Importance-Truncated No-Core Shell Model for Ab-Initio Nuclear Structure

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From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

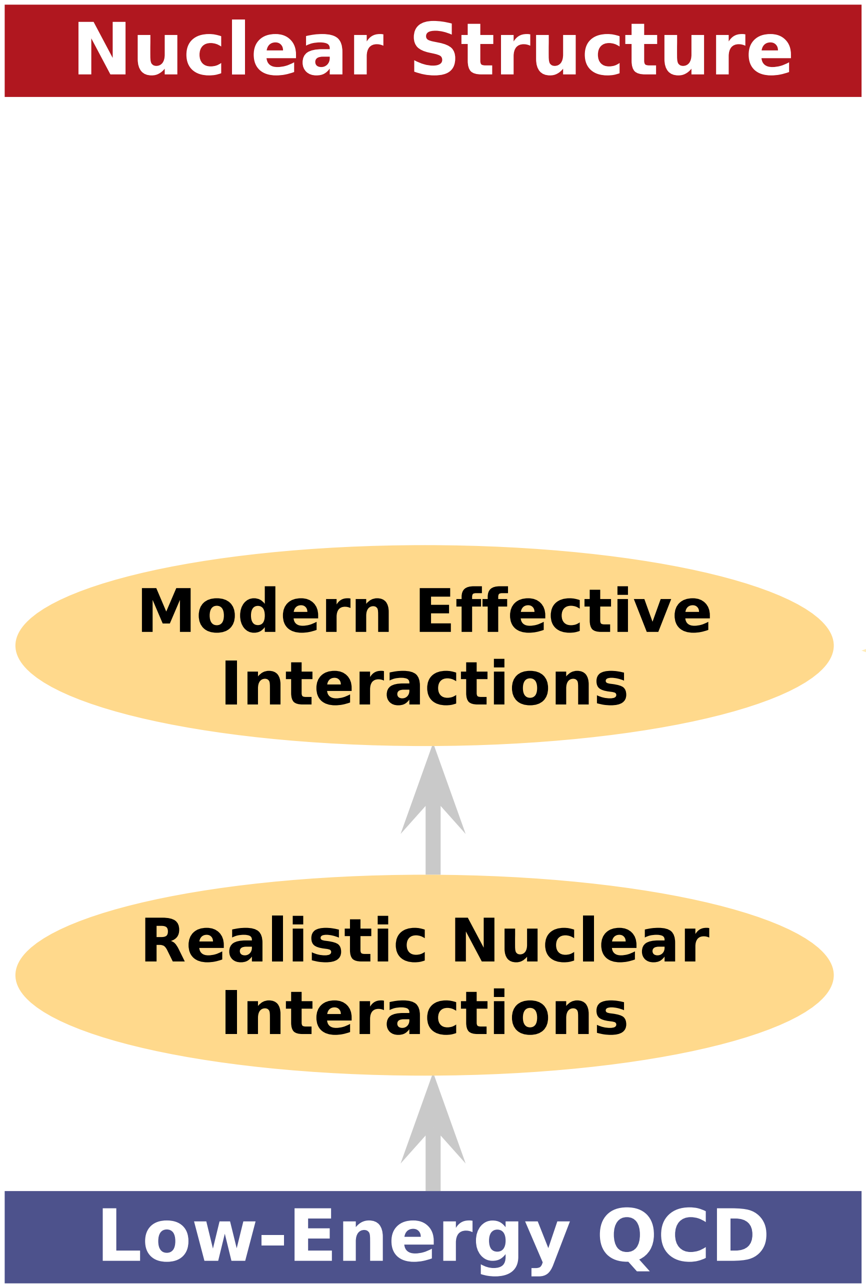
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

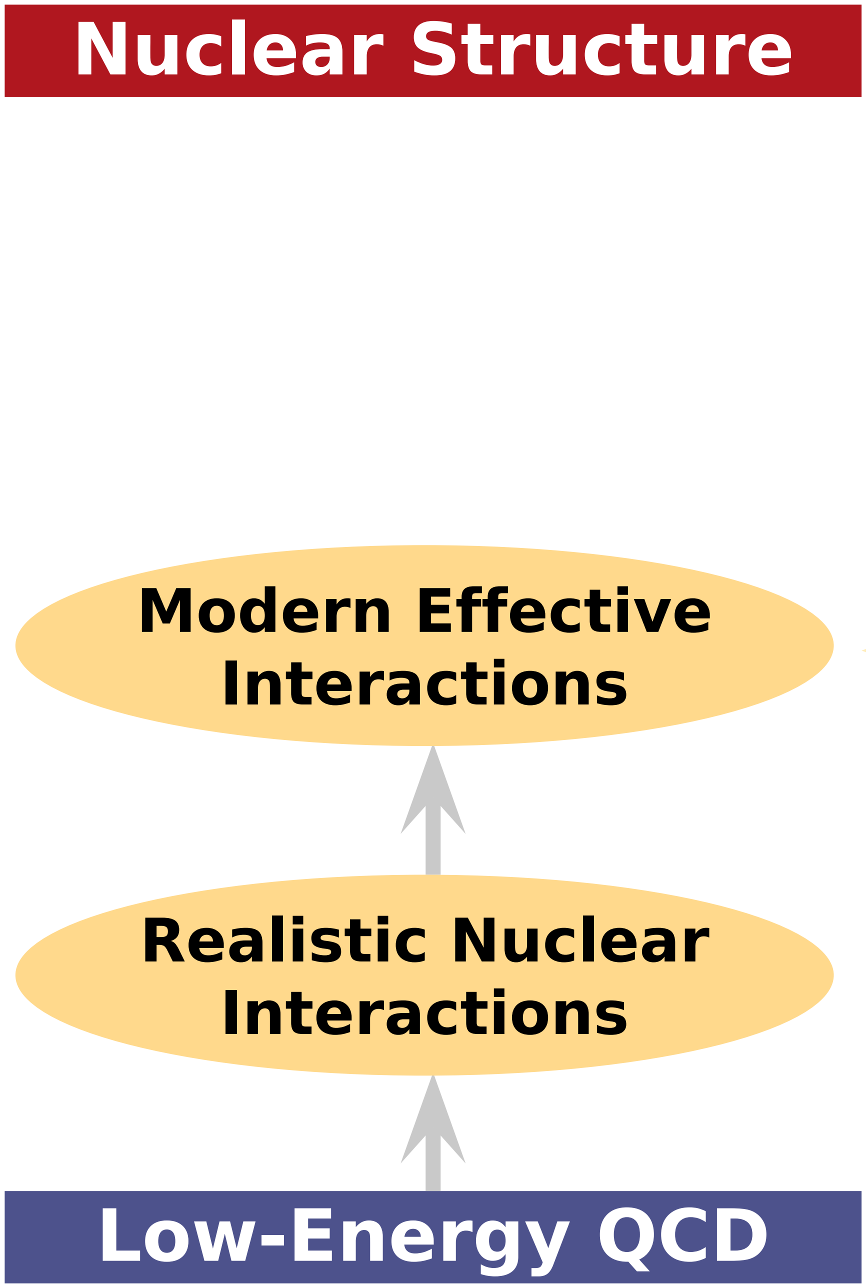
- chiral EFT interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations

