Normal-ordering approximation in particle-number-breaking theories

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[J. Ripoche, A. Tichai, T. Duguet, 2019, in prep.]

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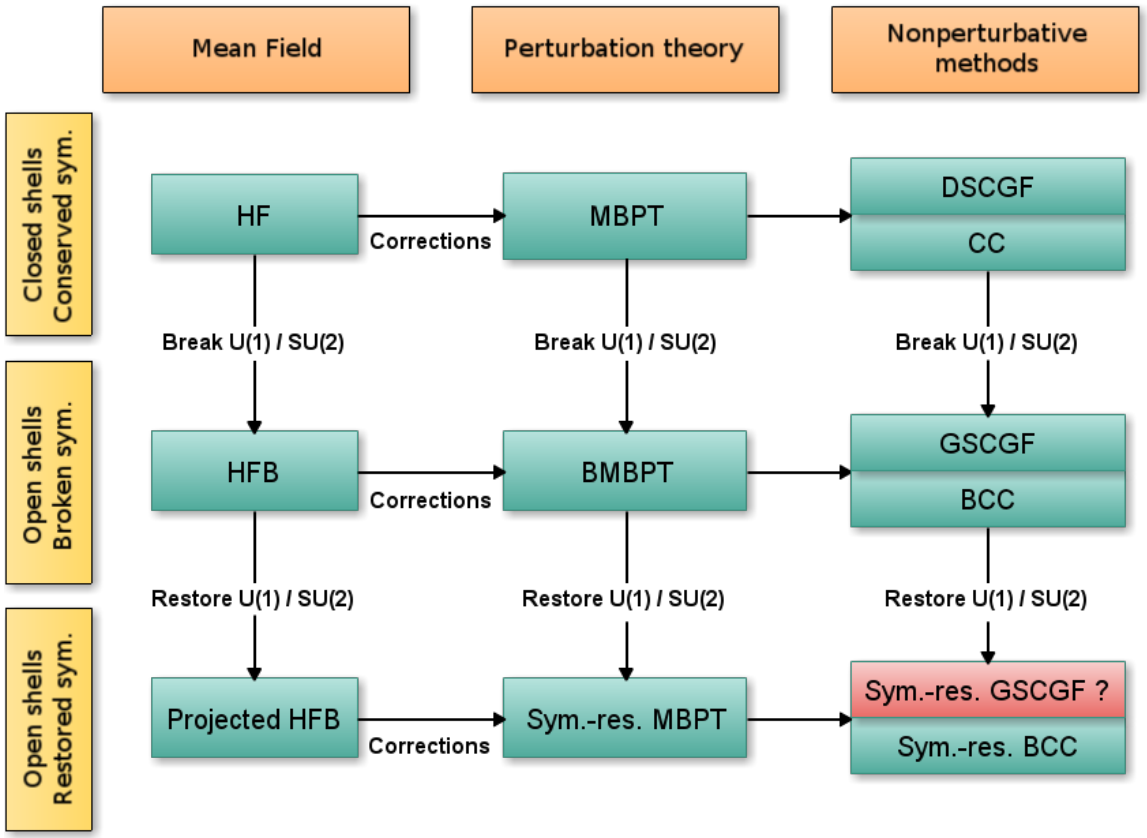
Outline

Outline

Ab Initio symmetry-breaking many-body methods

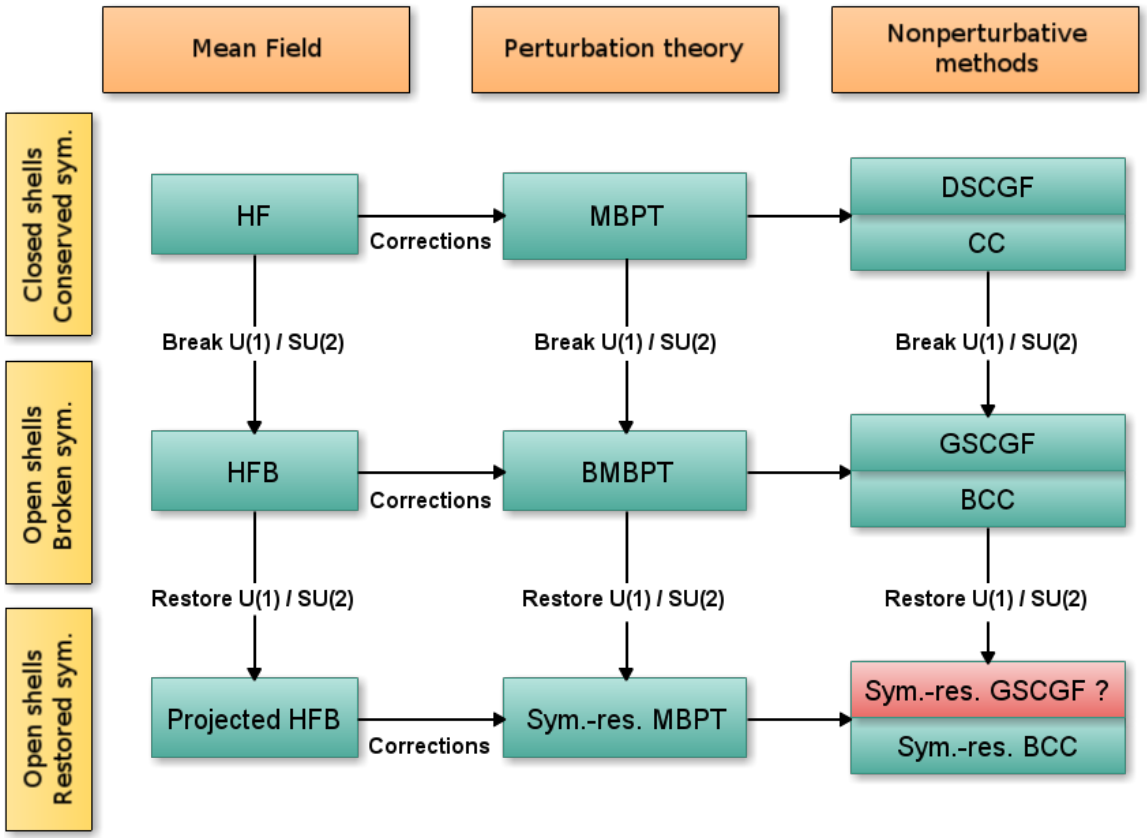


Courtesy of P. Arthuis, T. Duguet

New methods recently proposed and implemented

- BMBPT [Duguet *et al.* 2017, Tichai *et al.* 2018, Arthuis *et al.* 2019, Demol *et al.* 2019]
- PBMBPT [Duguet *et al.* 2017, Ripoche *et al.* 2019, Tichai *et al.* 2019]
- GSCGF [Somà *et al.* 2011]

Ab Initio symmetry-breaking many-body methods



Courtesy of P. Arthuis, T. Duguet

New methods recently proposed and implemented

- BMBPT → See Mikael's talk !
- PBMBPT → See Alexander's talk !
- GSCGF → See Vittorio's talk !

