

Ab Initio Nuclear Structure from Chiral NN+3N Hamiltonians

Robert Roth



TECHNISCHE
UNIVERSITÄT
DARMSTADT

From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

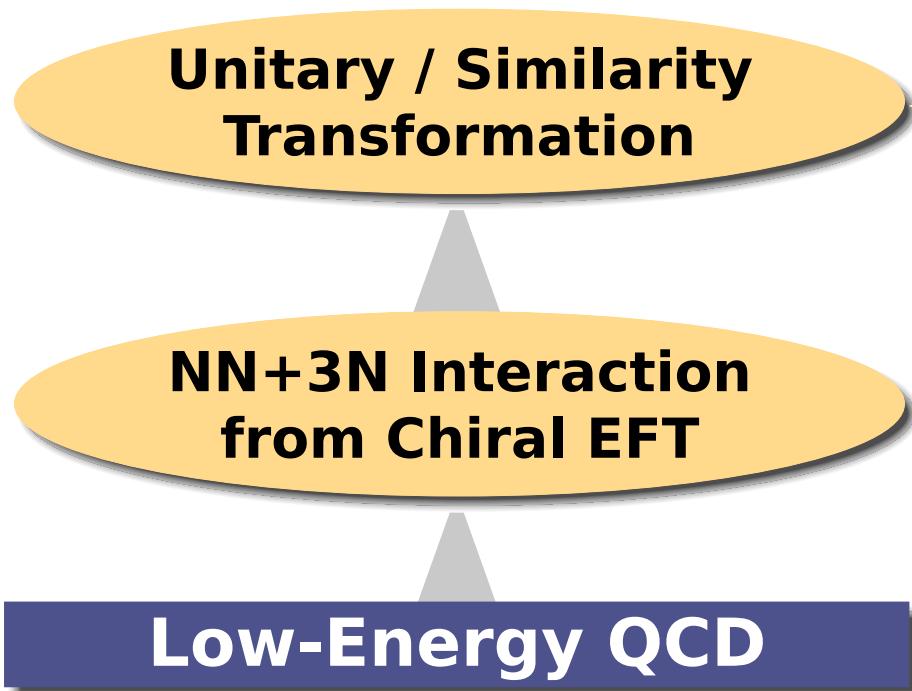
**NN+3N Interaction
from Chiral EFT**

Low-Energy QCD

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN, 3N,... interaction plus currents

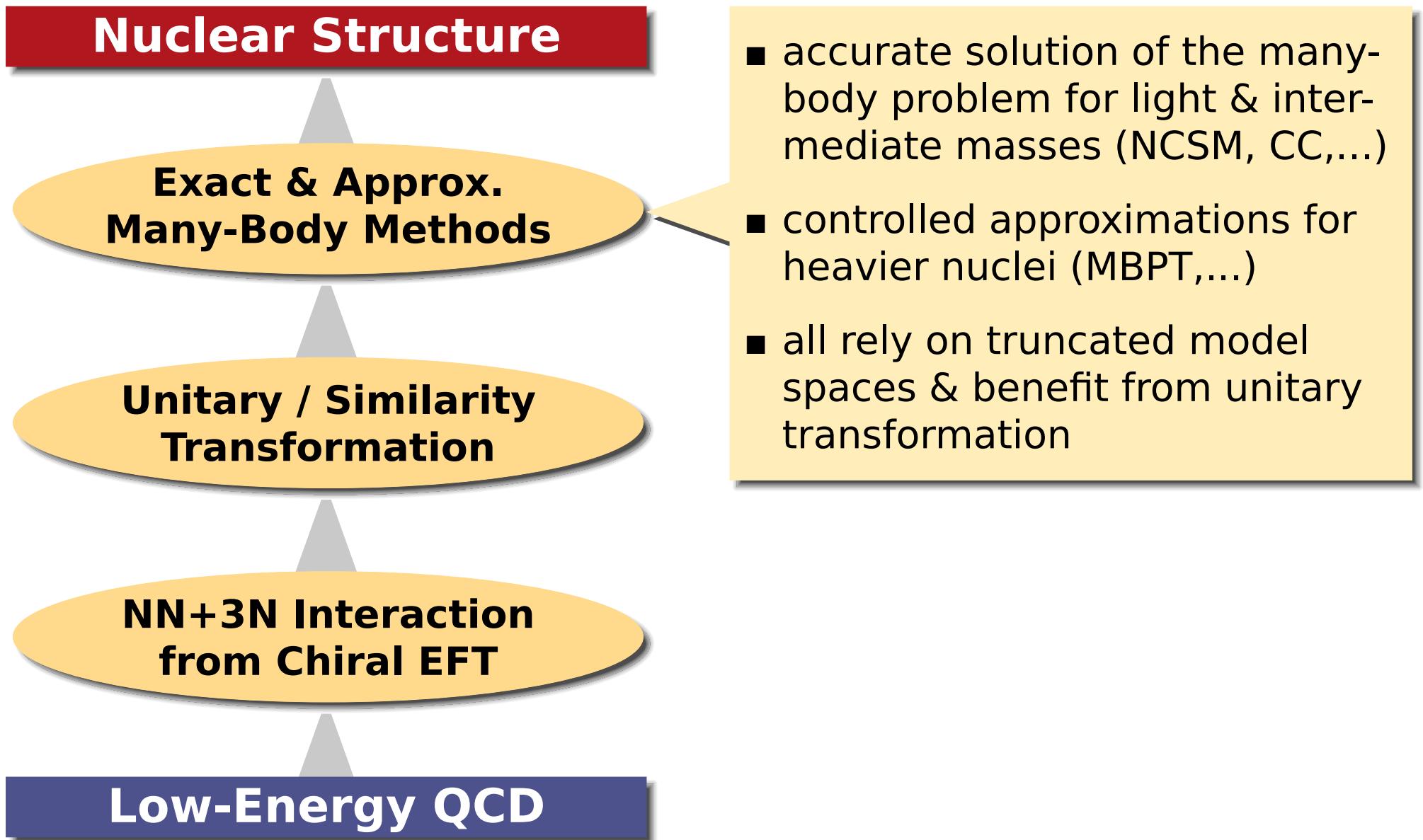
From QCD to Nuclear Structure

Nuclear Structure

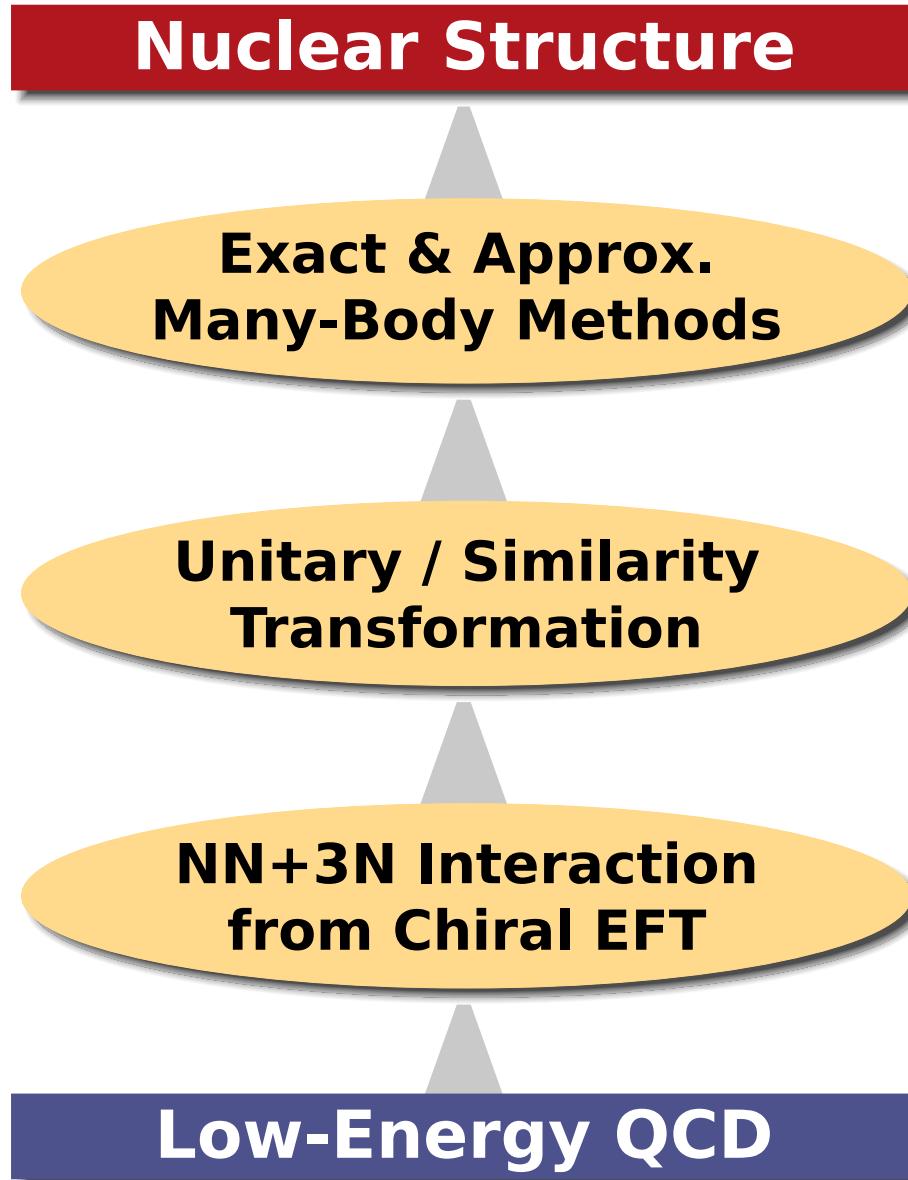


- adapt Hamiltonian to truncated low-energy model space
 - tame short-range correlations
 - improve convergence behavior
- transform Hamiltonian & observables consistently

From QCD to Nuclear Structure



From QCD to Nuclear Structure



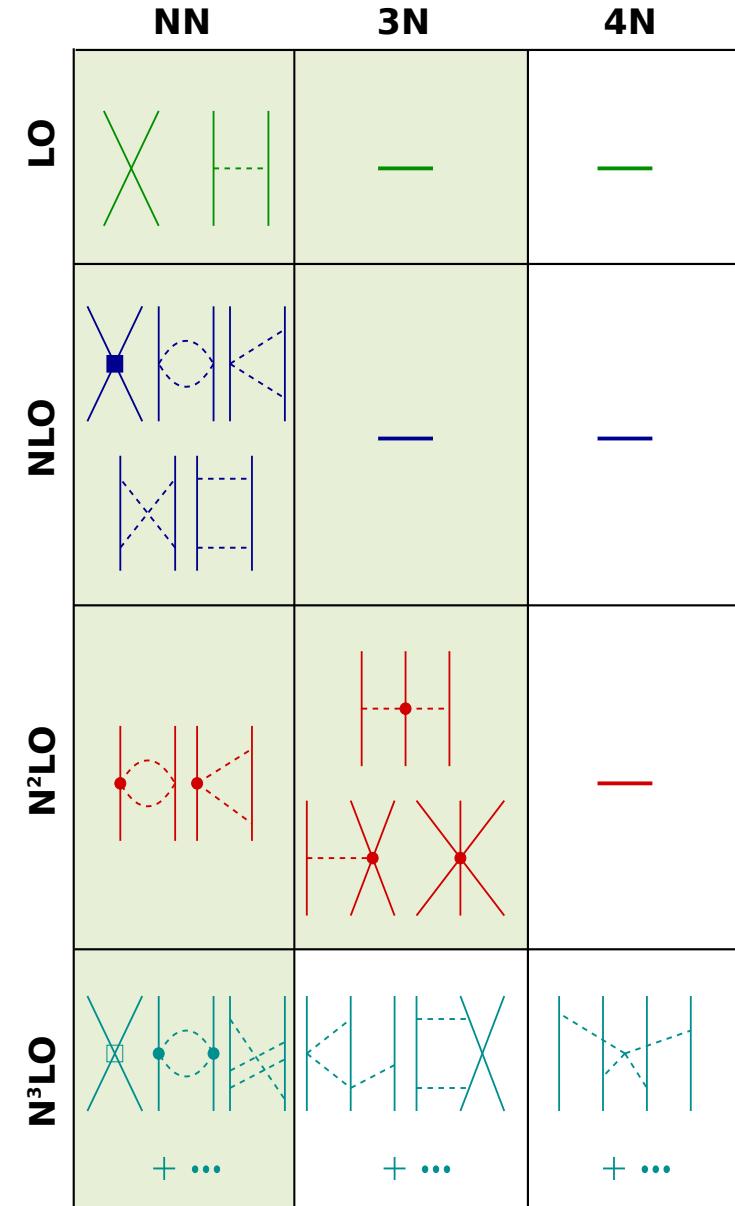
- How can we extend current ab-initio methods to describe open-shell and deformed nuclei?
- How can we include the effects of three-nucleon forces in a computationally efficient manner?
- How can we describe the onset of pairing in nuclei within various ab-initio frameworks?
- Benchmarking and accuracy: can we develop reliable theoretical error estimates?
- How can we bridge structure and reactions in a consistent fashion?
- How can we generate reliable predictions for the drip-lines?

Nuclear Interactions from Chiral EFT

Nuclear Interactions from Chiral EFT

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

- low-energy **effective field theory**
for relevant degrees of freedom (π, N)
based on symmetries of QCD
- long-range **pion dynamics** explicitly
- short-range physics absorbed in **contact terms**, low-energy constants fitted to experiment ($NN, \pi N, \dots$)
- hierarchy of **consistent NN, 3N, ... interactions** (plus currents)
- many **ongoing developments**
 - 3N interaction at N3LO, N4LO, ...
 - explicit inclusion of Δ -resonance
 - YN - & YY -interactions
 - formal issues: power counting, renormalization, cutoff choice, ...



Chiral NN+3N Hamiltonians

■ standard Hamiltonian:

- NN at N3LO: Entem / Machleidt, 500 MeV cutoff
- 3N at N2LO: Navrátil, local, 500 MeV cutoff, fit to $T_{1/2}(^3\text{H})$ and $E(^3\text{H}, ^3\text{He})$

■ standard Hamiltonian with modified 3N:

- NN at N3LO: Entem / Machleidt, 500 MeV cutoff
- 3N at N2LO: Navrátil, local, with modified LECs and cutoffs, refit to $E(^4\text{He})$

■ consistent N2LO Hamiltonian:

- NN at N2LO: Epelbaum et al., 450,...,600 MeV cutoff
- 3N at N2LO: Epelbaum et al., nonlocal, 450,...,600 MeV cutoff

■ consistent N3LO Hamiltonian:

- coming soon...

Similarity Renormalization Group

- Roth, Calci, Langhammer, Binder — in preparation (2013)
Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Roth, Reinhardt, Hergert — Phys. Rev. C 77, 064033 (2008)
Hergert, Roth — Phys. Rev. C 75, 051001(R) (2007)

Similarity Renormalization Group

Wegner, Glazek, Wilson, Perry, Bogner, Furnstahl, Hergert, Roth, Jurgenson, Navratil,...

continuous transformation driving
Hamiltonian to band-diagonal form
with respect to a chosen basis

- **unitary transformation** of Hamiltonian:

$$\tilde{H}_\alpha = U_\alpha^\dagger H U_\alpha$$

simplicity and flexibility
are great advantages of
the SRG approach

- **evolution equations** for \tilde{H}_α and U_α :

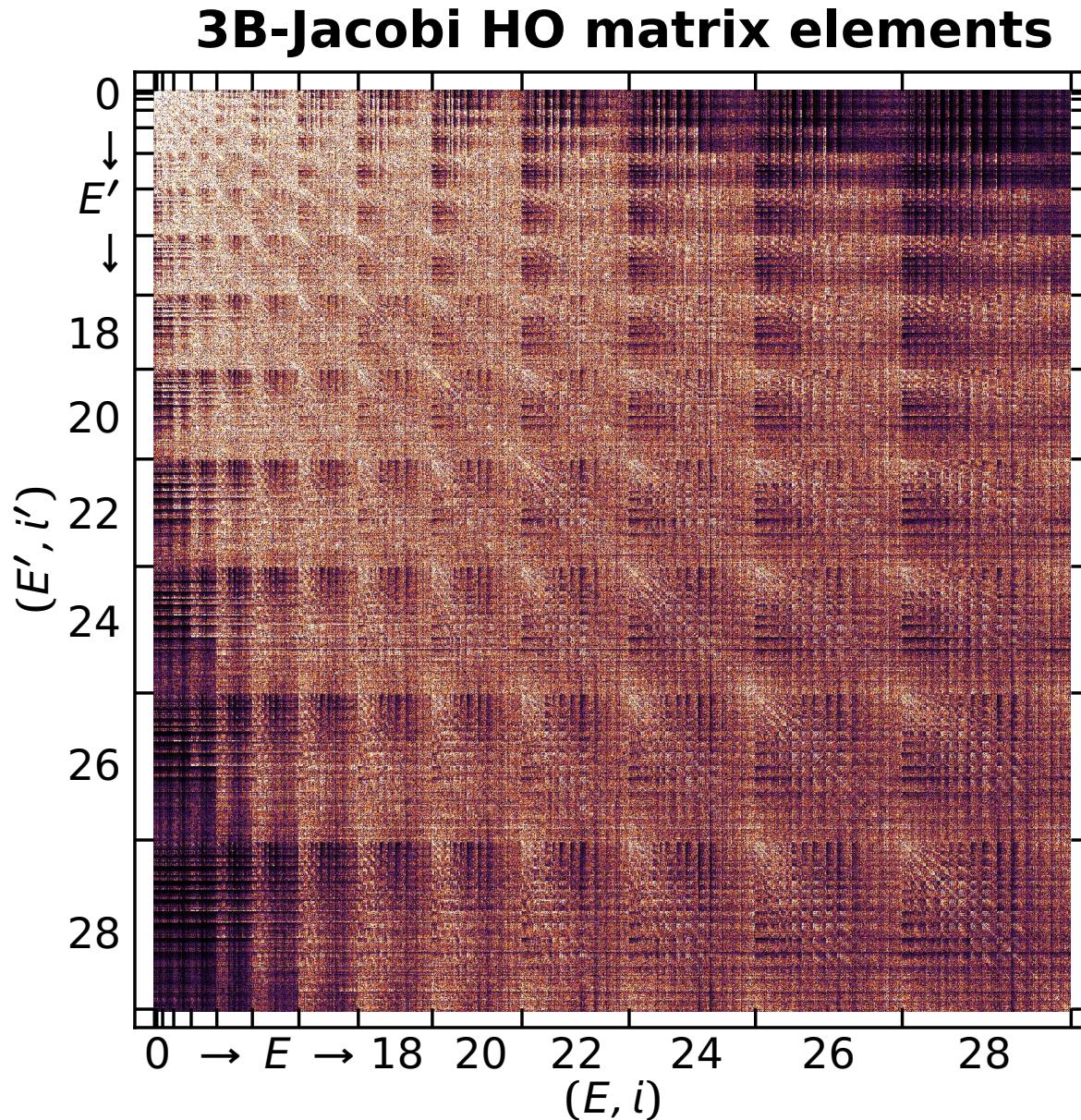
$$\frac{d}{d\alpha} \tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha]$$

solve SRG evolution
equations using two-,
three- & four-body matrix
representation

