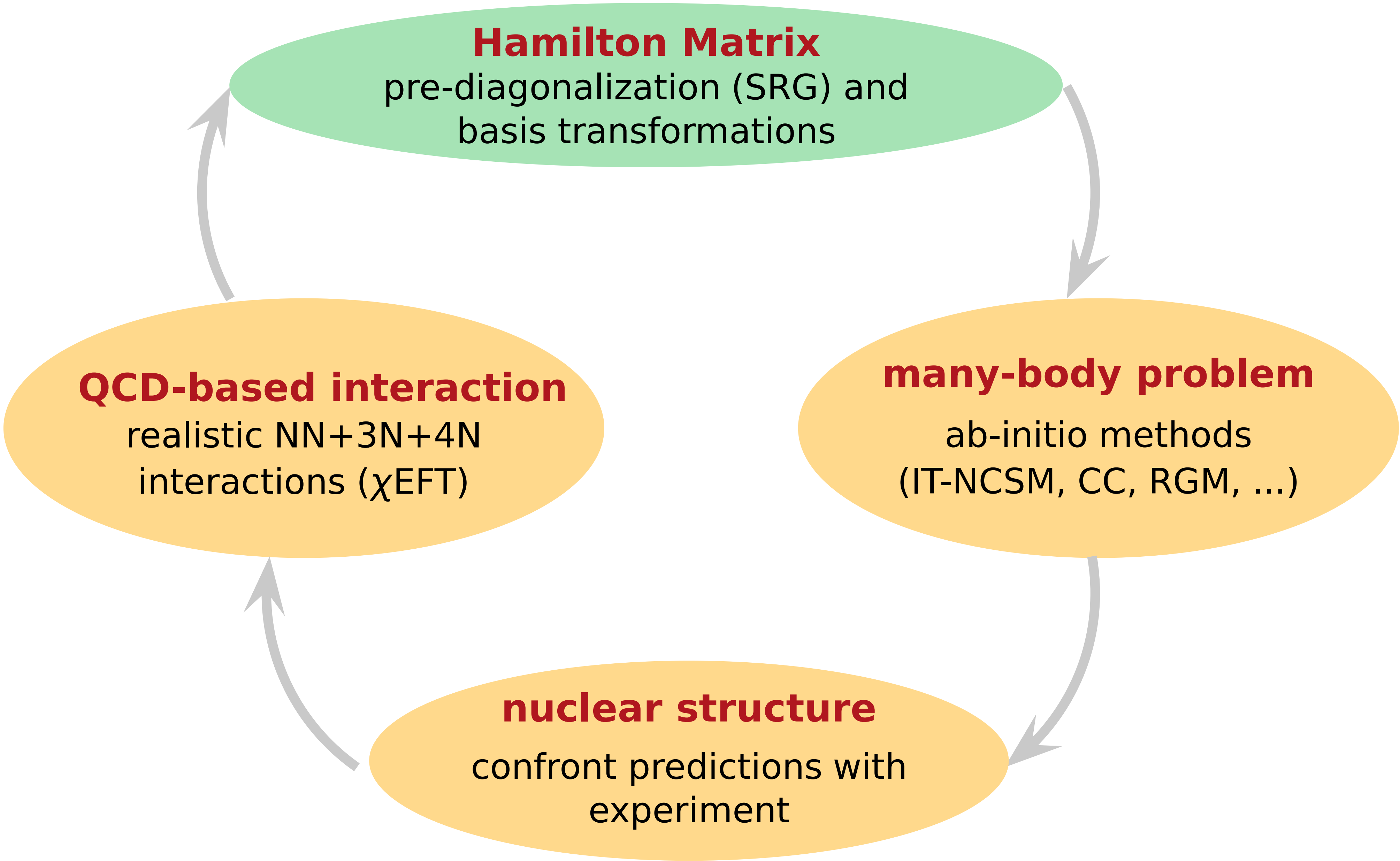
Introduction



New Directions

Applications to Nuclear Spectra
spectroscopy and sensitivity on 3N

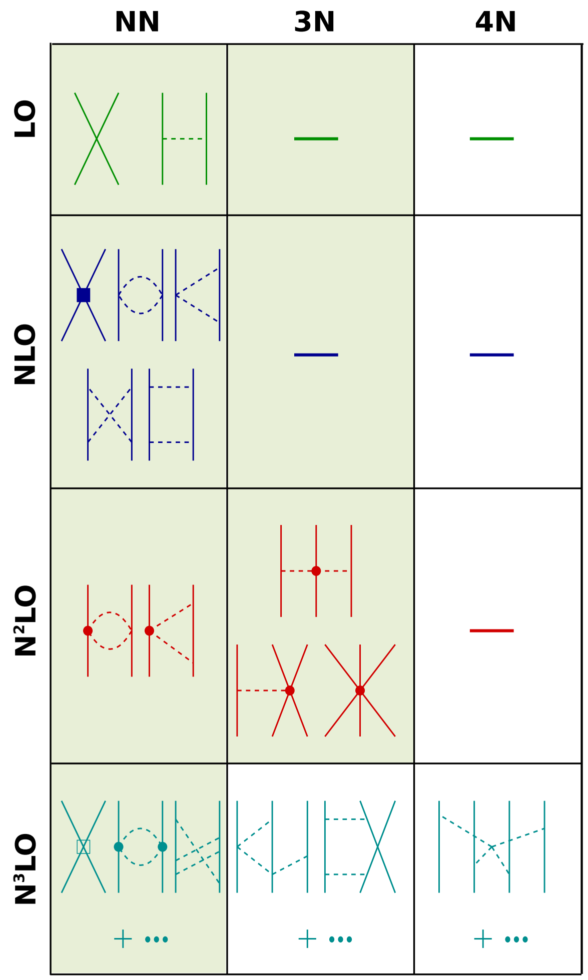
Probe Next-Generation Chiral Potentials
with ab-initio nuclear structure

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

- **standard Interaction:**
  - NN N^{3}LO: Entem&Machleidt, 500 MeV cutoff
  - 3N N^{2}LO: Navrátil, local, 500 MeV cutoff, fitted to Triton
- **standard Interaction with modified 3N:**
  - NN N^{3}LO: Entem&Machleidt, 500 MeV cutoff
  - 3N N^{2}LO: Navrátil, local, with modified LECs and cutoffs, fitted to ^{4}He
- **consistent N^{2}LO Interaction:**
  - NN N^{2}LO: Epelbaum et al., 450, . . . , 600 MeV cutoff
  - 3N N^{2}LO: Epelbaum et al., 450, . . . , 600 MeV cutoff, nonlocal
- **consistent N^{3}LO 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**

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

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 $1 \longleftrightarrow 2$:

$$|\alpha\rangle = |[(N_1 L_1, S_1)J_1, (N_2 L_2, S_2)J_2]JM_J, (T_1, T_2)TM_T\rangle$$

  - completely antisymmetric:

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

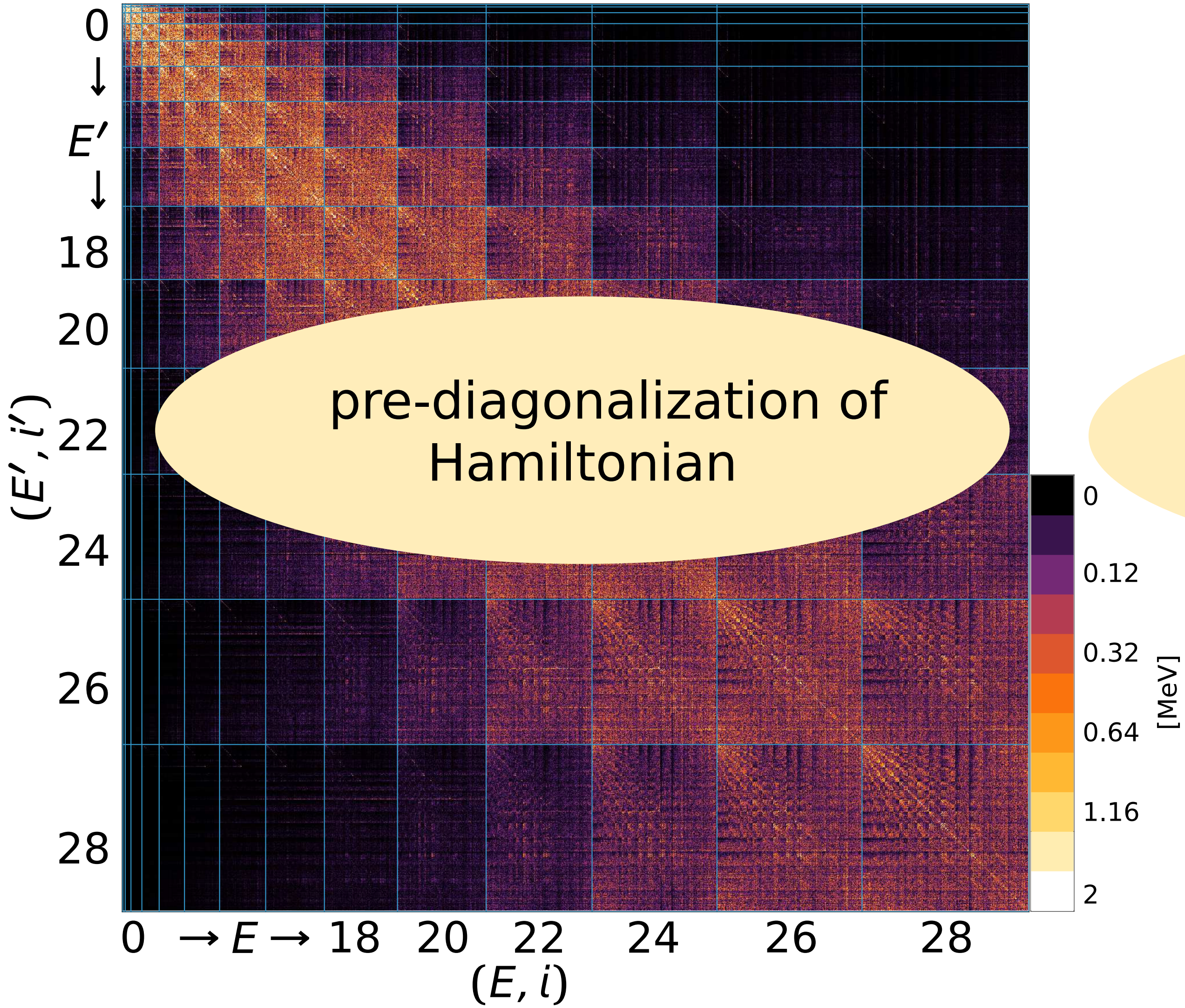
sizable **reduction** of basis dimension