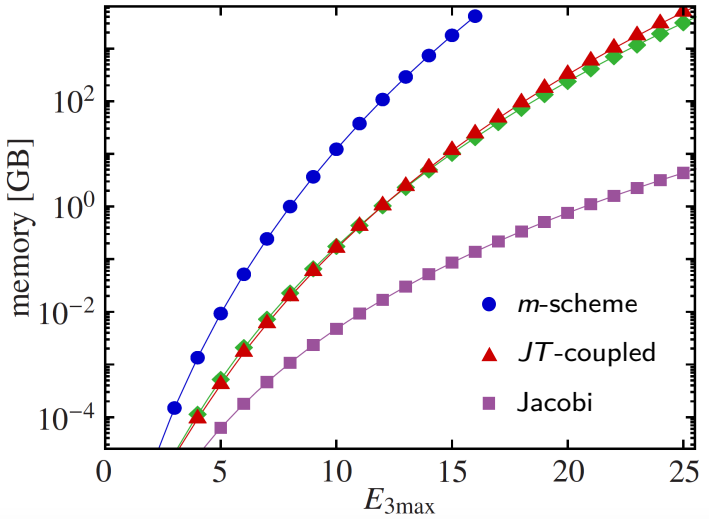
Nuclear physics and three-body forces

Nuclear physics requires (at least) a three-body Hamiltonian

$$H \equiv h^{11} + h^{22} + h^{33} = \sum_{i=1}^{3} \frac{1}{i!i!} \sum_{l_1 \ldots l_{2i}} h^{ii}_{l_1 \ldots l_i l_{i+1} \ldots l_{2i}} \; c^\dagger_{l_1} \ldots c^\dagger_{l_i} c_{l_{2i}} \ldots c_{l_{i+1}}$$

Three-body forces are very hard to handle

- Mode-6 tensor $\rightarrow$ memory challenge
- Compute and store ($\neq$ EDF)



[R. Roth *et al.* 2013]

In realistic model space ($e_{max} = 12$)

- Spherical reduction of tensors [J. Ripoche *et al.* 2019]
- (A priori) truncation $E3_{max} = 14 \ll 3e_{max}$ (20Gb)
- Larger model space for heavier nuclei

➔ Need to reduce the dimensionality

Many-body methods and three-body forces

Three-body Hamiltonian need to be fed into the Schrödinger equation

- Formalism with explicit three-body force $\rightarrow$ Formal challenge
- A lot of effort already generated to handle three-body
  - ◇ BMBPT [P. Arthuis *et al.* 2019]
  - ◇ CC [S. Binder *et al.* 2013]
  - ◇ SCGF [A. Carbone *et al.* 2013, F. Raimondi *et al.* 2018]

All what is covered next is relevant for all these methods (and more)

- Focus on CC and BCC

The N-body Hamiltonian

The N-body Hamiltonian is particle-number conserving ($[H, A] = 0$)

$$H \equiv h^{11} + h^{22} + h^{33} + \ldots + h^{NN} \,,$$

in which the i-body part h^{ii} is given by

$$h^{ii} = \frac{1}{i!\,i!} \sum_{l_1 \ldots l_{2i}} h^{ii}_{l_1 \ldots l_i\, l_{i+1} \ldots l_{2i}}\; c^\dagger_{l_1} \ldots c^\dagger_{l_i} c_{l_{2i}} \ldots c_{l_{i+1}} \,.$$

$\{c, c^\dagger\}, \lvert 0\rangle$	-6	-4	-2	0	$+2$	$+4$	$+6$
$h^{[0]}$				h^{00}			
$h^{[2]}$				h^{11}			
$h^{[4]}$				h^{22}			
$h^{[6]}$				h^{33}			

Contributions to the three-body operator H

Normal-ordering in single-particle basis

In normal-ordered form, the N-body Hamiltonian reads

$$H = \Lambda^{00} + \Lambda^{11} + \Lambda^{22} + \Lambda^{33} + \ldots + \Lambda^{NN} \, ,$$

in which the i-body field Λ^{ii} is given by

$$\Lambda^{ii} = \frac{1}{i!\,i!} \sum_{l_1 \ldots l_{2i}} \Lambda^{ii}_{l_1 \ldots l_i \, l_{i+1} \ldots l_{2i}} \;\; : c^\dagger_{l_1} \ldots c^\dagger_{l_i} c_{l_{2i}} \ldots c_{l_{i+1}} : \; .$$

$\{c, c^\dagger\}, \lvert SD\rangle$	-6	-4	-2	0	$+2$	$+4$	$+6$
$\Lambda^{[0]}$				Λ^{00}			
$\Lambda^{[2]}$				Λ^{11}			
$\Lambda^{[4]}$				Λ^{22}			
$\Lambda^{[6]}$				Λ^{33}			

Contributions to the three-body operator H

Normal-ordering in single-particle basis

Effective zero-body part of H

$$\Lambda^{00} = \sum_i h^{11}_{ii} + \frac{1}{2}\sum_{ij} h^{22}_{ijij} + \frac{1}{6}\sum_{ijk} h^{33}_{ijkijk}$$

Effective one-body part of H

$$\Lambda^{11}_{pq} = h^{11}_{pq} + \sum_i h^{22}_{piqi} + \frac{1}{2}\sum_{ij} h^{33}_{pijqij}$$

Effective two-body part of H

$$\Lambda^{22}_{pqrs} = h^{22}_{pqrs} + \sum_i h^{33}_{pqirsi}$$

Effective three-body part of H

$$\Lambda^{33}_{pqrstu} = h^{33}_{pqrstu}$$

Normal-ordering in single-particle basis

Effective zero-body part of H

$\Lambda^{00} = E_0^{\mathrm{HF}}$ (If $|\Phi\rangle$ is solution of HF)

Effective one-body part of H

$\Lambda^{11}_{pq} = 0$ (If $|\Phi\rangle$ is solution of HF)

Effective two-body part of H

$\Lambda^{22}_{pqrs} = h^{22}_{pqrs} + \sum_i h^{33}_{pqirsi}$

Effective three-body part of H

$\Lambda^{33}_{pqrstu} = h^{33}_{pqrstu}$

Many-body methods and three-body forces

A typical many-body formalism is about computing tensor network

➔ Contraction of Hamiltonian tensor and many-body tensors

Coupled Cluster energy equation with explicit three-body

$$E_0^{\mathrm{CCSDT}} = \Lambda^{00} + \sum_{ia} \Lambda^{11}_{ia} U^a_i + \frac{1}{2} \sum_{ijab} \Lambda^{22}_{ijab} U^a_i U^b_j + \frac{1}{4} \sum_{ijab} \Lambda^{22}_{ijab} U^{ab}_{ij} + \frac{1}{6} \sum_{ijkabc} \Lambda^{33}_{ijkabc} U^a_i U^b_j U^c_k + \frac{1}{4} \sum_{ijkabc} \Lambda^{33}_{ijkabc} U^{ab}_{ij} U^c_k + \frac{1}{36} \sum_{ijkabc} \Lambda^{33}_{ijkabc} U^{abc}_{ijk}$$

Problem: Three-body force requires coupling to triples (mode-6 tensor)

➔ Store: Both Λ^{33} and U_3 (even copy and update it iteratively)

➔ CPU time: E^{CCSDT} equation is a N^6 process (E^{CCSD} equation is N^4)

Can I get away with a two-body-like appoximation ?

YES: Normal-ordering two-body (NO2B) approximation [R. Roth *et al.* 2011]

Reduction of the storage ($e_{max} = 12$)

- ➔ **20Gb** for three-body operator ($E3_{max} = 14$)
- ➔ **250Mb** for NO2B operator
- ➔ For only 1% of error on the energy

Reduction of the cost

- ➔ Reduces to a $\mathbf{N^4}$ process (previously $\mathbf{N^6}$ process)

Intermediate step between

1. Full three-body mean-field (MF) calculation
2. Effective two-body beyond MF (BMF) calculation

NO2B approximation wrt a Slater Determinant (SD)

Normal-ordered three-body Hamiltonian with respect to a SD

$$H = \Lambda^{00} + \Lambda^{11} + \Lambda^{22} + \Lambda^{33} = \sum_{i=0}^{3} \sum_{l_1 \ldots l_{2i}} \Lambda^{ii}_{l_1 \ldots l_i l_{i+1} \ldots l_{2i}} : c^\dagger_{l_1} \ldots c^\dagger_{l_i} c_{l_{2i}} \ldots c_{l_{i+1}} :$$

