Bogoliubov Many-Body Perturbation Theory for Open-Shell Nuclei

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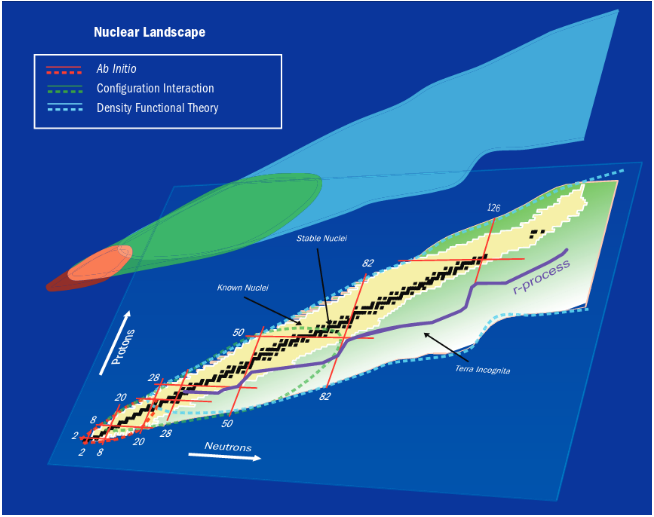
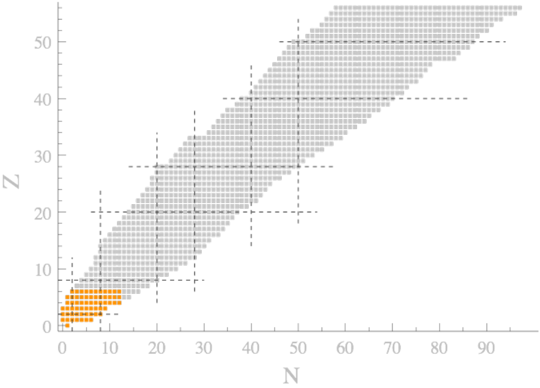
Café du DPhN
CEA Saclay - February 12th 2018

On Nuclear Structure Theory

Different methods to treat the whole nuclear chart:



Evolution of the ab initio reach

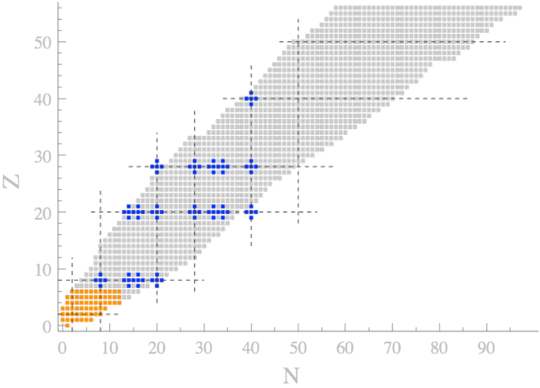


Courtesy of V. Soma, T. Duguet

"Exact" *ab initio* methods

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

Evolution of the ab initio reach

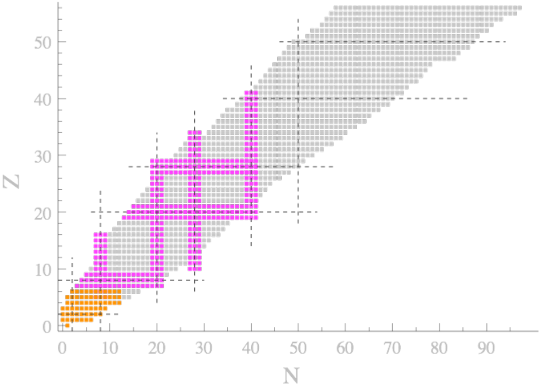


Courtesy of V. Soma, T. Duguet

***Ab initio* approaches for closed-shell nuclei**

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

Evolution of the ab initio reach

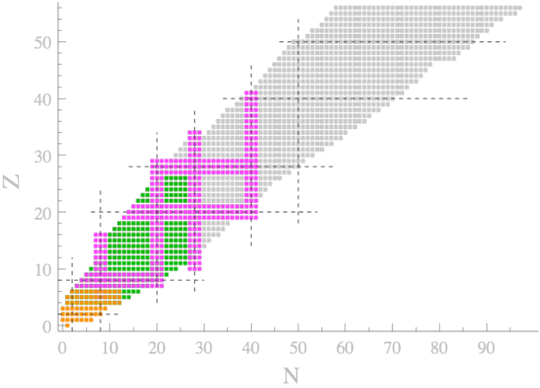


Courtesy of V. Soma, T. Duguet

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 or IMSRG

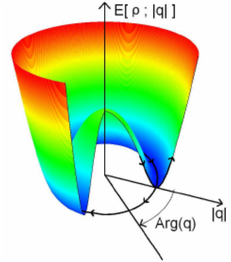
On symmetry breaking

Symmetry breaking helps incorporating non-dynamical correlations:

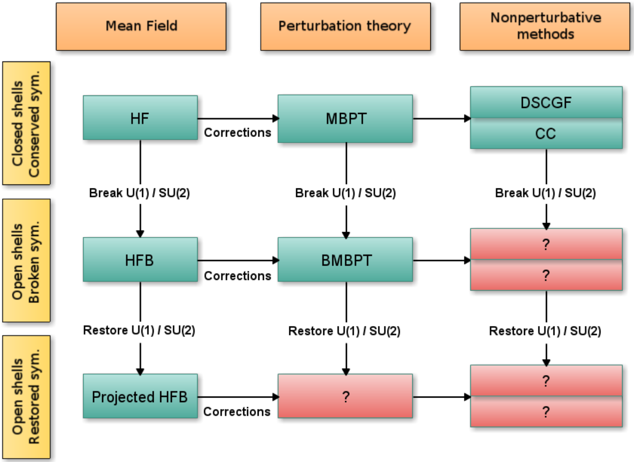
- Superfluid character: $U(1)$ (particle number)
- Deformations: $SU(2)$ (angular momentum)

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

$\Rightarrow$ Symmetries must eventually be restored

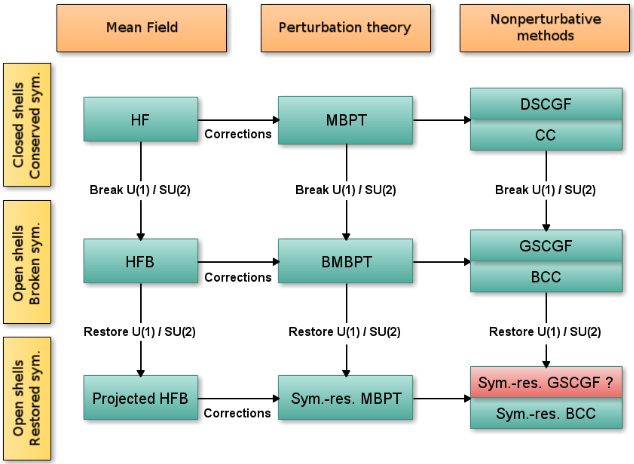


Quantum many-body methods



Expansion methods around unperturbed product state

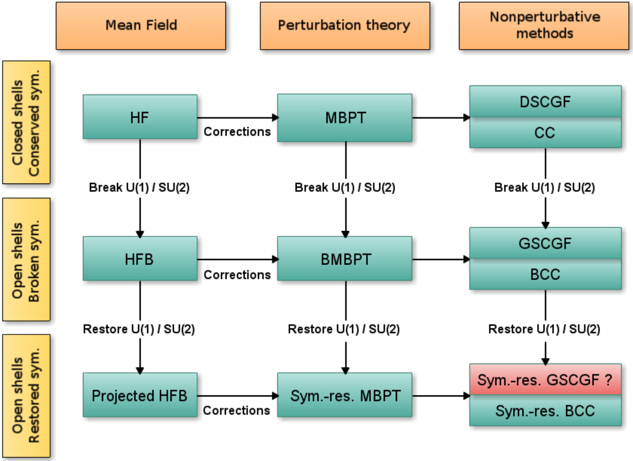
Quantum many-body methods



New methods recently proposed and implemented

- GSCGF, BCC [Somà *et al.* 2011, Signoracci *et al.* 2014]
- Sym.-res. BCC & sym.-res. BMBPT [Duguet 2015, Duguet & Signoracci 2017, Qiu *et al.* 2017]

Quantum many-body methods



MBPT reimplemented using SRG-evolved H [Tichai *et al.* 2016]

➥ MBPT competes with non-perturbative methods

The BMBPT project

Particle-number-restored BMBPT formalism

Exact diagrammatic expansion with symmetry breaking *and* restoration

[Duguet and Signoracci, *J. Phys. G* **44**, 2017]