From QCD to Nuclear Structure



- 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

From QCD to Nuclear Structure



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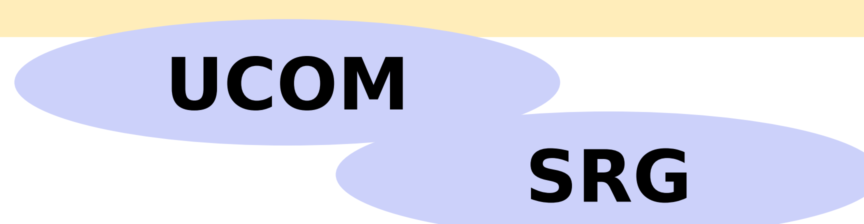
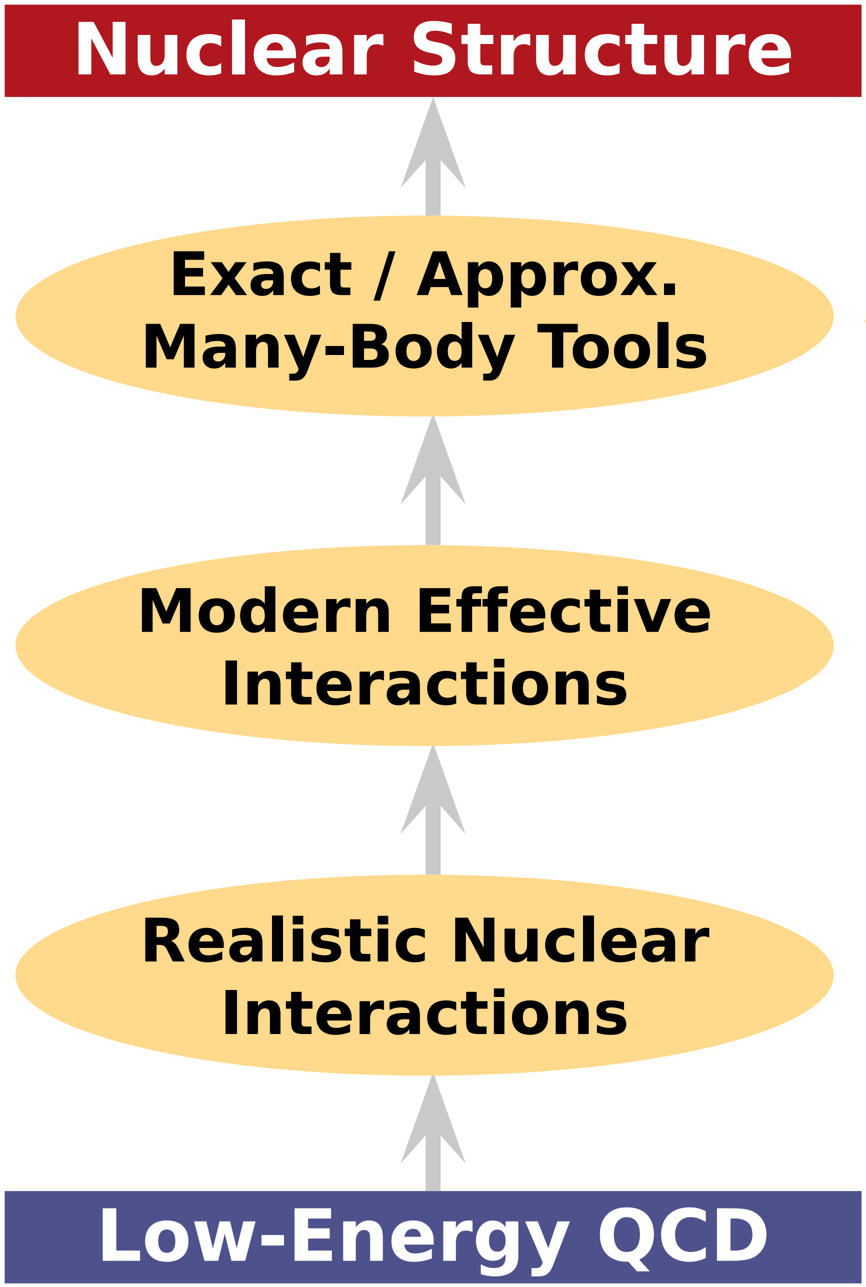


From QCD to Nuclear Structure



- ‘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

Nuclear Structure

↑

Exact / Approx. Many-Body Tools

↑

Modern Effective Interactions

↑

Realistic Nuclear Interactions

↑

Low-Energy QCD

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this talk: **NCSM**

more on other methods in **HK 83.2**

No-Core Shell Model: Basics

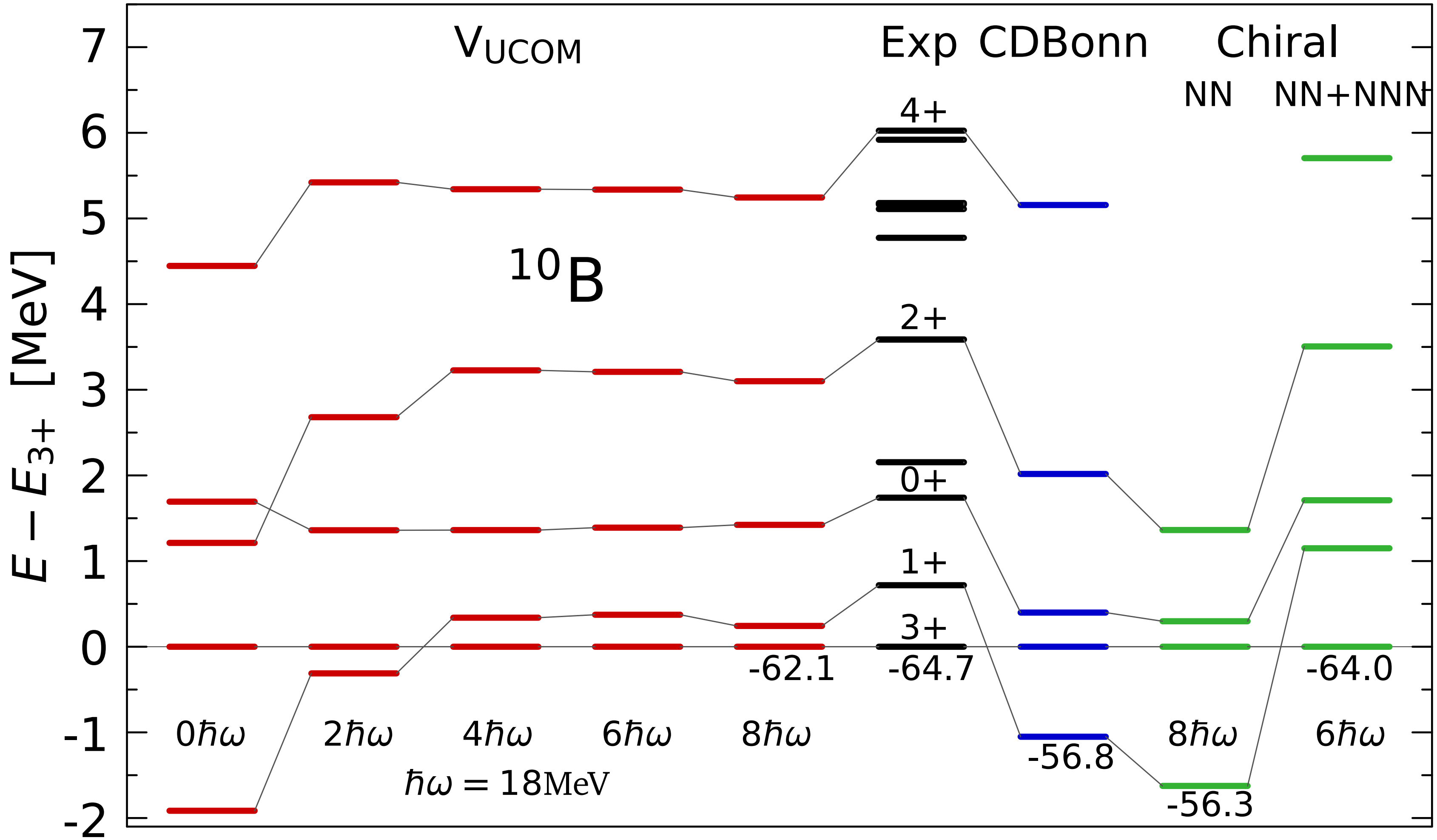
- special case of a **full configuration interaction (CI)** scheme
- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