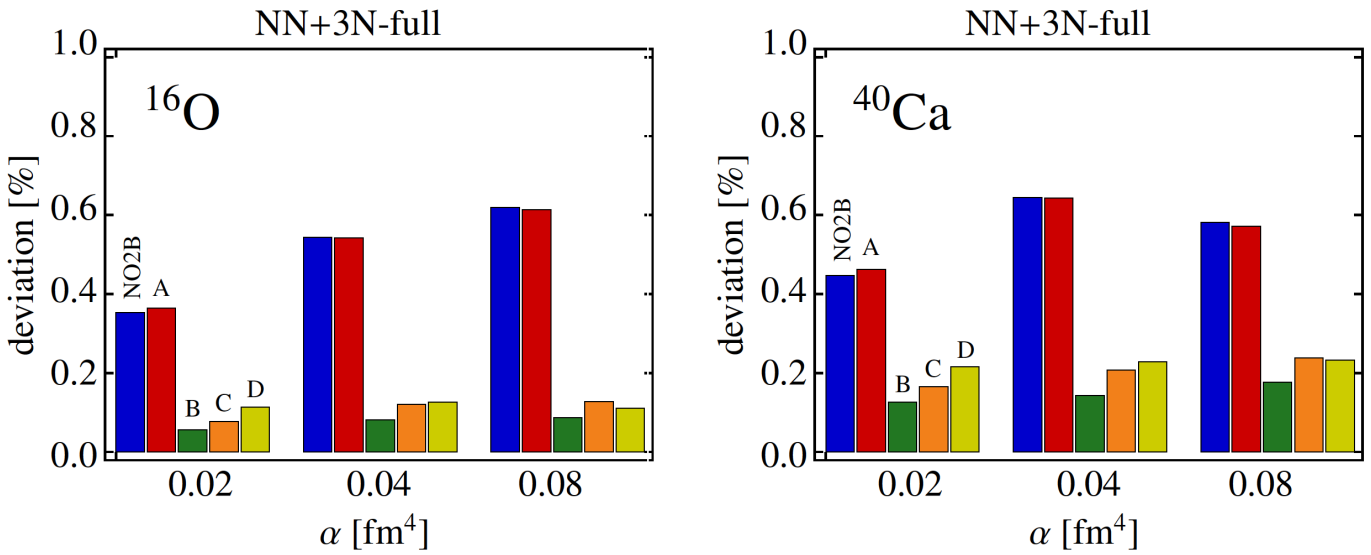
NO2B approximation

1. Put the three-body field Λ^{33} to zero (N^6)
2. 0,1,2-fields Λ^{00}, Λ^{11}, Λ^{22} (N^4) contain parts of h^{33}

NO2B Hamiltonian operator

➔ $H^{\mathrm{NO2B}} = \Lambda^{00} + \Lambda^{11} + \Lambda^{22}$

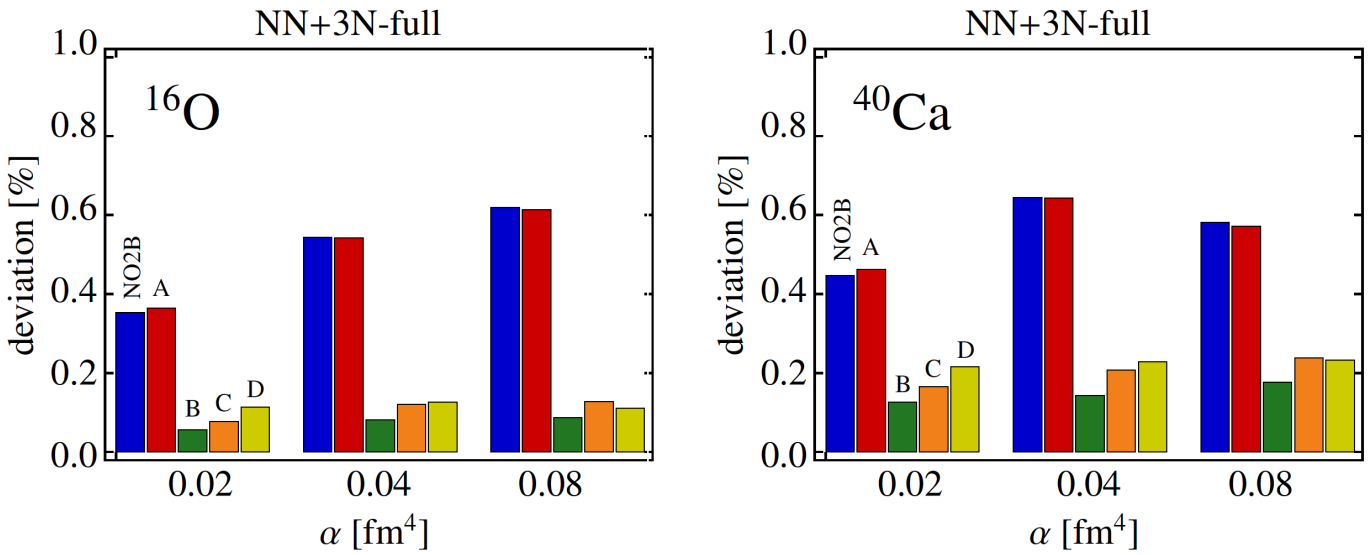
NO2B approximation for CC with three-body forces



[S. Binder *et al.* 2013]

- ➔ Deviation due to NO2B approximation is $< 1\%$
- ➔ Very good description at a manageable storage and CPU cost

NO2B approximation for CC with three-body forces



[S. Binder *et al.* 2013]

- ➔ Deviation due to NO2B approximation is $< 1\%$
- ➔ Very good description at a manageable storage and CPU cost

But what about symmetry-breaking many-body methods ?

Wick's theorem wrt a Bogoliubov vacuum

Bogoliubov transformation

$$\beta_k \equiv \sum_l U^*_{lk} c_l + V^*_{lk} c^\dagger_l$$

$$\beta^\dagger_k \equiv \sum_l U_{lk} c^\dagger_l + V_{lk} c_l$$

Bogoliubov vacuum

$$|\Phi\rangle \equiv \mathcal{C} \prod_k \beta_k |0\rangle$$

Elementary contractions

$$\rho_{l_1 l_2} \equiv \langle\Phi|c^\dagger_{l_2} c_{l_1}|\Phi\rangle / \langle\Phi|\Phi\rangle$$

$$\kappa_{l_1 l_2} \equiv \langle\Phi|c_{l_2} c_{l_1}|\Phi\rangle / \langle\Phi|\Phi\rangle$$

$$\kappa^*_{l_1 l_2} \equiv \langle\Phi|c^\dagger_{l_1} c^\dagger_{l_2}|\Phi\rangle / \langle\Phi|\Phi\rangle \,.$$

Wick's theorem

$$o^{nn} = \frac{1}{n!n!} \sum_{l_1 \ldots l_{2n}} o^{nn}_{l_1 \ldots l_{2n}} c^\dagger_{l_1} \ldots c^\dagger_{l_n} c_{l_{2n}} \ldots c_{l_{n+1}}$$

$$= \frac{1}{n!n!} \sum_{l_1 \ldots l_{2n}} o^{nn}_{l_1 \ldots l_{2n}} \Big[: c^\dagger_{l_1} \ldots c^\dagger_{l_n} c_{l_{2n}} \ldots c_{l_{n+1}} :$$

$$+ \rho_{l_{2n} l_n} : c^\dagger_{l_1} \ldots c^\dagger_{l_{n-1}} c_{l_{2n-1}} \ldots c_{l_{n+1}} : + \ldots$$

$$+ \kappa^*_{l_{n-1} l_n} : c^\dagger_{l_1} \ldots c^\dagger_{l_{n-2}} c_{l_{2n}} \ldots c_{l_{n+1}} : + \ldots$$

$$+ \kappa_{l_{2n-1} l_{2n}} : c^\dagger_{l_1} \ldots c^\dagger_{l_n} c_{l_{2n-2}} \ldots c_{l_{n+1}} : + \ldots$$

$$+ \ldots \Big]$$

- ➔ Apparition of anomalous contraction κ
- ➔ More terms appear in Wick's theorem

