Ab Initio Calculations Beyond the p-Shell

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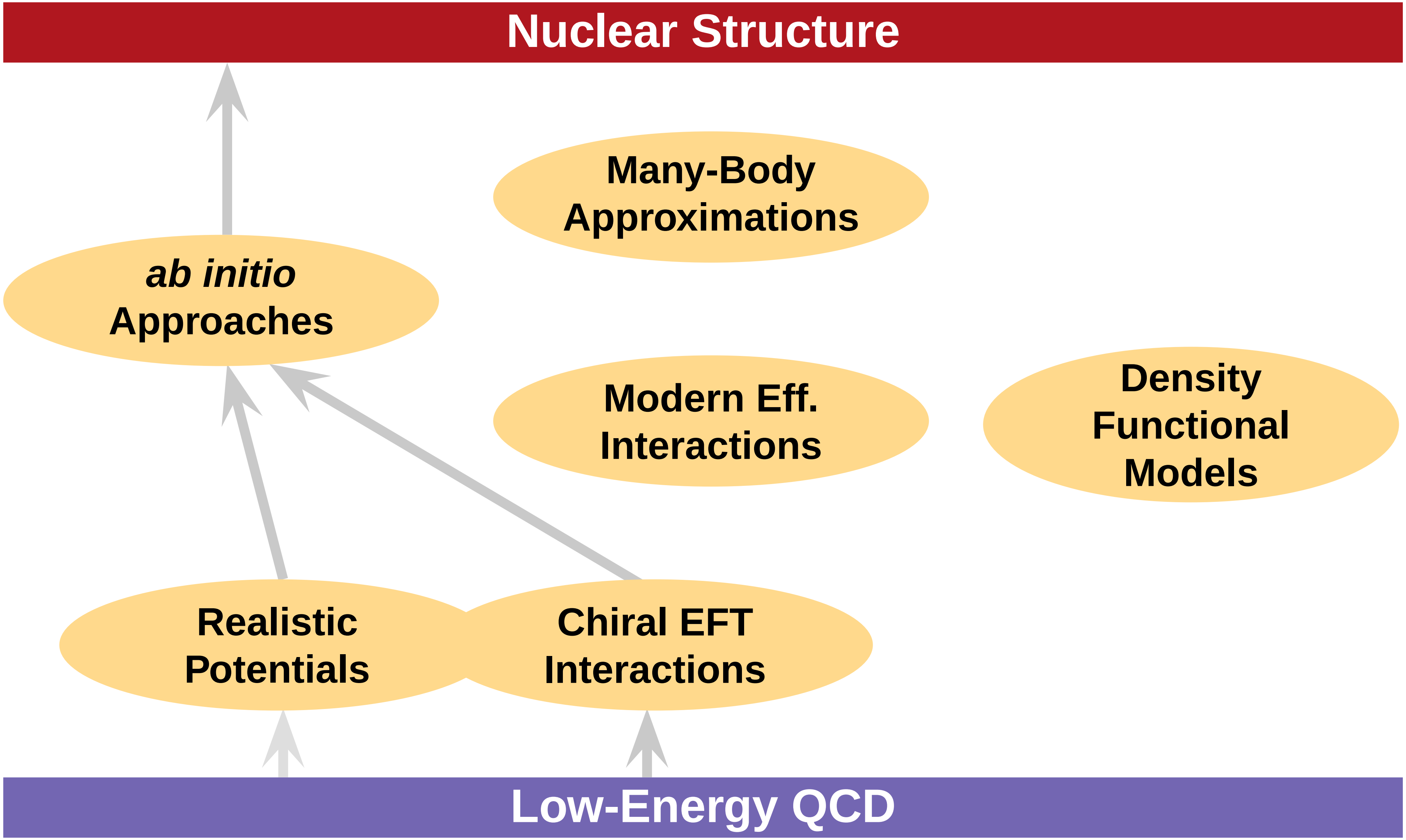
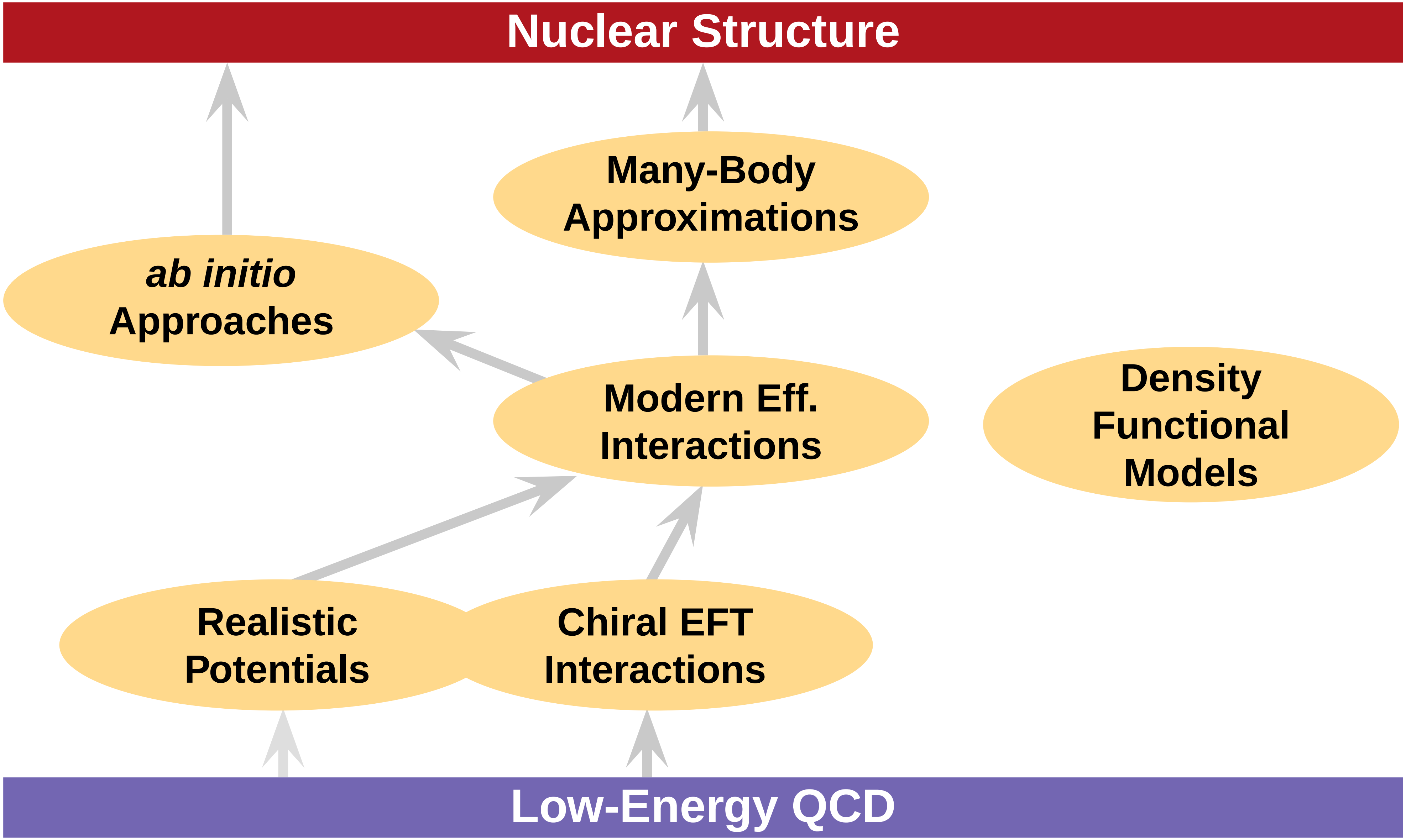
Overview

- Reminder: Modern Effective Interactions
- No-Core Shell Model
- Importance Truncated NCSM
- Conclusions & Perspectives

Modern Nuclear Structure Theory



Modern Nuclear Structure Theory



Unitary Correlation Operator Method

Correlation Operator

define an unitary operator C to describe the effect of short-range correlations

$$\mathrm{C} = \exp[-\mathrm{i}\,\mathrm{G}] = \exp\Big[-\,\mathrm{i}\sum_{i<j}\mathrm{g}_{ij}\Big]$$

