High-Order Many-Body Bogoliubov Perturbation Theory

Mikael FROSINI
CEA/DPhN, Saclay, France

Colloque GANIL
09/12/2019

P. Demol, M. Frosini, A. Tichai, J. Ripoche, V. Somà, T. Duguet
2019 in preparation
Introduction

Formalism

- Wave-functions and observables

Applications

- Resummed observables
  - A posteriori corrections

Conclusions
**Ab initio nuclear chart**

- **Approximate methods for doubly closed-shells**
  - Since 2000’s
  - MBPT, SCGF, CC, IMSRG
  - Polynomial scaling

- **Approximate methods for singly open-shell**
  - Since 2010’s
  - BMBPT, GGF, BCC, MR-IMSRG, MCPT
  - Polynomial scaling

- **Hybrid methods (ab initio shell model)**
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- **“Exact” methods**
  - Since 1980’s
  - Monte Carlo, CI, FY...
  - Factorial scaling
Single-reference expansion many-body methods

**Many-body problem**

\[ H |\Psi^A_k \rangle = E^A_k |\Psi^A_k \rangle \]

**U(1) Symmetry**

\[ [H, A] = 0 \]

A-Body Hamiltonian

\[ H = T + V^{2N} + V^{3N} + \ldots + V^{AN} \]

A-Body wave-function

5 variables, A nucleons
Single-reference expansion many-body methods

**Many-body problem**

\[ H |\Psi_k^A\rangle = E_k^A |\Psi_k^A\rangle \]

- A-Body Hamiltonian: \( H = T + V^{2N} + V^{3N} + \cdots + V^{AN} \)
- A-Body wave-function: 5 variables, A nucleons

**U(1) Symmetry**

\[ [H, A] = 0 \]

**Symmetry conserving expansion**

\[ H = H_0 + H_1 \] such that
\[ [H_0, A] = 0 \]
\[ [H_1, A] = 0 \]

**Full** \(|\Psi_n^A\rangle\) as perturbed eigenstate.

**Closed-shell**

**Open-shell**

**Non-degenerate**

**Degenerate**

Good starting point  Improper starting point
Single-reference expansion many-body methods

Many-body problem
\[ H \Psi_k^A = E_k^A \Psi_k^A \]

A-Body Hamiltonian
\[ H = T + V^{2N} + V^{3N} + \cdots + V^{AN} \]

A-Body wave-function
5 variables, A nucleons

\[ [H, A] = 0 \]

U(1) Symmetry

Symmetry conserving expansion
\[ H = H_0 + H_1 \quad \text{such that} \quad [H_0, A] = 0, \quad [H_1, A] = 0 \]

Closed-shell
Open-shell

Full \( \Psi^A_n \) as perturbed eigenstate.

Symmetry breaking expansion
\[ H = H'_0 + H'_1 \quad \text{such that} \quad [H'_0, A] \neq 0, \quad [H'_1, A] \neq 0 \]

Open-shell

- Static / dynamical correlations
- Polynomial cost at given order
- Truncated expansions break symmetry

Non-degenerate
Degenerate
Non-degenerate

Good starting point
Improper starting point
Proper starting point
Particle number corrections in BMBPT

\[ E_{gs} \text{ [MeV]} \]

HFB
2\textsuperscript{nd} order
3\textsuperscript{rd} order
High order constrained BMBPT

Constrained BMBPT
- Constrain average A at each order P.
- Convergence?

Workaround
- Numerically costly.
- A posteriori correction.

Toward high orders
- Series behavior? => resummation
- Particle number asymptotic restoration?
- Check low orders

Order P constraint

$|\Psi_0^{[P]}\rangle \xrightarrow{\text{BMBPT}(P)} A^{[P]}_0, E^{[P]}_0$

Observables

$A^{[P]}_0 = A_{\text{target}}? \xrightarrow{\text{no}} \text{HFB}$

Result

$\Omega_P, \Omega_{0,P}, \Omega_{1,P}$

Intrinsically iterative

Particle number adjusted at each working order P.

Truncation

$H^1$
$e_{\text{max}} 2, 4, 6$
$H^N$
$SD(T)(Q)$

Building CI Matrix.

