EENEN'10 Workshop

Importance Truncated NCSM for Ab Initio Spectroscopy

Robert Roth
Institut für Kernphysik

TECHNISCHE UNIVERSITÄT DARMSTADT

Strategy: QCD-based Nuclear Structure

Experimental Observables

'Exact' Ab Initio Methods	**Approximate Methods**
▪ exact numerical solution of many-body problem	▪ approximate treatment of many-body problem
▪ rigorous nuclear structure predictions for given Hamiltonian	▪ addressing specific observables & nuclei
▪ computationally demanding	▪ feasible for all masses

Unitarily Transformed Interactions

- account for short-range correlations by phase-shift conserving unitary transformation
- improve convergence & control 3N interactions

QCD-based Nuclear Interactions

Unitarily Transformed Interactions

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)
Roth et al. — Phys. Rev. C 72, 034002 (2005)
Roth et al. — Nucl. Phys. A 745, 3 (2004)

Unitary Correlation Operator Method

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

Static Unitary Transformation

$$\widetilde{\mathrm{H}} = \mathrm{C}_r^\dagger \mathrm{C}_\Omega^\dagger \,\mathrm{H}\, \mathrm{C}_\Omega \mathrm{C}_r \qquad \text{with} \qquad \mathrm{C}_\circ = \exp\Big(-\mathrm{i} \sum_{i<j} \mathrm{g}_{\circ,ij}\Big)$$

Central Correlator C_r

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

$$\mathrm{g}_r = \frac{1}{2}\big[s(\mathrm{r})\,\mathrm{q}_r + \mathrm{q}_r\, s(\mathrm{r})\big]$$

Tensor Correlator C_Ω

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

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

- $s(r)$ and $\vartheta(r)$ are optimized for the initial potential

Similarity Renormalization Group

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

Dynamic Flow Equation

- evolution equation for Hamiltonian

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

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

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

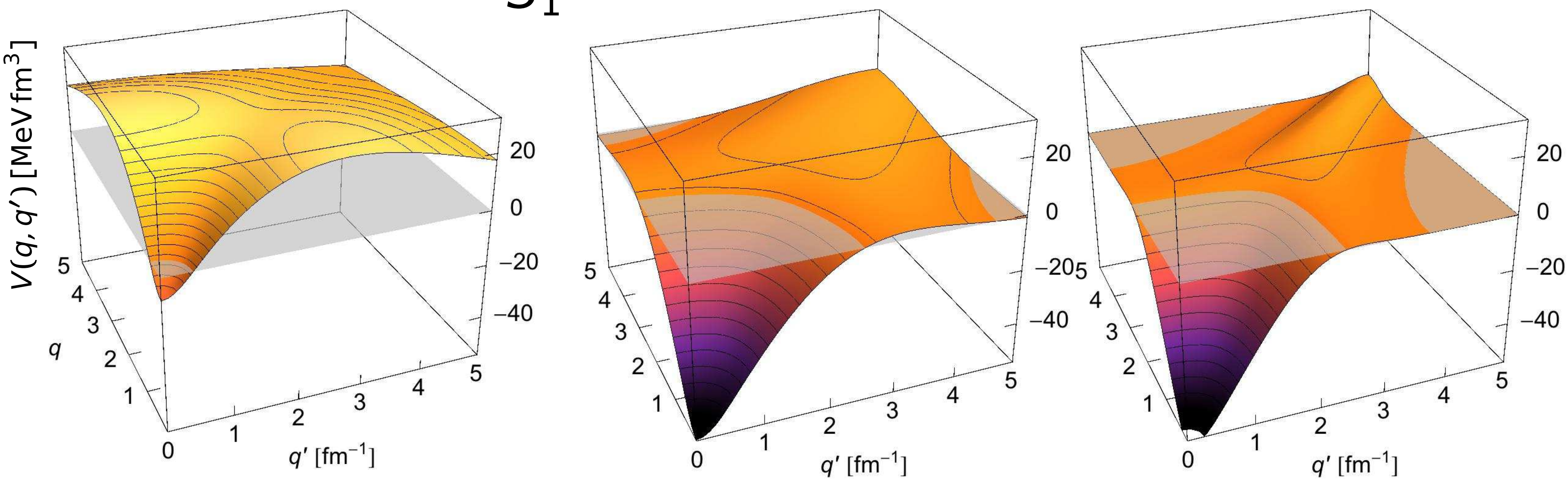
UCOM vs. SRG

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

Momentum-Space Matrix Elements

V_{AV18} | V_{UCOM} MIN, $I_\vartheta = 0.09\,\text{fm}^3$ | V_{SRG} $\bar{\alpha} = 0.03\,\text{fm}^4$

$^3S_1$



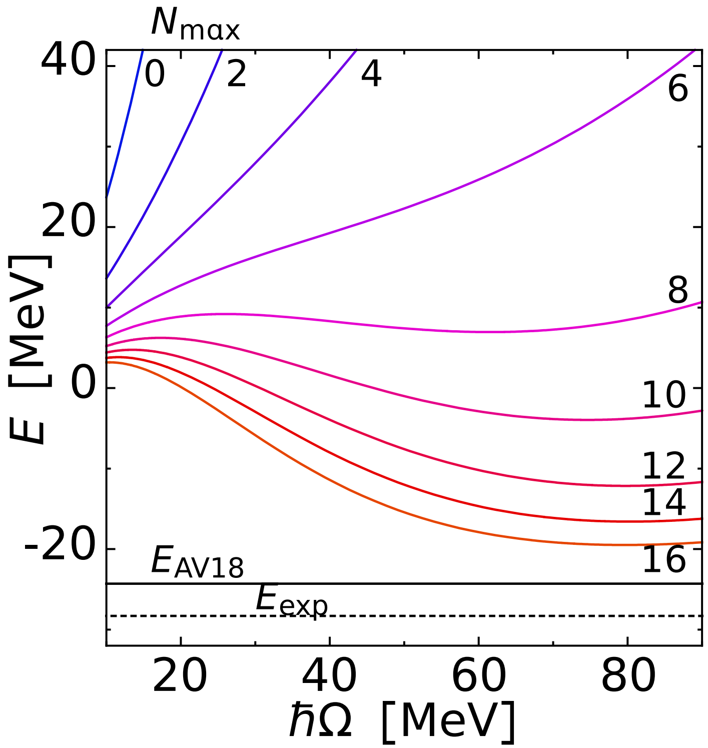
- suppression of off-diagonal matrix elements → pre-diagonalization