Formalism actualization

Expand off-diagonal kernels

$\langle \Psi | H | \Phi(\phi) \rangle$

$\langle \Psi | \Phi(\phi) \rangle$

Symmetry restoration

Diagonal reduction

$\langle \Psi | H | \Phi \rangle$

$\langle \Psi | \Phi \rangle$

No symmetry restoration

Ab initio

Realist H

High order

Energy Density Functional

Effective H

Low order

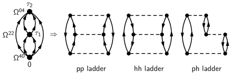
Diagonal implementation

$\langle \Psi | H | \Phi \rangle$

$\langle \Psi | \Phi \rangle$

Manual derivation of order 3

Check against MBPT limit



Automatic derivation

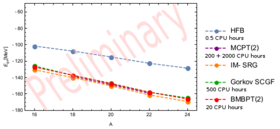
[PA, Duguet, Tichai, Lasseri, Ebran, in prep.]

Ab initio

Realist H

High order

Numerical implementation



[PA, Tichai, Hergert, Roth, Duguet, in prep.]

Bogoliubov Many-Body Perturbation Theory

- Quasiparticle creation and annihilation operators

$$\beta_k = \sum_p U^*_{pk}\, c_p + V^*_{pk}\, c^\dagger_p$$

$$\beta^\dagger_k = \sum_p U_{pk}\, c^\dagger_p + V_{pk}\, c_p$$

- Bogoliubov vacuum $|\Phi\rangle$, $\beta_k|\Phi\rangle = 0\, \forall k$

- Grand potential operator $\Omega \equiv H - \lambda A$ in quasiparticle basis

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

Bogoliubov Many-Body Perturbation Theory

- Perturbative expansion of ground-state energy ($\Omega = \Omega_0 + \Omega_1$)

$$\mathrm{E}_0 = \langle\Phi|\Big\{\Omega(0) - \int_0^\infty d\tau_1 \mathsf{T}\left[\Omega_1(\tau_1)\Omega(0)\right] + \frac{1}{2!}\int_0^\infty d\tau_1 d\tau_2 \mathsf{T}\left[\Omega_1(\tau_1)\,\Omega_1(\tau_2)\Omega(0)\right] + \ldots\Big\}|\Phi\rangle_c$$

- Propagators

$$G^{+-(0)}_{k_1 k_2}(\tau_1,\tau_2) \equiv \frac{\langle\Phi|\mathsf{T}[\beta^\dagger_{k_1}(\tau_1)\beta_{k_2}(\tau_2)]|\Phi\rangle}{\langle\Phi|\Phi\rangle} = -G^{-+(0)}_{k_2 k_1}(\tau_2,\tau_1)$$

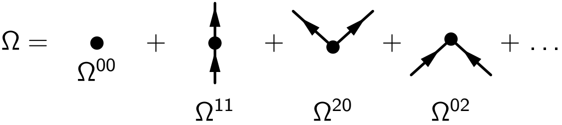
- Apply Wick theorem... Obtain lots of terms

Is there a more convenient way to proceed?

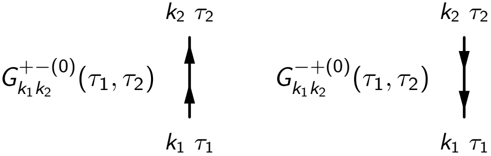
Yes: Express everything in terms of diagrams

Building blocks of the diagrammatic

- Normal-ordered form of Ω with respect to Φ



- Propagators



- Main diagrammatic rules
  - ◇ Wick theorem
  - ◇ No external legs
  - ◇ No oriented loop between vertices
  - ◇ No self-contraction
  - ◇ Propagators go out of the Ω vertex at time 0

The BMBPT project: Low-order derivation

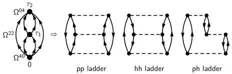
Diagonal implementation

$\langle \Psi | H | \Phi \rangle$

$\langle \Psi | \Phi \rangle$

Manual derivation of order 3

Check against MBPT limit



Automatic derivation

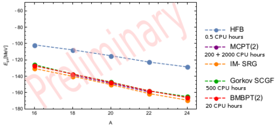
[PA, Duguet, Tichai, Lasseri, Ebran, in prep.]

Ab initio

Realist H

High order

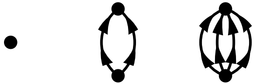
Numerical implementation



[PA, Tichai, Hergert, Roth, Duguet, in prep.]