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

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\text{max}}\hbar\omega$
  - important difference to conventional CI, where model space is defined by a truncation of the single-particle basis
- numerical solution of **eigenvalue problem** for the Hamiltonian H_{int} within truncated model space via Lanczos methods
- model spaces of **up to 10^9 basis states** are used routinely

No-Core Shell Model: Applications

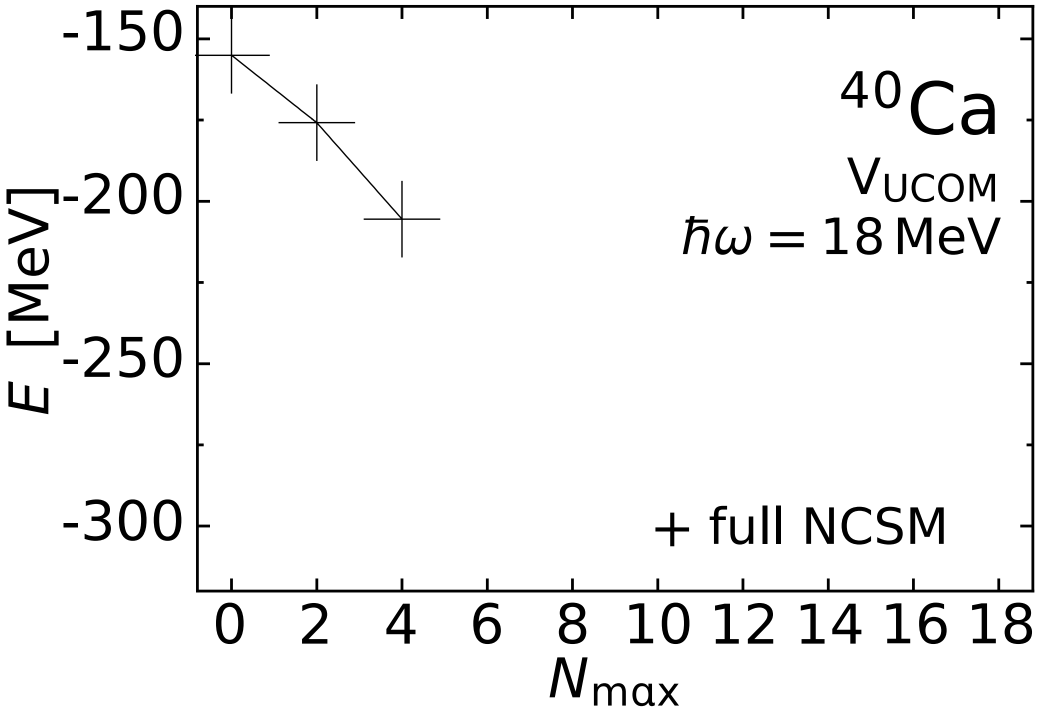
- typical domain of the NCSM are **nuclei with $A \lesssim 13$**
- Lee-Suzuki transformation used to enhance convergence



Importance-Truncated NCSM

- the **model-space dimension** is the single limiting factor for the NCSM

- full $6\hbar\omega$ calculation for ^{40}Ca presently not feasible (basis dimension $\sim 10^{10}$)



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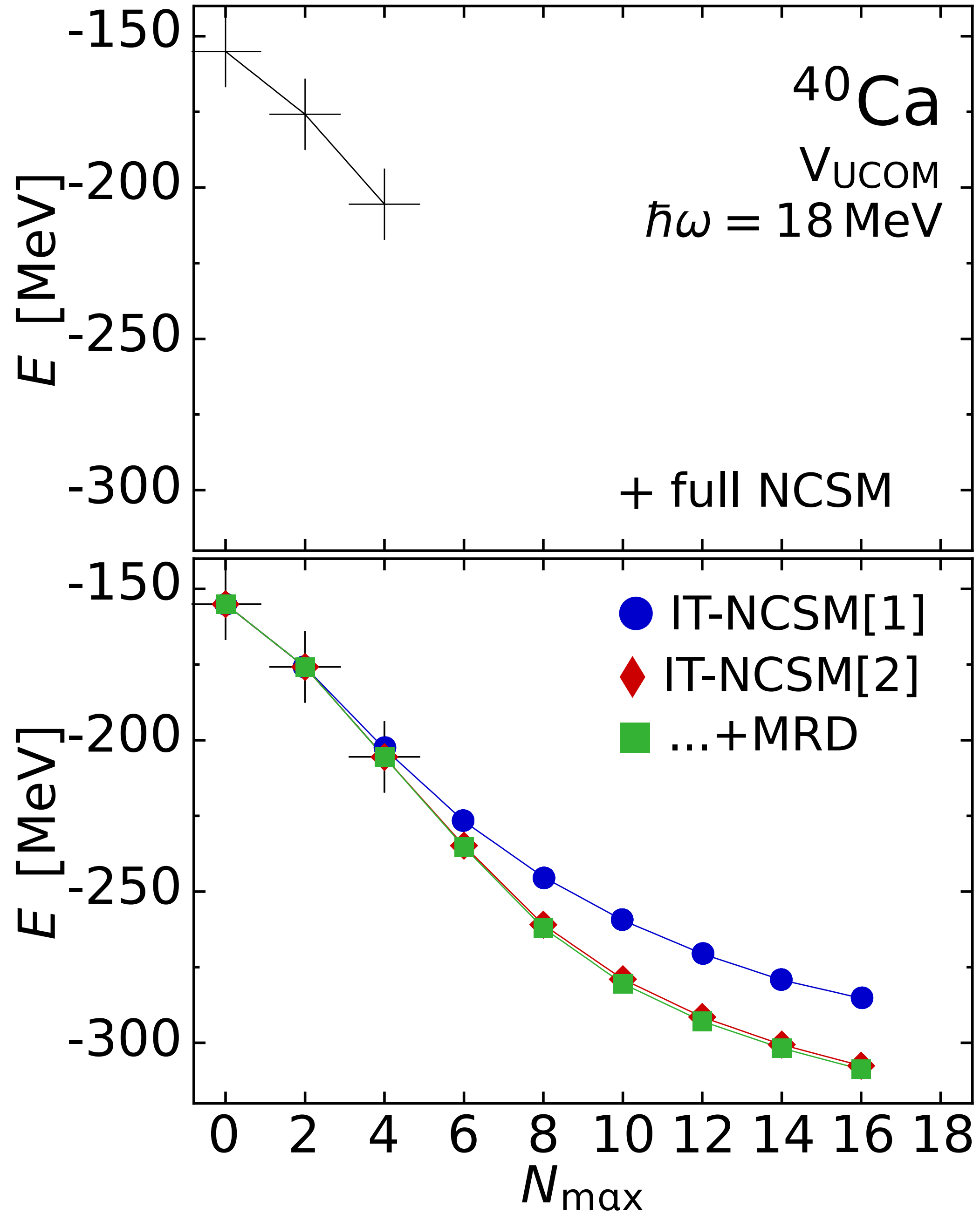
Importance Truncation

