Ab Initio Nuclear Structure from Chiral NN+3N Hamiltonians

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From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

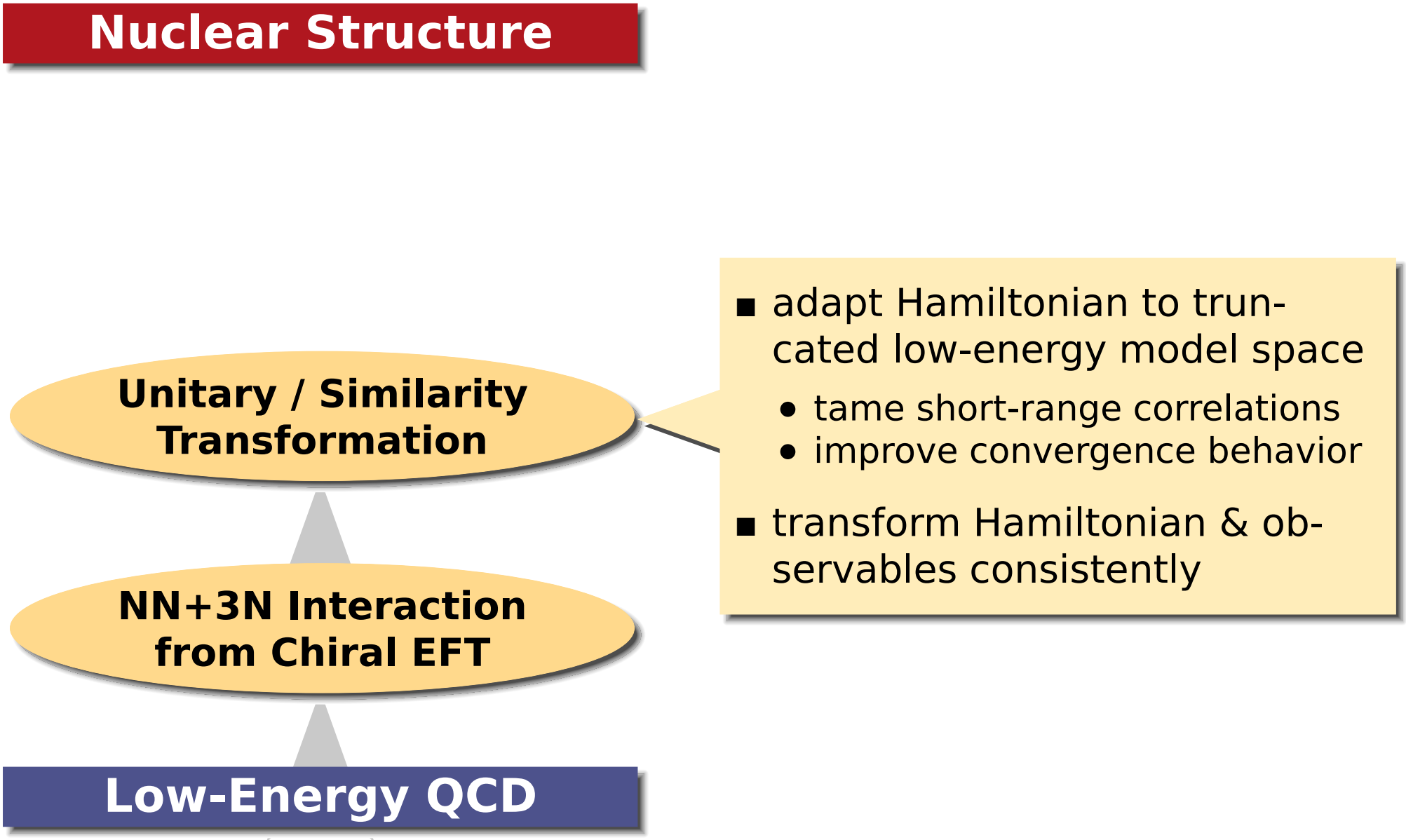
Nuclear Structure

NN+3N Interaction from Chiral EFT

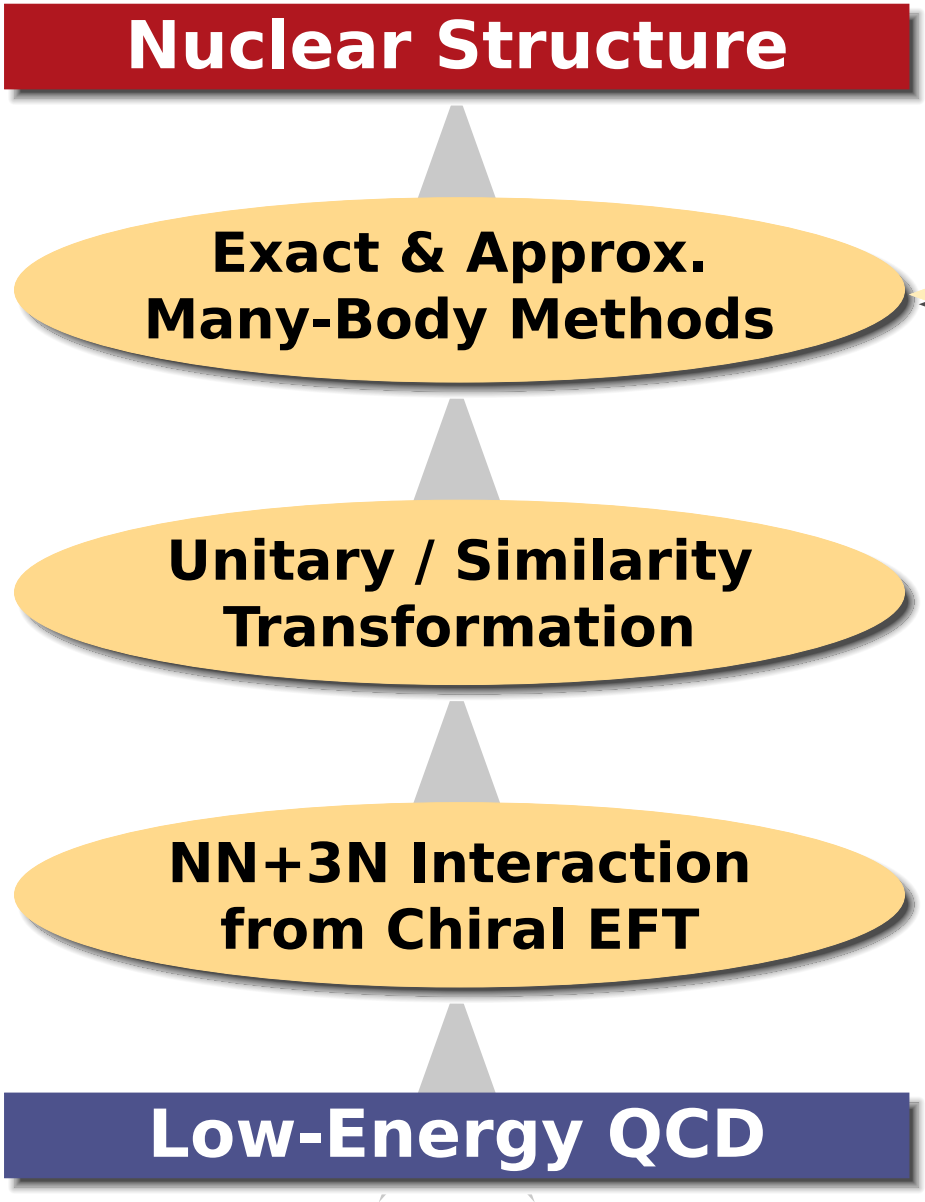
- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN, 3N,... interaction plus currents

Low-Energy QCD

From QCD to Nuclear Structure

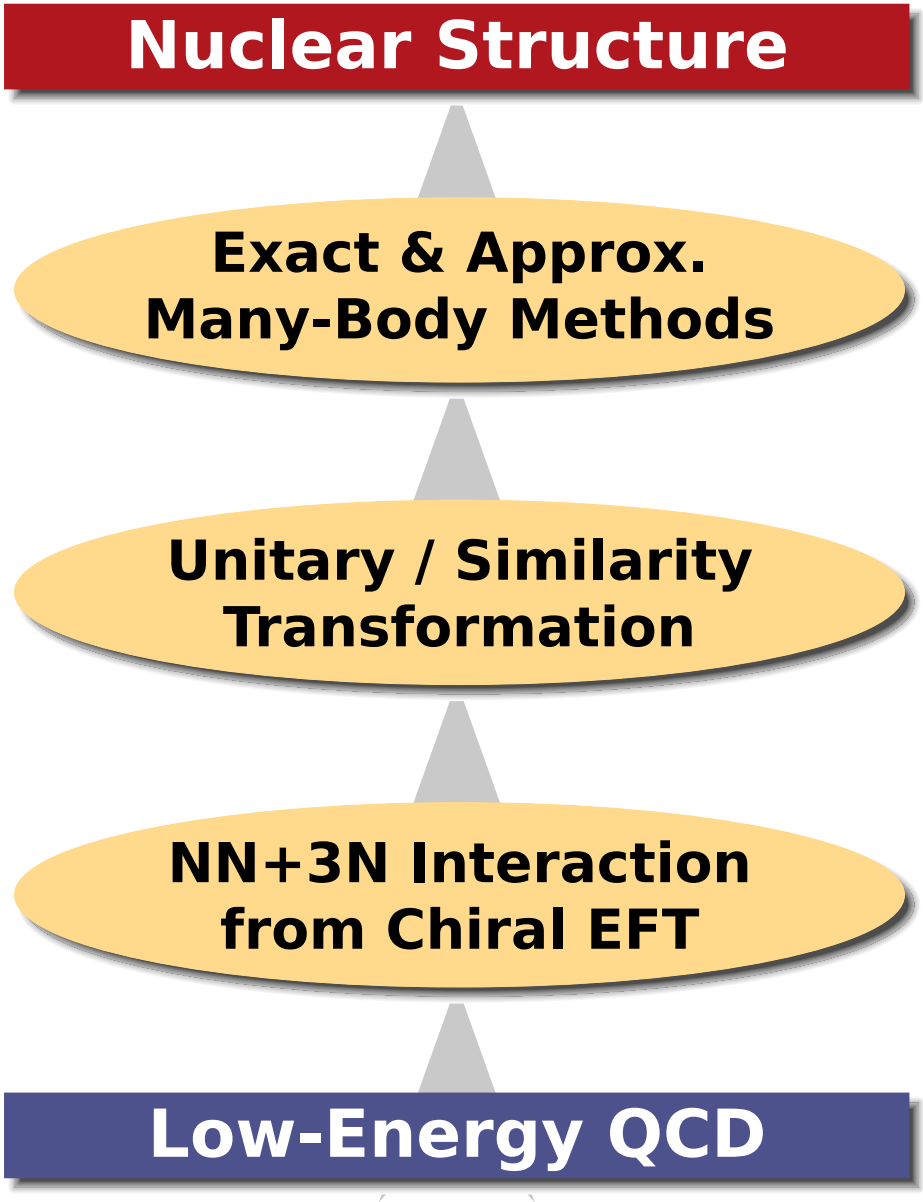


From QCD to Nuclear Structure



- accurate solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
- controlled approximations for heavier nuclei (MBPT,...)
- all rely on truncated model spaces & benefit from unitary transformation

From QCD to Nuclear Structure



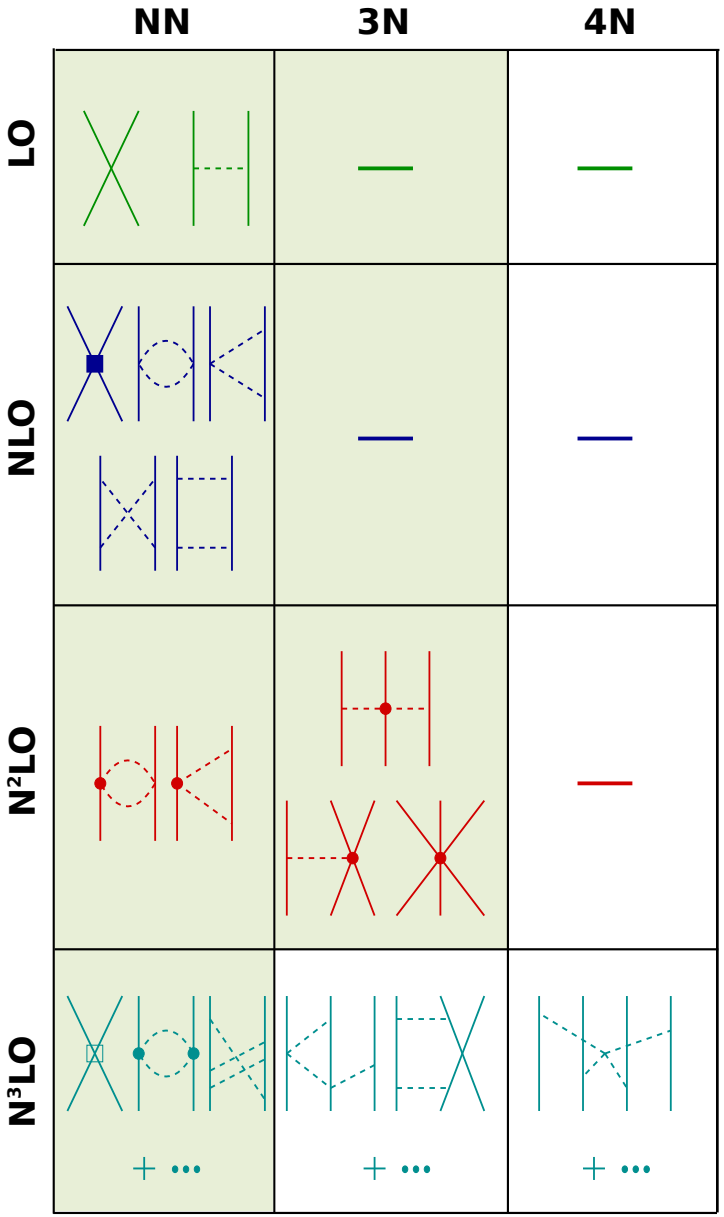
- How can we extend current ab-initio methods to describe open-shell and deformed nuclei?
- How can we include the effects of three-nucleon forces in a computationally efficient manner?
- How can we describe the onset of pairing in nuclei within various ab-initio frameworks?
- Benchmarking and accuracy: 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, πN,...)
- 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 $T_{1/2}(^3\mathrm{H})$ and $E(^3\mathrm{H}, ^3\mathrm{He})$
- **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 $E(^4\mathrm{He})$
- **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 Hami