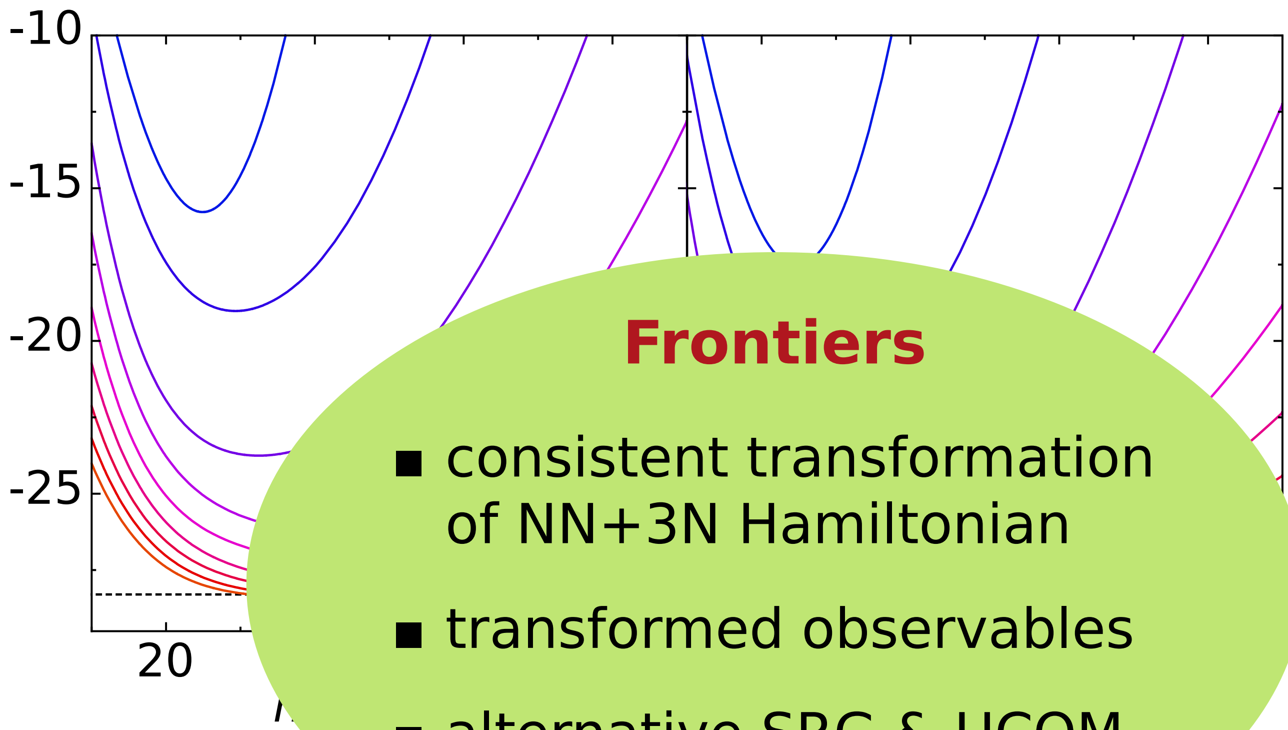
Convergence Properties: NCSM for ^{4}He

V_{AV18}

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

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





Frontiers

- consistent transformation of NN+3N Hamiltonian
- transformed observables
- alternative SRG & UCOM generators

- I_ϑ or $\bar{\alpha}$ adjusted such that ^{4}He binding … oduced

Importance Truncated No-Core Shell Model

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)

Importance Truncated NCSM

- converged NCSM calcu-
lations are essentially re
stricted to low
- full 10 o
for ^{16}O r
(basis dim

