Bogoliubov coupled cluster theory for open-shell nuclei

Workshop on Progress in Ab Initio Nuclear Theory

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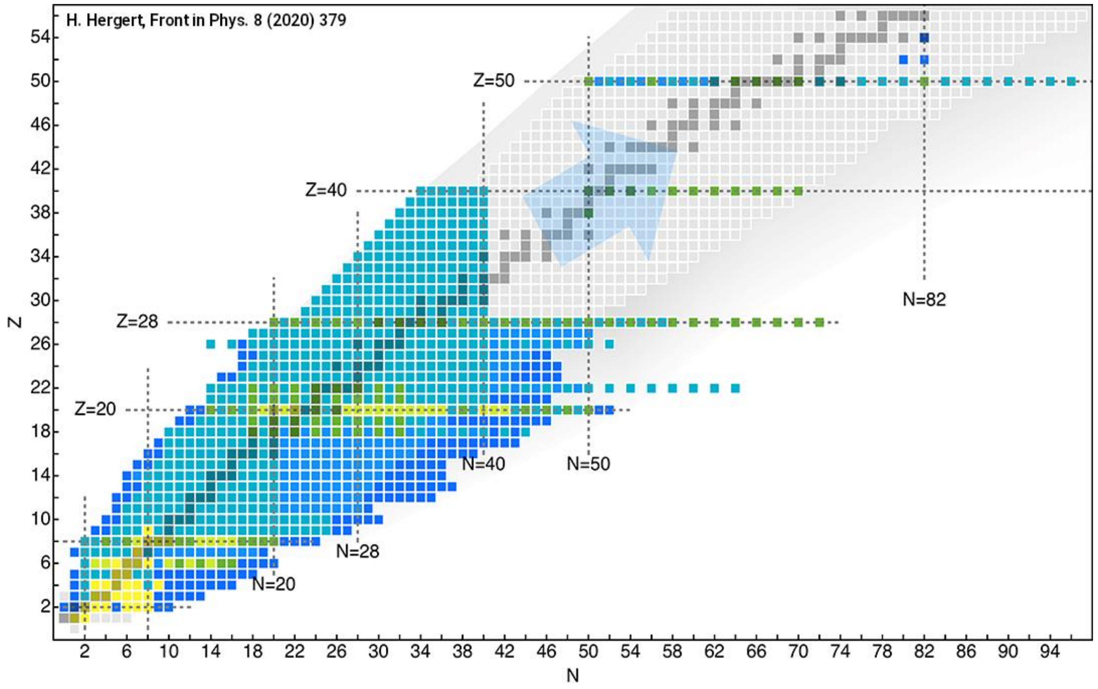
Open-shell frontier of ab initio many-body methods

- Open-shell nuclei
  - **Vast majority**
  - Strongly correlated
- Existing methods target mostly ground state
  - **Open-shell spectroscopy** at very frontier
- Push to heavier systems
  - **Polynomial** expansion methods required
  - Reduced storage schemes
- Single-refence symmetry-conserving approaches fail
  - Multi-reference techniques
  - Valence-space methods
  - **Symmetry-breaking approaches**
- Singly open-shell nuclei break particle-number symmetry
  - **Bogoliubov quasi-particle** framework
  - Grand canonical potential $\Omega \equiv H - \lambda A$



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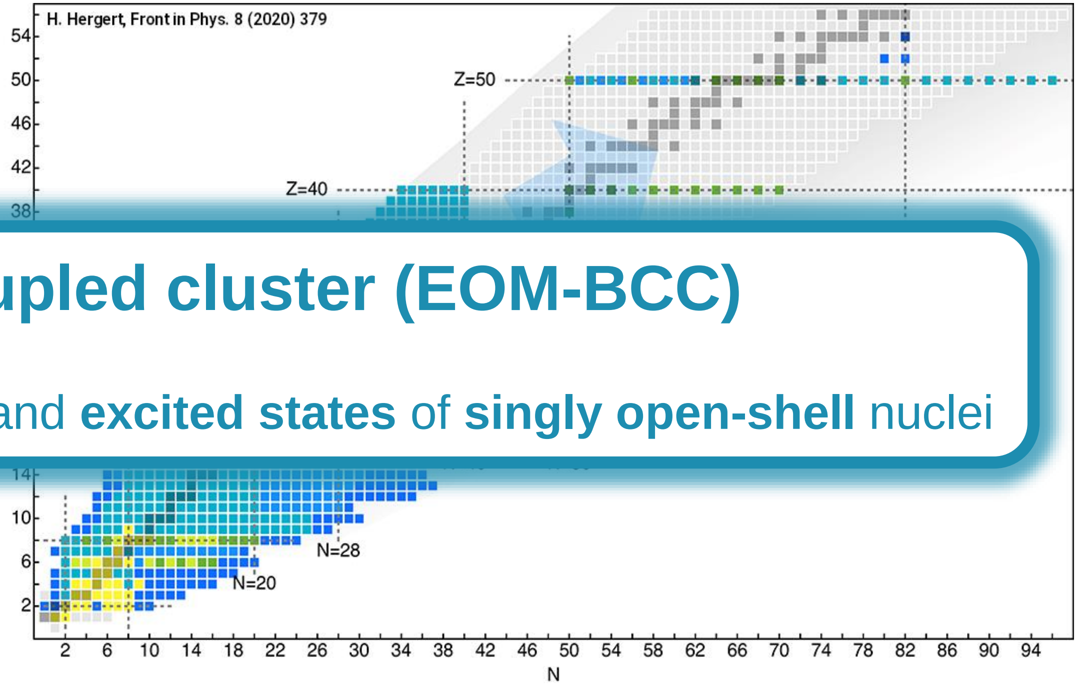

