Recent developments in Bogoliubov Many-Body Perturbation Theory

Pierre Arthuis
IRFU, CEA, Université Paris - Saclay

Doctoral Training Program
ECT*, Trento - June 23rd 2017

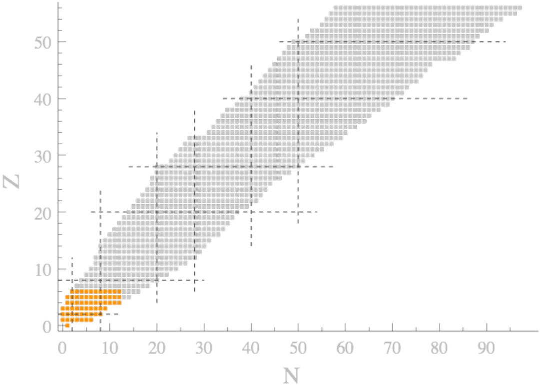
Outline

1. On ab initio methods and symmetry breaking
2. On Bogoliubov Many-Body Perturbation Theory
3. Recent progress
    - Validation of the formalism
    - First calculations
    - To higher orders

Outline

1. On ab initio methods and symmetry breaking
2. On Bogoliubov Many-Body Perturbation Theory
3. Recent progress
   - Validation of the formalism
   - First calculations
   - To higher orders

Evolution of the ab initio reach

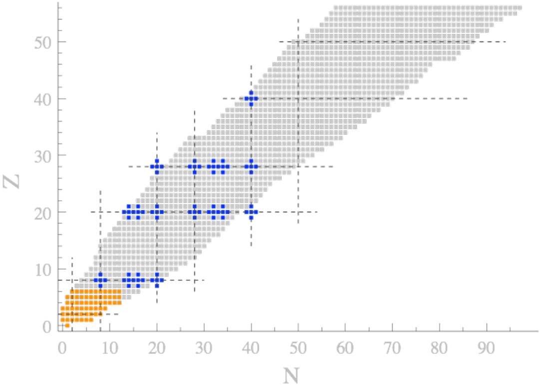


Courtesy of V. Soma, T. Duguet

"Exact" *ab initio* methods

- Since the 80's
- GFMC, NCSM, FY

Evolution of the ab initio reach

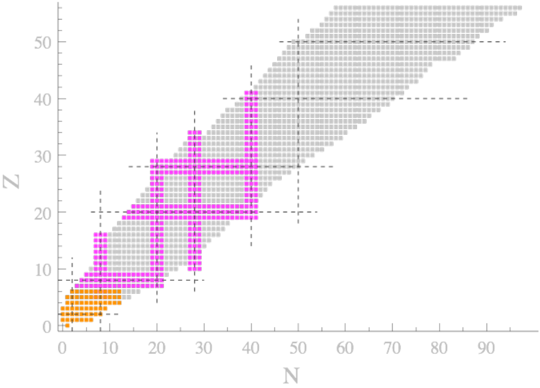


Courtesy of V. Soma, T. Duguet

Ab initio approaches for closed-shell nuclei

- Since the 2000's
- DSCGF, CC, IMSRG

Evolution of the ab initio reach

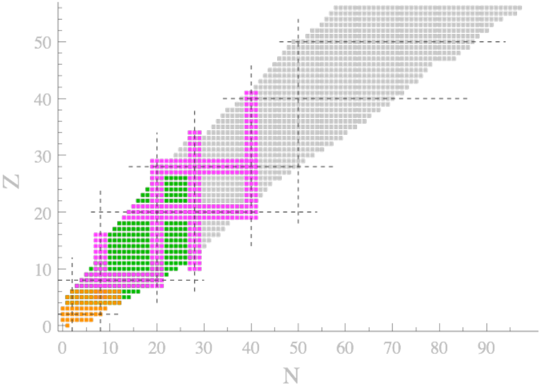


Courtesy of V. Soma, T. Duguet

Non-perturbative *ab initio* approaches for open-shell nuclei

- Since the 2010's
- GSCGF, BCC, MR-IMSRG

Evolution of the ab initio reach



Courtesy of V. Soma, T. Duguet

Ab initio shell model

- Since 2014
- Effective interaction via CC/IMSRG

What makes a method *ab initio*

1. Consider point-like nucleons as appropriate degrees of freedom
2. Use interactions rooted in underlying theory (i.e. QCD)
3. Expand the many-body Schrödinger equation systematically
4. Truncate at a given order and solve using computational methods
5. Estimate systematic error