Normal-ordering in single-particle basis

In normal-ordered form, the N-body Hamiltonian reads

$$H = \Lambda^{00} + \Lambda^{20} + \Lambda^{11} + \Lambda^{02} + \ldots + \Lambda^{NN} \, ,$$

in which the (i,j)-field Λ^{ij} is given by

$$\Lambda^{ij} = \frac{1}{i!j!} \sum_{l_1 \ldots l_{i+j}} \Lambda^{ij}_{l_1 \ldots l_i l_{i+1} \ldots l_{i+j}} \; : c^\dagger_{l_1} \ldots c^\dagger_{l_i} c_{l_{i+j}} \ldots c_{l_{i+1}} : \; .$$

$\{c, c^\dagger\}, \lvert\Phi\rangle$	-6	-4	-2	0	$+2$	$+4$	$+6$
$\Lambda^{[0]}$				Λ^{00}			
$\Lambda^{[2]}$			Λ^{02}	Λ^{11}	Λ^{20}		
$\Lambda^{[4]}$			Λ^{13}	Λ^{22}	Λ^{31}		
$\Lambda^{[6]}$				Λ^{33}			

Contributions to the three-body operator H

Normal-ordering in single-particle basis

Effective zero-body part of H

$$\Lambda^{00} = h^{00} + \mathrm{tr}[h^{11}\rho] + \frac{1}{2}\mathrm{tr}[h^{22}\rho\rho] + \frac{1}{4}\mathrm{tr}[h^{22}\kappa^*\kappa] + \frac{1}{6}\mathrm{tr}[h^{33}\rho\rho\rho] + \frac{1}{4}\mathrm{tr}[h^{33}\kappa^*\kappa\rho]$$

Effective one-body part of H

$$\Lambda^{11}_{l_1 l_2} = h^{11}_{l_1 l_2} + \mathrm{tr}[h^{22}\rho]_{l_1 l_2} + \frac{1}{2}\mathrm{tr}[h^{33}\rho\rho]_{l_1 l_2} + \frac{1}{4}\mathrm{tr}[h^{33}\kappa^*\kappa]_{l_1 l_2}$$

$$\Lambda^{20}_{l_1 l_2} = \frac{1}{2}\mathrm{tr}[h^{22}\kappa]_{l_1 l_2} + \frac{1}{2}\mathrm{tr}[h^{33}\kappa\rho]_{l_1 l_2}$$

$$\Lambda^{02}_{l_1 l_2} = \frac{1}{2}\mathrm{tr}[h^{22}\kappa^*]_{l_1 l_2} + \frac{1}{2}\mathrm{tr}[h^{33}\kappa^*\rho]_{l_1 l_2}$$

Effective two-body part of H

$$\Lambda^{22}_{l_1 l_2 l_3 l_4} = h^{22}_{l_1 l_2 l_3 l_4} + \mathrm{tr}[h^{33}\rho]_{l_1 l_2 l_3 l_4}$$

$$\Lambda^{31}_{l_1 l_2 l_3 l_4} = \frac{1}{2}\mathrm{tr}[h^{33}\kappa]_{l_1 l_2 l_3 l_4}$$

$$\Lambda^{13}_{l_1 l_2 l_3 l_4} = \frac{1}{2}\mathrm{tr}[h^{33}\kappa^*]_{l_1 l_2 l_3 l_4}$$

Effective three-body part of H

$$\Lambda^{33}_{l_1 l_2 l_3 l_4 l_5 l_6} = h^{33}_{l_1 l_2 l_3 l_4 l_5 l_6}$$

Normal-ordering in quasi-particle basis

In normal-ordered form, the N-body Hamiltonian reads

$$H = H^{00} + H^{20} + H^{11} + H^{02} + \ldots + H^{NN} \, ,$$

in which the (i,j)-part H^{ij} is given by

$$H^{ij} = \frac{1}{i!j!} \sum_{k_1 \ldots k_{i+j}} H^{ij}_{k_1 \ldots k_i k_{i+1} \ldots k_{i+j}} \, \beta^\dagger_{k_1} \ldots \beta^\dagger_{k_i} \beta_{k_{i+j}} \ldots \beta_{k_{i+1}} \, .$$

$\{\beta, \beta^\dagger\}, \lvert\Phi\rangle$	-6	-4	-2	0	$+2$	$+4$	$+6$
$H^{[0]}$				H^{00}			
$H^{[2]}$			H^{02}	H^{11}	H^{20}		
$H^{[4]}$		H^{04}	H^{13}	H^{22}	H^{31}	H^{40}	
$H^{[6]}$	H^{06}	H^{15}	H^{24}	H^{33}	H^{42}	H^{51}	H^{60}

Contributions to the three-body operator H

Normal-ordering in quasi-particle basis

Effective zero-body part of H

$$H^{00} = \Lambda^{00}$$

Effective one-body part of H

$$H^{20}_{k_1 k_2} = \sum_{l_1 l_2} \Lambda^{11}_{l_1 l_2} U^*_{l_1 k_1} V^*_{l_2 k_2} - \Lambda^{11}_{l_1 l_2} V^*_{l_2 k_1} U^*_{l_1 k_2} + \Lambda^{20}_{l_1 l_2} U^*_{l_1 k_1} U^*_{l_2 k_2} - \Lambda^{02}_{l_1 l_2} V^*_{l_1 k_1} V^*_{l_2 k_2}$$

$$H^{11}_{k_1 k_2} = \sum_{l_1 l_2} \Lambda^{11}_{l_1 l_2} U^*_{l_1 k_1} U_{l_2 k_2} - \Lambda^{11}_{l_1 l_2} V^*_{l_2 k_1} V_{l_1 k_2} + \Lambda^{20}_{l_1 l_2} U^*_{l_1 k_1} V_{l_2 k_2} - \Lambda^{02}_{l_1 l_2} V^*_{l_1 k_1} U_{l_2 k_2}$$

$$H^{02}_{k_1 k_2} = \sum_{l_1 l_2} \Lambda^{11}_{l_1 l_2} U_{l_2 k_1} V_{l_1 k_2} - \Lambda^{11}_{l_1 l_2} V_{l_1 k_1} U_{l_2 k_2} - \Lambda^{20}_{l_1 l_2} V_{l_1 k_1} V_{l_2 k_2} + \Lambda^{02}_{l_1 l_2} U_{l_1 k_1} U_{l_2 k_2}$$

Effective two-body part of H

$$\begin{aligned}
H^{40}_{k_1 k_2 k_3 k_4} = \sum_{l_1 l_2 l_3 l_4} \Lambda^{22}_{l_1 l_2 l_3 l_4} \Big(& - U^*_{l_1 k_1} U^*_{l_2 k_2} V^*_{l_3 k_3} V^*_{l_4 k_4} + U^*_{l_1 k_1} V^*_{l_3 k_2} U^*_{l_2 k_3} V^*_{l_4 k_4} \\
& - U^*_{l_1 k_1} V^*_{l_3 k_2} V^*_{l_4 k_3} U^*_{l_2 k_4} - V^*_{l_3 k_1} U^*_{l_1 k_2} U^*_{l_2 k_3} V^*_{l_4 k_4} \\
& + V^*_{l_3 k_1} U^*_{l_1 k_2} V^*_{l_4 k_3} U^*_{l_2 k_4} - V^*_{l_3 k_1} V^*_{l_4 k_2} U^*_{l_1 k_3} U^*_{l_2 k_4} \Big) \\
+ \Lambda^{31}_{l_1 l_2 l_3 l_4} \Big(& + U^*_{l_1 k_1} U^*_{l_2 k_2} U^*_{l_3 k_3} V^*_{l_4 k_4} - U^*_{l_1 k_1} U^*_{l_2 k_2} V^*_{l_4 k_3} U^*_{l_3 k_4} \\
& + U^*_{l_1 k_1} V^*_{l_4 k_2} U^*_{l_2 k_3} U^*_{l_3 k_4} - V^*_{l_4 k_1} U^*_{l_1 k_2} U^*_{l_2 k_3} U^*_{l_3 k_4} \Big) \\
+ \Lambda^{13}_{l_1 l_2 l_3 l_4} \Big(& - U^*_{l_1 k_1} V^*_{l_5 k_2} V^*_{l_6 k_3} V^*_{l_2 k_4} + V^*_{l_5 k_1} U^*_{l_1 k_2} V^*_{l_6 k_3} V^*_{l_2 k_4} \\
& - V^*_{l_5 k_1} V^*_{l_6 k_2} U^*_{l_1 k_3} V^*_{l_2 k_4} + V^*_{l_5 k_1} V^*_{l_6 k_2} V^*_{l_2 k_3} U^*_{l_1 k_4} \Big)
\end{aligned}$$

$$H^{31}_{k_1 k_2 k_3 k_4} = \dots$$

Normal-ordering in quasi-particle basis

Effective zero-body part of H

$H^{00} = E_0^{\mathrm{HFB}}$ (If $|\Phi\rangle$ is solution of HFB)