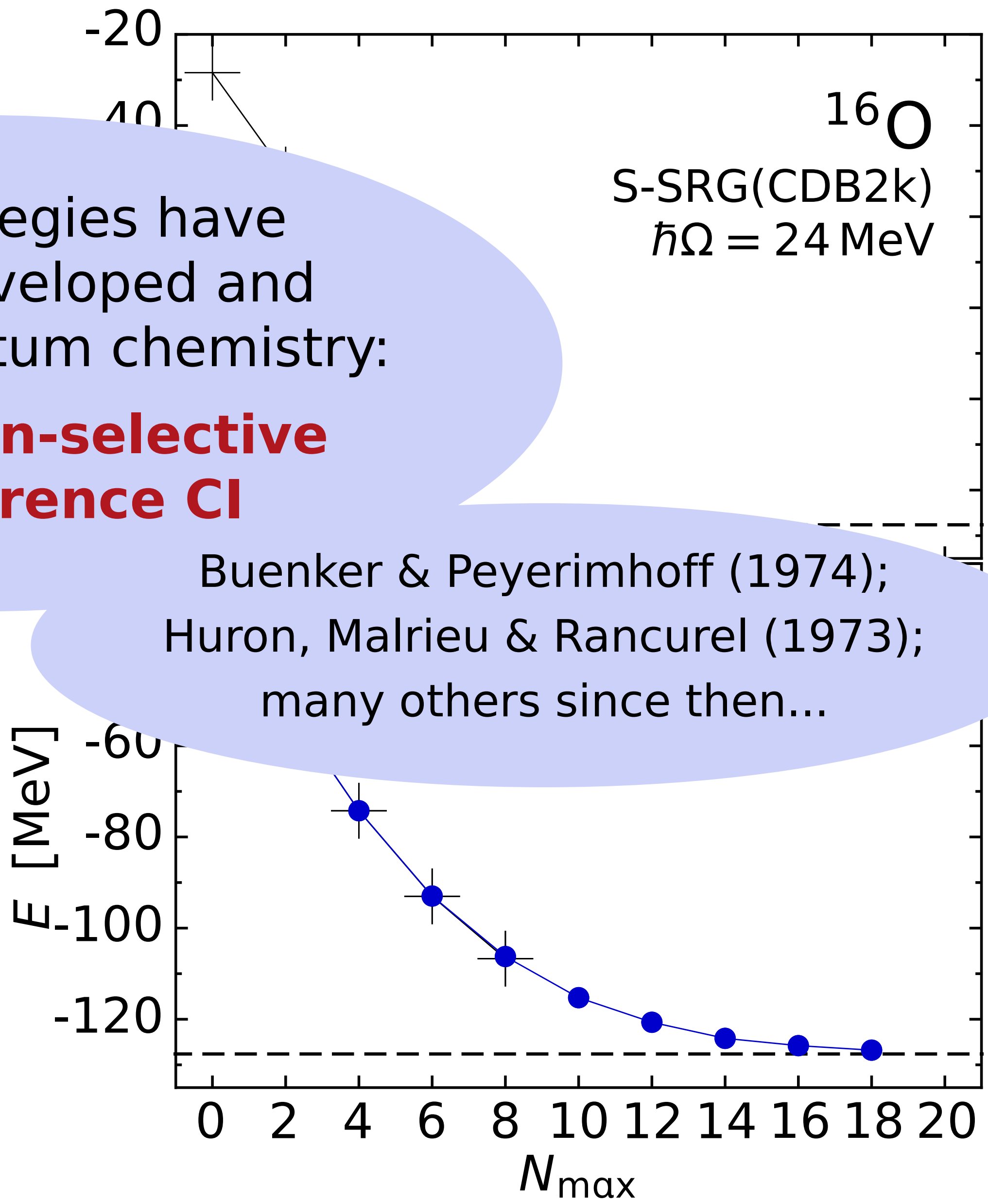
similar strategies have
first been developed and
applied in quantum chemistry:

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



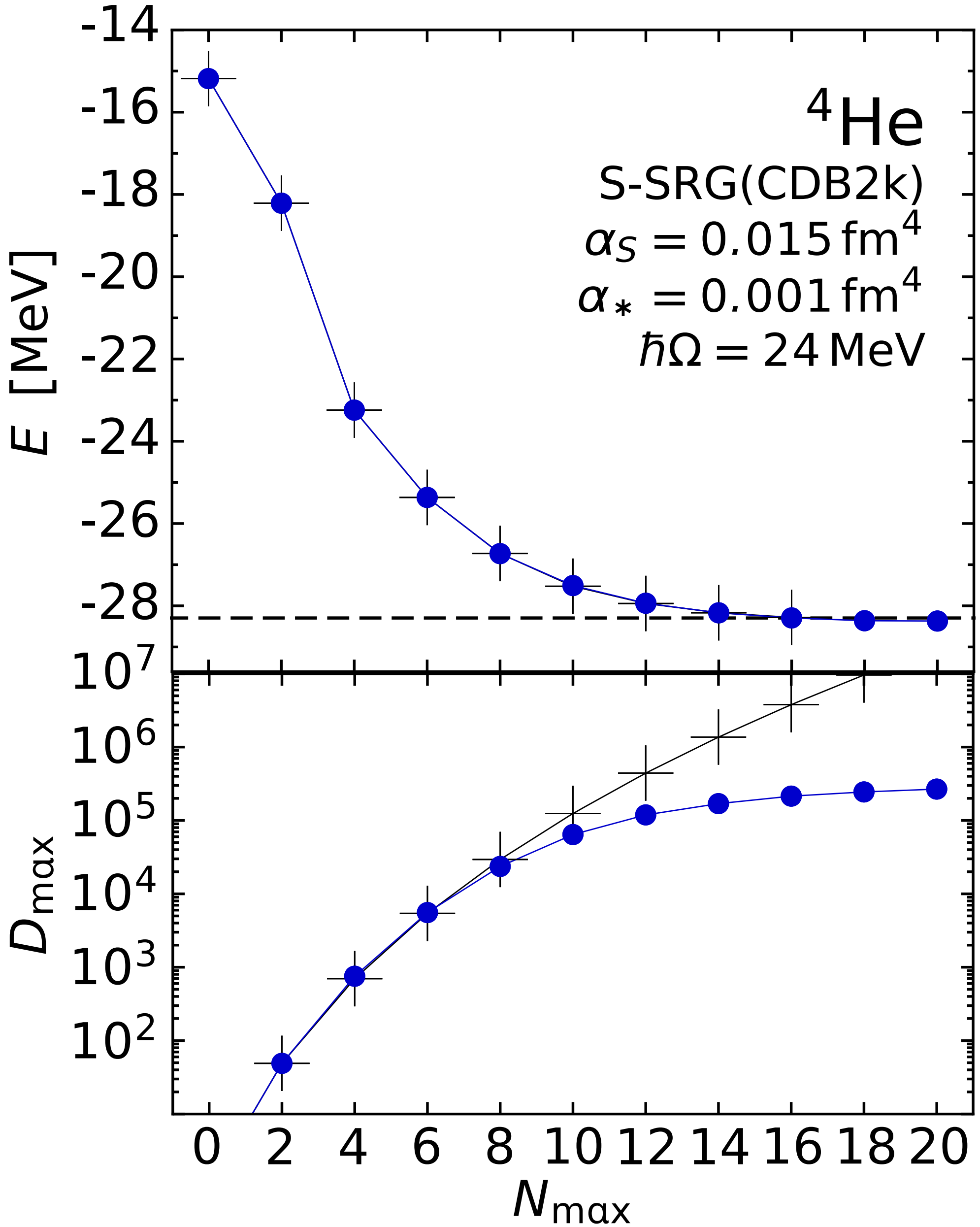
Importance Truncation: General Idea

- given an initial approximation $|\Psi_{\text{ref}}\rangle$ for the **target state**
- **measure the importance** of individual basis state $|\Phi_\nu\rangle$ via first-order multiconfigurational perturbation theory