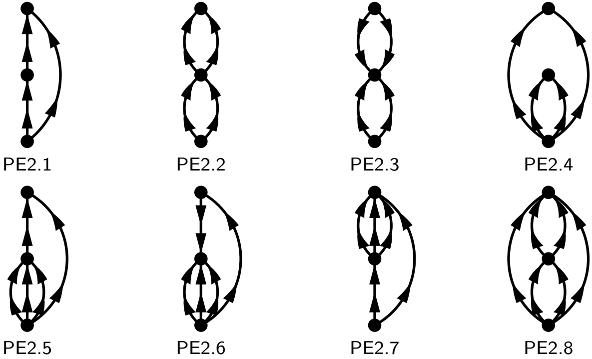
Low-order diagrams

- First- and second-order diagrams [Duguet and Signoracci, *J. Phys. G* **44**, 2017]



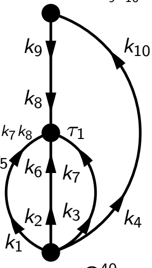
PE0.1 PE1.1 PE1.2

- Third-order diagrams



Validation of the manual derivation by checking the MBPT limit

Derivation of a third-order diagram



Feynman (time-dependent) and Goldstone (time-integrated) expressions:

$$\text{PE2.6} = -\frac{1}{3!} \sum_{k_1 k_2 k_3 k_4 k_8} \Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{04}_{k_1 k_2 k_3 k_8} \breve{\Omega}^{11}_{k_8 k_4} \int_0^\infty \mathrm{d}\tau_1 \mathrm{d}\tau_2 \theta(\tau_1 - \tau_2) e^{-\tau_1 \left(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_8} \right)} e^{\tau_2 \left(E_{k_8} - E_{k_4} \right)}$$

$$= -\frac{1}{3!} \sum_{k_1 k_2 k_3 k_4 k_8} \frac{\Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{04}_{k_1 k_2 k_3 k_8} \breve{\Omega}^{11}_{k_8 k_4}}{\left(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4} \right) \left(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_8} \right)}$$

Status of manual derivation and implementation

- All diagrams derived and numerically implemented up to order 3

  [PA, Tichai, Ebran, Duguet]

- Ab initio approach $\rightarrow$ Go to highest possible order
  - ◇ At least up to order 4 to check convergence patterns
  - ◇ Derivation time-consuming
  - ◇ Derivation error-prone

Develop automatic tool

- ◇ To generate all possible connected diagrams at order n
- ◇ To extract associated time-integrated expressions
- ◇ To be both quick and safe

The BMBPT project: Automatic derivation

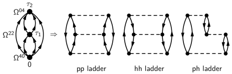
Diagonal implementation
$\langle \Psi | H | \Phi \rangle$
$\langle \Psi | \Phi \rangle$

Ab initio

Realist H
High order

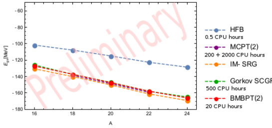
Manual derivation of order 3

Check against MBPT limit



Automatic derivation
[PA, Duguet, Tichai, Lasseri, Ebran, in prep.]

Numerical implementation



[PA, Tichai, Hergert, Roth, Duguet, in prep.]

Why and how?

Our goal

An automatic and systematic way of producing diagrams

Our tool

Adjacency matrices in graph theory

Our challenge

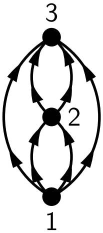
From BMBPT diagrammatic rules to constraints on matrices

Graphs and adjacency matrix

Each Feynman diagram to be represented by an adjacency matrix

- a_{ij} indicate the number of edges going from node i to node j

$$A = \begin{pmatrix} 0 & 2 & 2 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix} \Leftrightarrow$$



  - ◇ Carry detailed information for directed graphs
  - ◇ Symmetry properties and connectivity properties directly readable

- Only two propagators, readable as one once reading direction is fixed
  - ◇ Perfectly adapted for diagonal BMBPT
  - ◇ Extension needed for off-diagonal diagrams with anomalous propagator

Constraints from the diagrammatic rules

Each vertex belongs to $\Omega^{[2]}$ or $\Omega^{[4]}$

For each vertex i, $\sum_j (a_{ij} + a_{ji})$ is 2 or 4

No self-contraction (not the case for off-diagonal theory)

Every diagonal element is zero

Every propagator coming out of the vertex at time 0 goes upward

First column of the matrix is zero

No oriented loop between vertices

Can restrict to upper triangular matrices

Generate BMBPT diagrams

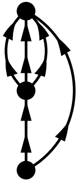
- Generate all upper triangular matrices for BMBPT diagrams at order n
  - Fill the matrices "vertex-wise"
  - Check the degree of each vertex before moving on