Effective one-body part of H

$H^{20}_{k_1 k_2} = 0$ (If $|\Phi\rangle$ is solution of HFB)

$H^{11}_{k_1 k_2} = 0$ (If $|\Phi\rangle$ is solution of HFB)

$H^{02}_{k_1 k_2} = 0$ (If $|\Phi\rangle$ is solution of HFB)

Effective two-body part of H

$$
\begin{aligned}
H^{40}_{k_1 k_2 k_3 k_4} = \sum_{l_1 l_2 l_3 l_4} \Lambda^{22}_{l_1 l_2 l_3 l_4} \Big(& - U^*_{l_1 k_1} U^*_{l_2 k_2} V^*_{l_3 k_3} V^*_{l_4 k_4} + U^*_{l_1 k_1} V^*_{l_3 k_2} U^*_{l_2 k_3} V^*_{l_4 k_4} \\
& - U^*_{l_1 k_1} V^*_{l_3 k_2} V^*_{l_4 k_3} U^*_{l_2 k_4} - V^*_{l_3 k_1} U^*_{l_1 k_2} U^*_{l_2 k_3} V^*_{l_4 k_4} \\
& + V^*_{l_3 k_1} U^*_{l_1 k_2} V^*_{l_4 k_3} U^*_{l_2 k_4} - V^*_{l_3 k_1} V^*_{l_4 k_2} U^*_{l_1 k_3} U^*_{l_2 k_4} \Big) \\
+ \Lambda^{31}_{l_1 l_2 l_3 l_4} \Big(& + U^*_{l_1 k_1} U^*_{l_2 k_2} U^*_{l_3 k_3} V^*_{l_4 k_4} - U^*_{l_1 k_1} U^*_{l_2 k_2} V^*_{l_4 k_3} U^*_{l_3 k_4} \\
& + U^*_{l_1 k_1} V^*_{l_4 k_2} U^*_{l_2 k_3} U^*_{l_3 k_4} - V^*_{l_4 k_1} U^*_{l_1 k_2} U^*_{l_2 k_3} U^*_{l_3 k_4} \Big) \\
+ \Lambda^{13}_{l_1 l_2 l_3 l_4} \Big(& - U^*_{l_1 k_1} V^*_{l_5 k_2} V^*_{l_6 k_3} V^*_{l_2 k_4} + V^*_{l_5 k_1} U^*_{l_1 k_2} V^*_{l_6 k_3} V^*_{l_2 k_4} \\
& - V^*_{l_5 k_1} V^*_{l_6 k_2} U^*_{l_1 k_3} V^*_{l_2 k_4} + V^*_{l_5 k_1} V^*_{l_6 k_2} V^*_{l_2 k_3} U^*_{l_1 k_4} \Big)
\end{aligned}
$$

$H^{31}_{k_1 k_2 k_3 k_4} = \dots$

NO2B approximation wrt a Bogoliubov state

Normal-ordered three-body Hamiltonian wrt a Bogoliubov state

$$H = H^{00} + \{H^{20} + H^{11} + H^{02}\} + \{H^{40} + H^{31} + H^{22} + H^{13} + H^{04}\} + H^{[6]}$$

Bogoliubov Coupled Cluster (BCC) energy equation

$$E_0^{\mathrm{BCCSDT}} = H^{00} + \frac{1}{2!}\mathrm{tr}[H^{02}U^{20}] + \frac{1}{8}\mathrm{tr}[H^{04}U^{20}U^{20}] + \frac{1}{4!}\mathrm{tr}[H^{04}U^{40}] + \frac{1}{48}\mathrm{tr}[H^{06}U^{20}U^{20}U^{20}] + \frac{1}{48}\mathrm{tr}[H^{06}U^{40}U^{20}] + \frac{1}{6!}\mathrm{tr}[H^{06}U^{60}]$$

NO2B approximation

1. Put the three-body part H^{06} (Λ^{33}) to zero
2. 0,1,2-body parts H^{00}, H^{02}, H^{04} contain parts of h^{33}

NO2B approximation wrt a Bogoliubov state

Normal-ordered three-body Hamiltonian wrt a Bogoliubov state

$$H = H^{00} + \{H^{20} + H^{11} + H^{02}\} + \{H^{40} + H^{31} + H^{22} + H^{13} + H^{04}\} + H^{[6]}$$

Bogoliubov Coupled Cluster (BCC) energy equation

$$E_0^{\mathrm{BCCSDT}} = H^{00} + \frac{1}{2!}\mathrm{tr}[H^{02}U^{20}] + \frac{1}{8}\mathrm{tr}[H^{04}U^{20}U^{20}] + \frac{1}{4!}\mathrm{tr}[H^{04}U^{40}] + \frac{1}{48}\mathrm{tr}[H^{06}U^{20}U^{20}U^{20}] + \frac{1}{48}\mathrm{tr}[H^{06}U^{40}U^{20}] + \frac{1}{6!}\mathrm{tr}[H^{06}U^{60}]$$

NO2B approximation

1. Put the three-body part H^{06} (Λ^{33}) to zero
2. 0,1,2-body parts H^{00}, H^{02}, H^{04} contain parts of h^{33}

This approximation is actually not well behaved !

Single projection vs double projection

Particle-number projection operator P^{A} (where $R(\varphi) \equiv e^{iA\varphi}$)

$$P^{\mathrm{A}} \equiv \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-i\varphi \mathrm{A}} R(\varphi)$$

