Importance Truncated No-Core Shell Model

for Nuclear Structure

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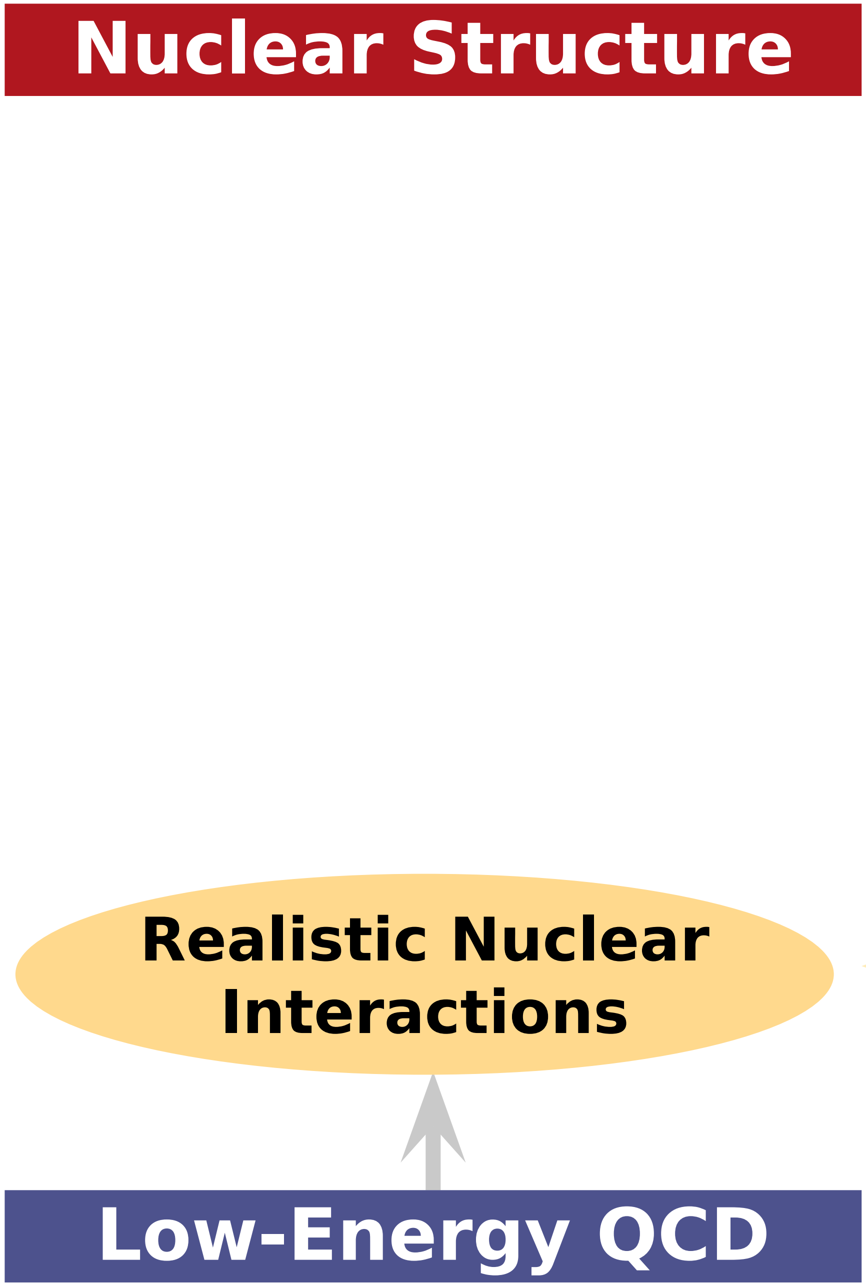
From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure



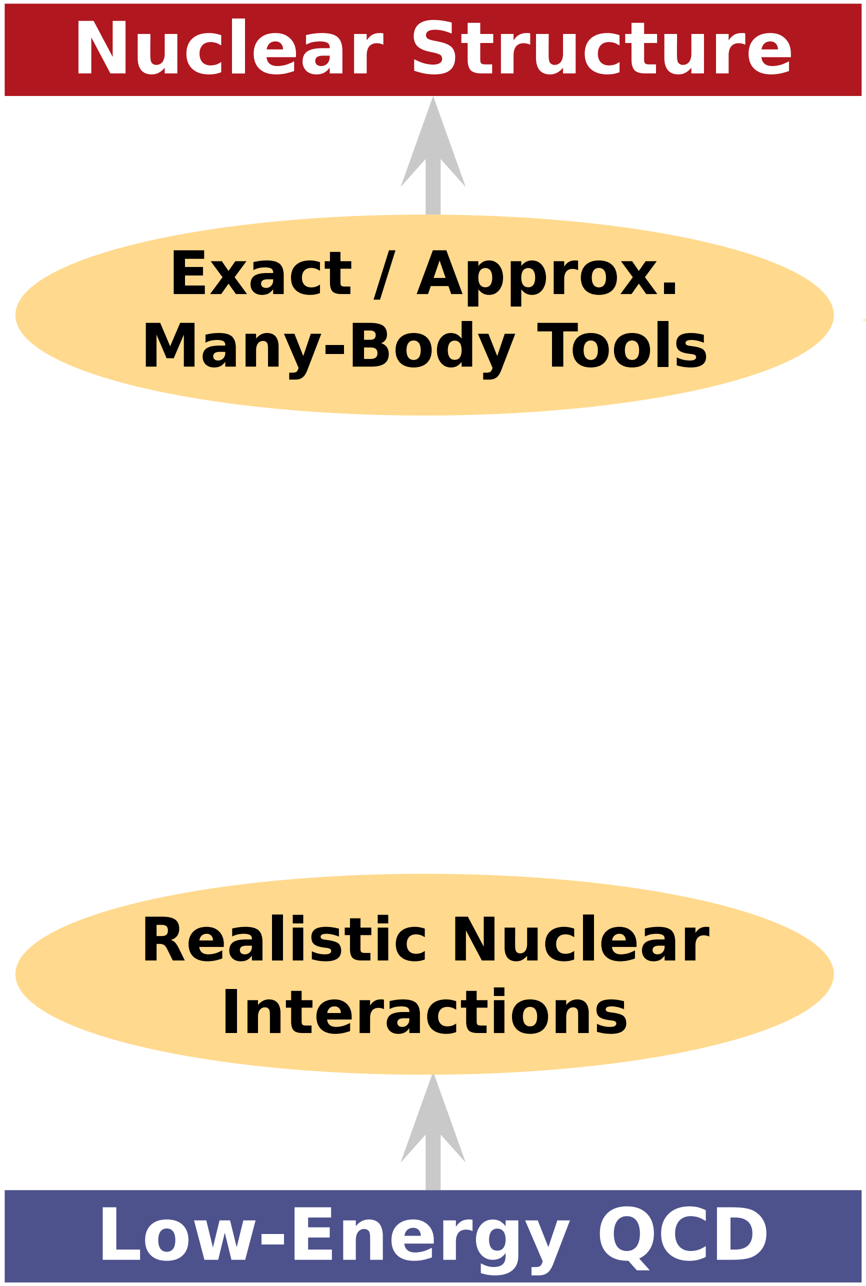
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

- chiral EFT interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations

From QCD to Nuclear Structure


Nuclear Structure

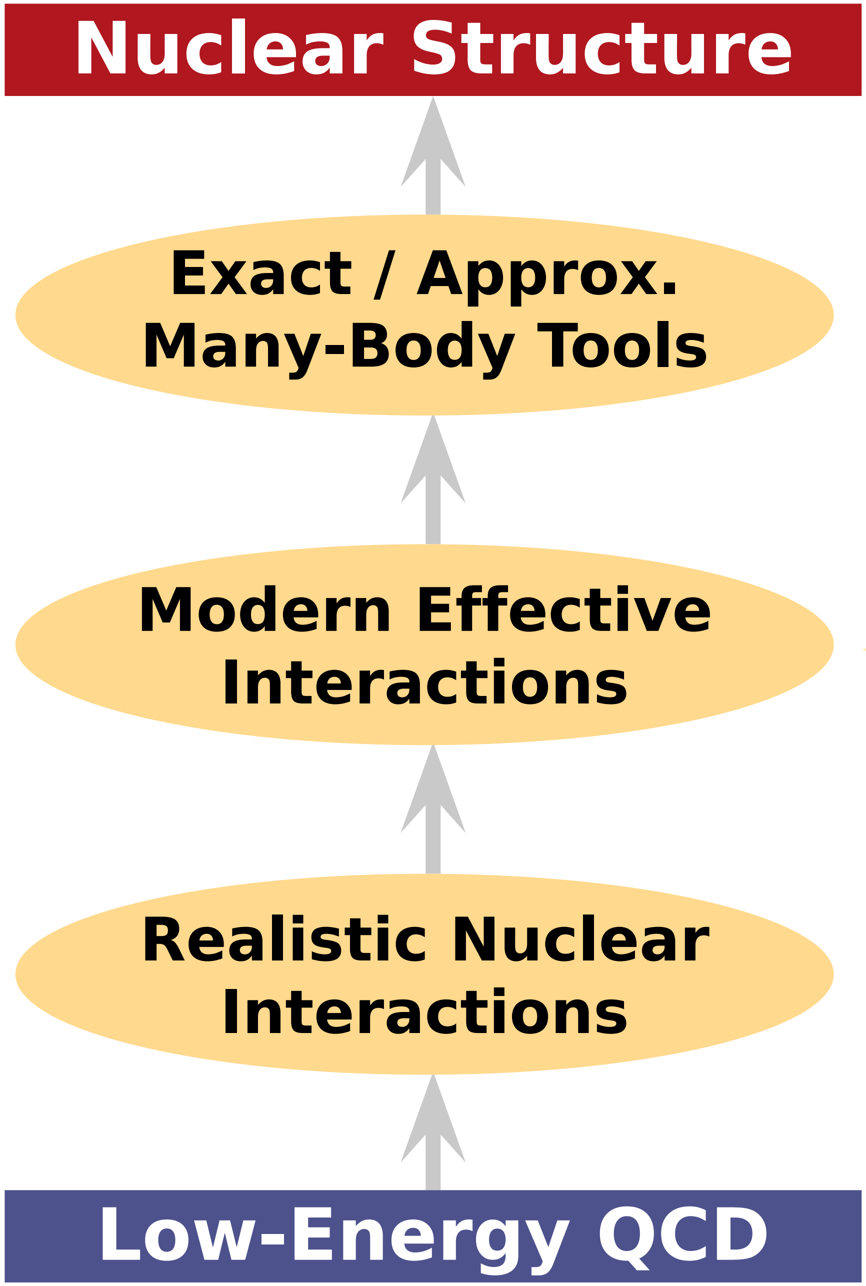
Exact / Approx. Many-Body Tools

Realistic Nuclear Interactions

Low-Energy QCD

- ‘exact’ solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
- controlled approximations for heavier nuclei (HF & MBPT,...)
- rely on restricted model spaces of tractable size
- not suitable for the description of short-range correlations

From QCD to Nuclear Structure



Nuclear Structure

Exact / Approx. Many-Body Tools

Modern Effective Interactions

Realistic Nuclear Interactions

Low-Energy QCD

- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts & deuteron)
  - generate new realistic int.
- need consistent effective interaction & effective operators
- unitary transformations most convenient (UCOM, SRG,...)