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

simplicity and flexibility are great advantages of the SRG approach

- **evolution equations** for $\tilde{H}_\alpha$ and U

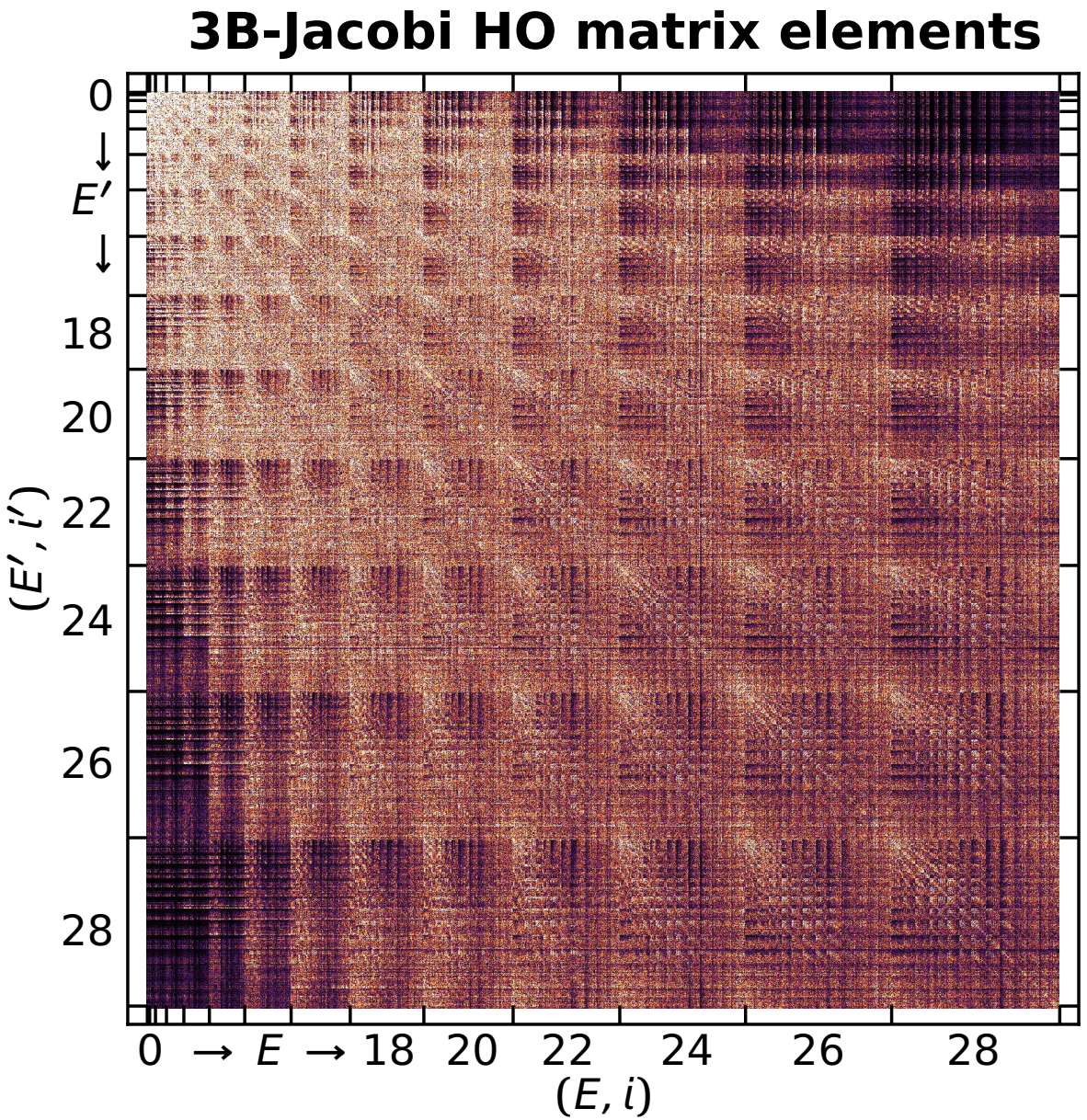
$$\frac{d}{d\alpha}\tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha]$$

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

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

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

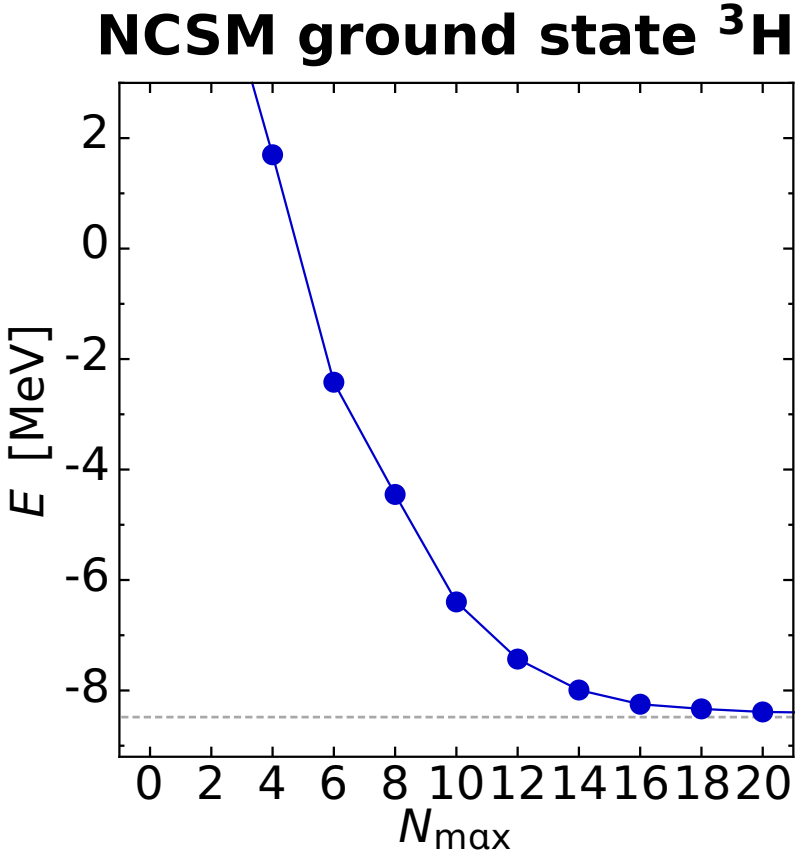
SRG Evolution in Three-Body Space



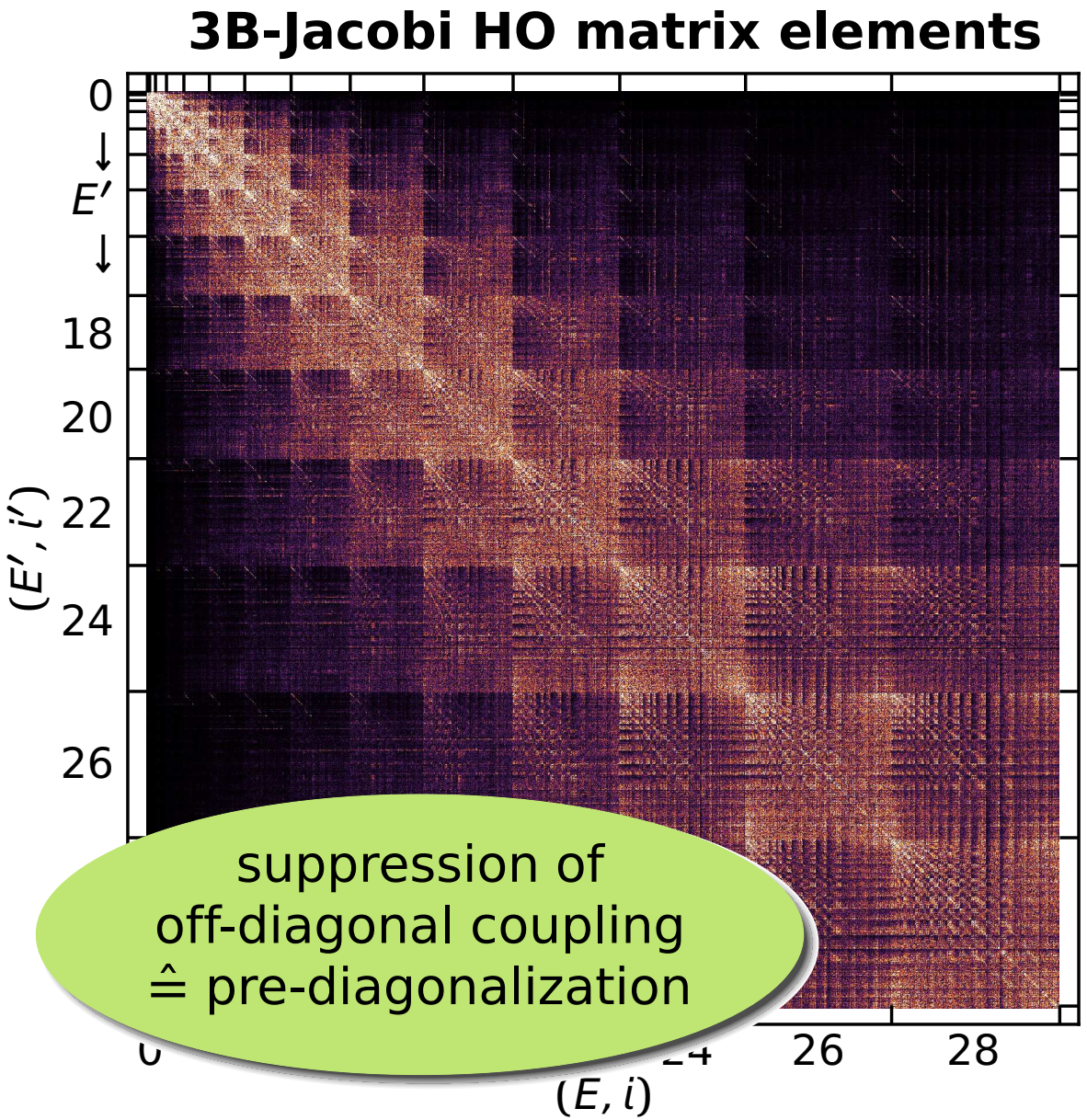
$$\alpha = 0.000\,\mathrm{fm}^4$$

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

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



SRG Evolution in Three-Body Space

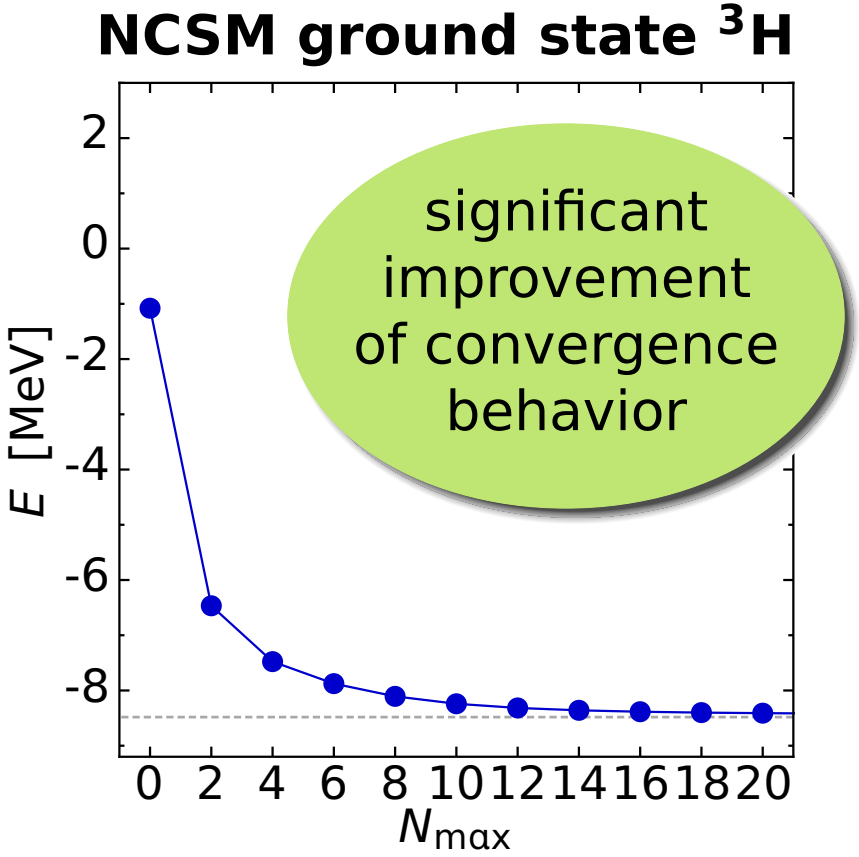


suppression of off-diagonal coupling ≙ pre-diagonalization

$\alpha = 0.320\,\mathrm{fm}^4$

$\Lambda = 1.33\,\mathrm{fm}^{-1}$

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



significant improvement of convergence behavior

Hamiltonian in *A*-Body Space

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

$$\widetilde{\mathrm{H}}_\alpha = \widetilde{\mathrm{H}}_\alpha^{[1]} + \widetilde{\mathrm{H}}_\alpha^{[2]} + \widetilde{\mathrm{H}}_\alpha^{[3]} + \widetilde{\mathrm{H}}_\alpha^{[4]} + \ldots$$

- 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 Ham[illegible] keep two- and induced three-body terms
- **NN+3N-full**: start with NN+3[illegible] 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 $E_{3\,\mathrm{max}} = 16$ 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 $E_{3\,\mathrm{max}} = 16$ 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 N_{max}
- full N_{max} for ^{16}O v (basis dim

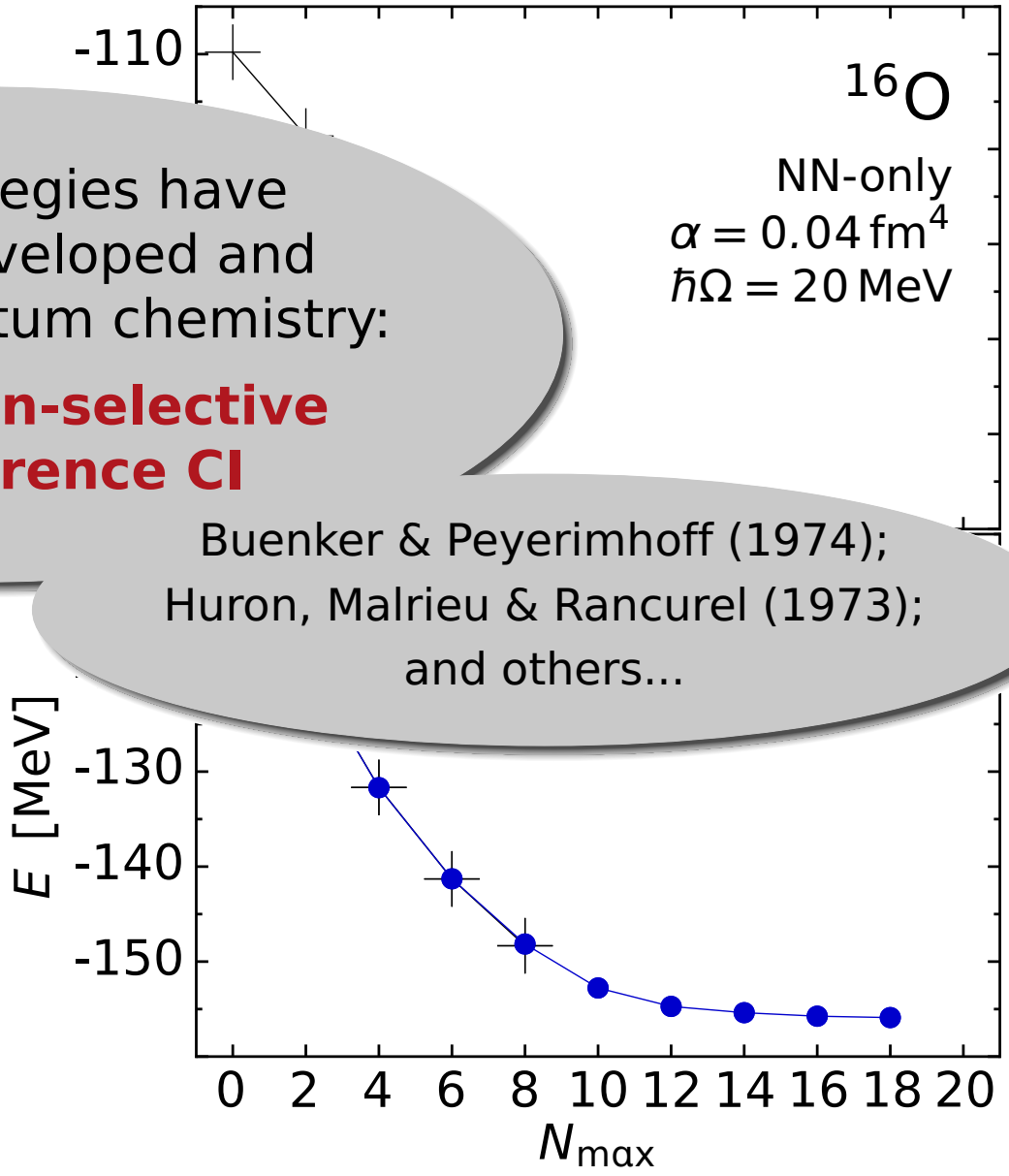
similar strategies have first been developed and applied in quantum chemistry:

configuration-selective multireference CI

Buenker & Peyerimhoff (1974); Huron, Malrieu & Rancurel (1973); and others...