If an operator O commutes with A, it must also commute with P^{A}

$$P^{\mathrm{A}} O = P^{\mathrm{A}} O P^{\mathrm{A}}$$

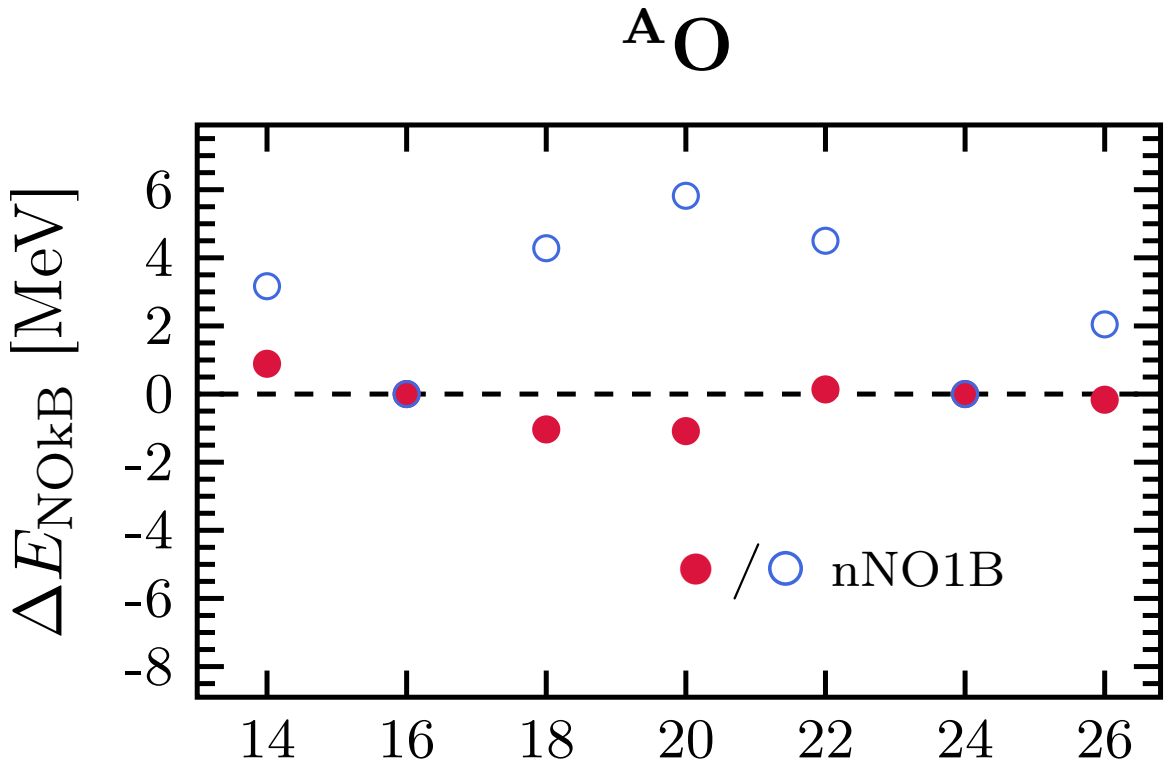
Projected mean-field quantities

- Single projection $O_{\Phi}^{\mathrm{A(s)}} = \langle \Phi | P^{\mathrm{A}} O | \Phi \rangle$
- Double projection $O_{\Phi}^{\mathrm{A(d)}} = \langle \Phi | P^{\mathrm{A}} O P^{\mathrm{A}} | \Phi \rangle$

If the operator O is

- Particle-number conserving $\Rightarrow O_{\Phi}^{\mathrm{A(s)}} = O_{\Phi}^{\mathrm{A(d)}}$
- Particle-number violating $\Rightarrow O_{\Phi}^{\mathrm{A(s)}} \neq O_{\Phi}^{\mathrm{A(d)}}$

Single projection vs double projection

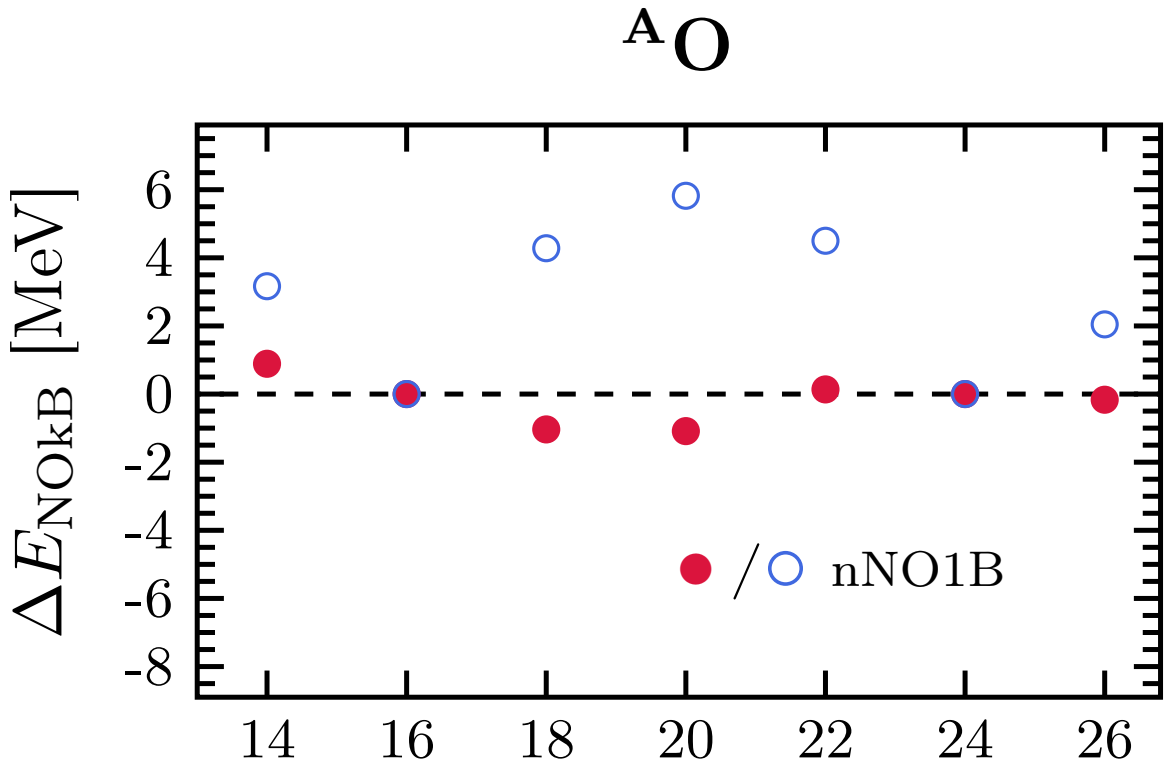


[J. Ripoche, A. Tichai, T. Duguet, in prep.]

- Filled (empty) symbol for single (double) projection
- Single and double projection different for nNO1B

What does it tell us ?

Single projection vs double projection



[J. Ripoche, A. Tichai, T. Duguet, in prep.]

- Filled (empty) symbol for single (double) projection
- Single and double projection different for nNO1B

What does it tell us ?

The approximate operator does not commute with A !

Outline

Motivation

The N-body Hamiltonian in different forms

$$\begin{aligned} H &\equiv h^{00} + h^{11} + h^{22} + h^{33} + \ldots + h^{NN} \\ &= \Lambda^{00} + \Lambda^{20} + \Lambda^{11} + \Lambda^{02} + \ldots + \Lambda^{NN} \\ &= H^{00} + H^{20} + H^{11} + H^{02} + \ldots + H^{NN} \, . \end{aligned}$$

Requirements of the approximation

1. Throw normal-ordered pieces Λ^{ij} (H^{ij}) of H with $i + j > k$
2. Get an approximate operator that still is particle-number conserving

For the naive extension of NOkB approximation

➔ First requirement is fulfilled but not the second one

➔ To do both requires to further approximate fields Λ^{ij} with $i + j \leq k$

Particle-number conserving NOkB approximation

The particle-number conserving NOkB (PNOkB) Hamiltonian operator

$$H^{\text{PNOkB}} \equiv \tilde{o}^{00} + \tilde{o}^{11} + \tilde{o}^{22} + \tilde{o}^{33} + \ldots = \sum_{n=0}^{k} \tilde{o}^{nn}$$

with

$$\tilde{o}^{nn} \equiv \frac{1}{n!n!} \sum_{l_1 \ldots l_{2n}} \tilde{o}^{nn}_{l_1 \ldots l_{2n}} c^\dagger_{l_1} \ldots c^\dagger_{l_n} c_{l_{2n}} \ldots c_{l_{n+1}}$$

and where $\tilde{o}^{nn}_{l_1 \ldots l_{2n}}$ $(n \leq k)$ are recursively defined in decreasing order by

$$\tilde{o}^{kk}_{l_1 \ldots l_{2k}} \equiv \Lambda^{kk}_{l_1 \ldots l_{2k}}$$

$$\tilde{o}^{nn}_{l_1 \ldots l_{2n}} \equiv \Lambda^{nn}_{l_1 \ldots l_{2n}} - \sum_{m=n+1}^{k} \tilde{\Lambda}^{nn(mm)}_{l_1 \ldots l_{2n}} \text{ for } n < k$$

Leading argument

- ➔ Same normal fields $\tilde{\Lambda}^{nn} = \Lambda^{nn}$
- ➔ For details on the derivation [J. Ripoche, A. Tichai, T. Duguet, in prep.]