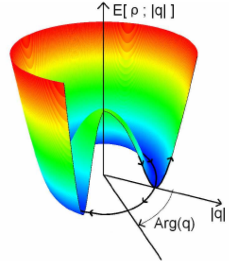
On symmetry breaking

Symmetry breaking helps incorporating non-dynamical correlations:

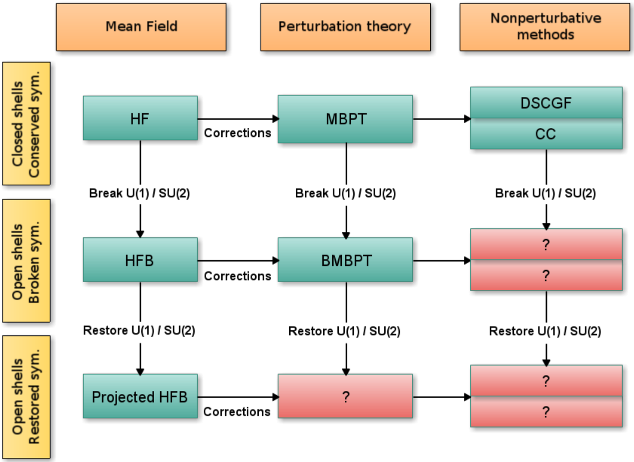
- Superfluid character: $U(1)$ (particle number)
- Deformations: $SU(2)$ (angular momentum)

But nuclei carry good quantum numbers (e.g. number of particles)

$\Rightarrow$ Symmetries must eventually be restored

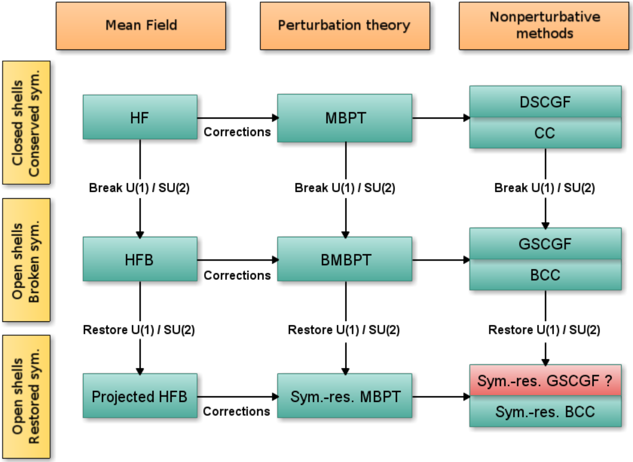


Quantum many-body methods



Expansion methods around unperturbed product state

Quantum many-body methods

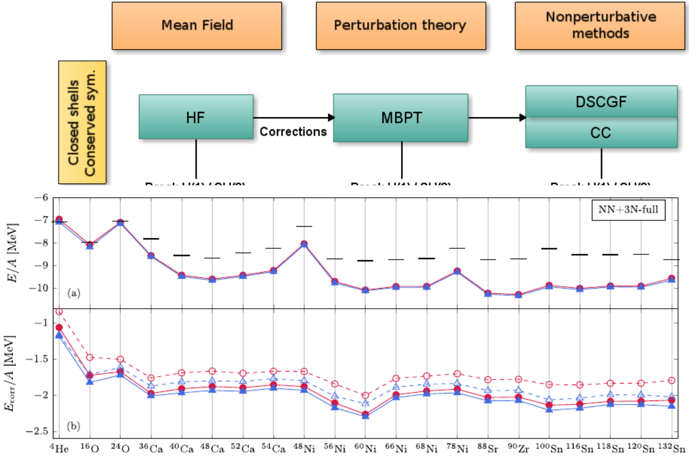


MBPT: Recently (re)implemented with SRG-evolved H [Tichai *et al.* 2016]

GSCGF, BCC: Recently proposed and implemented [Somà *et al.* 2011, Signoracci *et al.* 2014]

Sym.-res. BCC & sym.-res. BMBPT: Recently proposed [Duguet 2015, Duguet & Signoracci 2016]

Quantum many-body methods



MBPT: Recently (re)implemented with SRG-evolved H [Tichai *et al.* 2016]

GSCGF, BCC: Recently proposed and implemented [Somà *et al.* 2011, Signoracci *et al.* 2014]

Sym.-res. BCC & sym.-res. BMBPT: Recently proposed [Duguet 2015, Duguet & Signoracci 2016]

