Importance Truncated No-Core Shell Model

for Ab Initio Nuclear Structure

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Overview

- Motivation
- Unitarily Transformed Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Computational Many-Body Methods
  - No-Core Shell Model
  - Importance Truncated NCSM
  - Center-of-Mass Diagnostics

From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

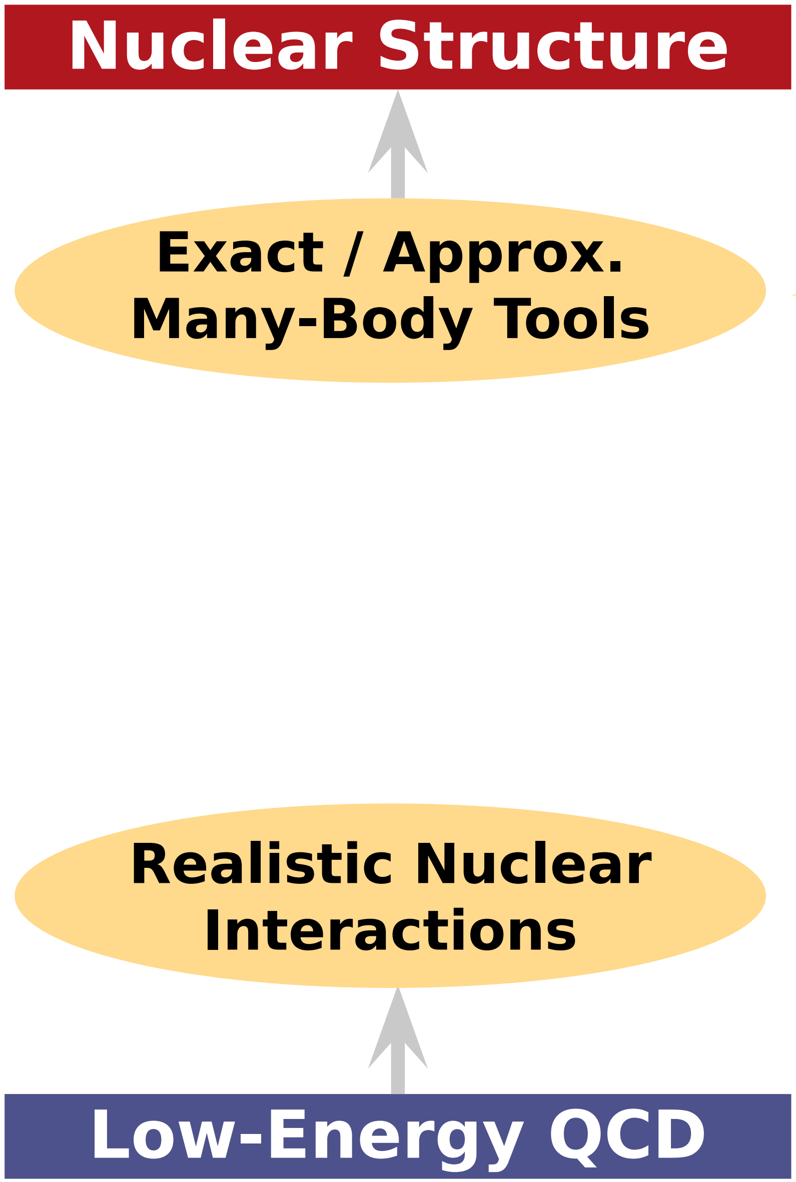
Realistic Nuclear Interactions

↑

Low-Energy QCD

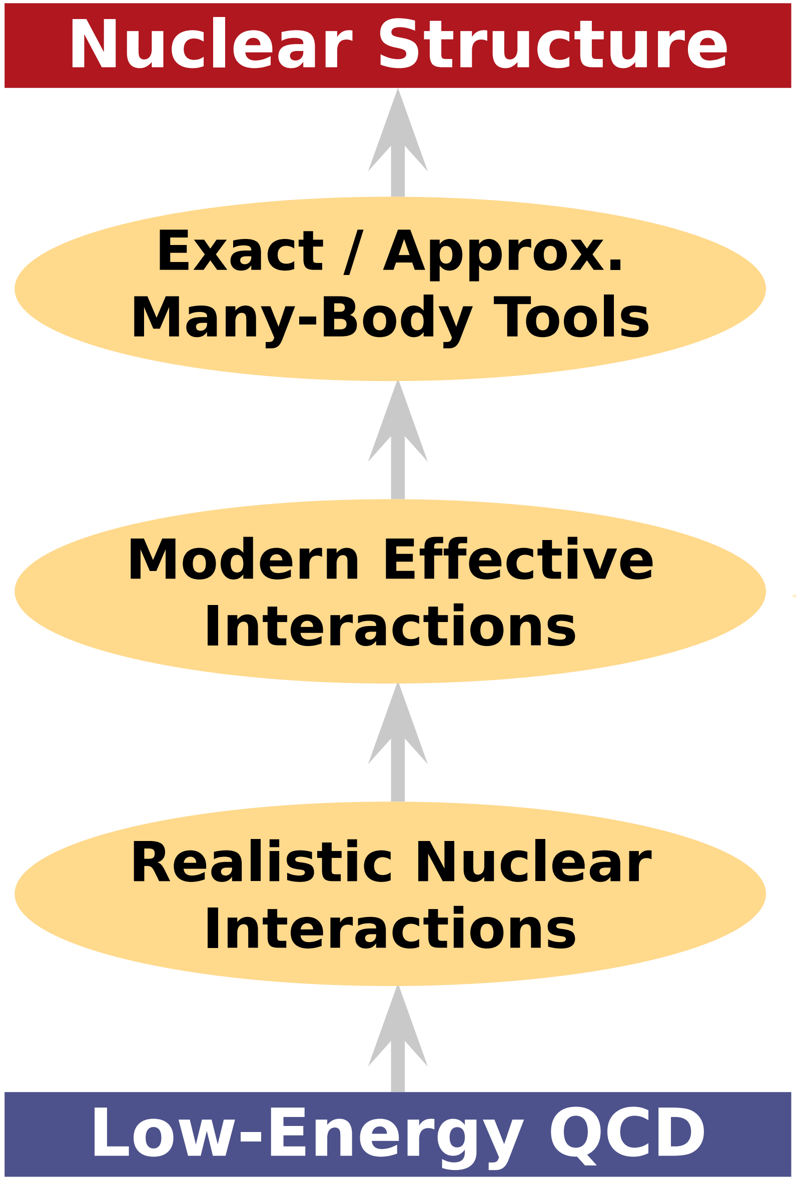
- chiral EFT interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations

From QCD to Nuclear Structure



- ‘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



- 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,...)

Unitarily Transformed Interactions

Unitary Correlation Operator Method (UCOM)

H. Feldmeier et al. — Nucl. Phys. A 632 (1998) 61

T. Neff et al. — Nucl. Phys. A713 (2003) 311

R. Roth et al. — Nucl. Phys. A 745 (2004) 3

R. Roth et al. — Phys. Rev. C 72, 034002 (2005)

Unitary Correlation Operator Method

explicit ansatz for unitary transformation operator **motivated by the physics of short-range correlations**

Central Correlator C_r

- radial distance-dependent shift in the relative coordinate of a nucleon pair

$$g_r = \frac{1}{2}\big[s(r)\, q_r + q_r\, s(r)\big]$$

$$q_r = \tfrac{1}{2}\big[\tfrac{\vec{r}}{r}\cdot\vec{q} + \vec{q}\cdot\tfrac{\vec{r}}{r}\big]$$

Tensor Correlator C_Ω

- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

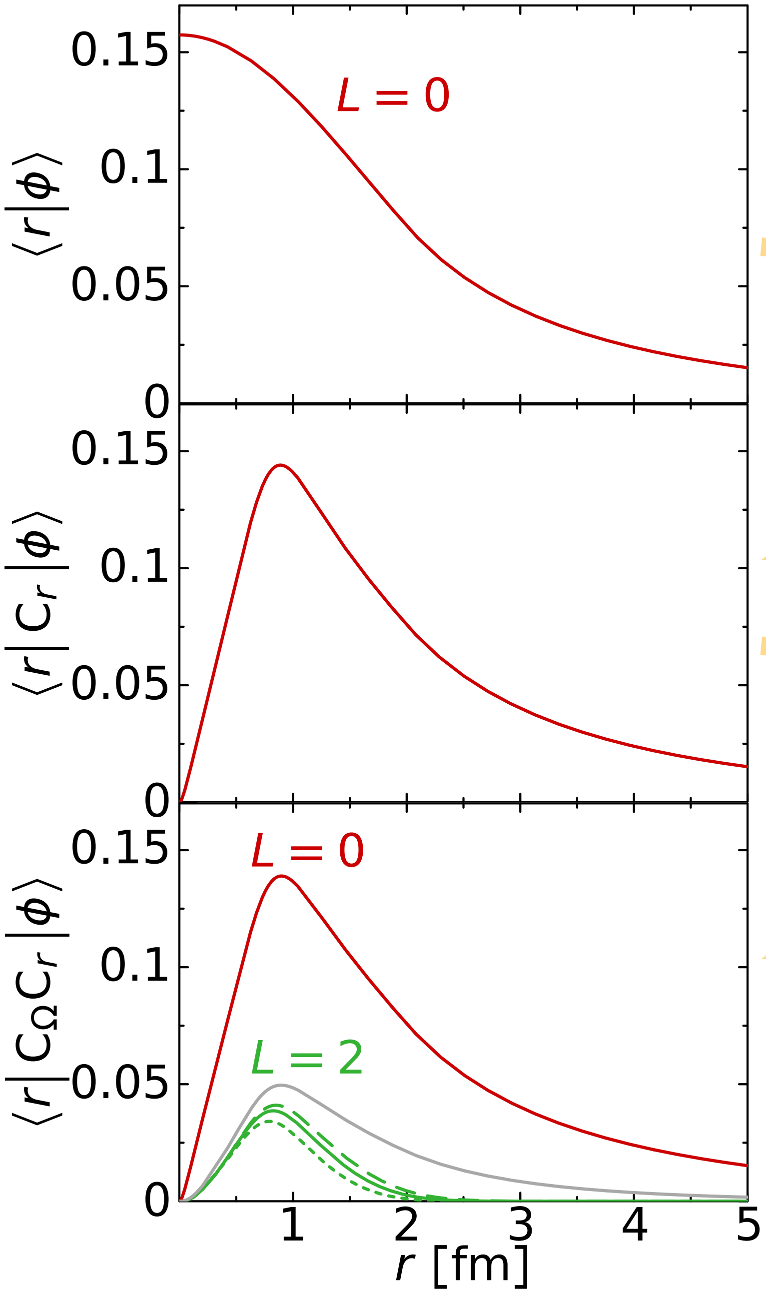
$$g_\Omega = \frac{3}{2}\vartheta(r)\big[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\leftrightarrow\vec{q}_\Omega)\big]$$

$$\vec{q}_\Omega = \vec{q} - \tfrac{\vec{r}}{r}\, q_r$$

$$C = C_\Omega C_r = \exp\Big(-\mathrm{i}\sum_{i<j} g_{\Omega,ij}\Big)\exp\Big(-\mathrm{i}\sum_{i<j} g_{r,ij}\Big)$$

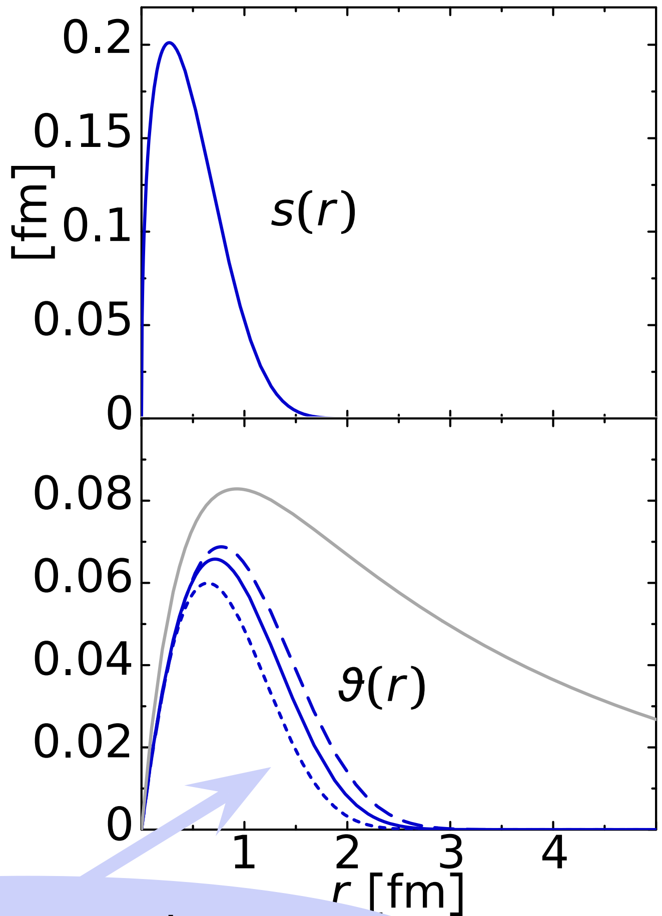
- $s(r)$ and $\vartheta(r)$ depend on & are optimized for initial potential