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 $\mathcal{M}_{\text{ref}}$

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

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

$$\frac{\langle \Phi_{\nu}| H |\Psi_{\text{ref},m}\rangle}{\epsilon_{\nu}}$$

- co… …from all basis states

- **solve eigenvalue problem** in … $\mathcal{M}_{\text{IT}}(\kappa_{\text{min}})$ and obtain improved approximation of target state

importance measure only probes 2p2h excitations on top of $\mathcal{M}_{\text{ref}}$ 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 $|\Psi_{\text{ref},m}\rangle$

  - ❶ 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 $\mathcal{M}_{\text{IT}}$

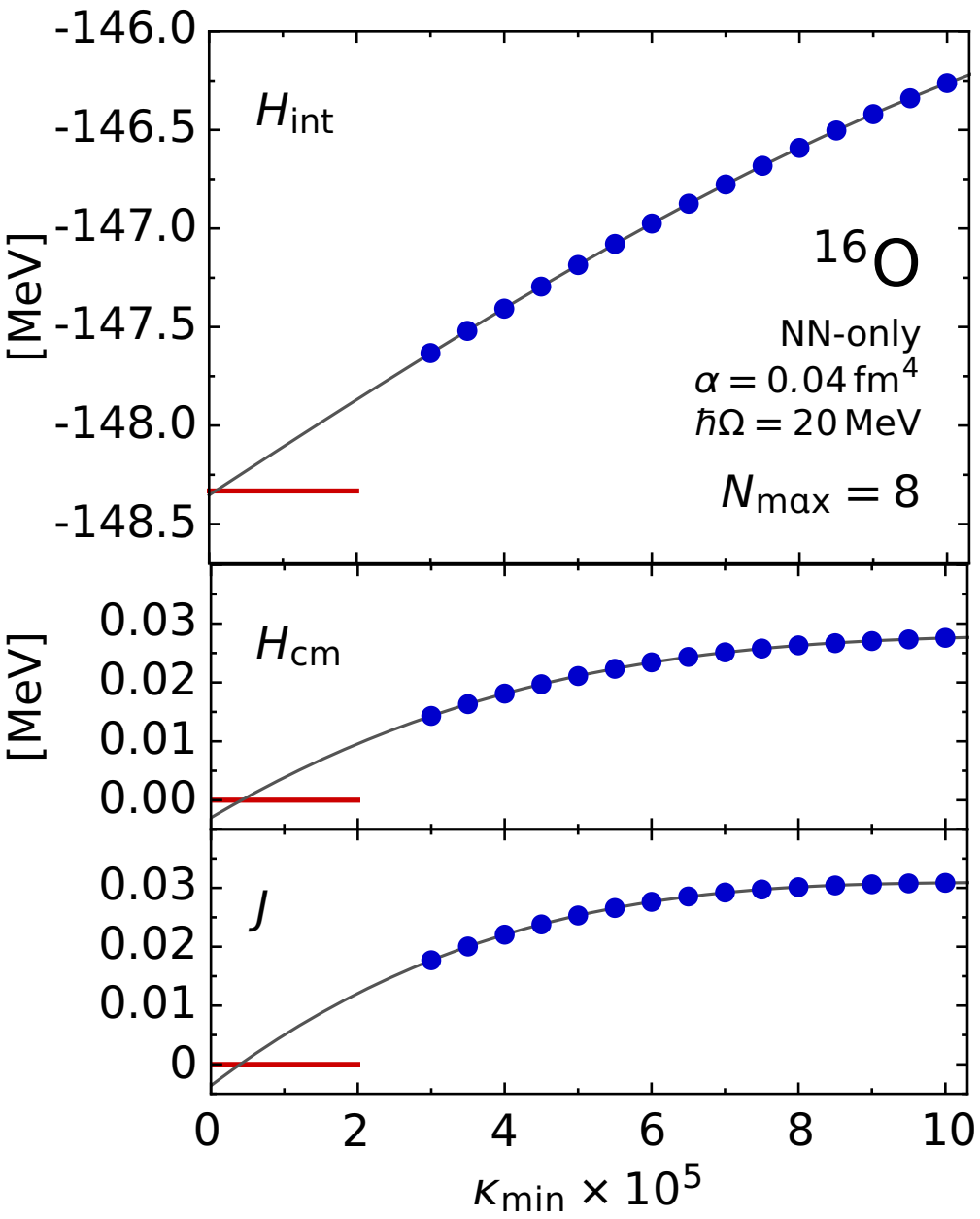
  - ❷ solve eigenvalue problem in $\mathcal{M}_{\text{IT}}$

  - ❸ use components of eigensta

  - ❹ goto ❶

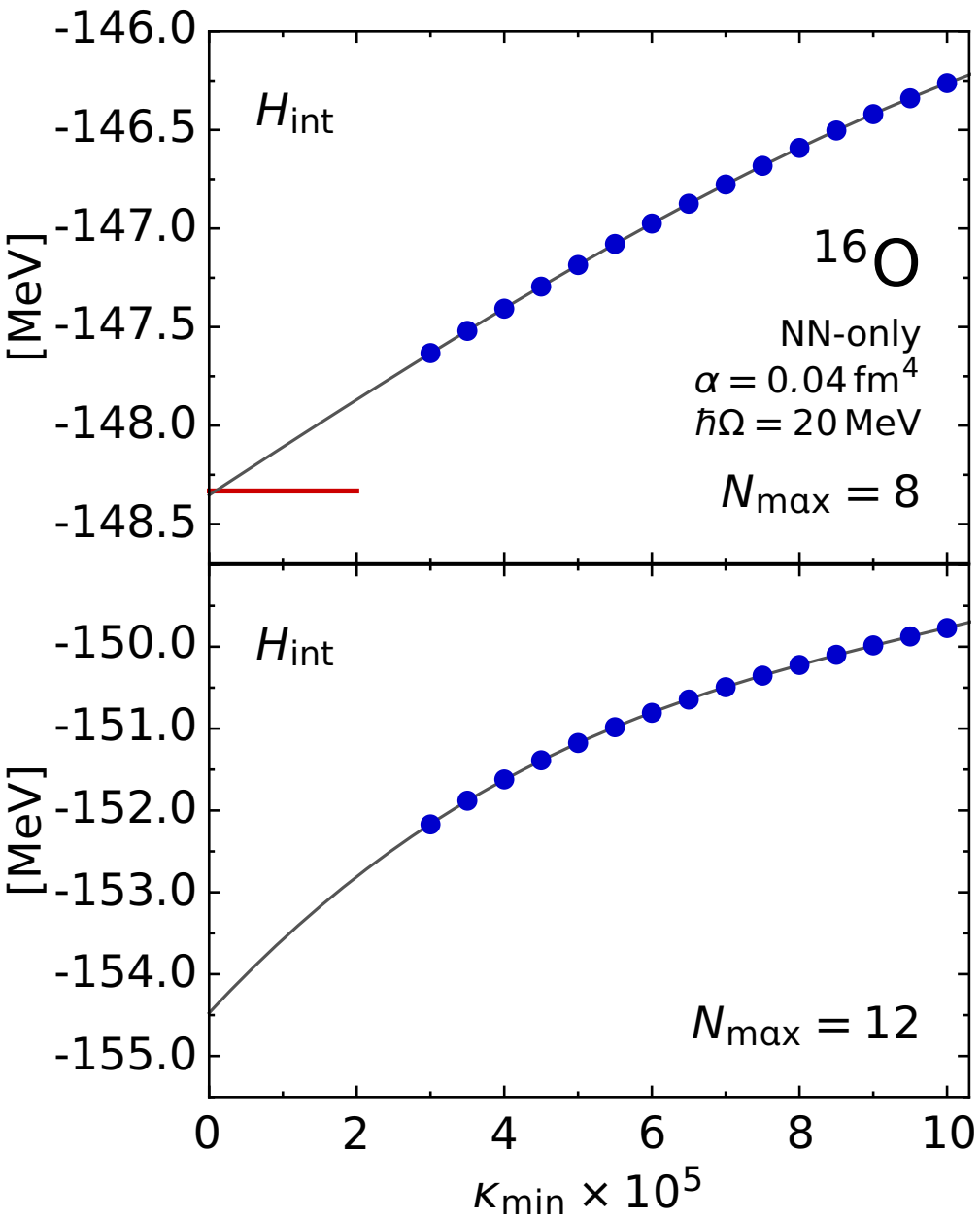
full NCSM space is recovered in the limit $(\kappa_{\min}, C_{\min}) \to 0$

Threshold Extrapolation



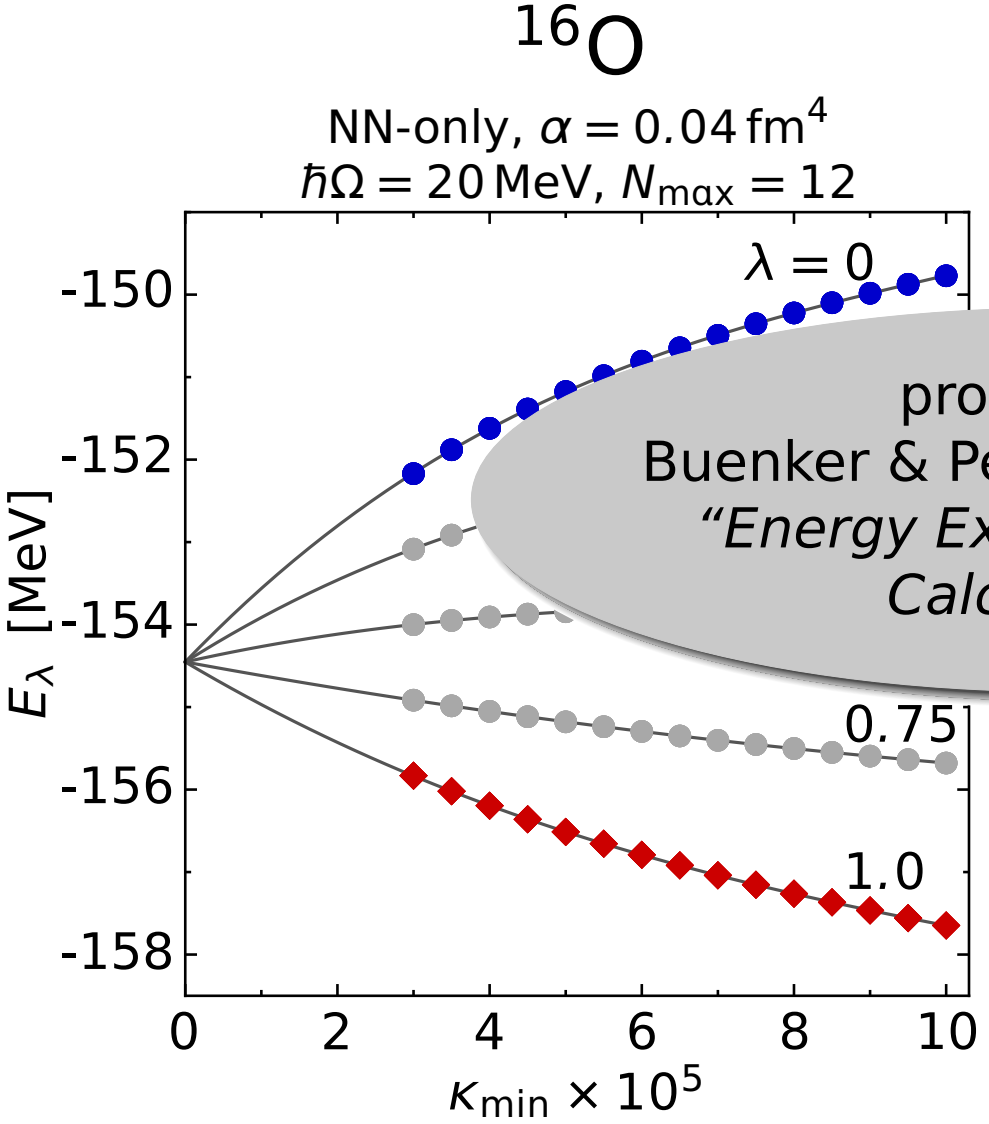
- repeat calculations for a **sequence of importance thresholds** κ_{min}
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $\kappa_{min} \rightarrow 0$ of observables to account for effect of excluded configurations

Threshold Extrapolation



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

Constrained Threshold Extrapolation



proposed by
Buenker & Peyerimhoff (1975):
"Energy Extrapolation in CI Calculations"

- for free: importance selection gives perturbative energy correction $\Delta_{\mathrm{excl}}(\kappa_{\min})$ accounting for **excluded states**

$\kappa_{\min} \to 0$

…ameter λ defining a family of energy sequences

$$E_\lambda(\kappa_{\min}) = E(\kappa_{\min}) + \lambda \Delta_{\mathrm{excl}}(\kappa_{\min})$$

- **simultaneous extrapolation** for family of λ-values with constraint $E_\lambda(0) = E_{\mathrm{extrap}}$