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

coefficients of fractional parentage (CFPs) by P. Navrátil

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



pre-diagonalization of Hamiltonian

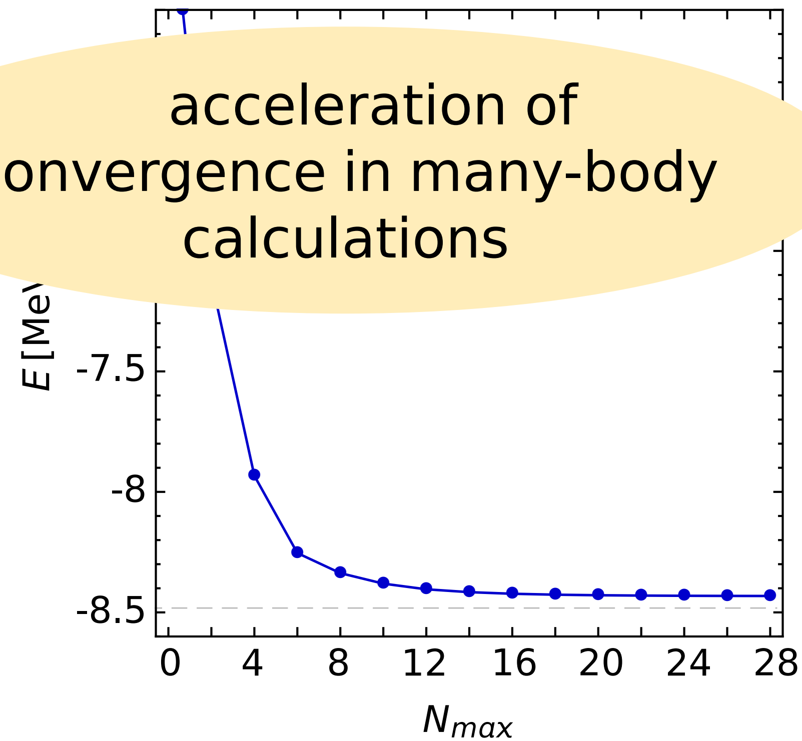
$$\alpha = 0.16\,\mathrm{fm}^4$$

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

$$\langle E'i'JT | \tilde{H}_\alpha - T_{int} | EiJT \rangle$$

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

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)

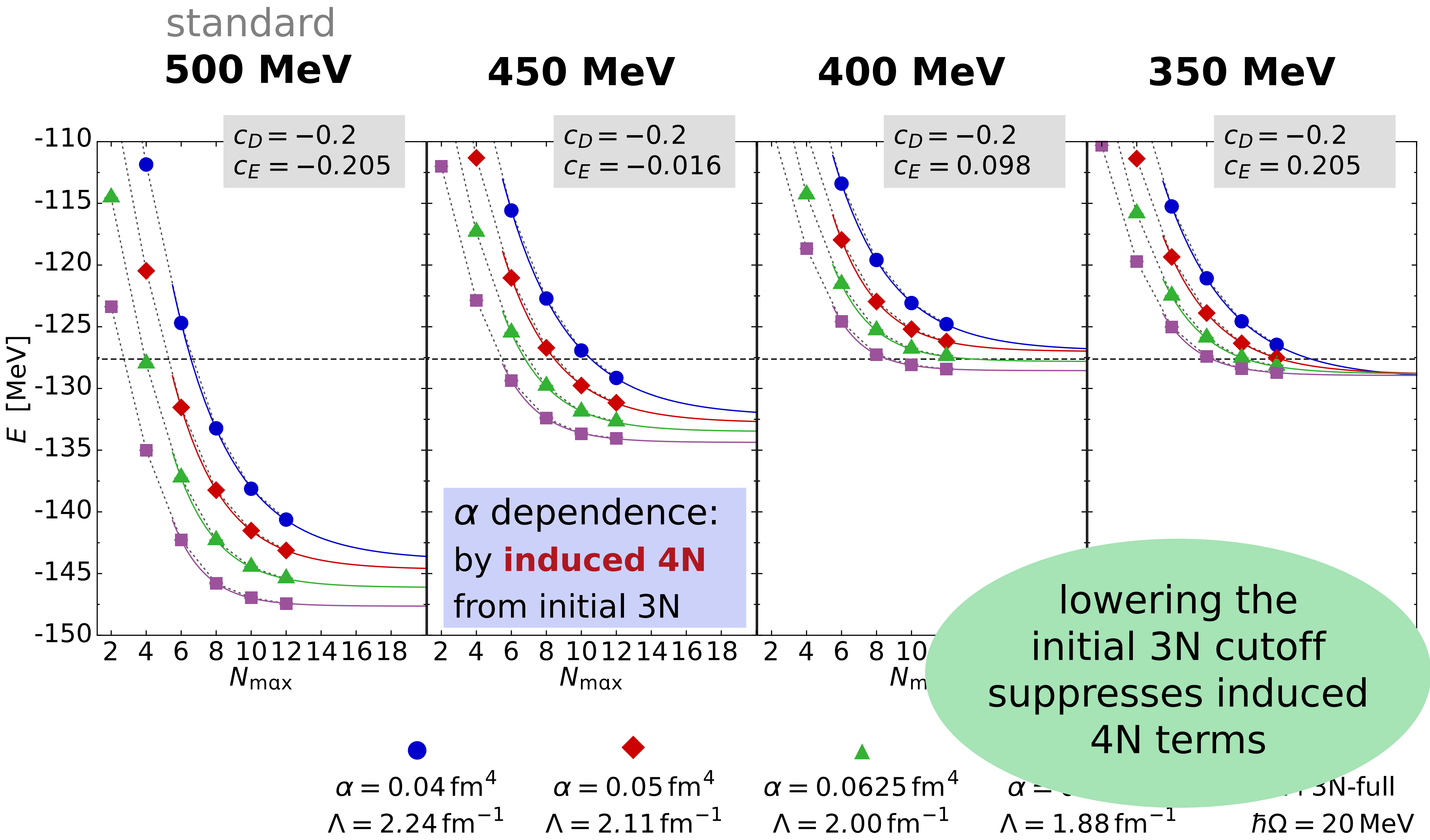
transformation from Jacobi into $\mathcal{J}T$-coupled scheme