- **dynamic generator**: commutator with the operator in whose eigenbasis H shall be diagonalized

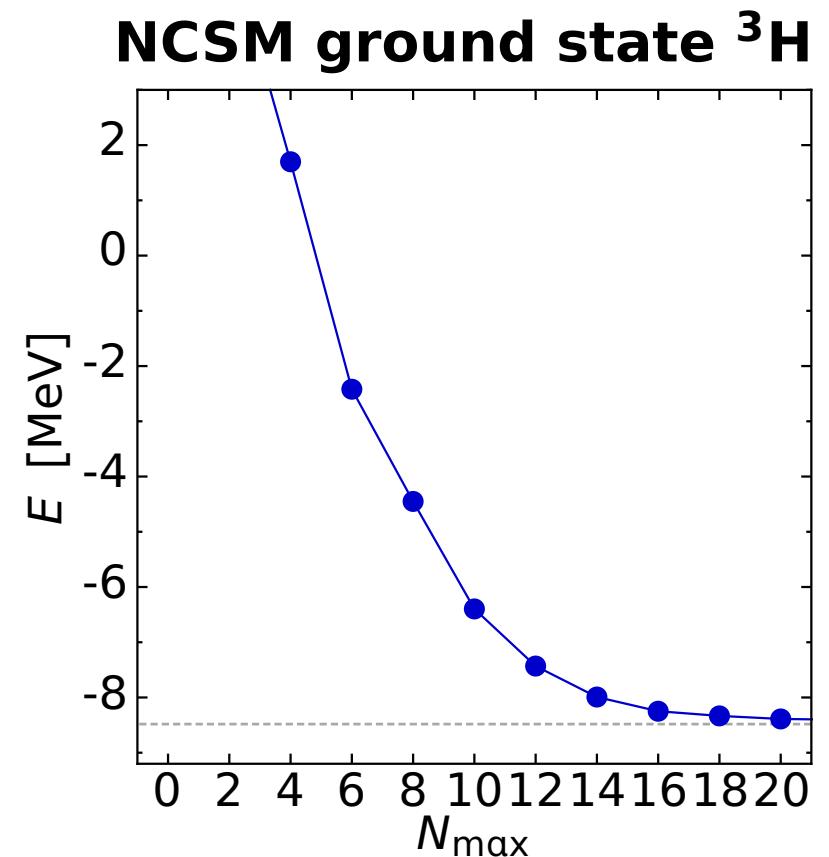
$$\eta_\alpha = (2\mu)^2 [T_{\text{int}}, \tilde{H}_\alpha]$$

SRG Evolution in Three-Body Space



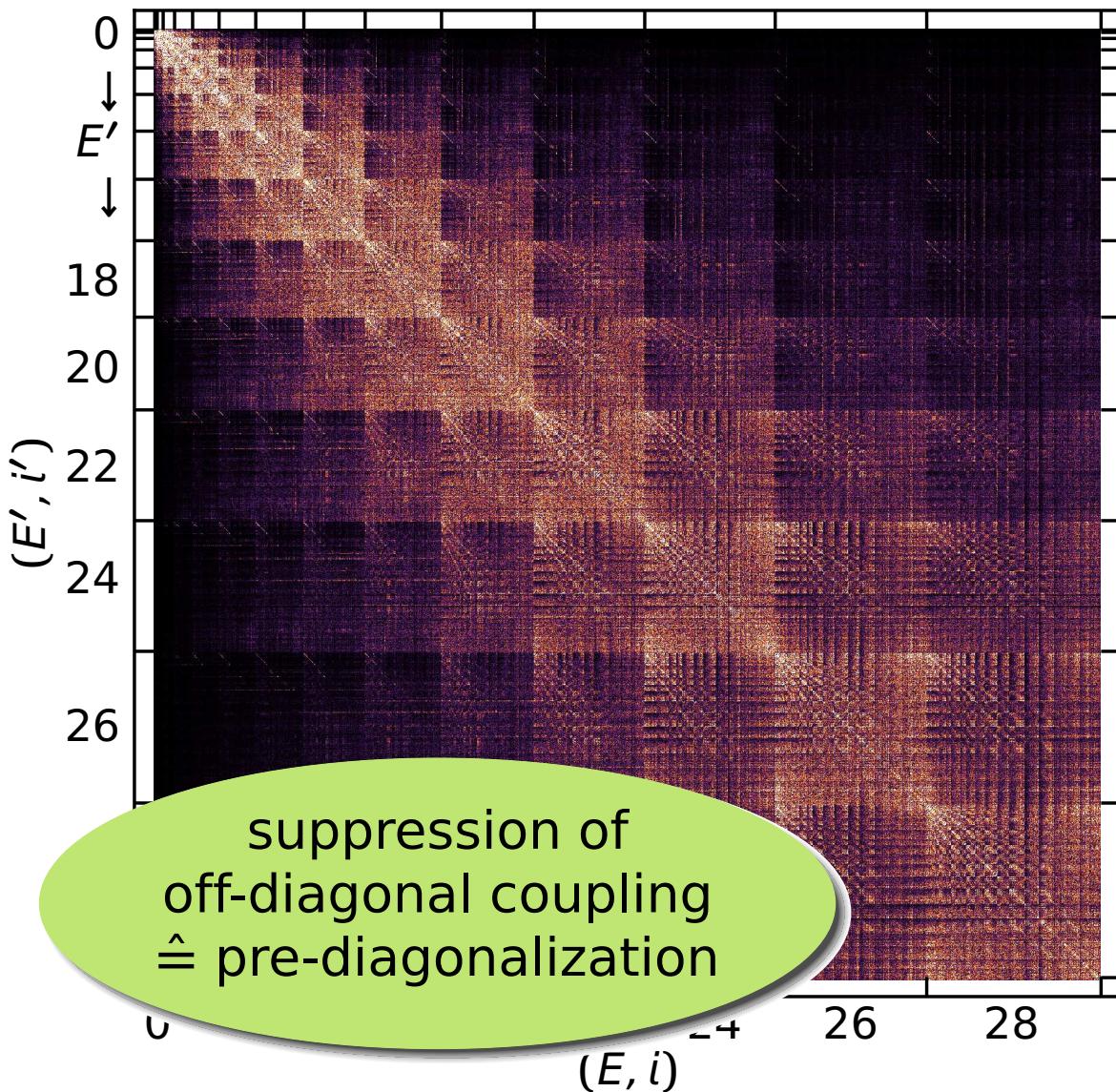
$\alpha = 0.000 \text{ fm}^4$
 $\Lambda = \infty \text{ fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28 \text{ MeV}$



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

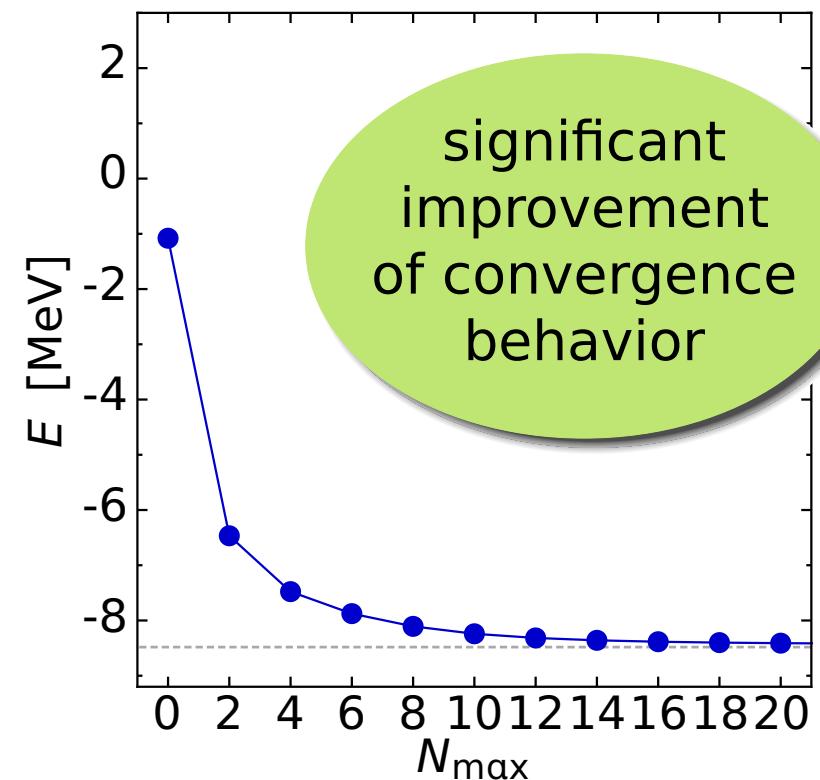


$$\alpha = 0.320 \text{ fm}^4$$

$$\Lambda = 1.33 \text{ fm}^{-1}$$

$$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28 \text{ MeV}$$

NCSM ground state ${}^3\text{H}$



Hamiltonian in A-Body Space

- evolution **induces n -body contributions** $\tilde{H}_\alpha^{[n]}$ to Hamiltonian

$$\tilde{H}_\alpha = \tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]} + \tilde{H}_\alpha^{[3]} + \tilde{H}_\alpha^{[4]} + \dots$$

- truncation of cluster series inevitable — formally destroys unitarity and invariance of energy eigenvalues (independence of α)

SRG-Evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and induced three-body terms
- **NN+3N-full**: start with NN+3N initial Hamiltonian and all three-body terms

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

Sounds easy, but...

❶ initial 3B-Jacobi HO matrix elements of chiral 3N interactions

- direct computation using Petr Navratil's ManyEff code (N2LO)
- conversion of partial-wave decomposed moment-space matrix elements of Epelbaum et al. (N2LO, N3LO,...)

❷ SRG evolution in 2B/3B space and cluster decomposition

- efficient implementation using adaptive ODE solver & BLAS;
largest JT-block takes a few hours on single node

❸ transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation

- transform directly into JT-coupled scheme; highly efficient implementation; can handle $E_{3\max} = 16$ in JT-coupled scheme

❹ data management and on-the-fly decoupling in many-body codes

- optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_{3\max} = 16$ in memory; suitable for GPUs

Importance Truncated No-Core Shell Model

- Roth, Calci, Langhammer, Binder — in preparation (2013)
- Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
- Navrátil, Roth, Quaglioni — Phys. Rev. C 82, 034609 (2010)
- Roth — Phys. Rev. C 79, 064324 (2009)
- Roth, Gour & Piecuch — Phys. Lett. B 679, 334 (2009)
- Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)
- Roth, Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

No-Core Shell Model

Barrett, Vary, Navratil, Maris, Nogga, Roth,...

NCSM is one of the most powerful and universal exact ab-initio methods

- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **all relevant observables** can be computed from the eigenstates
- range of applicability limited by **factorial growth** of basis with N_{\max} & A
- adaptive **importance truncation** extends the range of NCSM by reducing the model space to physically relevant states

Importance Truncated NCSM

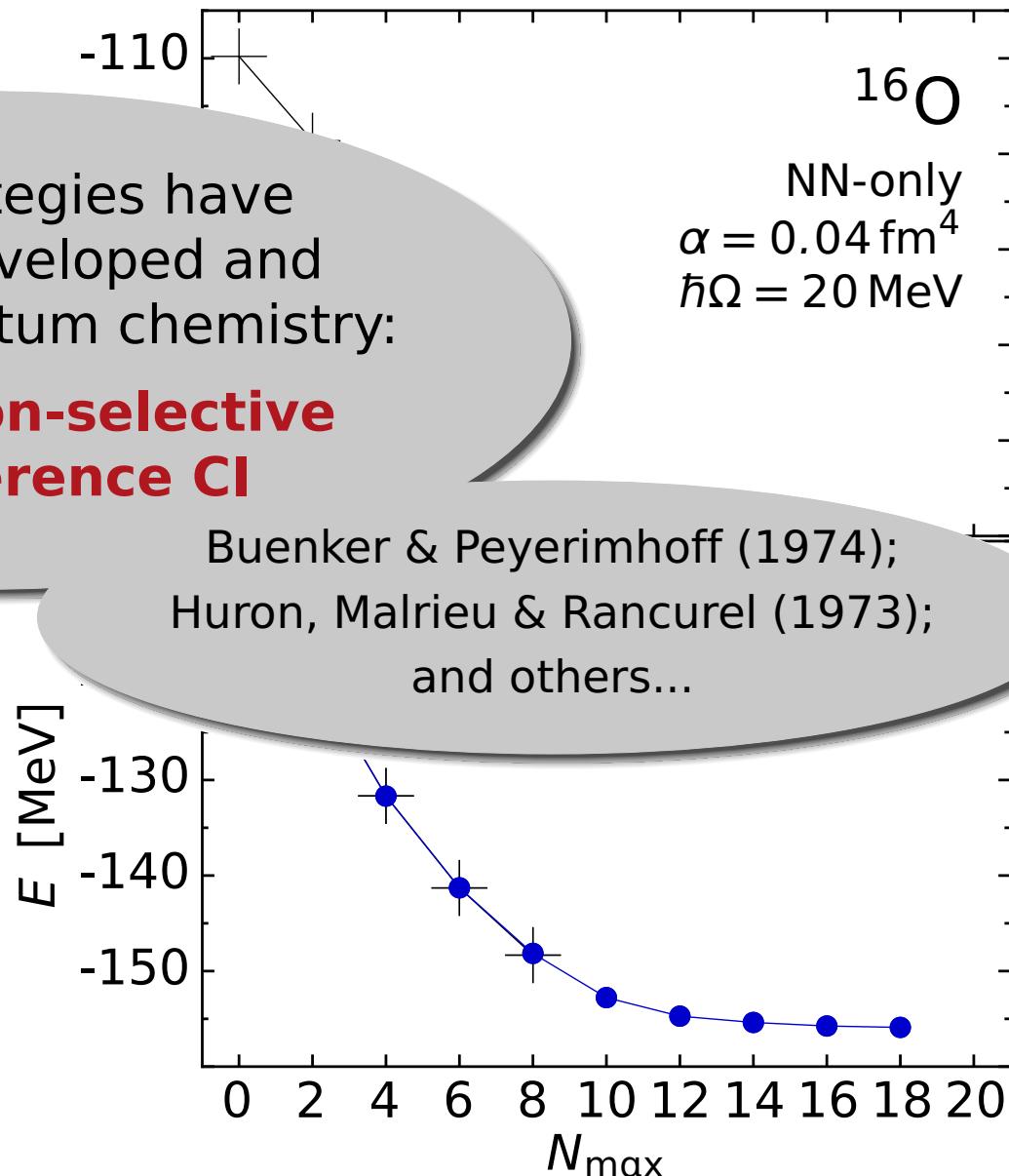
Roth, PRC 79, 064324 (2009); PRL 99, 092501 (2007)

- converged NCSM calculations essentially restricted to lower/mid range of N_{max}
- full N_{max} for ^{16}O via (basis dir.)

similar strategies have first been developed and applied in quantum chemistry:
configuration-selective multireference CI

Importance Truncation

reduce model space to the relevant basis states using an **a priori importance measure** derived from MBPT



Importance Truncation: Basic Idea

- **starting point:** approximation $|\Psi_{\text{ref},m}\rangle$ for the **target states** within a limited reference space \mathcal{M}_{ref}

$$|\Psi_{\text{ref},m}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C_{\nu}^{(\text{ref},m)} |\Phi_{\nu}\rangle$$

- **measure the importance** of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

- consider excited states
 - **solve eigenvalue problem** in $\mathcal{M}_{\text{IT}}(K_{\min})$ and obtain improved approximation of target state
- importance measure only probes 2p2h excitations on top of \mathcal{M}_{ref} for a two-body Hamiltonian