NCSM Toolbox

Nuclear Hamiltonian: Basics

- nucleus is a **self-bound object**: intrinsic properties are independent of center-of-mass state
  - factorization of intrinsic and CM components of many-body state and translational invariance are crucial
- translationally invariant **intrinsic Hamiltonian**

$$\begin{aligned} H_{\text{int}} &= (T - T_{\text{cm}}) + V_{NN} + V_{NNN} + \cdots \\ &= \qquad T_{\text{int}} \qquad + V_{NN} + V_{NNN} + \cdots \end{aligned}$$

- realistic **NN and NNN interactions**
  - use realistic interaction directly
  - employ unitary transformation to construct universal phase-shift equivalent soft interaction (UCOM, SRG,...)
  - construct effective model-space interaction via similarity transformation (Lee-Suzuki)

No-Core Shell Model: Basics

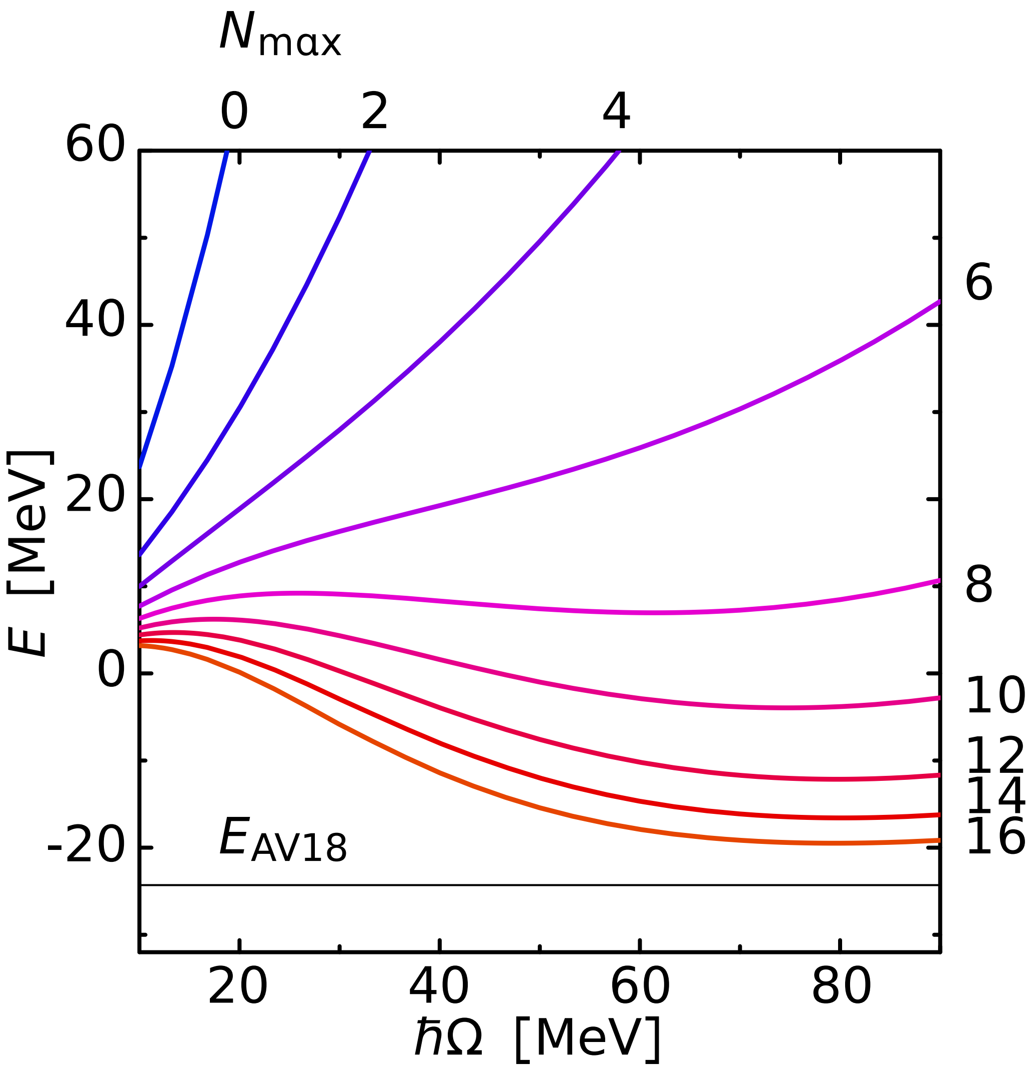
- special case of a **full configuration interaction (CI)** scheme
- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

$$|\Psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\max}\hbar\Omega$
  - ► **exact factorization** of intrinsic and CM component is possible
- numerical solution of **eigenvalue problem** for $\mathrm{H}_{\mathrm{int}}$ within $N_{\max}\hbar\Omega$ model space via Lanczos methods
  - ► model spaces of **up to 10^9 basis states** are used routinely
- increase $N_{\max}$ until **covergence** is observed

^{4}He: NCSM Convergence

V_{AV18}



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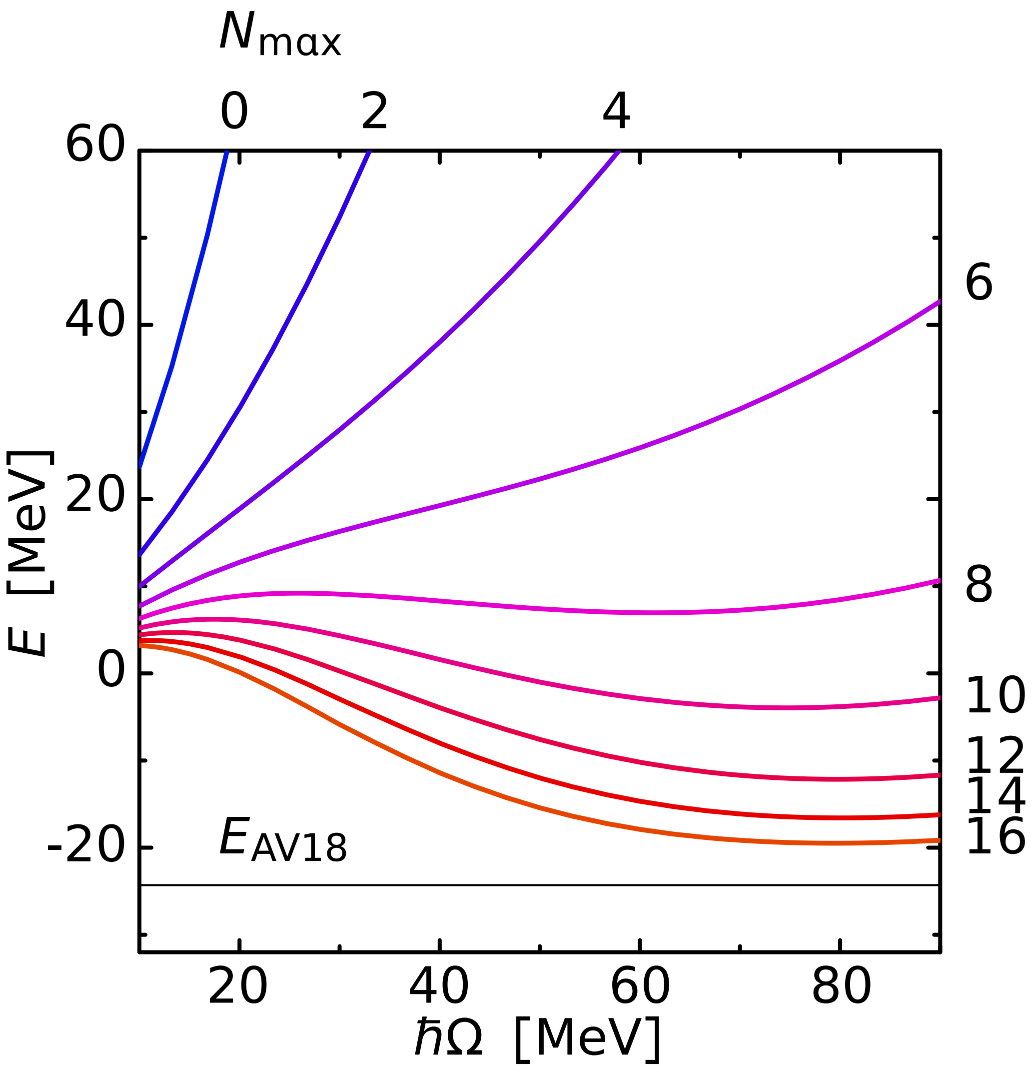
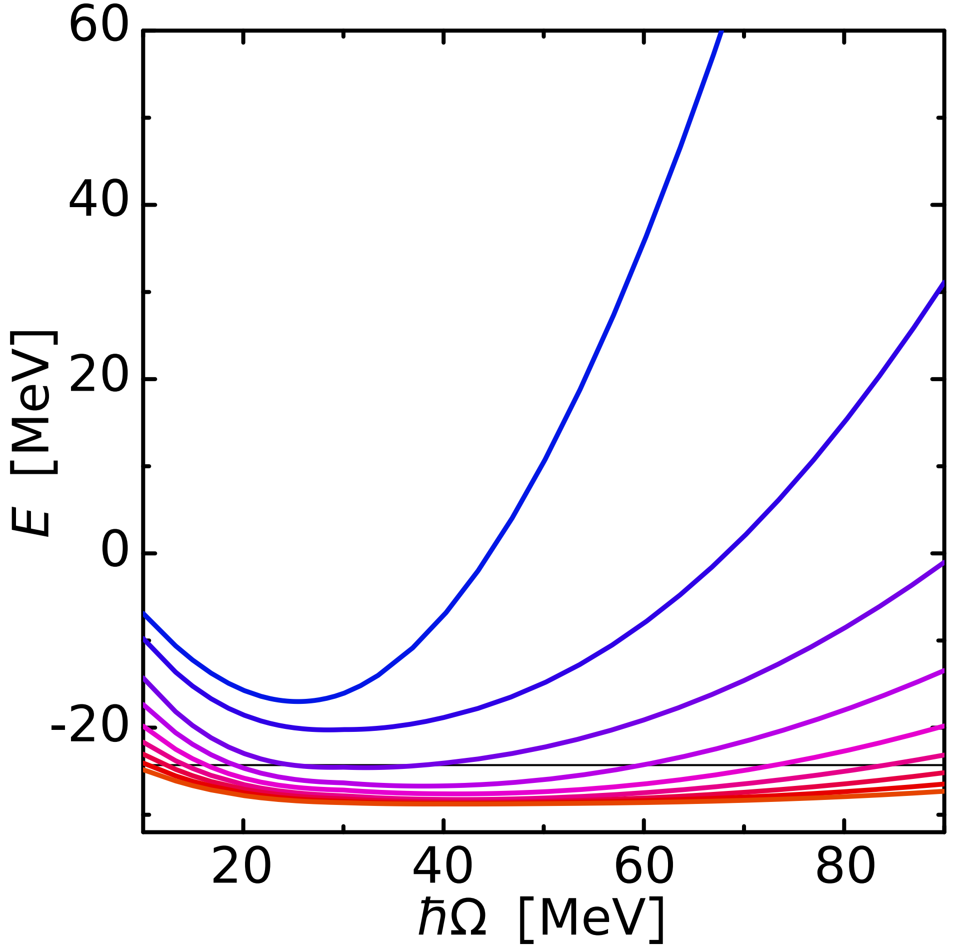
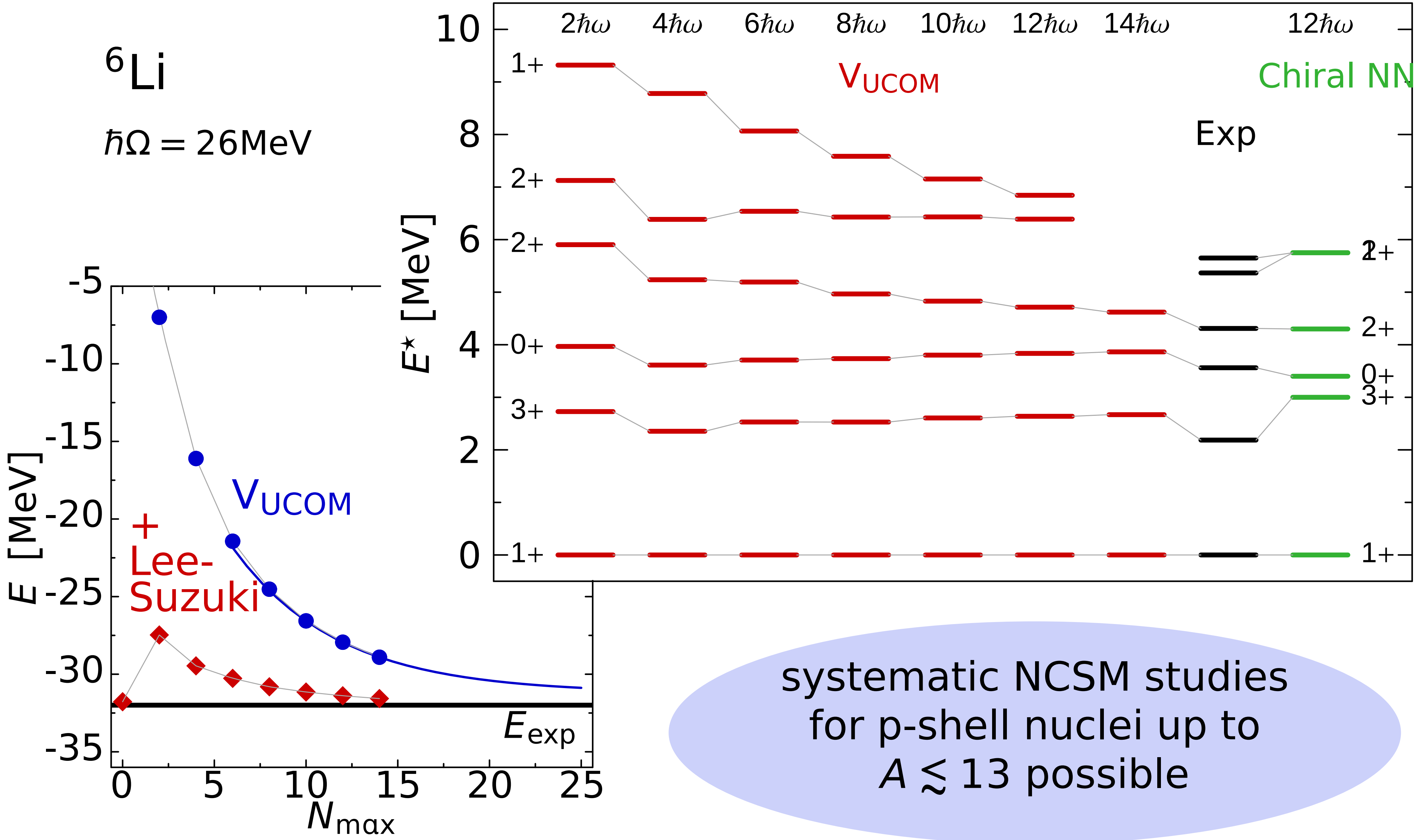