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

decoupling on the fly

ab-initio many-body calculation

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

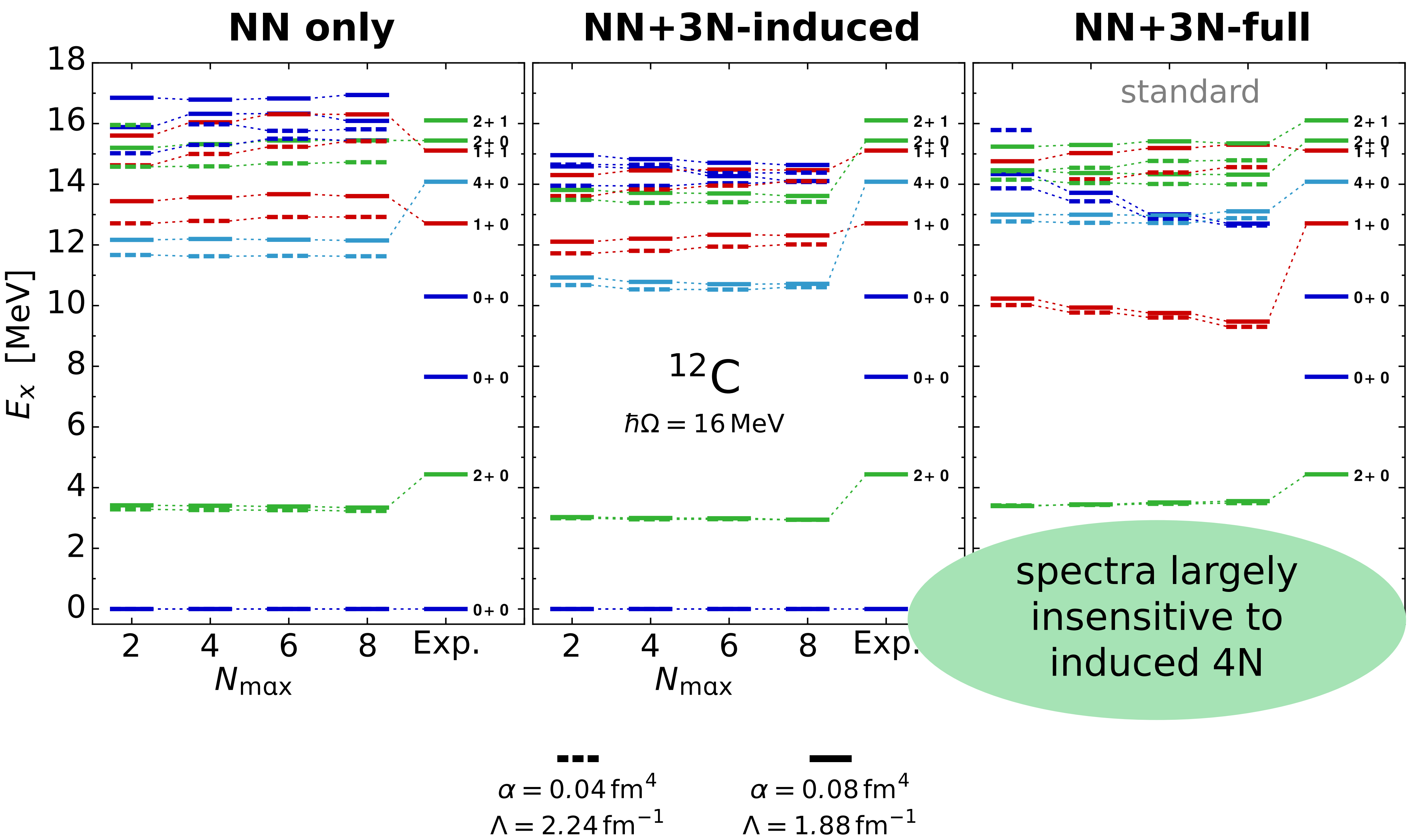


α dependence: by **induced 4N** from initial 3N

lowering the initial 3N cutoff suppresses induced 4N terms

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

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

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

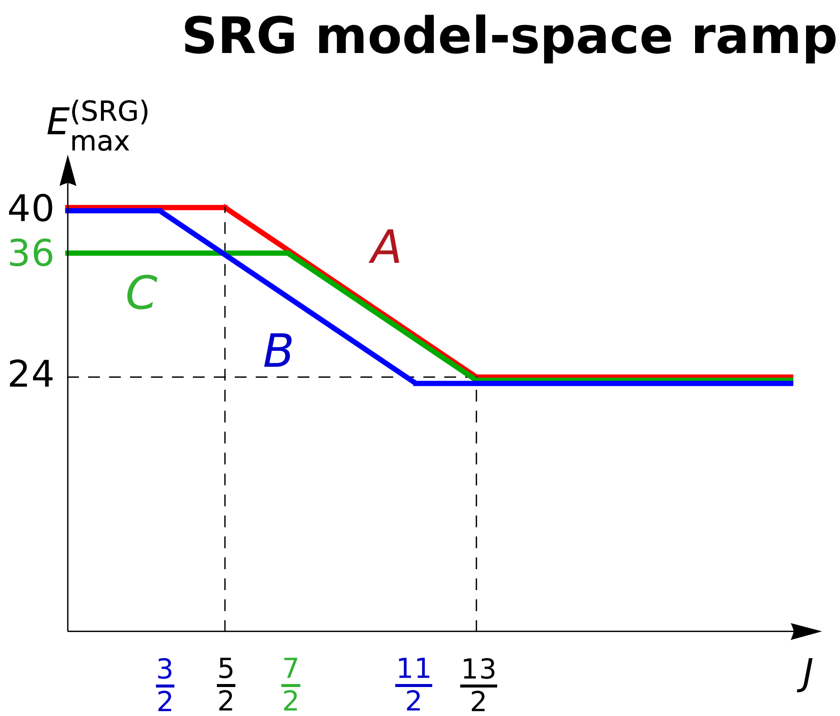
$$-2\langle E'i'JT|\,\widetilde{\mathrm{H}}_\alpha\,|E''i''JT\rangle\langle E''i''JT|\,\mathrm{T}_{\mathrm{int}}\,|E'''i'''JT\rangle\langle E'''i'''JT|\,\widetilde{\mathrm{H}}_\alpha\,|EiJT\rangle$$

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

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

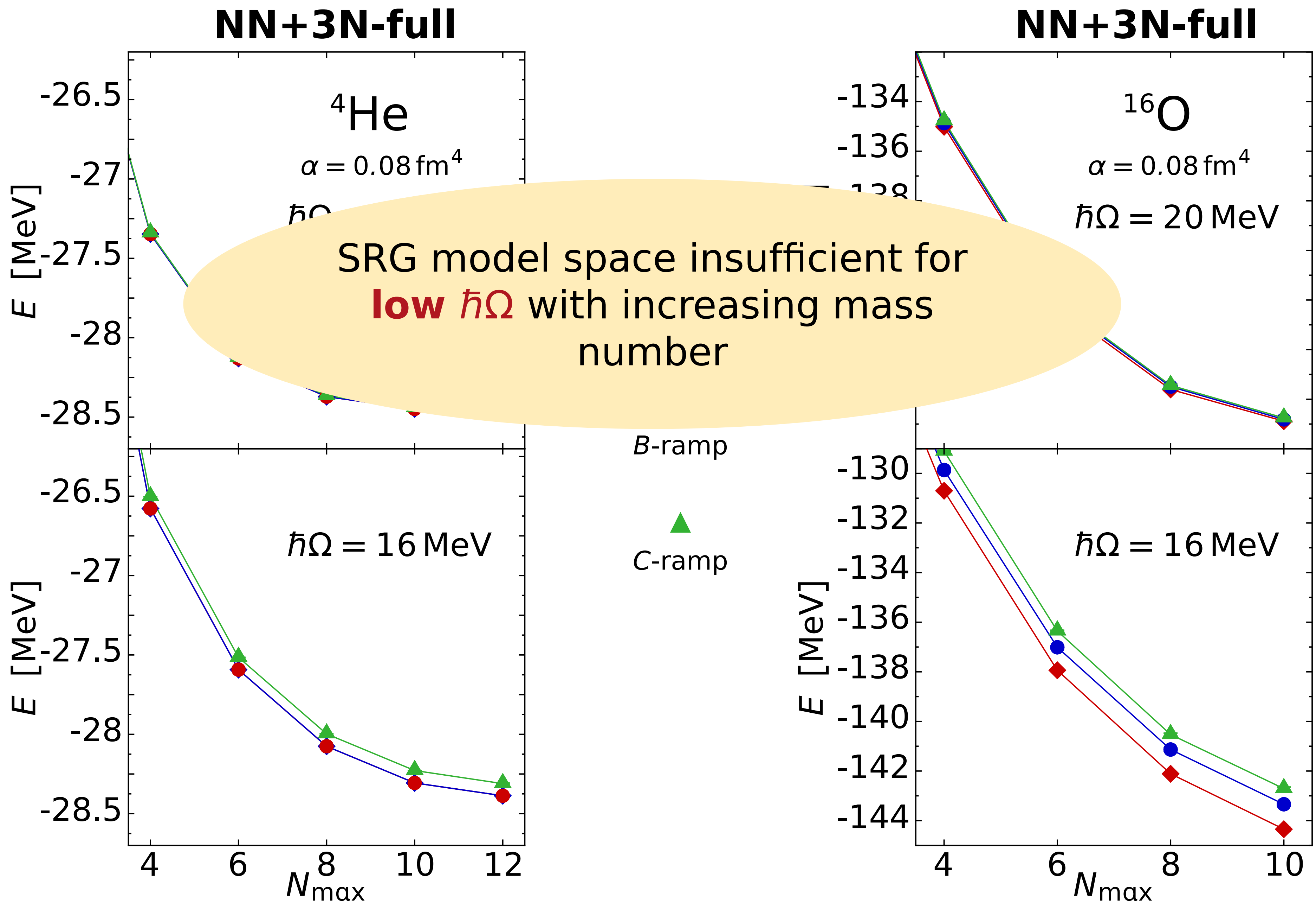
SRG Model Space

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



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

SRG Model Space: ^{4}He & ^{16}O Ground-State



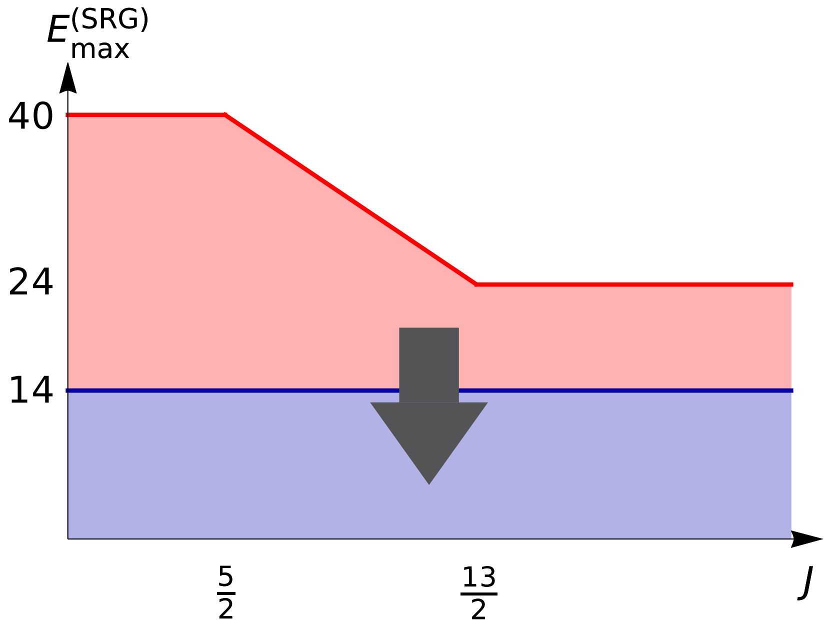
SRG model space insufficient for **low $\hbar\Omega$** with increasing mass number