Outline

1. On ab initio methods and symmetry breaking

2. On Bogoliubov Many-Body Perturbation Theory

3. Recent progress
   - Validation of the formalism
   - First calculations
   - To higher orders

Bogoliubov Many-Body Perturbation Theory

1. Use a Bogoliubov vacuum $|\Phi\rangle$ with $\beta_k|\Phi\rangle = 0$ for all k
2. Define grand potential operator Ω from chiral interaction

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

then normal-order and split: $\Omega = \Omega_0 + \Omega_1$

3. Define evolved state in imaginary time

$$|\Psi(\tau)\rangle \equiv \mathcal{U}(\tau)|\Phi\rangle = e^{-\tau\Omega_0} \mathrm{T} e^{-\int_0^\tau d\tau \Omega_1(\tau)}|\Phi\rangle$$

4. Expand and truncate the grand potential kernel $\Omega(\tau) \equiv \langle\Psi(\tau)|\Omega|\Phi\rangle$...
...and the norm kernel $N(\tau) \equiv \langle\Psi(\tau)|\Phi\rangle$

5. Extract ground state energy via

$$\mathrm{E}_0 = \lim_{\tau\to\infty} \frac{\Omega(\tau)}{N(\tau)} = \lim_{\tau\to\infty} \omega(\tau)$$

Expansion of the grand potential kernel

Inserting the operator Ω at time 0 and expanding

$$
\begin{aligned}
\mathrm{E}_0 &= \lim_{\tau\to\infty} \frac{\langle\Psi(\tau)|\Omega|\Phi\rangle}{\langle\Psi(\tau)|\Phi\rangle} \\
&= \langle\Phi|\Big\{\Omega(0) - \int_0^\infty d\tau_1 \mathrm{T}\left[\Omega_1(\tau_1)\Omega(0)\right] \\
&\qquad + \frac{1}{2!}\int_0^\infty d\tau_1 d\tau_2 \mathrm{T}\left[\Omega_1(\tau_1)\,\Omega_1(\tau_2)\Omega(0)\right] + \ldots\Big\}|\Phi\rangle_c
\end{aligned}
$$

Then expressing the grand potential in the qp basis

$$
\Omega = \Omega^{00} + \frac{1}{1!}\sum_{k_1 k_2} \Omega^{11}_{k_1 k_2}\beta^\dagger_{k_1}\beta_{k_2} + \frac{1}{2!}\sum_{k_1 k_2}\left\{\Omega^{20}_{k_1 k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + \Omega^{02}_{k_1 k_2}\beta_{k_2}\beta_{k_1}\right\} + \ldots
$$

Expansion of the grand potential kernel

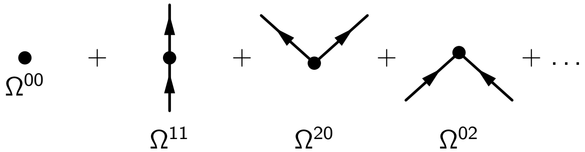
$$
\begin{aligned}
\mathrm{E}_0 = \sum_{p=0}^{\infty} \frac{(-1)^p}{p!} \sum_{\substack{i_0+j_0=2,4 \\ \vdots \\ i_p+j_p=2,4}} \int_0^{\infty} d\tau_1 \dots d\tau_p \\
\times \sum_{\substack{k_1 \dots k_{i_1} \\ k_{i_1+1} \dots k_{i_1+j_1} \\ \vdots \\ l_1 \dots l_{i_p} \\ l_{i_p+1} \dots l_{i_p+j_p}}} \frac{\Omega^{i_1 j_1}_{k_1 \dots k_{i_1}\, k_{i_1+1} \dots k_{i_1+j_1}}}{(i_1)!(j_1)!} \dots \frac{\Omega^{i_p j_p}_{l_1 \dots l_{i_p}\, l_{i_p+1} \dots l_{i_p+j_p}}}{(i_p)!(j_p)!} \frac{\Omega^{i_0 j_0}_{m_1 \dots m_{i_0}\, m_{i_0+1} \dots m_{i_0+j_0}}}{(i_0)!(j_0)!} \\
\times \langle \Phi | \mathrm{T} \Big[\beta^{\dagger}_{k_1}(\tau_1) \dots \beta^{\dagger}_{k_{i_1}}(\tau_1)\, \beta_{k_{i_1+j_1}}(\tau_1) \dots \beta_{k_{i_1+1}}(\tau_1) \dots \\
\dots \beta^{\dagger}_{l_1}(\tau_p) \dots \beta^{\dagger}_{l_{i_p}}(\tau_p)\, \beta_{l_{i_p+j_p}}(\tau_p) \dots \beta_{l_{i_p+1}}(\tau_p) \\
\times \beta^{\dagger}_{m_1}(0) \dots \beta^{\dagger}_{m_{i_0}}(0) \beta_{m_{i_0+j_0}}(0) \dots \beta_{m_{i_0+1}}(0) \Big] | \Phi \rangle_c
\end{aligned}
$$