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



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Importance Truncation

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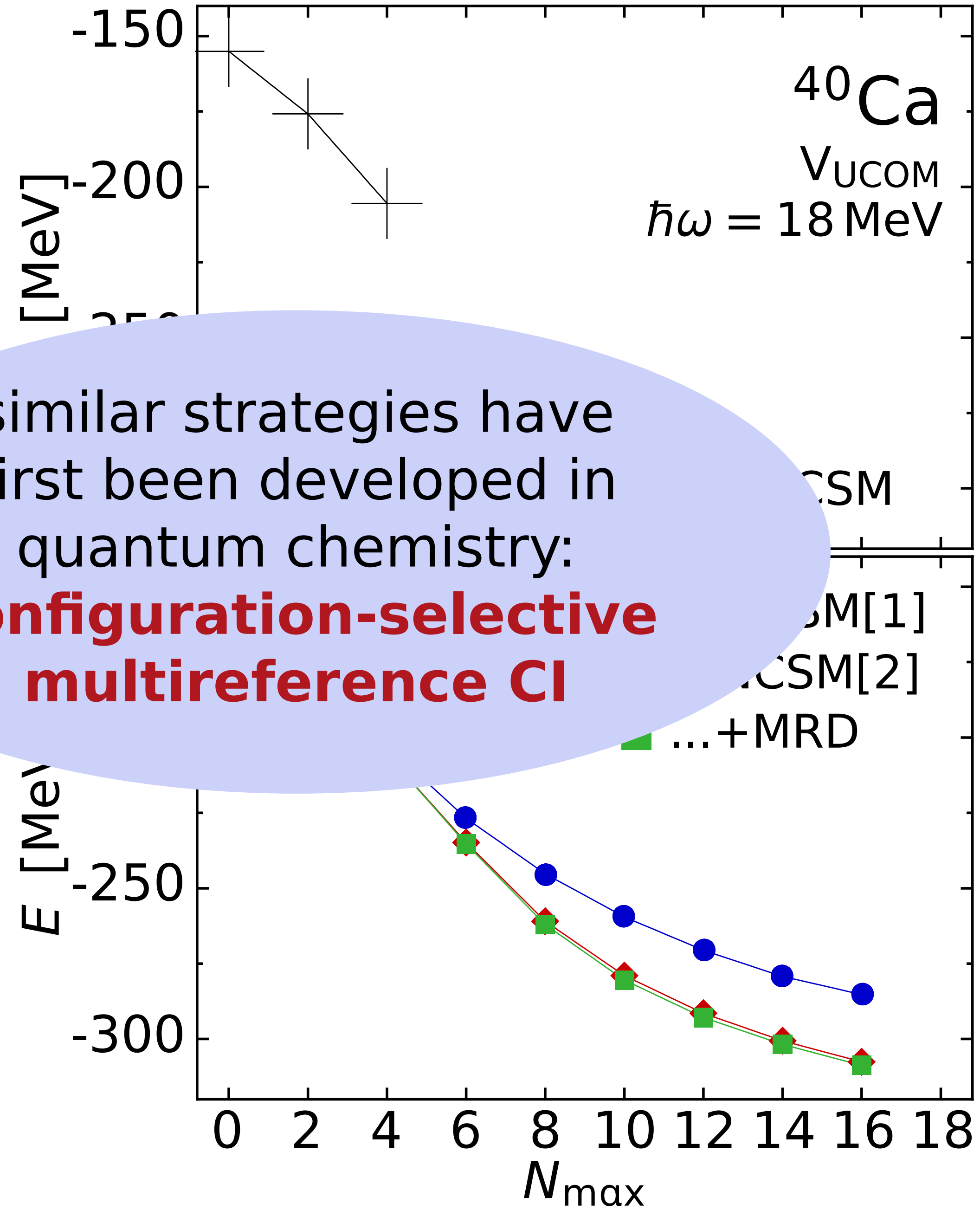
similar strategies have first been developed in quantum chemistry: **configuration-selective multireference CI**