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & a_{12} & a_{13} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & a_{12} & a_{13} \\ 0 & 0 & a_{23} \\ 0 & 0 & 0 \end{pmatrix}$$

- Discard matrices leading to topologically identical diagrams

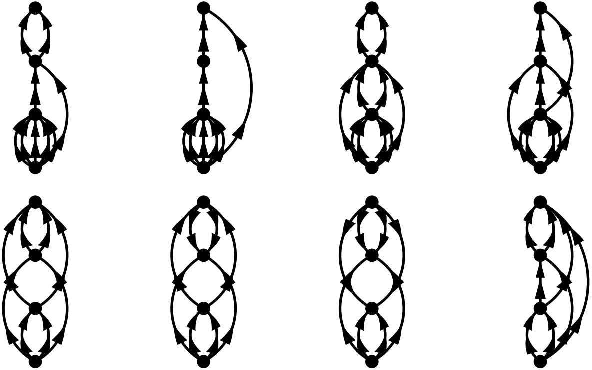
- Read the matrix and translate it into drawing instructions

```
\begin{fmfgraph*}(60,60)
\fmftop{v2}\fmfbottom{v0}
\fmf{phantom}{v0,v1}
\fmfv{d.shape=circle,d.filled=full,d.size=3thick}{v0}
\fmf{phantom}{v1,v2}
\fmfv{d.shape=circle,d.filled=full,d.size=3thick}{v1}
\fmfv{d.shape=circle,d.filled=full,d.size=3thick}{v2}
\fmffreeze
\fmf{prop_pm}{v0,v1}
\fmf{prop_pm,right=0.6}{v0,v2}
\fmf{prop_pm}{v1,v2}
\fmf{prop_pm,left=0.5}{v1,v2}
\fmf{prop_pm,right=0.5}{v1,v2}
\end{fmfgraph*}
```



Time to cook some diagrams

Run the code at order 4 with 2N and 3N interactions, obtain...



...and 388 others!

Status of the numerical derivation

- Number of diagrams with 2N interactions (using an HFB vacuum)
  - 8 (1) diagrams at order 3
  - 59 (10) diagrams at order 4
  - 568 (82) diagrams at order 5
  - 6 805 (938) diagrams at order 6
- Number of diagrams with 2N and 3N interactions (using an HFB vacuum)
  - 23 (8) diagrams at order 3
  - 396 (177) diagrams at order 4
  - 10 716 (5 055) diagrams at order 5
  - 100 000+ diagrams at order 6?
- Obtained in only a few minutes...

Automated expression derivation

All BMBPT diagrams produced automatically at a given order

➥ Need to derive automatically the diagrams' expressions

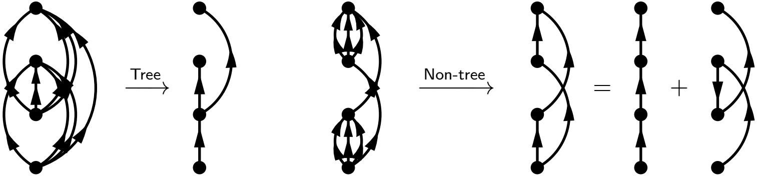
- Feynman diagrams recast different time-orderings
  - ✔ Less diagrams to set up
  - ✘ But time-integrated (Goldstone) expressions are to be coded
- Goldstone diagrams capture each time ordering separately
  - ✔ Time-integrated expressions obtained directly from diagrammatic rules
  - ✘ Many more diagrams to consider

Challenge: Extract Goldstone expressions from Feynman diagrams

- ◇ Capture all time ordering at once
- ◇ Challenging because of structure of corresponding time integrals
- ◇ Undone task to our knowledge (even for standard diagrammatic)

Time-structure diagrams [PA, Duguet, Tichai, Lasseri, Ebran, in prep.]

- Determine the time-structure diagram (TSD) associated to BMBPT one
  - ◇ Propagators carry time-ordering relations
  - ◇ Ω vertex at time 0 is a lower limit for time
  - ◇ One TSD recast several Feynman, even more Goldstone



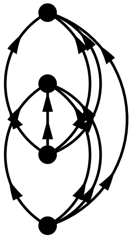
- Extraction of the time-integrated expression depends on TSD
  - ◇ If tree, apply the Goldstone-like algorithm based on subdiagrams
  - ◇ If non-tree, decompose the diagram in a sum of tree TSDs