All contributions computable algebraically and diagramatically

First- and second-order diagrams

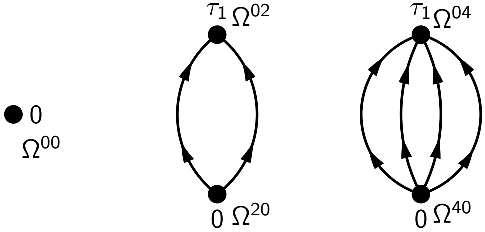
Diagrammatic representation of the grand potential Ω

$\Omega =$



Extracting and applying diagrammatic rules

$\mathrm{E}_0^{(1+2)} =$



Outline

1. On ab initio methods and symmetry breaking
2. On Bogoliubov Many-Body Perturbation Theory
3. Recent progress
   - Validation of the formalism
   - First calculations
   - To higher orders

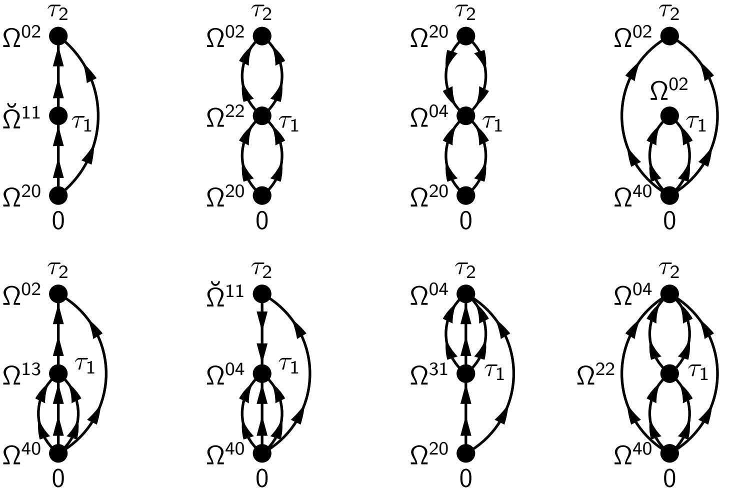
Outline

1. On ab initio methods and symmetry breaking

2. On Bogoliubov Many-Body Perturbation Theory

3. Recent progress
   - Validation of the formalism
   - First calculations
   - To higher orders

Third-order diagrams



Derivation of all diagrams up to third order

Validation of formal derivation

BMBPT must match standard MBPT in Slater determinant limit

$\rightarrow$ Matching must be true at each order

$\rightarrow$ Proof of consistent formalism for BMBPT

Validation of formal derivation

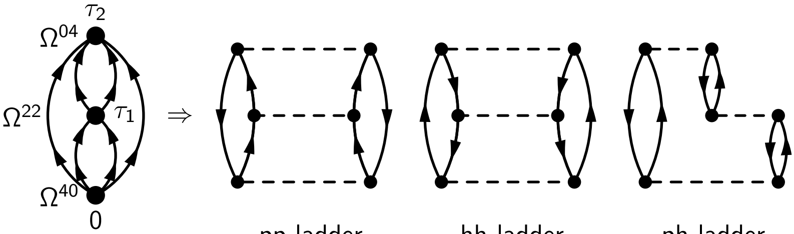
BMBPT must match standard MBPT in Slater determinant limit

$\rightarrow$ Matching must be true at each order

$\rightarrow$ Proof of consistent formalism for BMBPT

BMBPT(3) diagrams match MBPT(3) ones exactly

Canonical HF-MBPT diagrams were recovered from only one BMBPT



pp ladder hh ladder ph ladder

Outline

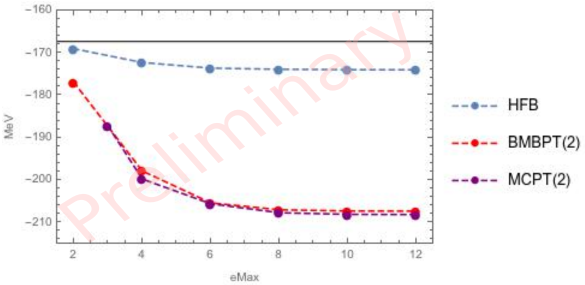
1. On ab initio methods and symmetry breaking