Uncertainty Quantification in the IT-NCSM

Uncertainty Quantification

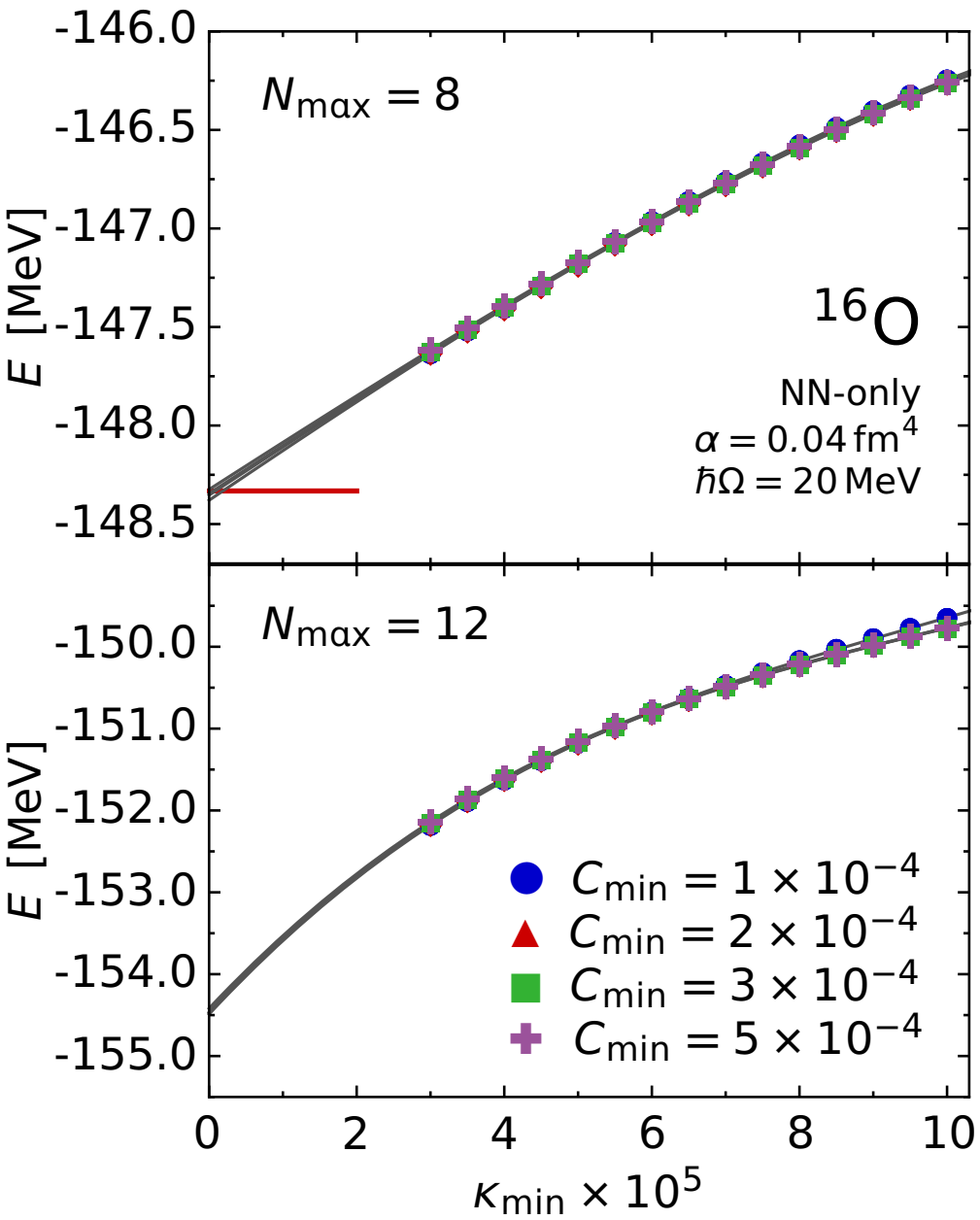
Importance Truncation

- use sequence of $(C_{\min}, \kappa_{\min})$-truncated model spaces
- extrapolate to $\kappa_{\min} \to 0$ using poynomial 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 $N_{\max} \to \infty$ using exponential ansatz or more elaborate extrapolation schemes
- uncertainty estimate derived from extrapolation protocol
- same **extrapolation uncertainties** as in full NCSM

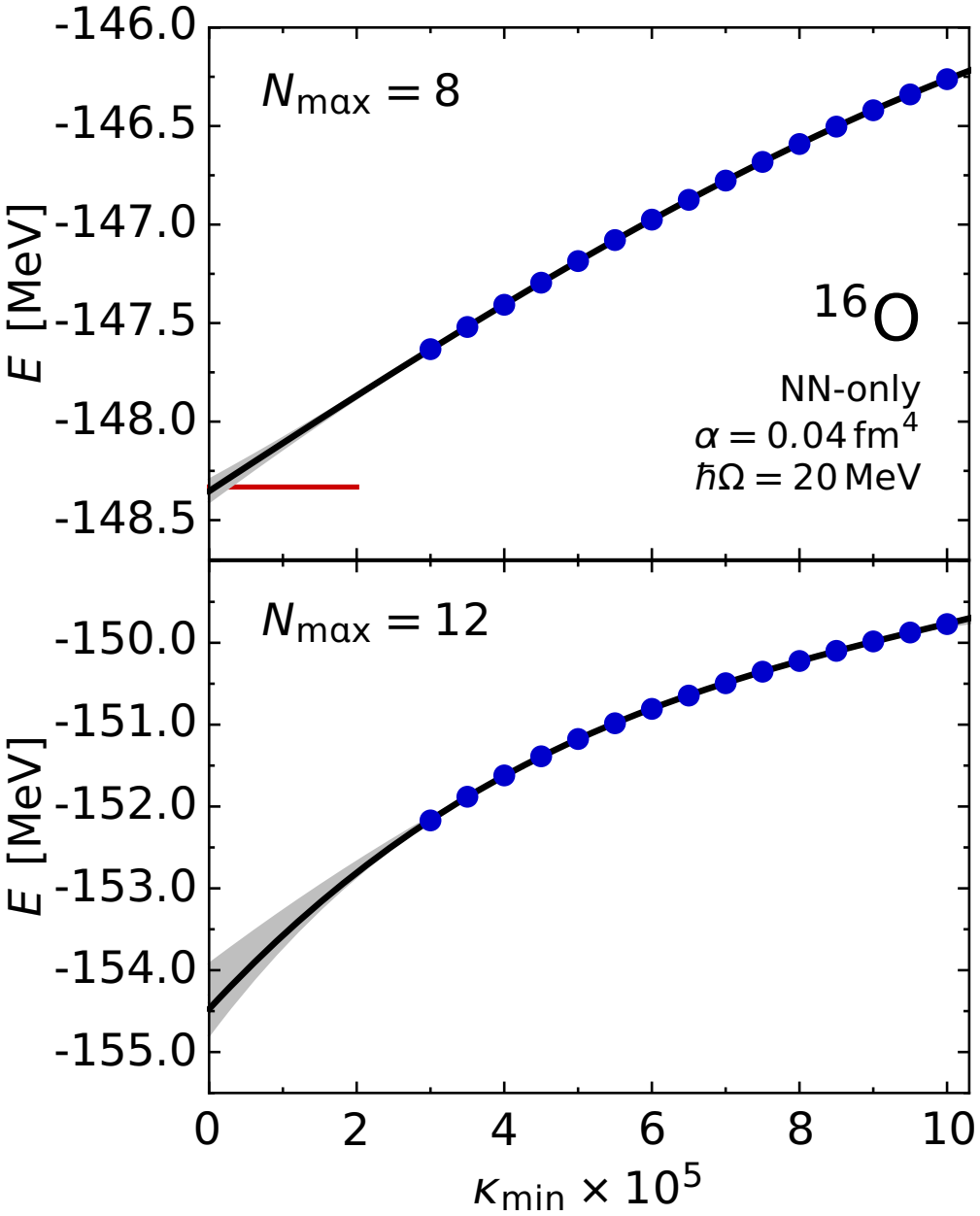
Comment on C_{min} Truncation



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

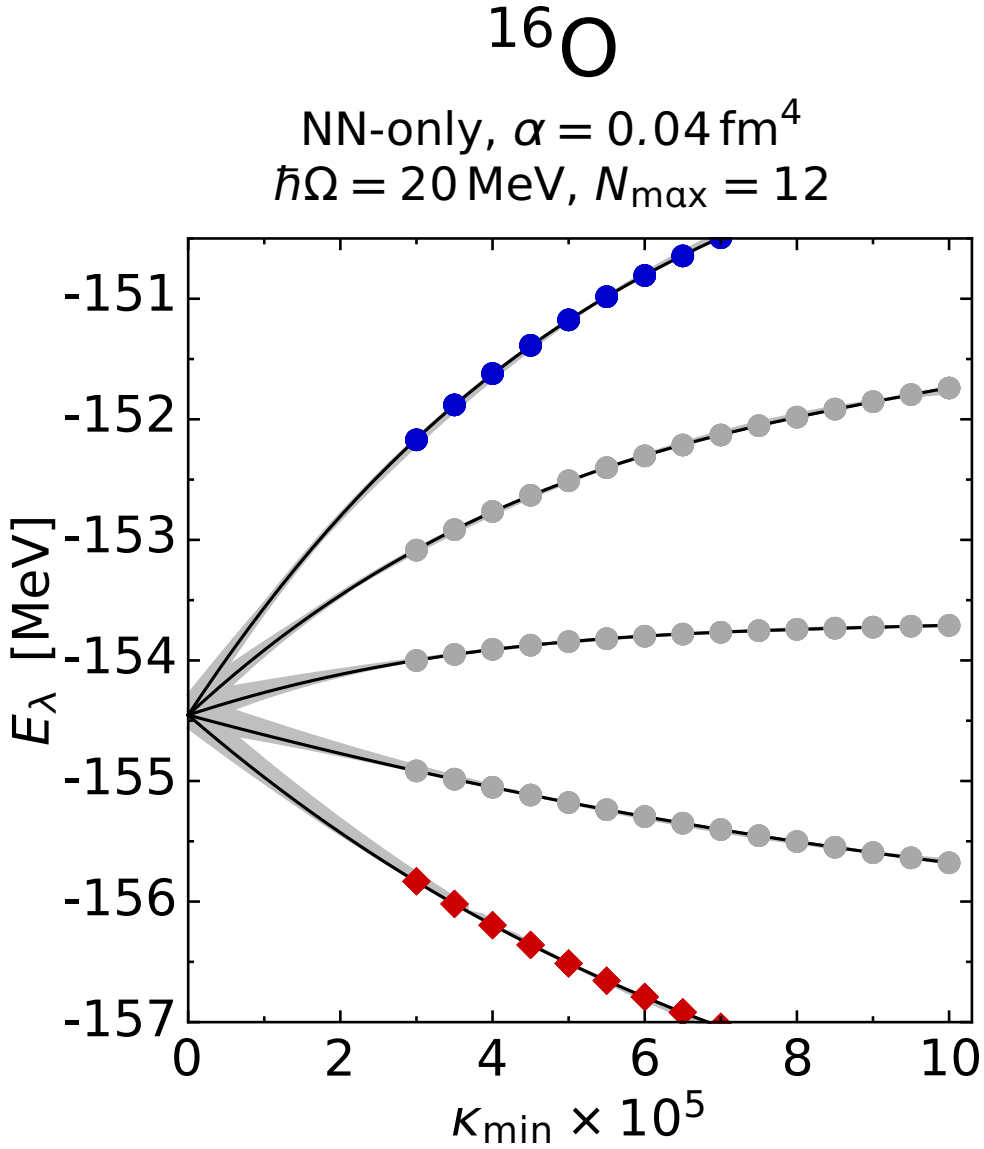
practically no influence on threshold extrapolated energies

Protocol: Simple $\kappa_{\min}$ Extrapolation



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

Protocol: Constrained $\kappa_{\min}$ Extrapolation



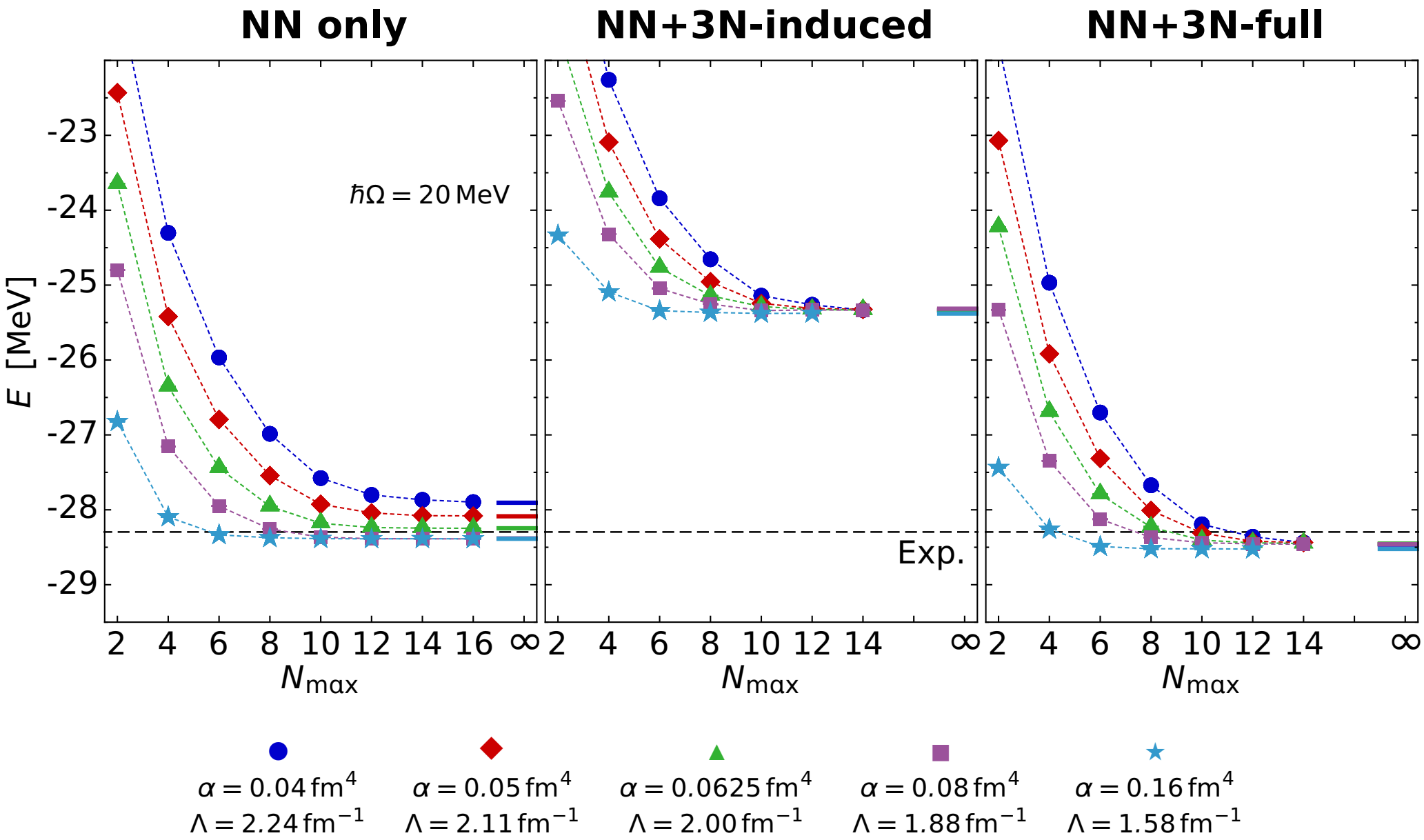
- select a few λ-values to get symmetrical approach towards common $E_{\mathrm{extrap}} = E_\lambda(\kappa_{\min} = 0)$
- constrained simultaneous extrapolation $\kappa_{\min} \to 0$ using polynomial $P_p(\kappa_{\min})$, typically of order $p = 3$
- generate uncertainty band from set of constrained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