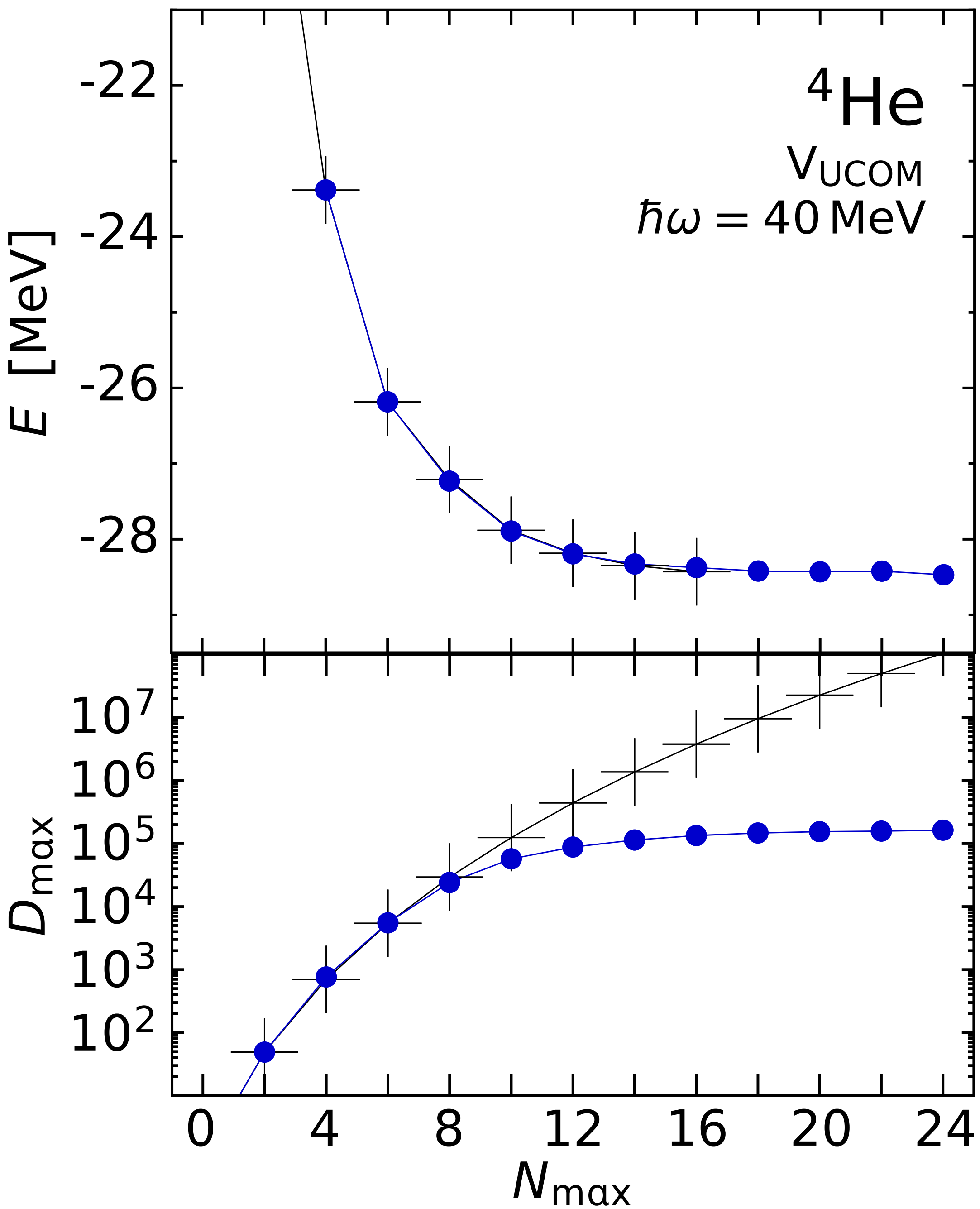
Importance Truncation: General Idea

- 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 $|\Psi_{\text{ref}}\rangle$
- **threshold extrapolations** and **perturbative corrections** can be used to account for discarded basis states

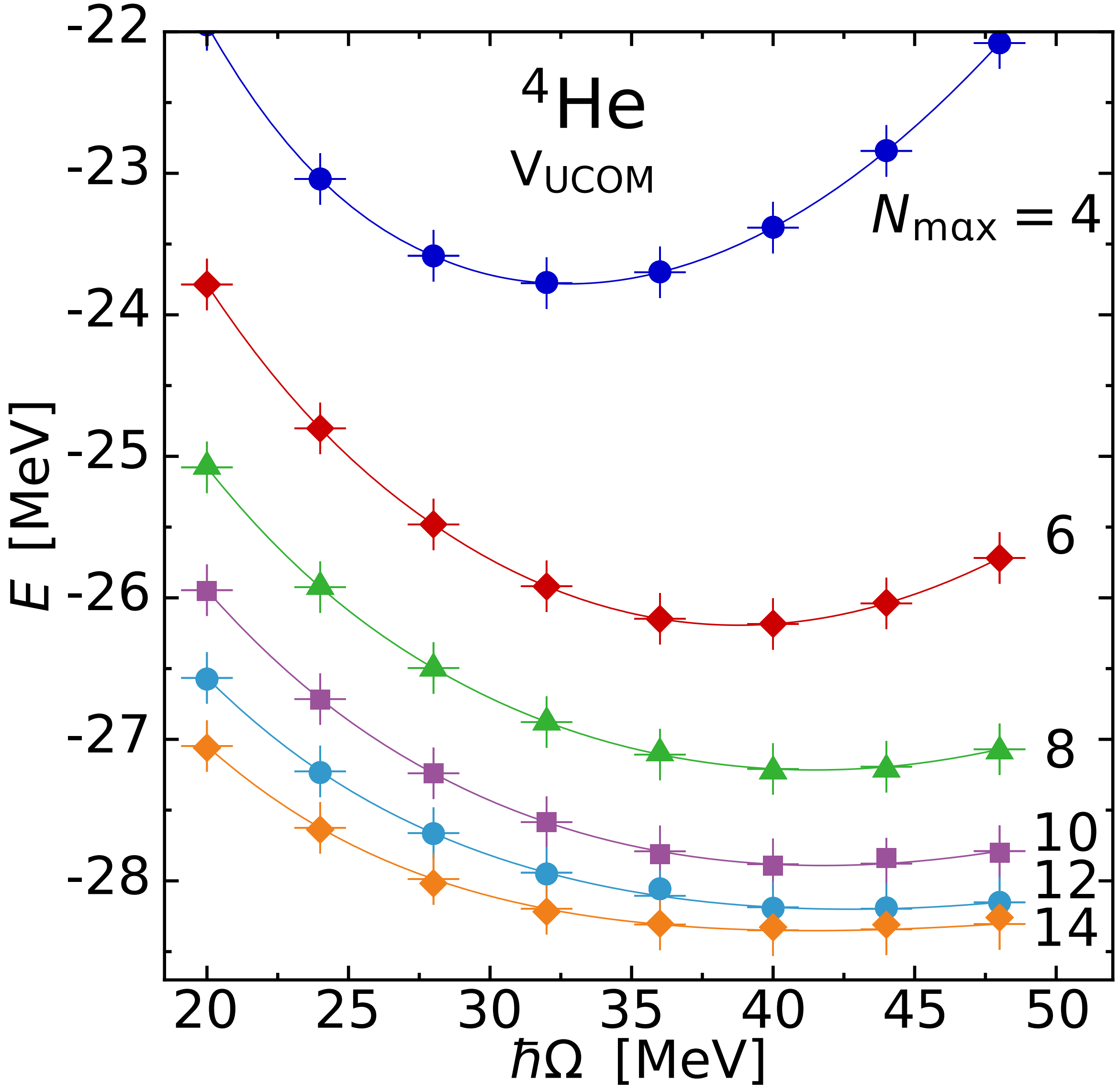
^{4}He: Importance-Truncated NCSM



- **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)