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

- construct **importance truncated space** spanned by basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$ and solve eigenvalue problem
- **iterative scheme**: repeat construction of importance truncated model space using eigenstate as improved reference $|\Psi_{\text{ref}}\rangle$
- a posteriori **threshold extrapolation** and **perturbative correction** used to recover contribution from discarded basis states

^{4}He: Importance-Truncated NCSM

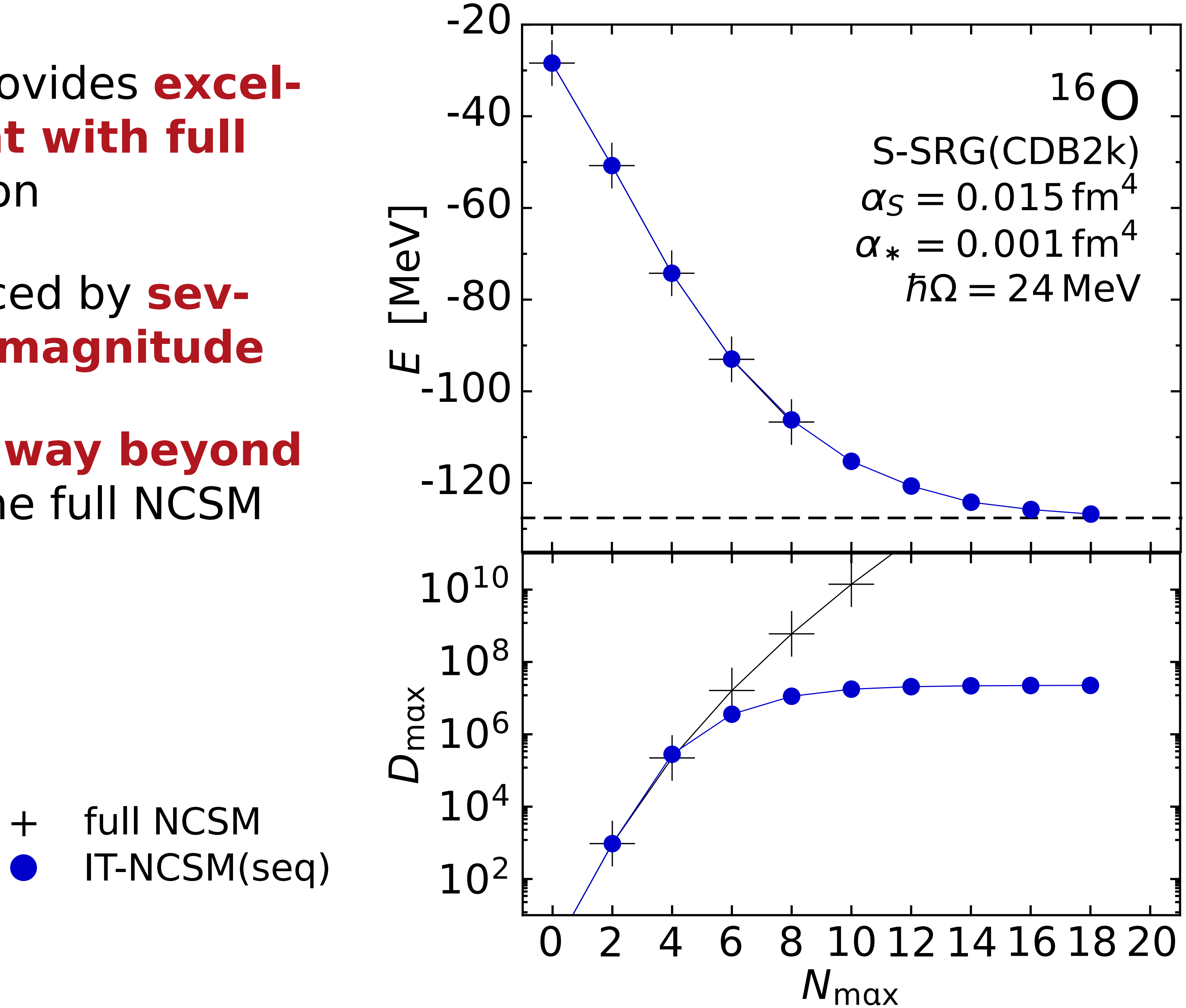


- **IT-NCSM(seq)**: $(N_{\text{max}} - 2)\hbar\Omega$ eigenstate used as reference for constructing importance truncated $N_{\text{max}}\hbar\Omega$ space
- **reproduces exact NCSM result** for all N_{max}
- reduction of basis by more than two orders of magnitude w/o loss of precision