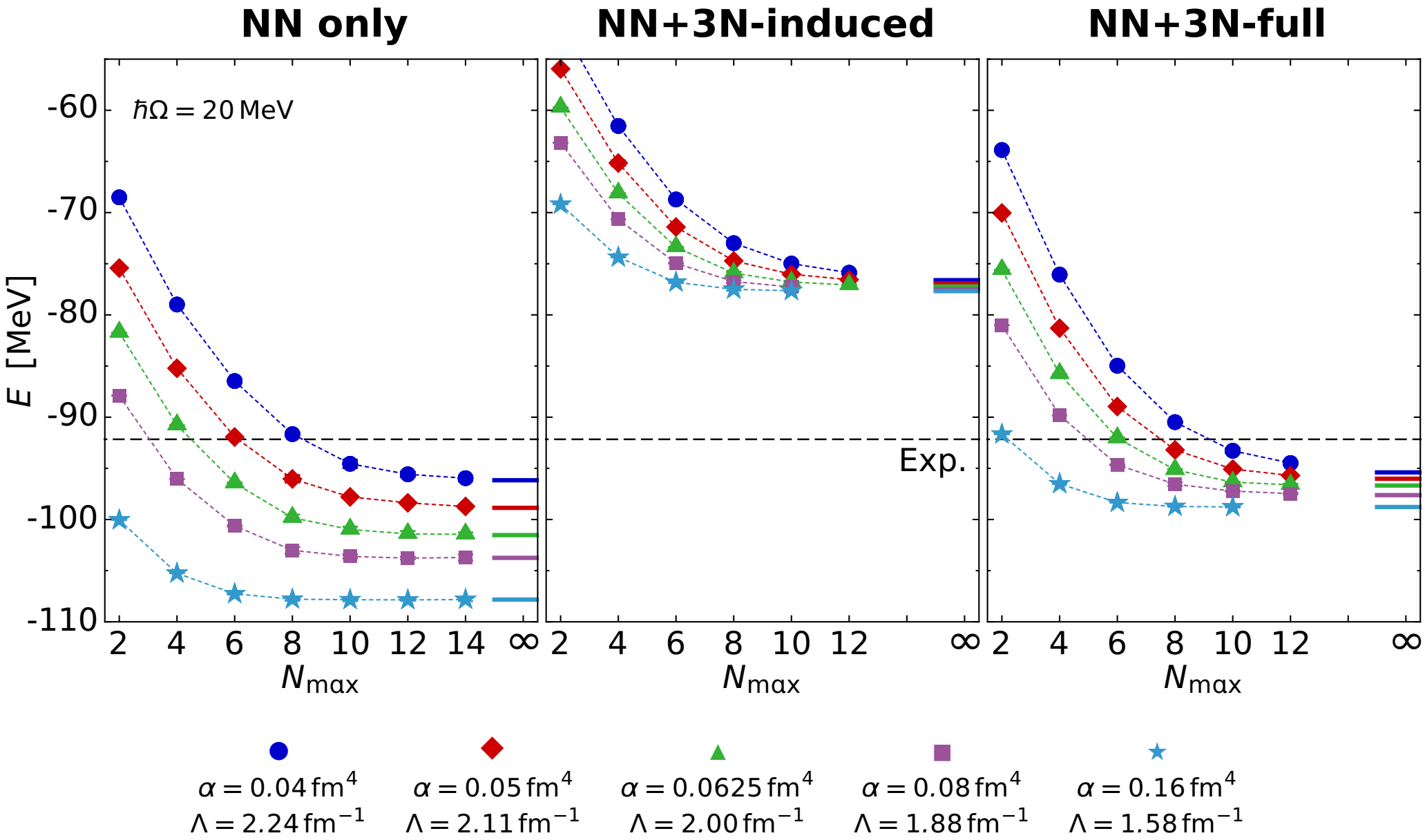
^{4}He: Ground-State Energies

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



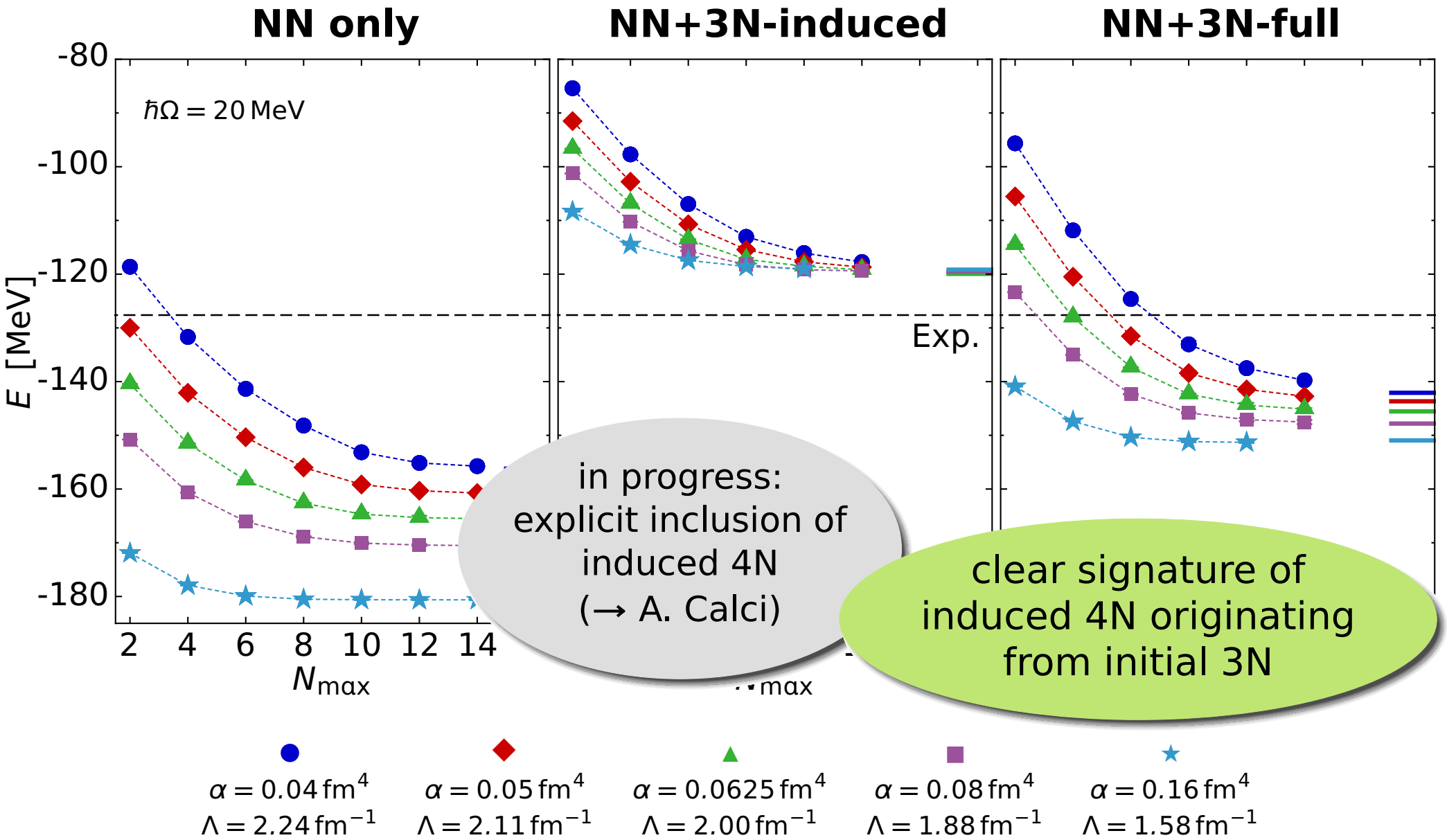
^{12}C: Ground-State Energies

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

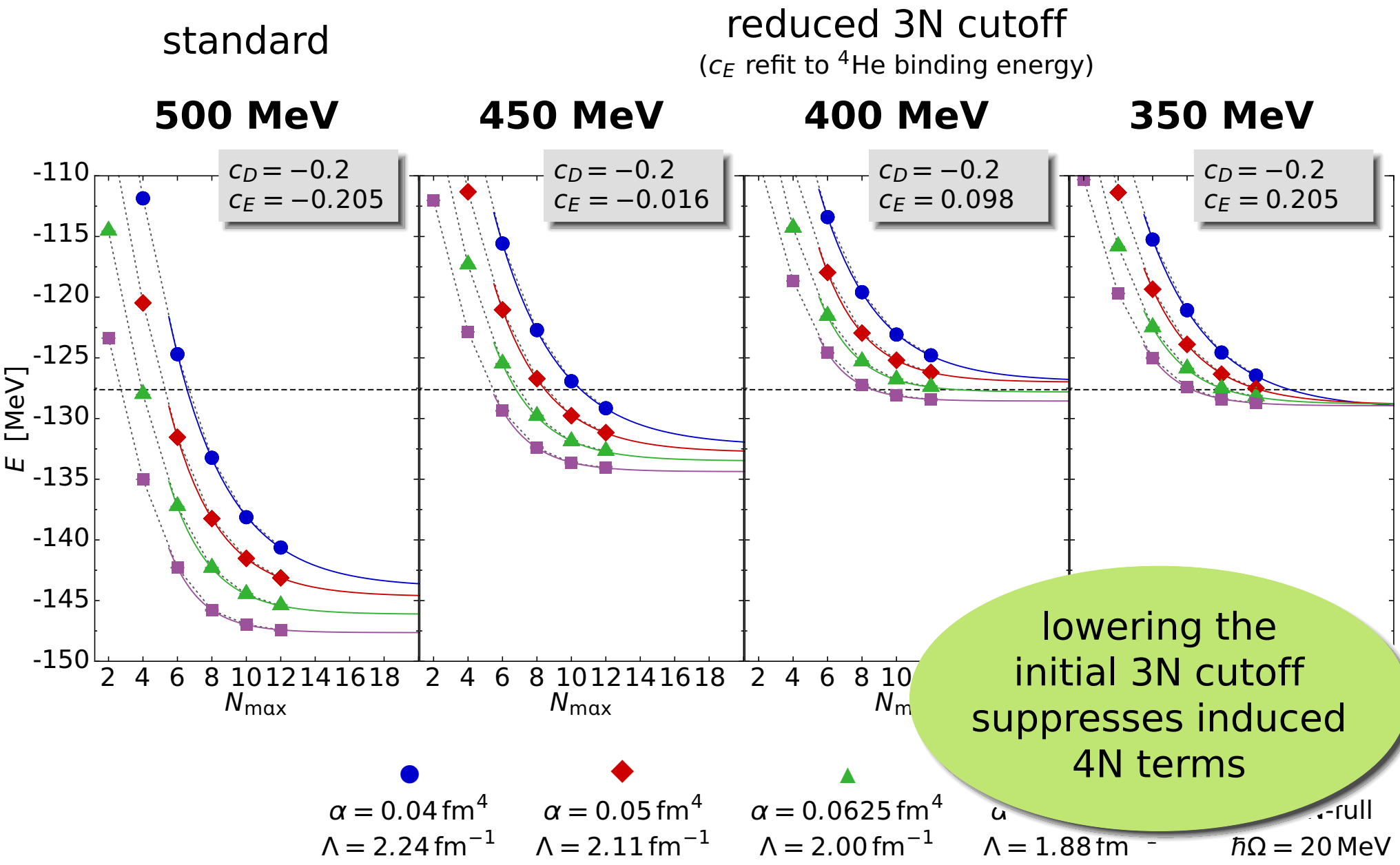


^{16}O: Ground-State Energies

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

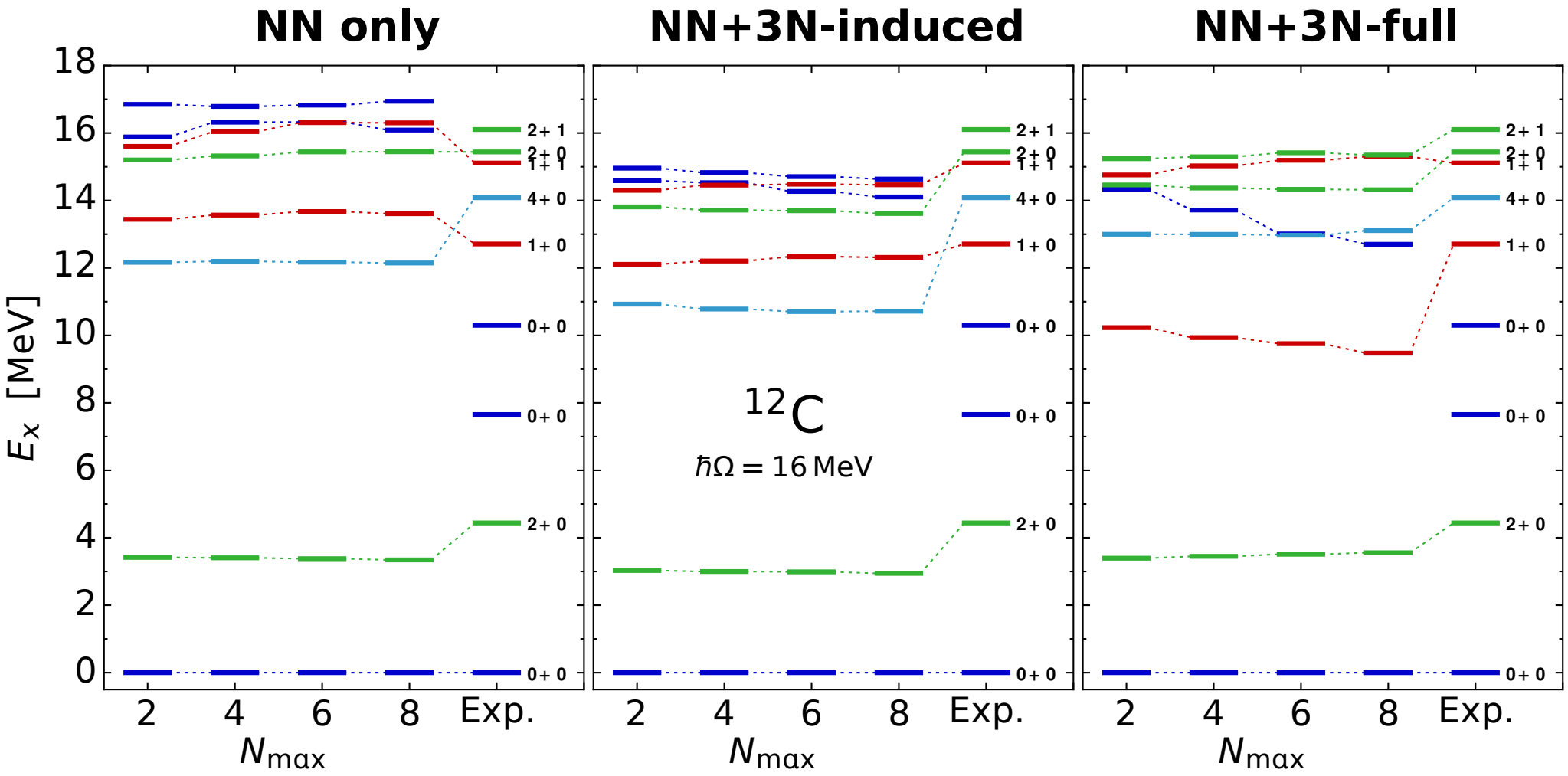


^{16}O: Lowering the Initial 3N Cutoff