Frequency Conversion

Idea:

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

Model Space: SRG → Many-Body



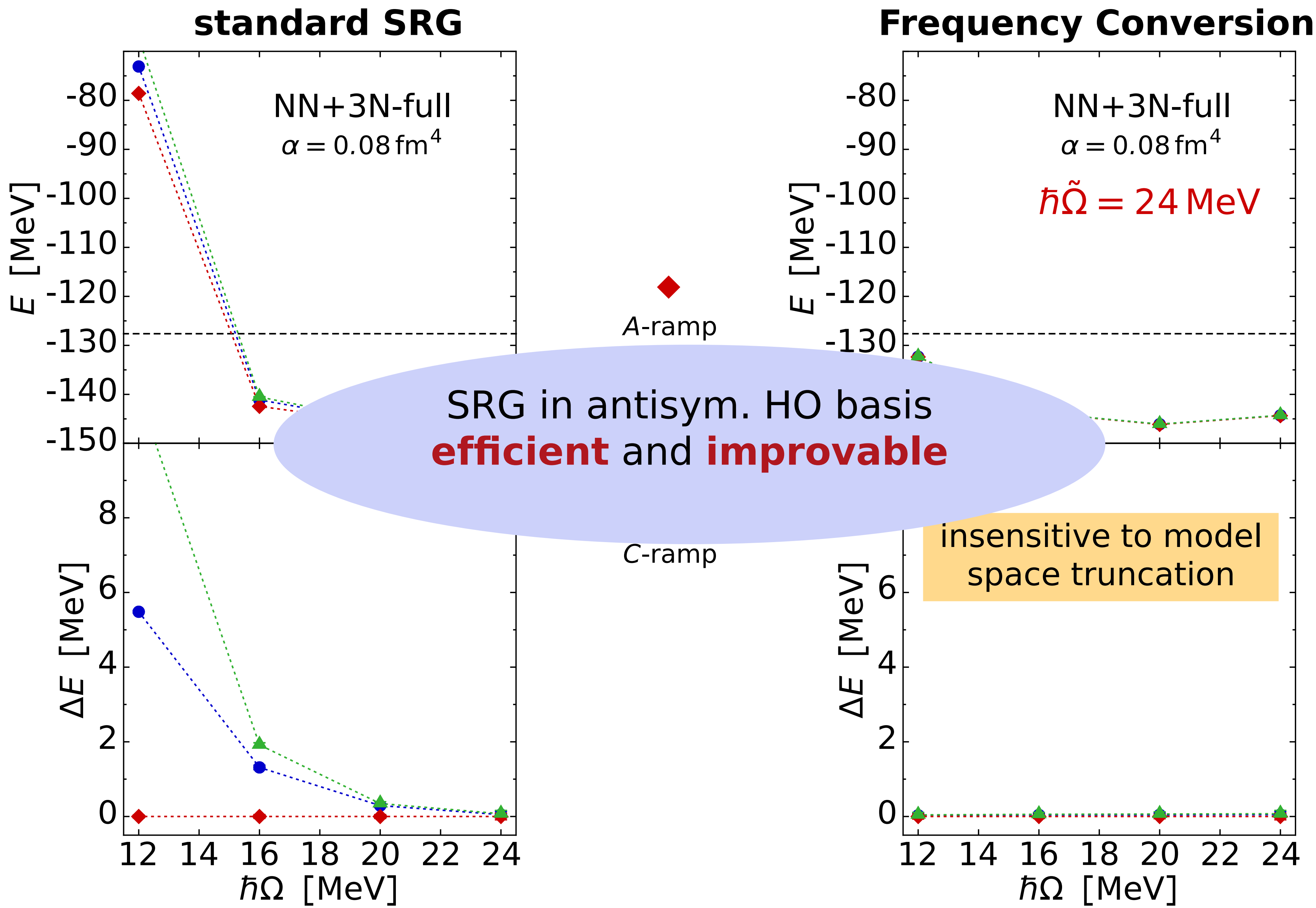
- benefits

  simple & efficient access to low frequencies

- limitation

  conversion becomes inaccurate if $\hbar\tilde{\Omega} - \hbar\Omega$ large

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^{2}LO

- why this is interesting:
  - **impact of N^{3}LO contributions**: some N^{3}LO diagrams can be absorbed into the N^{2}LO 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 variations of the c_i from different extractions (also affects N...

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

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

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

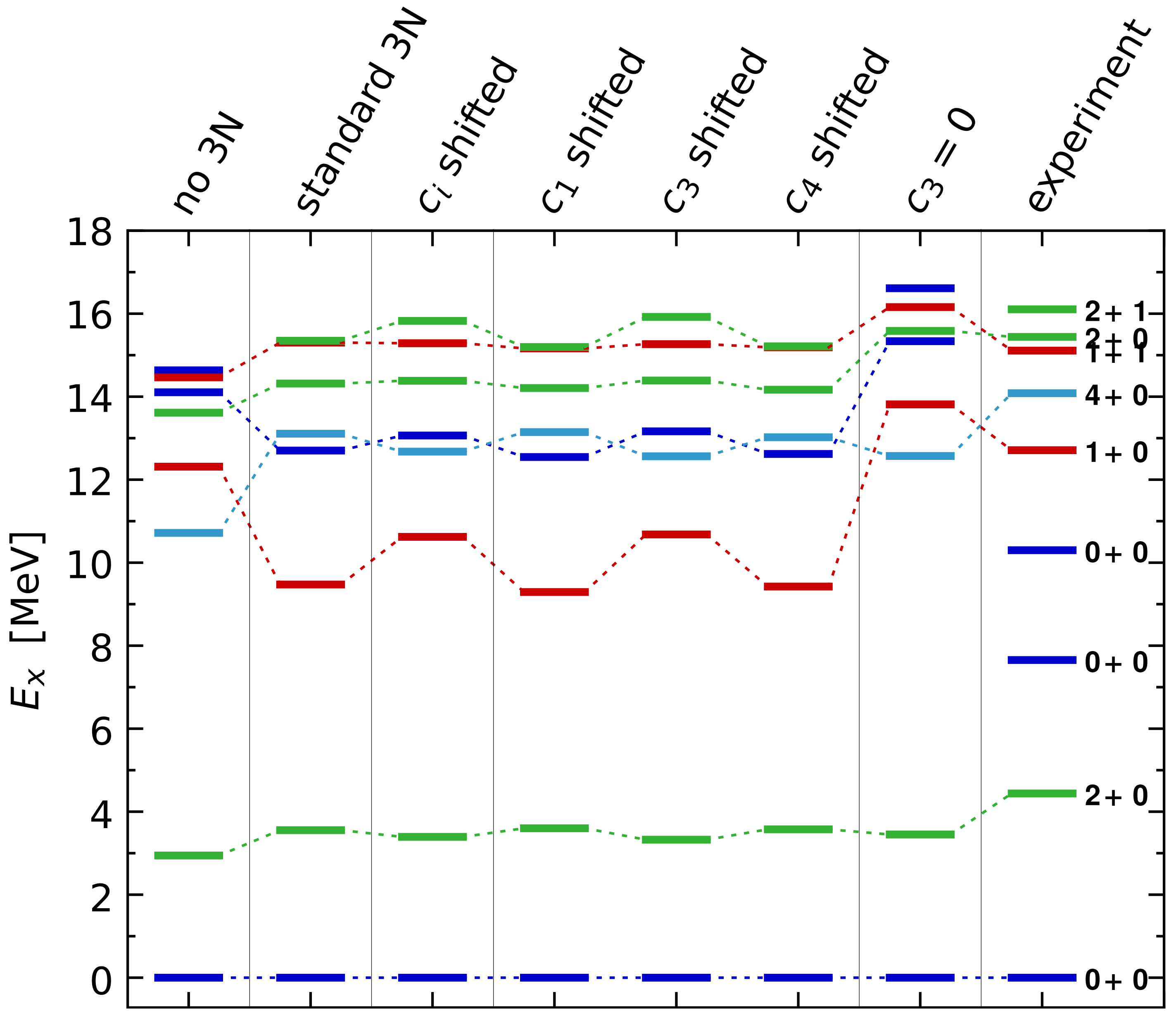
Sensitivity of Spectra on 3N Interactions