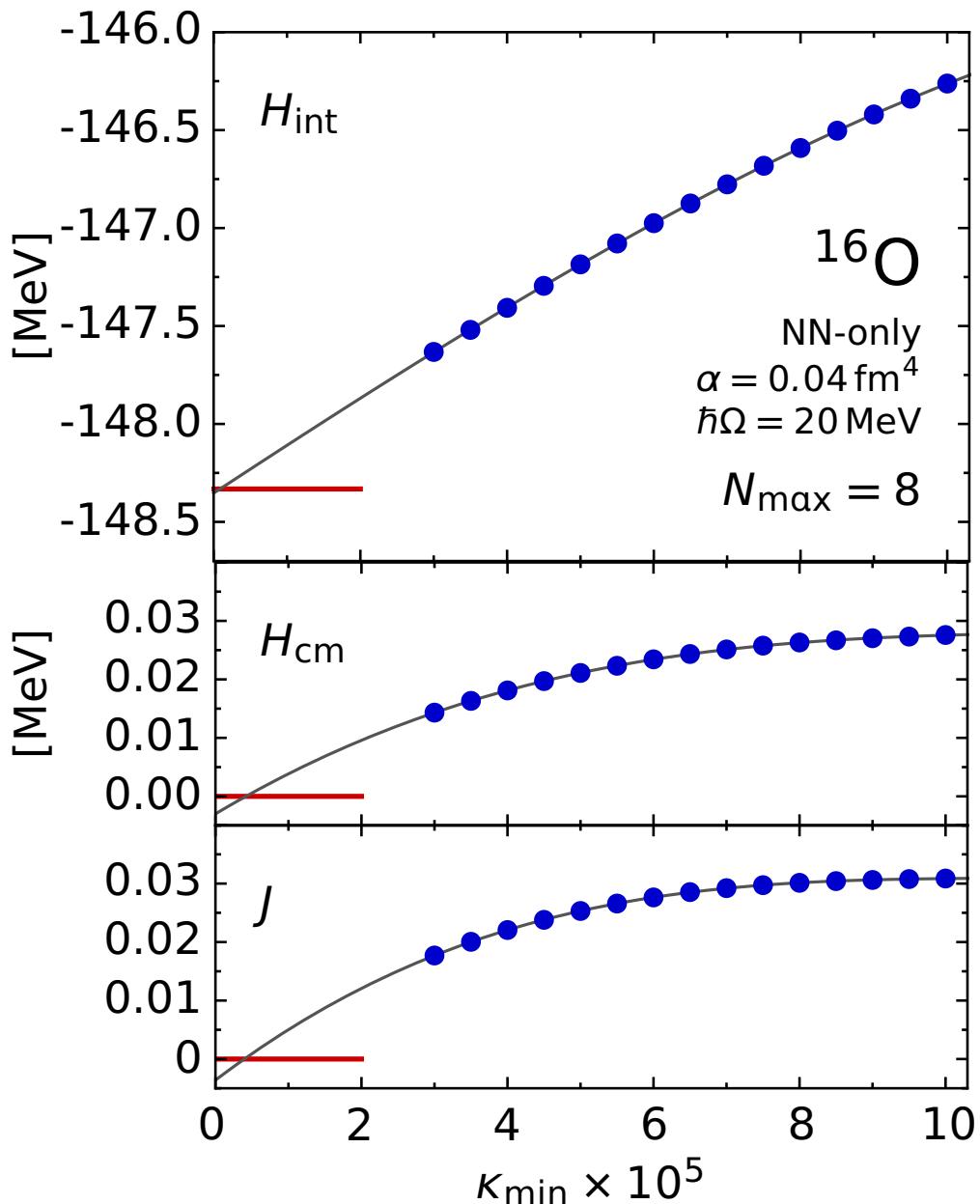
embed into iterative scheme to access full model space

Importance Truncation: Iterative Scheme

- **property of N_{\max} -truncated space:** step from N_{\max} to $N_{\max} + 2$ requires 2p2h excitations at most
- **sequential calculation** for a range of $N_{\max}\hbar\Omega$ spaces:
 - do full NCSM calculations up to a convenient N_{\max}
 - use components of eigenstates with $|C_\nu^{(m)}| \geq C_{\min}$ as initial $|\Psi_{\text{ref},m}\rangle$
 - ① consider all states $|\Phi_\nu\rangle \notin \mathcal{M}_{\text{ref}}$ from an $N_{\max} + 2$ space and add those with $|\kappa_\nu^{(m)}| \geq \kappa_{\min}$ to importance-truncated space \mathcal{M}_{IT}
 - ② solve eigenvalue problem in \mathcal{M}_{IT}
 - ③ use components of eigenstates with $|\kappa_\nu^{(m)}| \geq \kappa_{\min}$ as initial $|\Psi_{\text{ref},m}\rangle$
 - ④ goto ①

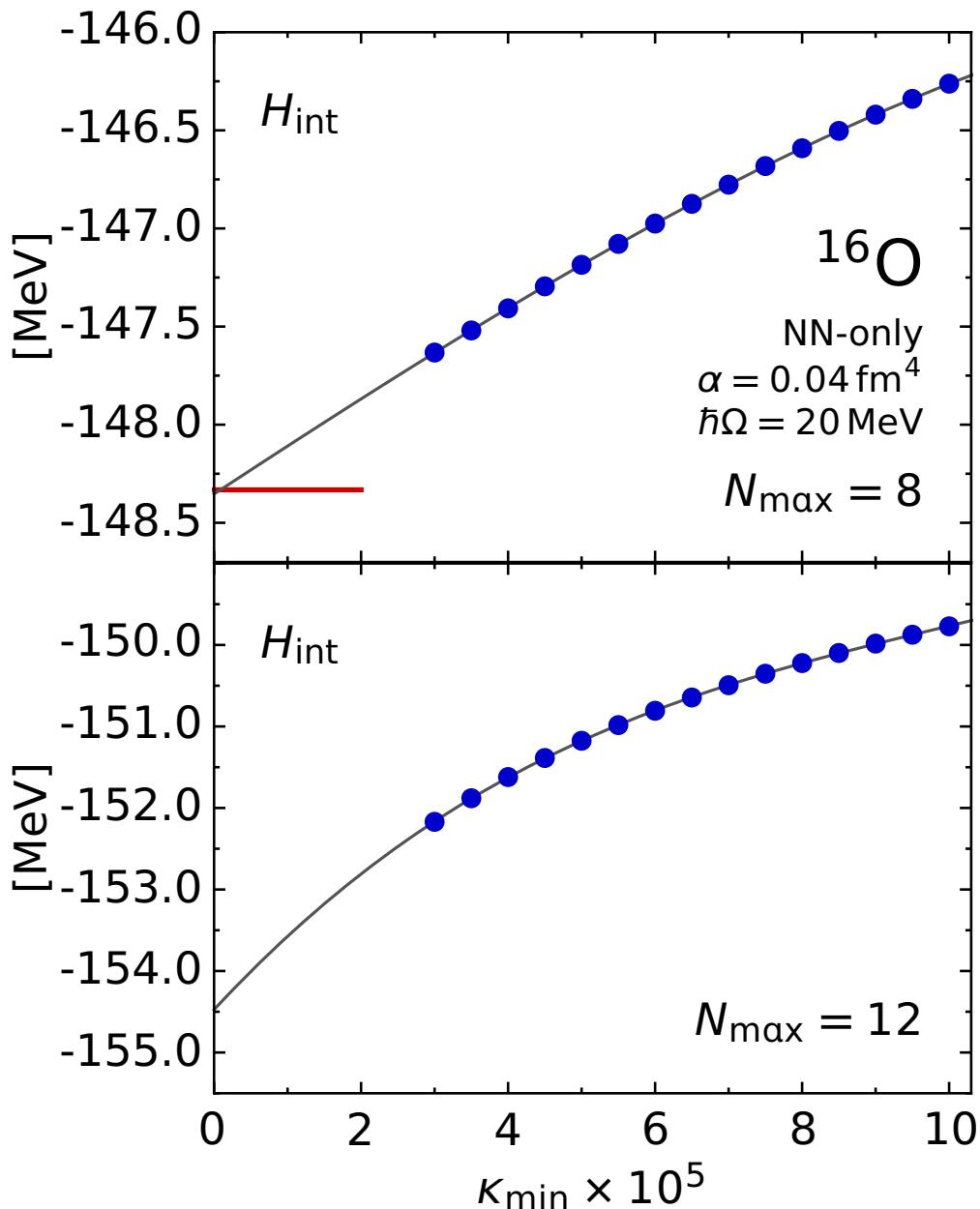
full NCSM space is
recovered in the limit
 $(\kappa_{\min}, C_{\min}) \rightarrow 0$

Threshold Extrapolation



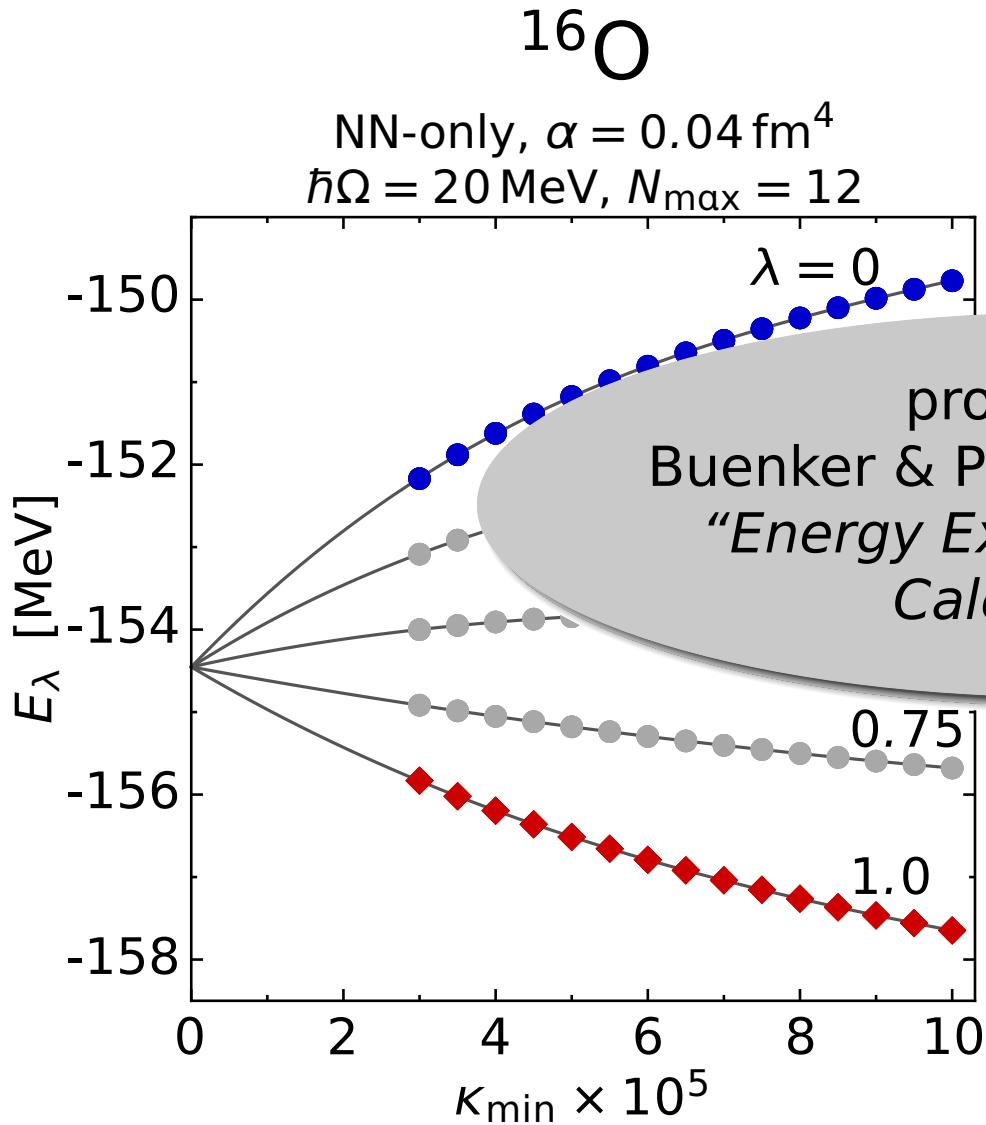
- repeat calculations for a **sequence of importance thresholds** κ_{\min}
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $\kappa_{\min} \rightarrow 0$ of observables to account for effect of excluded configurations

Threshold Extrapolation



- repeat calculations for a **sequence of importance thresholds** K_{min}
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $K_{\text{min}} \rightarrow 0$ of observables to account for effect of excluded configurations

Constrained Threshold Extrapolation



- for free: importance selection gives perturbative energy correction $\Delta_{\text{excl}}(\kappa_{\min})$ accounting for **excluded states**
- $\kappa_{\min} \rightarrow 0$
- diameter λ defining a family of energy sequences
- $$E_\lambda(\kappa_{\min}) = E(\kappa_{\min}) + \lambda \Delta_{\text{excl}}(\kappa_{\min})$$
- **simultaneous extrapolation** for family of λ -values with constraint $E_\lambda(0) = E_{\text{extrap}}$

Uncertainty Quantification in the IT-NCSM

Uncertainty Quantification

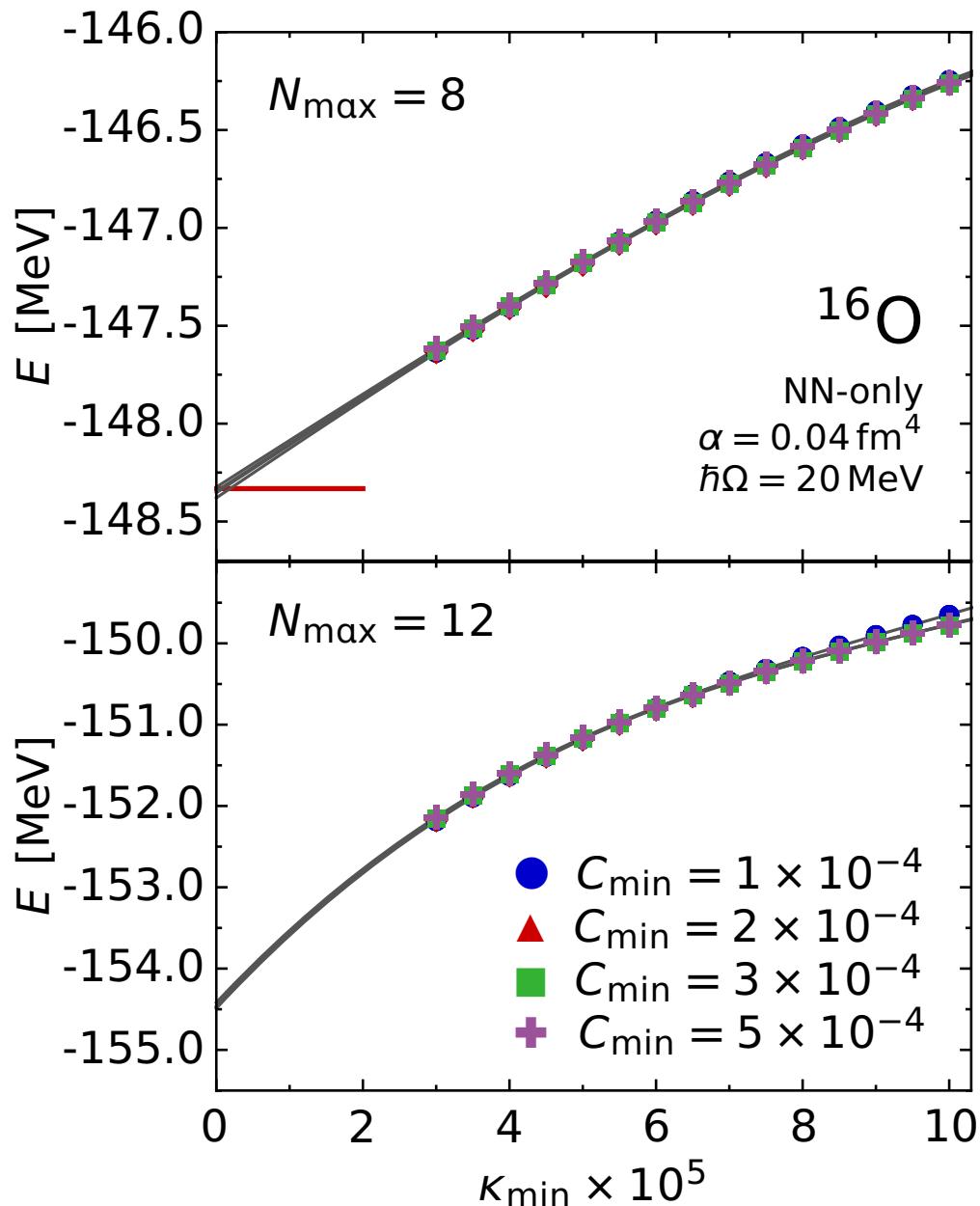
Importance Truncation

- use sequence of $(C_{\min}, \kappa_{\min})$ -truncated model spaces
- extrapolate to $\kappa_{\min} \rightarrow 0$ using polynomial ansatz or more refined constrained extrapolation scheme
- uncertainty estimate derived from extrapolation protocol
- **systematic uncertainty** absent in full NCSM

Model-Space Truncation

- use sequence of N_{\max} -truncated model spaces
- extrapolate to $N_{\max} \rightarrow \infty$ using exponential ansatz or more elaborate extrapolation schemes
- uncertainty estimate derived from extrapolation protocol
- same **extrapolation uncertainties** as in full NCSM

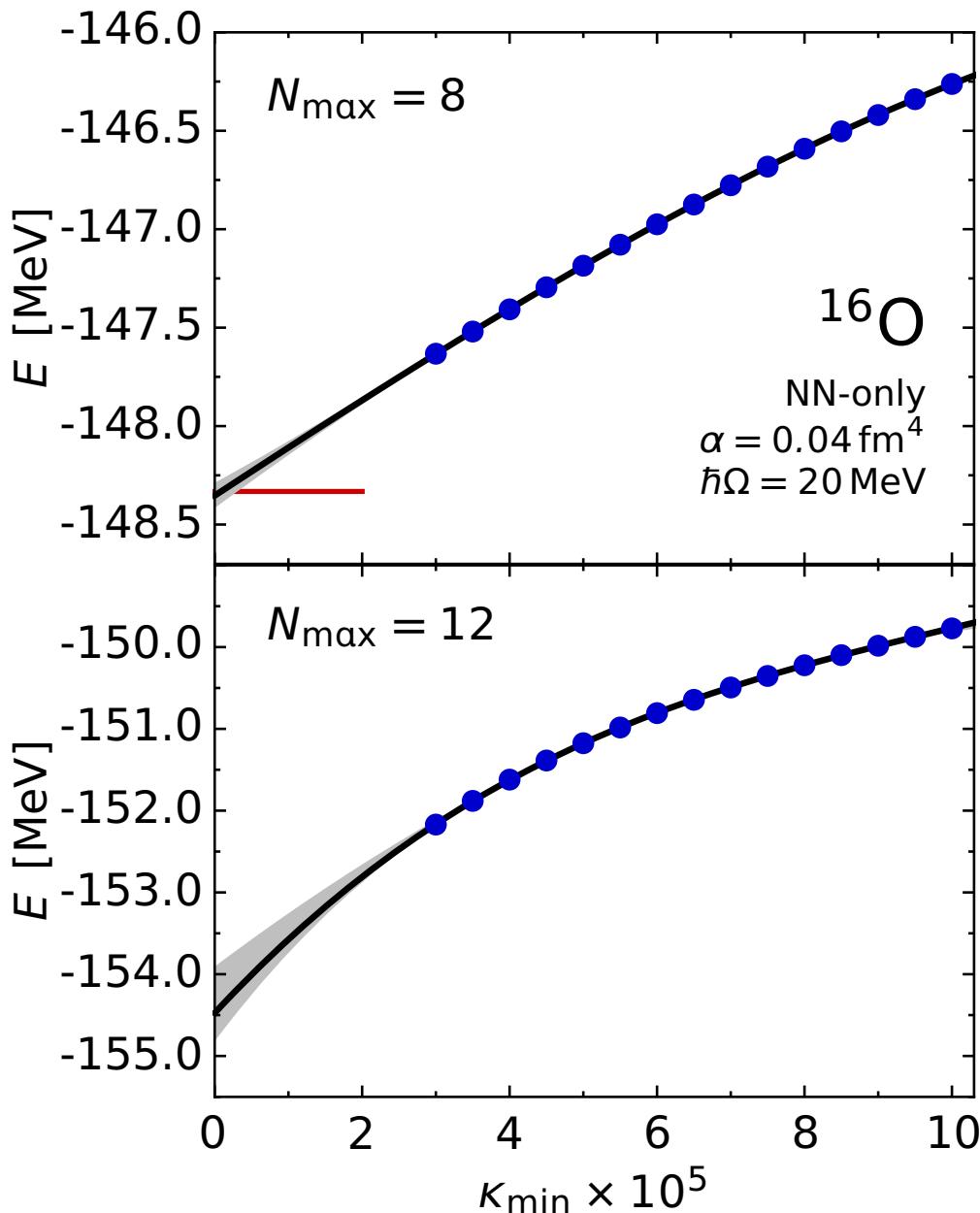
Comment on C_{\min} Truncation



- truncation of reference state to components with $|C_\nu| \geq C_{\min}$
- technical reason: importance selection phase scales with $(\dim \mathcal{M}_{\text{ref}})^2$
- typically $C_{\min} = 2 \times 10^{-4}$