Spectroscopy of ^{12}C

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



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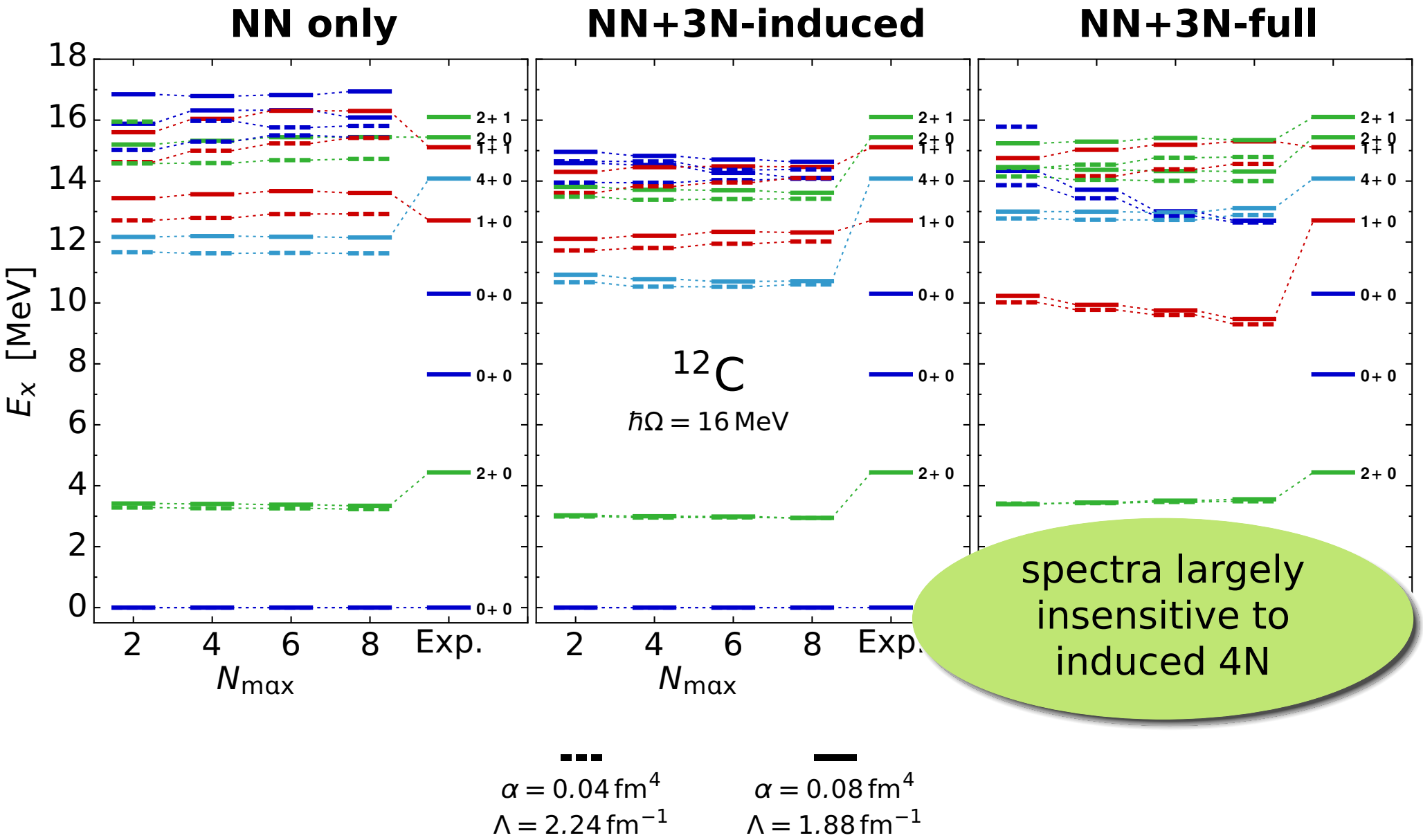
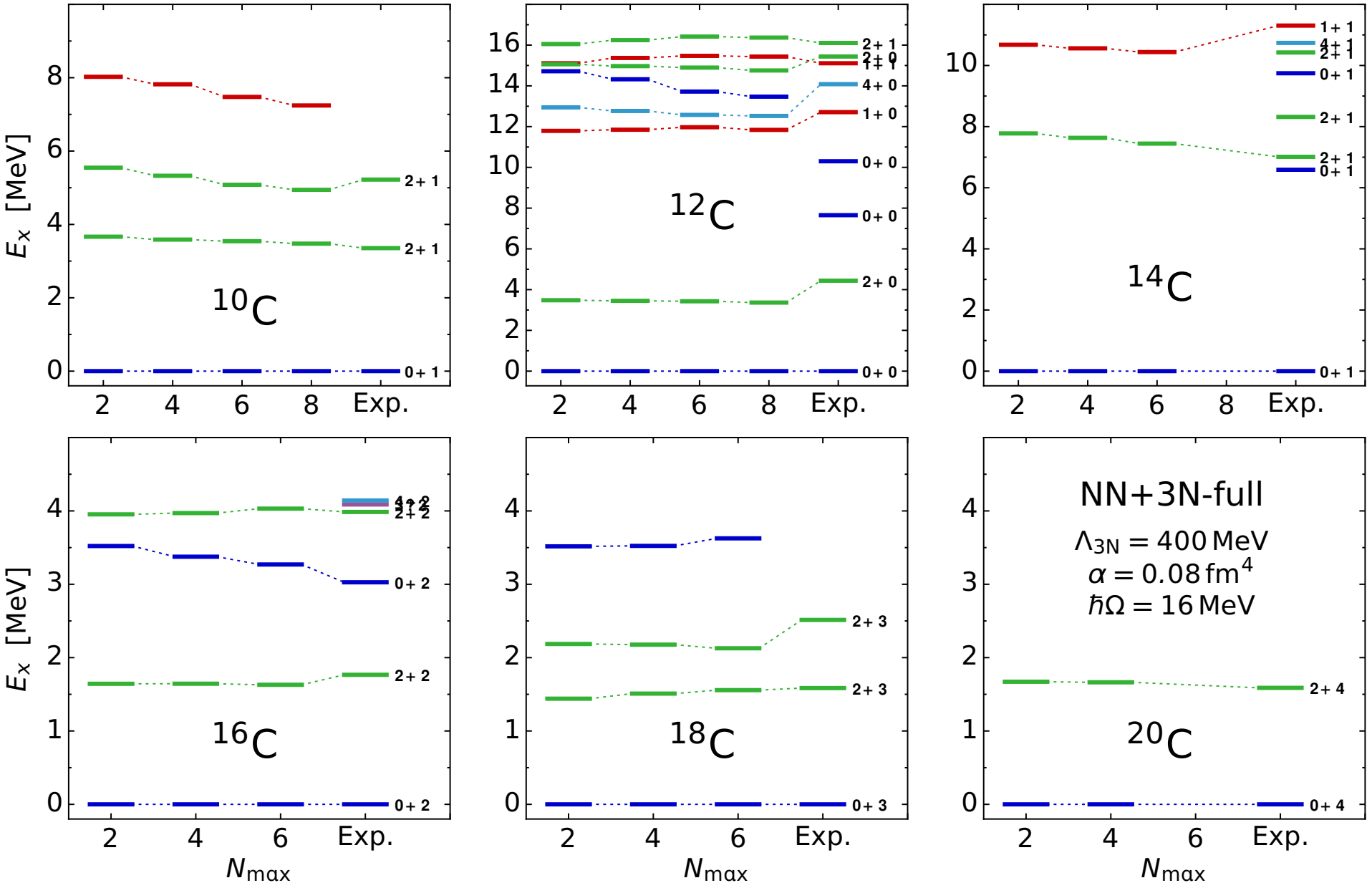


Ab Initio IT-NCSM Calculations for p- and sd-Shell Nuclei

Spectroscopy of Carbon Isotopes



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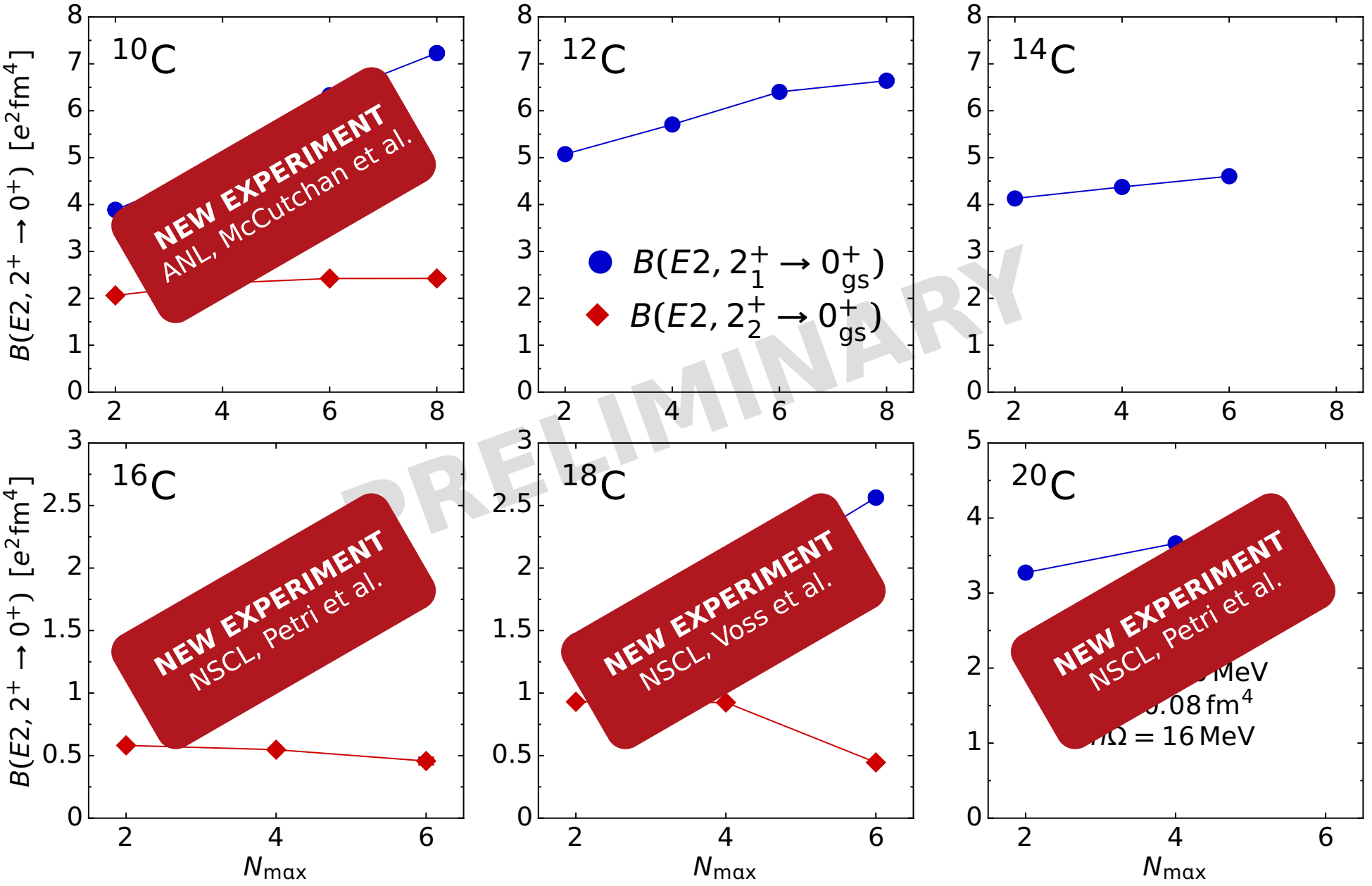
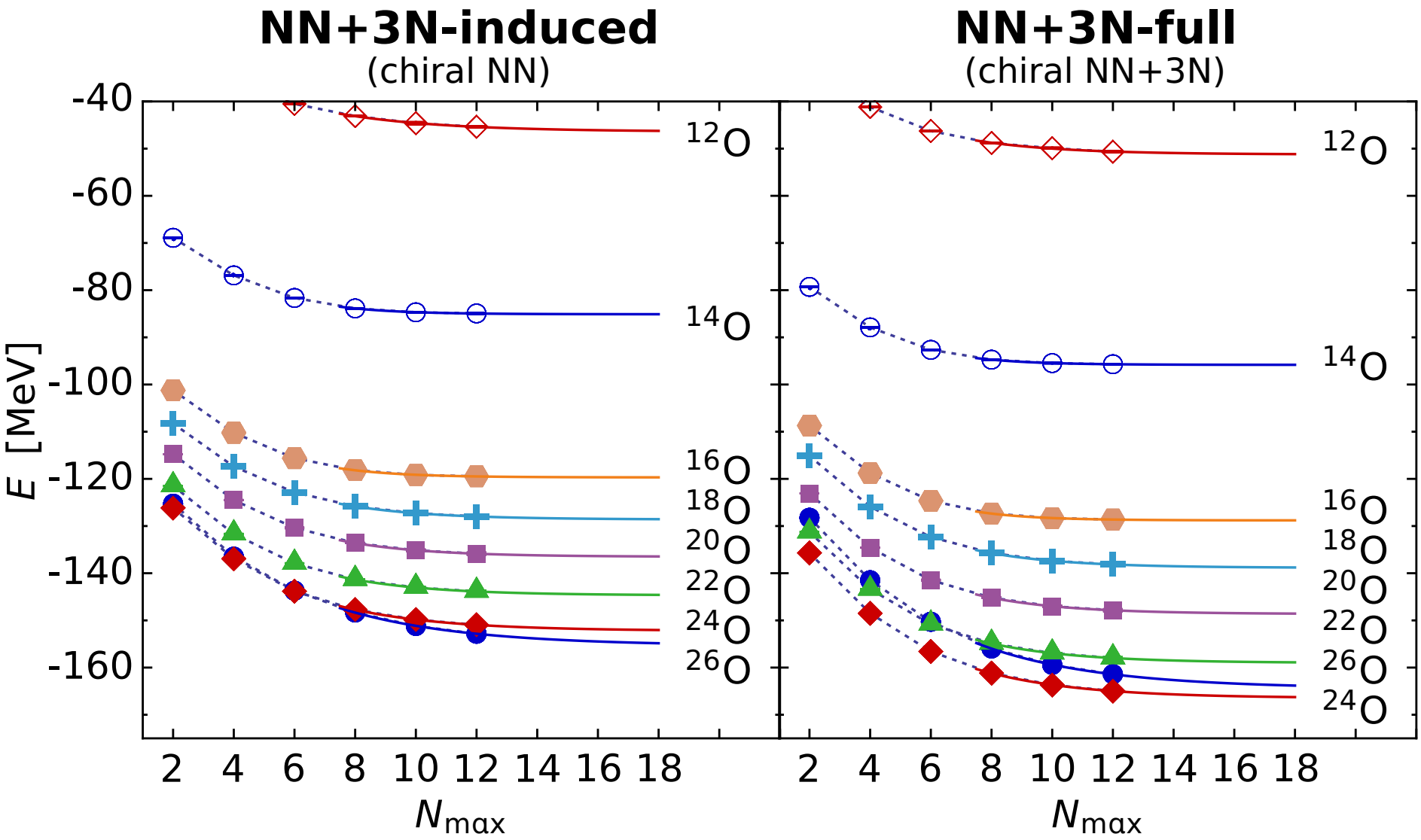


