

# Bogoliubov coupled cluster theory for open-shell nuclei

Workshop on Progress in Ab Initio Nuclear Theory

**Pepijn DEMOL**

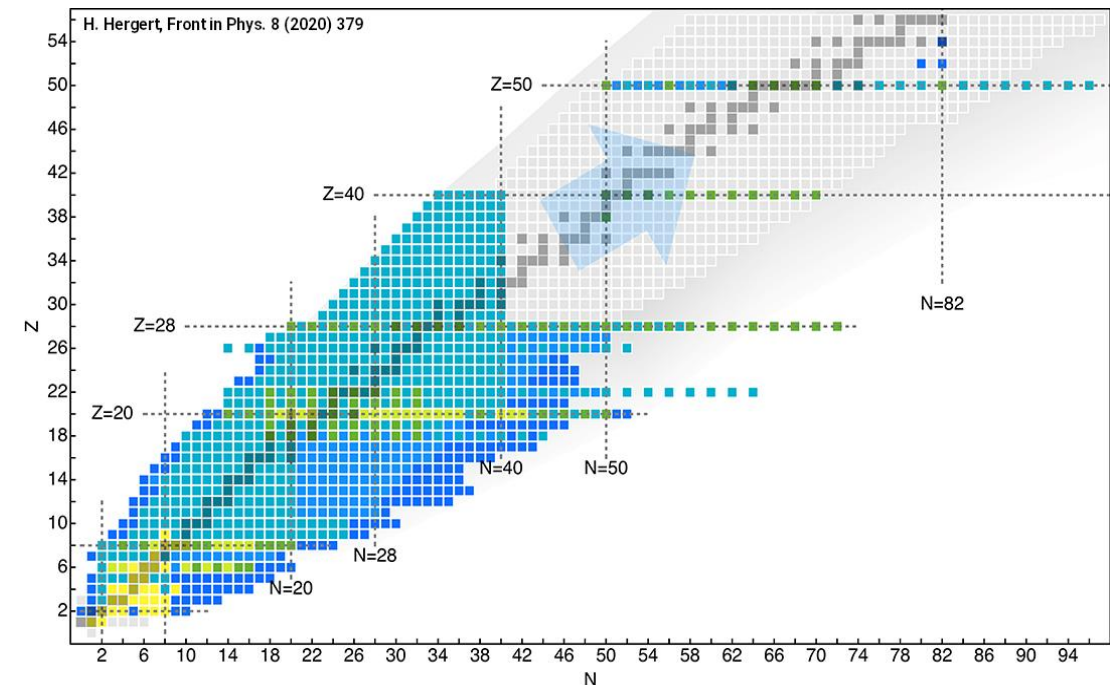
Supervisors **Thomas Duguet**  
**Riccardo Raabe**

Co-supervisor **Alexander Tichai**

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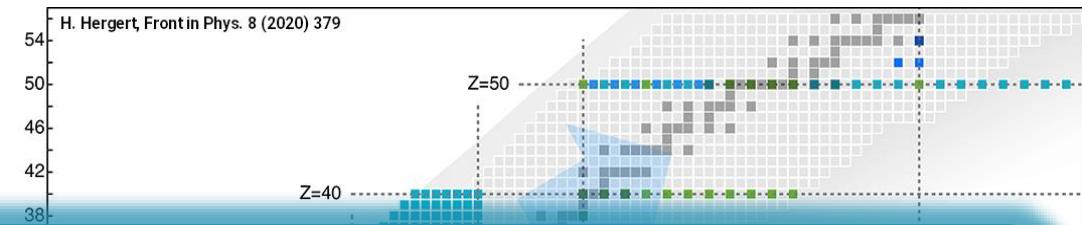
# Open-shell frontier of ab initio many-body methods

- 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-reference 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  $\Omega \equiv H - \lambda A$



# Open-shell frontier of ab initio many-body methods

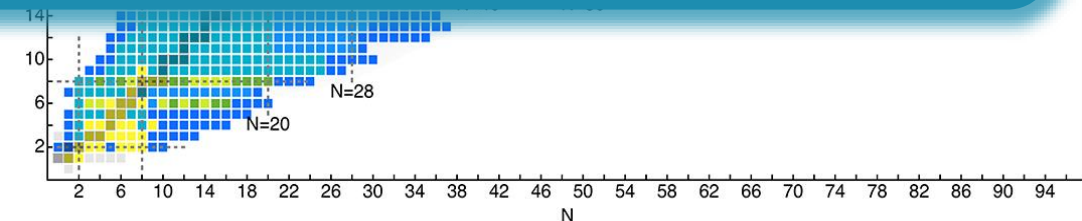
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## Equation-of-motion Bogoliubov coupled cluster (EOM-BCC)