- 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

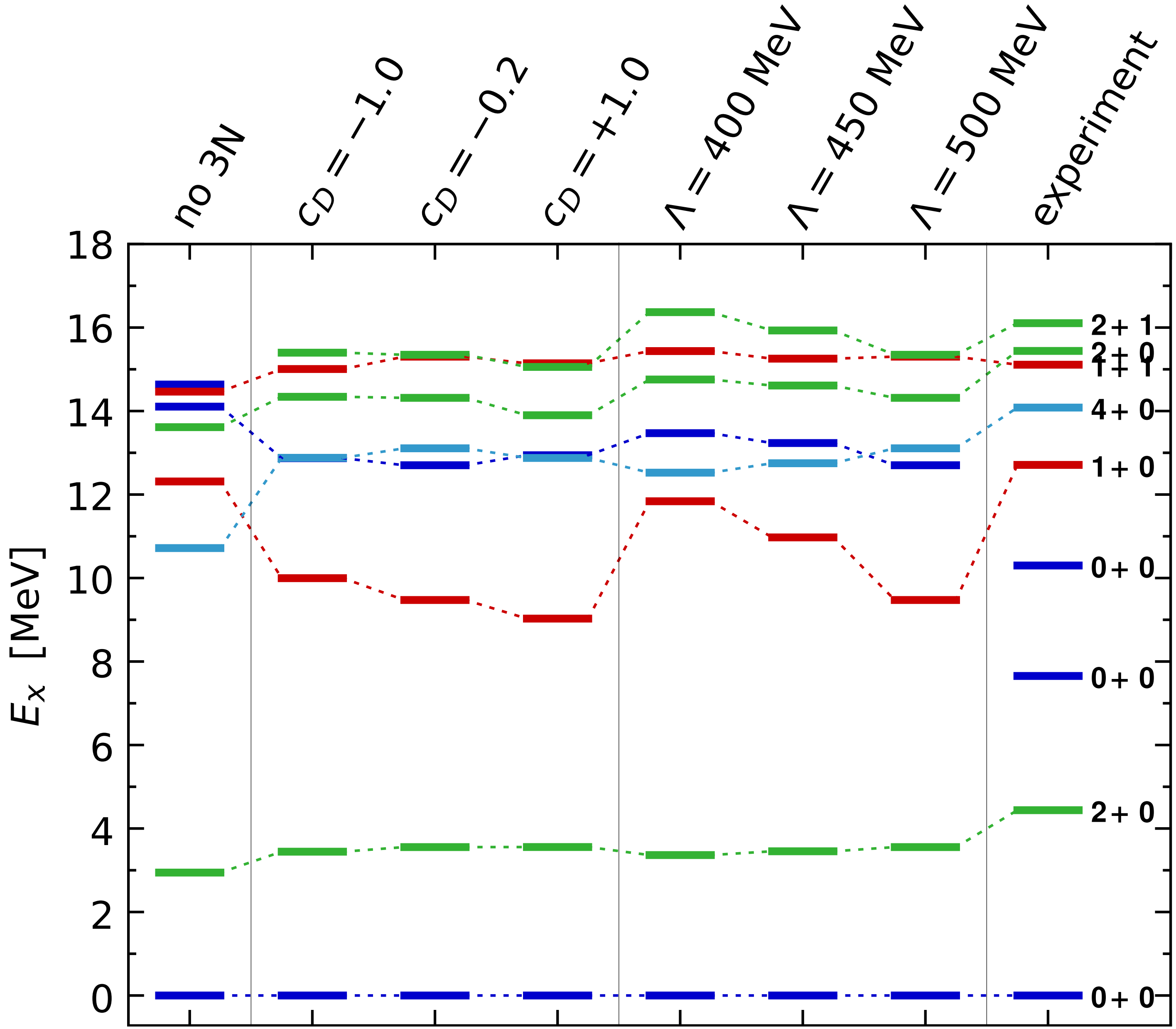
^{12}C : Sensitivity on c_i



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

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

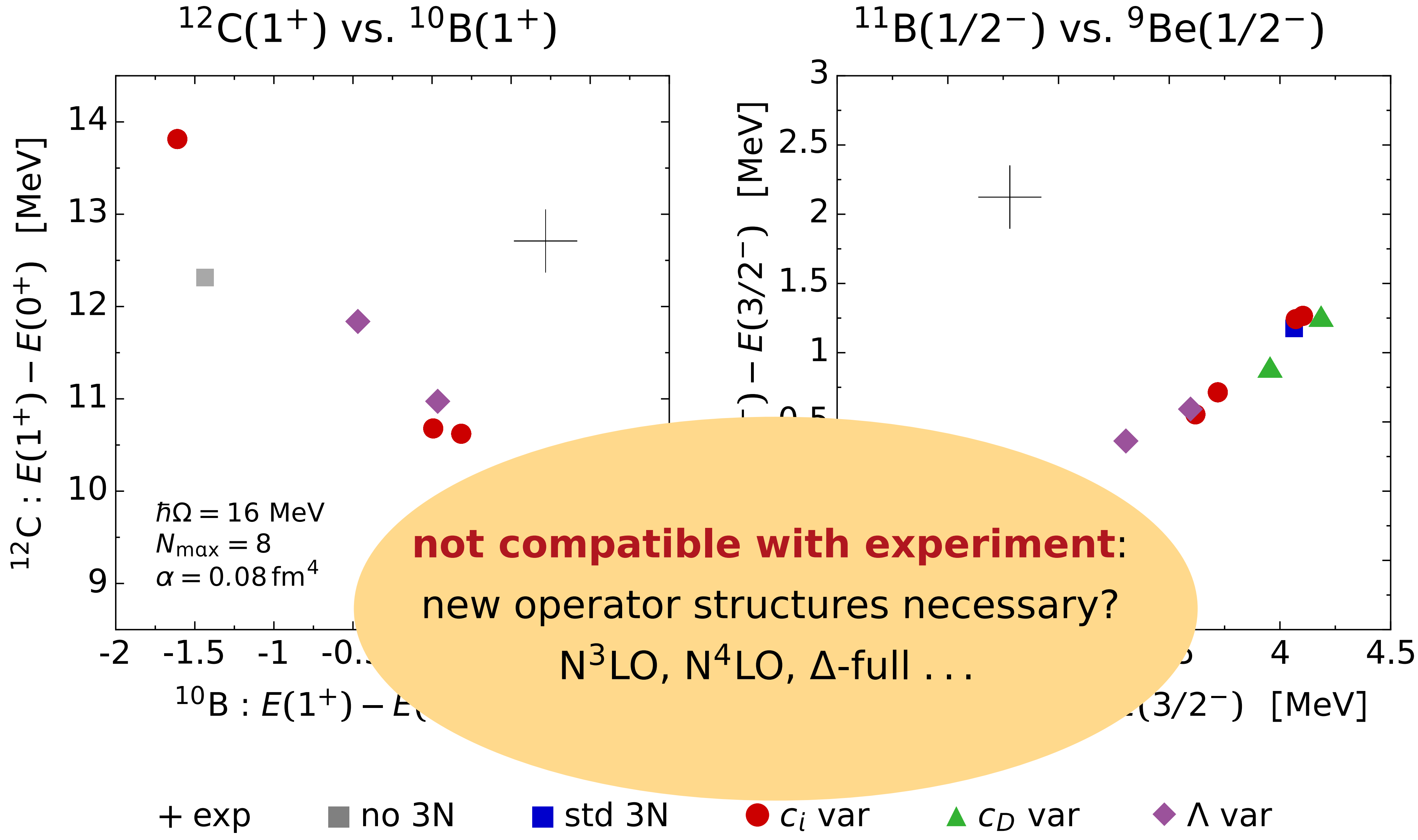
^{12}C : Sensitivity on c_D & Cutoff



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

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

Correlation Analysis



not compatible with experiment:
new operator structures necessary?
N^{3}LO, N^{4}LO, 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