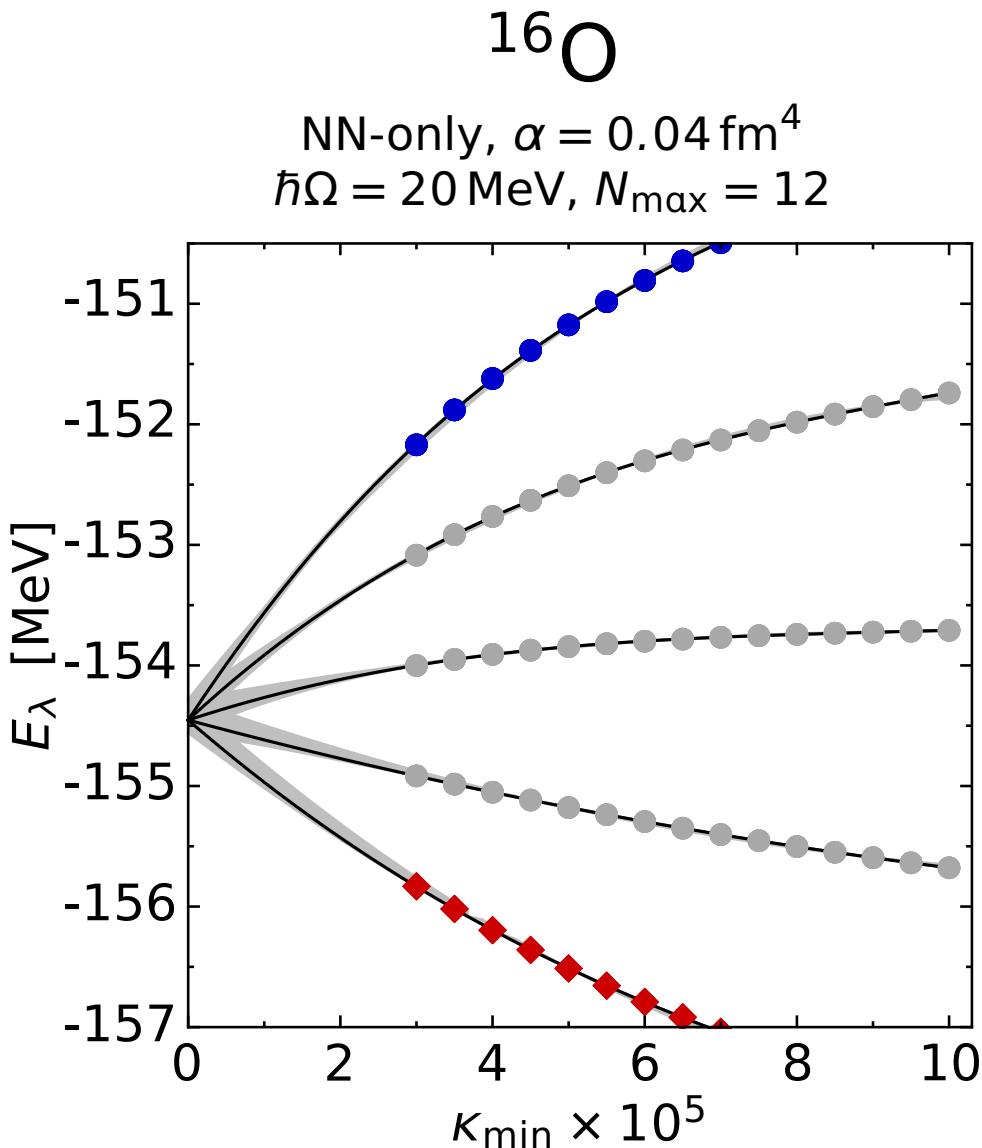
practically no influence on threshold extrapolated energies

Protocol: Simple K_{\min} Extrapolation



- perform IT-NCSM calculations for range of K_{\min} -values, typically $K_{\min} = 3, 3.5, \dots, 10 \times 10^{-5}$
- extrapolation $K_{\min} \rightarrow 0$ using polynomial $P_p(K_{\min})$ fit to full K_{\min} -set, typically of order $p = 3$
- generate uncertainty band from set of alternative extrapolations
 - P_{p-1} and P_{p+1} extrapolations using full K_{\min} -range
 - P_p extrapolations with lowest and lowest two K_{\min} -points dropped
- quote standard deviation as nominal uncertainty

Protocol: Constrained κ_{\min} Extrapolation



- select a few λ -values to get symmetrical approach towards common $E_{\text{extrap}} = E_\lambda(\kappa_{\min} = 0)$
- constrained simultaneous extrapolation $\kappa_{\min} \rightarrow 0$ using polynomial $P_p(\kappa_{\min})$, typically of order $p = 3$
- generate uncertainty band from set of constrained extrapolations
 - P_{p-1} and P_{p+1} extrapolations using full κ_{\min} -range
 - P_p extrapolations with lowest and lowest two κ_{\min} -points dropped
 - P_p extrapolations with smallest and largest λ -set dropped
- std. deviation gives uncertainty

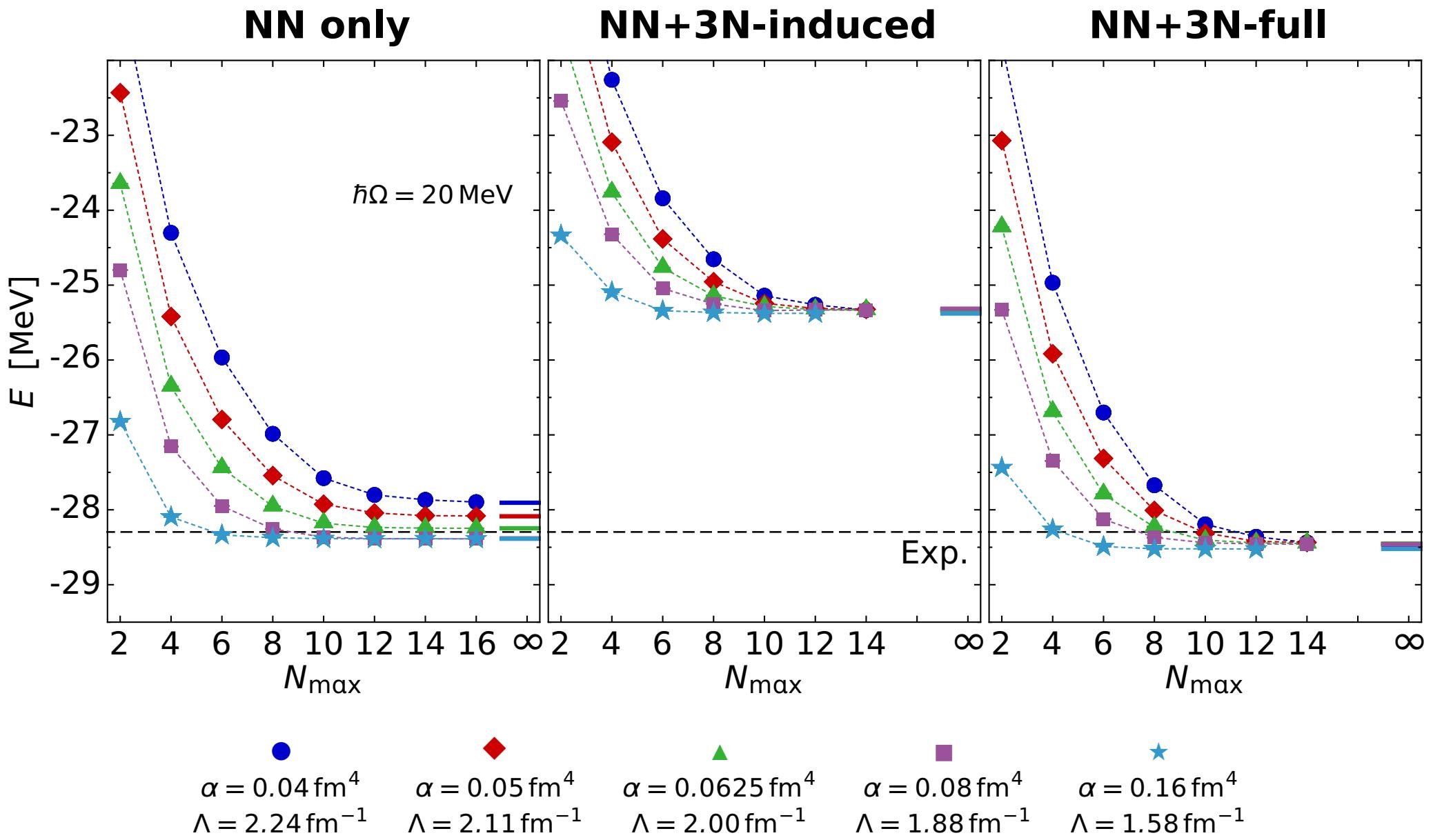
Characterization of SRG-Evolved NN+3N Hamiltonians

Roth, Calci, Langhammer, Binder — in preparation (2013)

Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)