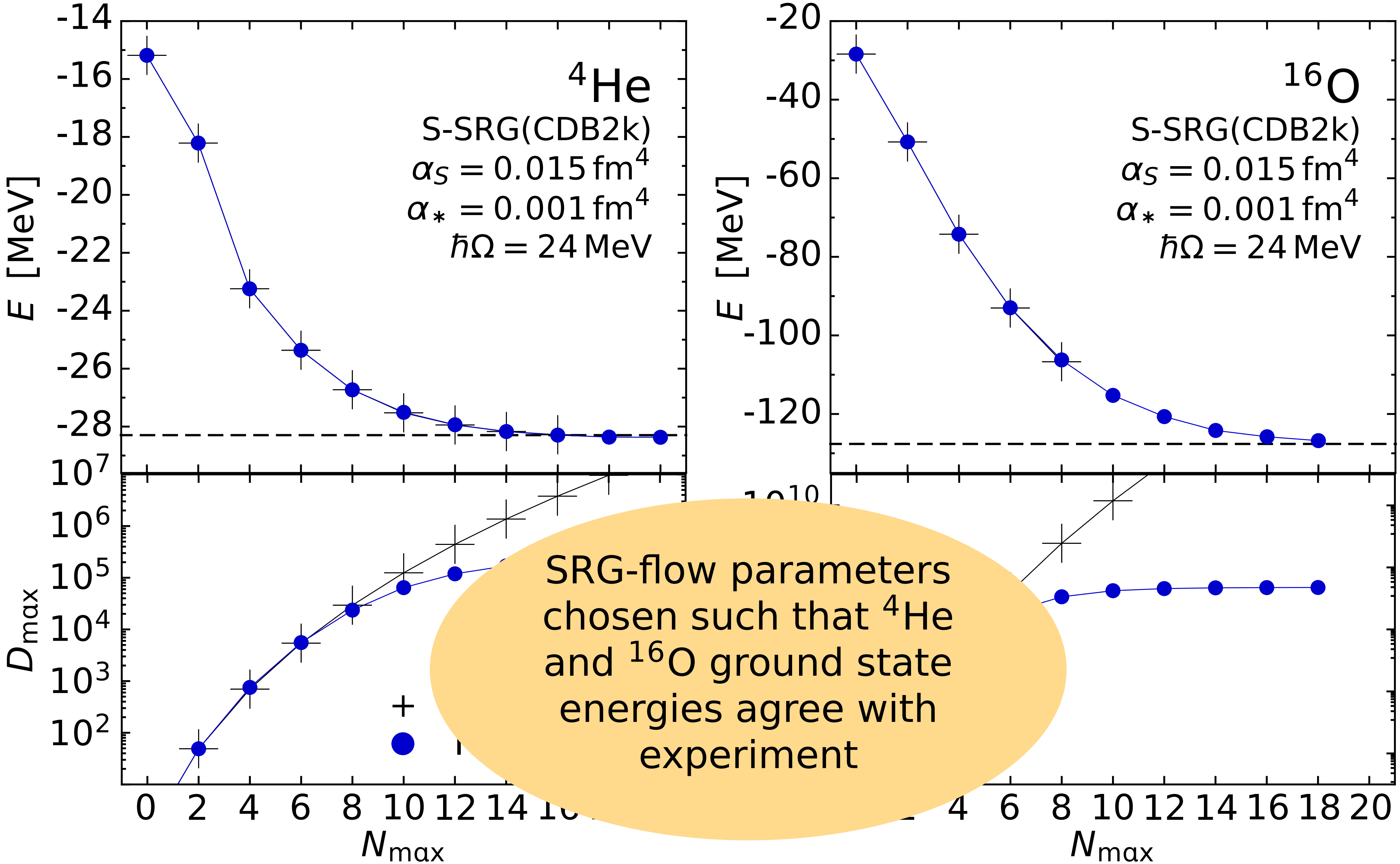
+ full NCSM
● IT-NCSM(seq)

^{16}O: Importance-Truncated NCSM

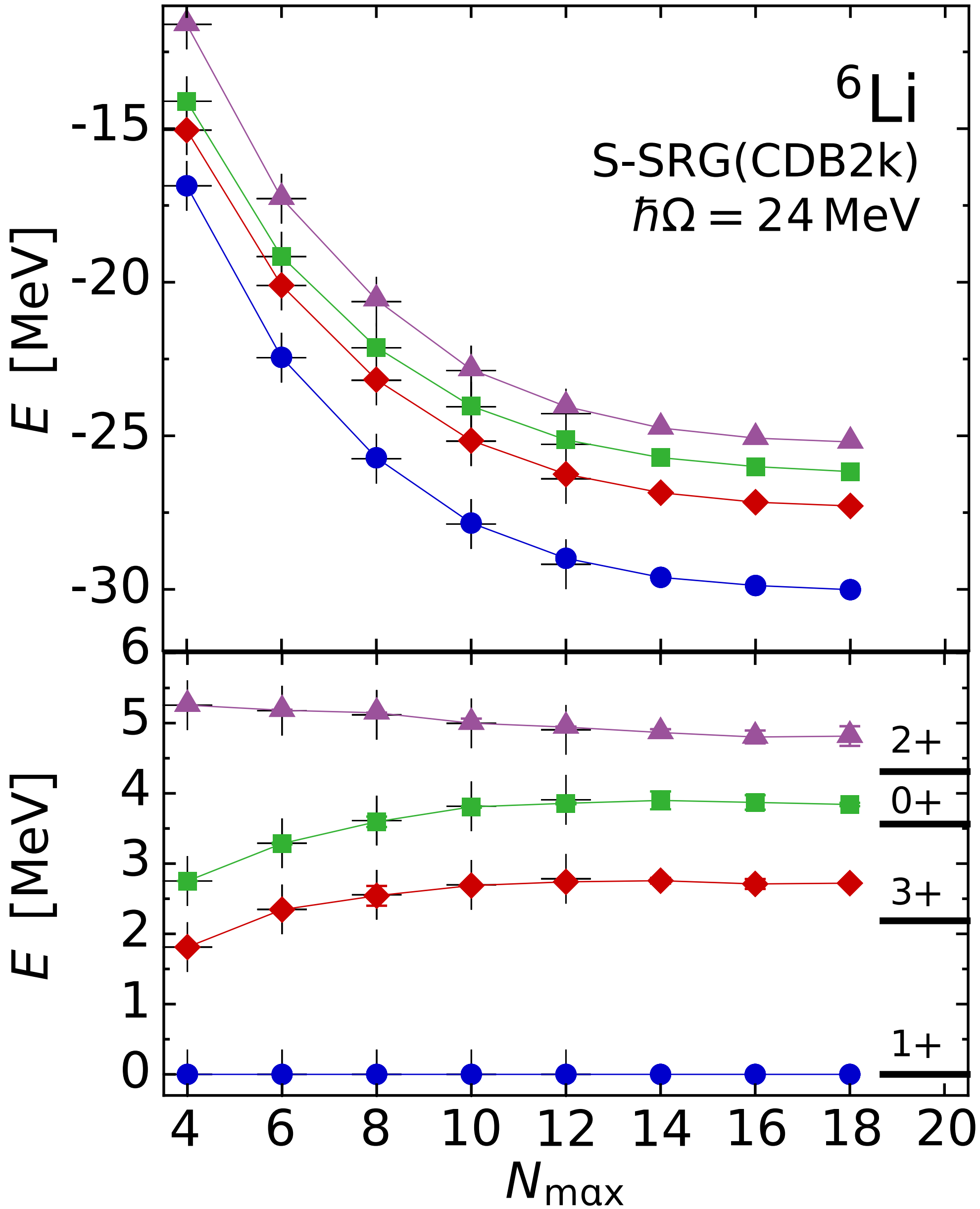
- IT-NCSM(seq) provides **excellent agreement with full NCSM** calculation
- dimension reduced by **several orders of magnitude**
- possibility to go **way beyond** the domain of the full NCSM