Toy Model / Proof of principle

Realistic interaction

Far from model space convergence

CI truncation contamination at high order

More informations than standard MBPT
Contents

● Introduction

● Formalism
  ○ Wave-functions and observables

● Applications
  ○ Resummed observables
  ○ \textit{A posteriori} corrections

● Conclusions
Time independent (un)constrained BMBPT

\[ \{a, a^\dagger\} \rightarrow \{\beta, \beta^\dagger\} \]

\[ |\Phi_P^{k_1 k_2 \cdots}\rangle \equiv \beta_{k_1}^\dagger \beta_{k_2}^\dagger \cdots |\Phi_P\rangle \]

\[ H \rightarrow \Omega_P \equiv H - \lambda_P A \]

\[ \Omega_P \equiv \Omega_{0,P} + \Omega_{1,P} \]

\[ \Omega_P(x) \equiv \Omega_{0,P} + x\Omega_{1,P} \]

\[ x \in [0, 1] \]

\[ \Omega_P(x)|\Psi_{n,P}(x)\rangle = \tilde{E}_{n,P}(x)|\Psi_{n,P}(x)\rangle \]
Time independent (un)constrained BMBPT

\[ \{a, a^\dagger\} \rightarrow \{\beta, \beta^\dagger\} \]

\[ |\Phi_P^{k_1 k_2 \cdots} \rangle \equiv \beta_{k_1}^\dagger \beta_{k_2}^\dagger \cdots |\Phi_P \rangle \]

\[ H \rightarrow \Omega_P \equiv H - \lambda_P A \]

\[ \Omega_P \equiv \Omega_{0,P} + \Omega_{1,P} \]

\[ \Omega_P(x) \equiv \Omega_{0,P} + x\Omega_{1,P} \quad x \in [0, 1] \]

\[ \langle \Phi_n | \Phi_n^{(p)} \rangle \equiv \delta_{np} \]

\[ \tilde{\mathcal{E}}_{n,P}^{(p)} = \langle \Phi_{n,P}^{(0)} | \Omega_{1,P} | \Phi_{n,P}^{(p-1)} \rangle \]

\[ |\Phi_{n,P}^{(p)} \rangle = \left( \Omega_P^{00} + \sum_{k \in n} E_k - \Omega_{0,P} \right)^{-1} \left[ \Omega_{1,P} |\Phi_{n,P}^{(p-1)} \rangle - \sum_{1 \leq j \leq p} \tilde{\mathcal{E}}_{n,P}^{(j)} |\Phi_{n,P}^{(p-j)} \rangle \right] \]
Contents

- Introduction
- Formalism
  - Wave-functions and observables
- Applications
  - Resummed observables
  - A posteriori corrections
- Conclusions
First results of unconstrained BMBPT

\[ E(\text{MeV}) \]

\[ \varepsilon(\text{MeV}) \]

Perturbative order \( P \)

\[ A \]

\[ \rho^2_A \]

Perturbative order \( P \)
Constrained BMBPT Taylor series

\[ E(\text{MeV}) \]

\[ \rho_A^2 \]

\[ A \]

\[ \text{Perturbative order } P \]
But series are diverging...
Analytic continuation


\[ |\Psi(c)\rangle = \sum_n \frac{c^n}{n!} |\Psi^{(n)}(0)\rangle \]

\[ |\Psi(x)\rangle = \sum_m \frac{(x-c)^m}{m!} |\Psi^{(m)}(x)\rangle \]

\[ |\Psi(x)\rangle = \sum_{nm} \frac{(x-c)^m c^n}{n!m!} |\Psi^{(m+n)}(0)\rangle \]
Eigen-vector continuation


\(|\Psi^{[P]}_n(x)\rangle\) visits a small space and is converging for small \(x\)

\[0 < x_0 < \cdots < x_P \ll 1\]