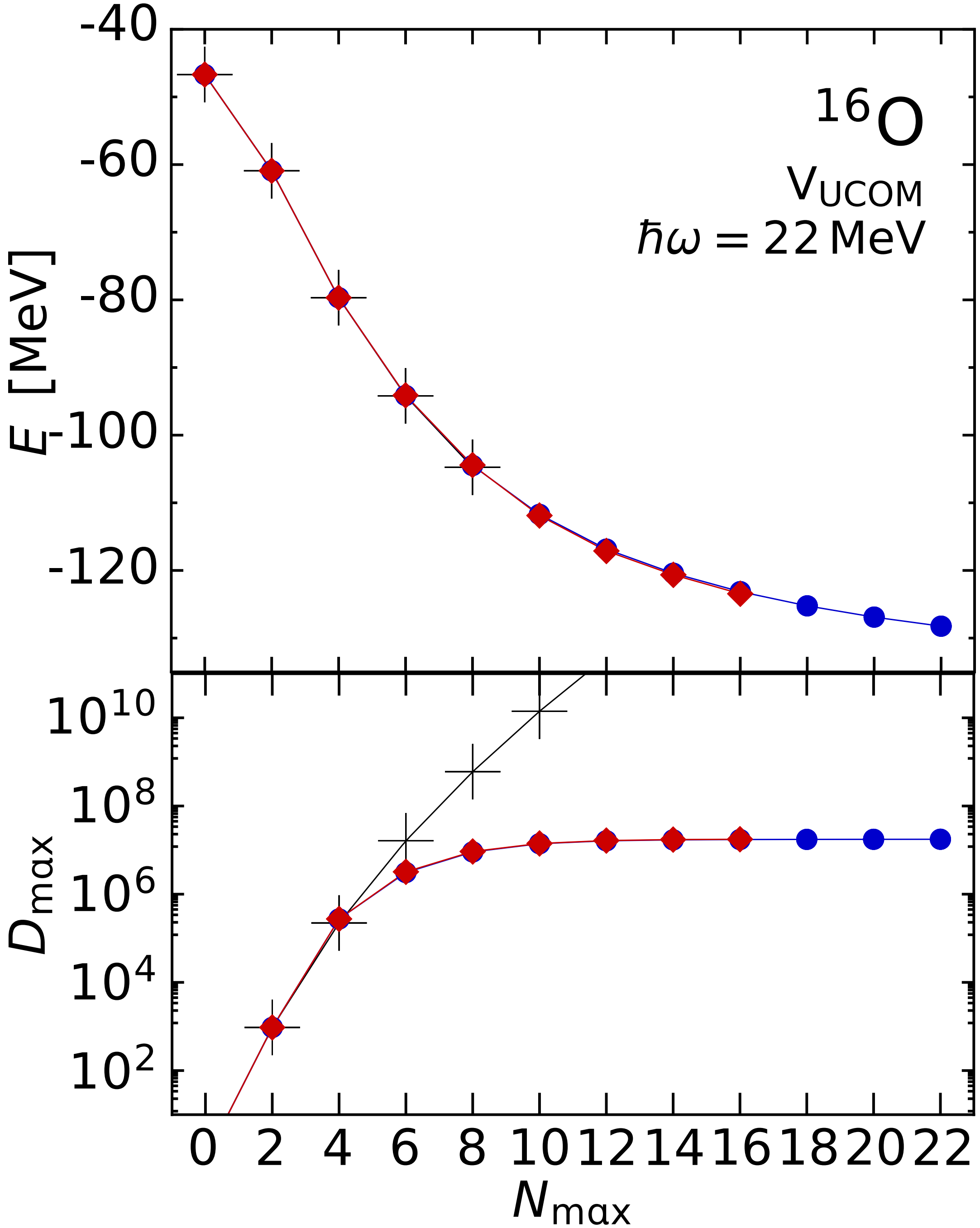
^{4}He: Importance-Truncated NCSM



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

+ full NCSM
● IT-NCSM(seq)