Correlated States

imprint short-range correlations onto uncorrelated many-body states

$$|\widetilde{\psi}\rangle = \mathrm{C}\;|\psi\rangle$$

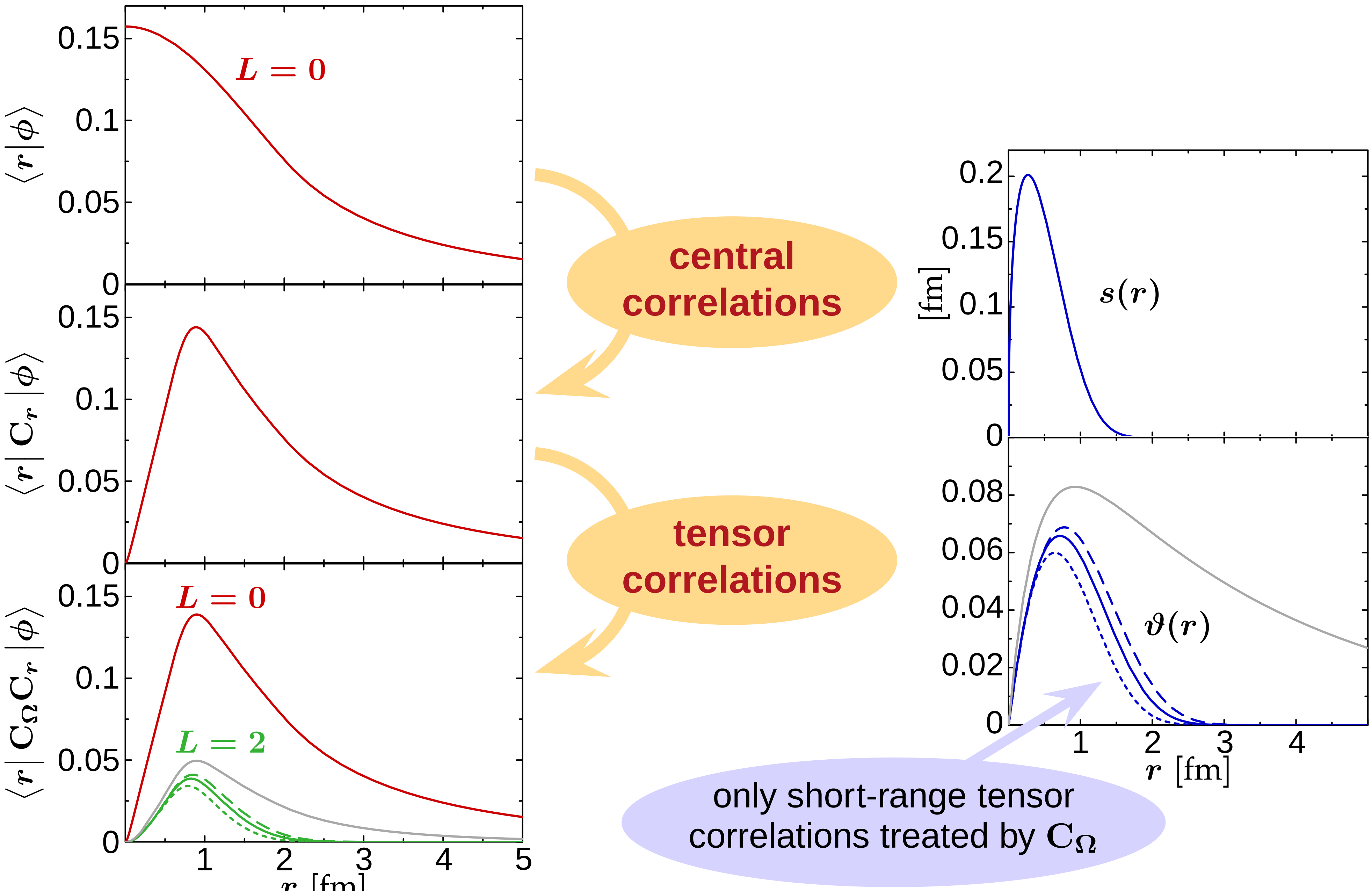
Correlated Operators

adapt Hamiltonian and all other observables to uncorrelated many-body space

$$\widetilde{\mathrm{O}} = \mathrm{C}^\dagger\;\mathrm{O}\;\mathrm{C}$$

$$\langle\widetilde{\psi}|\,\mathrm{O}\,|\widetilde{\psi}'\rangle = \langle\psi|\,\mathrm{C}^\dagger\;\mathrm{O}\;\mathrm{C}\,|\psi'\rangle = \langle\psi|\,\widetilde{\mathrm{O}}\,|\psi'\rangle$$

Correlated States: The Deuteron



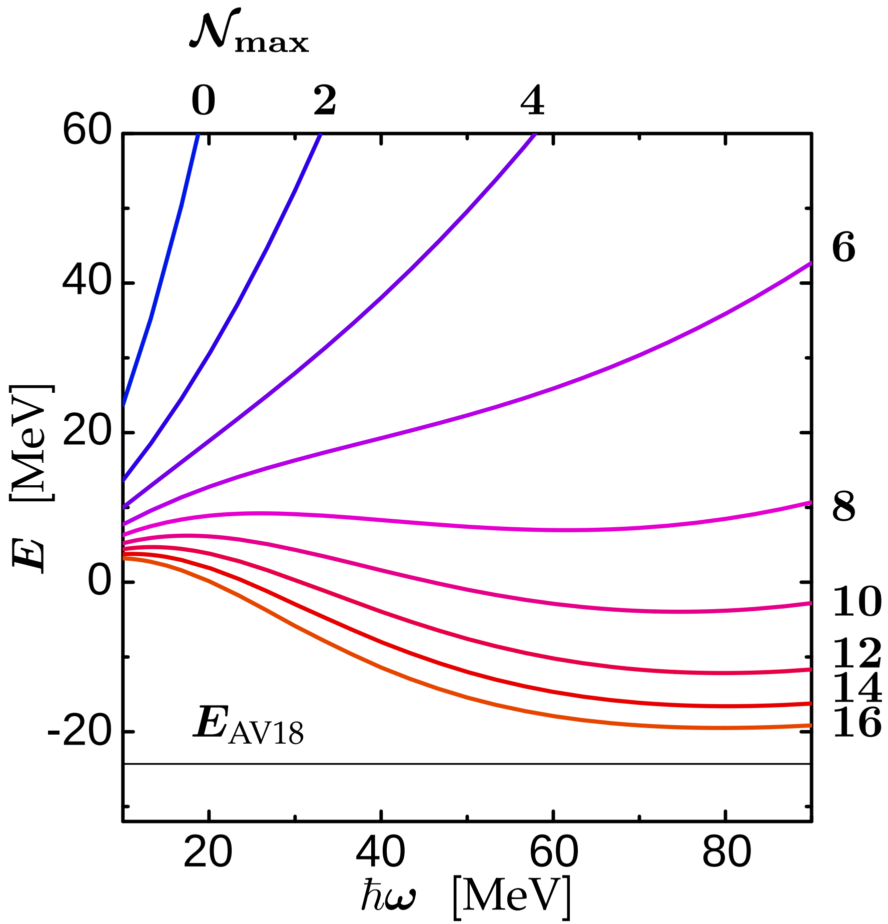
No-Core Shell Model

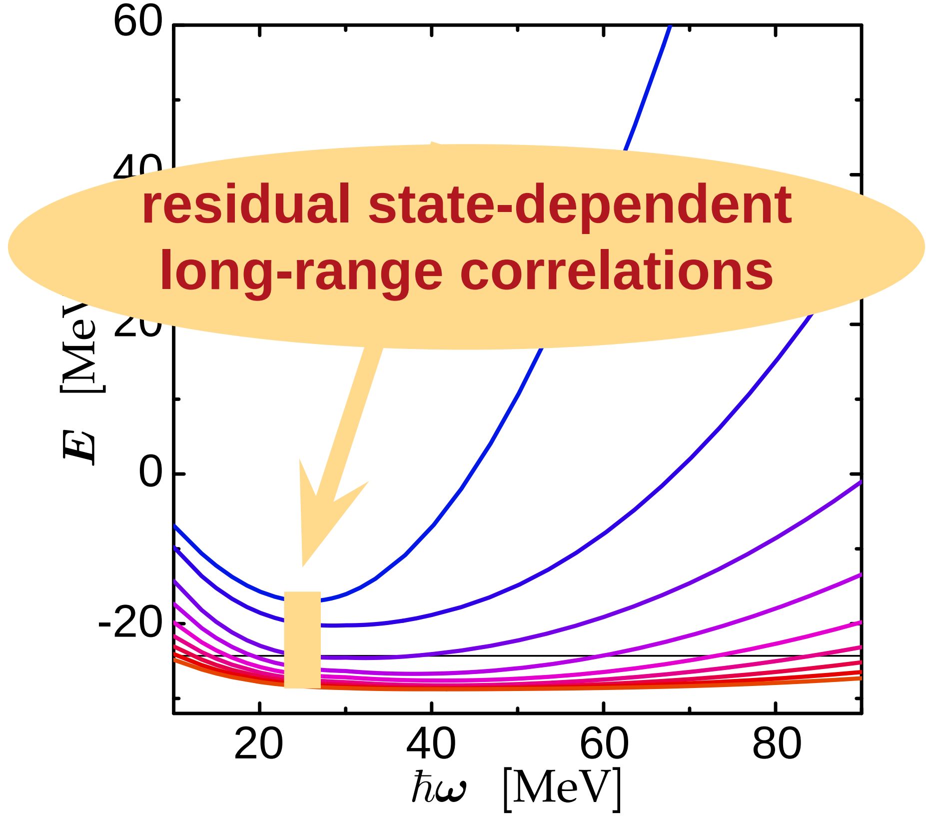
Roth et al. — Phys. Rev. C 72, 034002 (2005)
Roth & Navrátil — in preparation