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

- Many reference techniques
  - Valence-space methods
  - **Symmetry-breaking approaches**
- Singly open-shell nuclei break particle-number symmetry
    - **Bogoliubov quasi-particle** framework
    - Grand canonical potential  $\Omega \equiv H - \lambda A$



# 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  $\mathcal{T} \equiv \frac{1}{2!} \sum_{k_1 k_2} t_{k_1 k_2} \beta_{k_1}^\dagger \beta_{k_2}^\dagger + \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} t_{k_1 k_2 k_3 k_4} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3}^\dagger \beta_{k_4}^\dagger + \dots$

## 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**

$$\langle \Phi^{k_1 k_2 k_3 \dots} | \Omega e^{\mathcal{T}} | \Phi \rangle_C = 0$$

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

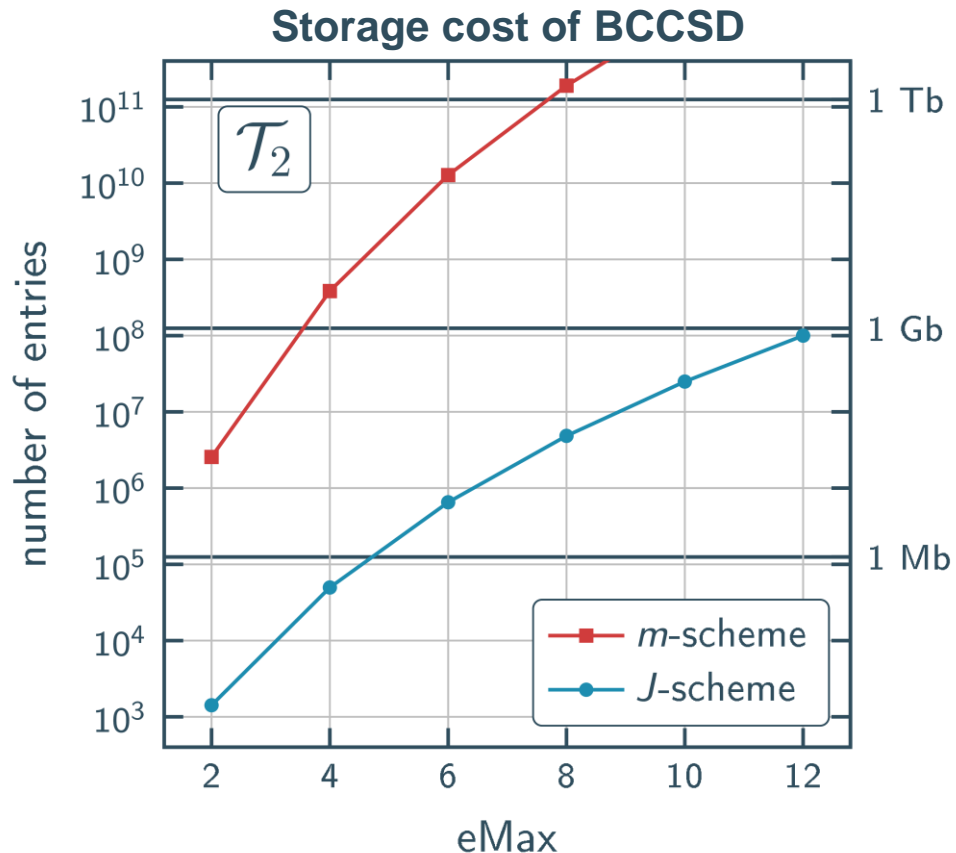
# Particle number constraint

*Details on poster*

## Outcomes:

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

# 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

# On my poster

**KU LEUVEN**
**fwo**

## Bogoliubov coupled cluster theory for open-shell nuclei

Pepijn DEMOL<sup>1</sup>, Alexander TICHAI<sup>2</sup>, Thomas DUGUET<sup>1,3</sup>

<sup>1</sup> KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium  
<sup>2</sup> Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany  
<sup>3</sup> CNRS, CEA, Université Paris-Saclay, F-91191 Orsay, France

### 1. 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
  - Polynomial expansion methods required
- Single-reference symmetry-conserving approaches fail
  - Multi-reference techniques
  - Variational space methods
  - Symmetry-breaking approaches
- Singly open-shell nuclei break particle-number symmetry
  - Bogoliubov quasi-particle framework

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

### 5. Angular-momentum reduction

**m-scheme BCC**

- Direct implementation of BCC Eqs.
- Storage cost of  $k_{i,j,k,l}$

**J-scheme BCC**

- Symmetry-reduced BCC Eqs.
- Storage cost of  $k_{i,j,k,l}(J,K,J')$

Automated angular-momentum coupling (amc) is:

```

graph LR
    Input[Input: Tensor contractions, m-scheme equations] --> AMC[AMC: Python package, Construct & reduce T-tensor graphs]
    AMC --> Output[Output: J-scheme equations]
    
```