V_{UCOM}



^{6}Li: NCSM throughout the p-Shell



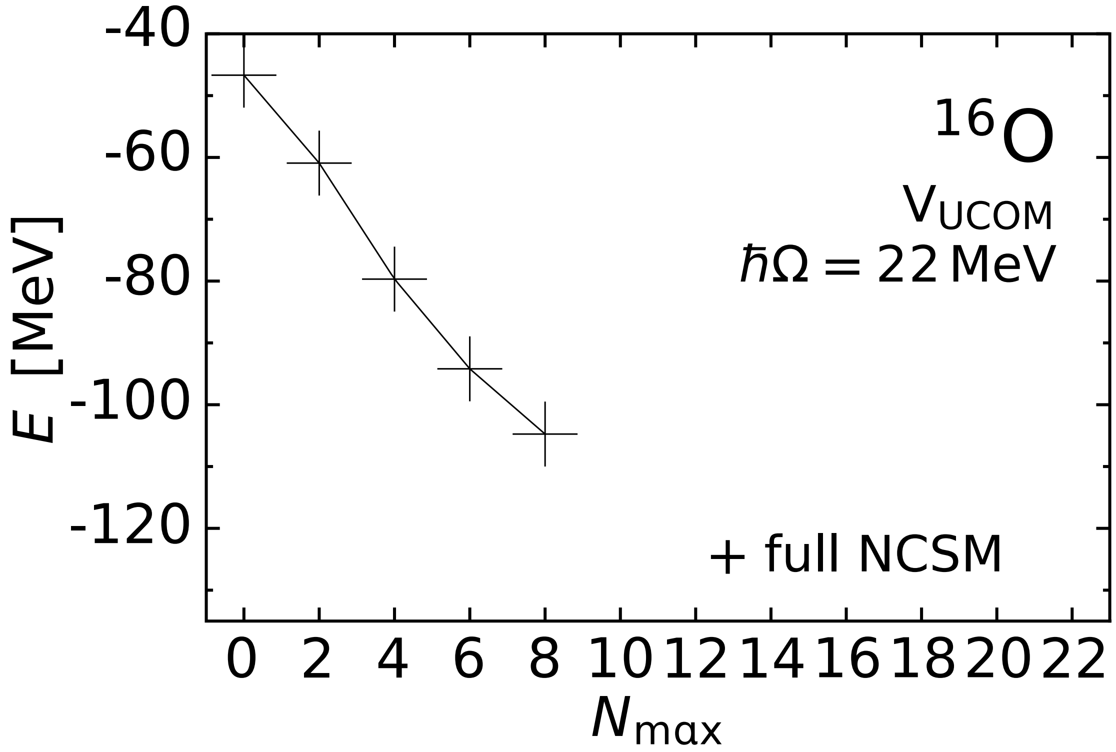
systematic NCSM studies for p-shell nuclei up to $A \lesssim 13$ possible

Importance Truncated No-Core Shell Model

Roth — Phys. Rev. C 79, 064324 (2009)
Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

Importance Truncated NCSM

- converged NCSM calculations are essentially restricted to p-shell
- full 10 or $12\hbar\Omega$ calculation for ^{16}O not yet feasible (basis dimension > 10^{10})



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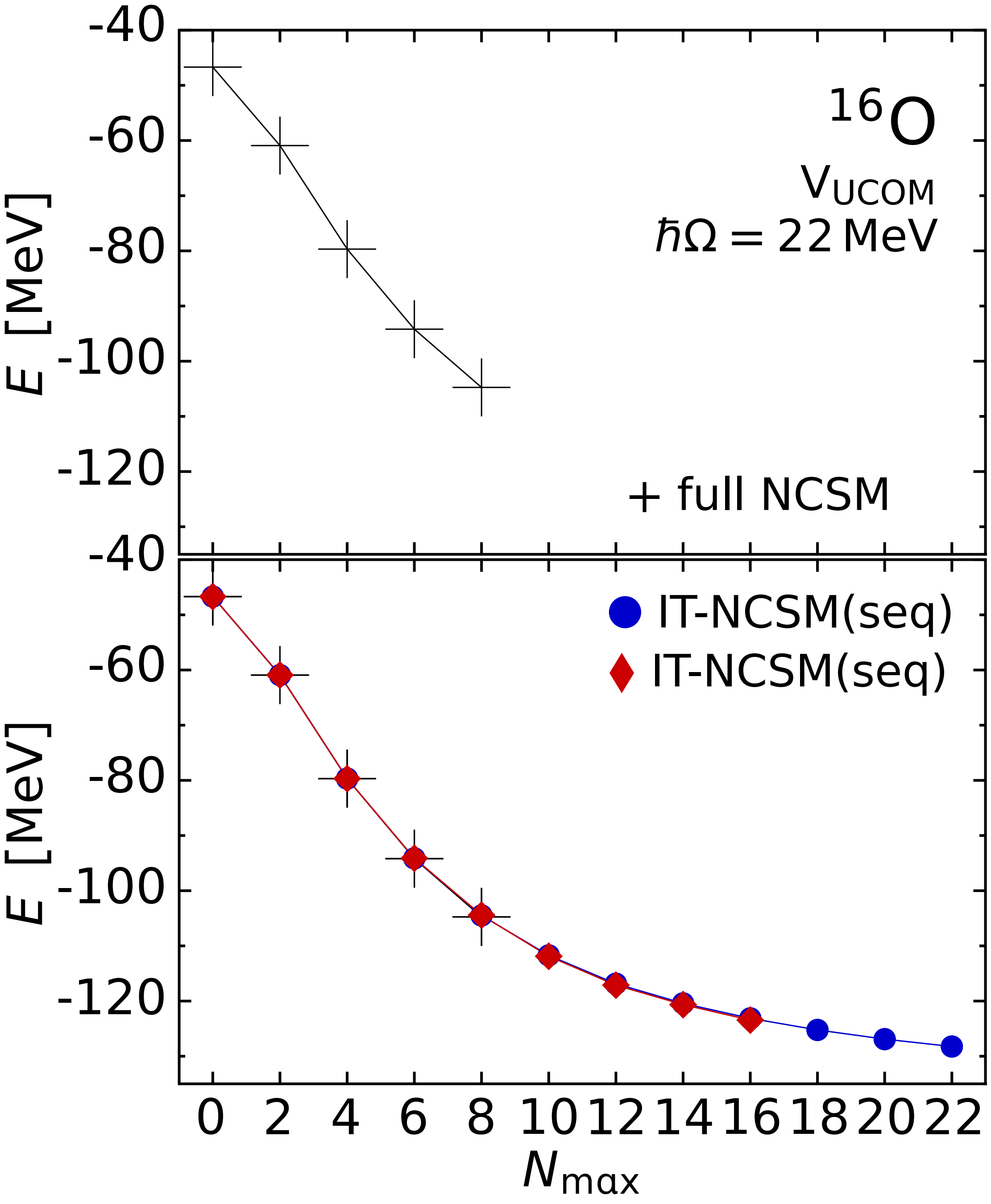
Importance Truncation

