Recent developments in Bogoliubov Many-Body Perturbation Theory

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Bridging nuclear ab-initio and energy-density-functional theories
IPN, Orsay - October 6th 2017

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

Diagonal version

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

$\langle \Psi | \Phi \rangle$

Off-diagonal version

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

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

Ab initio (This talk)

Realist H

High order

EDF (Thomas' talk)

Effective H

Low order

The BMBPT project

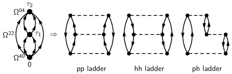
Diagonal implementation
$\langle \Psi | H | \Phi \rangle$
$\langle \Psi | \Phi \rangle$

Ab initio

Realist H
High order

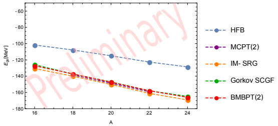
Manual derivation of order 3

Check against MBPT limit



Automatic derivation
[PA, Duguet, Ebran]

Numerical implementation



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

Outline

1. From BMBPT equations to diagrams...
   - Definition
   - Manual derivation up to third order

2. ...and from BMBPT diagrams back to equations
   - Automatic generation of connected diagrams
   - Automatic derivation of analytical formulas

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- Bogoliubov vacuum $|\Phi\rangle$, $\beta_k|\Phi\rangle = 0\,\forall k$
- Grand potential operator $\Omega \equiv H - \lambda A$ in quasiparticle basis

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

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

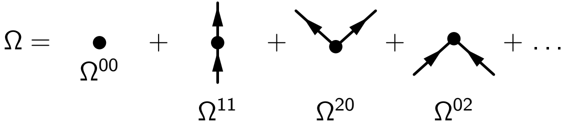
$$\mathrm{E}_0 = \langle\Phi|\Big\{\Omega(0) - \int_0^\infty d\tau_1 \mathrm{T}\left[\Omega_1(\tau_1)\Omega(0)\right] + \frac{1}{2!}\int_0^\infty d\tau_1 d\tau_2 \mathrm{T}\left[\Omega_1(\tau_1)\,\Omega_1(\tau_2)\Omega(0)\right] + \dots\Big\}|\Phi\rangle_c$$

- Propagators (also anomalous $G^{--(0)}$ for off-diagonal theory)

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

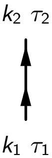
Building blocks of the diagrammatic

- Normal-ordered form of Ω with respect to Φ

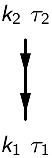


- Propagators

$G^{+-(0)}_{k_1 k_2}(\tau_1, \tau_2)$



$G^{-+(0)}_{k_1 k_2}(\tau_1, \tau_2)$



- Main diagrammatic rules
  - ◇ Wick theorem (off-diagonal Wick theorem for off-diagonal theory)
  - ◇ No external legs
  - ◇ No oriented loop between vertices
  - ◇ No self-contraction (anomalous one for off-diagonal theory)
  - ◇ Propagators go out of the Ω vertex at time 0
  - ◇ Equivalent lines
  - ◇ Discard topologically equivalent diagrams

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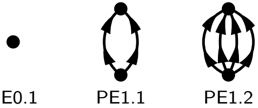
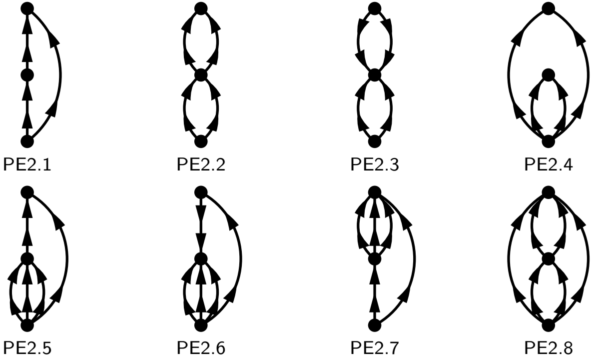
Low-order diagrams

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

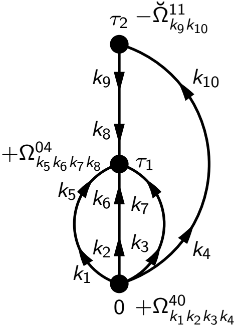


- Third-order diagrams



Validation of the manual derivation by checking the MBPT limit

Derivation of a third-order diagram



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

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

$$= -\frac{1}{3!} \sum_{k_1 k_2 k_3 k_4 k_5} \frac{\Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{04}_{k_1 k_2 k_3 k_5} \breve{\Omega}^{11}_{k_5 k_4}}{\left(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}\right) \left(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_5}\right)}$$

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

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Why and how?