Ground States of Oxygen Isotopes

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



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

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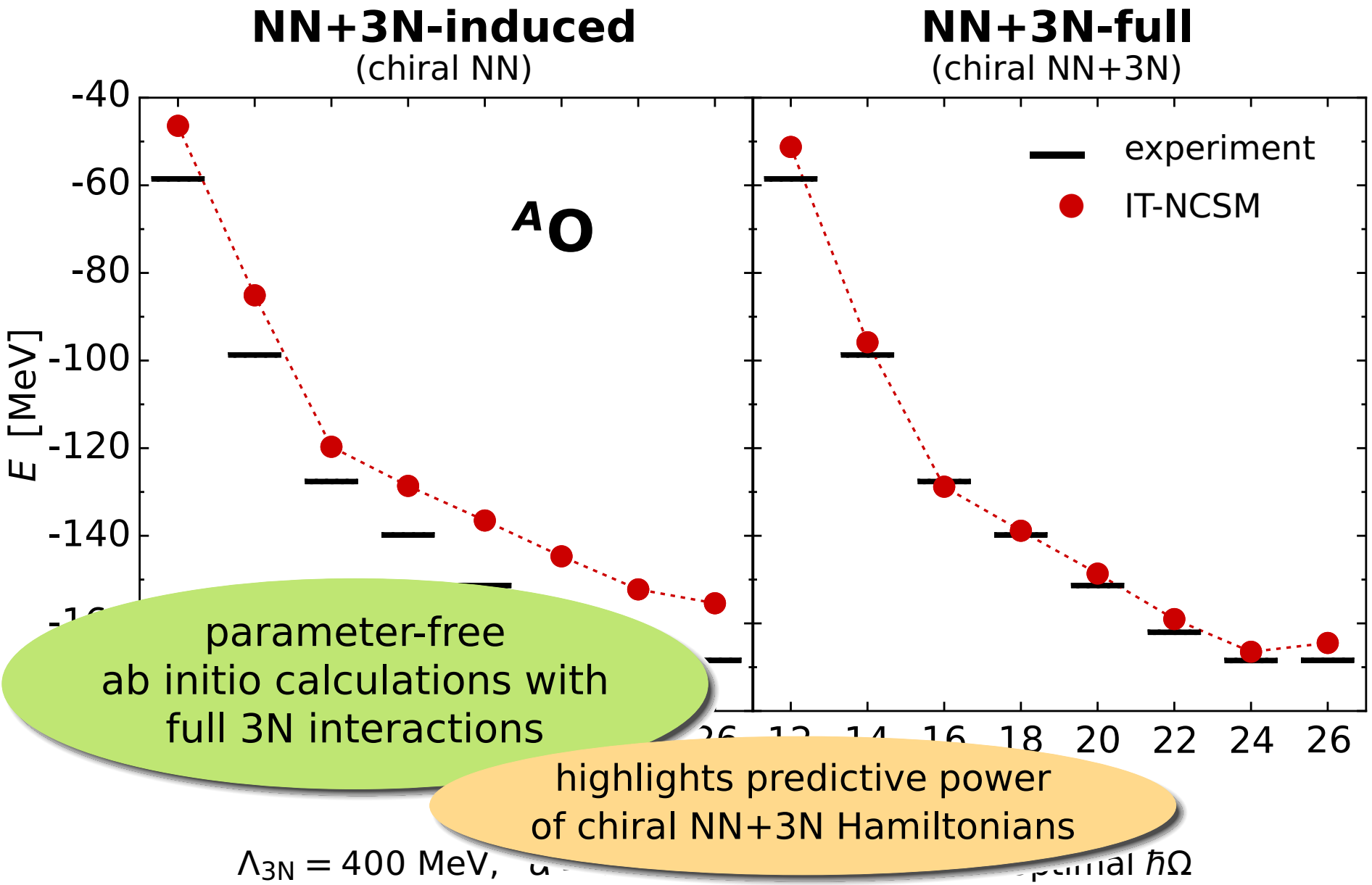


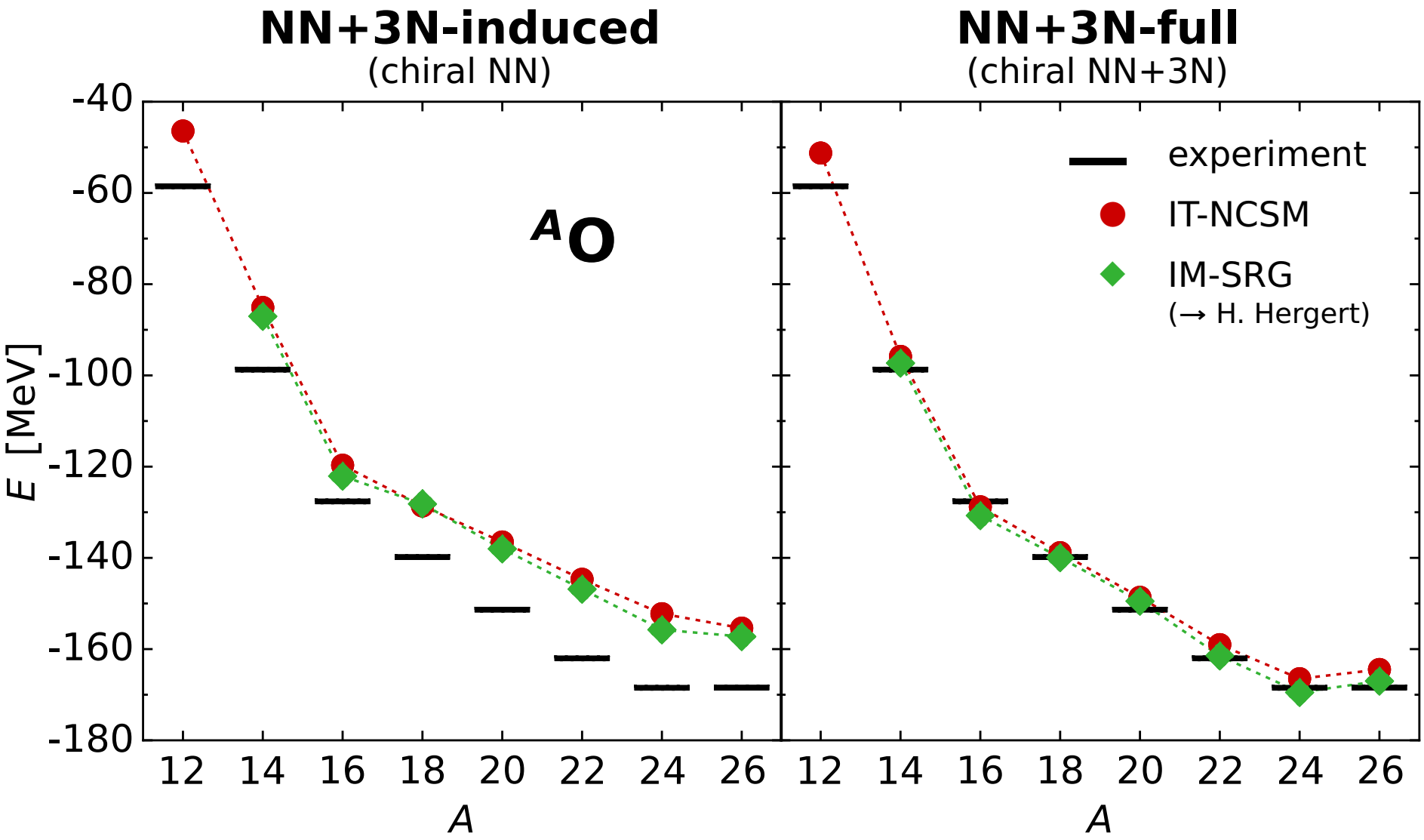
parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

$\Lambda_{3N} = 400$ MeV, [illegible] optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

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



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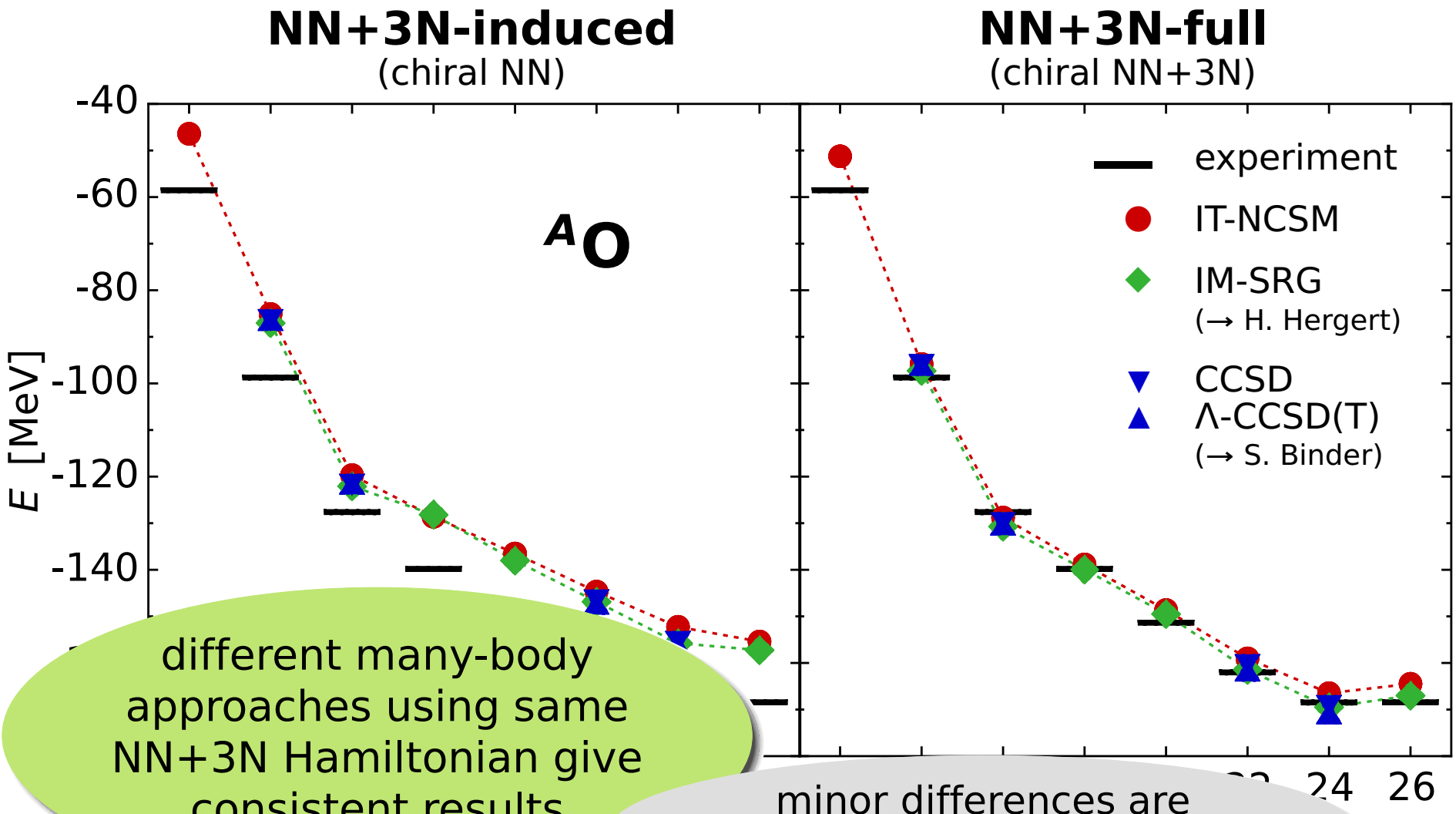


different many-body approaches using same NN+3N Hamiltonian give consistent results

minor differences are understood (NO2B, $E_{3\,max}$,...)

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^{-1}$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

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 (→ 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 $|0\rangle$

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

$$V^{abc}_{\bar{a}\bar{b}\bar{c}} = \langle abc | V_{3N} | \bar{a}\bar{b}\bar{c} \rangle \qquad A^{abc}_{\bar{a}\bar{b}\bar{c}} = a^\dagger_a a^\dagger_b a^\dagger_c \, a_{\bar{c}} a_{\bar{b}} a_{\bar{a}}$$

- **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 $|\Phi_{\mathrm{MR}}\rangle$

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

  where $\widetilde{A}^{\circ\circ\circ}_{\circ\circ\circ}$ 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 $|\Phi_{\mathrm{MR}}\rangle$

$$W = \frac{1}{36} \sum_{abc,\bar{a}\bar{b}\bar{c}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \, \rho^{abc}_{\bar{a}\bar{b}\bar{c}} \qquad W^{c}_{\bar{c}} = \frac{1}{4} \sum_{ab,\bar{a}\bar{b}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \, \rho^{ab}_{\bar{a}\bar{b}}$$

$$W^{bc}_{\bar{b}\bar{c}} = \sum_{a,\bar{a}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \, \rho^{a}_{\bar{a}} \qquad W^{abc}_{\bar{a}\bar{b}\bar{c}} = V^{abc}_{\bar{a}\bar{b}\bar{c}}$$

Multi-Reference Normal Ordering

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

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

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

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

with new matrix elements

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

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

Single-Reference Normal Ordering

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

$$\rho^{a}_{\bar{a}} = n_a \delta^{a}_{\bar{a}}$$
$$\rho^{ab}_{\bar{a}\bar{b}} = \rho^{a}_{\bar{a}}\,\rho^{b}_{\bar{b}} - \rho^{b}_{\bar{a}}\,\rho^{a}_{\bar{b}}$$
$$\rho^{abc}_{\bar{a}\bar{b}\bar{c}} = \ldots$$

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

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

with simplified matrix elements

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

IT-NCSM with MR-NO2B Approximation

❶ perform NCSM with explicit 3N interaction for small $N_{\max}$

- ground state defines the reference state $|\Phi_{\mathrm{MR}}\rangle$
- no explicit information on excited states enters