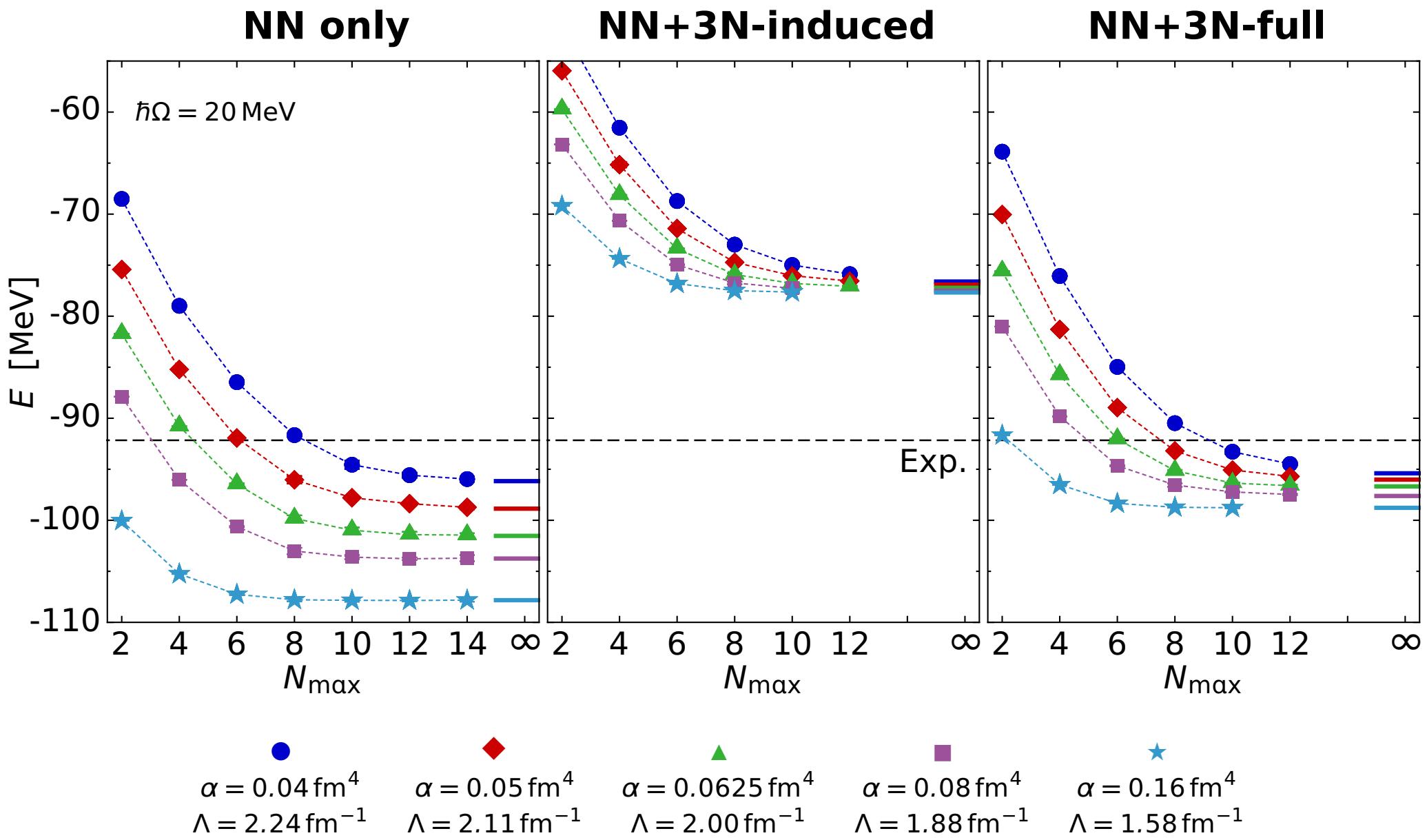
^4He : Ground-State Energies

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



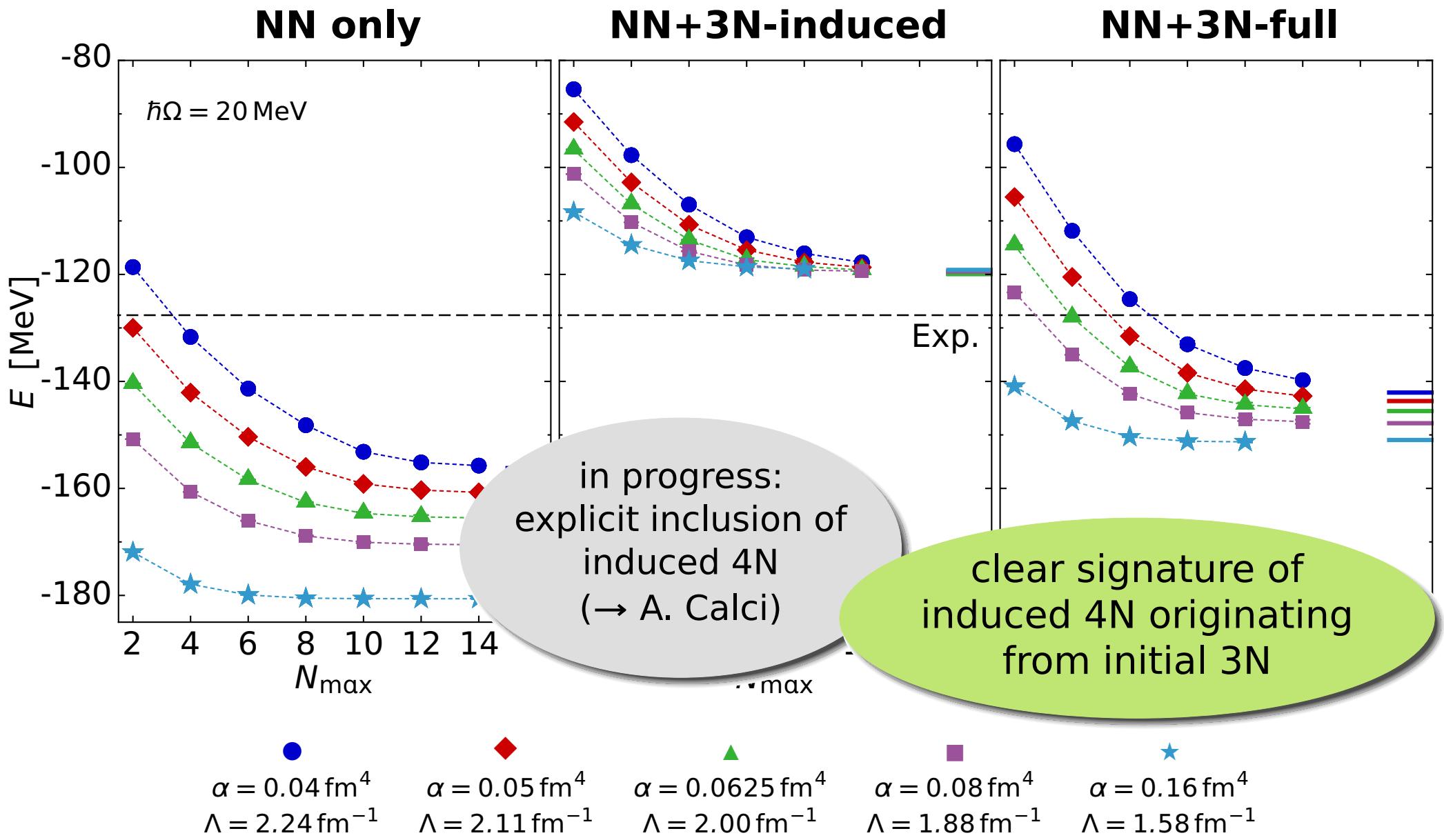
^{12}C : Ground-State Energies

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

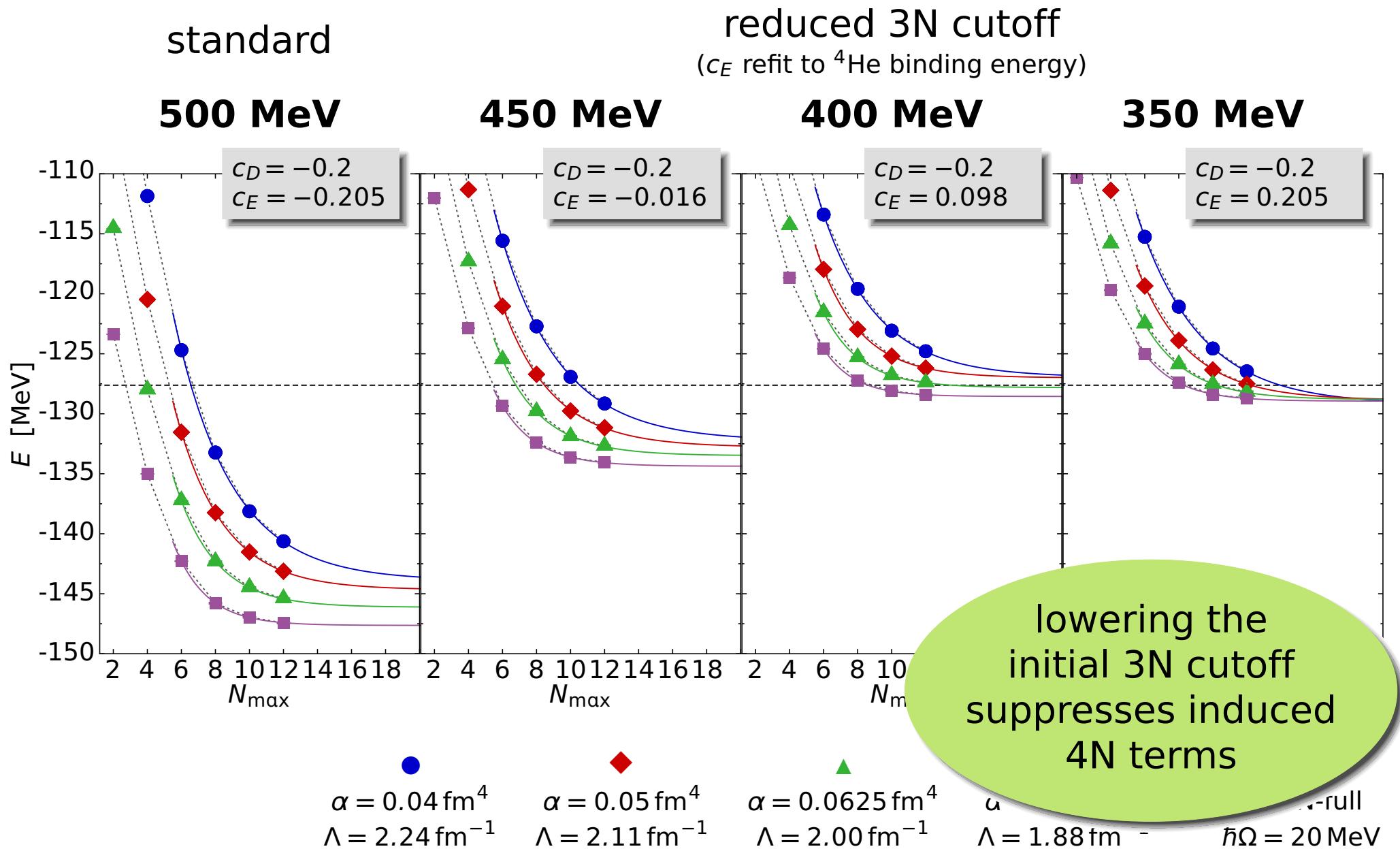


^{16}O : Ground-State Energies

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

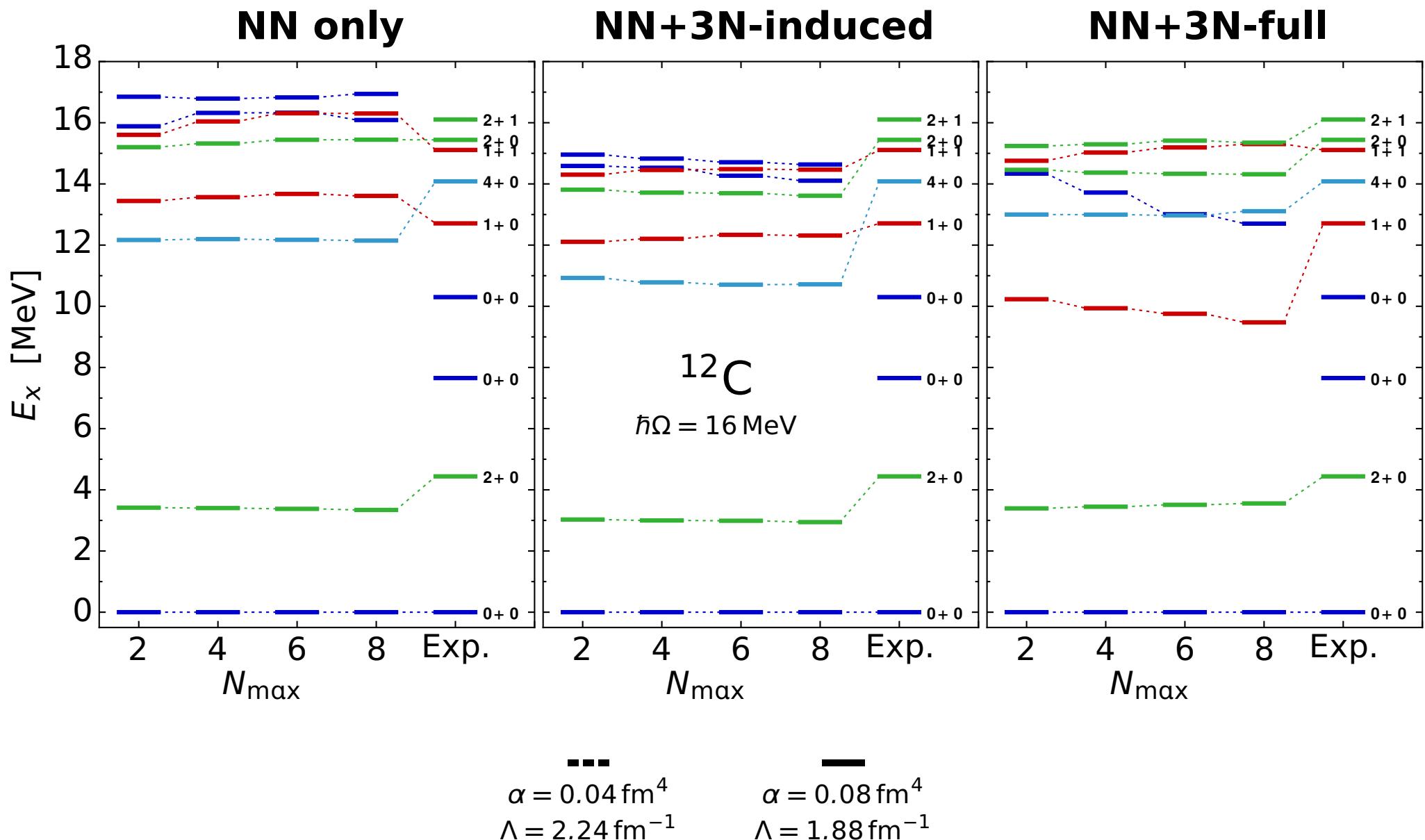


^{16}O : Lowering the Initial 3N Cutoff



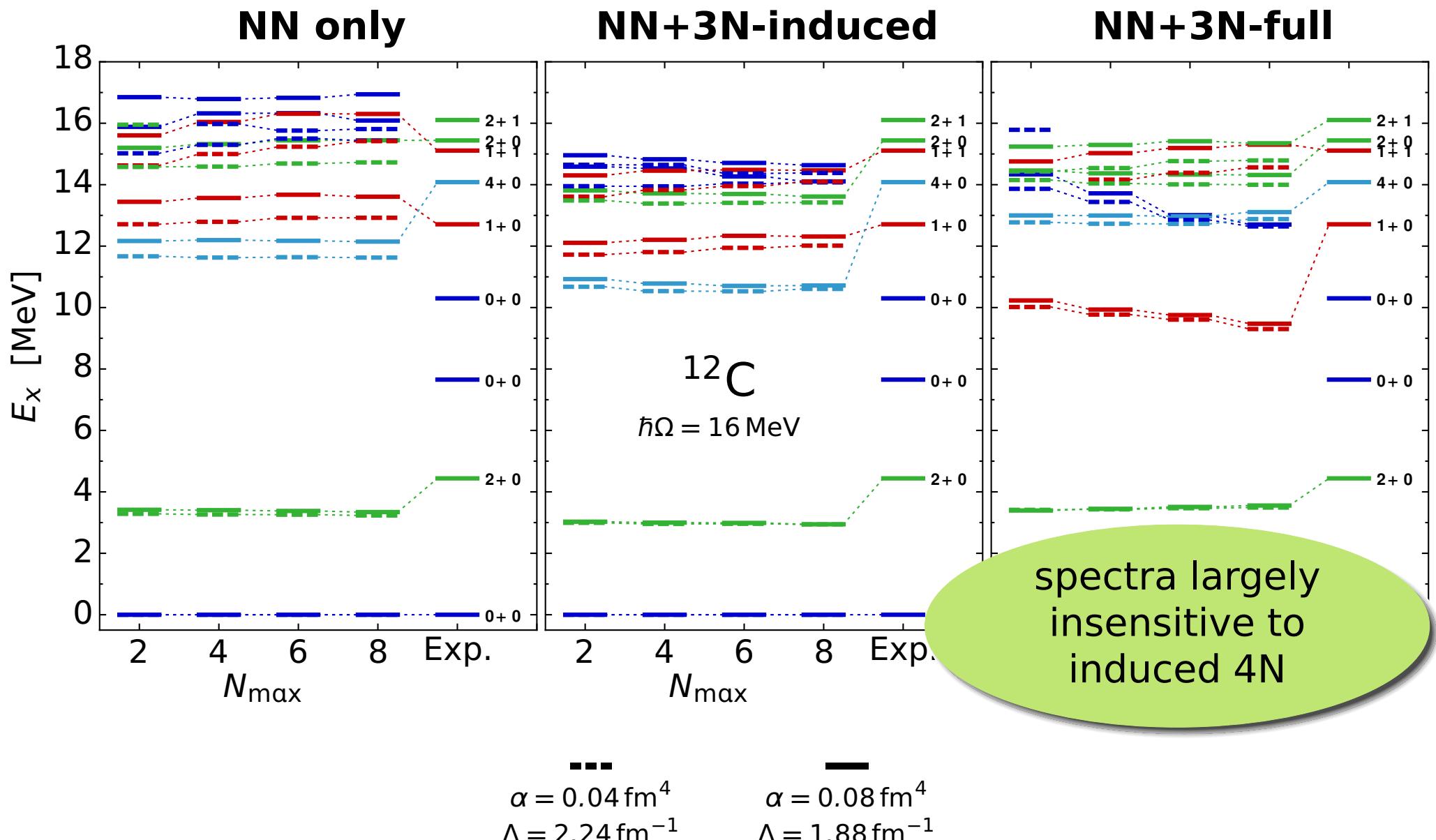
Spectroscopy of ^{12}C

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



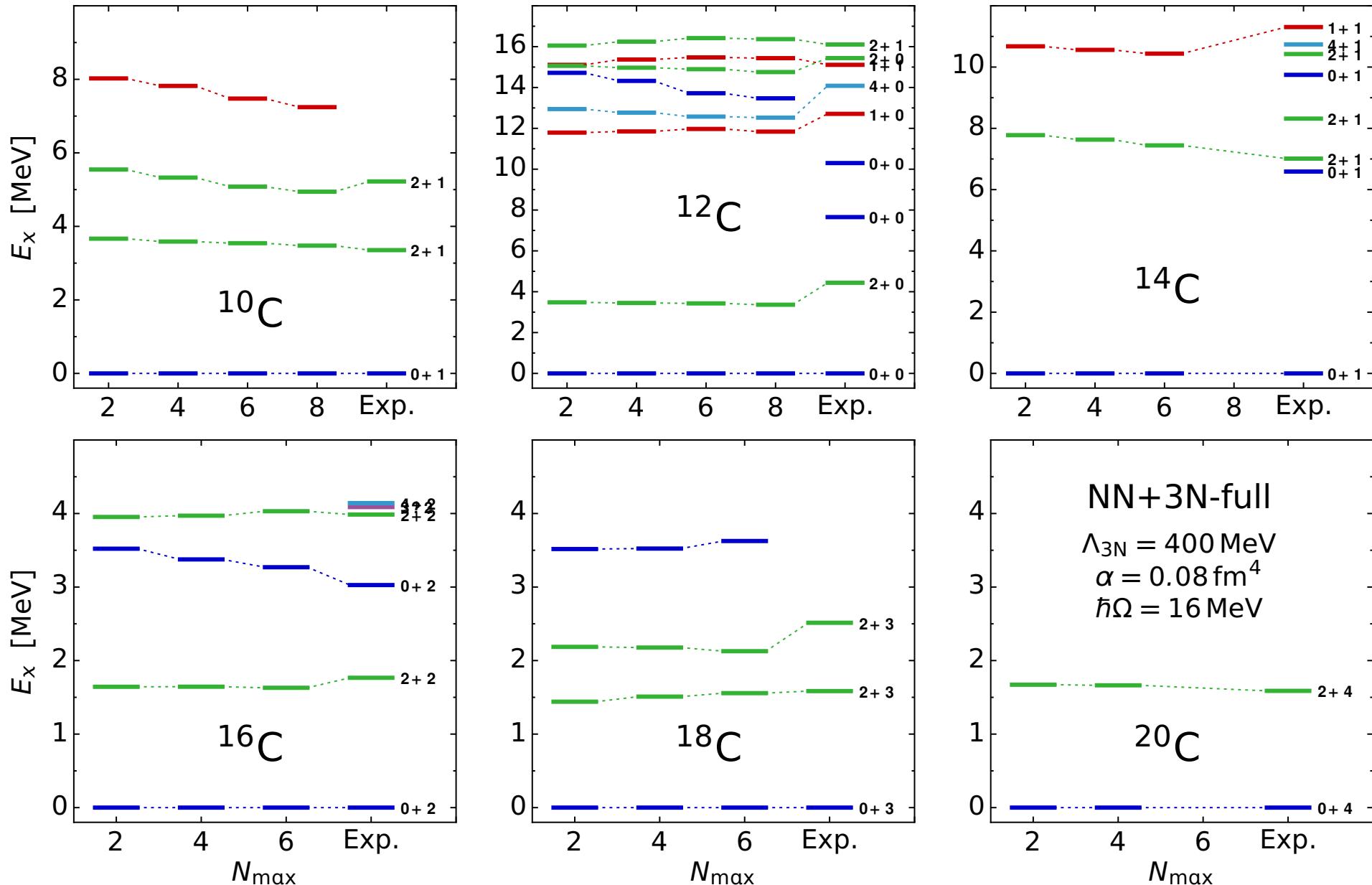
Spectroscopy of ^{12}C

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

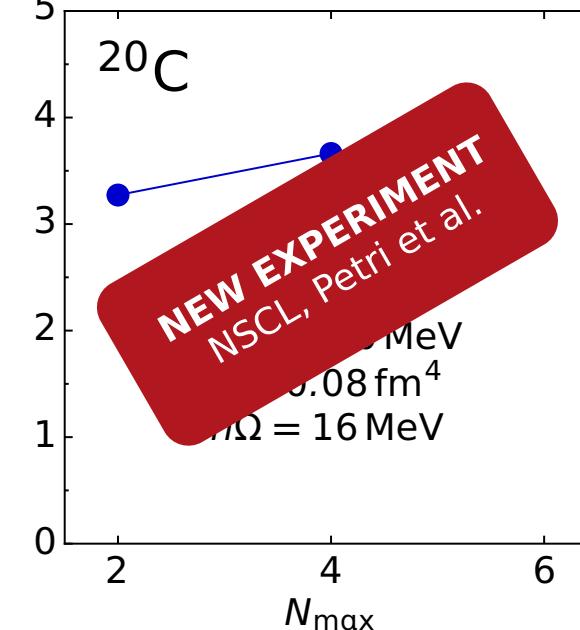
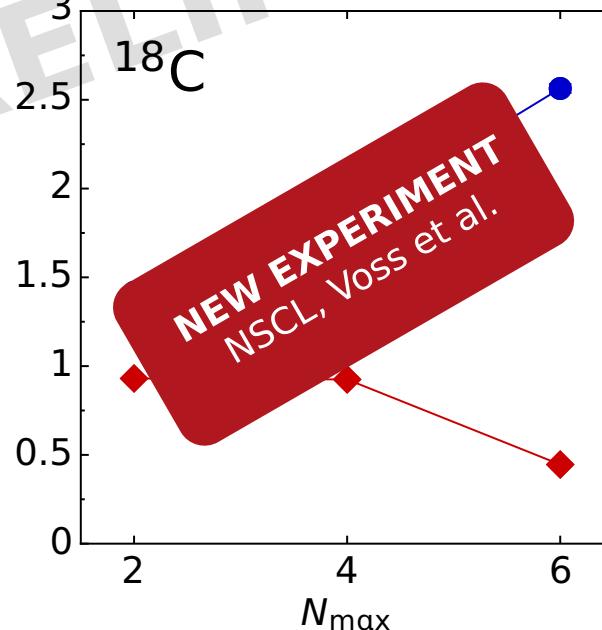
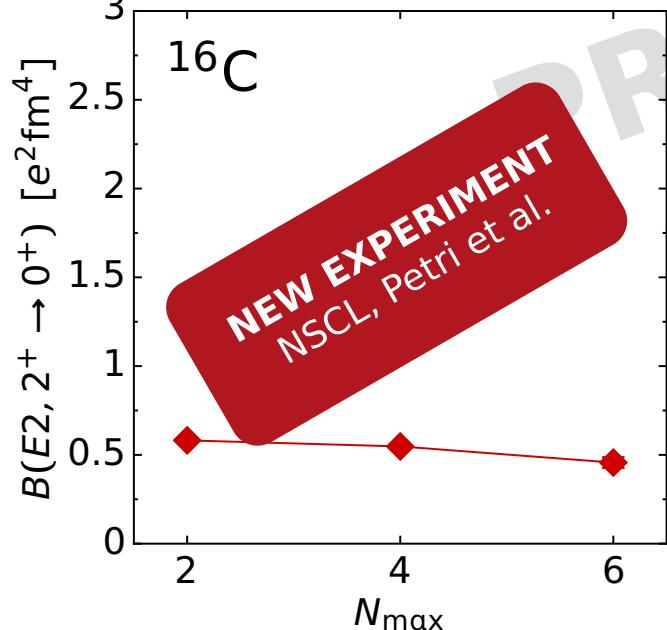
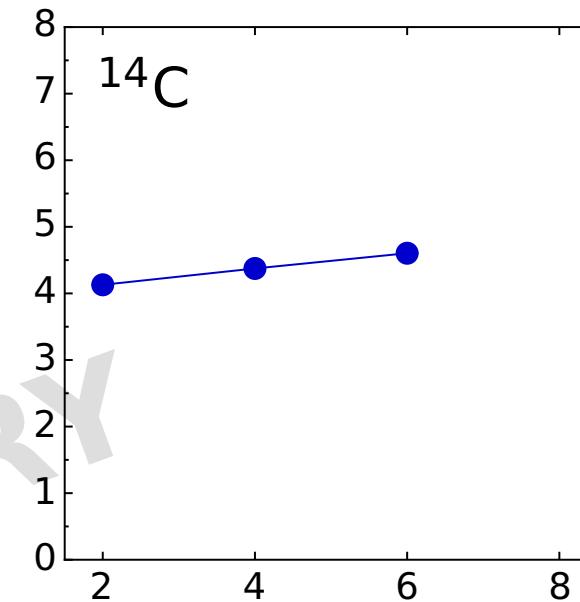