Correlated States: The Deuteron



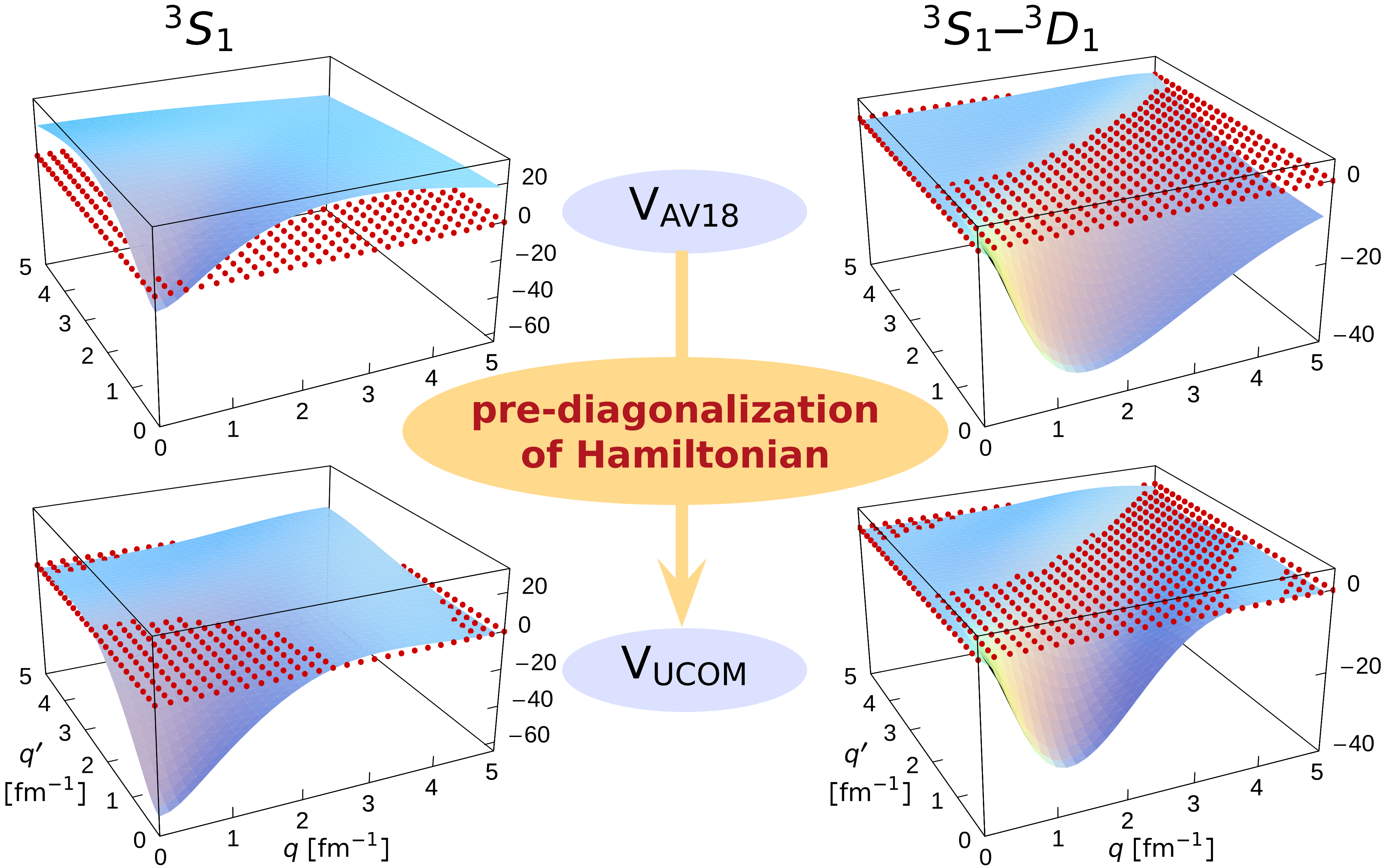
central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

Correlated Interaction: V_{UCOM}



Unitarily Transformed Interactions

Similarity Renormalization Group (SRG)

Hergert & Roth — Phys. Rev. C 75, 051001(R) (2007)
Bogner et al. — Phys. Rev. C 75, 061001(R) (2007)
Roth, Reinhardt, Hergert — Phys. Rev. C 77, 064033 (2008)

Similarity Renormalization Group

flow evolution of the **Hamiltonian to band-diagonal form** with respect to uncorrelated many-body basis

Flow Equation for Hamiltonian

- evolution equation for Hamiltonian

$$\widetilde{H}(\alpha) = C^{\dagger}(\alpha)\, H\, C(\alpha) \qquad \to \qquad \frac{d}{d\alpha}\widetilde{H}(\alpha) = \left[\eta(\alpha), \widetilde{H}(\alpha)\right]$$

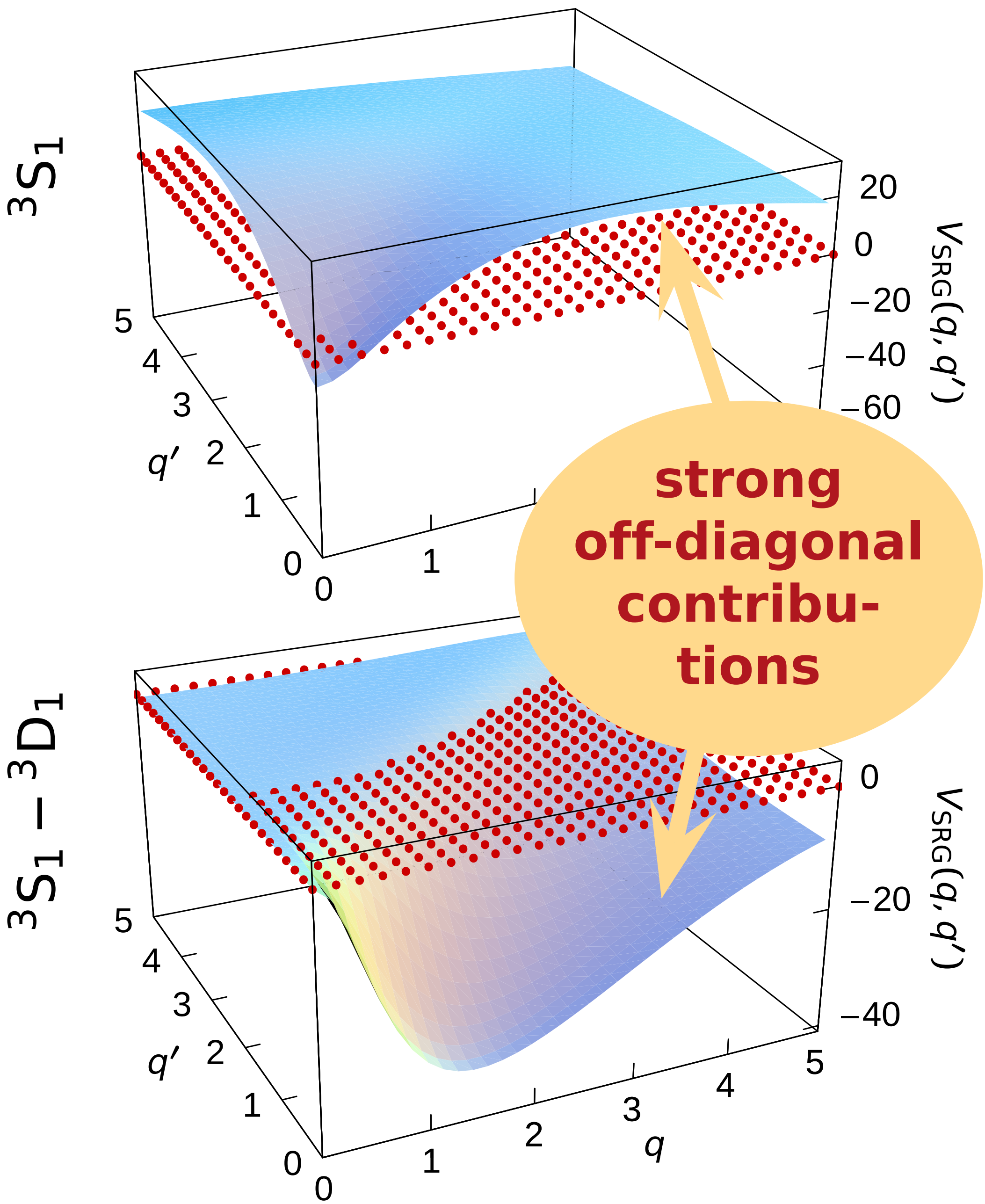
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

$$\eta(\alpha) \overset{2B}{=} \frac{1}{2\mu}\left[\vec{q}^{\,2}, \widetilde{H}(\alpha)\right]$$