Equation-of-motion Bogoliubov coupled cluster (EOM-BCC)

= **non-perturbative** correlation expansion method for ground and **excited states** of **singly open-shell** nuclei

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Bogoliubov coupled cluster (BCC)

- BCC extends standard CC to singly open-shell nuclei

- **Exponential Ansatz** $|\Psi_0^A\rangle = e^{\mathcal{T}}|\Phi\rangle$

  where $\mathcal{T} \equiv \frac{1}{2!}\sum_{k_1k_2} t_{k_1k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + \frac{1}{4!}\sum_{k_1k_2k_3k_4} t_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta^\dagger_{k_4} + \cdots$

Quasi-particle creation operators

Unitary mix of single-particle creation and annihilation operators $\{c_p^\dagger, c_p\}$

$\beta_k^\dagger = \sum_p U_{pk}c_p^\dagger + V_{pk}c_p$

Excitation amplitudes

Solutions of a set of **non-linear algebraic equations** which must be **solved iteratively**

$\left\langle \Phi^{k_1k_2k_3\cdots} \middle| \Omega\, e^{\mathcal{T}} \middle| \Phi \right\rangle_C = 0$

- In practice, truncate to **single** and **doubles** excitations (BCCSD) $\mathcal{T} \approx \mathcal{T}_1 + \mathcal{T}_2$

- Special care to constrain $\langle A\rangle$

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Particle number constraint

Details on poster

Outcomes:

- Computationally cheap
- Overall convergence accelerated
- Size of $\mathcal{T}_1$ reduced
- Extended to Bogoliubov many-body perturbation theory (BMBPT)

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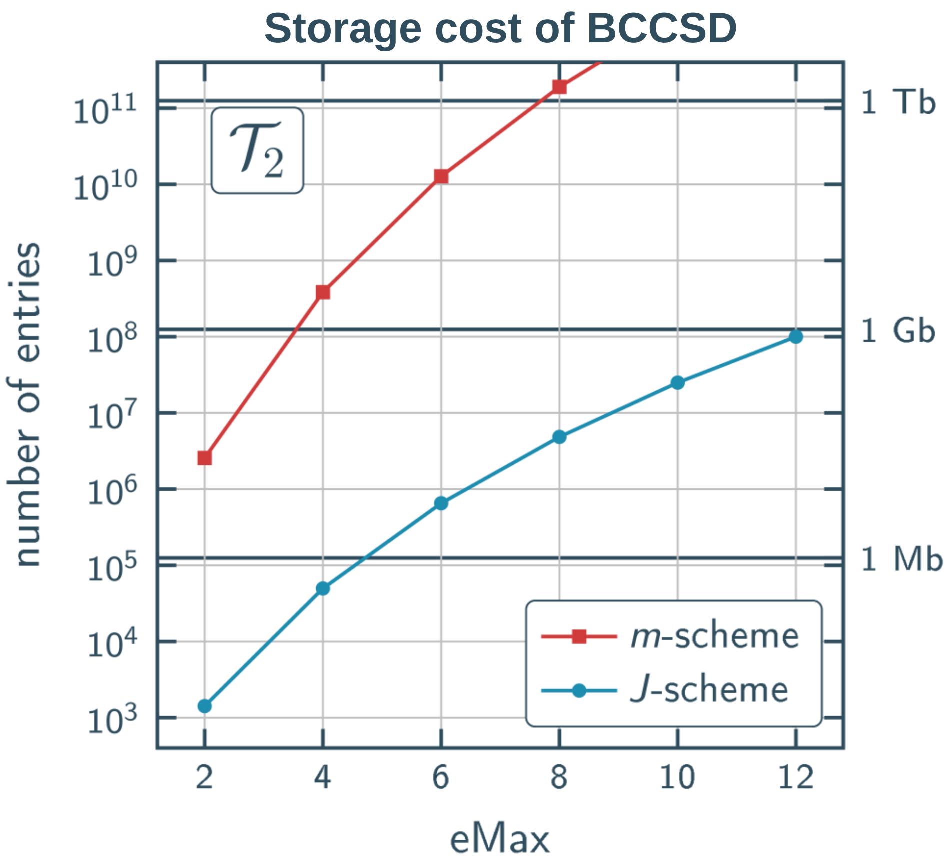
Angular-momentum reduction



m-scheme BCC

- Direct implementation of BCC Eqs.
- Storage cost of $t_{k_1 k_2 k_3 k_4}$ ✗

angular-momentum coupling

J-scheme BCC

- Symmetry-reduced BCC Eqs.
- Storage cost of $t_{\tilde{k}_1 \tilde{k}_2 \tilde{k}_3 \tilde{k}_4}(J_1 J_2)$ ✓

➔ **Immense memory reduction + speedup**

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On my poster

- First results of BCCSD in symmetry-restricted J-scheme form
  - Ground-state energies of Ca chain
  - χEFT NN+3N EM(1.8/2.0) in eMax10 E3Max12
- More details on
  - BCC formalism
  - Particle-number constraint
  - Angular momentum coupling (automatization)

outlook

- Ongoing calculations for **Sn isotopes** with eMax12 E3Max20 basis size
- Implementation of approximate triples correction for improved accuracy
- Access to **excited states** from equation-of-motion extension

➔ **Spectroscopy of singly open-shell isotopes from first principles**

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