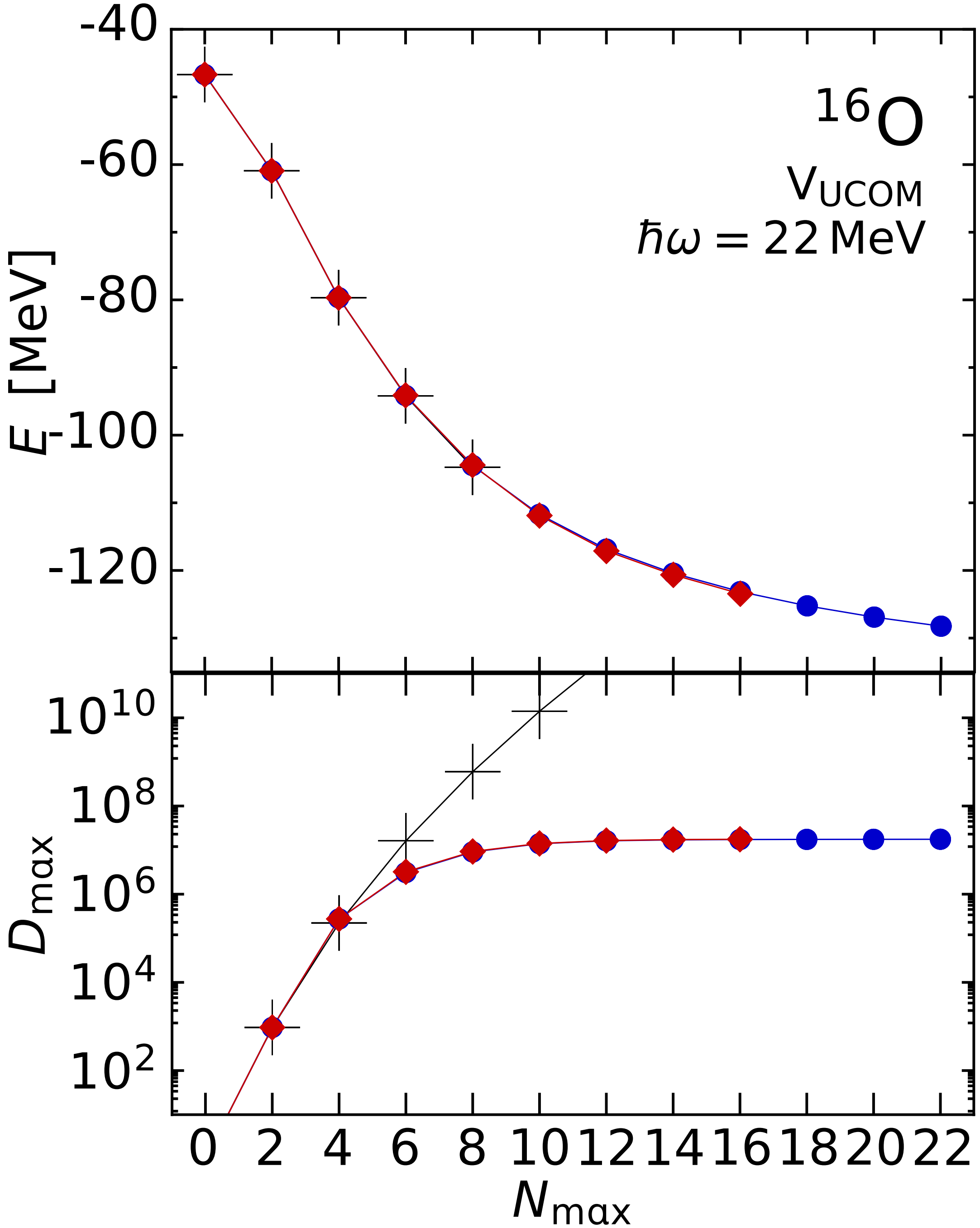
^{16}O: Importance-Truncated NCSM



- 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



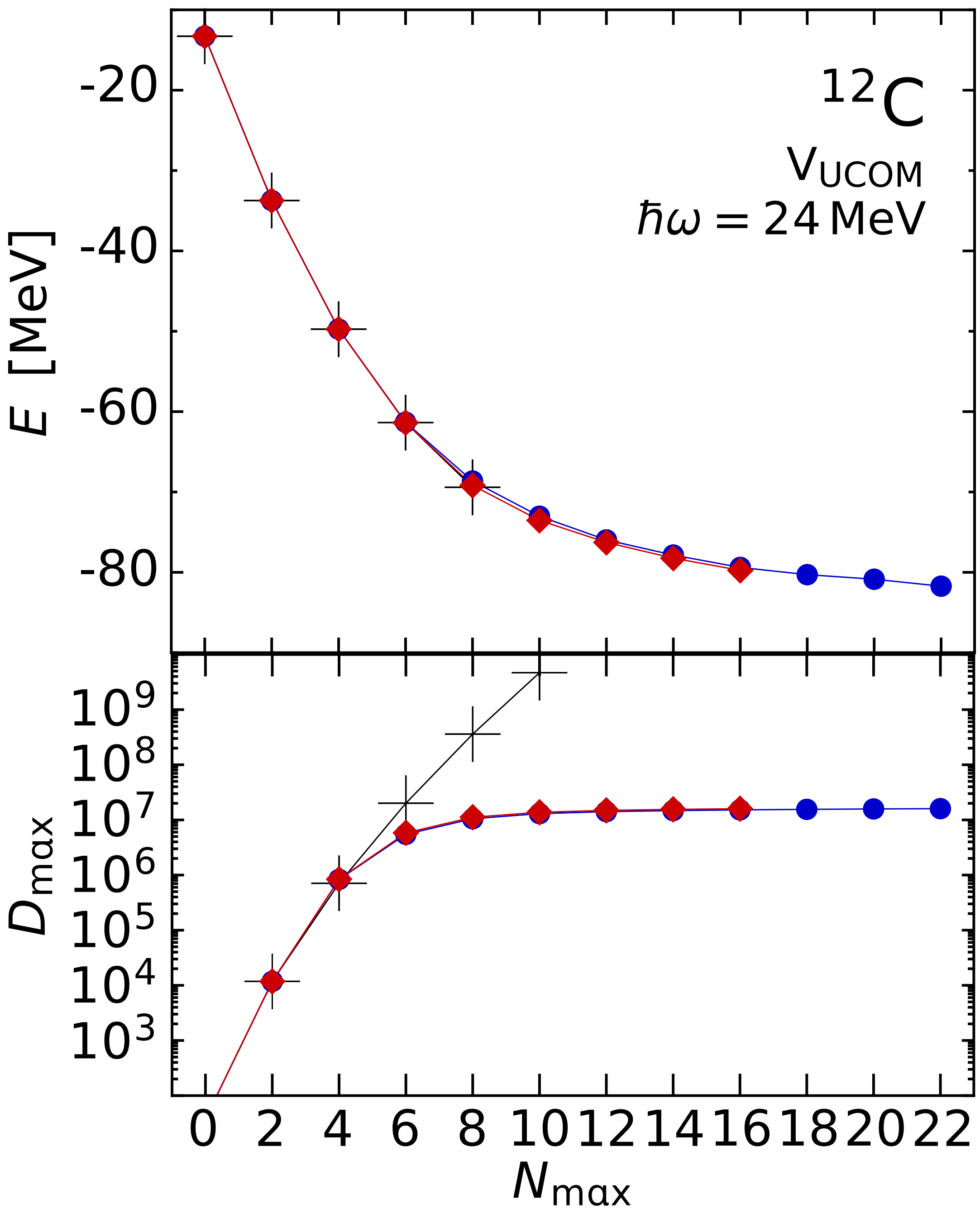
- extrapolation to $N_{max} \to \infty$

$$E_{\text{IT-NCSM(seq)}} = -133(3)\,\mathrm{MeV}$$
$$E_{exp} = -127.6\,\mathrm{MeV}$$

- V_{UCOM} predicts **reasonable binding energies** also for heavier nuclei
- slow non-exponential convergence makes precise extrapolation difficult

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

^{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 the available two-body matrix elements of V_{UCOM} only

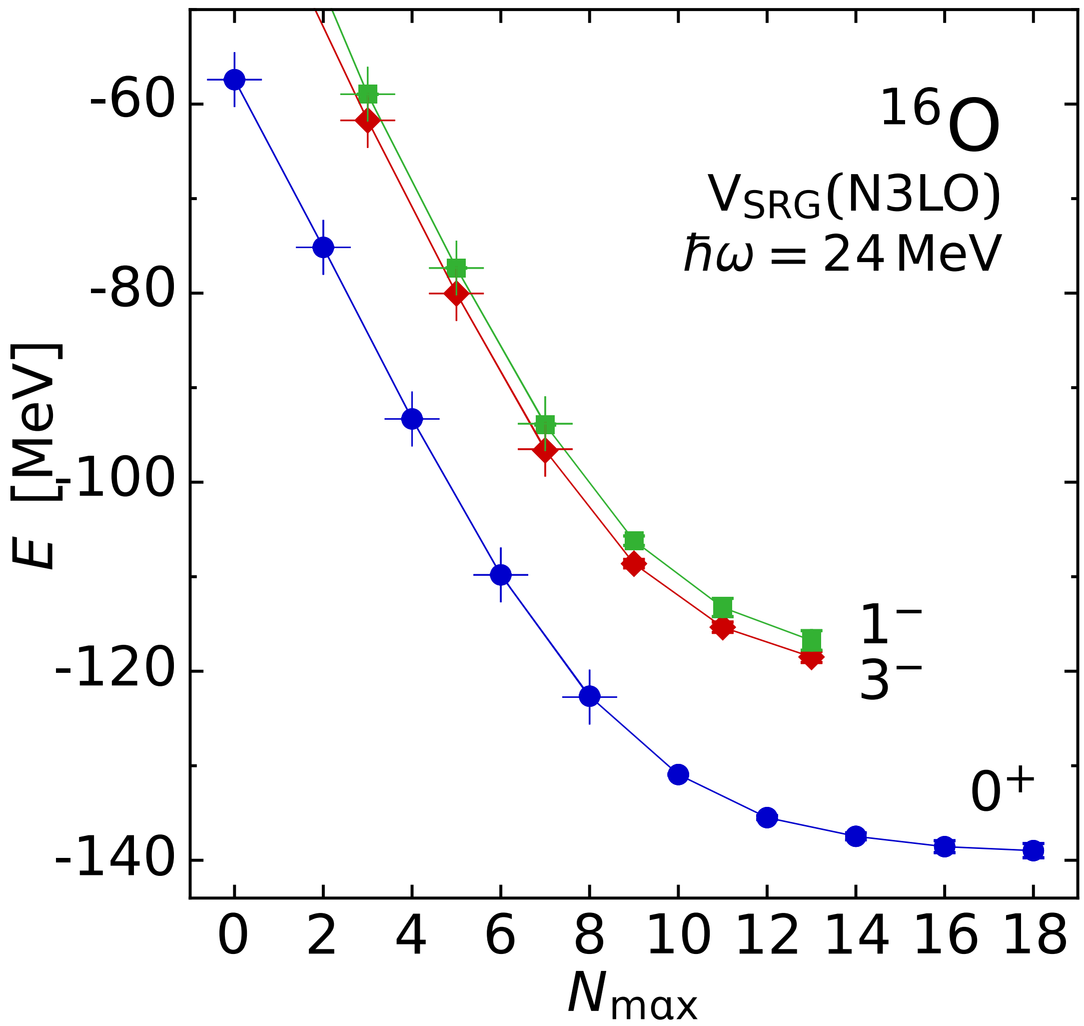
+ full NCSM
● IT-NCSM(seq), $C_{min} = 0.0005$
♦ IT-NCSM(seq), $C_{min} = 0.0003$