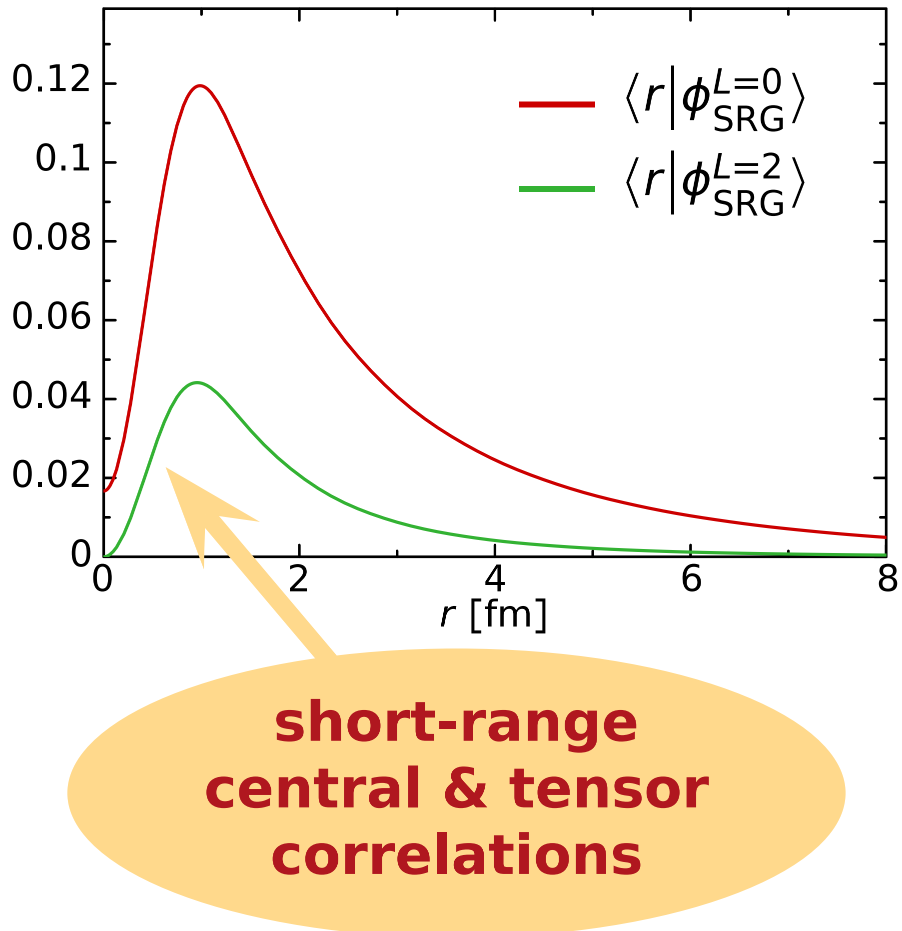
UCOM vs. SRG

$\eta(0)$ has the same structure as UCOM generators g_r & g_Ω

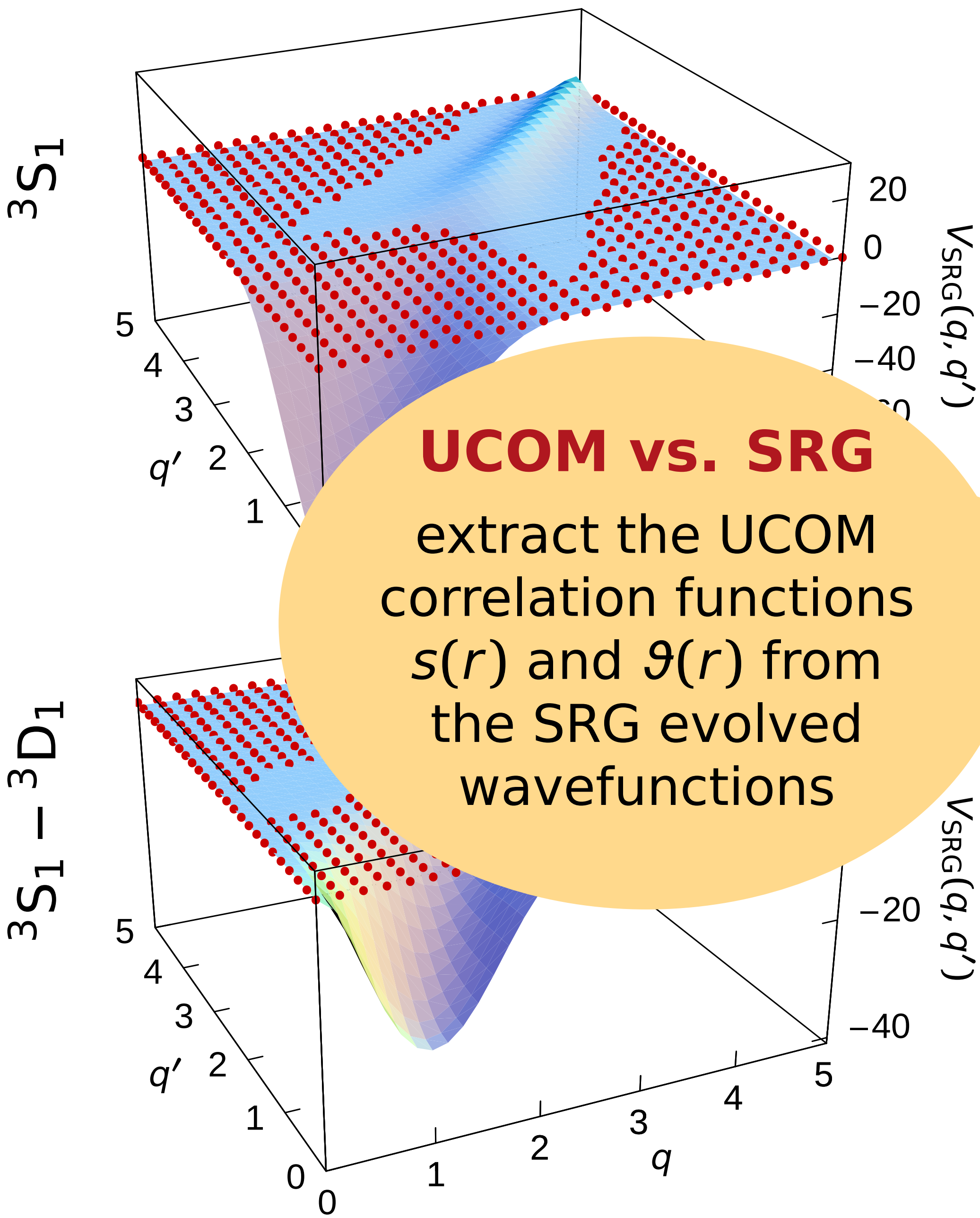
SRG Evolution: The Deuteron



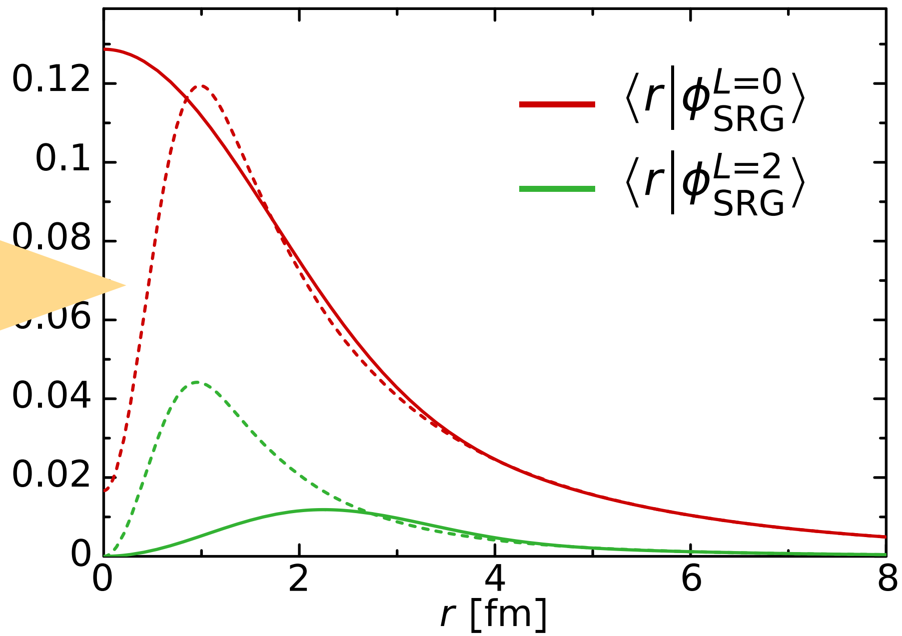
Argonne V18



SRG Evolution: The Deuteron



$\bar{\alpha} = 0.1000\,\text{fm}^4$



UCOM vs. SRG

extract the UCOM correlation functions $s(r)$ and $\vartheta(r)$ from the SRG evolved wavefunctions

Computational Many-Body Methods

No-Core Shell Model

Roth et al. — Phys. Rev. C 72, 034002 (2005)
Roth & Navrátil — in preparation

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

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

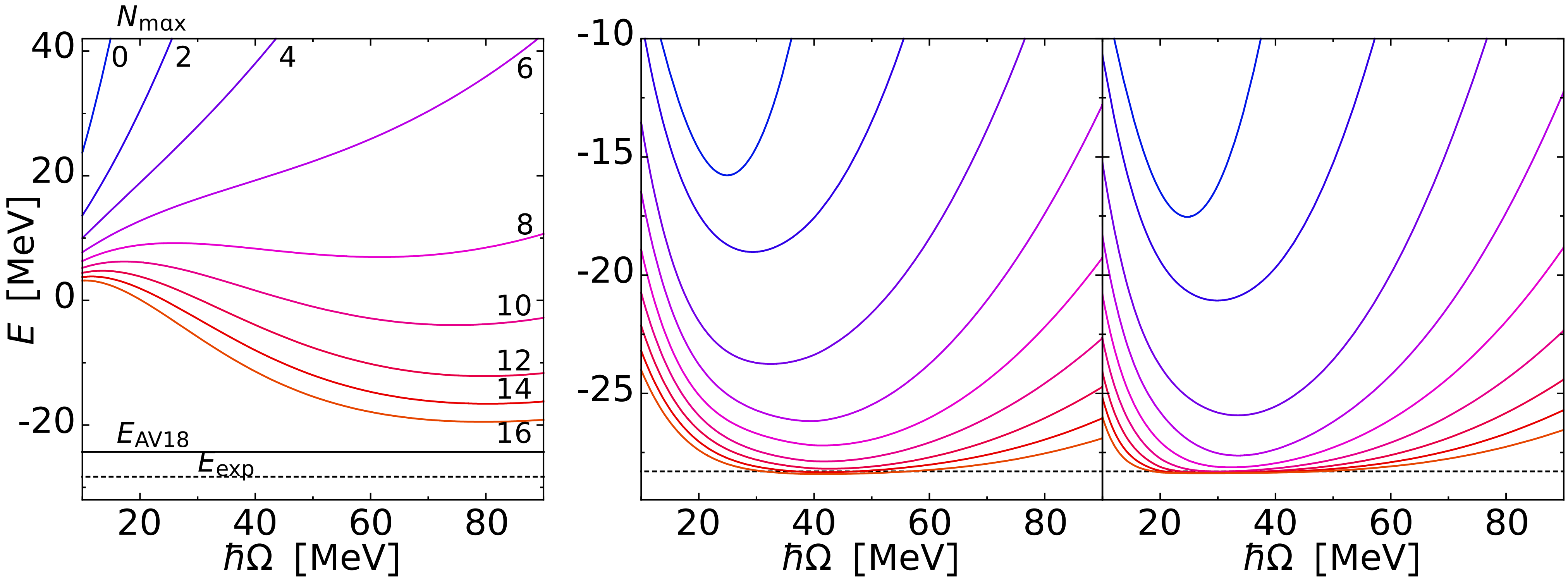
- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\max}\hbar\Omega$
  - ▸ **exact factorization** of intrinsic and CM component is possible
- numerical solution of **eigenvalue problem** for $\mathrm{H}_{\mathrm{int}}$ within $N_{\max}\hbar\Omega$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

^{4}He: NCSM Convergence

V_{AV18}

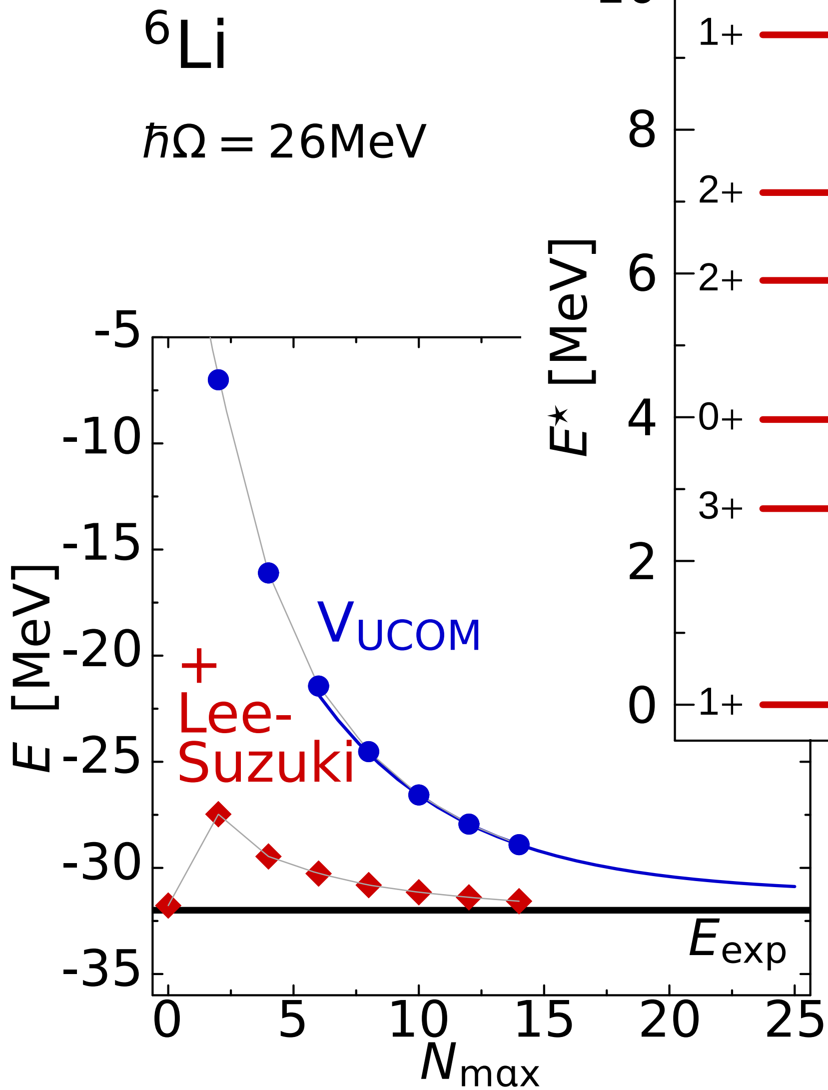
V_{UCOM}
MIN, $I_\vartheta = 0.09\,\mathrm{fm}^3$

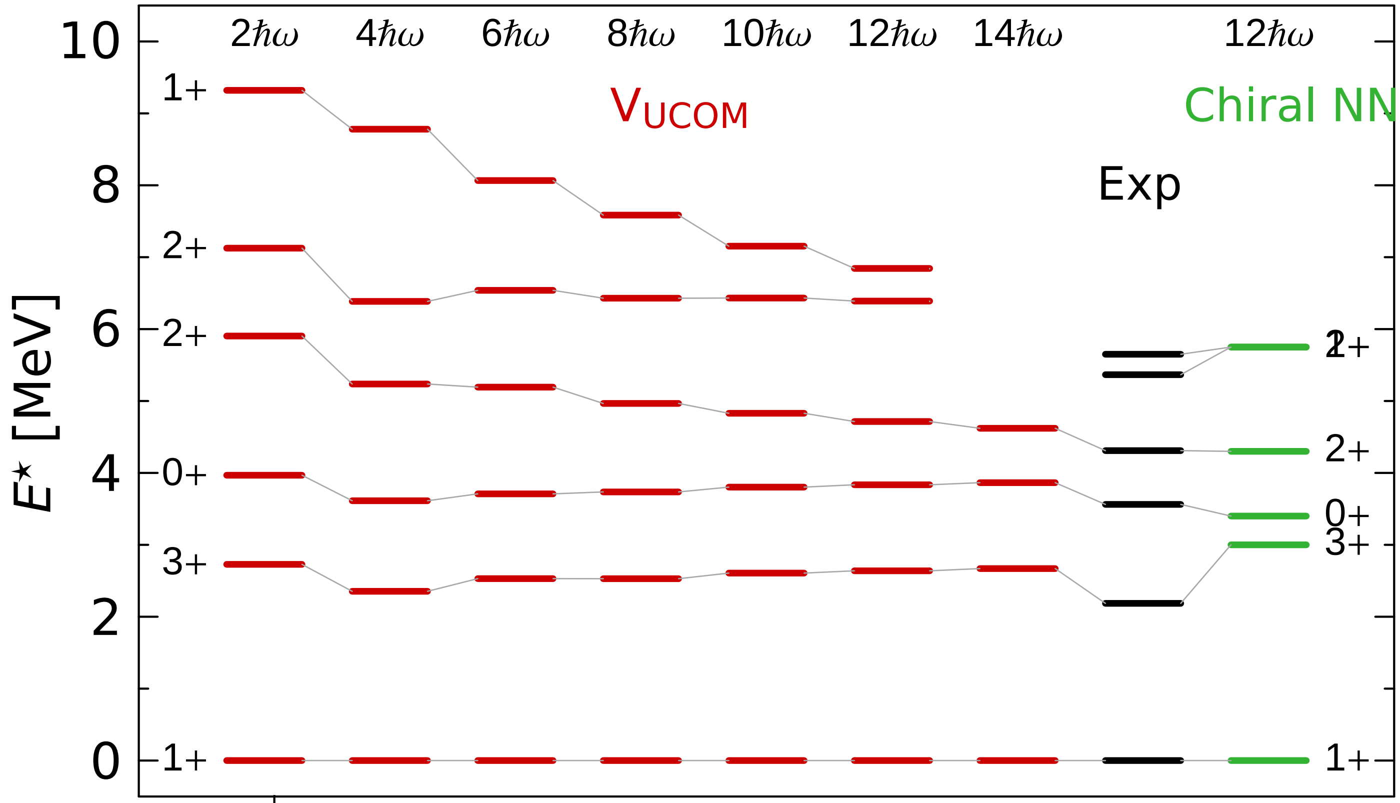
V_{SRG}
$\bar{\alpha} = 0.03\,\mathrm{fm}^4$