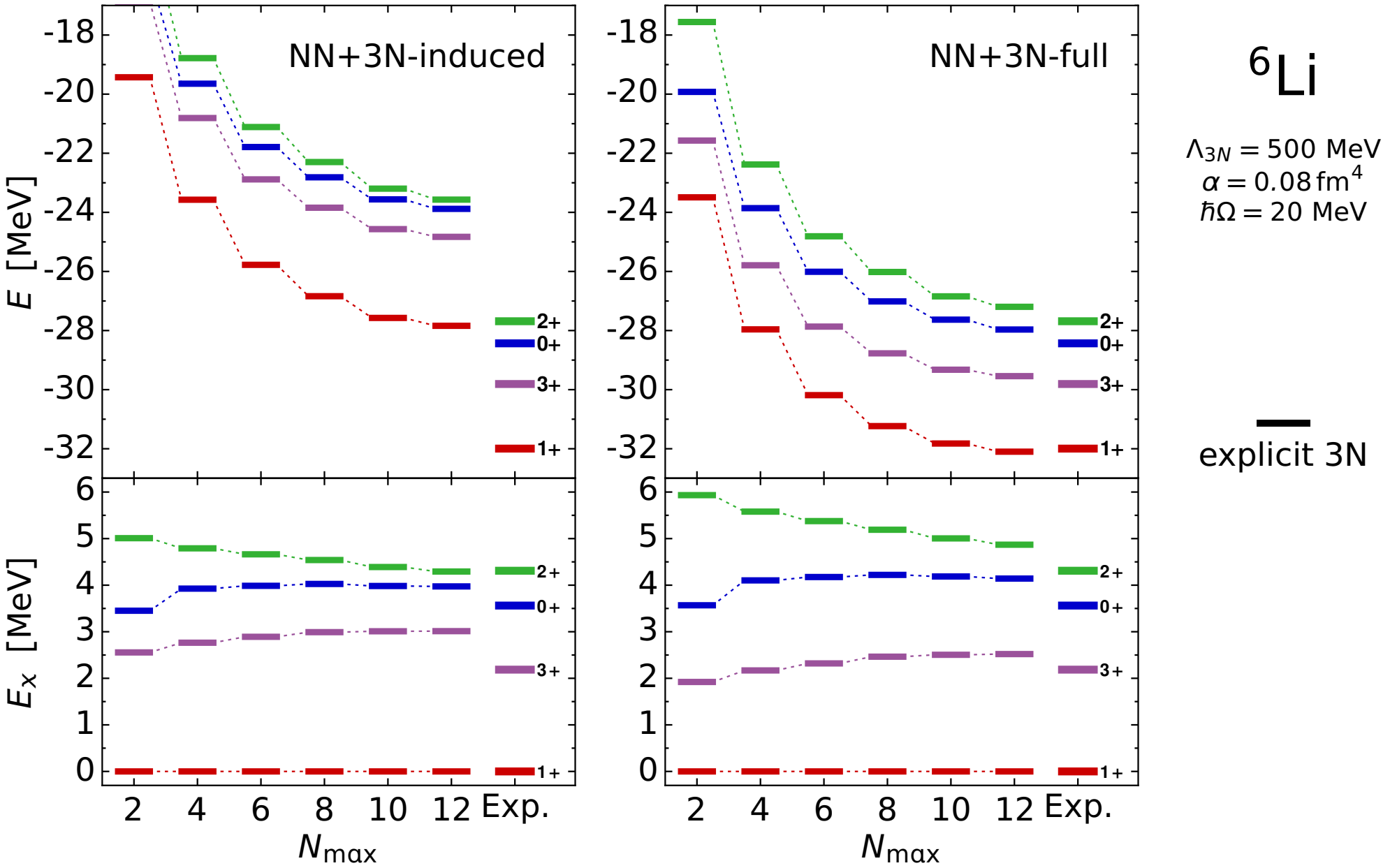
❷ compute zero-, one- and two-body matrix elements of MR-NO2B approximation

- density matrices for $|\Phi_{\mathrm{MR}}\rangle$ 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}Li

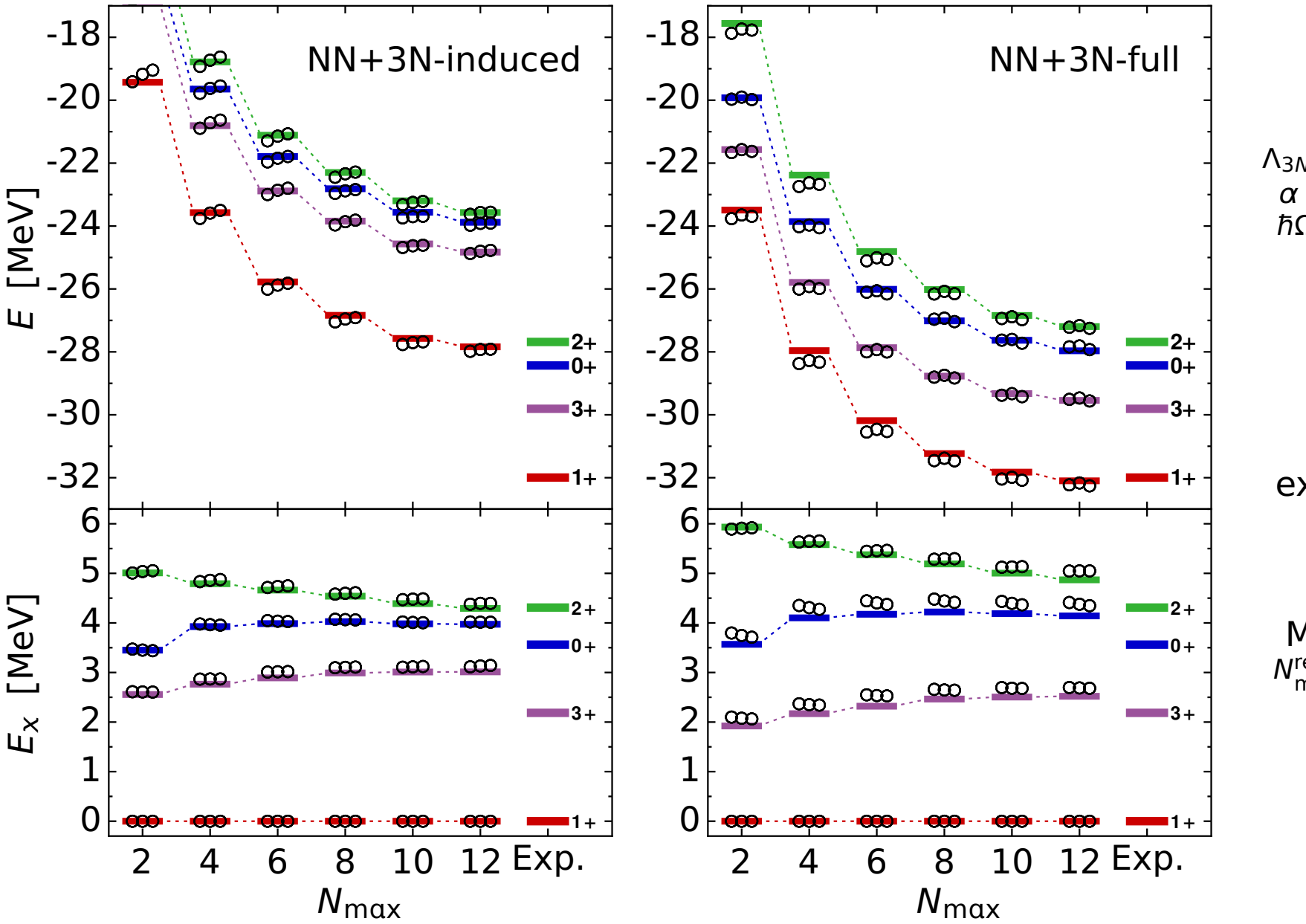


^{6}Li

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

explicit 3N

Benchmark: ^{6}Li



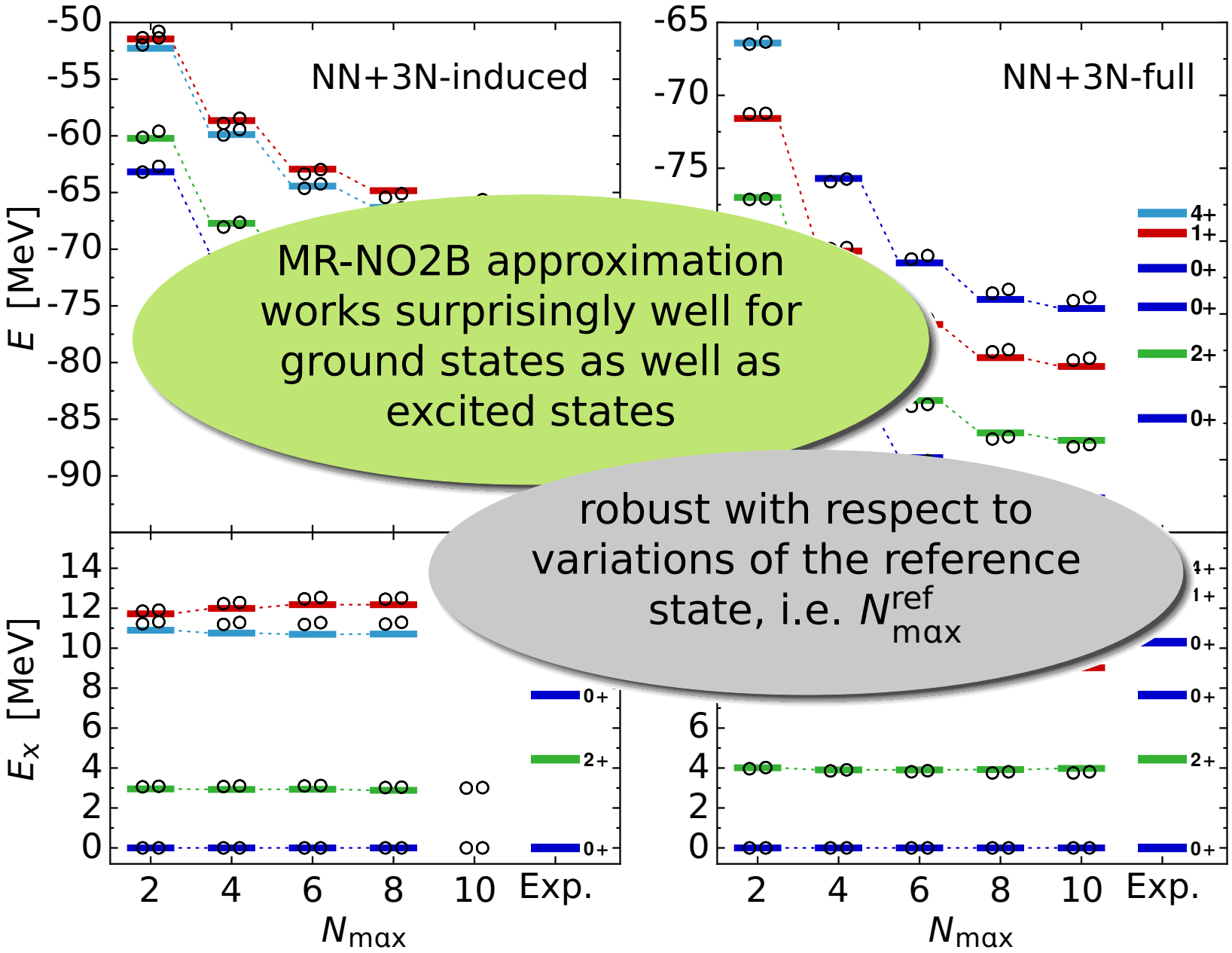
^{6}Li

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

explicit 3N

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

Benchmark: ^{12}C



MR-NO2B approximation works surprisingly well for ground states as well as excited states

robust with respect to variations of the reference state, i.e. $N_{\max}^{\text{ref}}$

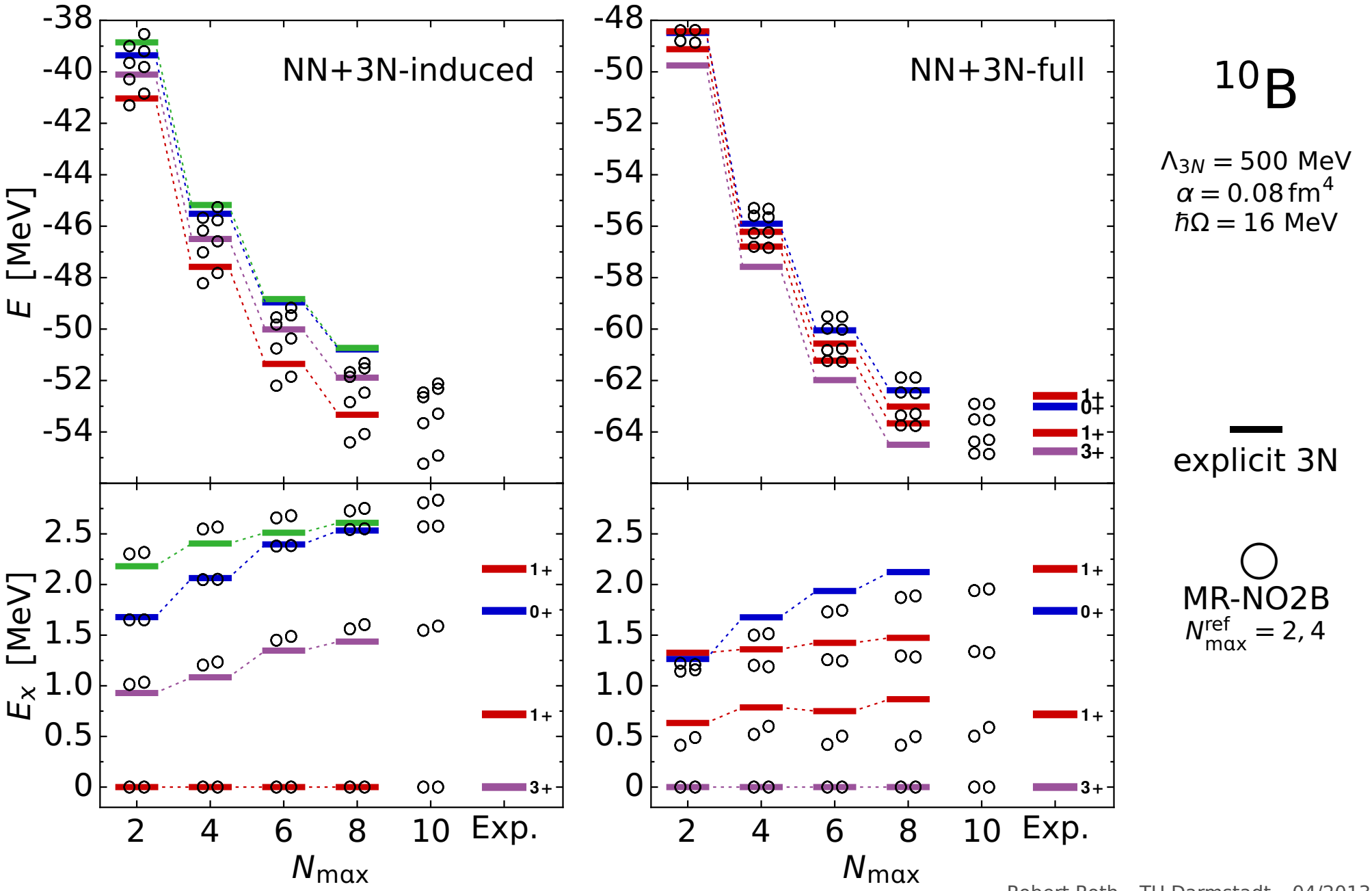
^{12}C

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

explicit 3N

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

Challenge: ^{10}B



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 (→ 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 ΛCCSD(T) is available with explicit 3N (→ 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 (→ P. Navratil)
- How can we generate reliable predictions for the drip-lines?
  - simply do all of the above...

Epilogue

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LOEWE
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