^{4}He & ^{16}O: Importance-Truncated NCSM



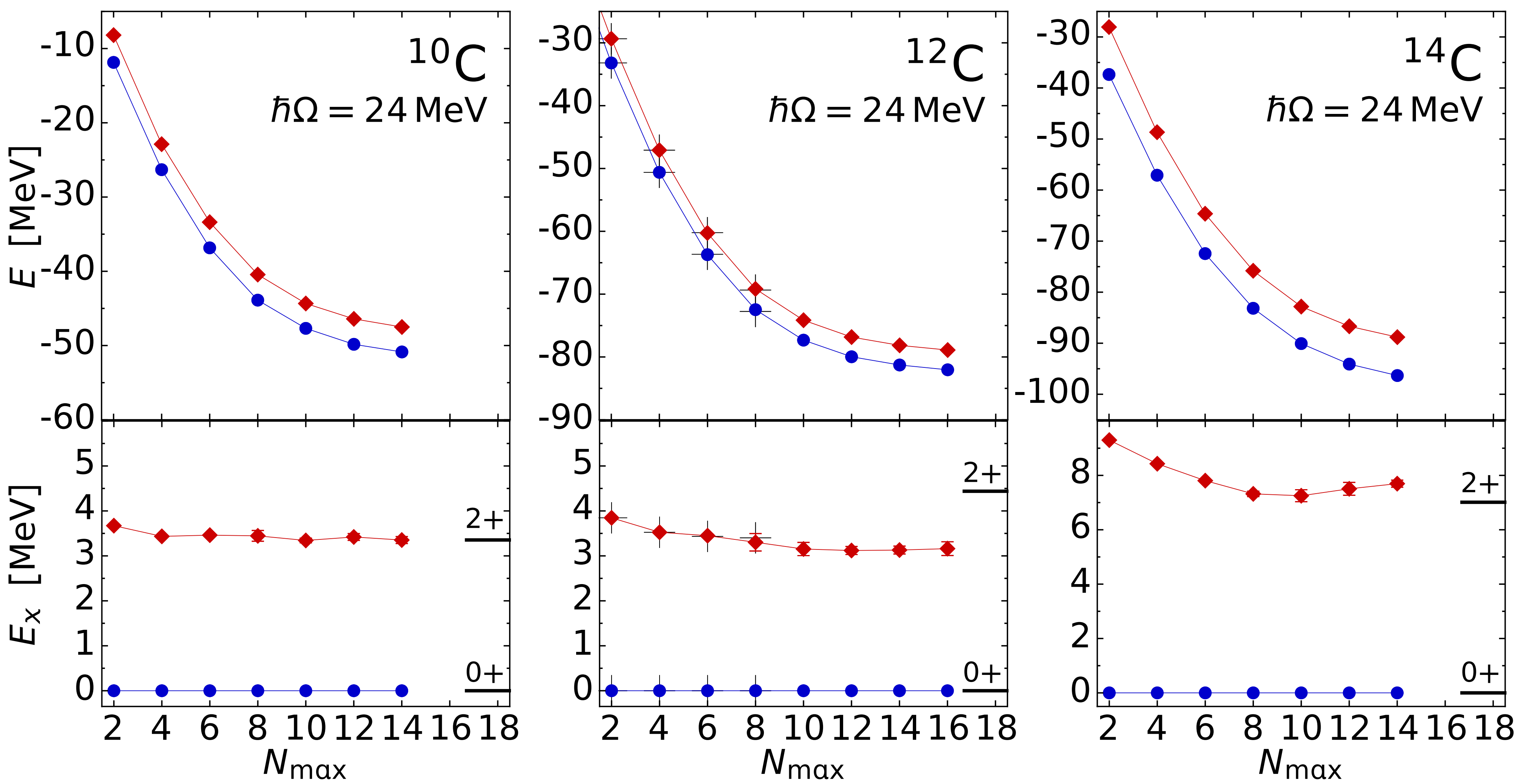
^{6}Li: IT-NCSM for Excited States



- **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

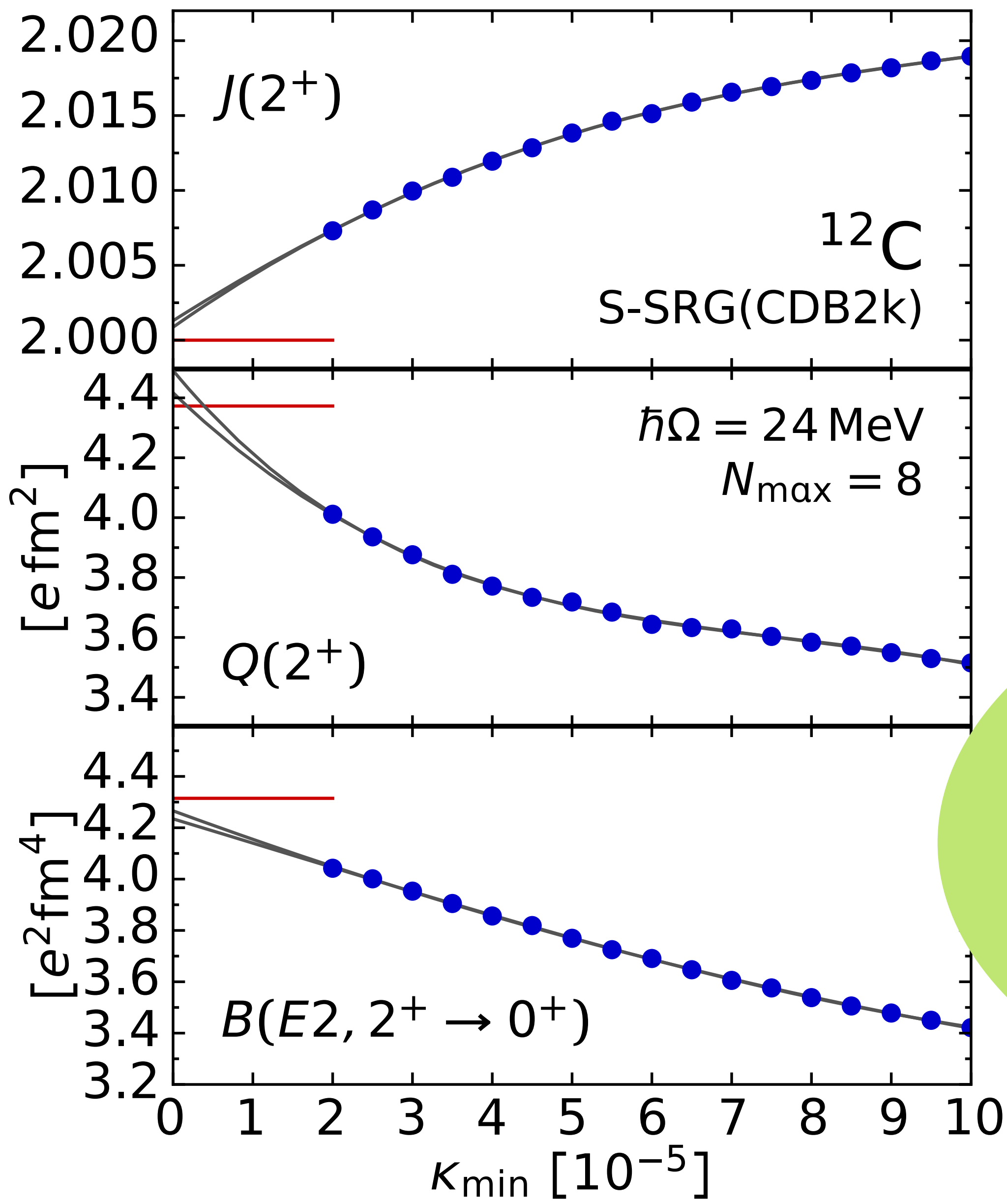
+ full NCSM
● IT-NCSM(seq)

Carbon Isotopes: 2^+ Systematics



- calculations for ^{16}C & ^{18}C are in progress... and non-trivial!

^{12}C: IT-NCSM for Spectroscopy



- access to **spectroscopic observables** via eigenstates
- multipole moments, transition strengths, transition formfactors, densities,...
- threshold extrapolation n... **full**