2. On Bogoliubov Many-Body Perturbation Theory

3. Recent progress
   - Validation of the formalism
   - First calculations
   - To higher orders

Proof of principle calculations

First BMBPT(2) proof of principle calculation of $^{20}\mathrm{O}$:



[Arthuis, Tichai, Hergert, Roth and Duguet, in prep.]
[Tichai, Gebrerufael and Roth, arXiv:1703.05664 (2017)]

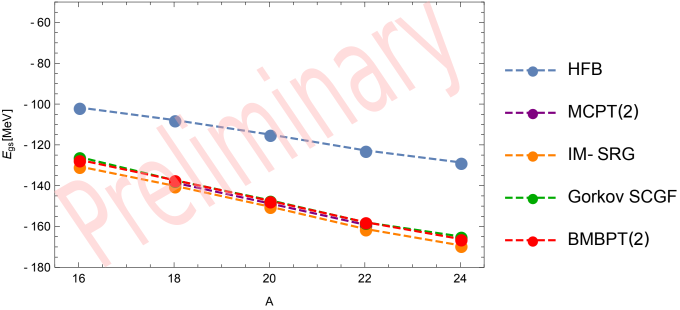
using NN SRG-evolved chiral interaction

On MCPT:

- Multi-configurational MBPT
- Alternative method for open-shell nuclei

Isotopic chains calculations at second order

First BMBPT(2) calculations on O, Ca, Ni and Sn isotopic chains



[Arthuis, Tichai, Hergert, Roth and Duguet, in prep.]
[Tichai, Gebrerufael and Roth, arXiv:1703.05664 (2017)]
[Hergert, Phys. Scripta 92 (2017)]
[Cipollone, Barbieri and Navràtil, Phys. Rev. C (2015)]

using NN and 3N SRG-evolved chiral interaction

Same chains under investigation at third order at the moment

Outline

1. On ab initio methods and symmetry breaking
2. On Bogoliubov Many-Body Perturbation Theory
3. Recent progress
   - Validation of the formalism
   - First calculations
   - To higher orders

Numerical derivation of higher orders

Have your computer do the diagrammatic work for you

- Produce the diagrams automatically
  - Diagrams are associated with adjacency matrices
  - Diagrammatic rules constrain the form of the matrices
  - Have your code generate all matrices, hence diagrams

- Extract their expression automatically as well
  - Read your diagrams (vertices, propagators, etc.)
  - Extract useful information from the structure
  - Retrieve the exact expression

Numerical derivation of higher orders

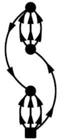
Produce higher orders diagrams

- 59 diagrams at order 4
- 568 diagrams at order 5

Extend to three-body diagrams

- 15 diagrams at order 3
- 337 diagrams at order 4
- 10 148 diagrams at order 5

$$\frac{-(-1)^3}{(3!)^2}\sum_{k_i}\frac{O^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_8}\Omega^{31}_{k_5k_6k_7k_4}\Omega^{13}_{k_8k_5k_6k_7}}{(+E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})(+E_{k_1}+E_{k_2}+E_{k_3}+E_{k_5}+E_{k_6}+E_{k_7})(+E_{k_1}+E_{k_2}+E_{k_3}+E_{k_8})}$$



Prospects

- Go up to fourth order
  - → Even better than other *ab initio* methods?
  - → Test for computational cost
- Push BMBPT to heavier nuclei
  - → Can go further than other *ab initio* methods
  - → Good test for the computational cost
- Implement particle-number restored BMBPT for the first time
  - → Required for precise study of open-shell nuclei
  - → Proof of concept of symmetry-restored BMBPT / BCC
- *Ab initio* driven EDF method [T. Duguet et al. (2015)]
  - → Safe/correlated/improvable off-diagonal EDF kernels
  - → Based on PNR-BMBPT

Conclusion

- MBPT and BMBPT are special among *ab initio* methods
  - ✔ Computationally friendlier
  - ✔ Potentially as precise as others when using SRG-evolved H

- BMBPT has been formulated and is being implemented
  - ✔ First derivation up to fourth order
  - ✔ First calculations up to third order
  - ✔ Appropriate framework to tackle open-shell nuclei
  - ✔ Systematic studies at third and fourth order to come

- Symmetry-restored BMBPT is the next step

Our collaborators

BMBPT Project

P. Arthuis
T. Duguet
J.-P. Ebran

A. Tichai
R. Roth

H. Hergert

On broader aspects

M. Drissi
J. Ripoche

R. Lasseri