- I_ϑ or $\bar{\alpha}$ adjusted such that ^{4}He binding energy is reproduced

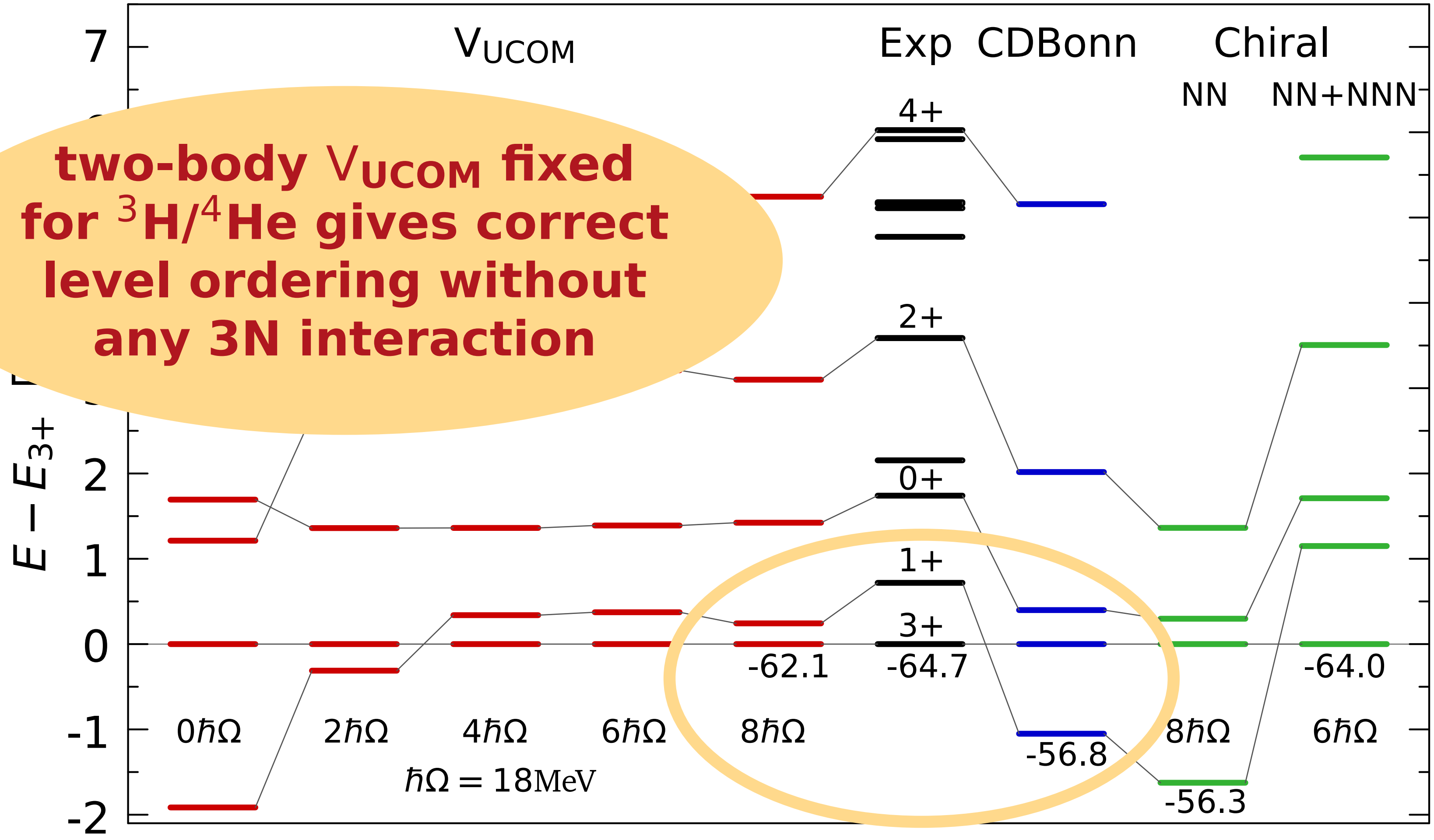
^{6}Li: NCSM throughout the p-Shell





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

^{10}B: Hallmark of a 3N Interaction?



two-body V_{UCOM} fixed for ^{3}H/^{4}He gives correct level ordering without any 3N interaction

Computational Many-Body Methods

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 calcu-
lations are essentially re-
stricted to p-sl
- full 10 o
for ^{16}O r
(basis din

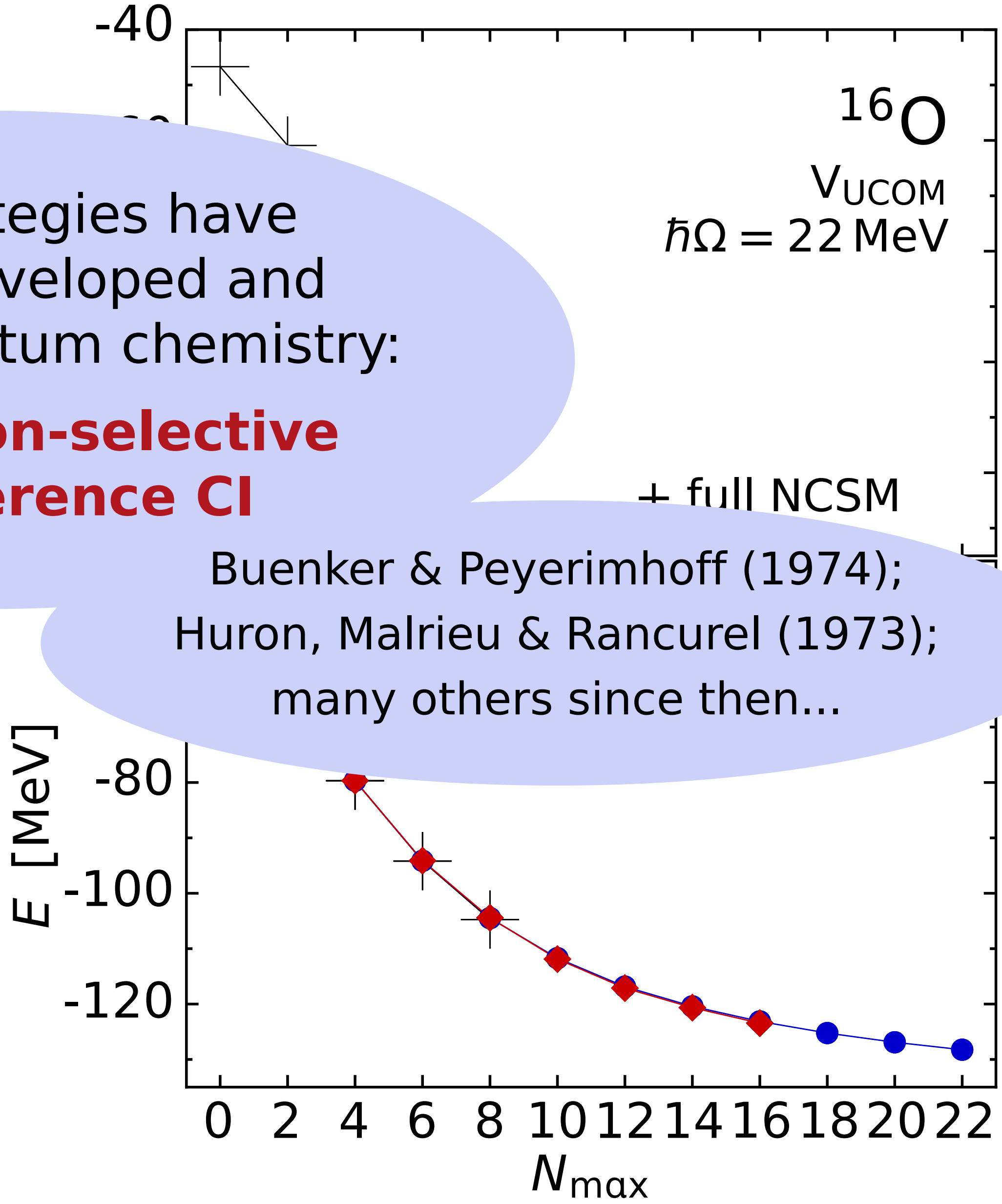
similar strategies have first been developed and applied in quantum chemistry:

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 $\left|\Psi_{\text{ref}}\right\rangle$ for the **target state** within a limited **reference space** $\mathcal{M}_{\text{ref}}$

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

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

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

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

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

Importance Truncation: Iterative Scheme

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

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

- simple iterative scheme for arbitrary many-body model spaces

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

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

❷ solve eigenvalue ...

❸ use dominant c... eigenstate ($|C_\nu|$ ... $|\Psi_{\mathrm{ref}}\rangle$, goto ❶

IT-NCSM(seq)

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

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

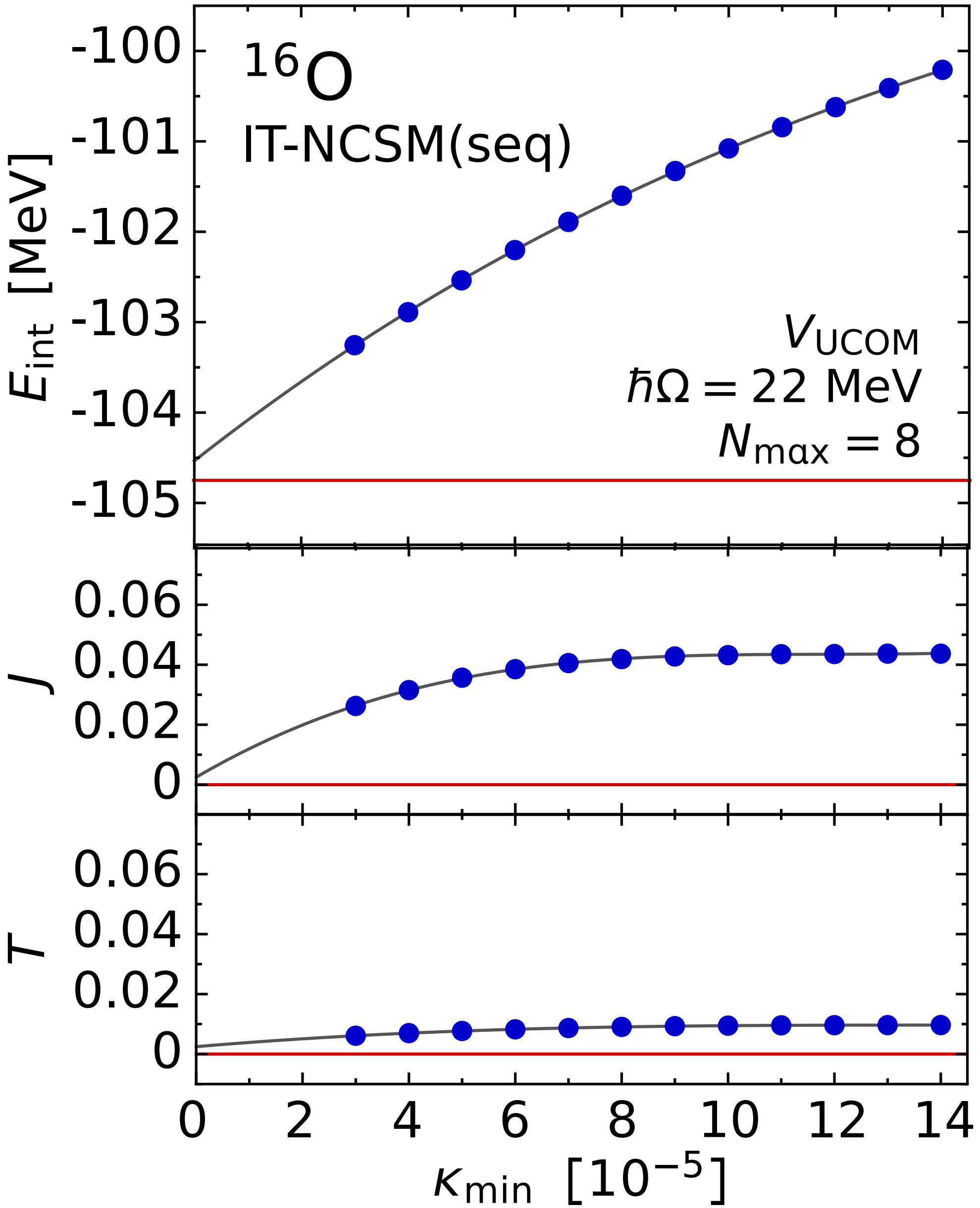
❶ construct importance truncated ... for $N_{\max} + 2$