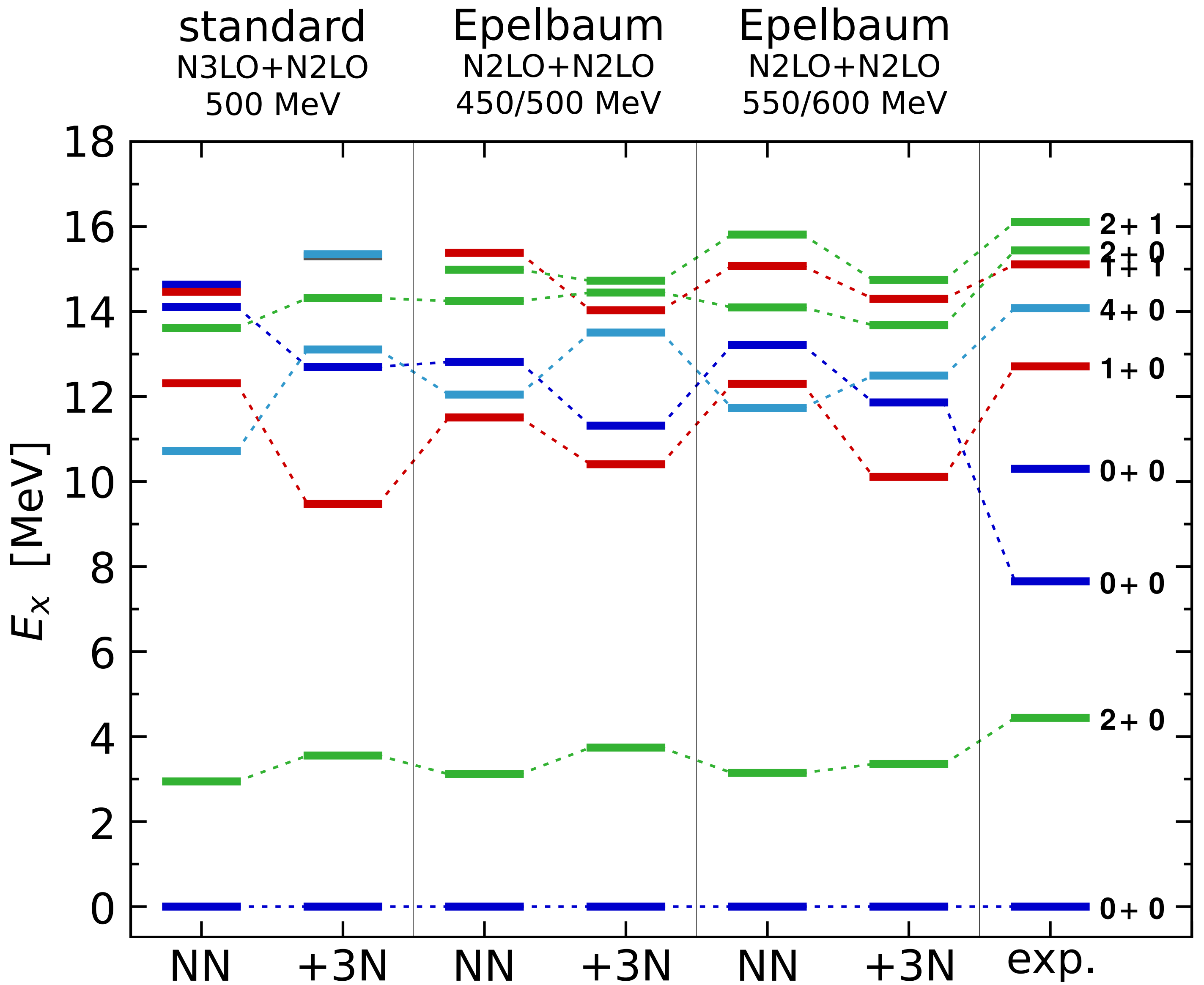
Machinery 3-Body Momentum Basis

Our Strategy:

- transform initial interaction to antisym. HO Jacobi basis
- use HO machinery afterwards (SRG; $\mathcal{J}, T$-coupled scheme;$\ldots$)
  - 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 $a(nd)$ and $E(^3\text{H})$, included up to J=7/2