^{4}He: Convergence

V_{AV18}

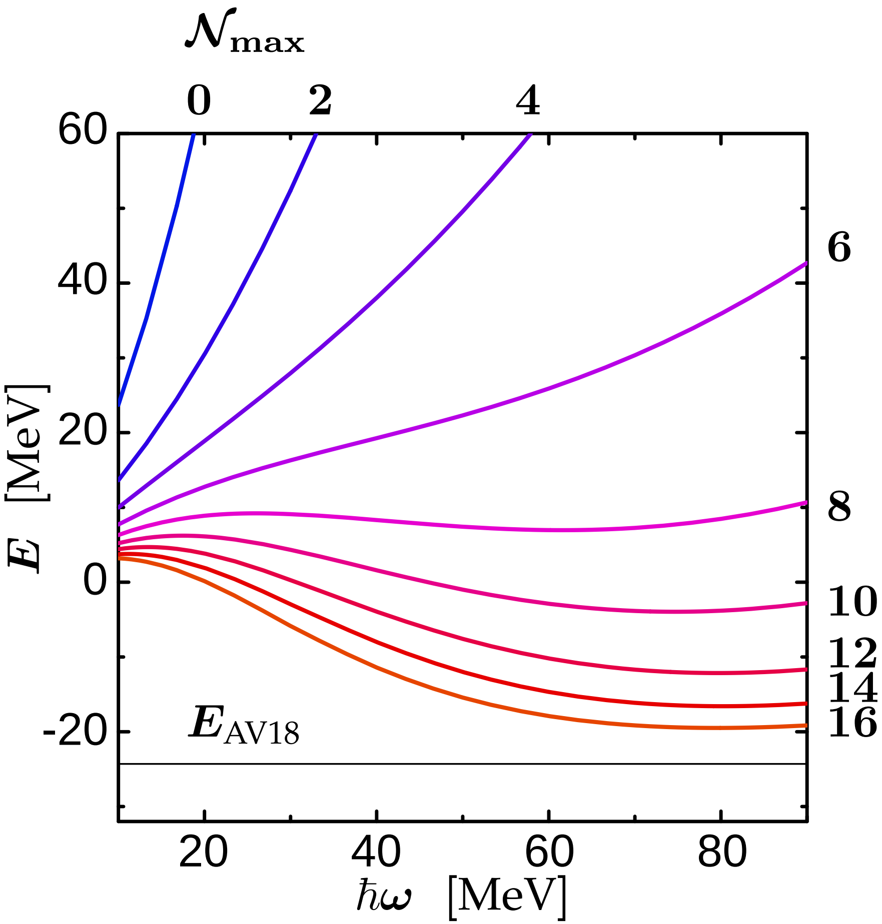
V_{UCOM}



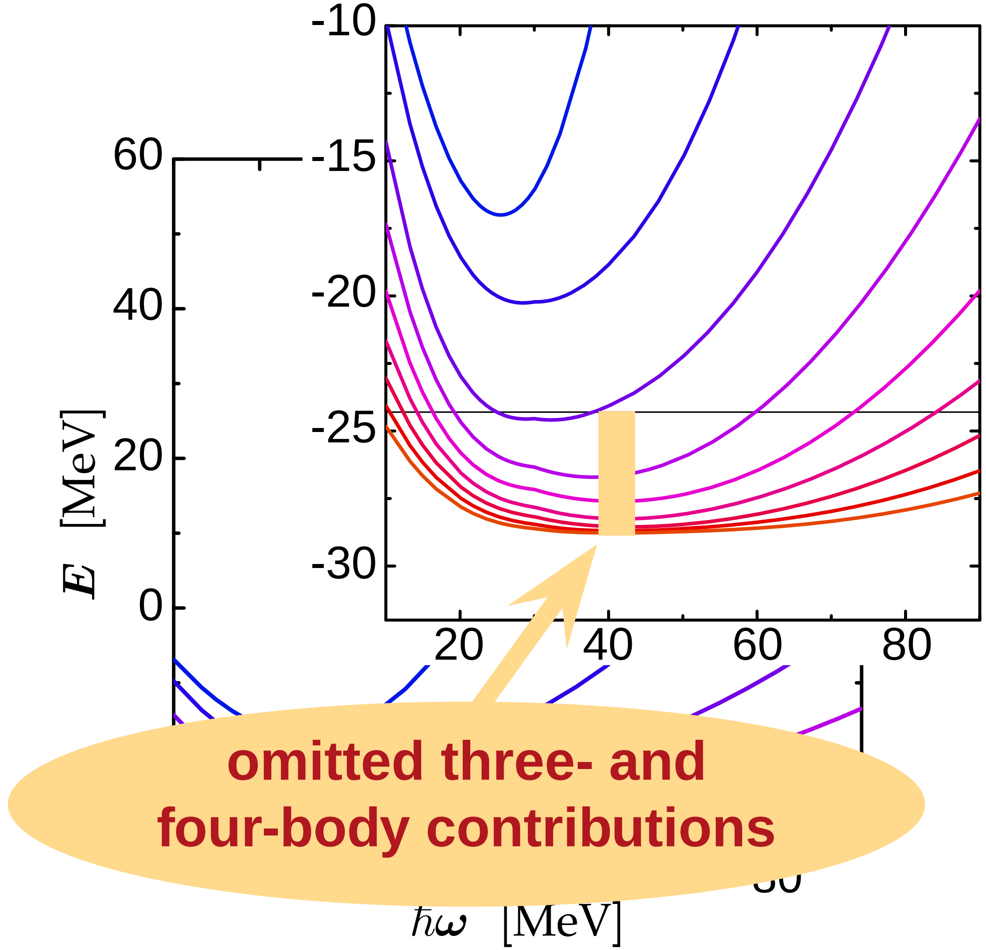


^{4}He: Convergence

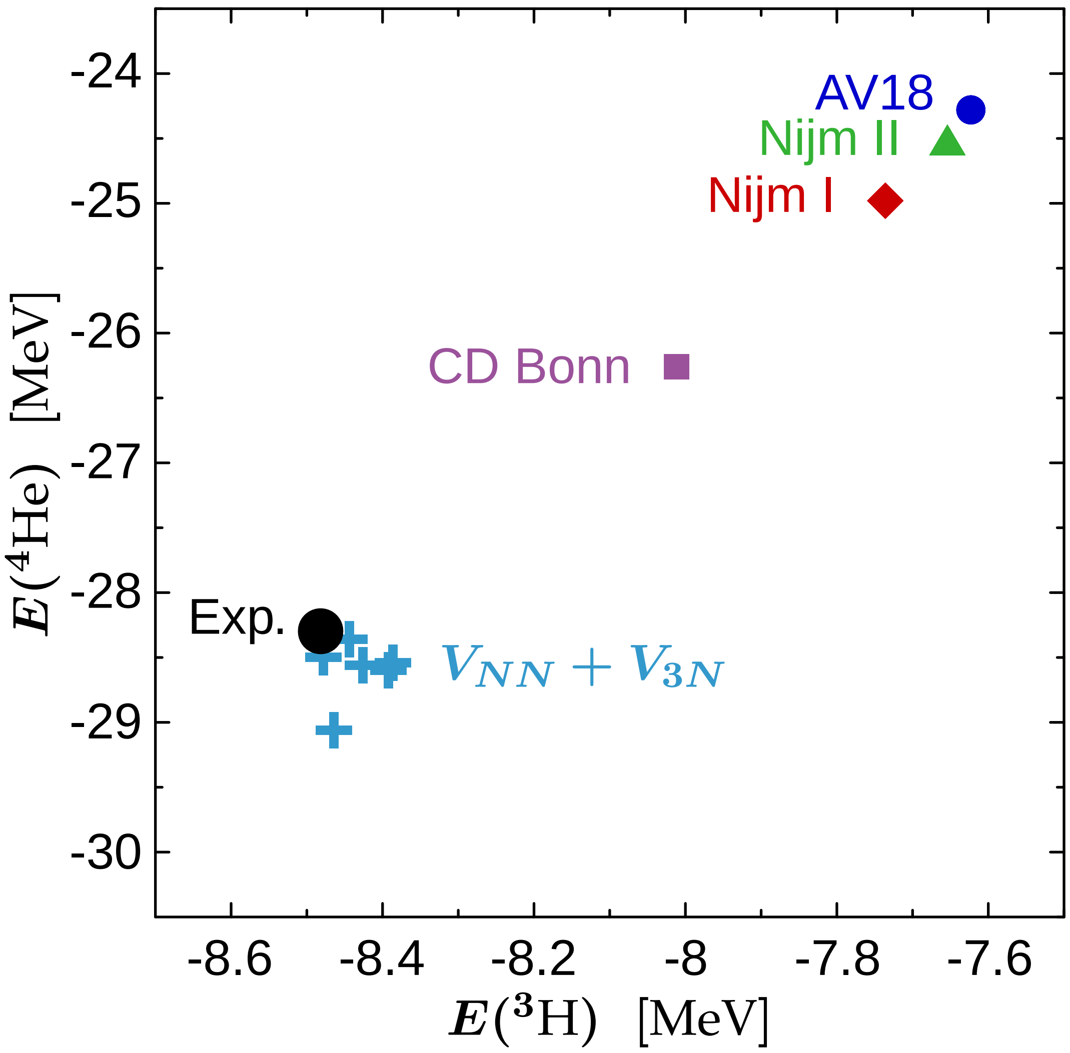
V_{AV18}



V_{UCOM}

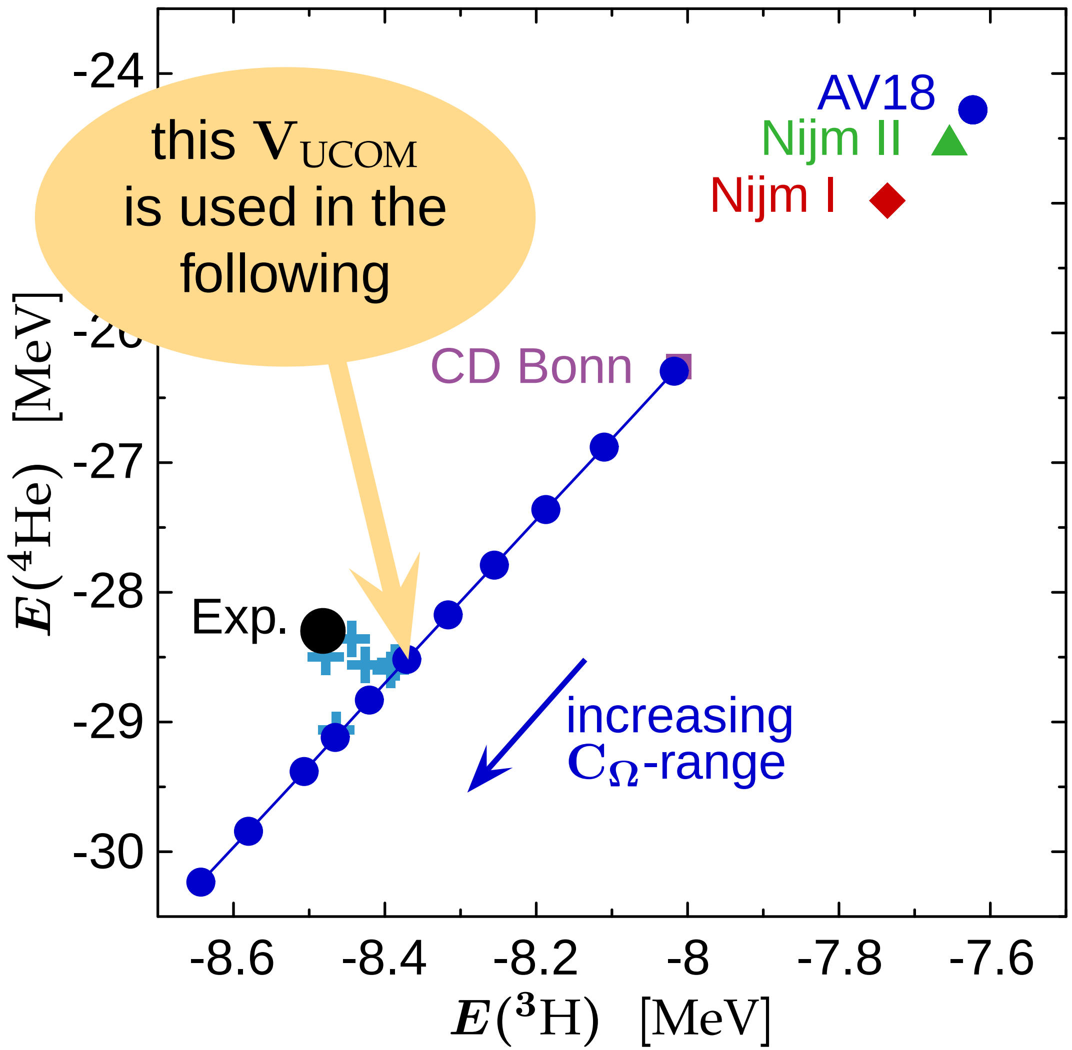


Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions

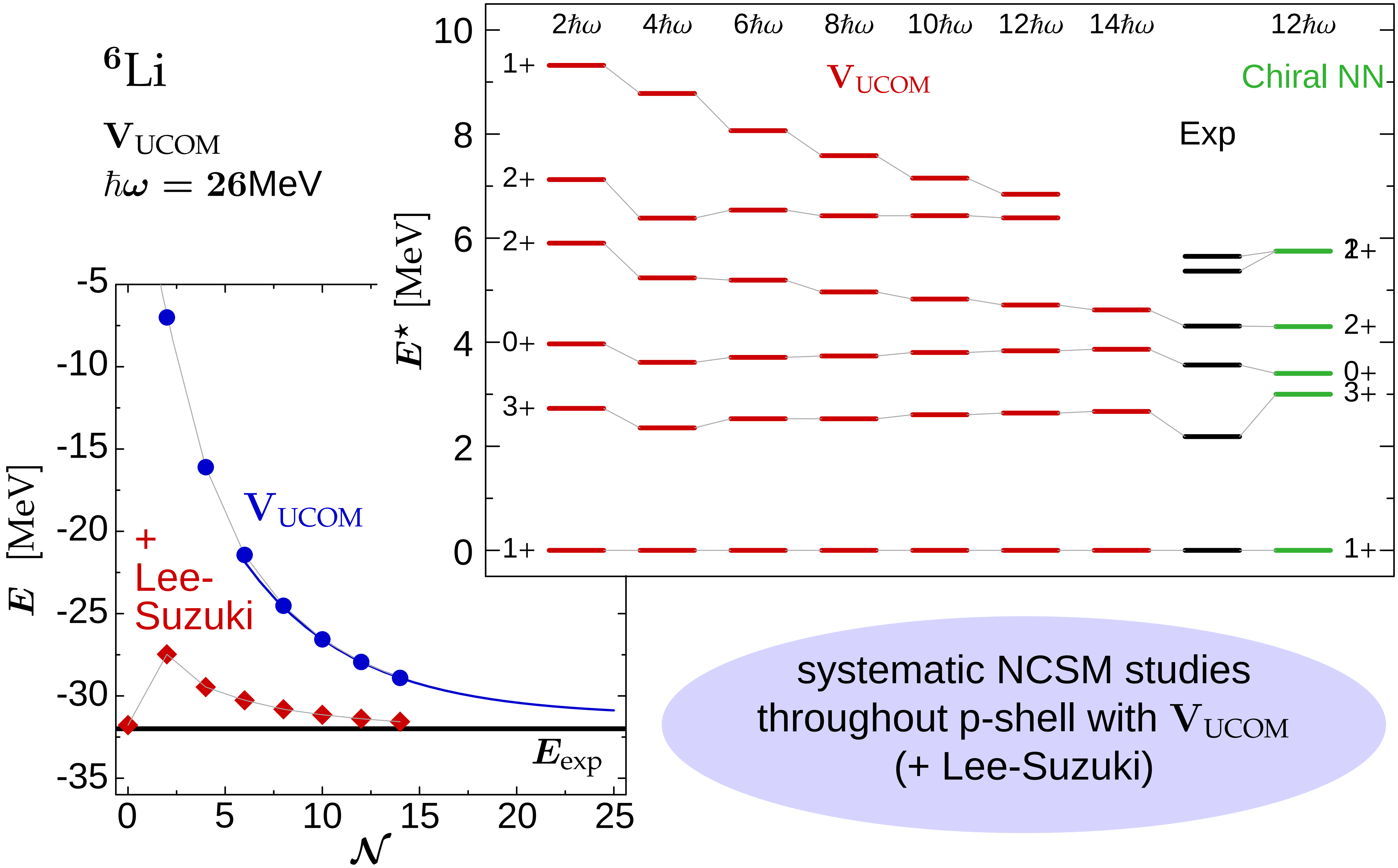
Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- change of C_{Ω}-correlator range results in shift along Tjon-line