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



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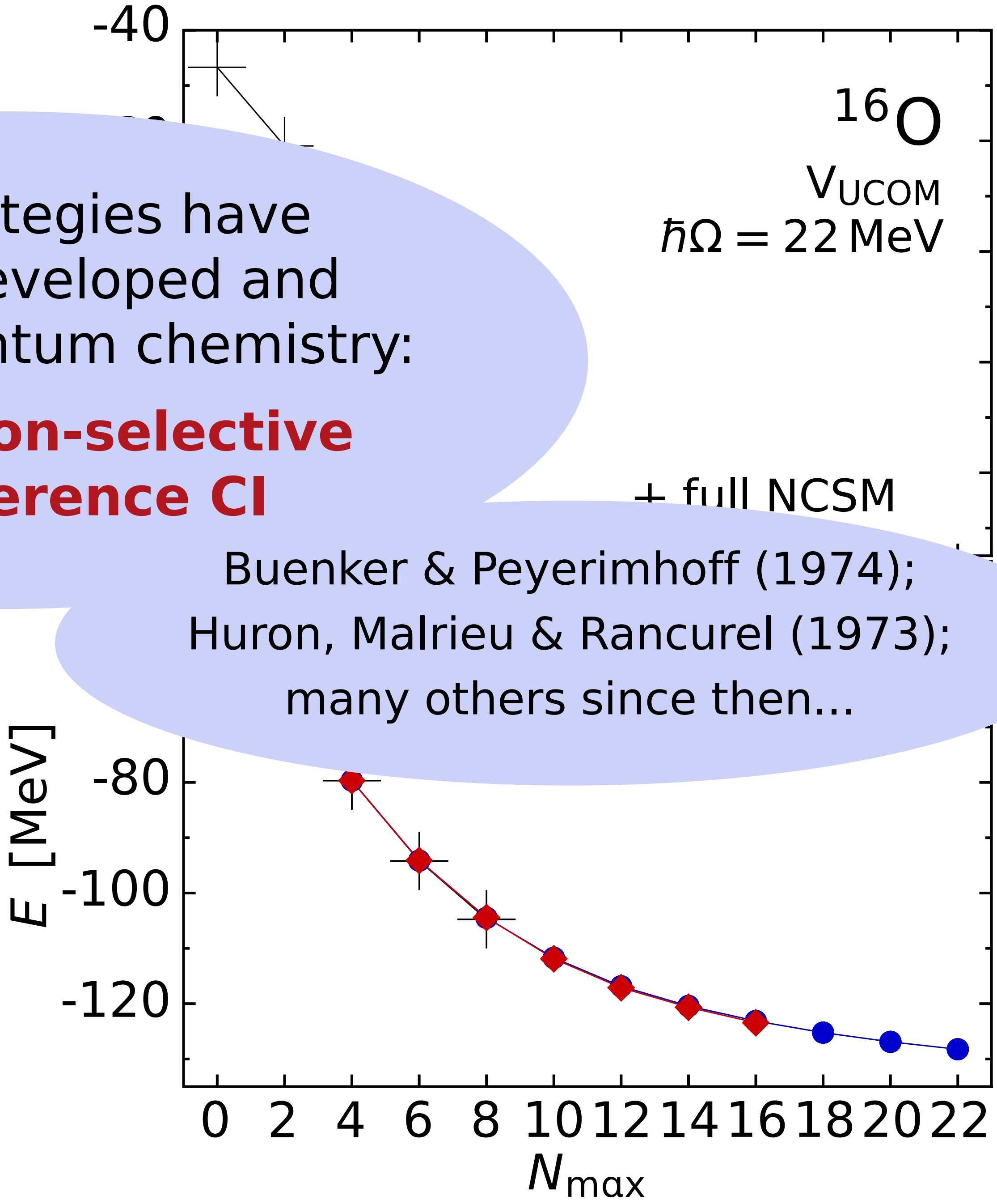

similar strategies have first been developed and applied in quantum chemistry:

configuration-selective multireference CI

Buenker & Peyerimhoff (1974);
Huron, Malrieu & Rancurel (1973);
many others since then...

Importance Truncation

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

Importance Truncation: General Idea

- given an initial approximation $|\Psi_{\text{ref}}\rangle$ for the **target state** within a limited **reference space** $\mathcal{M}_{\textbf{ref}}$

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

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

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

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

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

Importance Truncation: Iterative Scheme

- non-zero importance measure κ_ν only for states which **differ from $|\Psi_{\text{ref}}\rangle$ by 2p2h excitation** at most

IT-NCSM[*i*] or IT-CI[*i*]

- simple iterative scheme for a single $N_{\text{max}}\hbar\Omega$ model space

✪ start with $|\Psi_{\text{ref}}\rangle = |\Phi_0\rangle$

❶ construct importance truncated space containing up to 2p2h on top of $|\Psi_{\text{ref}}\rangle$

❷ solve eigenvalue problem

❸ use dominant components of eigenstate ($|C_\nu| \geq C_{\text{min}}$) as new $|\Psi_{\text{ref}}\rangle$, goto ❶

IT-NCSM(seq)

- sequential update scheme for a set of $N_{\text{max}}\hbar\Omega$ spaces

✪ start with $N_{\text{max}} = 2$ eigenstate from full NCSM as initial $|\Psi_{\text{ref}}\rangle$

❶ construct importance truncated space for $N_{\text{max}} + 2$

❷ solve eigenvalue problem

❸ use dominant components of eigenstate ($|C_\nu| \geq C_{\text{min}}$) as new $|\Psi_{\text{ref}}\rangle$, goto ❶

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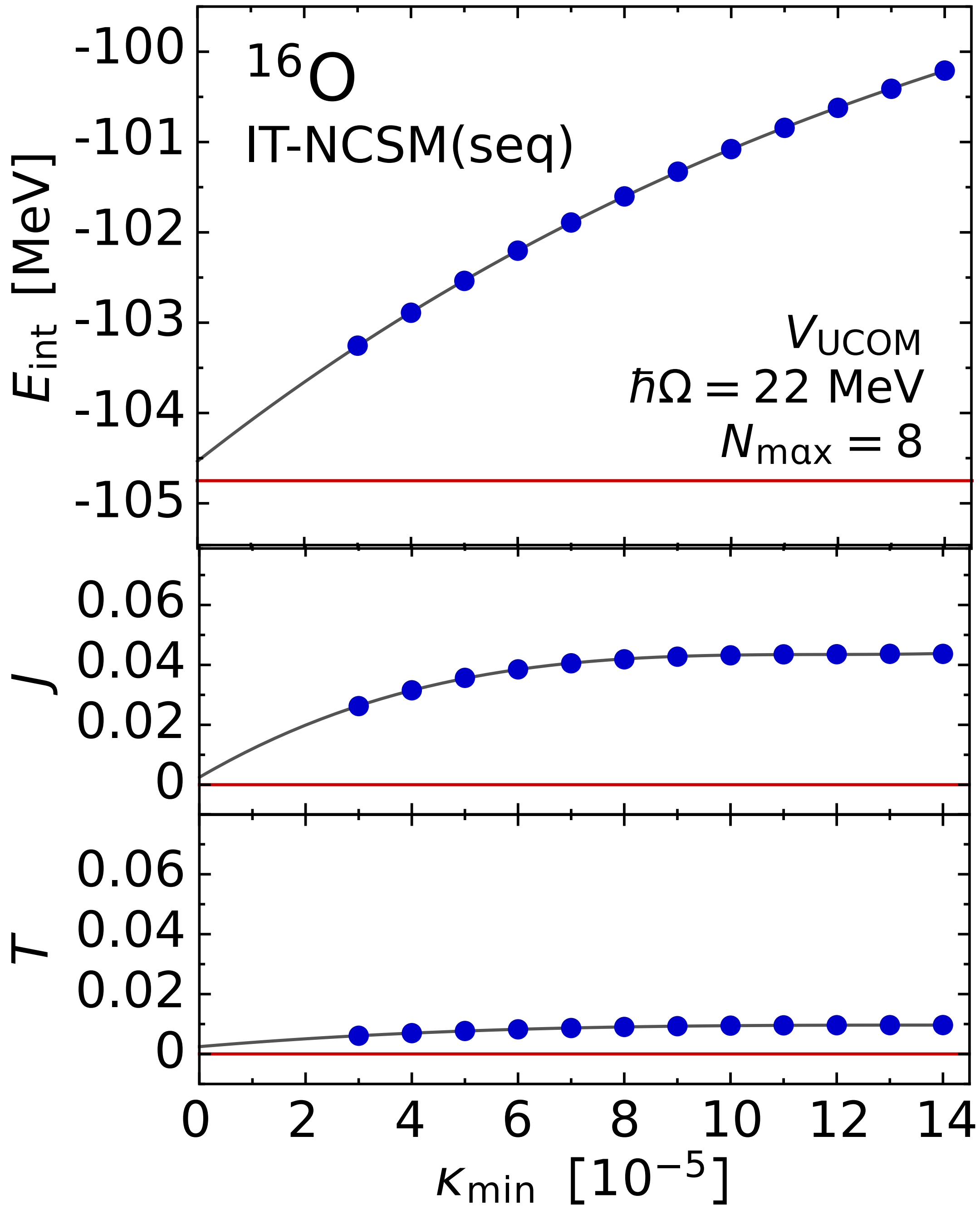
❶ construct importance truncated
r $N_{\max} + 2$