**Extrapolate** \(|\Psi^{[P]}_n\rangle\) by diagonalizing \(\Omega\) on \(|\Psi^{[P]}_n(x_0)\rangle, \cdots, |\Psi^{[P]}_n(x_P)\rangle\) or equivalently on \(|\Phi^{(0)}_n\rangle, \cdots, |\Phi^{(P)}_n\rangle\)

\[\Omega_{i,j,P} \equiv \langle \Phi^{(i)}_{n,P} | \Omega | \Phi^{(j)}_{n,P} \rangle\]

\[N_{i,j,P} \equiv \langle \Phi^{(i)}_{n,P} | \Phi^{(j)}_{n,P} \rangle.\]

**Generalized Eigenvalue Problem**

\[\Omega X = \lambda NX.\]

**Ground state**

\[|\tilde{\Psi}^{[P]}_{0,P,EC}(x)\rangle \equiv \text{argmin}_{\Psi} \frac{\langle \Psi | \Omega_{P} | \Psi \rangle}{\langle \Psi | \Psi \rangle}\]

P-order approx. of \(\Omega\) ground state connected to \(|\Phi_0\rangle\)

**Observables**

\[|O^{[P]}_{n,P,EC}\rangle \equiv \frac{\langle \Phi_n | O | \Psi^{[P]}_{n,P,EC} \rangle}{\langle \Phi_n | \Psi^{[P]}_{n,P,EC} \rangle}\]

**Remarks**

- No need of computing the vectors explicitly
- Increases complexity
- Valid also at low orders
- Variational: improves at each iteration
Resummed observables in unconstrained BMBPT

Still wrong particle number even in the limit...
Constrained BMBPT
**A posteriori correction**

**Goal**: Correct for the discrepancy in average neutron / proton number without constraining at order $P > 0$

\[
E_0^{[P]} \bigg|_{A_0} = \mathcal{E}_0^{[P]} + \lambda A_0. \\
E_0^{[P]} \bigg|_{A_0 + \delta A} \approx E_0^{[P]} \bigg|_{A_0} + \lambda \delta A
\]

\[
\tilde{E}_0^{[P]} \bigg|_A \equiv E_0^{[P]} \bigg|_{A^{[P]}} + \lambda \left( A - A^{[P]} \right) = \mathcal{E}_0^{[P]} \bigg|_{A^{[P]}} + \lambda A
\]

- No additional work (only one vacuum).
- Valid for small corrections.
- Apply to all computation methods of observables.
- Already used at order 3 in realistic calculations.
Comparison with constrained BMBPT
Contents

- Introduction
- Formalism
  - Wave-functions and observables
- Applications
  - Resummed observables
  - A posteriori corrections
- Conclusions
Conclusion

**Accurate results at low order**
- Standard projective approach accurate (divergence at high order).
- Significant contamination to A appear early.

**A posteriori corrections**
- Accurate workaround to constrained BMBPT.
- No additional cost.

**Resummation techniques**
- Pade does not help at low order.
- Eigenvector continuation: promising result.
- What about computational cost?
- Increases convergence rate.

**Particle number restoration**
- Need commutation between A and H...
- ... seem to appear at larger configuration space.
- SDT(Q)(P): higher order in PT with full operator.
- Underlines the need for projection techniques.
Thanks for your attention

- Pepijn Demol
- Julien Ripoche
- Alexander Tichai
- Thomas Duguet
- Vittorio Somà
Resummation of projective observables using Pade approximants

\[ O_{n,P}^{[P]}(x) = \sum_{p=0}^{P} x^p \langle \Phi_{n,P}^{(0)} | O | \Phi_{n,P}^{(p)} \rangle \]

How to deal with divergent partial sums at \( x=1 \)?

\[ O(x) = \sum o_i x^i \]

\[ O^{[M/N]}(x) = \frac{\sum_{i=1}^{M} a_i x^i}{1 + \sum_{i=1}^{N} b_i x^i} \]

so that

\[ \frac{d^k O^{[M/N]}(x)}{dx^k} \bigg|_{x=0} = \frac{d^k O(x)}{dx^k} \bigg|_{x=0} \quad \forall \ 0 \leq k \leq M + N. \]

Unconstrained: resummation of the projective truncated series.

Constrained: resummation of the partial sum at each order.

Remarks:

- Captures poles in the complex plane.
- Efficient at high order only: instabilities.
- No extra work: post-treatment only.
Importance truncation


P=2