✔ Algorithms implemented and used at all orders

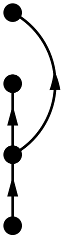
Algorithm for denominator extraction

For each perturbation vertex in the diagram with an associated tree TSD

1. Determine all its descendants using the TSD diagram
2. Form a subgraph using the vertex and its descendants
3. For all propagators entering the subgraph, add the associated qpe



$\leftrightarrow$



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

Algorithm for denominator extraction

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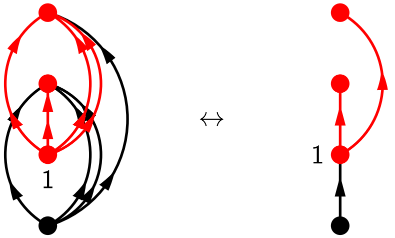

$$\frac{-(-1)^3}{(3!)^2} \sum_{k_i} \frac{\Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{40}_{k_5 k_6 k_7 k_8} \Omega^{04}_{k_5 k_1 k_2 k_3} \Omega^{04}_{k_6 k_7 k_8 k_4}}{(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_5})(E_{k_4}+E_{k_6}+E_{k_7}+E_{k_8})}$$

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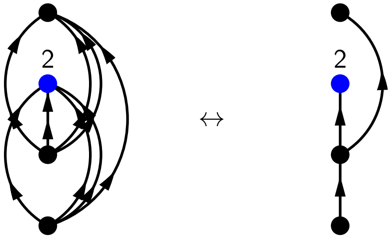

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Algorithm for denominator extraction

For each perturbation vertex in the diagram with an associated tree TSD

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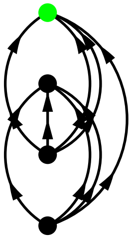
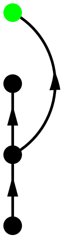


$\leftrightarrow$

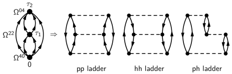


$$\frac{-(-1)^3}{(3!)^2} \sum_{k_i} \frac{\Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{40}_{k_5 k_6 k_7 k_8} \Omega^{04}_{k_5 k_1 k_2 k_3} \Omega^{04}_{k_6 k_7 k_8 k_4}}{(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_5})(E_{k_4}+E_{k_6}+E_{k_7}+E_{k_8})}$$

Diagonal implementation
$\langle\Psi|H|\Phi\rangle$
$\langle\Psi|\Phi\rangle$

Manual derivation of order 3

Check against MBPT limit



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Ab initio

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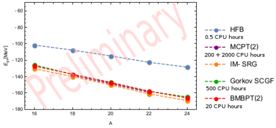
High order

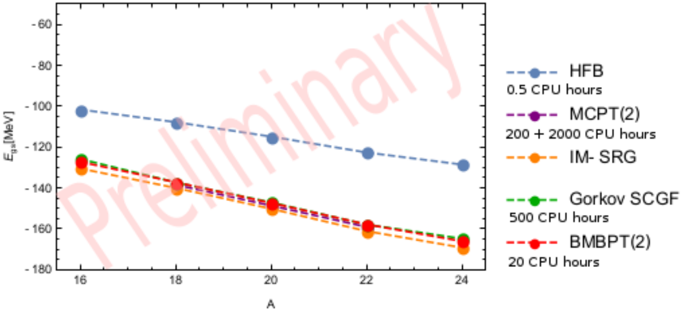
Numerical implementation



[PA, Tichai, Hergert, Roth, Duguet, in prep.]

Isotopic chains calculations at second order

- Test BMBPT(2) calculations on O (below), Ca, Ni and Sn 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

- Third-order calculations under way / fourth order in near future
- Systematic calculations to come

Conclusion

- BMBPT diagrams now generated automatically
  - ✔ Fast and error-safe
  - ✔ No intrinsic upper limit on the order
- BMBPT analytical expressions automatically derived to all order as well
  - ✔ Feynman and Goldstone expressions for all diagrams
  - ✔ Order 4 to be implemented in BMBPT code in near future
- Project still moving on
  - ◇ Code to be published
  - ◇ Open to collaborations regarding other diagrammatic methods
- Progress done in numerical implementation in the mean time

Perspectives

- Extend the scope of the automated diagram generator
  - Gorkov SCGF
  - Off-diagonal BMBPT
- Extend the scope of diagonal BMBPT
  - Excited states and new observables
  - Developments used in parallel in future BCC implementation
- Move towards symmetry-restored BMBPT
  - Extensive work on the theory
  - Automated diagram generation and derivation
  - Implementation in the BMBPT numerical code
- Move towards fully automated calculations?

Our collaborators

BMBPT Project

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