... e problem

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

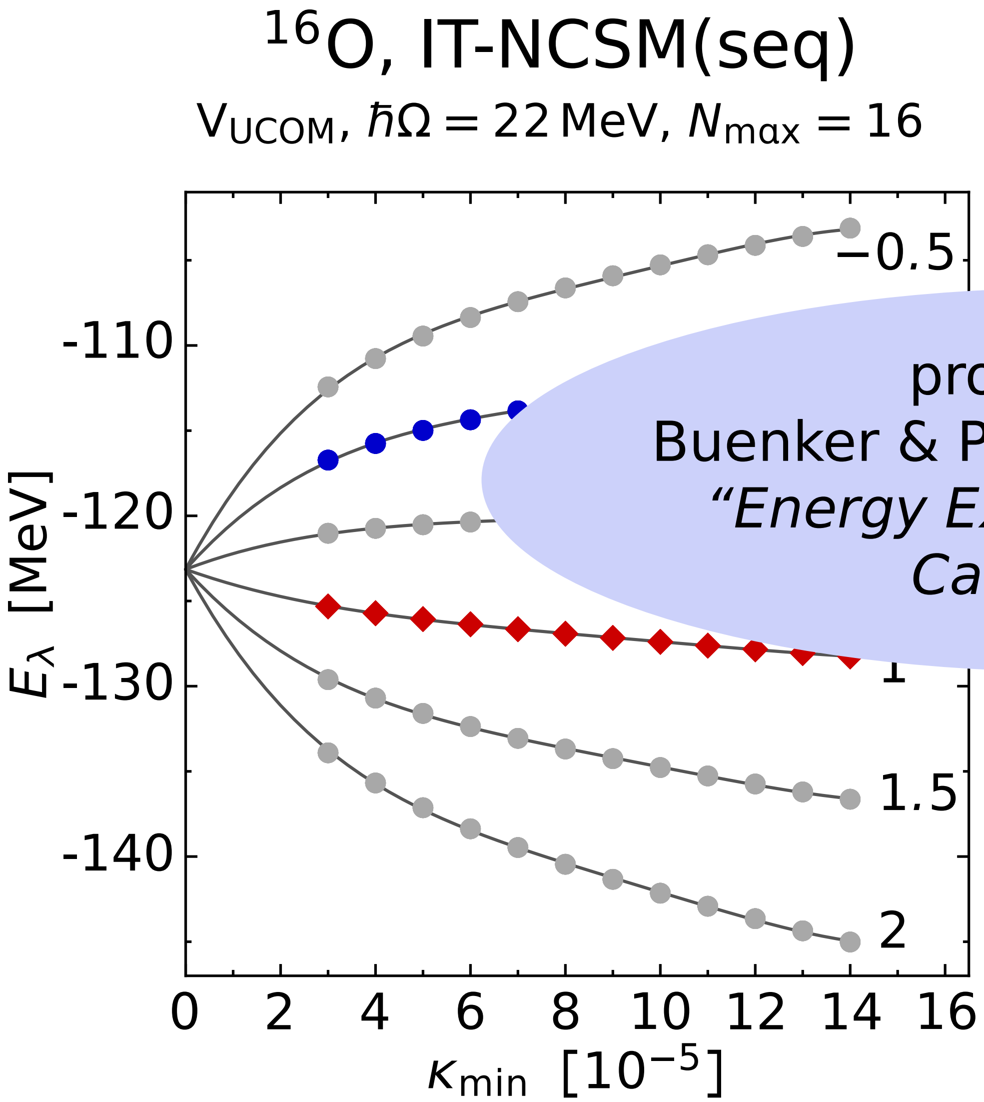
full NCSM model space is recovered in the limit $(\kappa_{\min}, C_{\min}) \to 0$ in IT-NCSM(seq) and IT-NCSM[i_{conv}]

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** $\kappa_{\text{min}} \to 0$ of observables to account for effect of excluded configurations

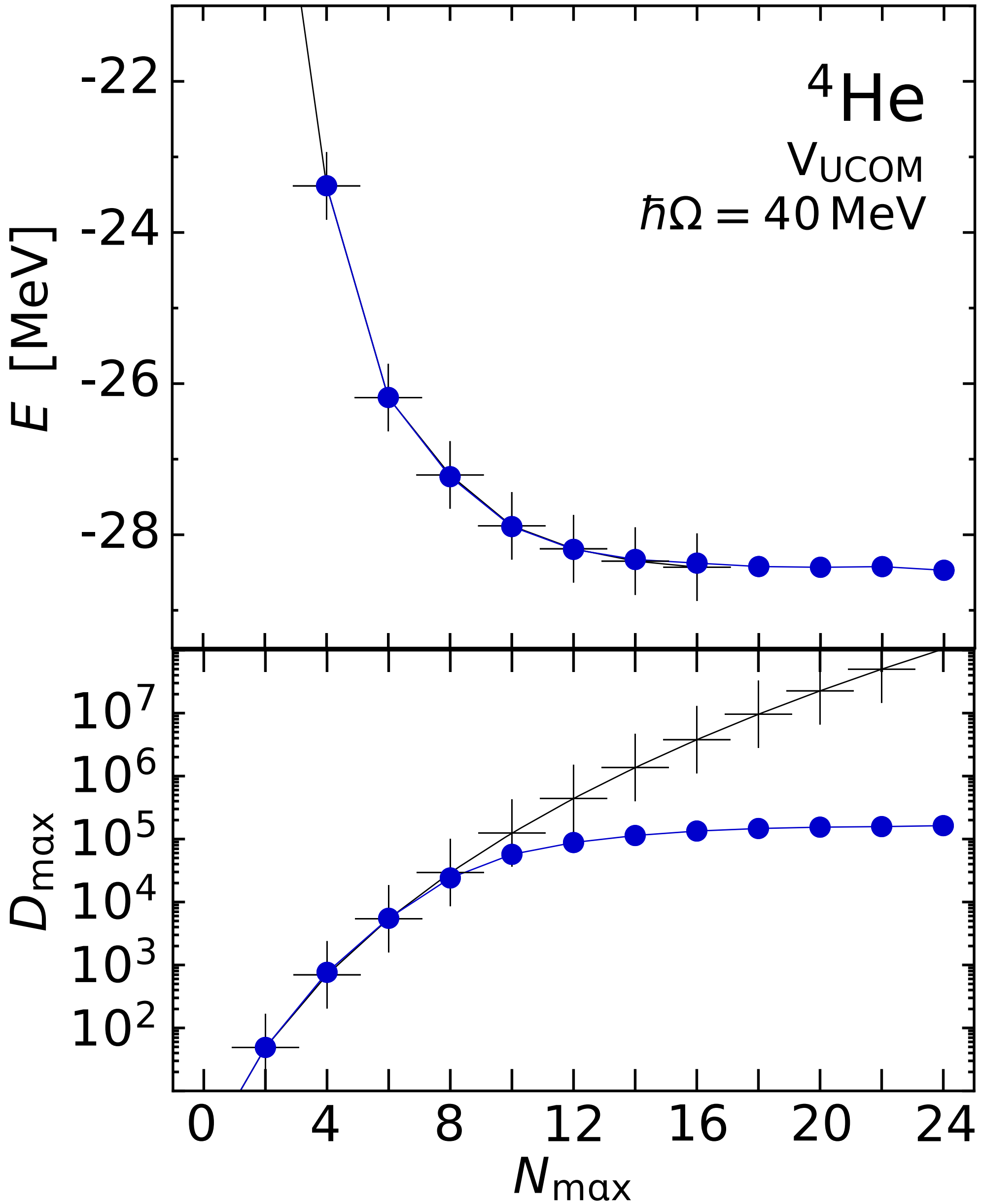
Constrained Threshold Extrapolation



- estimate energy contribution of **excluded states** perturbatively ➔ $\Delta_{excl}(\kappa_{min})$
- ... **eous fit** of combined ... $\lambda\Delta_{excl}(\kappa_{min})$ for set of λ-values with the constraint $E_\lambda(0) = E_{extrap}$
- **robust threshold extrapolation** with error bars determined by variation of the λ set

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

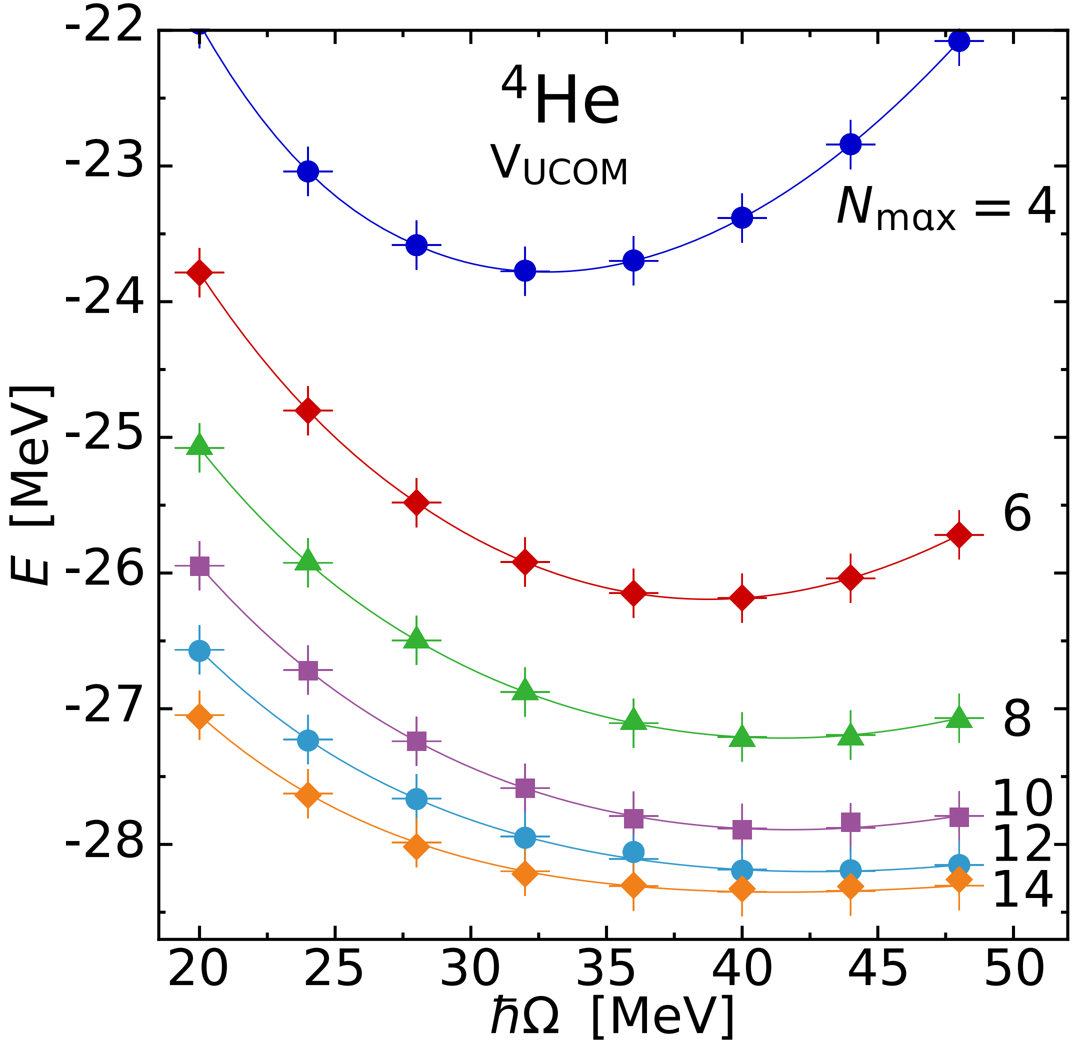
^{4}He: Importance-Truncated NCSM



- **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)