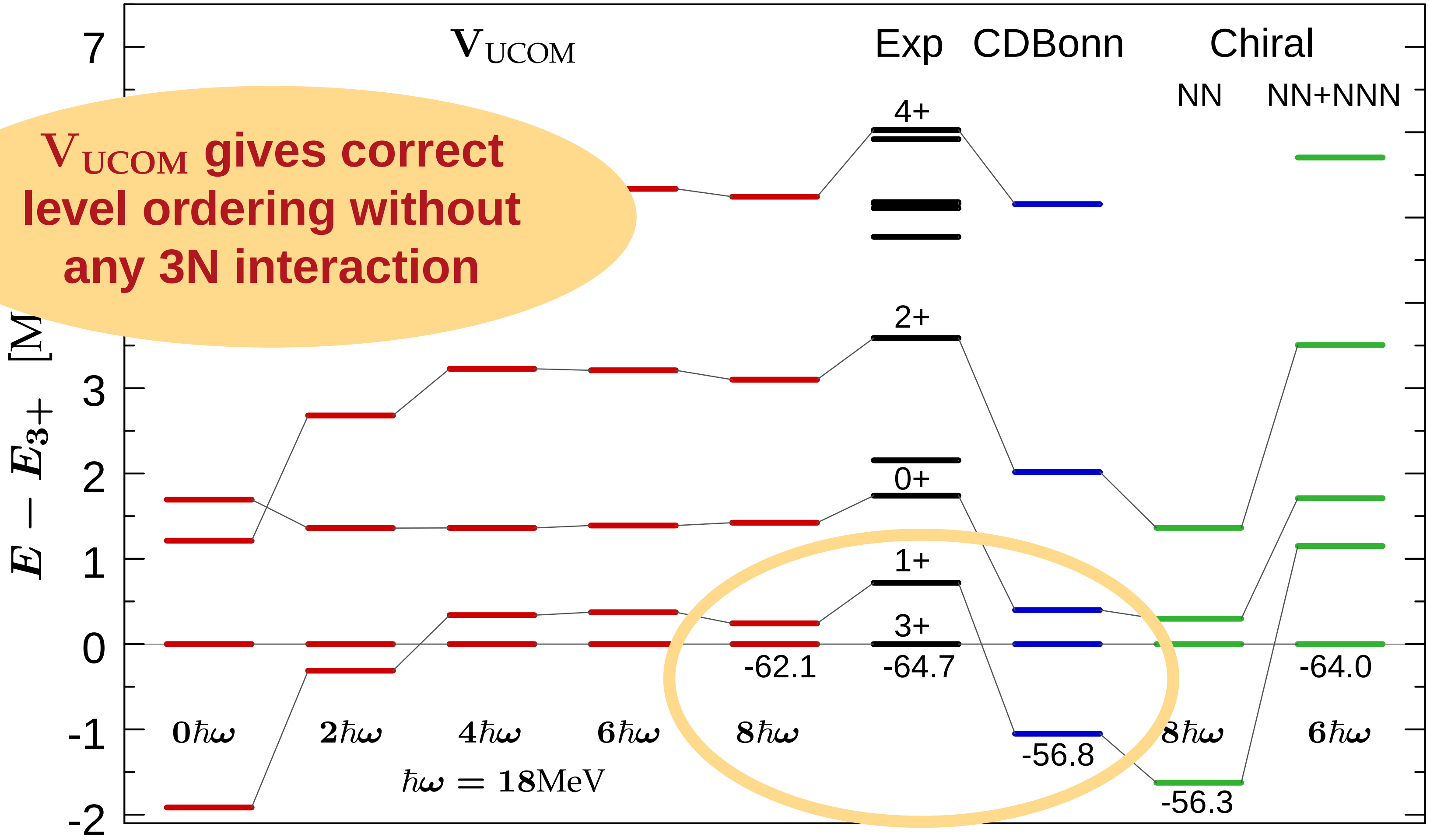
minimize net three-body force by choosing correlator with energies close to experimental value

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



systematic NCSM studies throughout p-shell with $\mathbf{V}_{\text{UCOM}}$ (+ Lee-Suzuki)

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



V_{UCOM} gives correct level ordering without any 3N interaction

Importance Truncated No-Core Shell Model

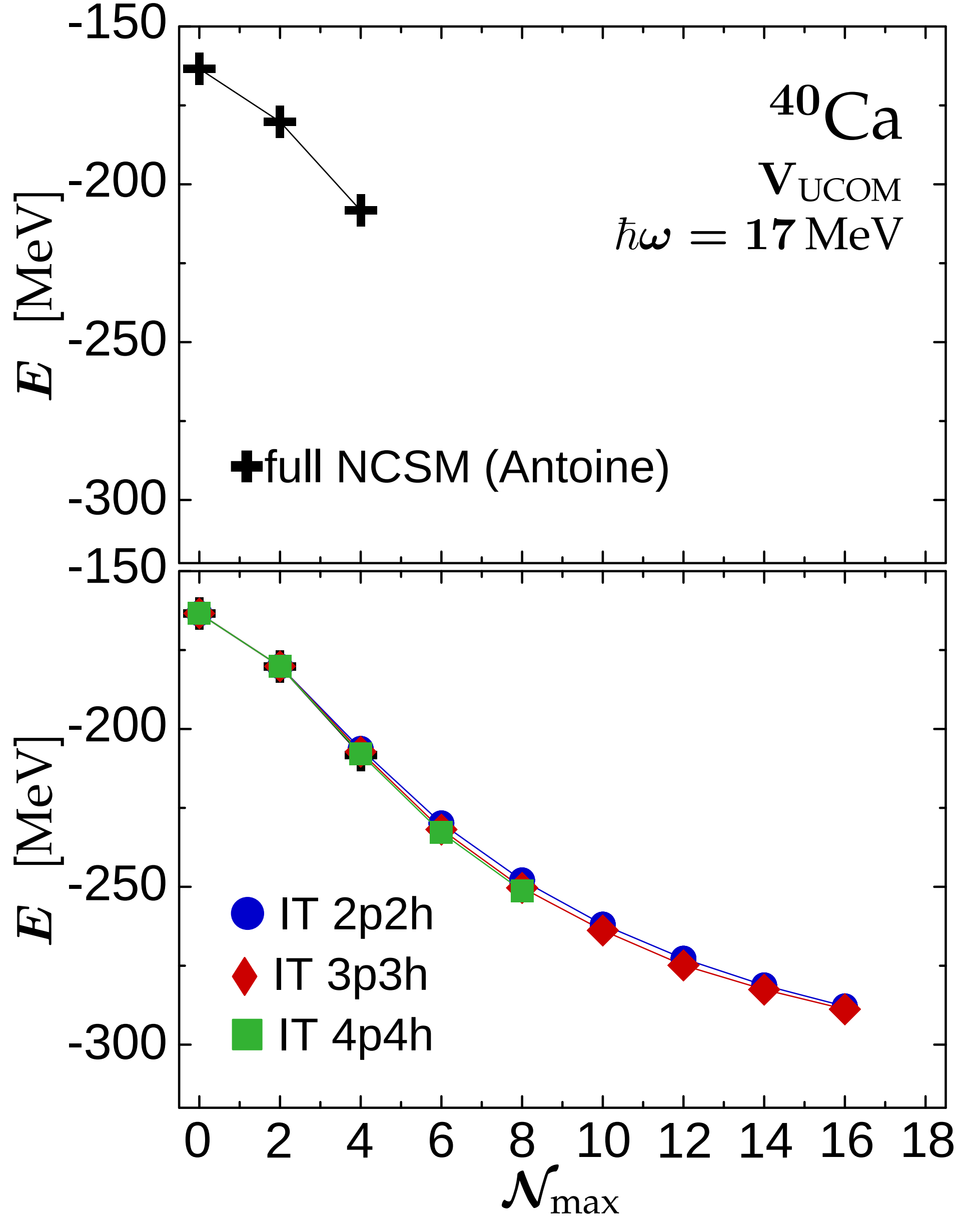
Roth & Navrátil — arXiv: 0705.4069

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to p-shell
- full $6\hbar\omega$ calculation for ^{40}Ca presently not feasible (basis dimension $\sim 10^{10}$)