Particle-number conserving NOkB approximation

PNOkB operator in its normal-ordered form in the single-particle basis

$$H^{\text{PNOkB}} = \sum_{i,j=0}^{\max(i,j)\leq k} \tilde{\Lambda}^{ij} = \sum_{i,j=0}^{\max(i,j)\leq k} \Lambda^{ij} + \breve{\Lambda}^{ij}$$

where the extra term $\breve{\Lambda}^{ij}$ are possibly non-vanishing for $i \neq j$ and $N \geq 4$

➔ For anomalous fields of an original four-body operator (or higher rank)

In practice the PNO2B approximation of a three-body Hamiltonian gives

$$H^{\text{PNO2B}} = \sum_{i,j=0}^{\max(i,j)\leq 2} \Lambda^{ij}$$

Naive vs Particle-number conserving extensions

(Naive ext. of) NOkB approximation

$$H^{\text{nNOkB}} = \sum_{i+j=0}^{i+j\leq k} \Lambda^{ij}$$

PNOkB approximation

$$H^{\text{PNOkB}} = \sum_{i+j=0}^{\max(i,j)\leq k} \tilde{\Lambda}^{ij}$$

NO2B approximation of a three-body operator

$$H^{\text{nNO2B}} = \Lambda^{00} + \Lambda^{20} + \Lambda^{11} + \Lambda^{02} + \Lambda^{31} + \Lambda^{22} + \Lambda^{13}$$

$$H^{\text{PNO2B}} = \Lambda^{00} + \Lambda^{20} + \Lambda^{11} + \Lambda^{02} + \Lambda^{22}$$

$$H^{\text{nNO2B}} = \tilde{o}^{00} + \tilde{o}^{20} + \tilde{o}^{11} + \tilde{o}^{02} + \tilde{o}^{31} + \tilde{o}^{22} + \tilde{o}^{13}$$

$$H^{\text{PNO2B}} = \tilde{o}^{00} + \tilde{o}^{11} + \tilde{o}^{22}$$

Naive vs Particle-number conserving extensions

(Naive ext. of) NOkB approximation

$$H^{\text{nNOkB}} = \sum_{i+j=0}^{i+j\leq k} \Lambda^{ij}$$

PNOkB approximation

$$H^{\text{PNOkB}} = \sum_{i+j=0}^{\max(i,j)\leq k} \tilde{\Lambda}^{ij}$$

NO1B approximation of a three-body operator

$$H^{\text{nNO1B}} = \Lambda^{00} + \Lambda^{20} + \Lambda^{11} + \Lambda^{02}$$

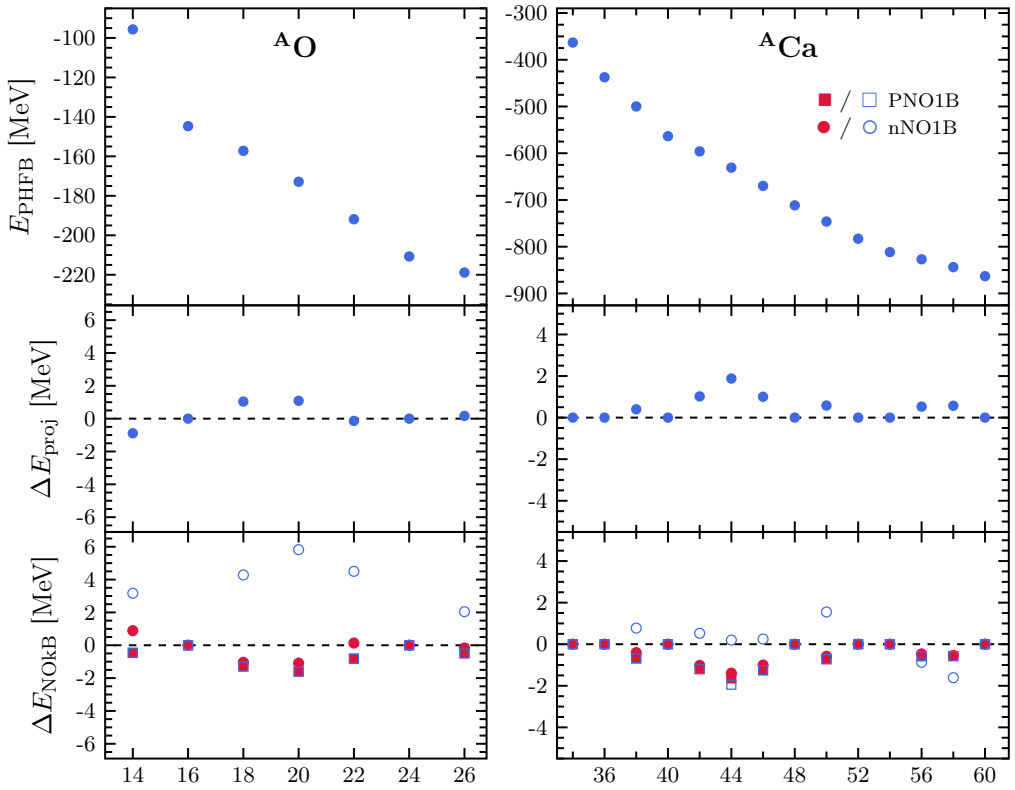
$$H^{\text{PNO1B}} = \Lambda^{00} + \Lambda^{11}$$

$$H^{\text{nNO1B}} = \tilde{o}^{00} + \tilde{o}^{20} + \tilde{o}^{11} + \tilde{o}^{02}$$

$$H^{\text{PNO1B}} = \tilde{o}^{00} + \tilde{o}^{11}$$

Outline

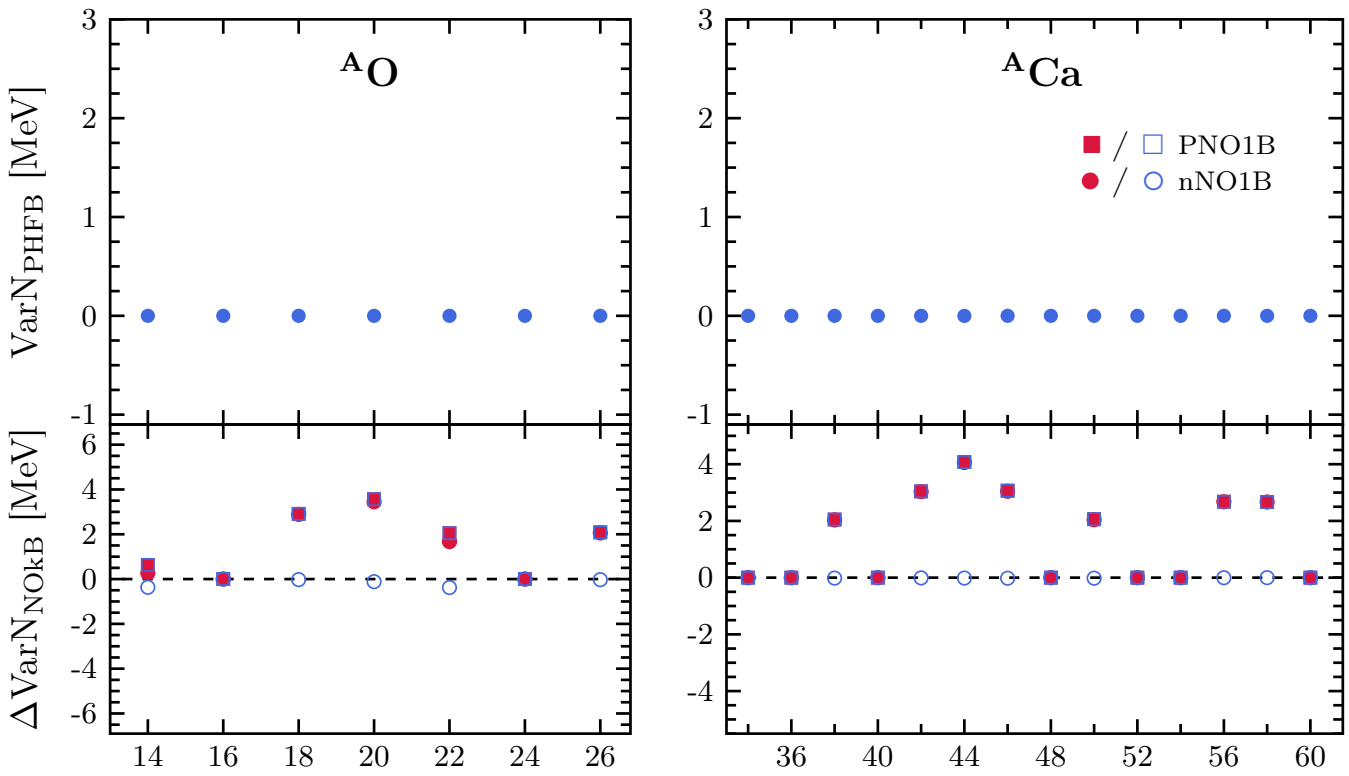
Projected energy for some isotopic chains



[J. Ripoche, A. Tichai, T. Duguet, in prep.]