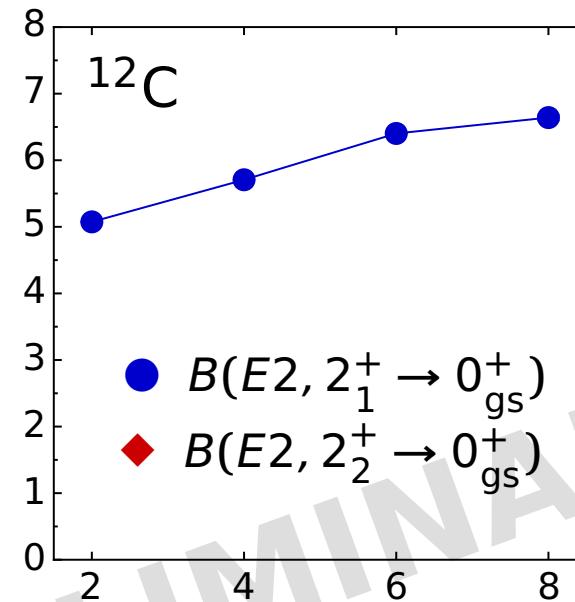
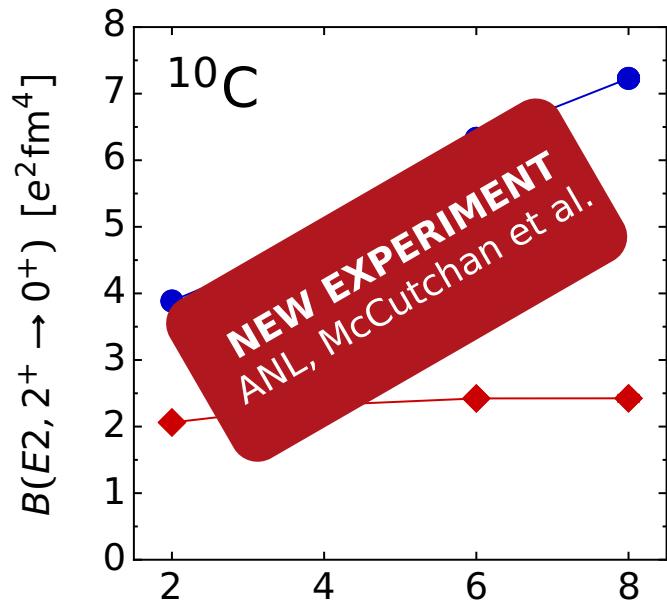


Ab Initio IT-NCSM Calculations for p- and sd-Shell Nuclei

Spectroscopy of Carbon Isotopes

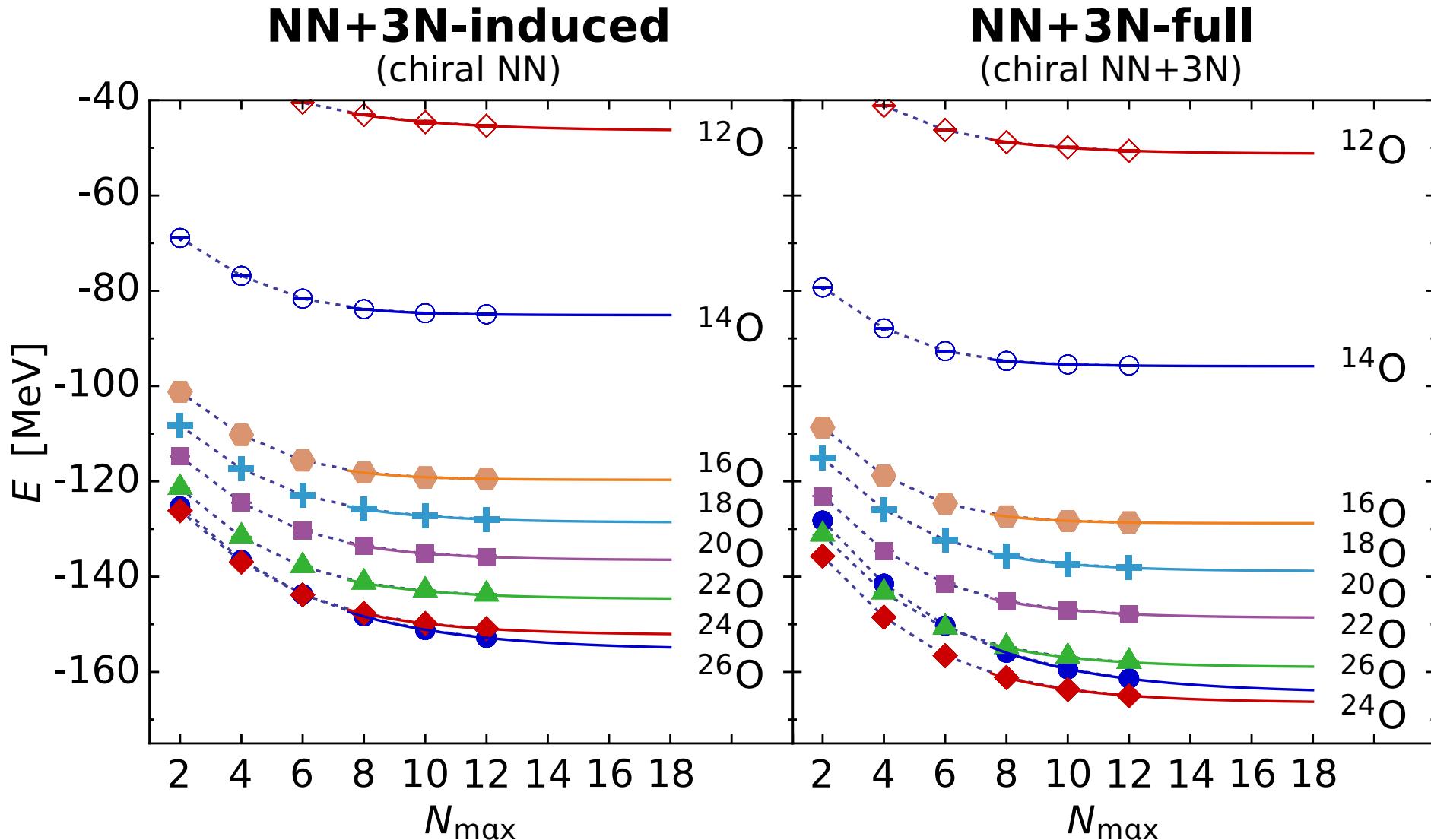


Spectroscopy of Carbon Isotopes



Ground States of Oxygen Isotopes

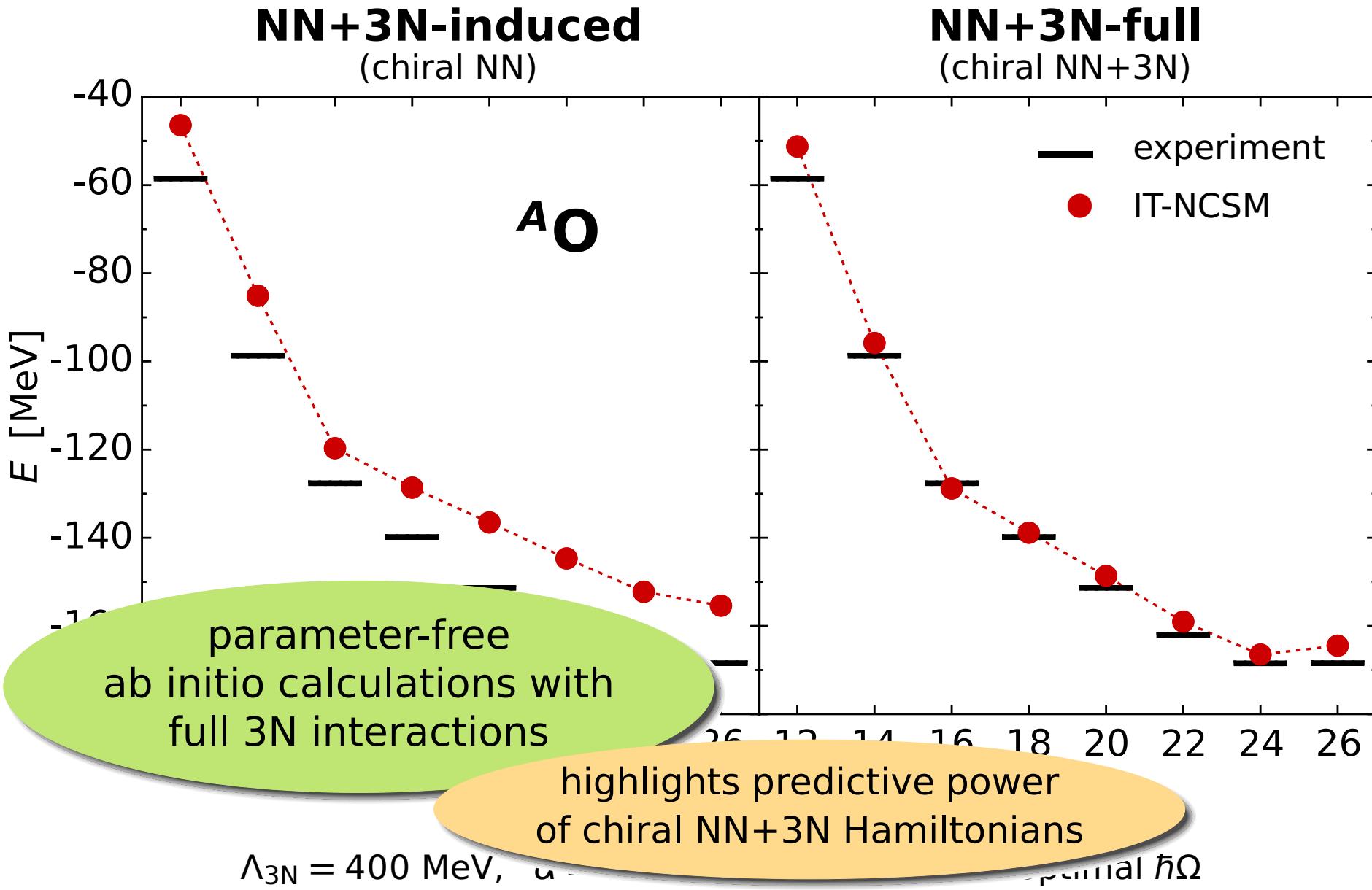
Hergert, Binder, Calci, Langhammer, Roth; arXiv:1302.7294



$$\Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\max} = 14, \quad \text{optimal } \hbar\Omega$$

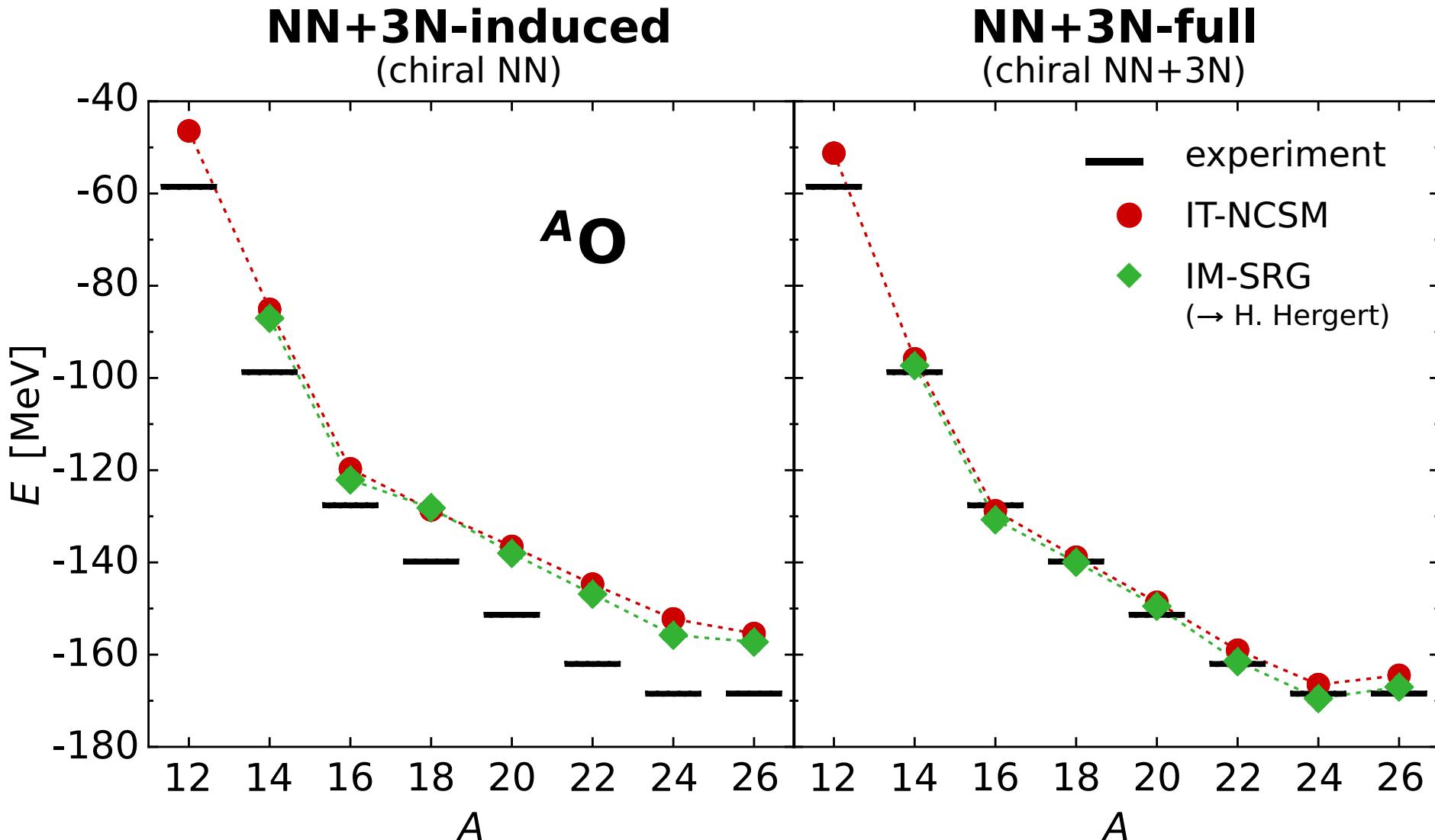
Ground States of Oxygen Isotopes

Hergert, Binder, Calci, Langhammer, Roth; arXiv:1302.7294



Ground States of Oxygen Isotopes

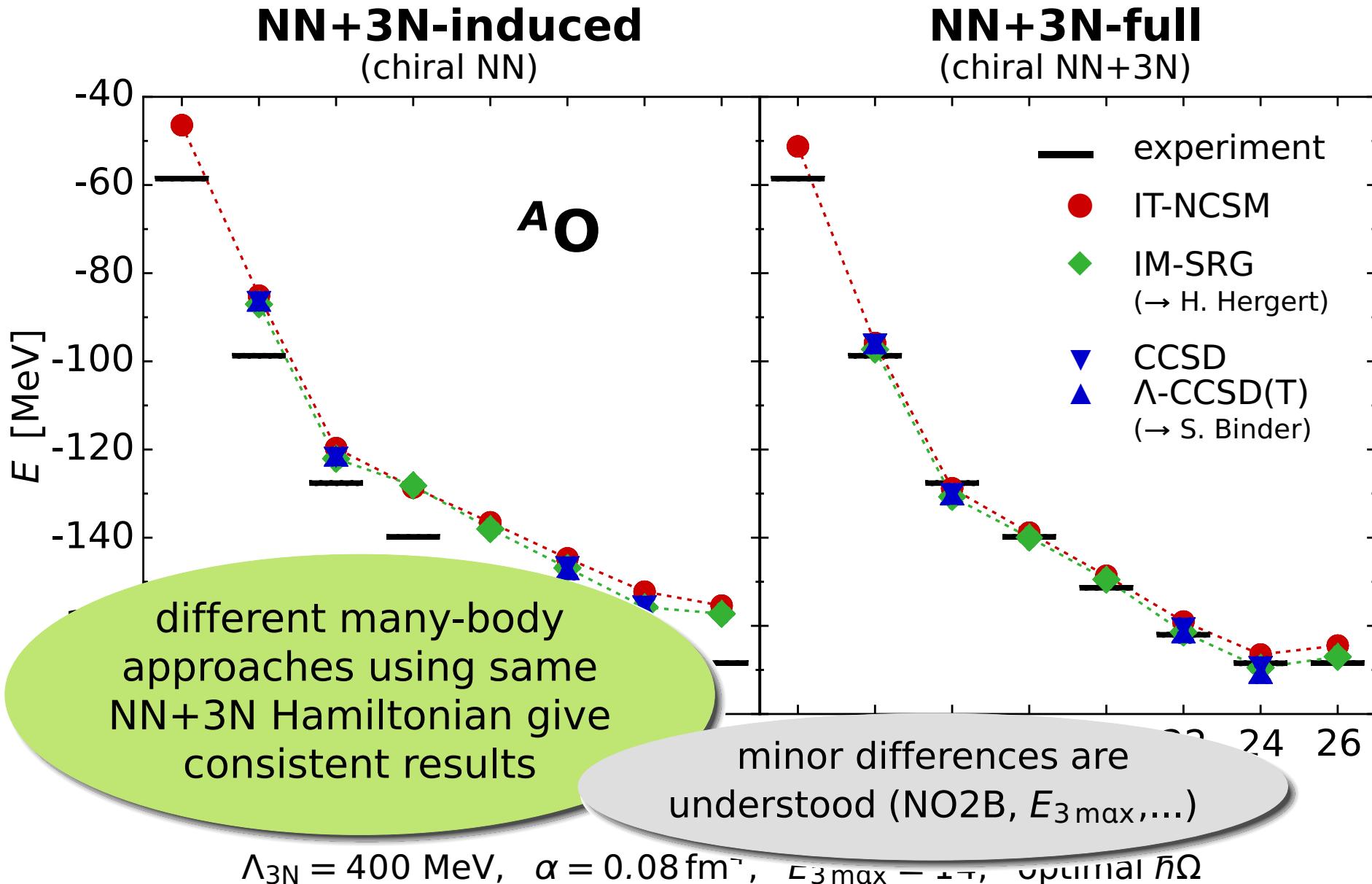
Hergert, Binder, Calci, Langhammer, Roth; arXiv:1302.7294



$$\Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\max} = 14, \quad \text{optimal } \hbar\Omega$$