Importance Truncation

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



General Idea

- given an intrinsic Hamiltonian

$$\mathbf{H}_{\text{int}} = \mathbf{T} - \mathbf{T}_{\text{cm}} + \mathbf{V} = \mathbf{H}_0 + \mathbf{H}'$$

  and an unperturbed Hamiltonian $\mathbf{H}_0$ with eigenstates $\left|\Phi_\nu\right\rangle$

- consider lowest-order **perturbation theory** to construct a correction $\left|\Psi^{(1)}\right\rangle$ to the unperturbed reference state $\left|\Psi^{(0)}\right\rangle$

$$\left|\Psi^{(0)}\right\rangle = \left|\Psi_{\text{ref}}\right\rangle = \left|\Phi_0\right\rangle \qquad \left|\Psi^{(1)}\right\rangle = \sum_{\nu \neq \text{ref}} \kappa_\nu \left|\Phi_\nu\right\rangle$$

- perturbative estimate of amplitudes serves as **measure for importance of individual basis states $\left|\Phi_\nu\right\rangle$**

$$\kappa_\nu = -\frac{\left\langle\Phi_\nu\right| \mathbf{H}' \left|\Psi_{\text{ref}}\right\rangle}{E_\nu^{(0)} - E_{\text{ref}}^{(0)}}$$

- restrict model space to **important configurations with $|\kappa_\nu| \geq \kappa_{\min}$** and solve eigenvalue problem

Iterative Construction of Model Space

❶ start with reference state $|\Psi_{\text{ref}}\rangle = |\Phi_0\rangle$ (simplest case)

❷ create 1p1h and 2p2h excitations of $|\Psi_{\text{ref}}\rangle$ and keep important basis states $|\Phi_\nu\rangle$ with $|\kappa_\nu| \geq \kappa_{\text{min}}$

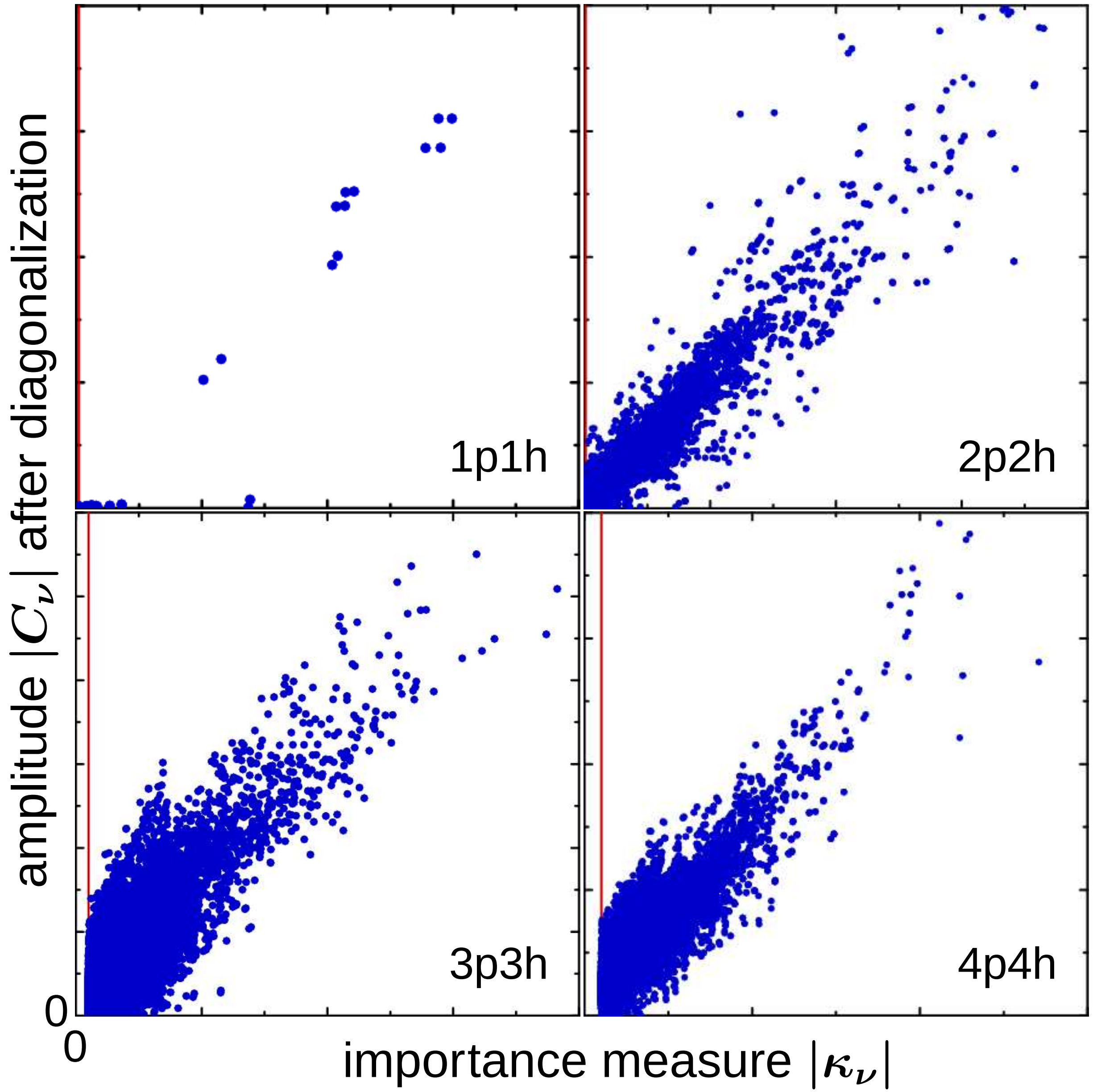
❸ solve the eigenvalue problem of H_{int} in this model space (up to 2p2h); ground state yields new reference state (dominant components)

❹ create 1p1h and 2p2h excitations of new $|\Psi_{\text{ref}}\rangle$ and keep the important basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$

❺ solve the eigenvalue problem of H_{int} in resulting model space (up to 4p4h)

...and so on...