→ OVERALL SPEEDUP ≈ 500

### 2. Quasi-particle formalism

- Quasi-particle (qp) operators defined via unitary Bogoliubov transformation
 
$$A = \sum_i c_i a_i + \sum_i d_i a_i^\dagger$$
- Corresponding vacuum functions as the reference state  $|0\rangle = C \prod_i |0_i\rangle$
- Grand potential operator  $\Omega$  expressed in qp basis
 
$$\Omega = H - \lambda(N + \tilde{N}) + \tilde{D}^2 + \tilde{D}^3 + \tilde{D}^4 + \tilde{D}^5 + \dots$$

where e.g.  $\tilde{D}^2 = \sum_{i,j} \tilde{D}_{ij}^{(2)} a_i^\dagger a_j a_i a_j^\dagger$

### 6. First J-scheme BCC calculations

- Total ground-state binding energy along Calcium chain comparing
  - naïve (non-Bogoliubov) HF
  - Bogoliubov many-body perturbation theory (BMPT(2,3))
  - BCCSD

- Particle number constraint extended to BMPT as
  - soft interaction, non-perturbative correlations required by BCC are small
  - BCC applicable independently of softness of interaction

### 3. Bogoliubov coupled cluster (BCC)

- BCC extends standard CC to singly open-shell nuclei
- Exponential Ansatz  $|\Psi\rangle = e^T |\Phi\rangle$ 

where  $T = \sum_{i,j} t_{ij} a_i^\dagger a_j + \sum_{i,j,k,l} t_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \dots$
- BCCSD truncate to single and doubles excitations,  $T = T_1 + T_2$
- Similarity-transformed grand potential operator  $\tilde{\Omega} = e^{-T} \Omega e^T$
- Ground-state energy  $E_0 = \langle \Phi | \tilde{\Omega} | \Phi \rangle = \langle \Phi | \tilde{H} | \Phi \rangle$
- Unknown  $t_{i,j,k,l}$  obtained from set of tensor equations  $\langle \Phi | \tilde{\Omega}^{(i)} | \Phi \rangle = 0$ 
  - Coupled non-linear equations solved iteratively  $T^{(n+1)} = T^{(n)} + K^{(n)}(\tilde{\Omega})$
  - Convergence accelerated using mixing, direct inversion of iterative subspace

### 4. Particle number constraint

- Update chemical potential at each BCC iteration  $\tilde{\Omega}^{(n)} = H - \lambda^{(n)} A$
- $\lambda^{(n)}$  determined by solving
 
$$\Delta \lambda^{(n)} = \langle \Phi | [T^{(n+1)}] \Phi \rangle = \langle \Phi | [T^{(n)} + K^{(n)}(\tilde{\Omega})] \Phi \rangle - \lambda^{(n)} \langle \Phi | A | \Phi \rangle = 0$$

**Outcomes**

- $\lambda$  constrained at each iteration
- Computationally cheap
- Overall convergence accelerated
- Size of  $T$  reduced

### 7. Conclusion and outlook

**Conclusion**

- Computationally efficient CC formalism applicable to open-shell nuclei
- Effective particle number constraint in BCC, applicable to BMPT
- First time implementation of BCCSD in symmetry-restricted J-scheme form

**Outlook**

- Ongoing calculations for Sn isotopes with eMax12 E3Max12 basis size
- Implementation of approximate singles correction for improved accuracy
- Access to excited states from equation-of-motion extension
- Implementation of electromagnetic observables

→ Spectroscopy of singly open-shell isotopes from first principles

<sup>(1)</sup> A. Spisak et al., Phys. Rev. C 91, 044328 (2015)  
<sup>(2)</sup> A. Tichai et al., Eur. Phys. J. A 46, 93 (2020) https://arxiv.org/abs/1908.02010  
<sup>(3)</sup> R. Heine et al., Phys. Lett. B 798, 226 (2018)  
<sup>(4)</sup> Heine et al., Phys. Rev. C 83, 024302 (2011)  
<sup>(5)</sup> Demol, P. Tichai, T. Duguet, in preparation (2022)  
<sup>(6)</sup> Tichai, P. Demol, T. Duguet, in preparation (2022)

- First results of BCCSD in symmetry-restricted J-scheme form
  - Ground-state energies of Ca chain
  - $\chi$ EFT 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**



# Collaboration



**T. Duguet**  
B. Bally  
J. P. Ebran  
M. Frosini  
A. Porro  
A. Roux  
A. Scalesi  
V. Somà  
G. Stellin



**A. Tichai**  
R. Roth



G. Hagen