e problem

nponents of
$\geq C_{\min}$) as new

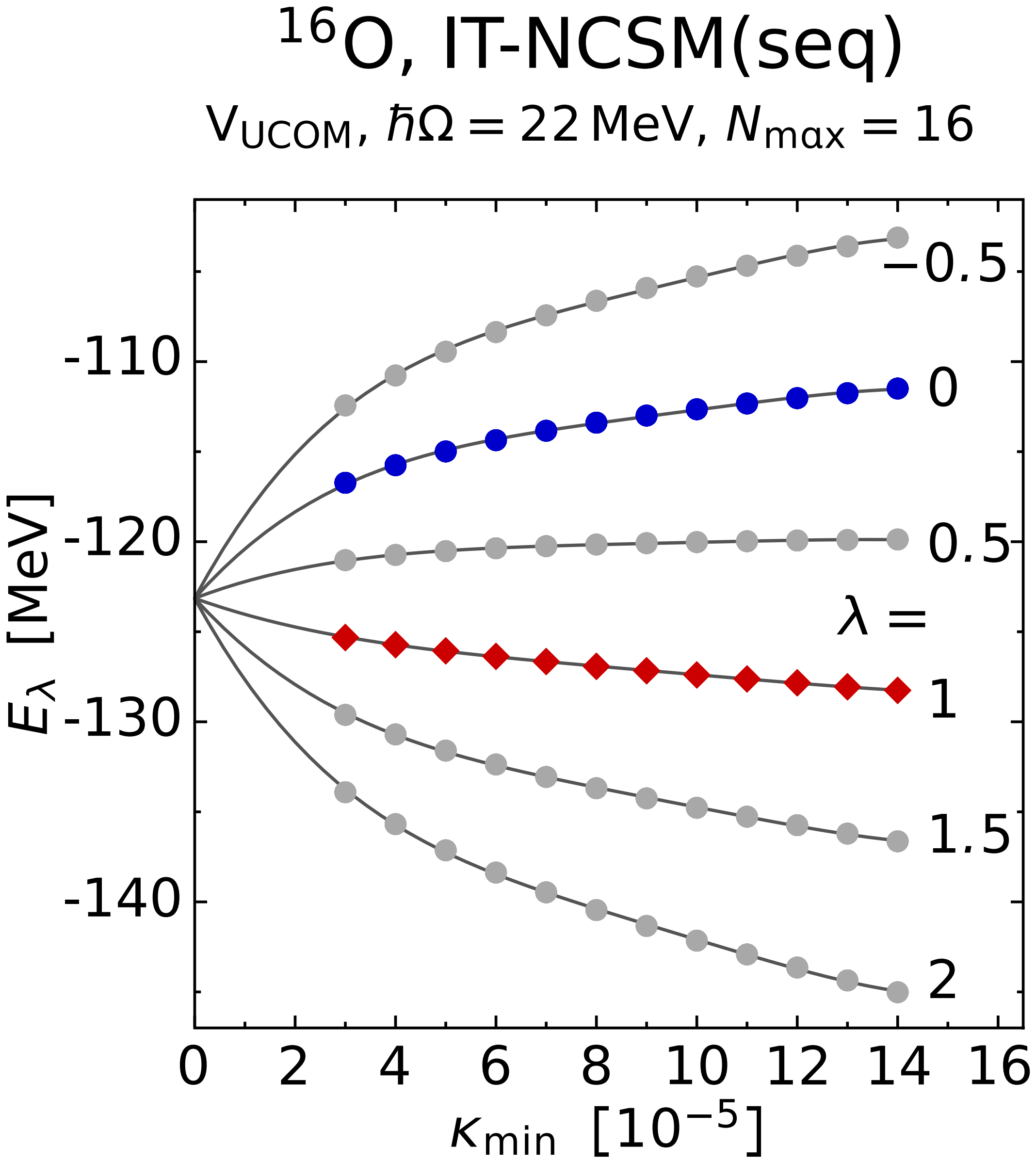
full NCSM model space is recovered in the limit $(\kappa_{\min}, C_{\min}) \to 0$ in IT-NCSM(seq) and IT-NCSM[i_{conv}]

Threshold Dependence



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

Constrained Threshold Extrapolation



- estimate energy contribution of **excluded states** perturbatively → $\Delta_{\mathrm{excl}}(\kappa_{\min})$
- **simultaneous fit** of combined energy

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

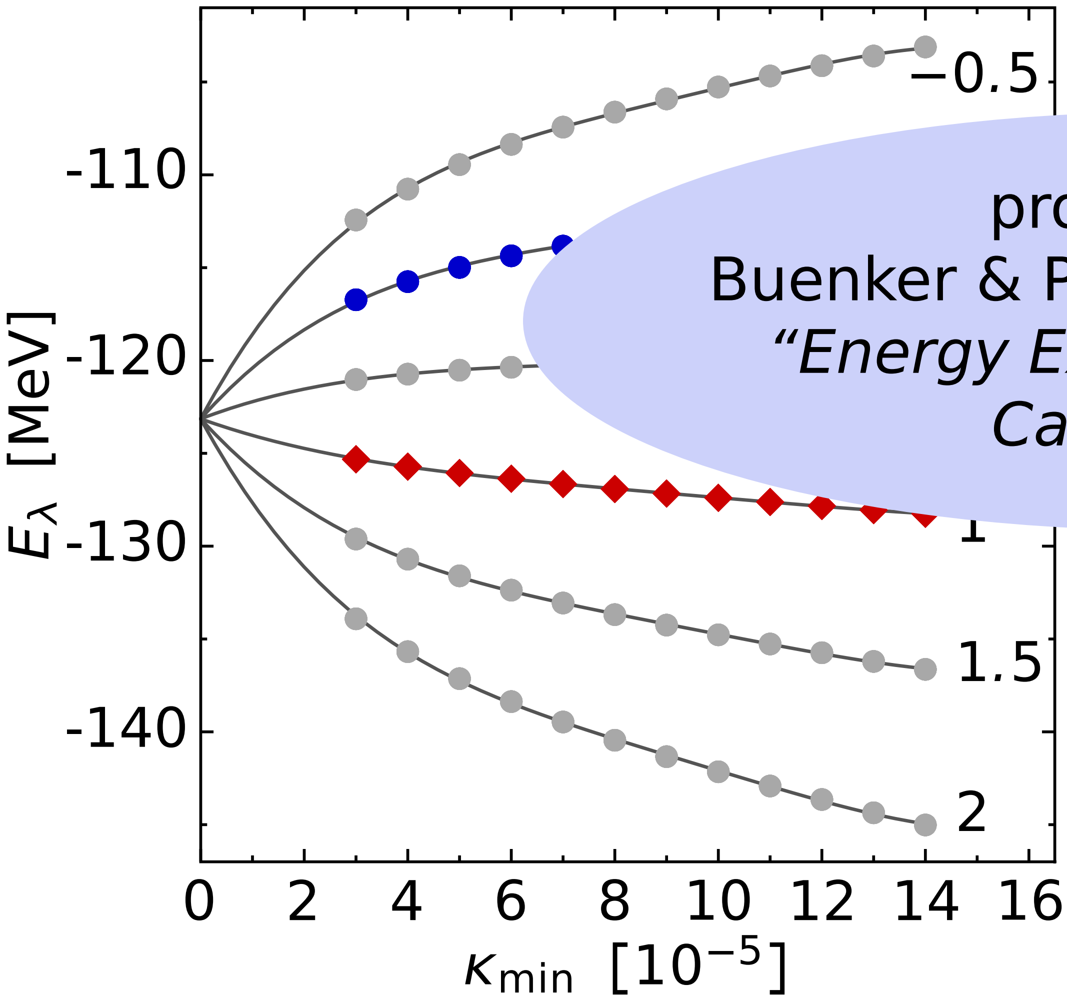
for set of λ-values with the constraint $E_\lambda(0) = E_{\mathrm{extrap}}$

- **robust threshold extrapolation** with error bars determined by variation of the λ set

Constrained Threshold Extrapolation

^{16}O, IT-NCSM(seq)

V_{UCOM}, $\hbar\Omega = 22\,\mathrm{MeV}$, $N_{\max} = 16$



- estimate energy contribution of **excluded states** perturbatively ➜ $\Delta_{\mathrm{excl}}(\kappa_{\min})$

ltaneous fit of combined

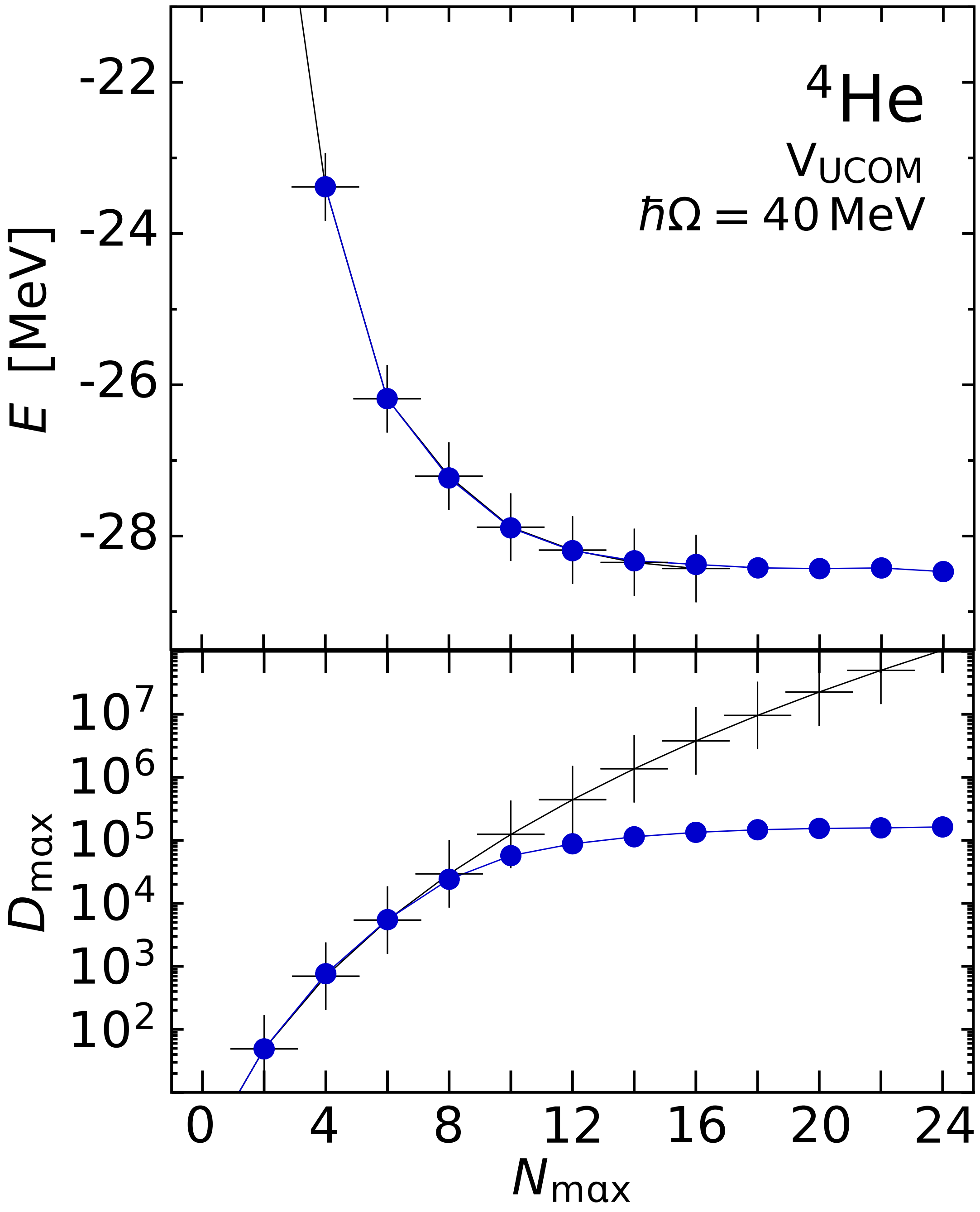
$\lambda\Delta_{\mathrm{excl}}(\kappa_{\min})$

for set of λ-values with the constraint $E_\lambda(0) = E_{\mathrm{extrap}}$

- **robust threshold extrapolation** with error bars determined by variation of the λ set

proposed by
Buenker & Peyerimhoff (1975):
“Energy Extrapolation in CI Calculation”