Our goal

An automatic and systematic way of producing diagrams

Our tool

Adjacency matrices in graph theory

Our challenge

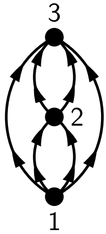
From BMBPT diagrammatic rules to constraints on matrices

Graphs and oriented adjacency matrix

Each Feynman diagram to be represented by an adjacency matrix

- $\tilde{a}_{ij}$ indicate the number of edges going from node i to node j

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



  - ◇ 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

No loop between two vertices

Either a_{ij} or a_{ji} is zero

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

First column of the matrix is zero

Generate BMBPT diagrams

- Generate all possible matrices associated with BMBPT diagrams at order n
  - Fill the matrices "vertex-wise"
  - Leave first column blank
  - Attribute a value to a_{ij} only if a_{ji} is zero
  - Check the degree of each vertex before moving on

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & a_{12} & a_{13} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & a_{12} & a_{13} \\ 0 & 0 & a_{23} \\ 0 & a_{32} & 0 \end{pmatrix}$$

- Run some checks to avoid
  - Matrices appearing twice
  - Matrices associated to vanishing graphs (e.g. loops between vertices)
  - Matrices associated to topologically identical diagrams

Draw the generated diagrams

- Matrices encode all the necessary information to draw your graph
  - ◇ Order n (i.e. number of vertices) determined by its size
  - ◇ a_{ij} gives the number of propagators to draw from vertex i to vertex j

- Run through 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*}
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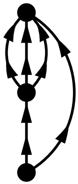
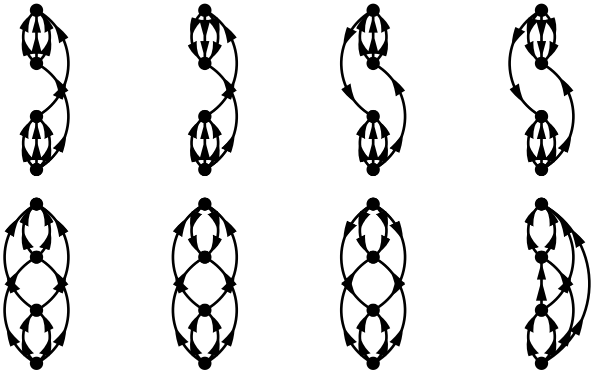


Time to cook some diagrams

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...

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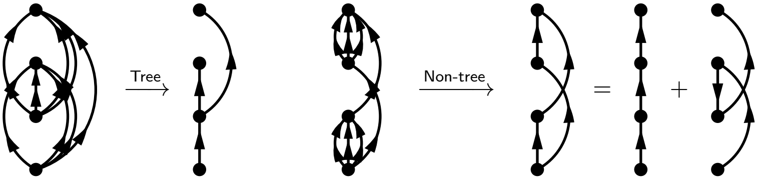
Why and how?

- 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 time-integrated 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 [*Automatic derivation of BMBPT diagrams*, PA, Duguet, 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



- Extraction of the time-integrated expression depends on TSD
  - ◇ If tree, apply the Goldstone-like algorithm based on subdiagrams
    ✔ Already implemented and used at all orders
  - ◇ If non-tree, decompose the diagram in a sum of tree TSDs
    ✔ Algorithm figured out at all orders, to be implemented
- One TSD recast several Feynman, even more Goldstone

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 expressions for all diagrams
  - ✔ Algorithm for Goldstone expressions of (non) tree diagrams (to be) coded
  - ✔ Order 4 to be implemented in BMBPT code in near future

- Project still moving on
  - ◇ Code to be published
  - ◇ To be extended for off-diagonal BMBPT
  - ◇ To be extended for Gorkov SCGF developments
  - ◇ Open to collaborations regarding other diagrammatic methods

- Progress done in numerical implementation in the mean time

Our collaborators

BMBPT Project

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On broader aspects

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