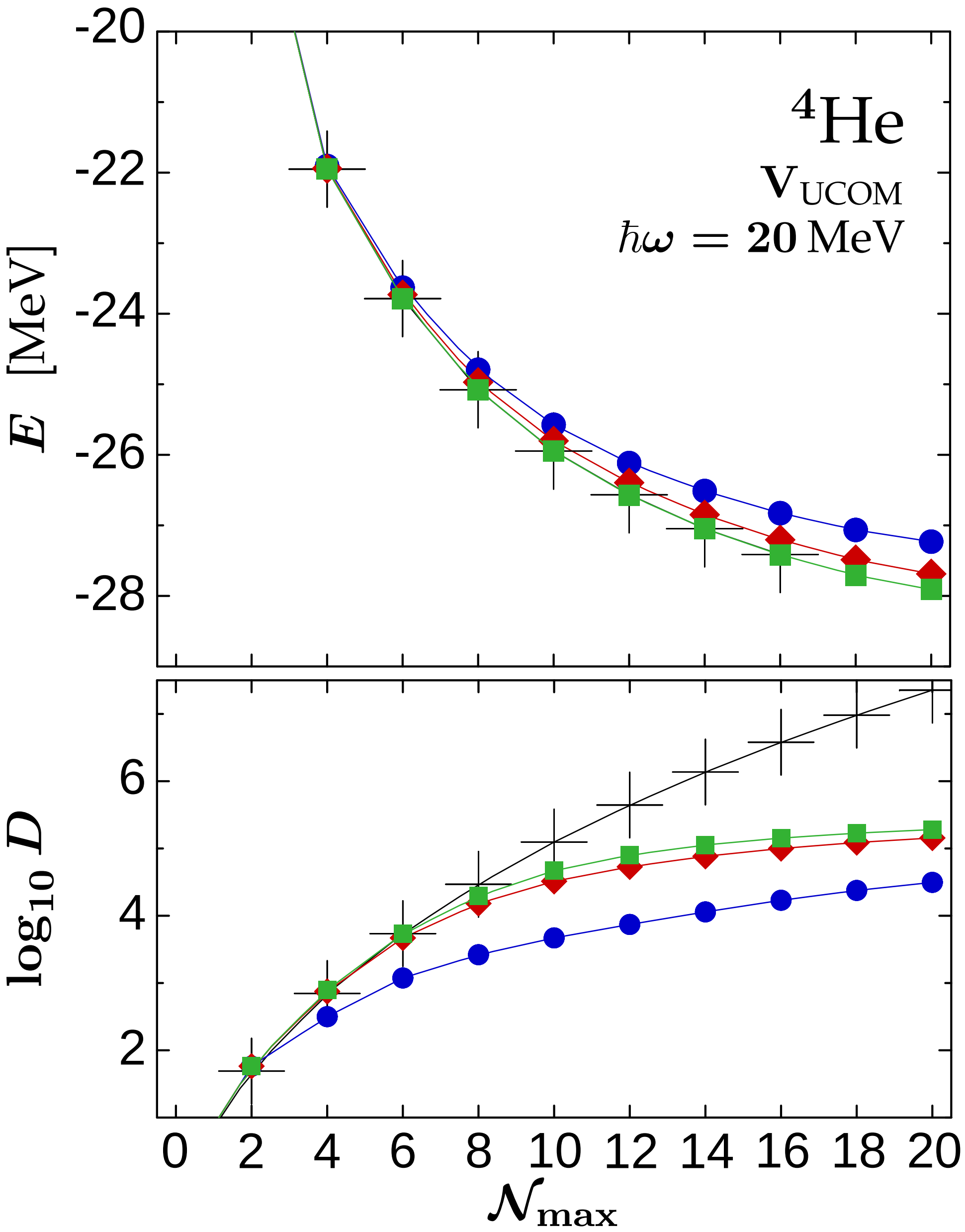
Importance Measure



- importance measure κ_ν provides **reliable a priori estimate** of the a posteriori amplitude C_ν obtained from diagonalization

^{16}O
$\mathbf{V}_{\text{UCOM}}$
$\hbar\omega = \mathbf{20}\,\text{MeV}$
$\mathcal{N}_{\mathbf{max}} = \mathbf{6}$

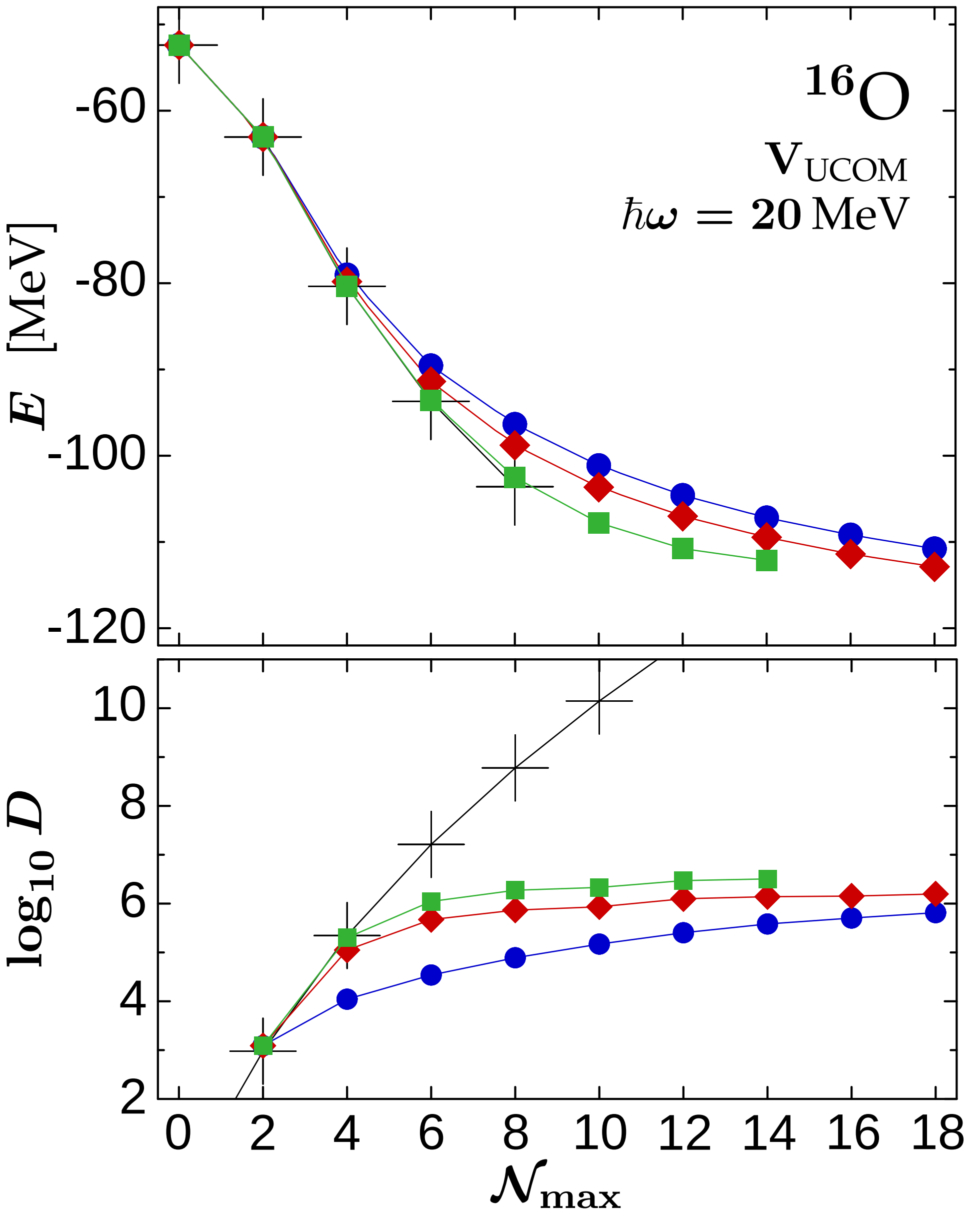
Benchmark: ^{4}He



- **reproduces exact NCSM result** with an importance truncated basis that is 2 orders of magnitude smaller than the full $\mathcal{N}_{max}\hbar\omega$ space

+ full NCSM (Antoine)
● IT-NCSM 2p2h
♦ IT-NCSM 3p3h
■ IT-NCSM 4p4h

Benchmark: ^{16}O

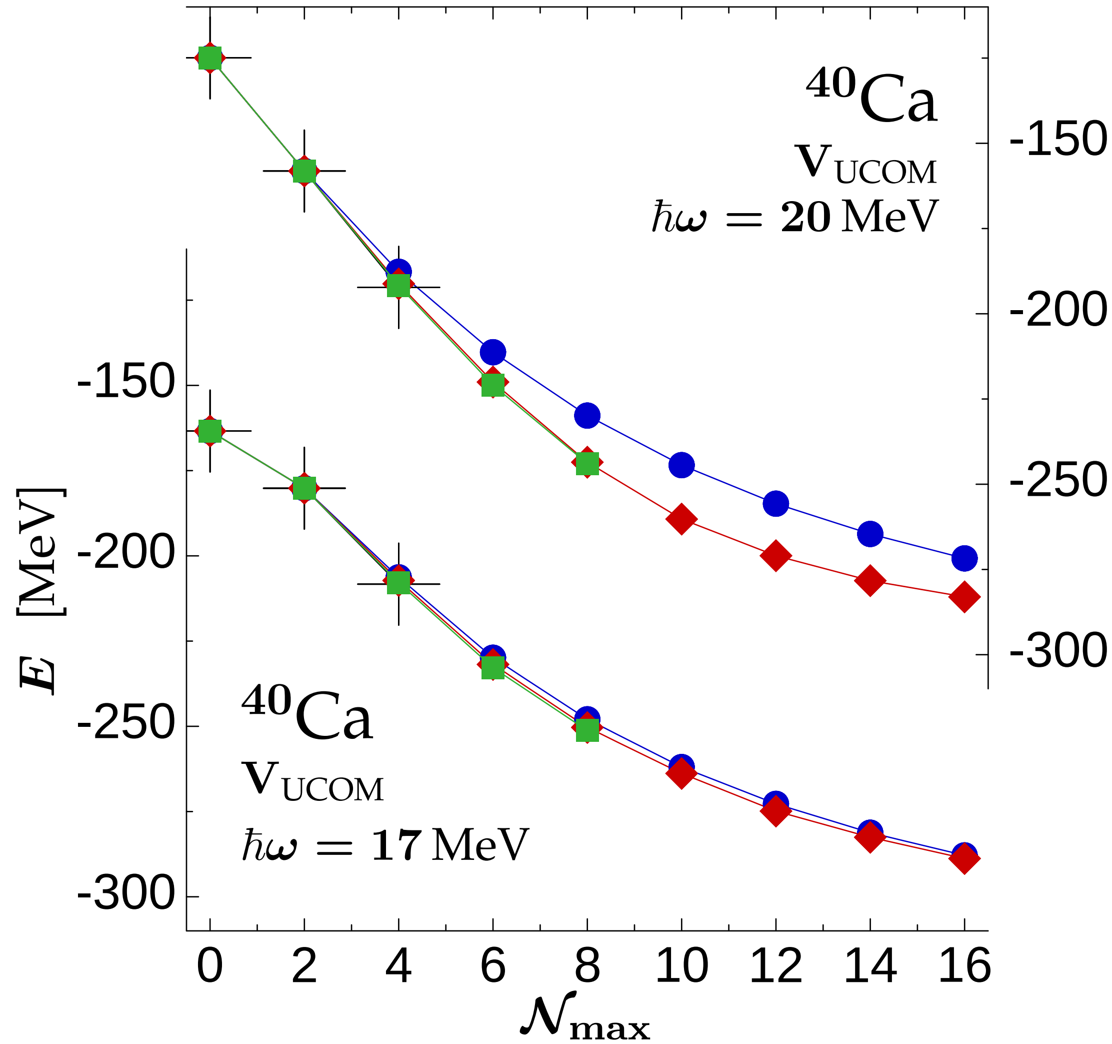


- **excellent agreement with full NCSM** calculation although configurations beyond 4p4h are not included

- dimension reduced by **several orders of magnitude**; possibility to go way beyond the domain of the full NCSM

+ full NCSM (Antoine)
● IT-NCSM 2p2h
♦ IT-NCSM 3p3h
■ IT-NCSM 4p4h

Benchmark: ^{40}Ca



- $16\hbar\omega$ calculations for ^{40}Ca are feasible
- extrapolation of ground state energy (3p3h, $\hbar\omega = \mathbf{17}\,\text{MeV}$) yields

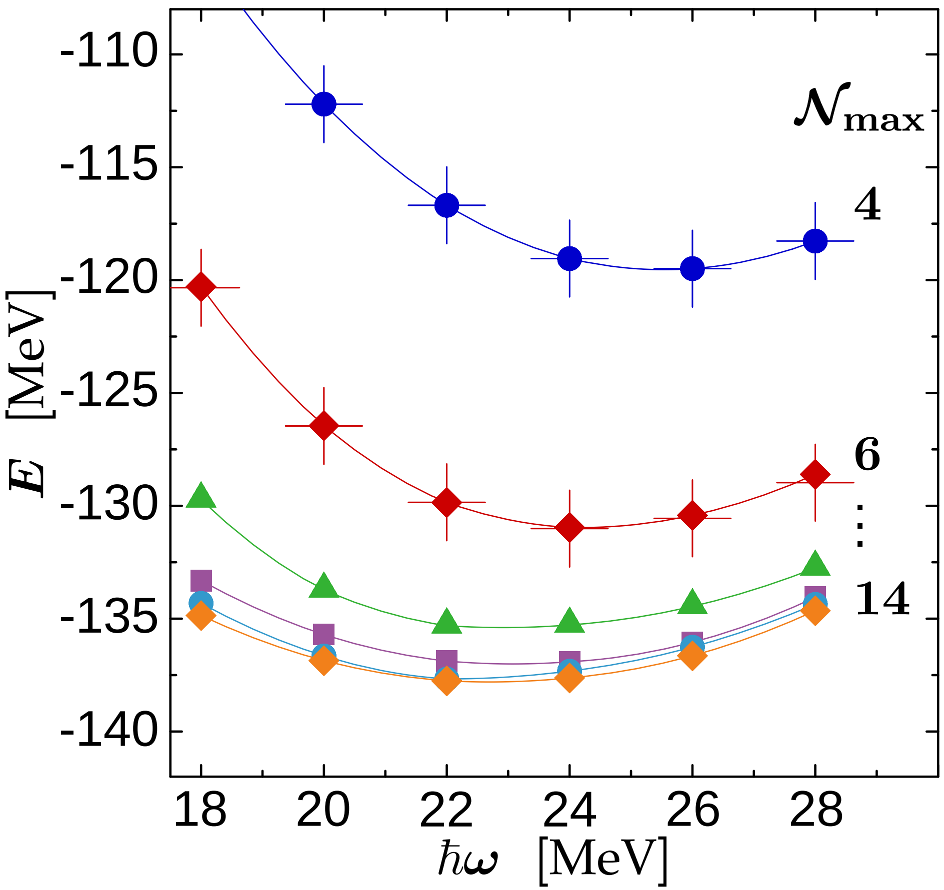
$$E_\infty \approx -\mathbf{316}\,\text{MeV}$$
$$E_{\text{exp}} = -\mathbf{342.05}\,\text{MeV}$$

+ full NCSM (Antoine)
● IT-NCSM 2p2h
♦ IT-NCSM 3p3h
■ IT-NCSM 4p4h

Benchmark Results for $V_{\text{low}k}$

$\mathbf{V}_{\text{low-}k}$
(AV18, $\Lambda = 2.1\,\text{fm}^{-1}$)

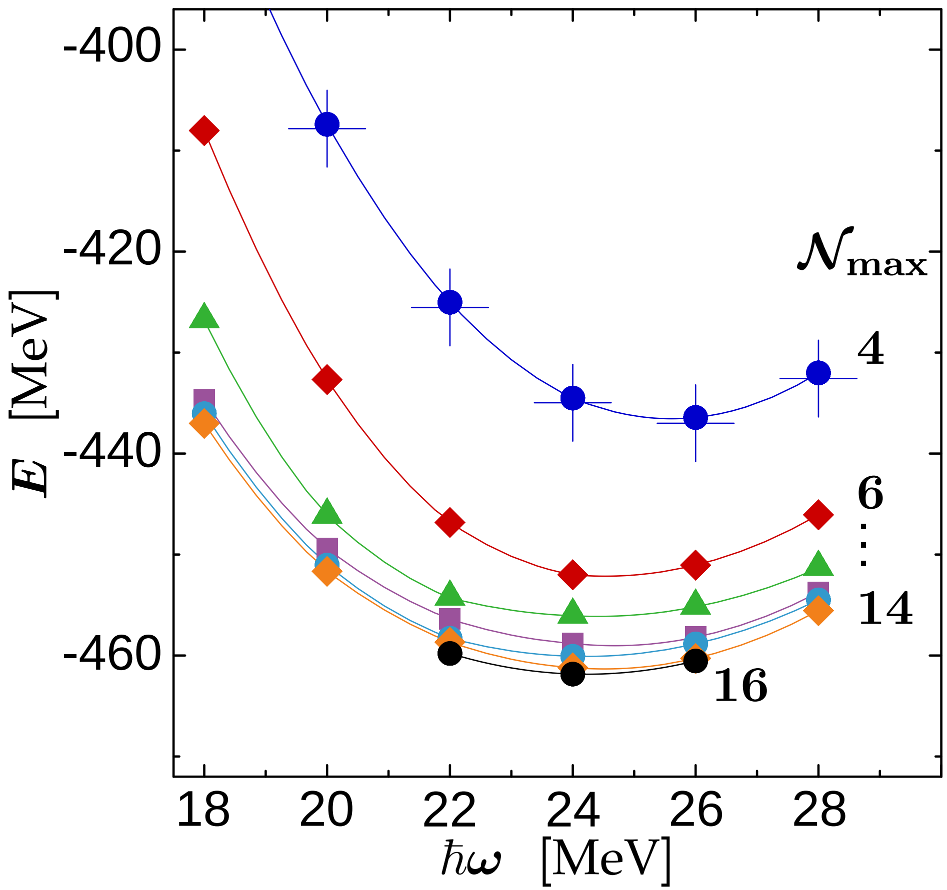
^{16}O
(up to 4p4h)



$E_\infty(\text{4p4h}) \approx -138\,\text{MeV}$

$R_{\text{rms}}(\text{4p4h}) = 2.03\,\text{fm}$

^{40}Ca
(up to 3p3h)



$E_\infty(\text{3p3h}) \approx -463\,\text{MeV}$

$R_{\text{rms}}(\text{3p3h}) = 2.27\,\text{fm}$

Conclusions

- importance truncation provides a **conceptually simple and universal tool** for large-scale eigenvalue problems
- **fully variational**: can be viewed as a variational calculation with an adaptive trial state
- very efficient in **reducing the model space** (by several orders of magnitude) to relevant states without loosing precision
- **no center-of-mass contaminations** ($< 100\,\mathrm{keV}$): importance truncation preserves properties of full $N_{\mathrm{max}}\hbar\omega$ space
- eigenstates in **shell-model representation** for free: convenient starting point for calculation of densities, form factors, etc.
- **computationally efficient** (need only a few processors)

Perspectives

- explicit inclusion of **configurations beyond 4p4h**
- **perturbative estimate** for contribution of configurations beyond 4p4h
- **alternative schemes** for construction of importance truncated space
- study of **excited states** with generalized reference states
- use of **Hartree-Fock single-particle states**
- use of **Lee-Suzuki transformed interactions**

exciting new tool
for ab initio calculations
beyond the p-shell

Epilogue

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