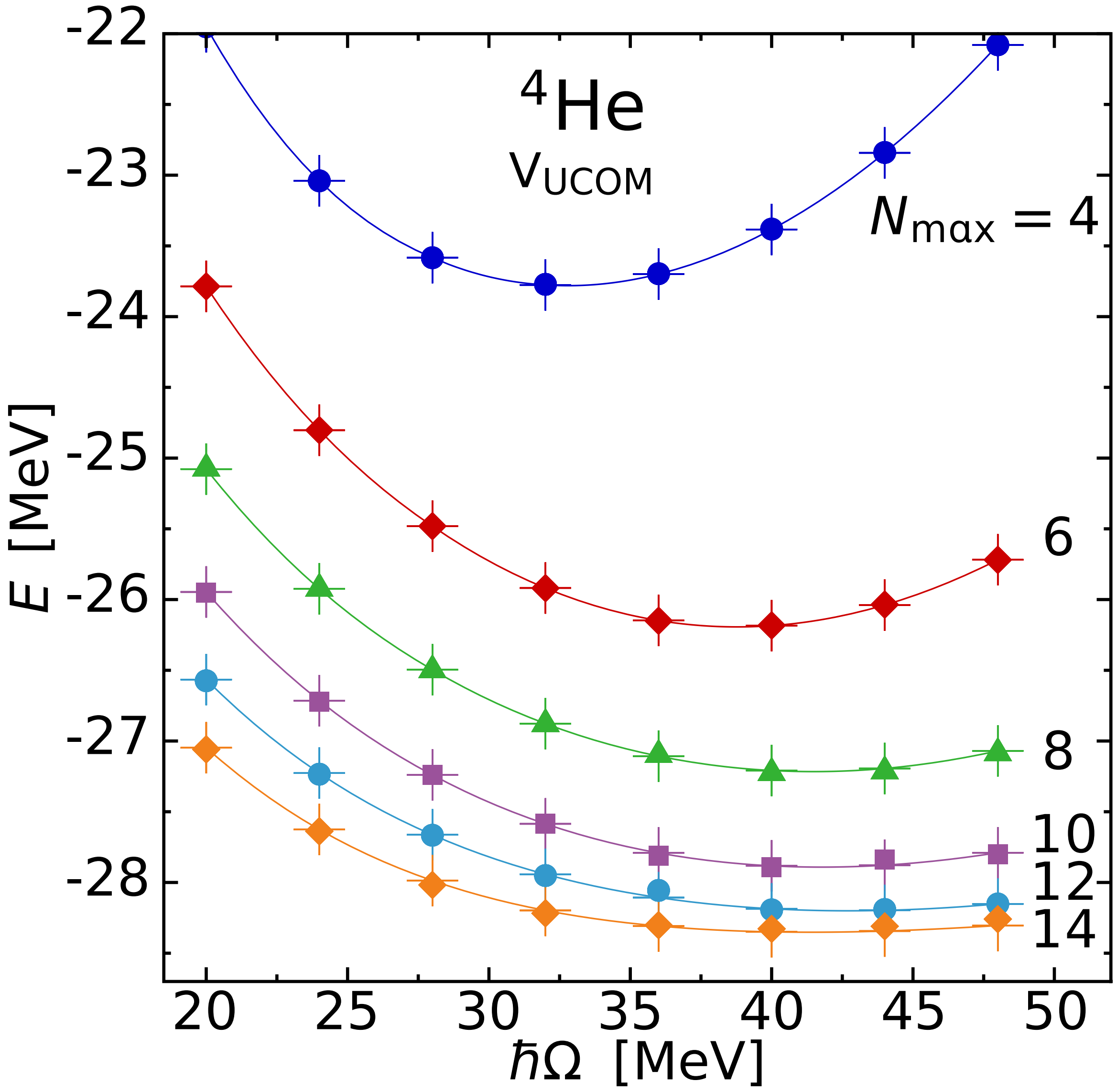
^{4}He: Importance-Truncated NCSM



- **sequential IT-NCSM(seq)**: single importance update using $(N_{\max}-2)\hbar\Omega$ eigenstate as reference
- **reproduces exact NCSM result** for all $N_{\max}$
- reduction of basis by more than two orders of magnitude w/o loss of precision

\+ full NCSM
● IT-NCSM(seq)

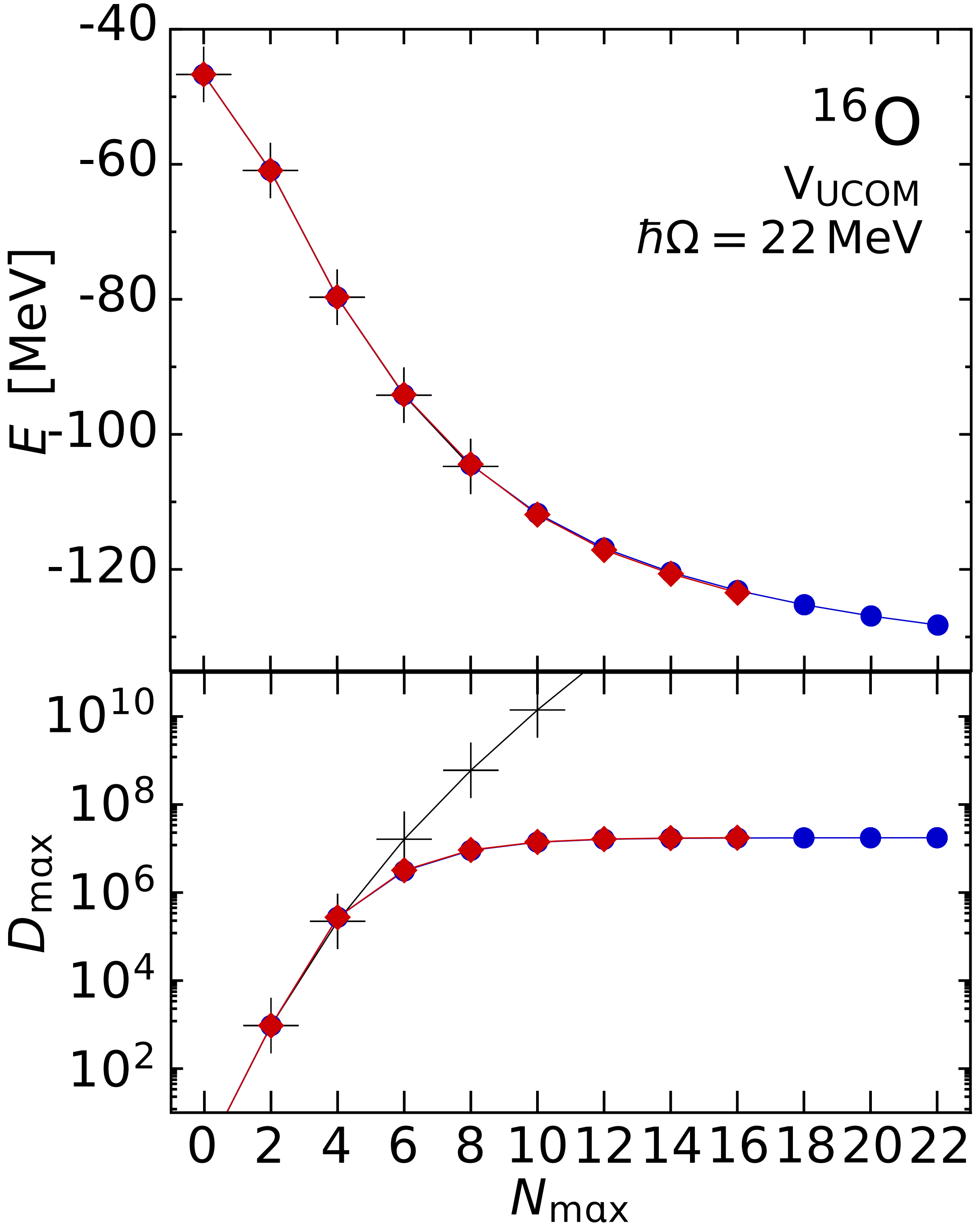
^{4}He: Importance-Truncated NCSM



- **reproduces exact NCSM result** for all $\hbar\Omega$ and N_{max}
- importance truncation & threshold extrapolation is robust
- **no center-of-mass contamination** for any N_{max} and $\hbar\Omega$

+ full NCSM
● IT-NCSM(seq)

^{16}O: Importance-Truncated NCSM



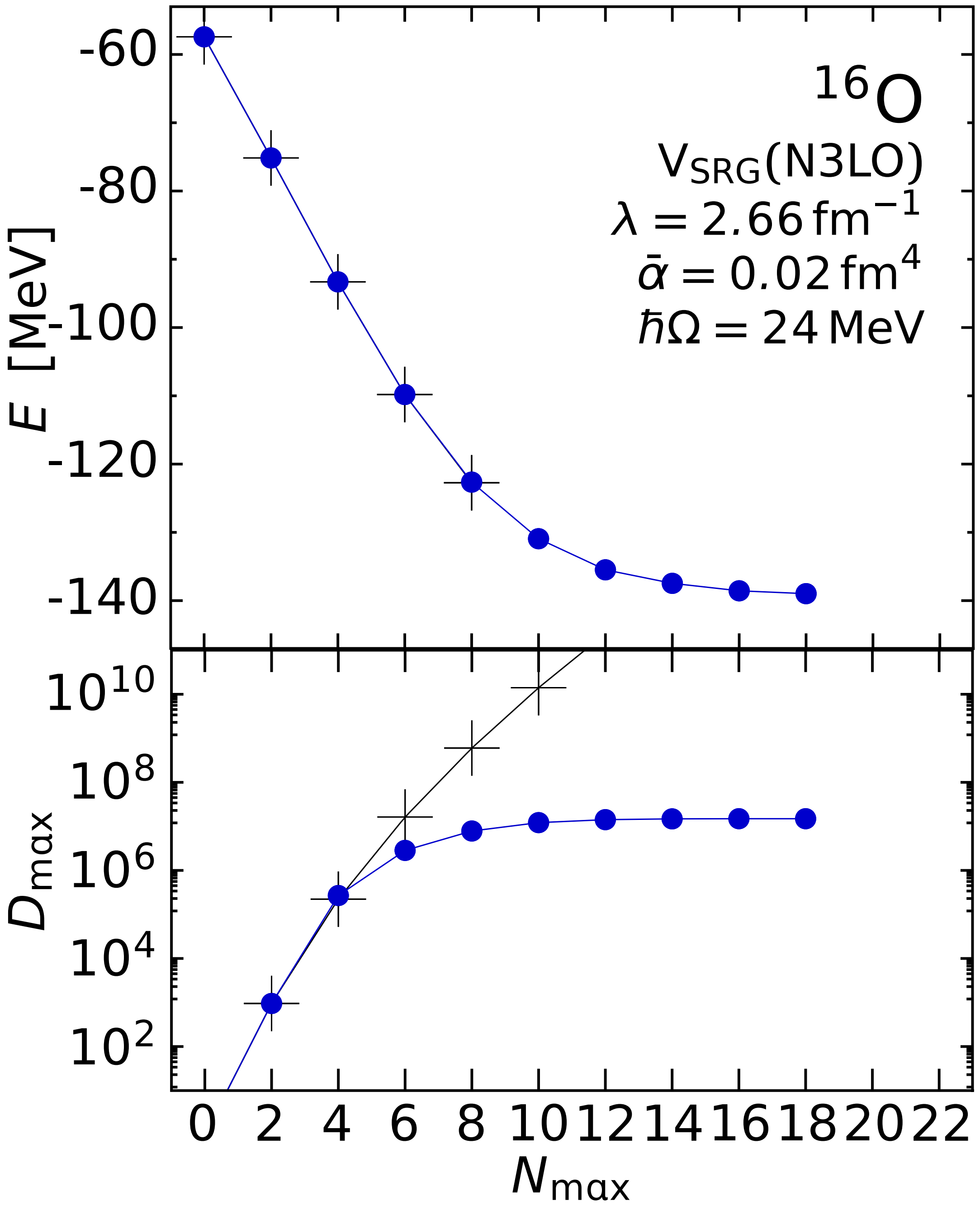
- IT-NCSM(seq) provides **excellent agreement with full NCSM** calculation