Ground States of Oxygen Isotopes

Hergert, Binder, Calci, Langhammer, Roth; arXiv:1302.7294



Multi-Reference Normal-Ordering Approximation

Motivation: Normal Ordering

avoid formal and computational challenges of including explicit 3N terms in many-body calculations

- circumvent **formal extension of many-body method** to include explicit 3N interactions
- avoid the **increase of computational cost** caused by inclusion of explicit 3N interactions
- **normal-ordered two-body approximation** works very well for closed-shell systems (\rightarrow S. Binder)
- can we do the same for **open-shell nuclei?**

Normal Ordering of 3N Interaction

- **starting point:** three-body operator in second-quantized form with respect to the zero-body vacuum $|0\rangle$

$$V_{3N} = \frac{1}{36} \sum_{abc, \bar{a}\bar{b}\bar{c}} V_{\bar{a}\bar{b}\bar{c}}^{abc} A_{\bar{a}\bar{b}\bar{c}}^{abc}$$

$$V_{\bar{a}\bar{b}\bar{c}}^{abc} = \langle abc | V_{3N} | \bar{a}\bar{b}\bar{c} \rangle \quad A_{\bar{a}\bar{b}\bar{c}}^{abc} = a_a^\dagger a_b^\dagger a_c^\dagger a_{\bar{c}} a_{\bar{b}} a_{\bar{a}}$$

- **single-reference normal ordering:** assume reference state $|\Phi_{SR}\rangle$ given by a single Slater determinant
 - standard toolbox: Wick theorem, contractions, etc.
- **multi-reference normal ordering:** assume reference state $|\Phi_{MR}\rangle$ given by a superposition of Slater determinants
 - generalized Wick theorem and n-tupel contractions proposed by Mukherjee & Kutzelnigg (1997)

Multi-Reference Normal Ordering

- **three-body operator in normal-ordered form** with respect to multi-reference state $|\Phi_{\text{MR}}\rangle$

$$V_{3N} = W + \sum_{c, \bar{c}} W_{\bar{c}}^c \tilde{A}_{\bar{c}}^c + \frac{1}{4} \sum_{bc, \bar{b}\bar{c}} W_{\bar{b}\bar{c}}^{bc} \tilde{A}_{\bar{b}\bar{c}}^{bc} + \frac{1}{36} \sum_{abc, \bar{a}\bar{b}\bar{c}} W_{\bar{a}\bar{b}\bar{c}}^{abc} \tilde{A}_{\bar{a}\bar{b}\bar{c}}^{abc}$$

where $\tilde{A}_{\circ\circ\circ}^{\circ\circ\circ}$ indicates multi-reference normal ordered string of creation and annihilation operators (abstract concept)

- matrix elements of **normal-ordered n -body contributions** involve one-, two- and three-body density matrices for $|\Phi_{\text{MR}}\rangle$

$$W = \frac{1}{36} \sum_{abc, \bar{a}\bar{b}\bar{c}} V_{\bar{a}\bar{b}\bar{c}}^{abc} \rho_{\bar{a}\bar{b}\bar{c}}^{abc}$$

$$W_{\bar{c}}^c = \frac{1}{4} \sum_{ab, \bar{a}\bar{b}} V_{\bar{a}\bar{b}\bar{c}}^{abc} \rho_{\bar{a}\bar{b}}^{ab}$$

$$W_{\bar{b}\bar{c}}^{bc} = \sum_{a, \bar{a}} V_{\bar{a}\bar{b}\bar{c}}^{abc} \rho_{\bar{a}}^a$$

$$W_{\bar{a}\bar{b}\bar{c}}^{abc} = V_{\bar{a}\bar{b}\bar{c}}^{abc}$$

Multi-Reference Normal Ordering

- discard normal-ordered three-body contribution to define the **normal-ordered two-body (NO2B) approximation**

$$V_{\text{NO2B}} = W + \sum_{c,\bar{c}} W_{\bar{c}}^c \tilde{A}_{\bar{c}}^c + \frac{1}{4} \sum_{bc,\bar{b}\bar{c}} W_{\bar{b}\bar{c}}^{bc} \tilde{A}_{\bar{b}\bar{c}}^{bc}$$

- converted back into **vacuum normal order** with respect to $|0\rangle$

$$V_{\text{NO2B}} = \bar{V} + \sum_{c,\bar{c}} \bar{V}_{\bar{c}}^c A_{\bar{c}}^c + \frac{1}{4} \sum_{bc,\bar{b}\bar{c}} \bar{V}_{\bar{b}\bar{c}}^{bc} A_{\bar{b}\bar{c}}^{bc}$$

with new matrix elements

$$\bar{V} = \frac{1}{36} \sum_{abc,\bar{a}\bar{b}\bar{c}} V_{\bar{a}\bar{b}\bar{c}}^{abc} \left(\rho_{\bar{a}\bar{b}\bar{c}}^{abc} - 18 \rho_{\bar{a}}^a \rho_{\bar{b}\bar{c}}^{bc} + 36 \rho_{\bar{a}}^a \rho_{\bar{b}}^b \rho_{\bar{c}}^c \right)$$

$$\bar{V}_{\bar{c}}^c = \frac{1}{4} \sum_{ab,\bar{a}\bar{b}} V_{\bar{a}\bar{b}\bar{c}}^{abc} \left(\rho_{\bar{a}\bar{b}}^{ab} - 4 \rho_{\bar{a}}^a \rho_{\bar{b}}^b \right)$$

$$\bar{V}_{\bar{b}\bar{c}}^{bc} = \sum_{a,\bar{a}} V_{\bar{a}\bar{b}\bar{c}}^{abc} \rho_{\bar{a}}^a$$

Single-Reference Normal Ordering

- **single-reference normal ordering** is recovered by putting in density matrices for a single Slater-determinant

$$\begin{aligned}\rho_{\bar{a}}^a &= n_a \delta_{\bar{a}}^a \\ \rho_{\bar{a}\bar{b}}^{ab} &= \rho_{\bar{a}}^a \rho_{\bar{b}}^b - \rho_{\bar{a}}^b \rho_{\bar{b}}^a \\ \rho_{\bar{a}\bar{b}\bar{c}}^{abc} &= \dots\end{aligned}$$

- three-body operator in **single-reference NO2B approximation** converted back into vacuum representation

$$V_{\text{NO2B}} = \bar{V} + \sum_{c,\bar{c}} \bar{V}_{\bar{c}}^c A_{\bar{c}}^c + \frac{1}{4} \sum_{bc,\bar{b}\bar{c}} \bar{V}_{\bar{b}\bar{c}}^{bc} A_{\bar{b}\bar{c}}^{bc}$$

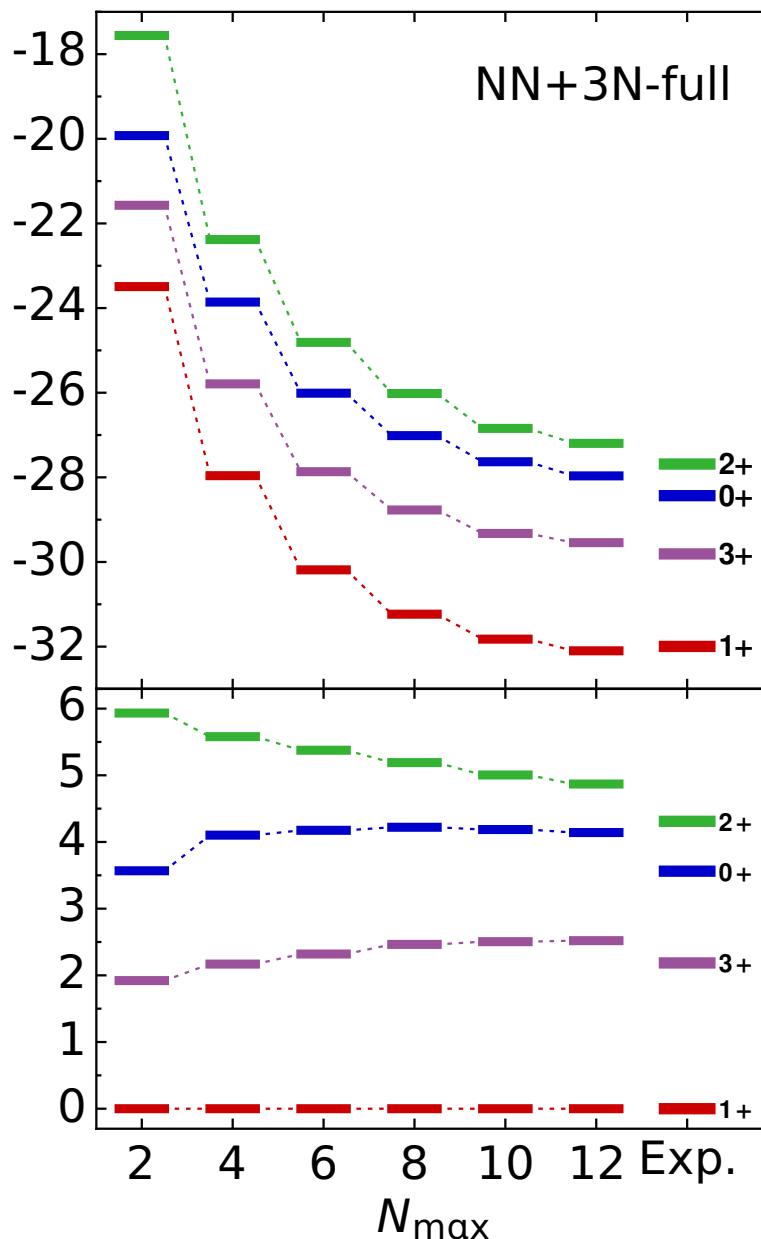
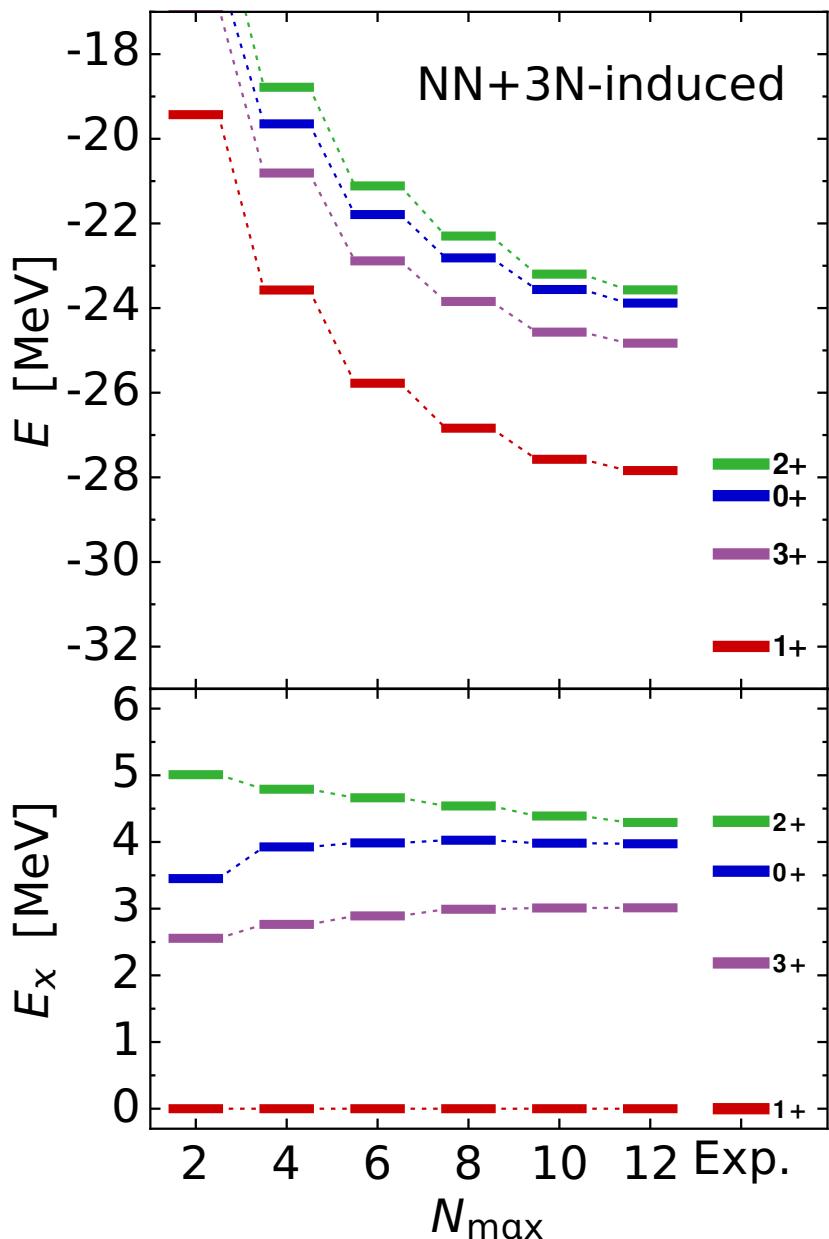
with simplified matrix elements

$$\bar{V} = \frac{1}{6} \sum_{abc} V_{abc}^{abc} n_a n_b n_c \quad \bar{V}_{\bar{c}}^c = -\frac{1}{2} \sum_{ab} V_{ab\bar{c}}^{abc} n_a n_b \quad \bar{V}_{\bar{b}\bar{c}}^{bc} = \sum_a V_{a\bar{b}\bar{c}}^{abc} n_a$$

IT-NCSM with MR-NO2B Approximation

- ❶ perform NCSM with explicit 3N interaction for small N_{\max}
 - ground state defines the reference state $|\Phi_{\text{MR}}\rangle$
 - no explicit information on excited states enters
- ❷ compute zero-, one- and two-body matrix elements of MR-NO2B approximation
 - density matrices for $|\Phi_{\text{MR}}\rangle$ can be precomputed and stored
 - three-body density matrix is not need explicitly
- ❸ perform NCSM or IT-NCSM calculation up to large N_{\max} using MR-NO2B approximation
 - same computational cost as a simple NN-only calculation
 - larger model spaces become accessible