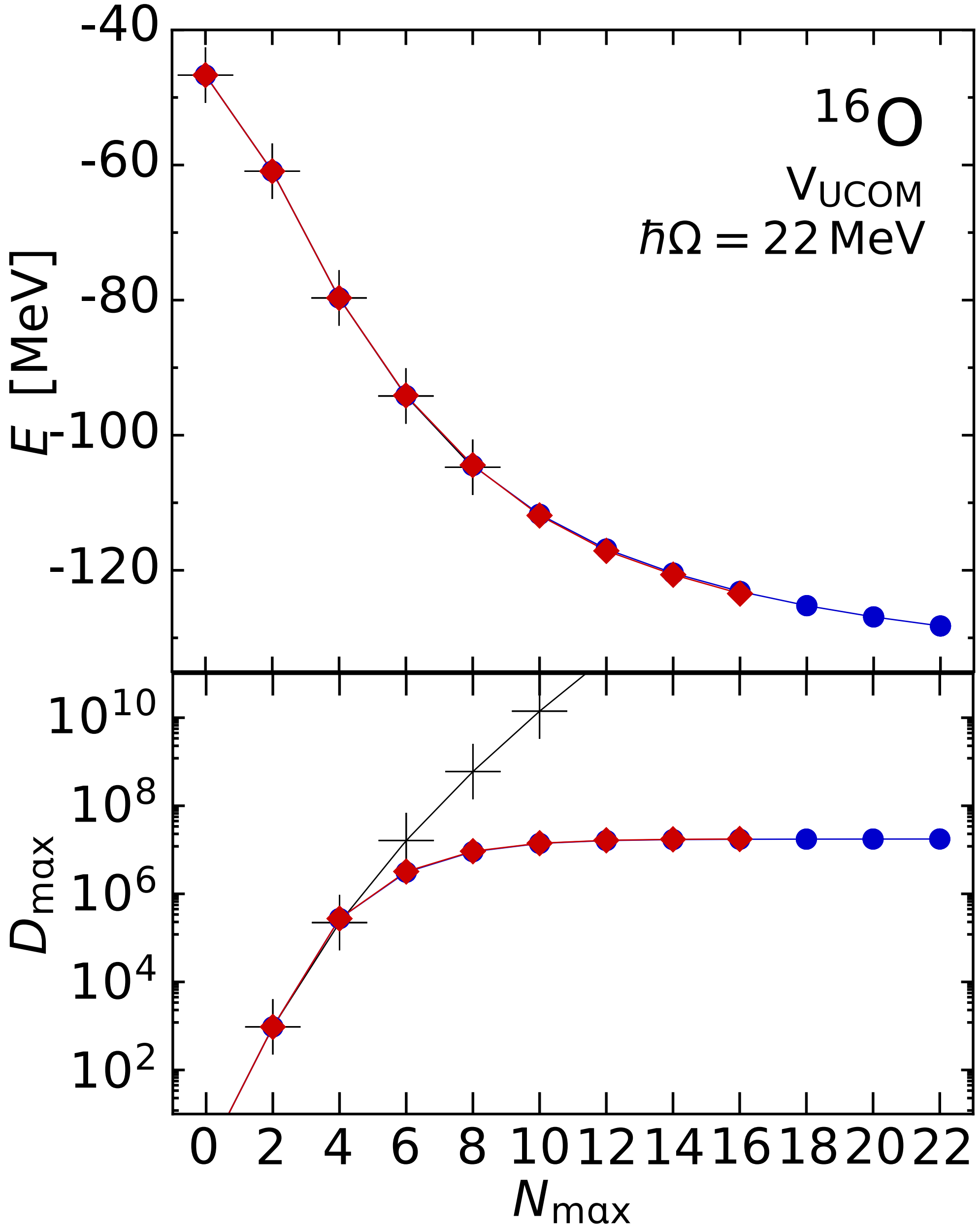
^{4}He: Importance-Truncated NCSM



- **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 $\hbar\Omega$

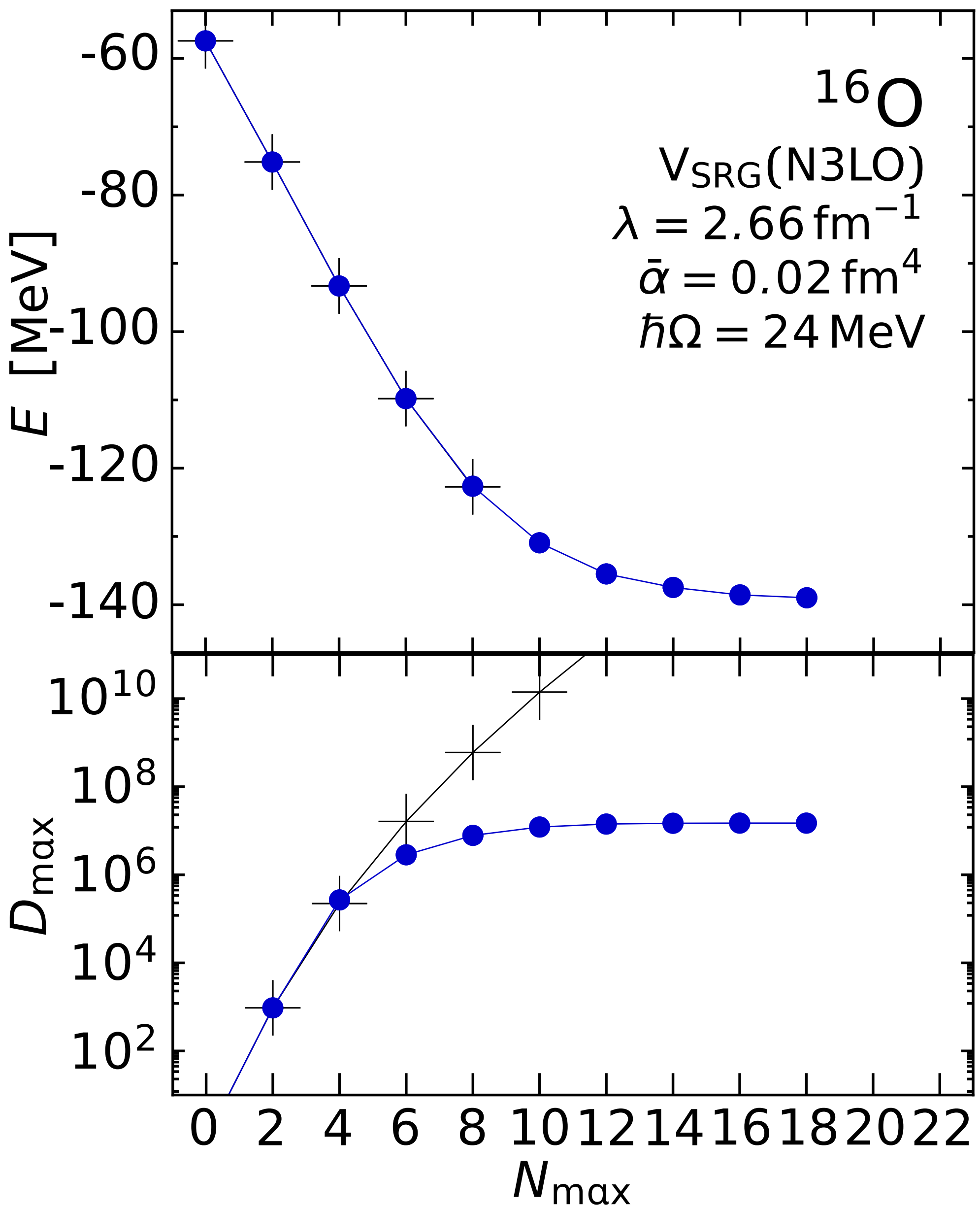
+ full NCSM
● IT-NCSM(seq)