- dimension reduced by **several orders of magnitude**

- possibility to go **way beyond** the domain of the full NCSM

+ full NCSM
● IT-NCSM(seq), $C_{min} = 0.0005$
♦ IT-NCSM(seq), $C_{min} = 0.0003$

^{16}O: Importance-Truncated NCSM

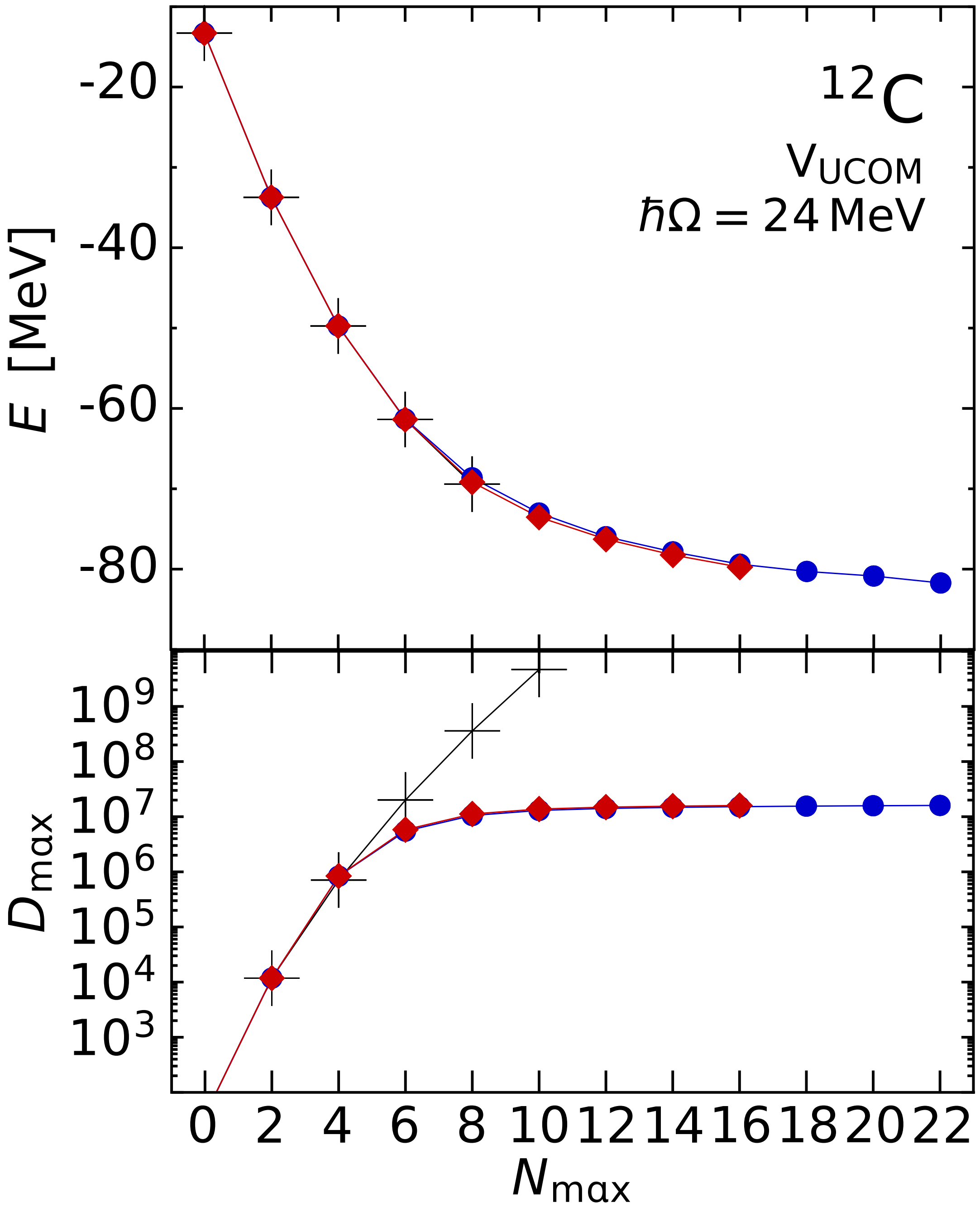


- **SRG-evolved N3LO potential** provides a much better convergence behavior
- nevertheless, $N_{max} \leq 8$ calculations are not sufficient
- non-exponential behavior observed with V_{UCOM} is really due to interaction

\+ full NCSM

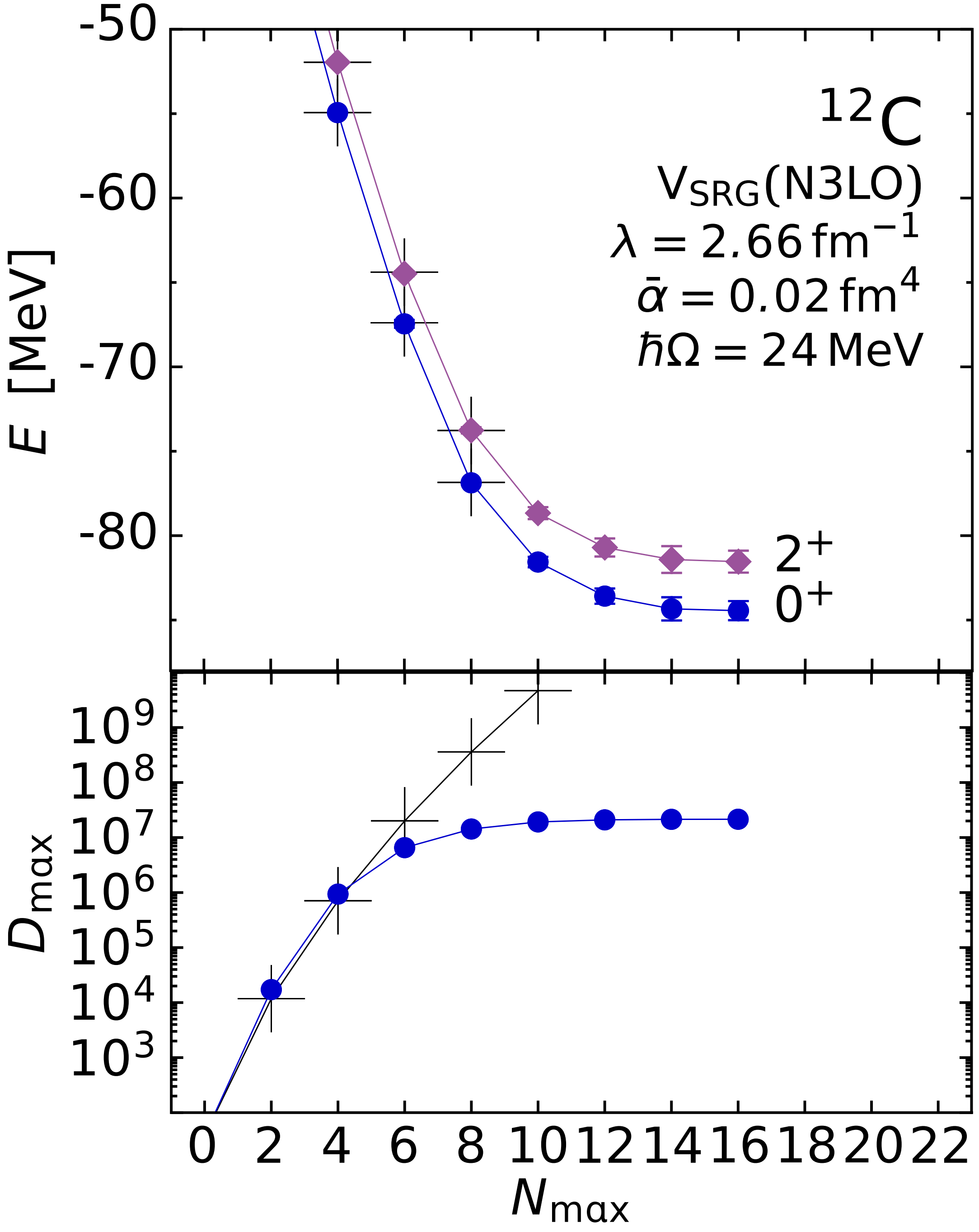
● IT-NCSM(seq), $C_{min} = 0.0005$

^{12}C: IT-NCSM for Open-Shell Nuclei



- **excellent agreement with full NCSM** calculations
- IT-NCSM(seq) works just as well for **non-magic / open-shell nuclei**
- all calculations limited by available two-body matrix elements & CPU time only