- Empty circle are farther to zero than filled ones
- Filled and empty squares lie on top of one another → PN conserving

Projected variance for some isotopic chains



[J. Ripoche, A. Tichai, T. Duguet, in prep.]

- Projected neutron-number variance is indeed vanishing
- Filled and empty squares lie on top of one another $\rightarrow$ PN conserving

Outline

Conclusions

Nuclear structure

- Three-body forces requirement
- Storage/cost problem

NOkB approximation

- Intermediate step between MF and BMF
- Powerful tool to reduce storage/cost

Extension to symmetry-breaking normal-ordering

- Naive extension leads to particle-number non-conserving operator
- Particle-number conserving extension needs further approximation

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BACK UP

Singly/doubly gauge-rotated mean-field kernels

Gauge-rotated Bogoliubov state

$$|\Phi(\varphi)\rangle \equiv R(\varphi)|\Phi\rangle\,.$$

Singly- and doubly-rotated mean-field norm kernels

$$\mathcal{N}^{(0)}(\varphi) \equiv \langle\Phi(\varphi)|\Phi\rangle\,,$$
$$\mathcal{N}^{(0)}(\varphi,\varphi') \equiv \langle\Phi(\varphi)|\Phi(\varphi')\rangle = \mathcal{N}^{(0)}(\varphi-\varphi')\,.$$

Singly- and doubly-rotated mean-field operator kernels

$$O^{(0)}(\varphi) \equiv \langle\Phi(\varphi)|O|\Phi\rangle\,,$$
$$O^{(0)}(\varphi,\varphi') \equiv \langle\Phi(\varphi)|O|\Phi(\varphi')\rangle\,.$$

Connected singly- and doubly-rotated mean-field operator kernels

$$o^{(0)}(\varphi) \equiv O^{(0)}(\varphi)/\mathcal{N}^{(0)}(\varphi)\,,$$
$$o^{(0)}(\varphi,\varphi') \equiv O^{(0)}(\varphi,\varphi')/\mathcal{N}^{(0)}(\varphi,\varphi')\,.$$

Single projection vs double projection

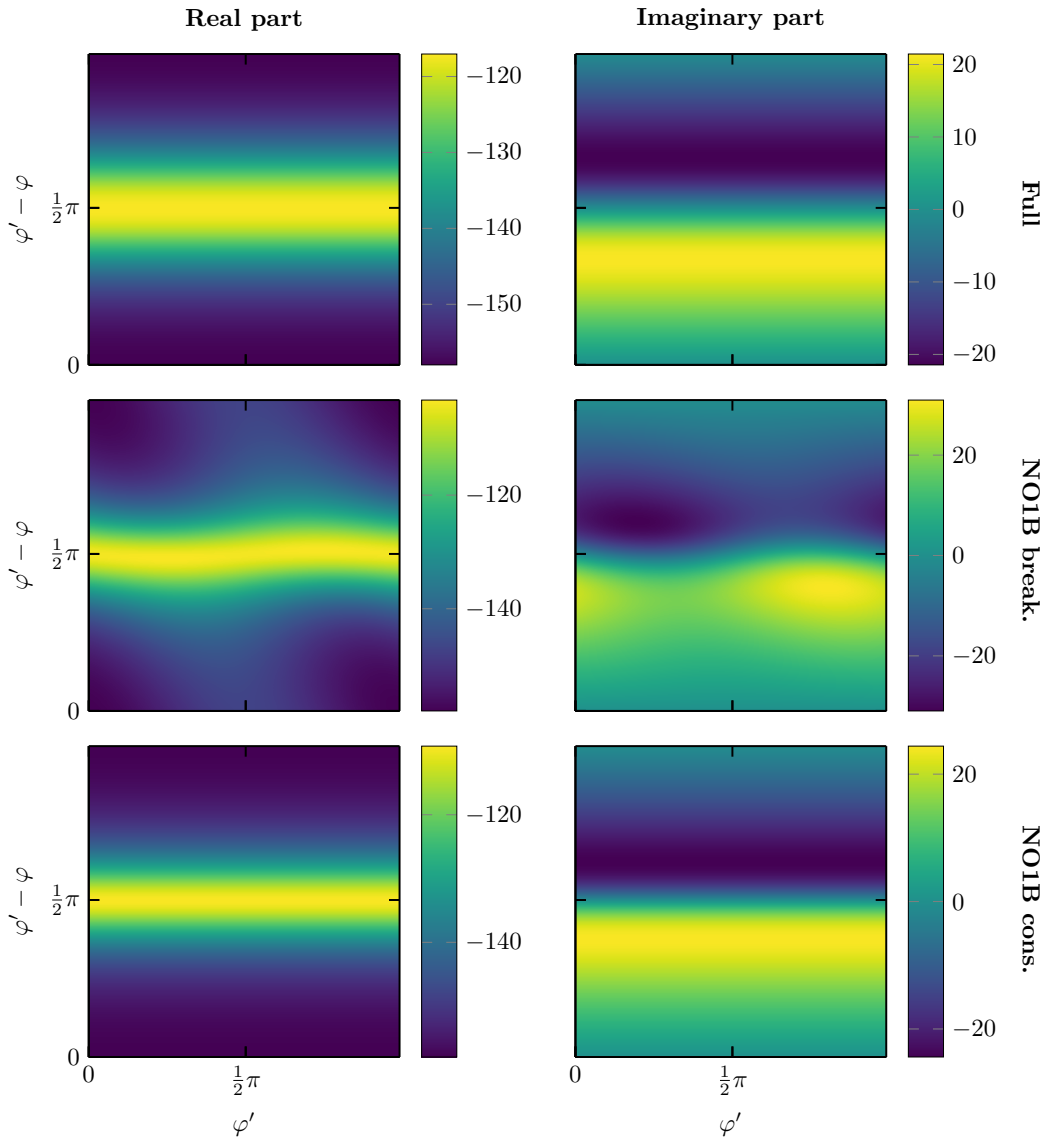
Single projection

$$O_{\Phi}^{\mathrm{A(s)}} \equiv \langle \Phi | P^{\mathrm{A}} O | \Phi \rangle = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{i\varphi \mathrm{A}} o^{(0)}(\varphi) \mathcal{N}^{(0)}(\varphi) \, .$$

Double projection

$$O_{\Phi}^{\mathrm{A(d)}} \equiv \langle \Phi | P^{\mathrm{A}} O P^{\mathrm{A}} | \Phi \rangle = \int_0^{2\pi} \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{d\varphi'}{2\pi} e^{i(\varphi - \varphi')\mathrm{A}} o^{(0)}(\varphi, \varphi') \mathcal{N}^{(0)}(\varphi - \varphi') \, .$$

Mean-field Hamiltonian kernel for O18



[J. Ripoche, A. Tichai, T. Duguet, in prep.]

Potentiel energy surface