Summary

- importance-truncation scheme extends the domain of ab-initio NCSM calculations to **much larger N_{max} and A**
  - $22\hbar\omega$ calculations for ^{12}C and ^{16}O done routinely
- IT-NCSM has **all the advantages of the full NCSM**
  - variational principle
  - no spurious center-of-mass contamination
  - applicable for closed and open-shell nuclei
  - ground and excited states are treated on the same footing
  - wave-functions for free
  - expectation values, transition matrix elements, densities and form-factors can be computed with standard shell-model technology
- implementation is different from standard NCSM & calculations are computationally demanding

Outlook

- further development of the **IT-NCSM technology**
- IT-NCSM as tool for **testing new interactions**
- **full spectroscopy** for low-lying states in nuclei with $A \lesssim 40$ in large $N_{\rm max}\hbar\omega$ spaces
- **nucleon-nucleus reactions** within the RGM approach using IT-NCSM wave functions (with P. Navrátil)



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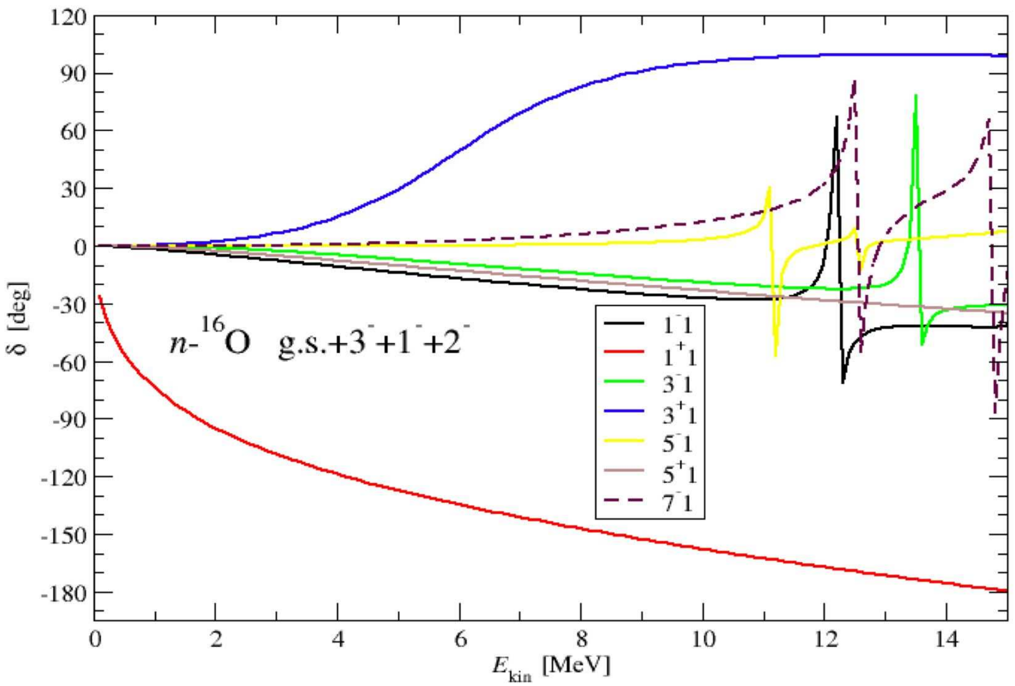

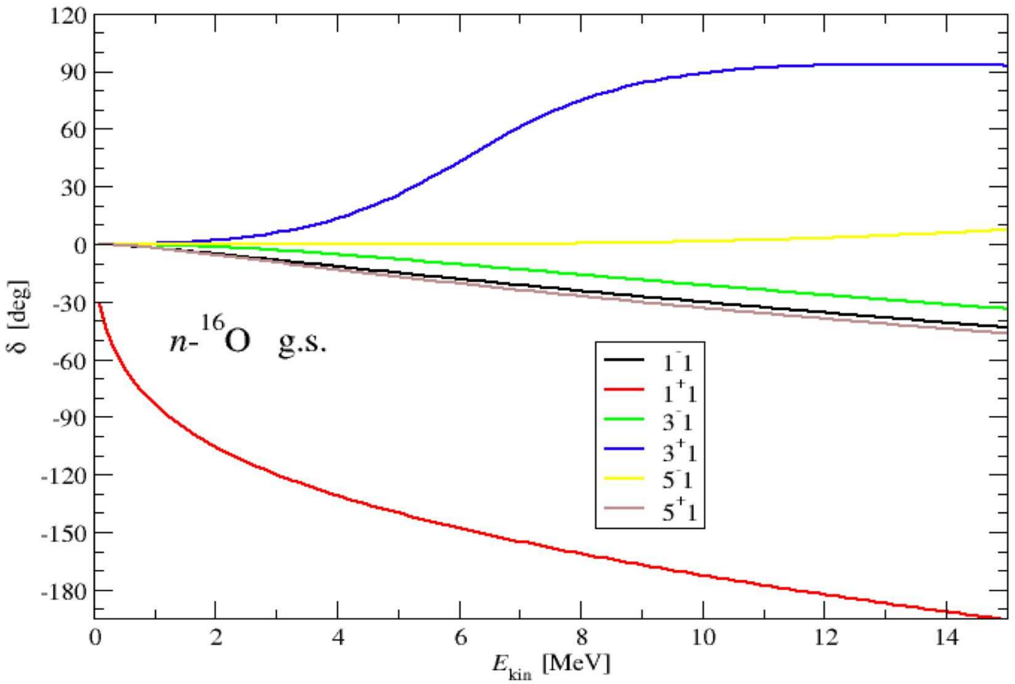

Epilogue

- **thanks to my group & my collaborators**
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