^{12}C: IT-NCSM for Excited States

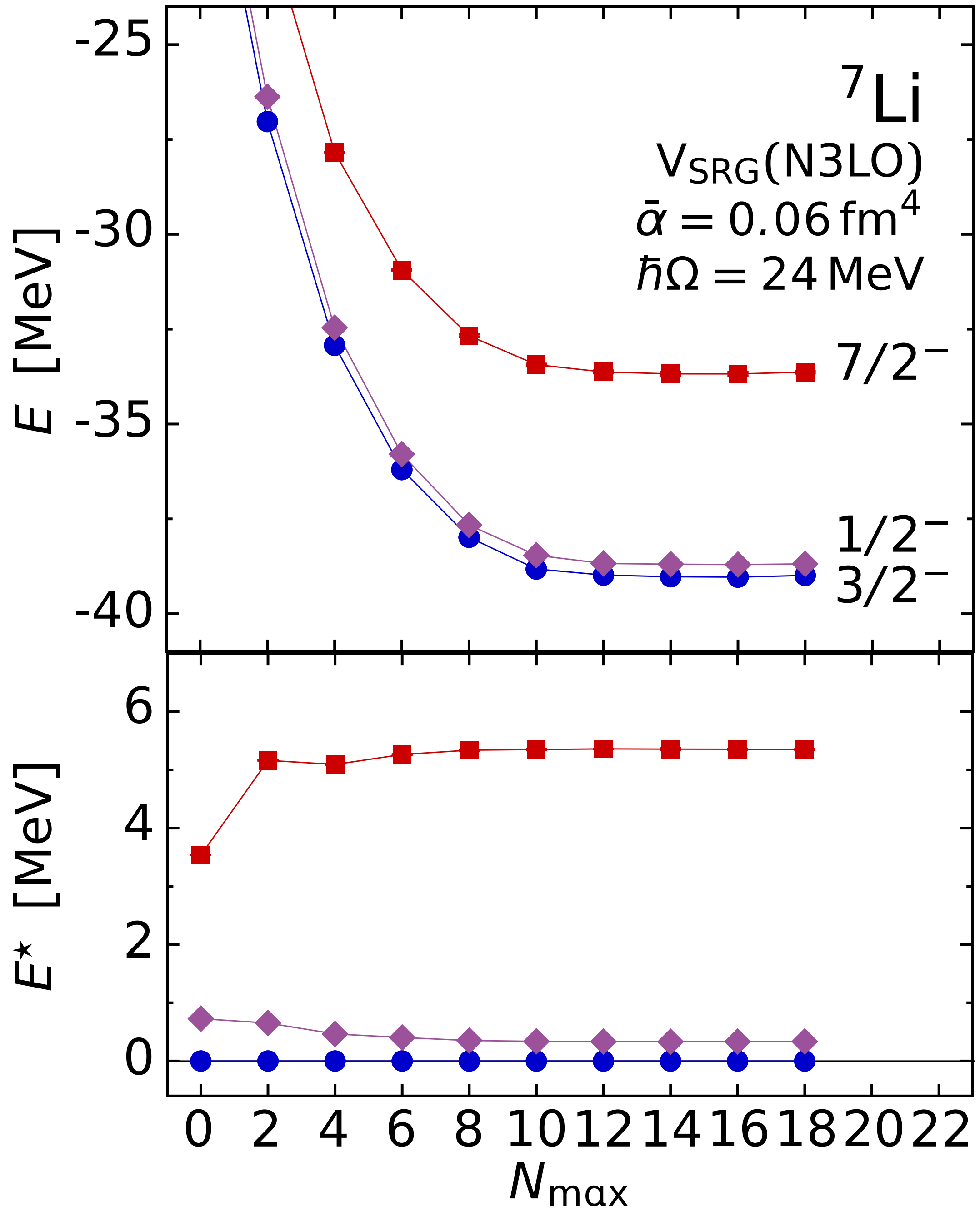


- **target ground & excited states** simultaneously
  - ► separate importance measure $\kappa_\nu^{(n)}$ for each target state
  - ► basis state is included if $|\kappa_\nu^{(n)}| \geq \kappa_{\min}$ for any n
- dimension of importance truncated space **grows linearly** with # of target states

+ full NCSM

●♦ IT-NCSM(seq), $C_{\min} = 0.0005$

^{7}Li: IT-NCSM for Odd Nuclei



- IT-NCSM(seq) can treat a ground state & few low-lying excited states **on the same footing**
- **excellent agreement with full NCSM** calculations also for excited states
- easy access to **full spectroscopy**

●♦■ IT-NCSM(seq), $C_{\min} = 0.0003$

IT-NCSM: Pros and Cons

- ✔ **fulfills variational principle** & Hylleraas-Undheim theorem
- ✔ **no center-of-mass contamination** induced by importance truncation in $N_{\mathrm{max}}\hbar\Omega$ space
- ✔ constrained **threshold extrapolation** $\kappa_{\mathrm{min}} \to 0$ recovers contribution of excluded configurations efficiently and accurately
- ✔ **open and closed-shell nuclei** with **ground and excited states** can be treated on the same footing
- ✔ **compatible with shell model**: compute any observable from wave functions in SM representation
- ✘ **only approximate size-extensivity** after threshold extrapolation in IT-NCSM(seq) or IT-NCSM[i_{conv}] – no explicit *npnh* truncation
- ✘ computationally still demanding

CM Diagnostics

- nucleus is a self-bound system: intrinsic and CM component of the many-body state have to factorize

$$\left|\Psi\right\rangle = \left|\psi_{\mathrm{int}}\right\rangle \otimes \left|\psi_{\mathrm{cm}}\right\rangle$$

- detect presence of an **unphysical coupling between intrinsic and CM degrees of freedom** by manipulating the CM spectrum and checking for the impact on the intrinsic state

- Lawson-modification of the Hamiltonian

$$\mathrm{H}_{\beta} = \mathrm{H}_{\mathrm{int}} + \beta\, \mathrm{H}_{\mathrm{cm}}$$

with harmonic oscillator Hamiltonian w.r.t. the CM

$$\mathrm{H}_{\mathrm{cm}} = \frac{1}{2mA}\vec{\mathrm{P}}^{2}_{\mathrm{cm}} + \frac{mA\Omega^{2}}{2}\vec{\mathrm{X}}^{2}_{\mathrm{cm}} - \frac{3}{2}\hbar\Omega\,.$$

whose exact ground state can be represented in the $0\hbar\Omega$ space

CM Diagnostics

- **analyze β-dependence of expectation values of $\mathrm{H}_{\mathrm{int}}$** computed with eigenstates of H_β

$$\langle \mathrm{H}_{\mathrm{int}} \rangle_\beta = \langle \Psi_\beta | \mathrm{H}_{\mathrm{int}} | \Psi_\beta \rangle$$

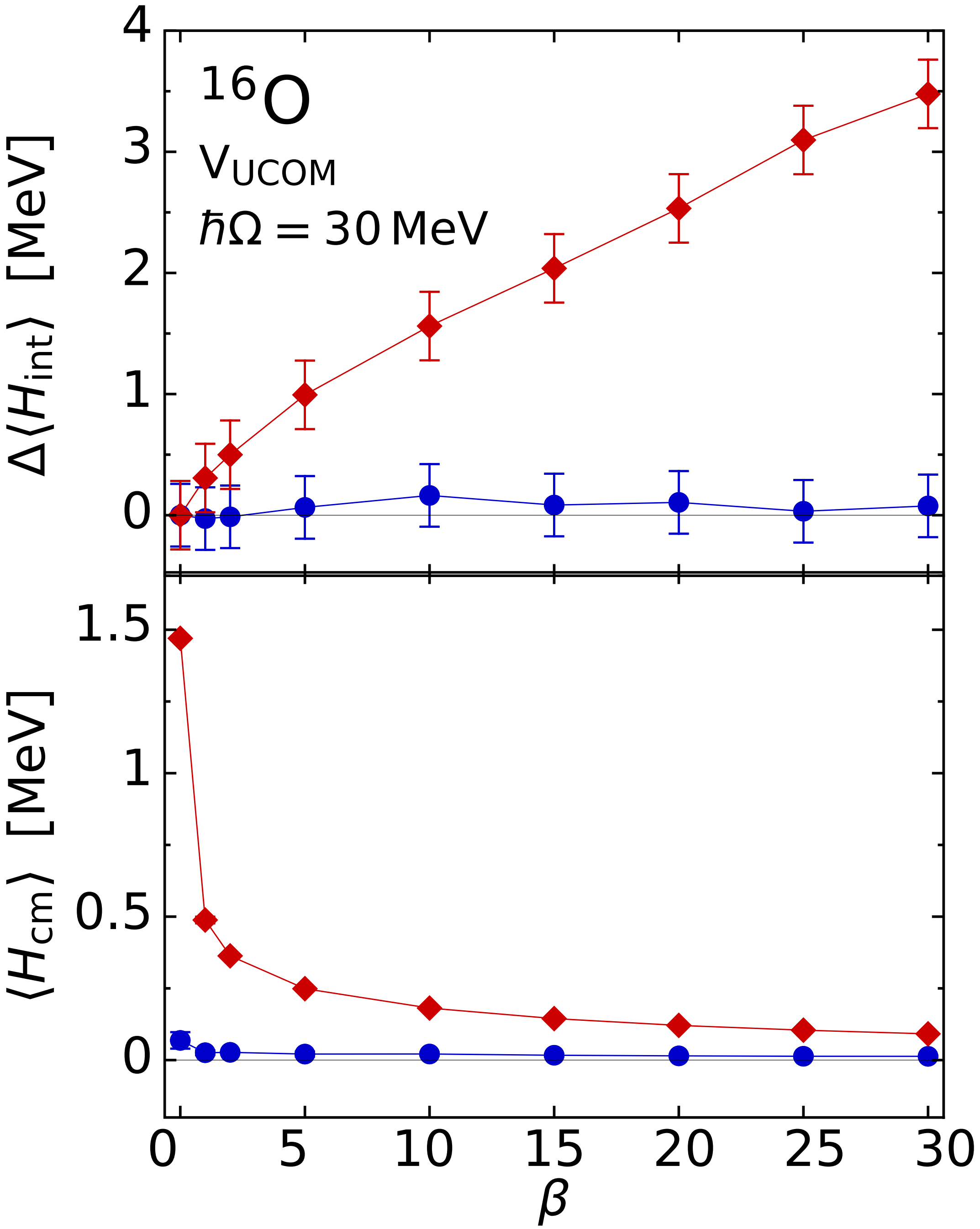
→ any dependence of $\langle \mathrm{H}_{\mathrm{int}} \rangle_\beta$ on β indicates an unphysical coupling between intrinsic and CM motion

- **analyze β-dependence of expectation values of H_{cm}** computed with eigenstates of H_β

$$\langle \mathrm{H}_{\mathrm{cm}} \rangle_\beta = \langle \Psi_\beta | \mathrm{H}_{\mathrm{cm}} | \Psi_\beta \rangle$$

→ any non-zero value of $\langle \mathrm{H}_{\mathrm{cm}} \rangle_\beta$ for $\beta > 0$ indicates an unphysical coupling between intrinsic and CM motion

CM Diagnostics: IT-NCSM(seq) vs. IT-CI[2]



- IT-NCSM(seq) – $N_{\mathrm{max}}\hbar\Omega$ trunc.
  - ► $\Delta\langle \mathrm{H_{int}}\rangle_\beta$ and $\langle \mathrm{H_{cm}}\rangle_\beta$ are practically zero for all $\beta > 0$
  - ► **CM is decoupled** to a very good approximation

- IT-CI[2] – single-particle trunc.
  - ► sizable dependence of $\Delta\langle \mathrm{H_{int}}\rangle_\beta$ on β and thus **sizable CM contamination**

● IT-NCSM(seq), $N_{\mathrm{max}} = 8$
♦ IT-CI[2], $e_{\mathrm{max}} = 5$

IT-NCSM: Perspectives

importance truncation extends the
range of applicability of the NCSM to
larger N_{max} and A while preserving
most of its advantages

- full **ab-initio spectroscopy** for low-lying states **in p- and sd-shell** ($A \lesssim 40$)
- use eigenstates as input for secondary calculation: **RGM for nucleon-nucleus phase shifts** (→ Petr Navrátil)
- include **three-body interactions**, at least approximately
- **algorithmic and conceptual improvements** to extend the mass range

Epilogue

- **thanks to my group & my collaborators**
  - S. Binder, A. Calci, B. Erler, A. Günther, H. Hergert, M. Hild, H. Krutsch, J. Langhammer, P. Papakonstantinou, S. Reinhardt, F. Schmitt, N. Vogelmann

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