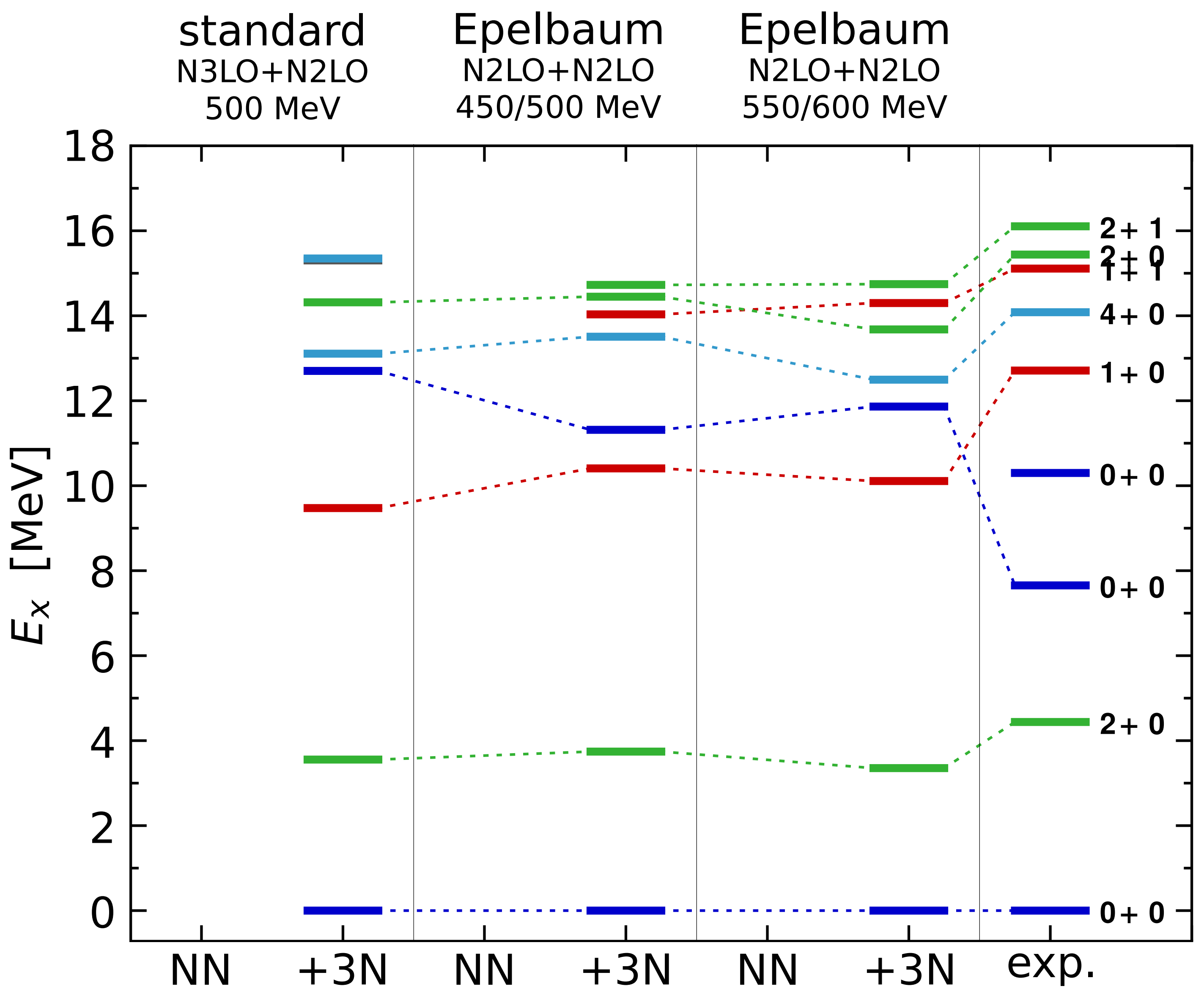
^{12}C : Consistent N^2LO Hamiltonians



- rather consistent description with different NN+3N Hamiltonians

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

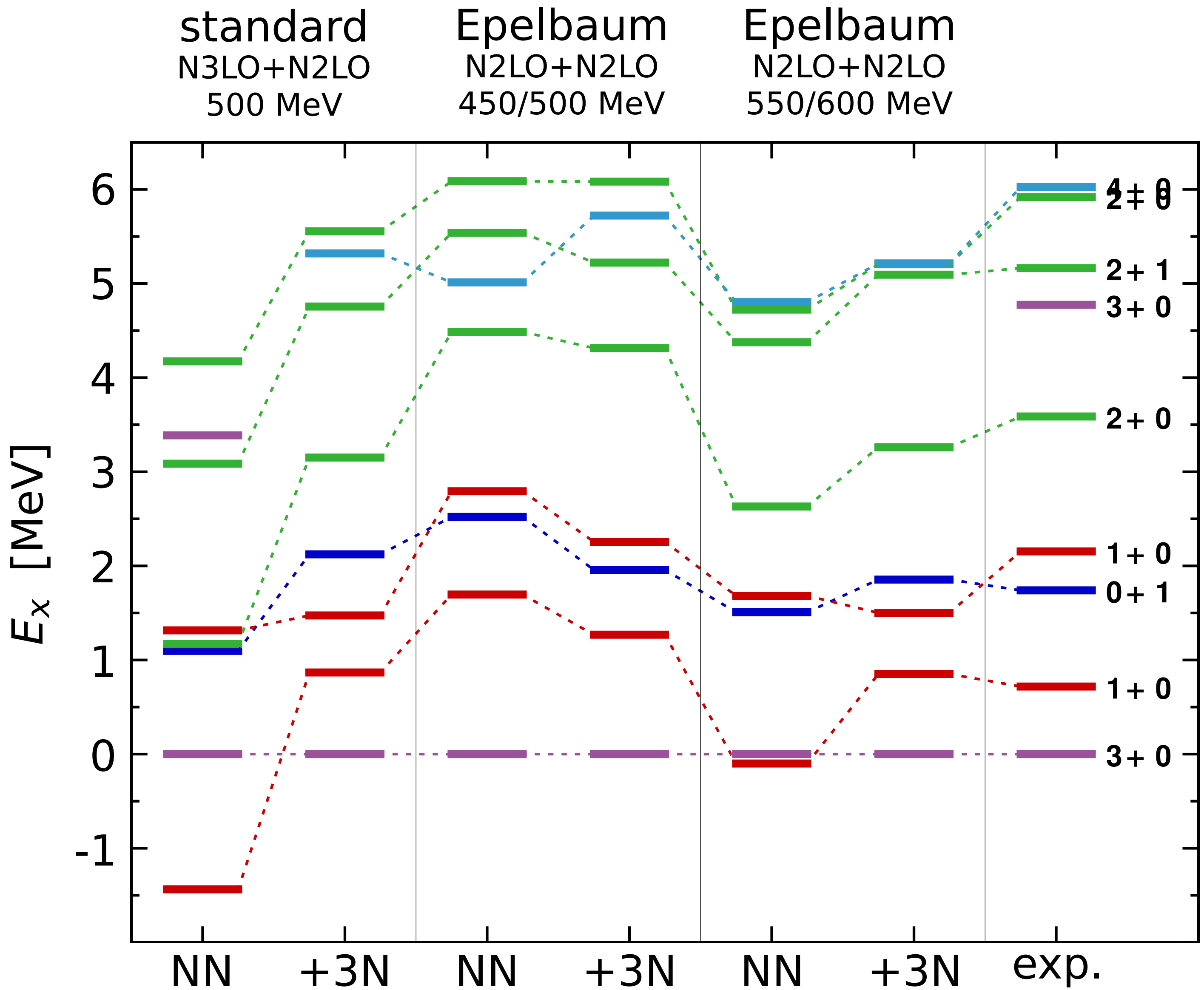
^{12}C : Consistent N^2LO Hamiltonians



- rather consistent description with different NN+3N Hamiltonians

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

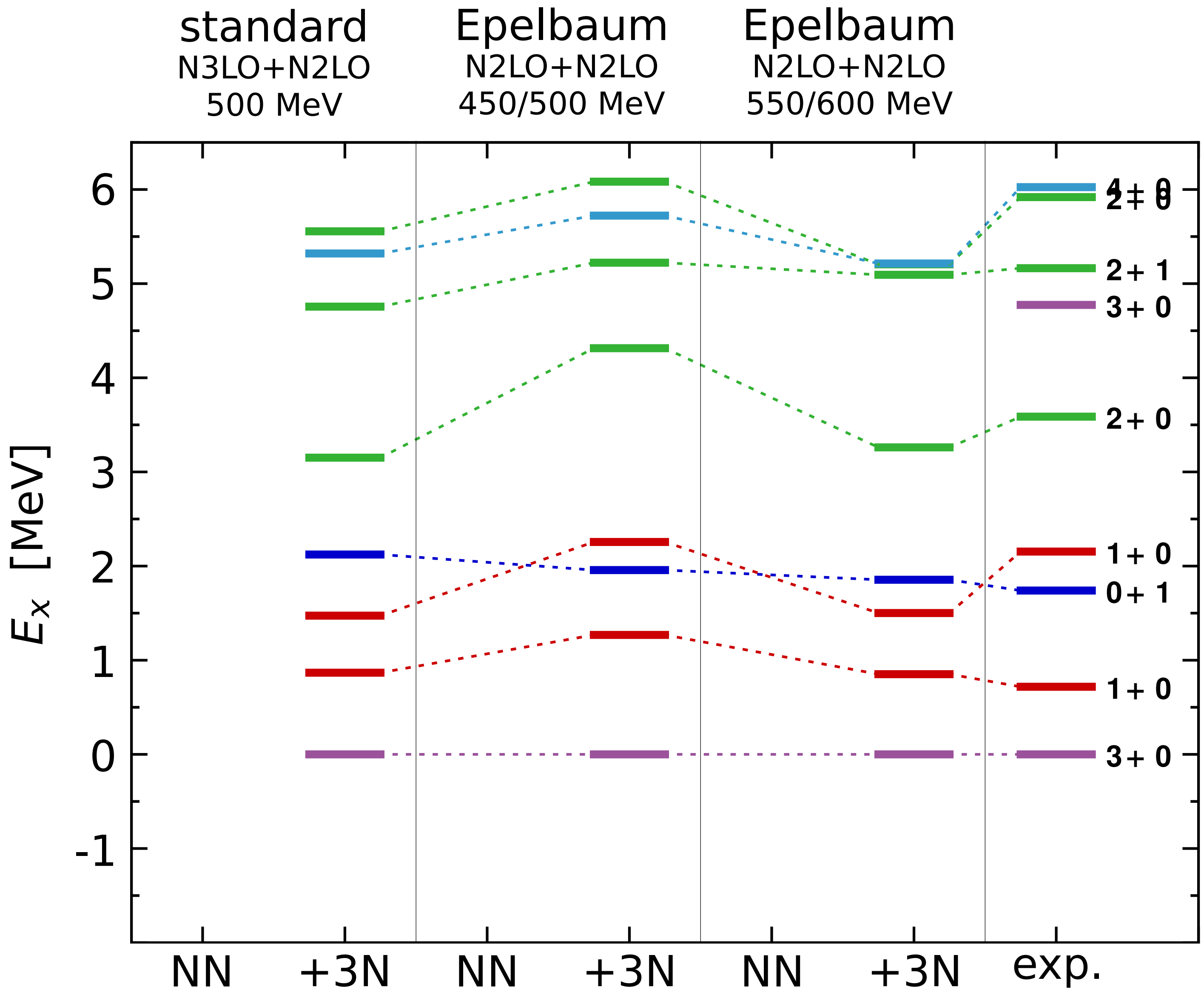
^{10}B : Consistent N^{2}LO Hamiltonians



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

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

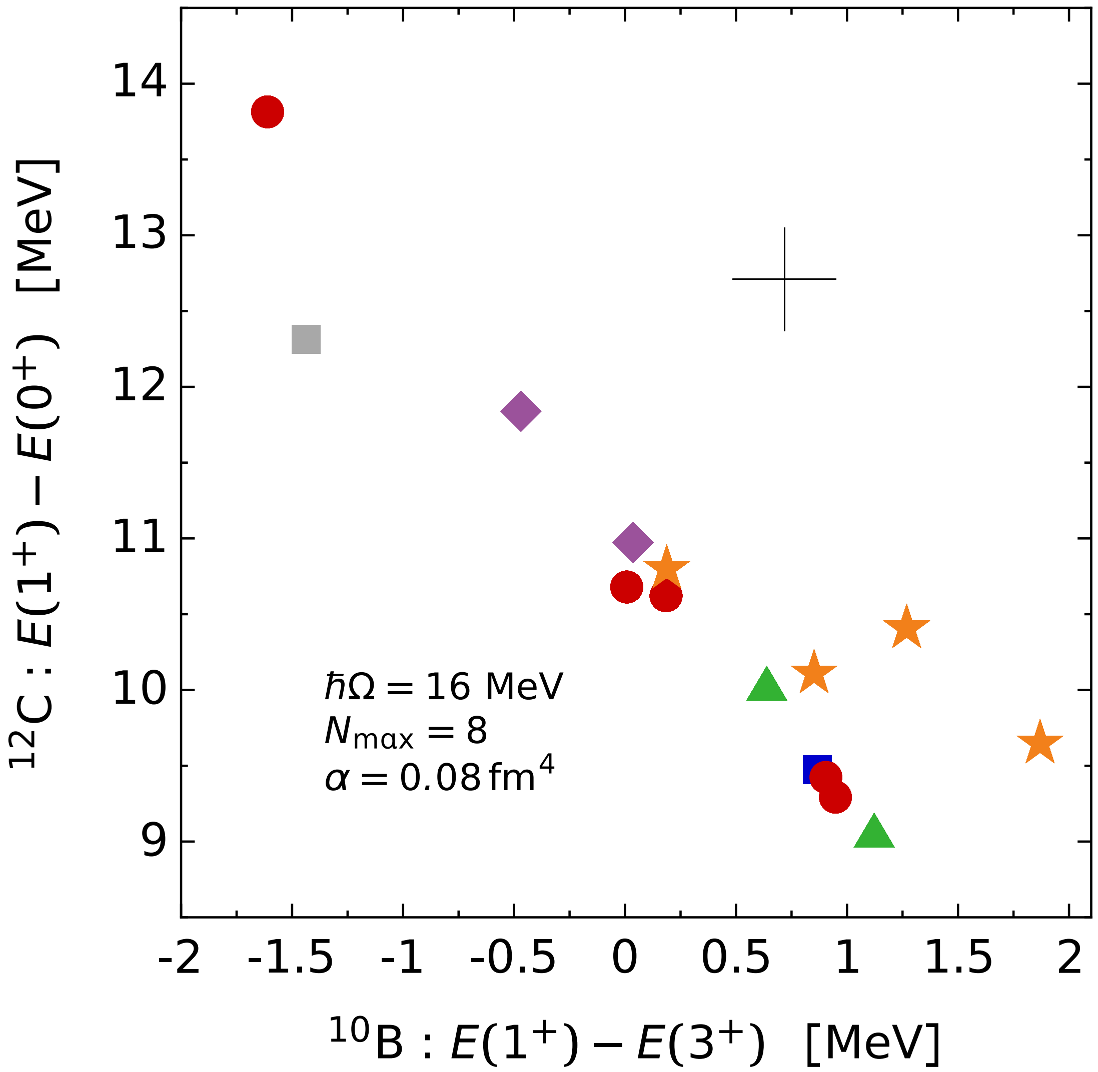
^{10}B : Consistent N^{2}LO Hamiltonians



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

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

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^{2}LO
- NN+3N

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)