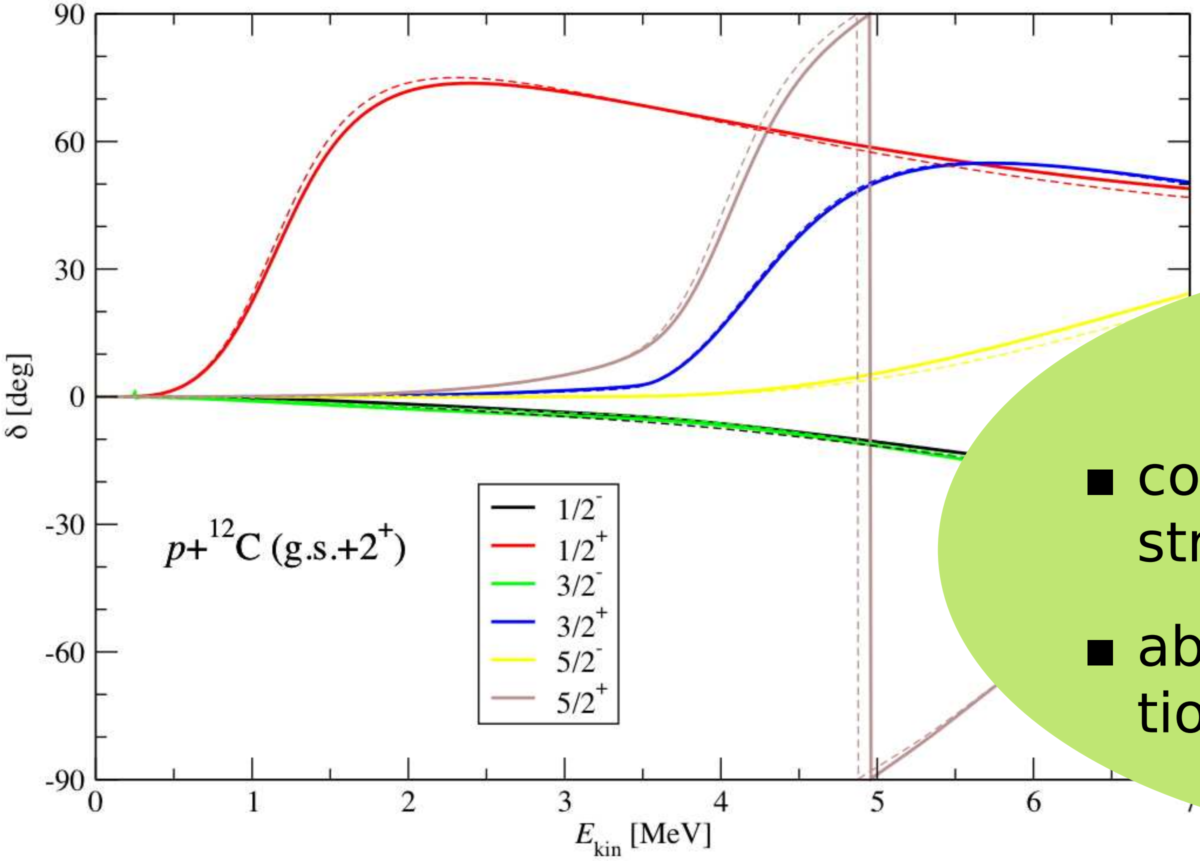
Frontiers

- p- and sd-shell nuclei in large $N_{max}\hbar\Omega$ spaces
- complete spectroscopy beyond the domain of the full NCSM

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



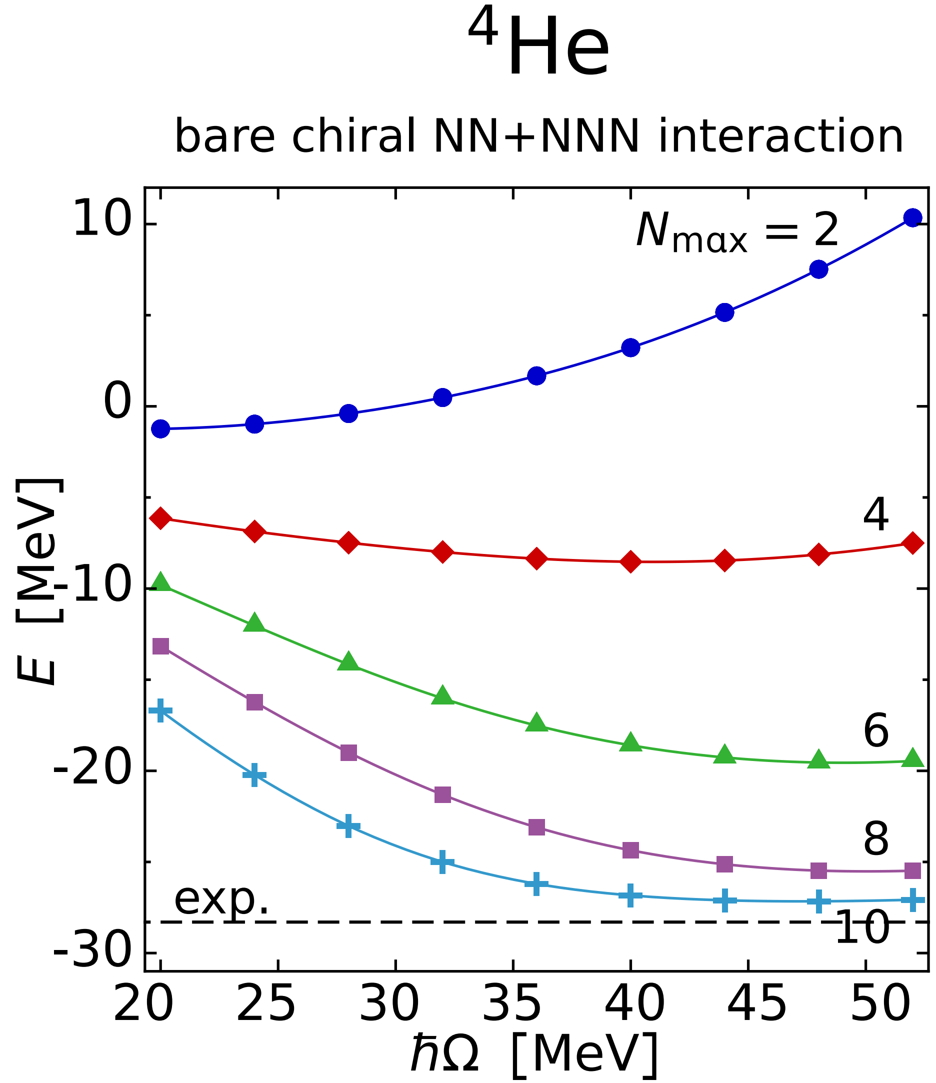
- phase-shifts for p + ^{12}C elastic scattering with SRG-transformed chiral N3LO ($\alpha = 0.02\,\mathrm{fm}^4$)
- ve func-
- in-

Frontiers

- coupling of ab initio structure & reactions
- ab initio low-energy reactions for p-shell & beyond

Next: IT-NCSM with 3N Interactions

- developed efficient code for computation of J-coupled 3N matrix elements of the chiral 3N interaction
- implemented full 3N capabilities into IT-NCSM code (no approximations)
- implemented consistent SRG-transformation of chiral NN+NNN Hamiltonian
- ready to go...



Epilogue

- **thanks to my group & my collaborators**
  - S. Binder, A. Calci, B. Erler, A. Günther, M. Hild, H. Krutsch, J. Langhammer, P. Papakonstantinou, S. Reinhardt, F. Schmitt
    Institut für Kernphysik, TU Darmstadt
  - P. Navrátil, S. Quaglioni
    Lawrence Livermore National Laboratory, USA
  - H. Hergert, P. Piecuch, J. Gour
    Michigan State University, USA
  - C. Forssén
    Chalmers University of Technology, Sweden
  - H. Feldmeier, T. Neff,...
    Gesellschaft für Schwerionenforschung (GSI)

Deutsche Forschungsgemeinschaft DFG

SFB 634

HIC for FAIR Helmholtz International Center

LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz