Multi-Configurational Many-Body Perturbation Theory

'Many-body perturbation theories in modern quantum chemistry and nuclear physics'

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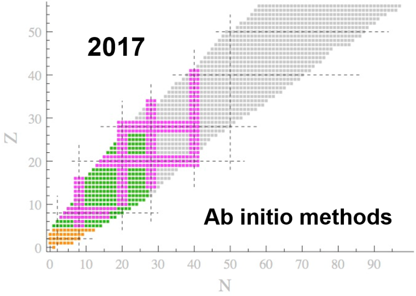
Overview

- Challenges in nuclear many-body theory
- Review of the nuclear Hamiltonian
- Merging CI and MBPT
- Multi-configurational many-body perturbation theory
    - Basic theory
    - Diagrams
    - Results
- Conclusion



Motivation

- **goal**: *ab initio* treatment for **degenerate medium-mass** Fermi systems

$$H|\psi\rangle = E|\psi\rangle$$

- **systematic uncertainties** coming from ...
  - nuclear input Hamiltonian
  - truncation error in many-body expansion
- open-shell systems require treatment of **static correlation effects**
  - effective Hamiltonian approaches
    CCEI, MBPT, VS-IMSRG
  - symmetry-broken reference states
    BMBPT, BCC, Gorkov-SCGF, $SU(2)$-CC
  - multi-configurational reference states
    NCSM-PT, MR-IMSRG, IM-NCSM
- **goal:** treat **even and odd nuclei** and **excited states** on equal footing
- **strategy:** combination of successful many-body techniques

$\Longrightarrow$ **hybrid *ab initio* approaches**

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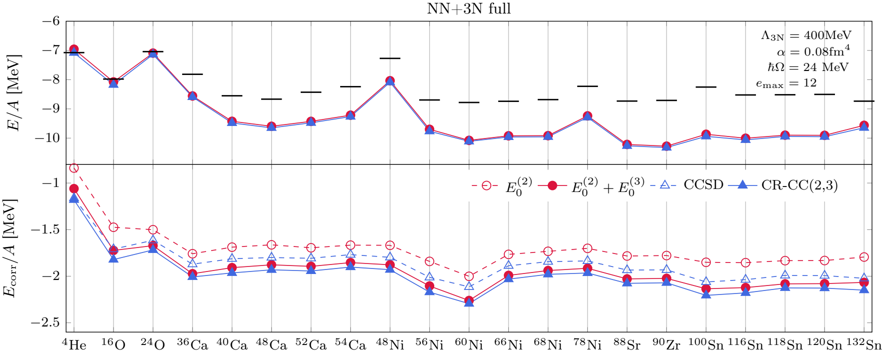
Novel approach:
Merge configuration interaction
with perturbation theory:
Perturbatively-Improved
No-Core Shell Model

Ab Initio?



A. Tichai, J. Langhammer, S. Binder, R. Roth, PLB **756** 283

- HF-MBPT can efficiently describe closed-shell systems
- comparable accuracy as **state-of-the-art CC models**
- only $1-3\%$ of computational resources required
- **defects in Hamiltonian** cause large deviation from experiment

The Nuclear Many-Body Problem — Why MBPT?

- typical s.p. basis contains $N \approx 2000$ states (***m*-scheme dimension**):

$$|k\rangle = \underbrace{|n_k, l_k, s_k, j_k, m_k\rangle}_{\textbf{spinorbitals}} \otimes \underbrace{|1/2, t_k\rangle}_{\textbf{isospin}}$$

- **problem:** non-perturbative approaches require handling of **large tensors**

CCD	t_{ij}^{ab}	$\rightarrow$	$N_o^2 N_v^2 \approx 80\ \ Gb$ storage
CCT	t_{ijk}^{abc}	$\rightarrow$	$N_o^3 N_v^3 \approx 10^6\, Gb$ storage

$\Longrightarrow$ **storage bottleneck**

- **solution: spherical framework** (analogue of symmetry restriction)

$$|\tilde{k}\rangle = |n_k, l_k, j_k, t_k\rangle \text{ with } \tilde{N} \approx 200$$

- milder scaling BUT restricted to even-even nuclei
- MBPT does not suffer from tensor storage

$\Longrightarrow$ **formulate open-shell MBPT in m-scheme**

Hamiltonian – Chiral Effective Field Theory

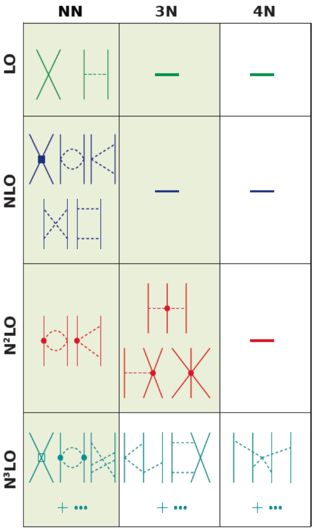
- Lagrangian consistent with **QCD symmetries**
- **effective d.o.f.** are pions and nucleons
- intrinsic hierarchy arises from:
  - **power-counting scheme**
  - **particle-rank** of operators
- goal: theory with **systematic uncertainties**

  ... current power counting not renormalizable
- state-of-the-art Hamiltonian:
  - NN interaction @ N3LO

    Entem, Machleidt, Phys.Rev C 68, 041001(R) (2003)
  - 3N interaction @ N2LO

    Navrátil, Few Body Systems 41, 117 (2007)

... no unique nuclear Hamiltonian!



Similarity Renormalization Group

- perform pre-diagonalization via **unitary transformation:** $\hat{H}_\alpha = \hat{U}^\dagger_\alpha \hat{H} \hat{U}_\alpha$
- solve **evolution equations** for anti-Hermitian **dynamic generator**

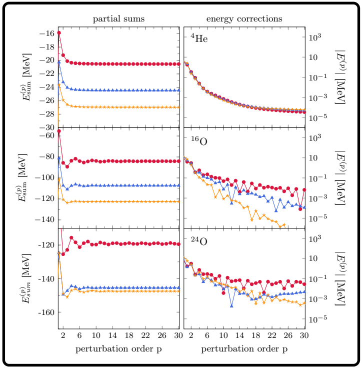
$$\frac{d}{d\alpha}\hat{H}_\alpha = \left[\hat{\eta}_\alpha, \hat{H}_\alpha\right] \quad \text{with} \quad \hat{\eta}_\alpha = (2\mu)^2 \left[\hat{T}_{\text{int}}, \hat{H}_\alpha\right]$$

- **advantage:** improved model-space convergence
- **tradeoff**: induces **many-body operators**

$$\hat{H}_\alpha = \hat{H}^{[2B]}_\alpha + \hat{H}^{[3B]}_\alpha + \underbrace{\hat{H}^{[4B]}_\alpha + \hat{H}^{[5B]}_\alpha + \dots}_{\text{discard!}}$$

- **violation of unitarity** in Fock space
- diagnostic tool: variation of flow parameter
- **soft interaction:** faster MBPT convergence

A. Tichai *et al.*, PLB **756** 283



Inclusion of 3B Forces

- explicit inclusion of 3B operators is **very expensive**
- use **normal ordering** of 3B operator with respect to *A*-body reference state

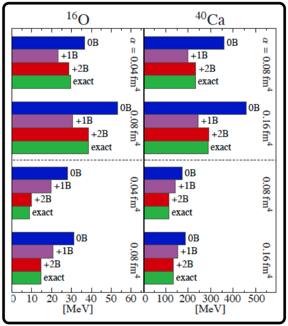
$$V_{3N} = \sum V^{3B}_{\circ\circ\circ\circ\circ\circ} a^\dagger_\circ a^\dagger_\circ a^\dagger_\circ a_\circ a_\circ a_\circ$$

$$= W^0 + \sum W^{1B}_{\circ\circ} \{a^\dagger_\circ a_\circ\} + \sum W^{2B}_{\circ\circ\circ\circ} \{a^\dagger_\circ a^\dagger_\circ a_\circ a_\circ\} + \sum W^{3B}_{\circ\circ\circ\circ\circ\circ} \{a^\dagger_\circ a^\dagger_\circ a^\dagger_\circ a_\circ a_\circ a_\circ\}$$

- discard residual three-body part

  $\Rightarrow$ **normal-ordering two-body approximation**

- three-body physics via two-body operators
- induced error: $\approx 1-3\%$
- extension to **arbitrary reference states**

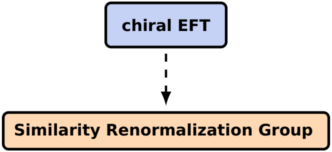


Roth *et al.*, PRL **109**, 052501 (2012)

MBPT in Nuclear Structure

chiral EFT

MBPT in Nuclear Structure



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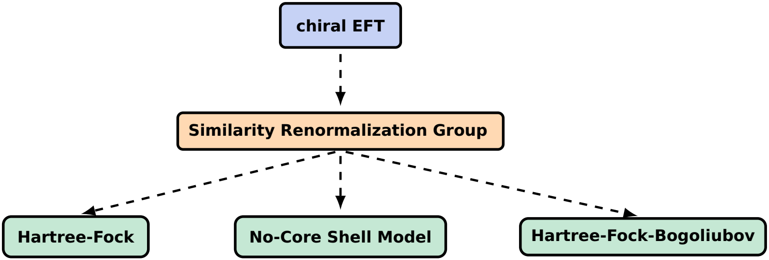

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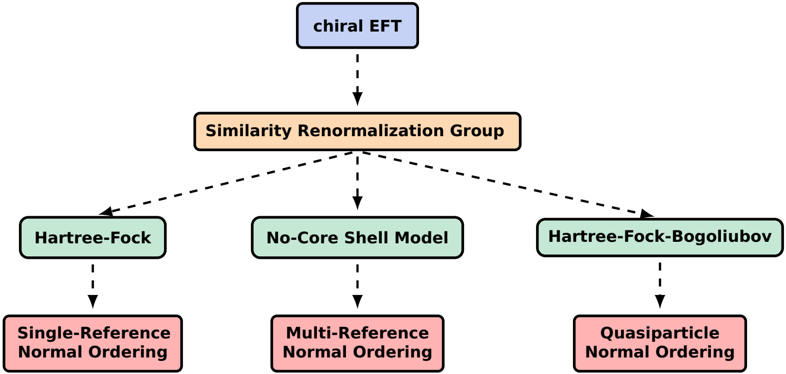

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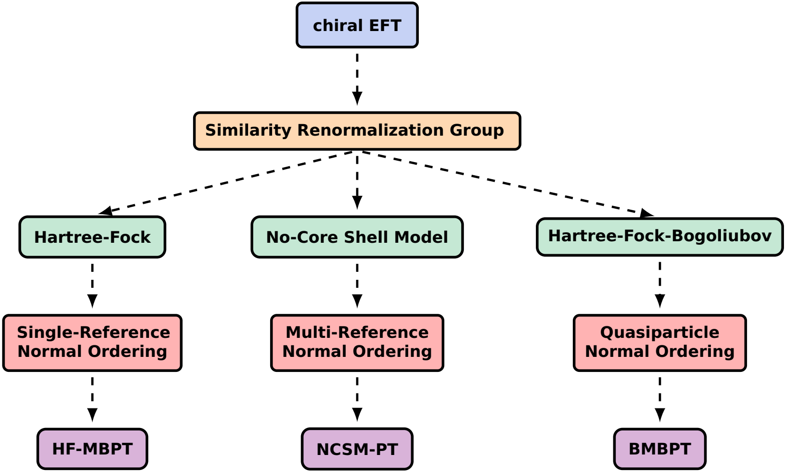

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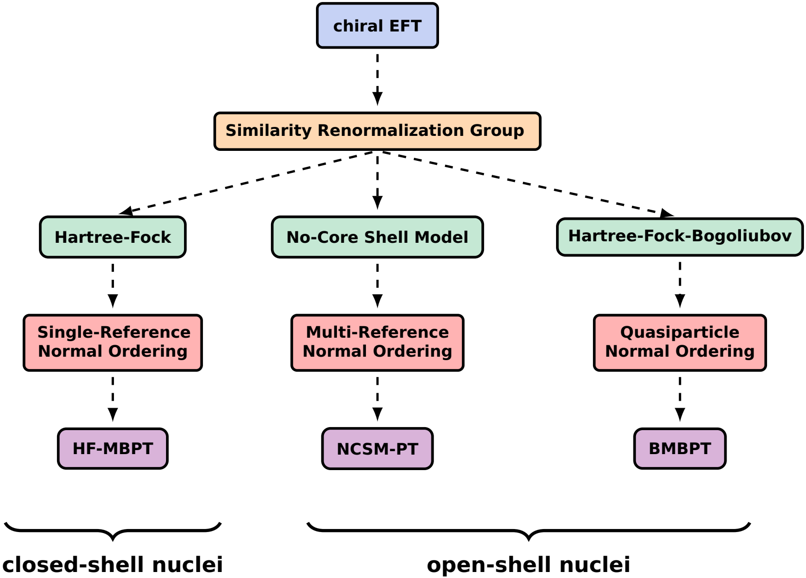
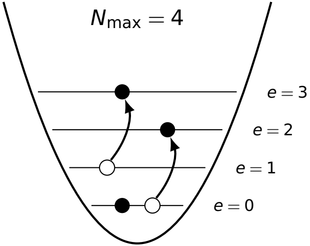


No-Core Shell Model

- construct **matrix representation** using Slater determinants w.r.t. HO/HF orbitals

$$H_{ij} = \langle \Phi_i | H | \Phi_j \rangle$$

- perform **large-scale diagonalization** in N_{max}-truncated model space
- all nucleons are active degrees of freedom
- **variational principle** holds for absolute binding energies
- storage of many-body Hamiltonian limits application to **light nuclei**
- adaptive **importance truncation** extends applicability up to medium-light systems
- particular variant of **CI method**



^{6}Li proton orbits

Hybrid Many-Body Theory

No-core shell model

- \+ variational approach
- \+ great flexibility
- − computationally demanding
- − limited to light nuclei

Perturbation theory

- \+ access large model spaces
- \+ computationally very efficient
- − requires proper reference state
- − convergence unclear

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reference state

parametrized by $\left(N_{\mathbf{max}}^{(\mathbf{ref})}, p\right)$

residual correlation effects

No-core shell model perturbation theory (NCSM-PT)

+ captures static correlation effects
+ systematically improvable reference states
+ NCSM-PT is exact in two limits
– convergence to be investigated

inspired by quantum chemistry

Surjan, Szabados, Rolik, Nakano, ...

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General properties → **Convergence behaviour** → **Low-order corrections**

Multi-Configurational MBPT

- **reference state** from diagonalization in a small model space $\mathcal{M}_{\text{ref}}$

$$|\psi_{\text{ref}}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} c_\nu |\phi_\nu\rangle$$

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$$H_0 = E^{(0)}_{\text{ref}} |\psi_{\text{ref}}\rangle\langle\psi_{\text{ref}}| + \sum_{I \neq |\psi_{\text{ref}}\rangle} E^{(0)}_I |\psi_I\rangle\langle\psi_I| + \sum_{\nu \notin \mathcal{M}_{\text{ref}}} E^{(0)}_\nu |\phi_\nu\rangle\langle\phi_\nu|$$

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- definition of **zeroth-order energies**

$$E^{(0)}_{\text{ref}} = \sum_p \epsilon_p \gamma_{pp} \qquad E^{(0)}_\nu = \sum_{i \in |\phi_\nu\rangle} \epsilon_i \qquad \gamma_{pq} = \langle\psi_{\text{ref}}| a^\dagger_p a_q |\psi_{\text{ref}}\rangle$$

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- generalization of Fock operator via correlated **1B density matrix**

$$f_{pq} = H^{[1]}_{pq} + \sum_i H^{[2B]}_{piqi} \quad \longrightarrow \quad f_{pq} = H^{[1B]}_{pq} + \sum_{rs} H^{[2B]}_{prqs} \cdot \gamma_{rs}$$

- define **single-particle energies** by $\epsilon_p = f_{pp}$

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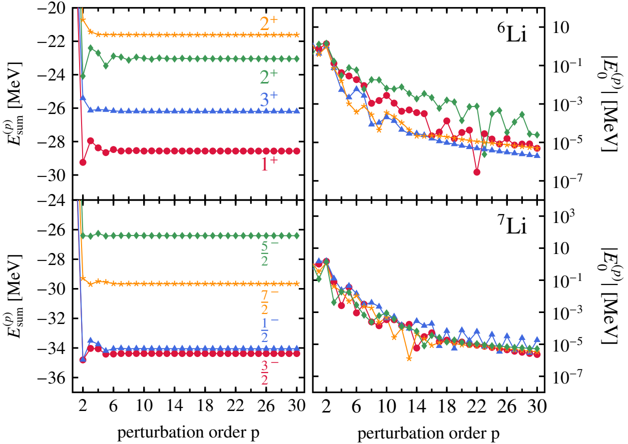
- define **single-particle energies** by $\epsilon_p = f_{pp}$
- **one-dimensional reference space:** reduction to single-determinantal MBPT

Convergence Behavior of NCSM-PT

NN+3N-full, $\Lambda_{3N} = 500\,\text{MeV}$



$\hbar\Omega = 20\,\text{MeV}$, $\alpha = 0.08\,\text{fm}^4$, $N_{\text{max}} = 4$, $N_{\text{max}}^{\text{ref}} = 0$

AT, Gebrerufael, Vobig, Roth arXiv: 1703.05664 (2016)

- perturbation series **converges exponentially** for all reference states
- different reference states have a **similar convergence pattern**
- low-order partial sums yield good approximation to converged result

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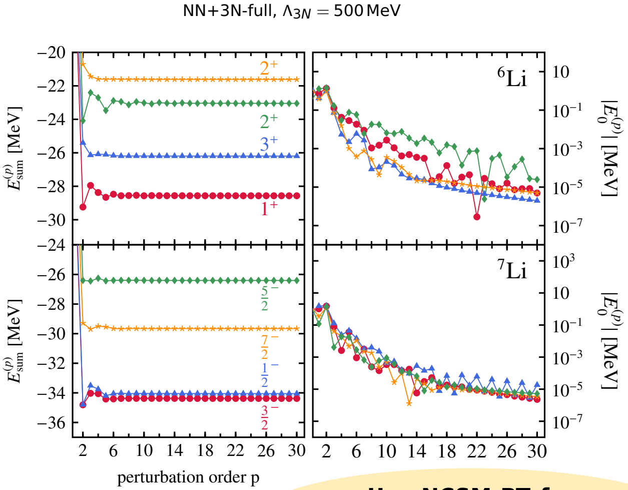

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Use NCSM-PT for heavier systems!

Low-order Energy Corrections

- second-order energy correction in **'sum-over-configurations'** form:

$$E^{(2)} = \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{|\langle \psi_{\text{ref}} | \hat{W} | \Phi_\nu \rangle|^2}{E_{\text{ref}} - E_\nu^{(0)}}$$

- **problem: size of many-body basis** limits configuration-driven approach

$\Longrightarrow$ derive **sum-over-orbital** formalism

- expand energy correction w.r.t. **Slater determinant components**

$$E^{(2)} = \sum_{\mu,\mu' \in \mathcal{M}_{\text{ref}}} c_{\mu'} c_\mu^\star \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{\langle \Phi_{\mu'} | \hat{W} | \Phi_\nu \rangle \langle \Phi_\nu | \hat{W} | \Phi_\mu \rangle}{E_{\text{ref}} - E_\nu^{(0)}}$$

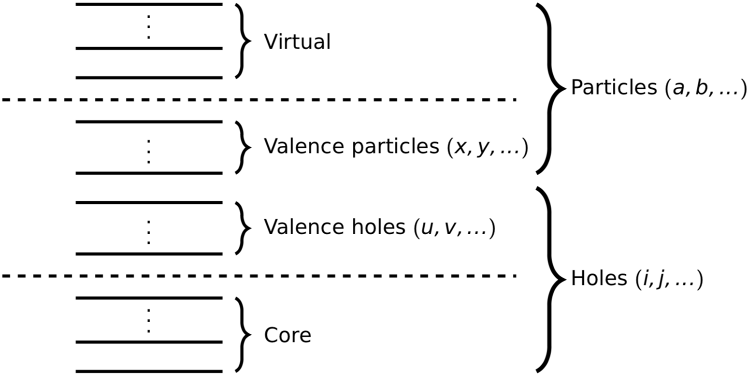
- interpret $\langle \Phi_{\mu'} |$ as ph excitation and apply **Wick's theorem**

$$\langle \Phi_{\mu'} | = \langle \Phi_\mu | \{ i_1^\dagger \cdots i_p^\dagger a_p \cdots a_1 \}_{|\Phi_\mu\rangle}$$

- **normal-ordered one-body part** depends on current Fermi vacuum

$$\langle p | \hat{h}_1^{(\mu)} | q \rangle = (H_{pq}^{[1B]} - \epsilon_p) \delta_{pq} + \frac{1}{2} \sum_{i \in |\Phi_\mu\rangle} H_{piqi}^{[2B]}$$

Classification of Single-Particle States



- particle-hole nature depends on **current Fermi vacuum**
- number of particle or holes is constant
- core states can be empty in the most general case

Diagrams

- development of **diagrammatic framework** to support Wick evaluation of

$$\langle \Phi_{\mu'} | \hat{W} | \Phi_\nu \rangle \langle \Phi_\nu | \hat{W} | \Phi_\mu \rangle$$

- classify diagrams according to **external excitation rank**
  - closed topologies: 2 diagrams (**non-canonical HF diagrams**)
  - single excitations: 6 diagrams
  - double excitations: 8 diagrams
  - triple excitations: 4 diagrams
  - quadruple excitations: 1 diagram

  } **wave-function diagrams**

- **NCSM reference state:** 1B part of perturbation operator not diagonal

$\Longrightarrow$ Brillouin's theorem does not hold

- resolvent operator yields **determinant-dependent denominator**

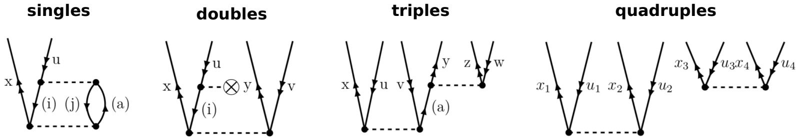
$$D_\mu = \epsilon^{ab\ldots}_{ij\ldots} + \Delta_\mu \qquad \text{with} \qquad \Delta_\mu = E^{(0)}_{\text{ref}} - E^{(0)}_\mu$$

Open Diagrams

- open diagrams appear for $\mu \neq \mu'$

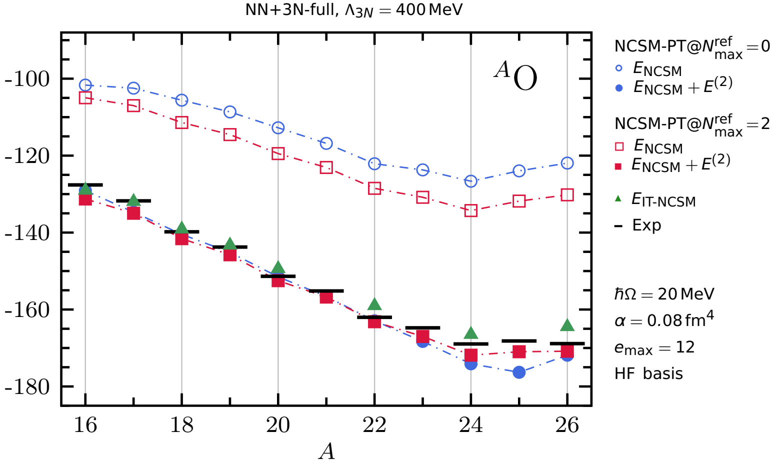
$$\langle \Phi_{\mu'} | \hat{W} | \Phi_\nu \rangle \langle \Phi_\nu | \hat{W} | \Phi_\mu \rangle$$

- open lines correspond to **valence particles**
- four different classes appear at second order (for 2B Hamiltonians)



- external lines require **permutation operators** (similar to CC theory)
- overall mixed computational scaling of diagrams
  - **closed diagrams:** $\sim \dim(\mathcal{M}_{\text{ref}}) \cdot N_p^2 \cdot N_h^2$
  - **open diagrams:** $\sim \dim(\mathcal{M}_{\text{ref}})^2 \cdot N_p^2 \cdot N_h$
- in applications reference space contains **millions of determinants**

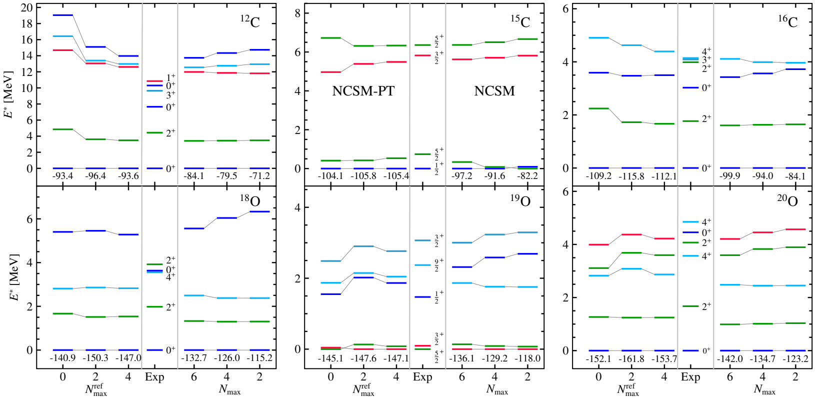
NCSM-PT – Oxygen Chain



- NCSM-PT accounts for a large part of **dynamical correlation**
- computationally **very cheap** technique (1-5% of diagonalization)
- small deviation due to **missing higher-order corrections** (and NO2B)

NCSM-PT – Excitation Energies

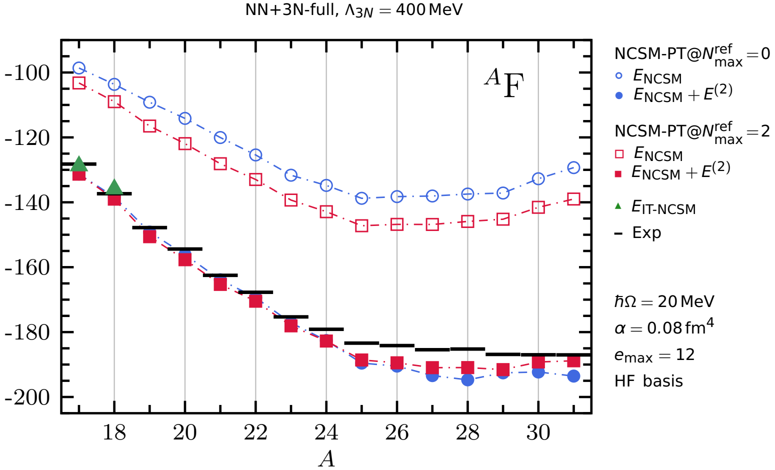
NN+3N-full, $\Lambda_{3N} = 400\,\text{MeV}$



$\hbar\Omega = 20\,\text{MeV}$, $\alpha = 0.08\,\text{fm}^4$, $e_{\text{max}} = 12$, HF basis

- correct **level ordering** when using $N_{\text{max}}^{\text{ref}} = 2$ reference states
- overall **good agreement** with NCSM spectra
- unsatisfactory description of second 0^+ state in ^{12}C (**clustering effects**)

NCSM-PT – New Frontiers



- extend the reach of **NCSM-based approaches** to heavier masses
- first *ab initio* calculations of **complete fluorine chain** in a no-core approach
- good reproduction of **experimental trend**

Limitations

- second-order effects are limited to **2p-2h excitations**
- challenging to describe **collective phenomena** in ph-picture
- **solution:** use complementary approaches
  - symmetry-broken MBPT (see talks by **P. Arthuis** and **T. Duguet**)
  - generalized multi-particle-multi-hole basis
- apply generalized normal ordering for arbitrary reference state

'Normal order and extended Wick theorem for a multiconfiguration reference wave function'
W. Kutzelnigg, D. Mukherjee, Journal of Chemical Physics **107** 432 (1997)

- was succesfully applied in open-shell extension of IM-SRG
- **challenge:** design a multi-particle-multi-hole flavour of MBPT
  - efficient handling of **overlap matrix**
  - treat redundant many-body basis states via SVD

Summary

- state-of-the-art nuclear Hamiltonians are very soft:

  ... use many-body perturbation theory!

- strongly-correlated systems require **generalized reference states**
  - Hartree-Fock-Bogoliubov vacua
  - multi-configurational vacua
  - generator-coordinate method
  - ...
- NCSM-PT yields **excellent agreement** with large-scale diagonalization
- only $1-5\%$ of computational resources required compared to FCI
- even and odd nuclei on equal footing in **no-core approach**
- immediate access to **excited states**
- **extends range of applicability** of NCSM-based techniques

Outlook

Improving accuracy ...

- perform **systematic studies** with respect to:
  - single-particle basis
  - choice of partitioning
  - size of reference state
- derive and implement **higher-order energy corrections**

  $\Rightarrow$ **automated diagram and code generation**

- implementation of **three-body operators** at second order

... and extending the framework

- calculating **other observables** via state corrections
- reference states from **truncated configuration interaction**

  $\Longrightarrow$ **higher mass numbers**

- derive **multi-particle-multi-hole** MBPT version

Epilogue

- **Thanks to my group**
  - P. Arthuis, M. Drissi, T. Duguet, V. Somà
    CEA, Saclay, France

- **Thanks to our collaborators**
  - J.-P. Ebran, J. Ripoche
    CEA DAM DIF, Arpajon, France
  - H. Hergert
    Michigan State University, USA
  - **R. Roth**
    Technische Universität Darmstadt, Germany

CURIE
TGCC

COMPUTING TIME