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

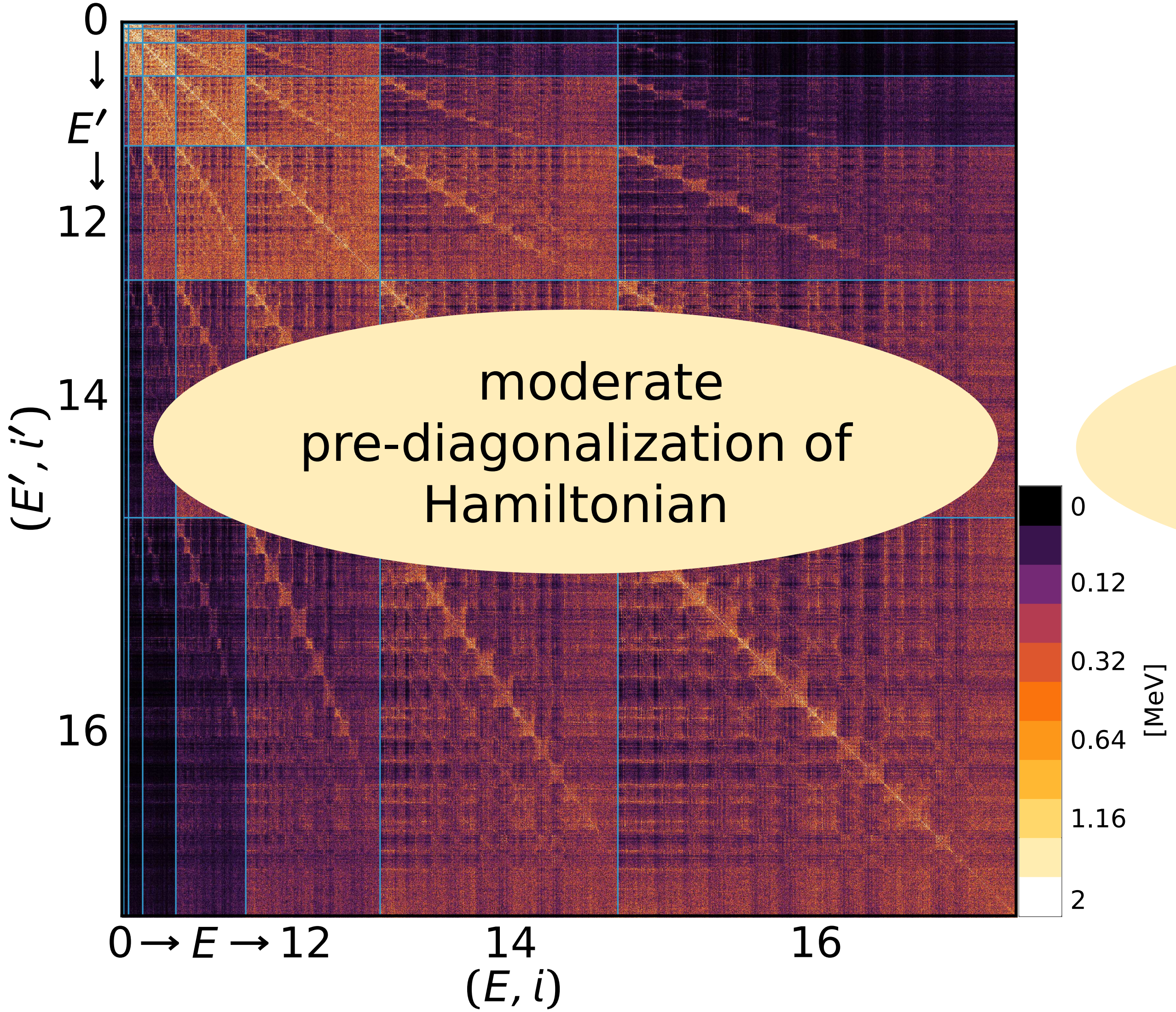
- antisym. Jacobi state

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

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

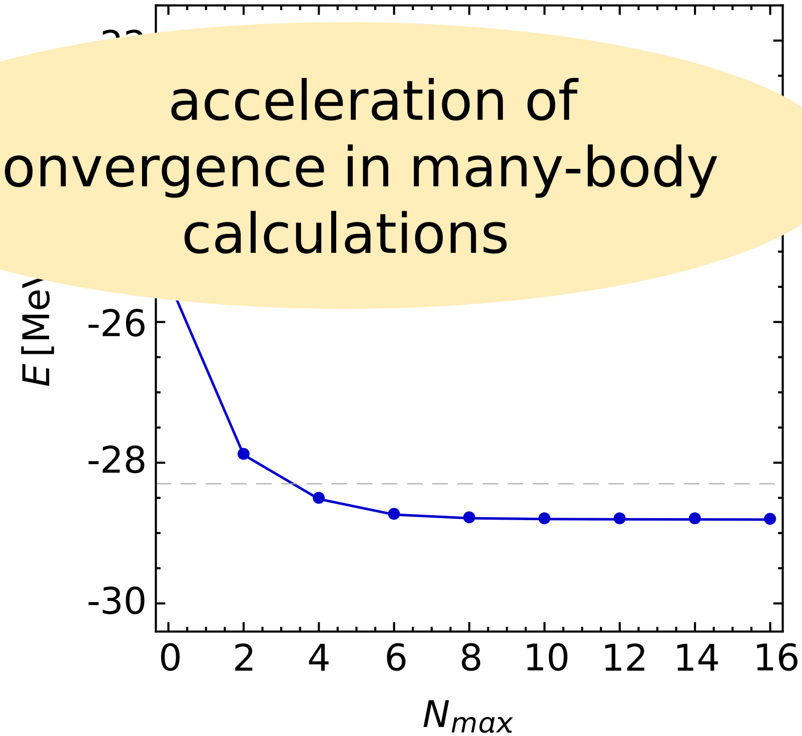
$$\alpha = 0.16\,\mathrm{fm}^4$$

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

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

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

NCSM ground state ^{4}He



acceleration of convergence in many-body calculations

First Shot: Sum over Fourth Particle

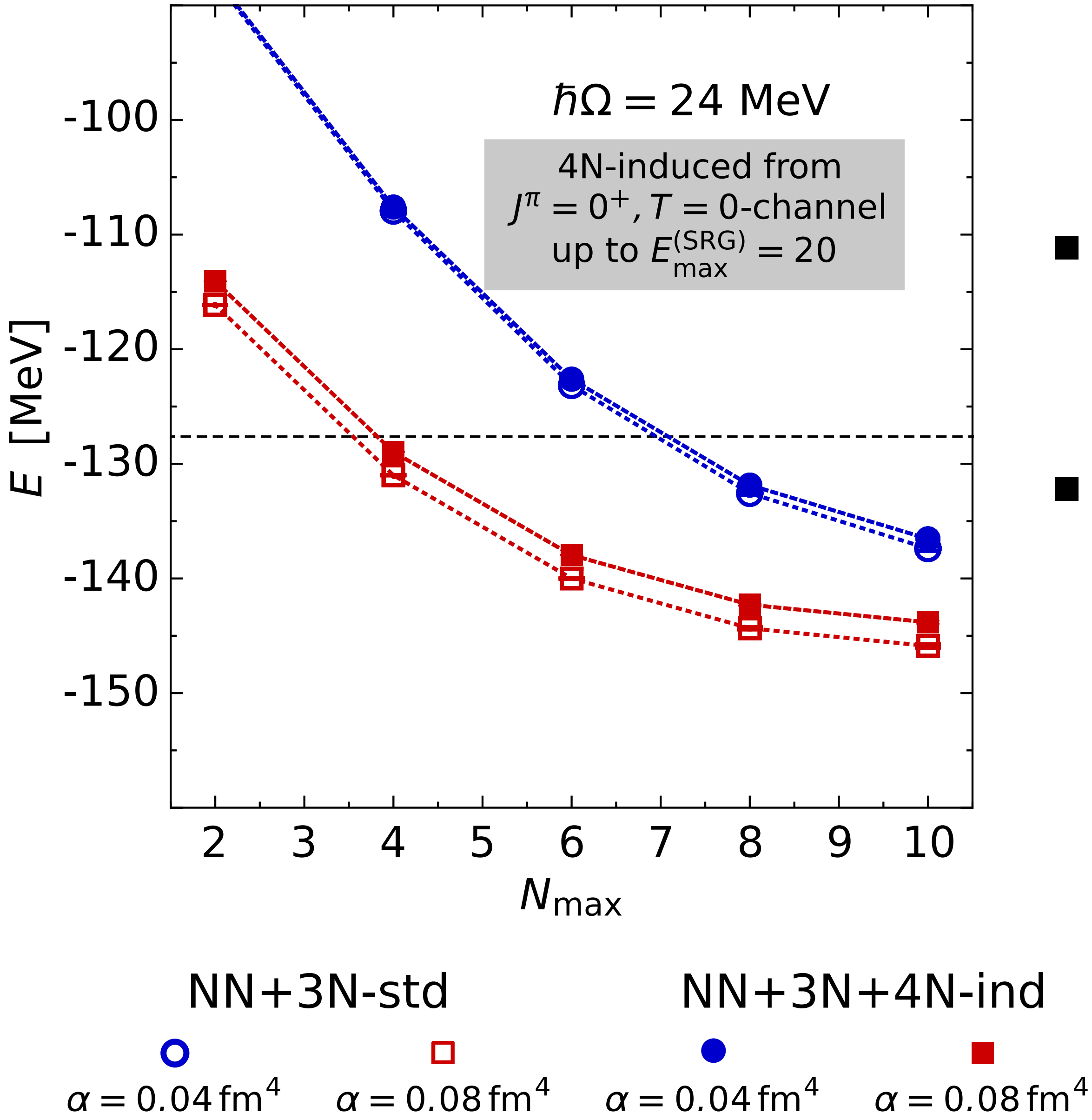
- transformation to **four-body m-scheme** basis and additional **normal-ordering** approximation in progress
- meanwhile:
  create **effective three-body interaction** in Jacobi basis
  - sum over fourth particle (unperturbed m-sheme state)
  - only consider equal J_{12}, T_{12} in Bra and Ket and average over projections
  - set three-body center of mass motion to ground-state

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

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

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

First Shot: ^{16}O Ground State



- correction by induced 4N in **right direction**, but **too small**
- **improvements**:
  - consider further 4N channels
  - increase $E^{(SRG)}_{max}$
  - 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**
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    Chalmers University, Sweden
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    GSI Helmholtzzentrum

SFB 634

Deutsche Forschungsgemeinschaft

DFG

HIC for FAIR

Helmholtz International Center

LOEWE

Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung

JUROPA — JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC — CSC Center for Scientific Computing Frankfurt

HOPPER — NERSC

COMPUTING TIME