Automated generation of Bogoliubov MBPT expressions

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TRIUMF Workshop
Vancouver, Canada - February 28th 2018

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

Bogoliubov Many-Body Perturbation Theory

- 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 ($\Omega = \Omega_0 + \Omega_1$)

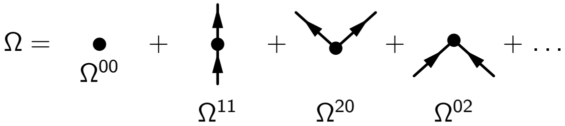
$$\mathrm{E}_0 = \langle\Phi|\Big\{\Omega(0) - \int_0^\infty d\tau_1 \mathrm{T}\left[\Omega_1(\tau_1)\Omega(0)\right] + \frac{1}{2!}\int_0^\infty d\tau_1 d\tau_2 \mathrm{T}\left[\Omega_1(\tau_1)\,\Omega_1(\tau_2)\Omega(0)\right] + \dots\Big\}|\Phi\rangle_c$$

- Propagators

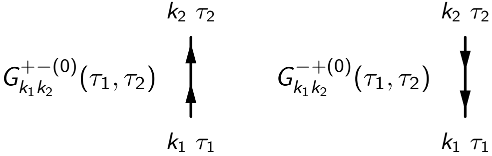
$$G^{+-(0)}_{k_1 k_2}(\tau_1,\tau_2) \equiv \frac{\langle\Phi|\mathrm{T}[\beta^\dagger_{k_1}(\tau_1)\beta_{k_2}(\tau_2)]|\Phi\rangle}{\langle\Phi|\Phi\rangle} = -G^{-+(0)}_{k_2 k_1}(\tau_2,\tau_1)$$

Building blocks of the diagrammatic

- Normal-ordered form of Ω with respect to Φ



- Propagators



- Main diagrammatic rules from 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: Current step

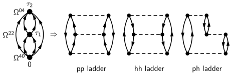
Diagonal implementation

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

$\langle \Psi | \Phi \rangle$

Manual derivation of order 3

Check against MBPT limit



Automatic derivation

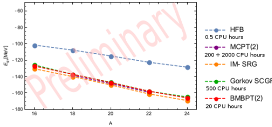
[PA, Duguet, Tichai, Lasseri, Ebran, in prep.]

Ab initio

Realist H

High order

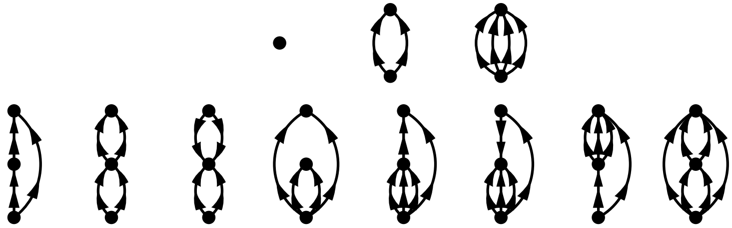
Numerical implementation



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

Status of manual derivation and implementation

- All diagrams derived and numerically implemented up to order 3



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

Develop automatic tool

- ◇ To generate all possible connected diagrams at order n
- ◇ To extract associated time-integrated expressions

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

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?
- See poster for details on the implementation

Automated expression derivation

All BMBPT diagrams produced automatically at a given order

➥ Need to derive automatically the diagrams' expressions

- BMBPT uses Feynman diagrams recasting different time-orderings
  - ✗ But time-integrated (Goldstone) expressions are to be coded
- Challenge: Extract Goldstone expressions from Feynman diagrams
  - ◇ Undone task to our knowledge (even for standard diagrammatic)

How did we do it?

See on poster!

The BMBPT project: First numerical results

Diagonal implementation

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

$\langle \Psi | \Phi \rangle$

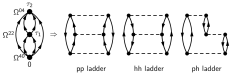
Ab initio

Realist H

High order

Manual derivation of order 3

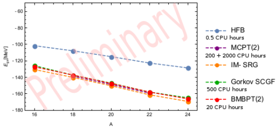
Check against MBPT limit



Automatic derivation

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

Numerical implementation



See A. Tichai's talk on Friday!

See you on Thursday!

Other BMBPT-related projects

Automated diagram generator

CEA: P. Arthuis, T. Duguet, J.-P. Ebran, A. Tichai

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