Benchmark: ${}^6\text{Li}$

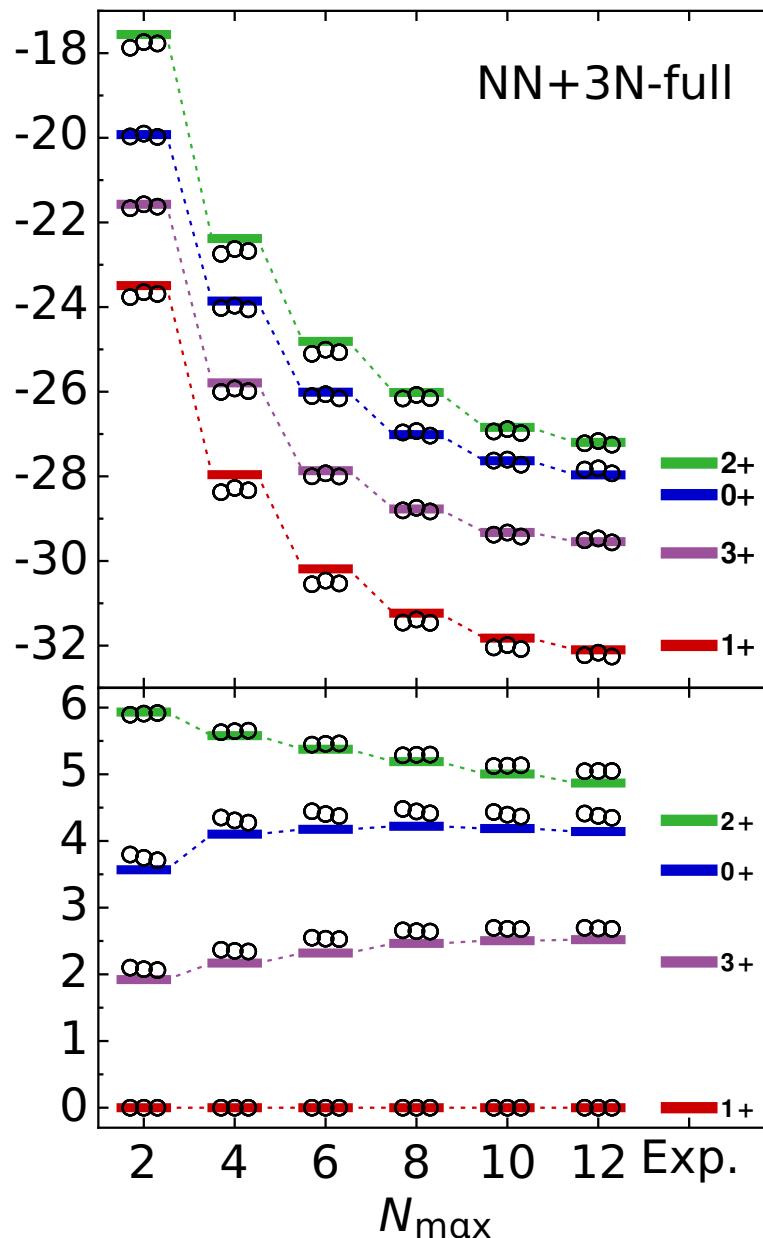
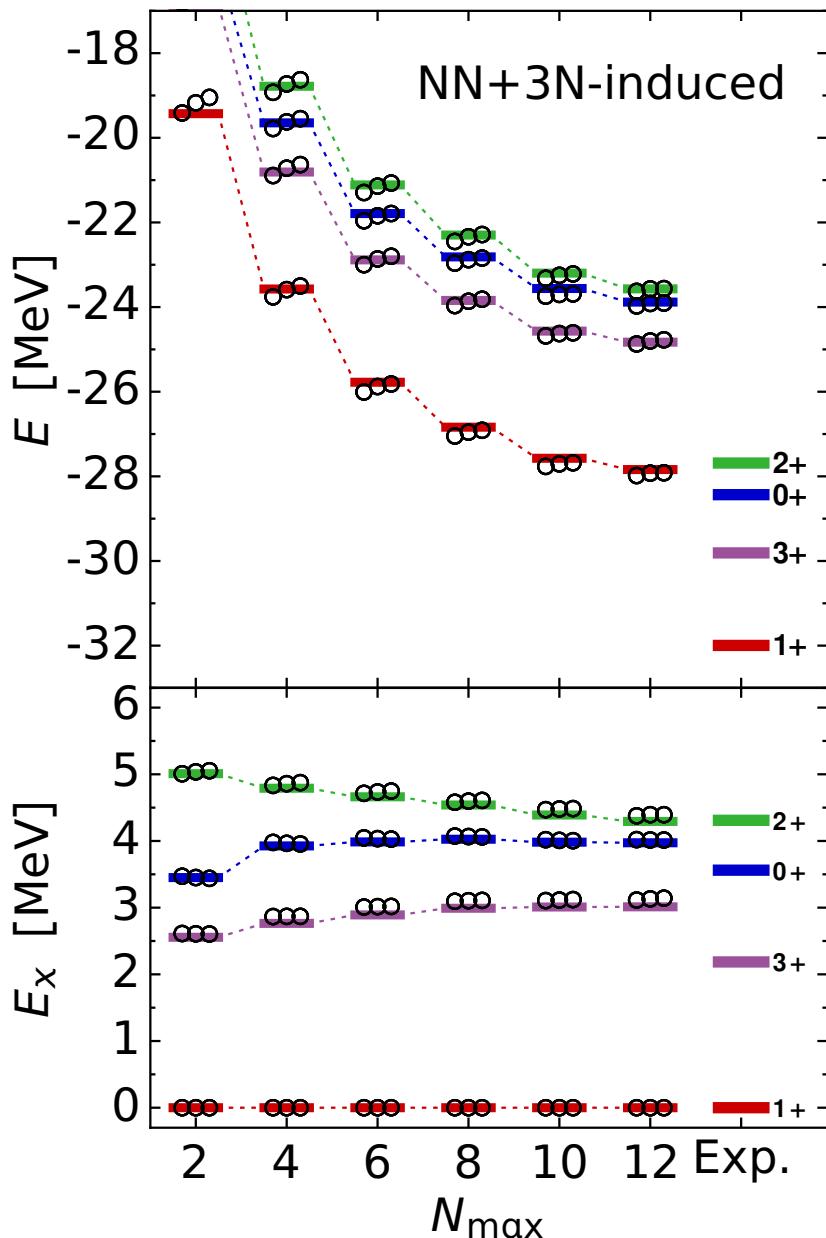


${}^6\text{Li}$

$\Lambda_{3N} = 500 \text{ MeV}$
 $\alpha = 0.08 \text{ fm}^4$
 $\hbar\Omega = 20 \text{ MeV}$

— explicit 3N

Benchmark: ${}^6\text{Li}$



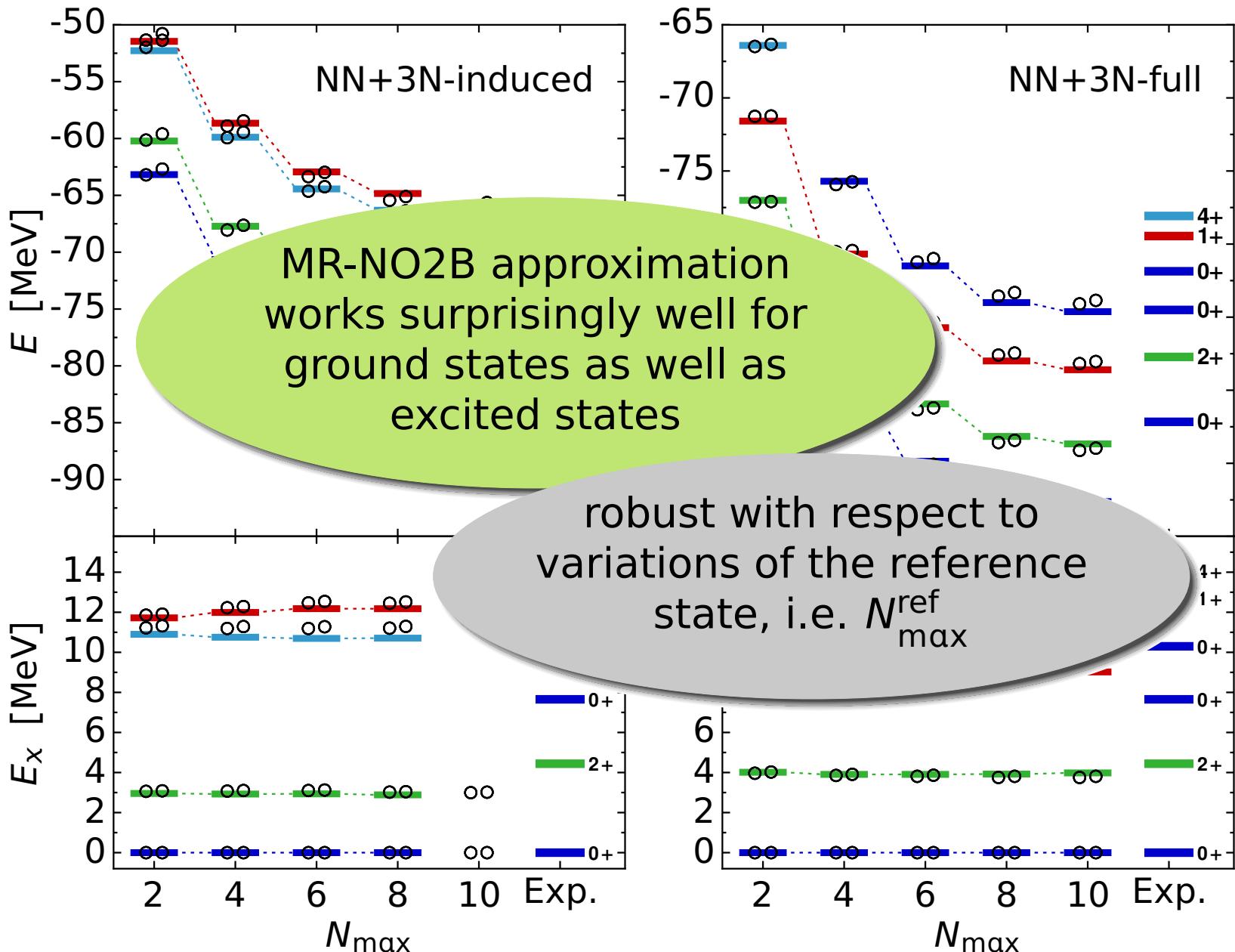
${}^6\text{Li}$

$\Lambda_{3N} = 500 \text{ MeV}$
 $\alpha = 0.08 \text{ fm}^4$
 $\hbar\Omega = 20 \text{ MeV}$

— explicit 3N

MR-NO2B
 $N_{\max}^{\text{ref}} = 2, 4, 6$

Benchmark: ^{12}C



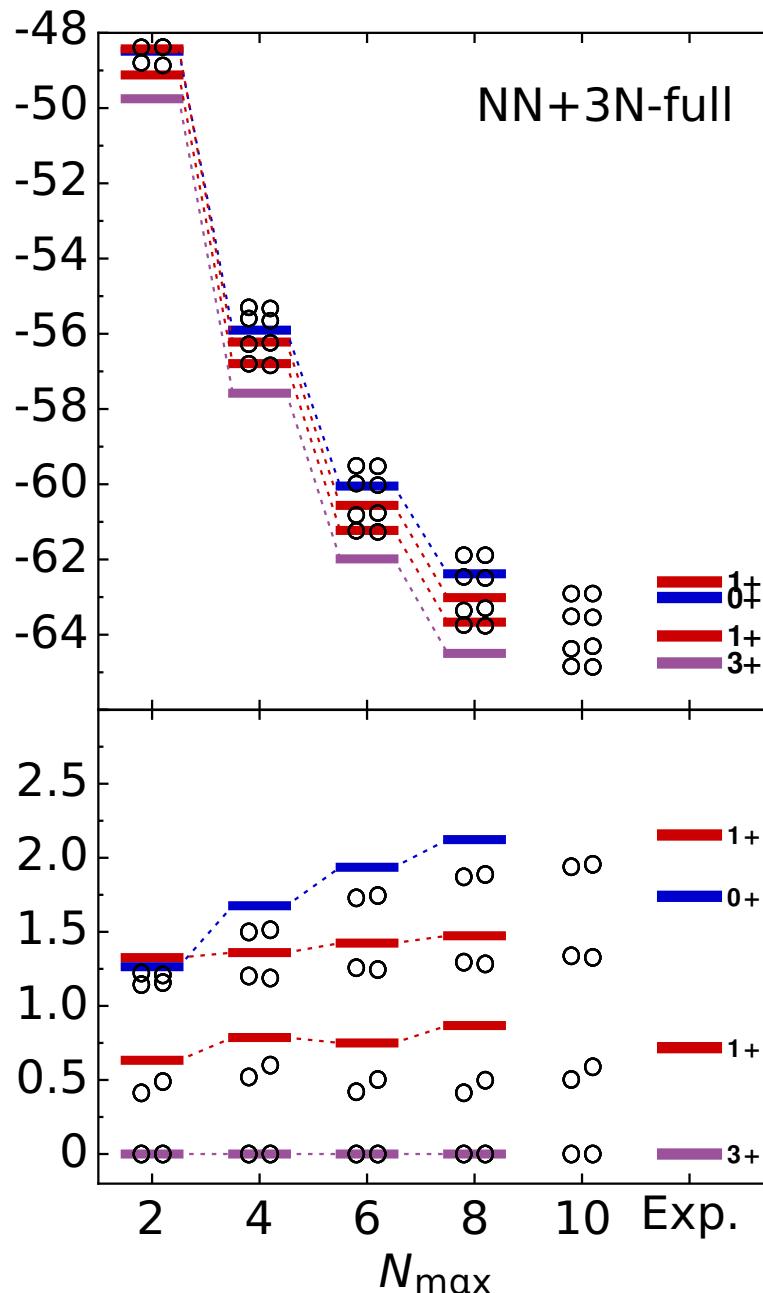
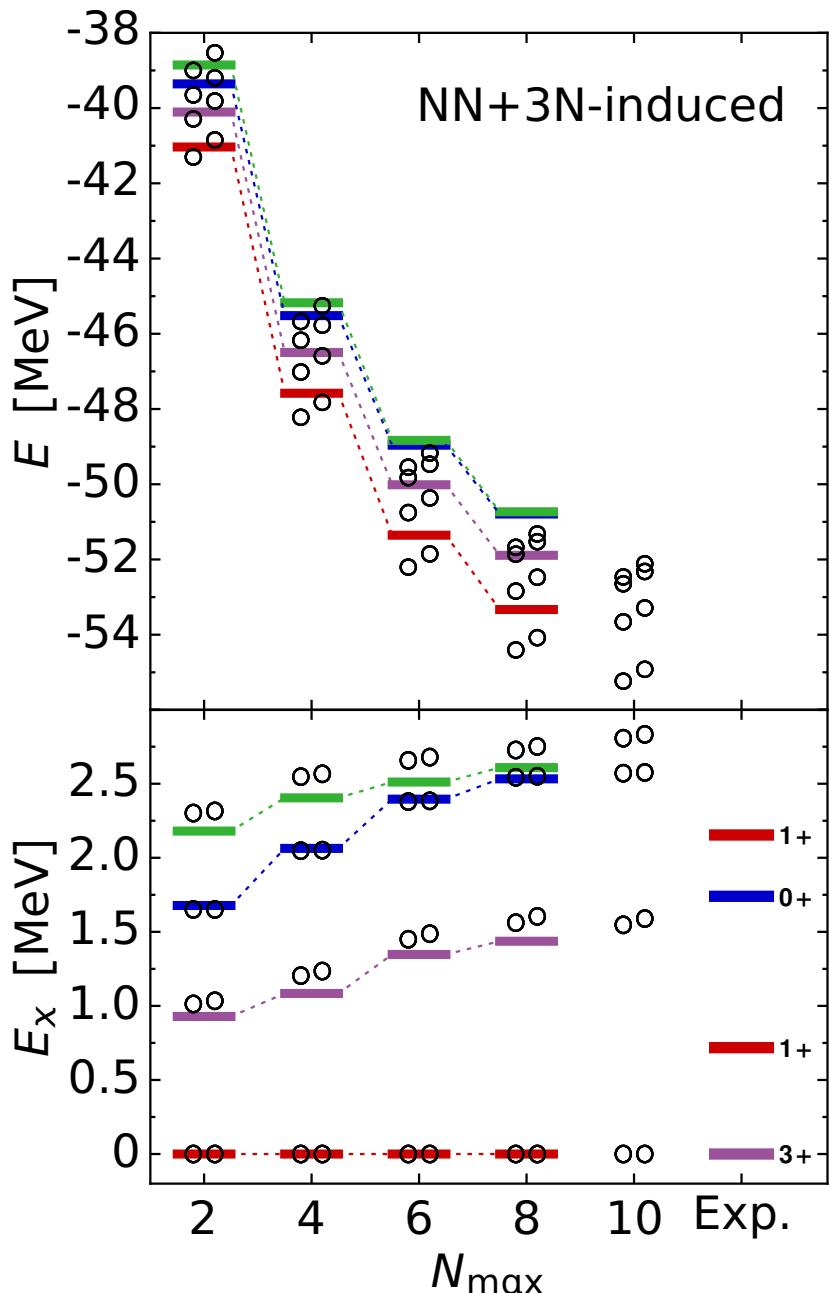
^{12}C

$\Lambda_{3N} = 500 \text{ MeV}$
 $\alpha = 0.08 \text{ fm}^4$
 $\hbar\Omega = 20 \text{ MeV}$

explicit 3N

○
 MR-NO2B
 $N_{\max}^{\text{ref}} = 2, 4$

Challenge: ^{10}B



^{10}B
 $\Lambda_{3N} = 500 \text{ MeV}$
 $\alpha = 0.08 \text{ fm}^4$
 $\hbar\Omega = 16 \text{ MeV}$
— explicit 3N
○ MR-NO2B
 $N_{\max}^{\text{ref}} = 2, 4$

Reflections

Questions I

- How can we extend current ab-initio methods to describe open-shell and deformed nuclei?
 - IT-NCSM describes open and closed-shell nuclei on the same footing
 - MR-IM-SRG is a true open-shell approach for medium/heavy masses (\rightarrow H. Hergert), others are following
- How can we include the effects of three-nucleon forces in a computationally efficient manner?
 - explicit 3N interactions are used in IT-NCSM very efficiently
 - CCSD and Λ CCSD(T) is available with explicit 3N (\rightarrow S. Binder)
 - single- and multi-reference normal ordering provide robust approximations at reduced cost
 - this does not imply that any kind of ‘summation over the third particle’ is accurate

Questions II

- How can we describe the onset of pairing in nuclei within various ab-initio frameworks?
 - any ab initio approach for open shells has to describe pairing
- Can we develop reliable theoretical error estimates?
 - defining element of any ab initio approach
 - uncertainty quantification case by case within the many-body approach, not just guessing
 - uncertainty quantification also necessary for the chiral EFT inputs
- How can we bridge structure and reactions in a consistent fashion?
 - NCSM/RGM and NCSMC with 3N are on their way (\rightarrow P. Navratil)
- How can we generate reliable predictions for the drip-lines?
 - simply do all of the above...

Epilogue

■ thanks to my group & my collaborators

- **S. Binder, A. Calci**, B. Erler, E. Gebrerufael,
H. Krutsch, **J. Langhammer**, S. Reinhardt, S. Schulz,
C. Stumpf, A. Tichai, R. Trippel, R. Wirth
Institut für Kernphysik, TU Darmstadt

- **P. Navrátil**

TRIUMF Vancouver, Can

- J. Vary, P. Ma

Iowa State Univ

- S. Quaglioni, U

LLNL Livermore, USA

- P. Piecuch

Michigan State University, USA

- **H. Hergert**, K. Hebeler

Ohio State University, USA

- G. Tsakonstantinou

Univ Bayreuth, F

- J. Jorssén

Chalmers University, Sweden

- H. Feldmeier, T. Neff

GSI Helmholtzzentrum

LENPIC

Low-Energy Nuclear
Physics International
Collaboration



COMPUTING TIME



Deutsche
Forschungsgemeinschaft

DFG

HIC | FAIR
for
Helmholtz International Center

 LOEWE

Exzellente Forschung für
Hessens Zukunft

 HELMHOLTZ
| GEMEINSCHAFT



Bundesministerium
für Bildung
und Forschung