^{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

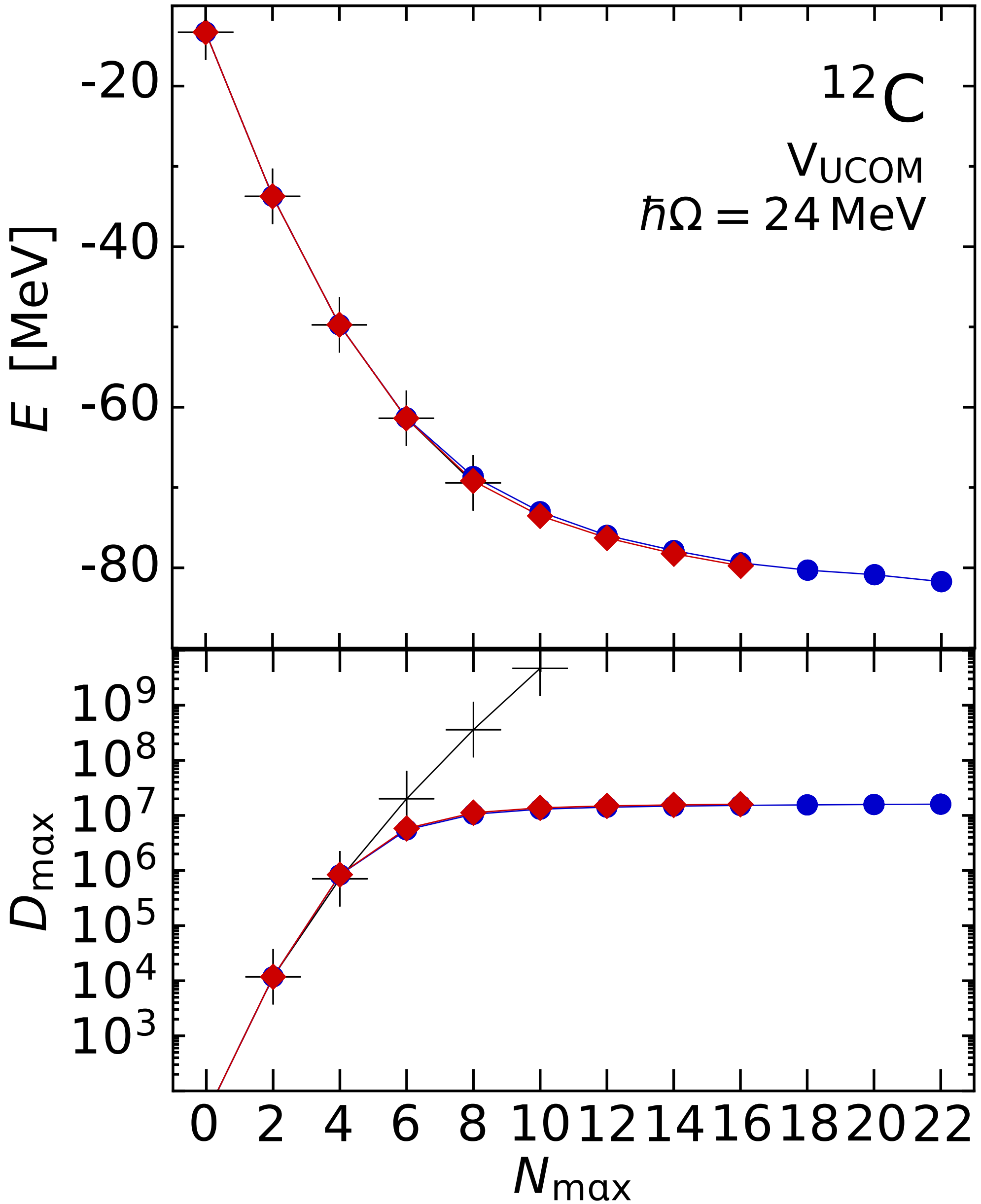
^{16}O: Importance-Truncated NCSM



- **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), $C_{min} = 0.0005$

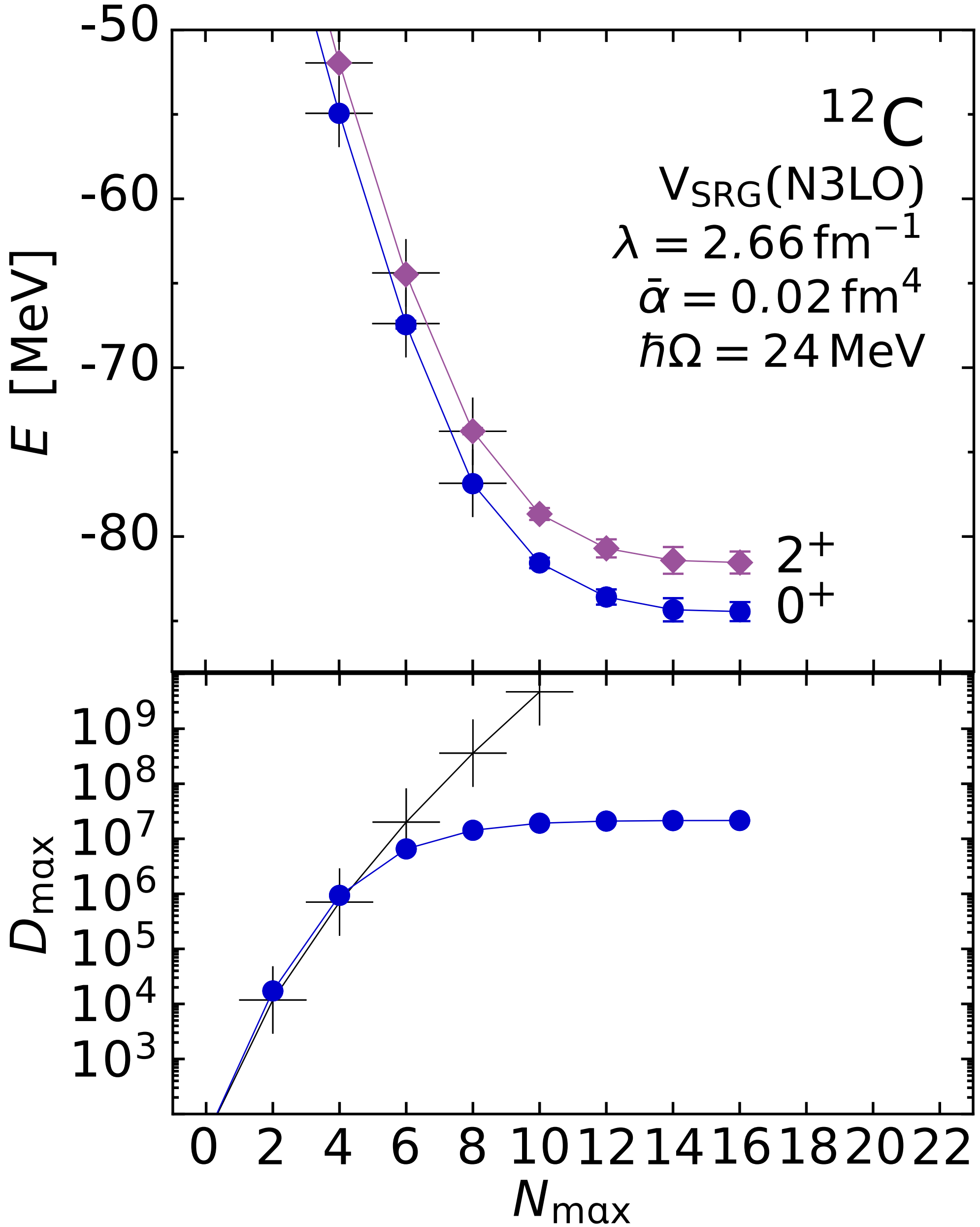
^{12}C: IT-NCSM for Open-Shell Nuclei



- **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

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

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

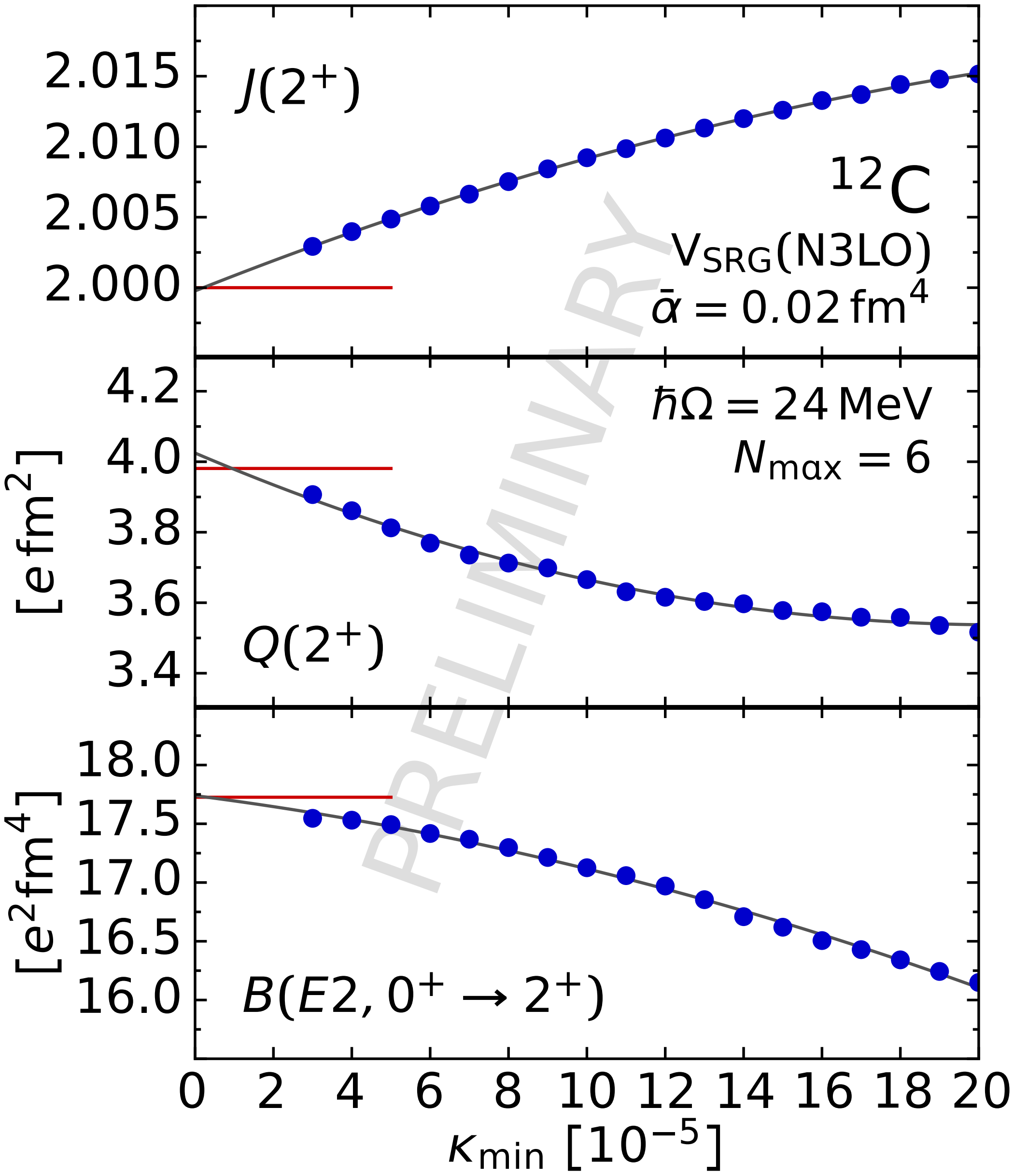


- **target ground & excited states** simultaneously
  - ► separate importance measure $\kappa_\nu^{(n)}$ for each target state
  - ► basis state is included if $|\kappa_\nu^{(n)}| \geq \kappa_{\text{min}}$ for any n
- dimension of importance truncated space **grows linearly** with # of target states

+ full NCSM

●♦ IT-NCSM(seq), $C_{\text{min}} = 0.0005$

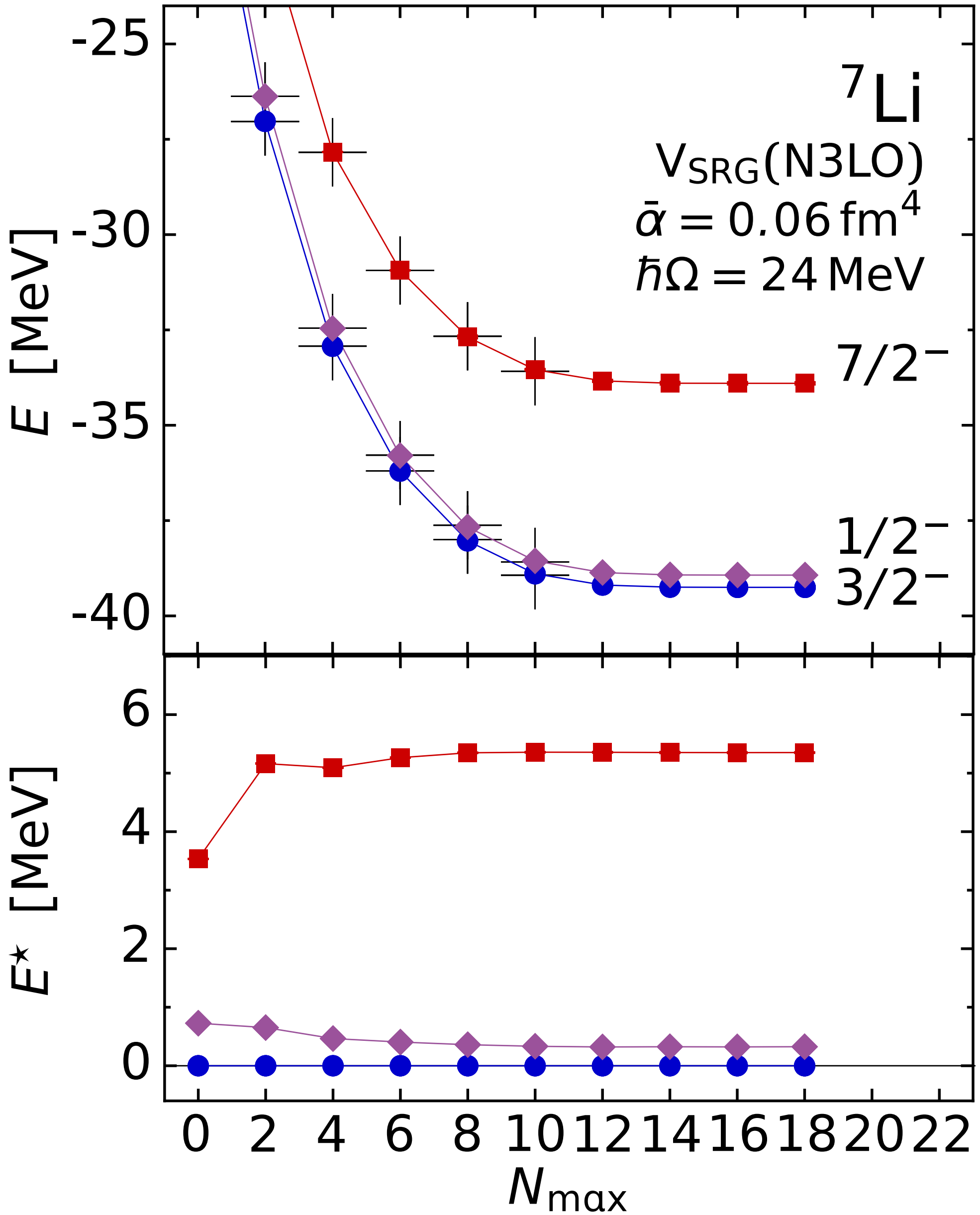
^{12}C: IT-NCSM for Spectroscopy



- access to **spectroscopic observables** via eigenstates
- multipole moments, transition strengths, transition formfactors, densities,...
- simple threshold extrapolation essentially **reproduces full NCSM results**

systematic spectroscopy in p- and sd-shell with large $N_{max}\hbar\Omega$ spaces

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



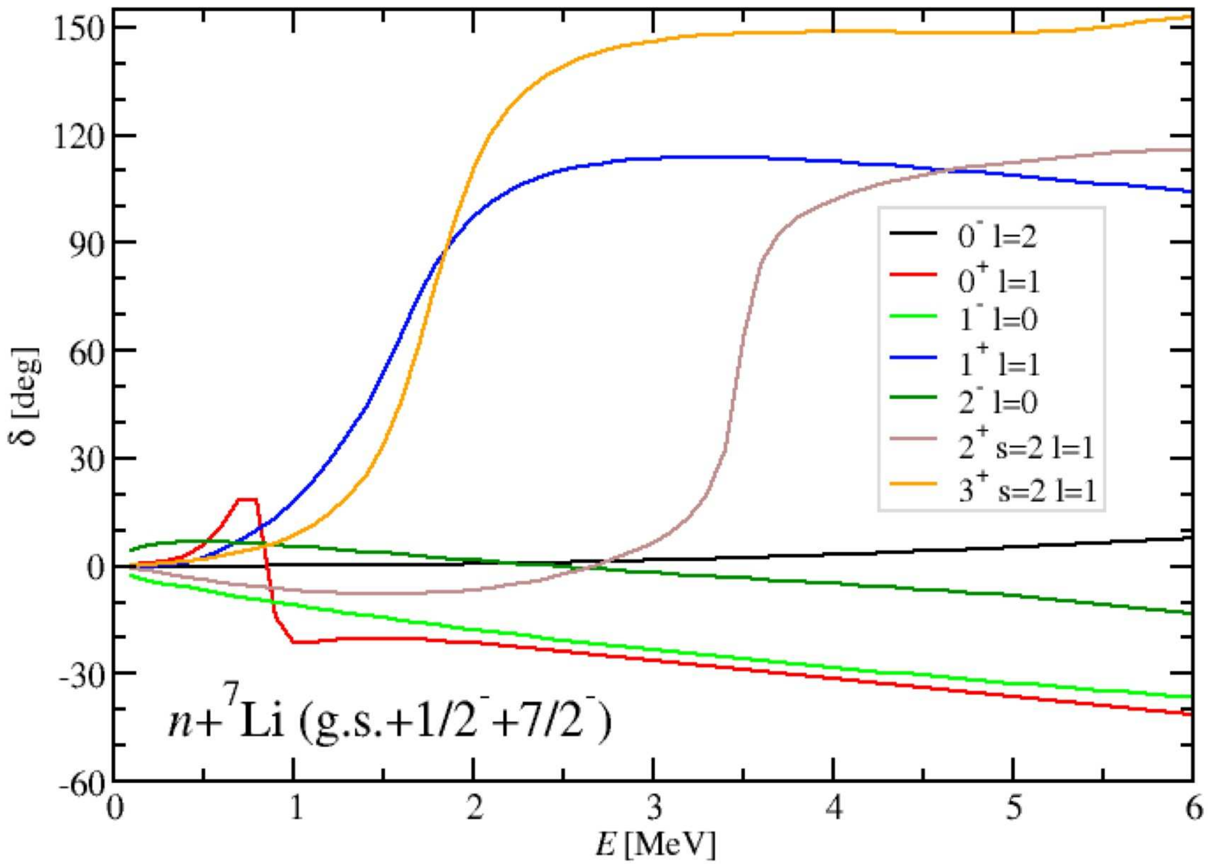
- IT-NCSM(seq) treats a ground state & low-lying excited states for open- and closed-shell nuclei **on the same footing**
- **excellent agreement with full NCSM** calculations in all cases

+ full NCSM
●♦■ IT-NCSM(seq), $C_{min} = 0.0002$

RGM & IT-NCSM: Ab Initio Reactions

with Petr Navrátil & Sofia Quaglioni (LLNL)

- **IT-NCSM wave function as input for RGM** (Resonating Group Method) calculations of low-energy nucleon-nucleus scattering



- using 3 lowest ^{7}Li states
- so-far up to $N_{max} = 14$, here $N_{max} = 8$
- phase-shifts with full NCSM and IT-NCSM input agree
- 2 bound states for ^{8}Li
- 4 resonances: 3^+ and 1^+ are known, 0^+ and 2^+ resonances are predictions

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** $\kappa_{\mathrm{min}} \rightarrow 0$ 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
- **approximate size-extensivity** after threshold extrapolation in IT-NCSM(seq) or IT-NCSM[i_{conv}] – **no explicit *npnh* truncation**
- ✘ computationally still demanding

Computational Many-Body Methods

Center-of-Mass Diagnostics

Roth, Gour & Piecuch — arXiv:0906.4276

Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)

CM Problem: Bane of Nuclear Structure

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

$$|\Psi\rangle = |\psi_{\text{int}}\rangle \otimes |\psi_{\text{cm}}\rangle$$

- factorization is manifest in Jacobi-coordinate methods

- Slater-determinant methods: only the $N_{\max}\hbar\Omega$ **space** build from **harmonic oscillator basis** allows for exact factorization

- for any other truncation or single-particle basis one has to ask:
  - Is there a **coupling** between intrinsic and CM component?
  - How strong is the **effect on observables** of interest?

- **CM diagnostics**: perturb CM part and check for effect on the intrinsic part via expectation values of intrinsic observables

CM Diagnostics

- consider model space built from **HO single-particle basis**

- solve many-body problem with **modified Hamiltonian** (following Palumbo, Gloeckner & Lawson)

$$H_\beta = H_{int} + \beta \, H_{cm}$$

  including additional HO Hamiltonian w.r.t. the CM

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

- Why this particular H_{cm} operator?
  - the exact ground state of H_{cm} can be represented in model space (embedded $0\hbar\Omega$ space)
  - if there is factorization, then H_{cm} will not induce a coupling

CM Diagnostics

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

$$\langle H_{\text{int}} \rangle_\beta = \langle \Psi_\beta | H_{\text{int}} | \Psi_\beta \rangle$$

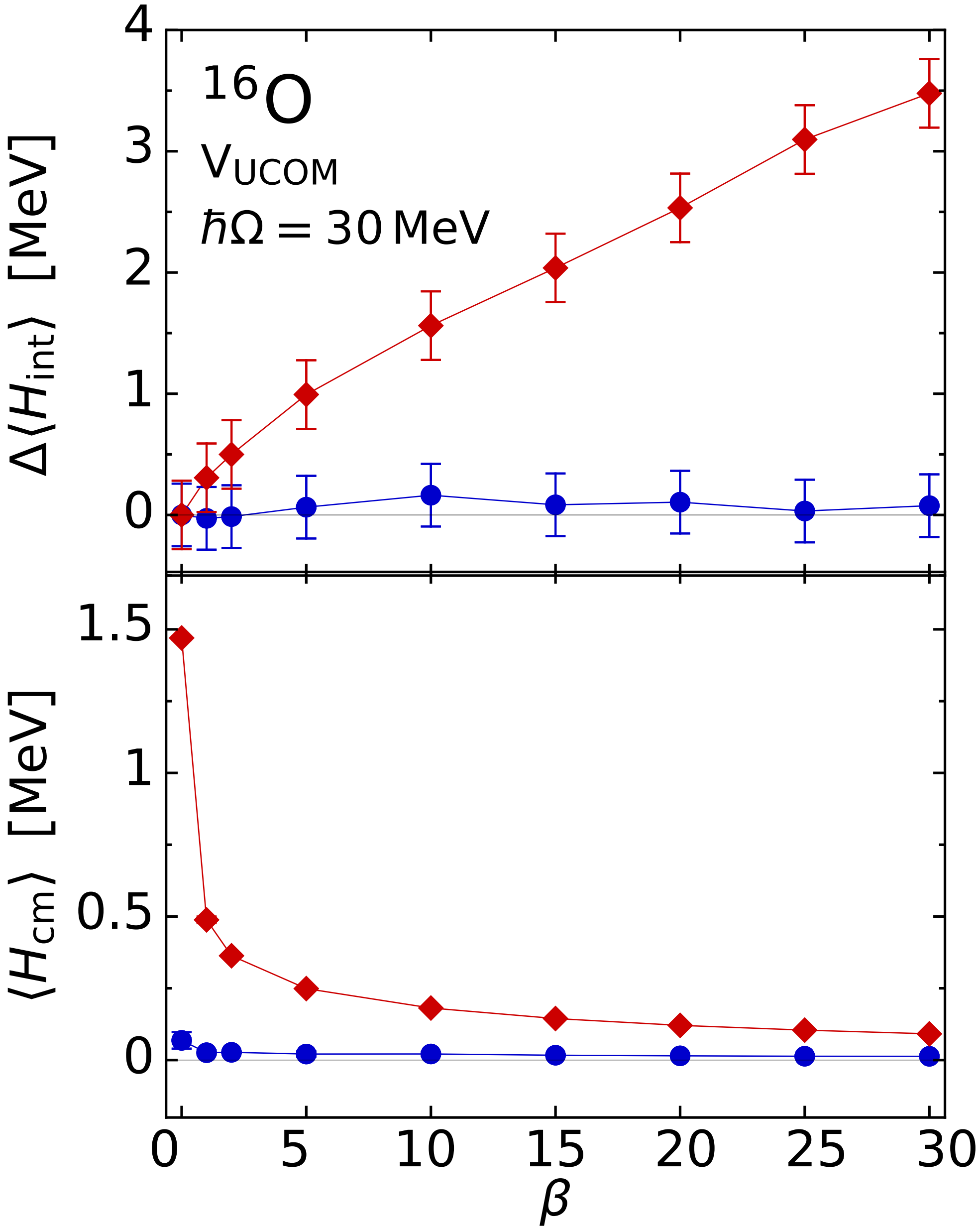
→ any dependence of $\langle H_{\text{int}} \rangle_\beta$ on β indicates an unphysical coupling between intrinsic and CM motion

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

$$\langle H_{\text{cm}} \rangle_\beta = \langle \Psi_\beta | H_{\text{cm}} | \Psi_\beta \rangle$$

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

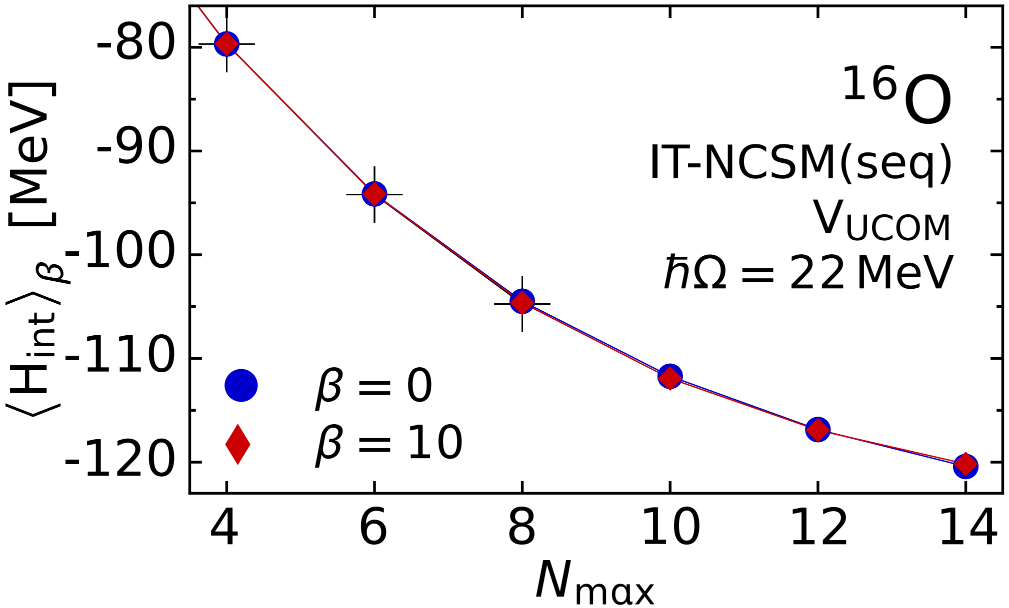
CM Diagnostics: IT-NCSM vs. IT-CI

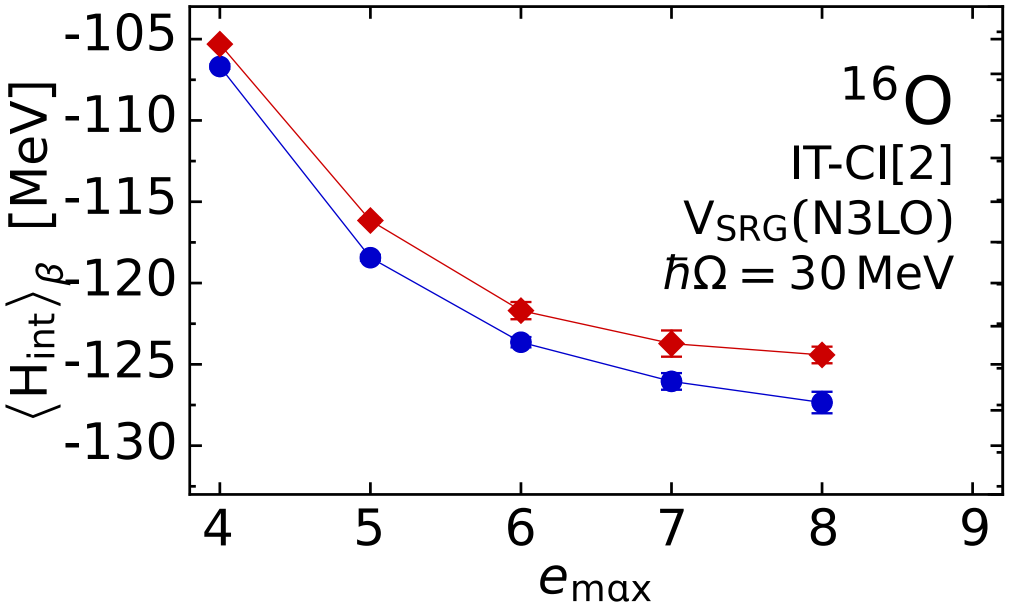


- IT-NCSM(seq) – $N_{max}\hbar\Omega$ trunc.
  - ▸ $\Delta\langle H_{int}\rangle_\beta$ and $\langle H_{cm}\rangle_\beta$ are practically zero for all $\beta > 0$
  - ▸ **CM is decoupled** to a very good approximation
- IT-CI[2] – single-particle trunc.
  - ▸ sizable dependence of $\Delta\langle H_{int}\rangle_\beta$ on β and thus **sizable CM contamination**

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

CM Diagnostics: IT-NCSM vs. IT-CI





- IT-NCSM shows excellent decoupling for all model spaces
  - ► importance truncation preserves the **translational invariance** of the $N_{max}\hbar\Omega$ space
- IT-CI exhibits **sizable coupling** which does not improve with increasing e_{max}

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**
- 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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  - P. Navrátil

    Lawrence Livermore National Laboratory, USA
  - P. Piecuch, J. Gour

    Michigan State University, USA
  - H. Feldmeier, T. Neff,...

    Gesellschaft für Schwerionenforschung (GSI)

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HIC for FAIR

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