Symmetry-Broken Many-Body Perturbation Theory

Progress in Ab Initio Techniques in Nuclear Physics
TRIUMF

with P. Arthuis, T. Duguet, J.-P. Ebran, H. Hergert and R. Roth

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Overview

- Current status of single-reference theory
- General aspects of symmetry breaking
- Bogoliubov many-body perturbation theory
  - Formal developments
  - Implementation
- Results
- Conclusion
Motivation

- **goal**: ab initio treatment for *degenerate medium-mass* Fermi systems

\[ H | \psi \rangle = E | \psi \rangle \]

- diversity of successful approaches
  - ‘exact’ approaches
    - GFMC, (IT-)NCSM, ...
  - equation-of-motion approaches
    - EOM-CC, EOM-IMSRG, ...
  - valence-space approaches
    - CCEI, IMSRG, MBPT, ...
  - multi-determinantal approaches
    - MR-IMSRG, IM-NCSM, NCSM-PT, ...

- complementary ansatz: symmetry-broken reference states
  \[ \Rightarrow \text{derive symmetry-broken correlation expansion} \]

- grasp **non-dynamical correlation** at single-reference level
  - applicable to arbitrary mass-numbers
  - symmetry must be restored eventually

- **symmetry-broken techniques** proved great power
  - Gorkov self-consistent Green’s function
  - Bogoliubov coupled cluster (realistic calculations yet awaiting)
  - Generalized truncated configuration interaction *(poster of J. Ripoche)*
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- **Novel approach**: Combine symmetry breaking with perturbation theory: **Bogoliubov MBPT**
Single-Reference Many-Body Theory

Mean field

Closed shell conserved sym.
HF

Break $U(1)$

Open shell broken sym.
HFB

Perturbation theory

MBPT

Non-perturbative methods

Dyson SCGF

CC

IMSRG

Gorkov SCGF

BCC

PNB-IMSRG

Sym.-res. BMBPT

Sym.-res. BCC

Sym.-res. GSCGF

MR-IMSRG

Open shell conserved sym.
Projected HFB

Restore $U(1)$
formal foundation of the framework already available

'Symmetry broken and restored coupled-cluster theory: II. global gauge symmetry and particle number'
T. Duguet, A. Signoracci, JPG 44 049601 (2016)

inspired similar development in quantum chemistry

'Projected coupled cluster theory'
Y. Qiu, T. Henderson, J. Zhao, G. Scuseria, JCP 147, 064111 (2017)

reference state breaks symmetry of the underlying Hamiltonian

\[ U(1) : \quad \text{global gauge symmetry} \quad \iff \quad \text{pairing correlations} \]
\[ SU(2) : \quad \text{angular-momentum symmetry} \quad \iff \quad \text{quadrupolar correlations} \]

replace Hamiltonian by grand potential \( \Omega = H - \lambda A \)
natural setting uses quasi-particle formulation

\[ \beta_k = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p \]
\[ \beta_k = \sum_p U_{pk}^* c_p^\dagger + V_{pk}^* c_p \]
particle-number-broken vacuum of HFB type: \( \{ U_k, V_k, E_k > 0 \} \)
BMBPT(n) reduces to HF-MBPT(n) for closed-shell nuclei
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\[
\begin{align*}
\beta^\dagger_k &= \sum_p U_{pk} c^\dagger_p + V_{pk} c_p \\
\beta_k &= \sum_p U^*_{pk} c_p + V^*_{pk} c^\dagger_p
\end{align*}
\]

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BMBPT – Time-Dependent Formalism

- Central quantity: **imaginary-time evolution operator**

\[ U(\tau) = e^{-\tau \Omega} \]

- Definition of partitioning \( \Omega = \Omega_0 + \Omega_1 \) fixes the unperturbed system

- Derive perturbation expansion for \( U(\tau) \)

\[ U(\tau) = \exp(-\tau \Omega_0) T \exp(-\int_0^\tau dt \Omega_1(t)) \]

- Introduction of unperturbed propagators

\[ G^0 = \begin{pmatrix} G^{+-}(0) & G^{--}(0) \\ G^{++}(0) & G^{+-}(0) \end{pmatrix}, \quad G^{+-}(0)(\tau_1, \tau_2) = \frac{\langle \Phi | T [\beta_{k_1}^\dagger(\tau_1) \beta_{k_2}(\tau_2)] | \Phi \rangle}{\langle \Phi | \Phi \rangle} \]

- Ground-state observables obtained by expanding operator kernels

\[ O = \lim_{\tau \to \infty} \langle \Phi | e^{-\tau \Omega_0} T e^{-\int_0^\tau dt \Omega_1(t)} O | \Phi \rangle \]

- Diagrammatic framework can be developed to support Wick evaluation
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diagrammatic framework can be developed to support **Wick evaluation**
tools for **automatic derivation of diagrams** (poster of P. Arthuis)
- results available to arbitrary orders
- inclusion of non-canonical diagrams
- full inclusion of three-body interaction

⇒ **public code available in near future**


derivation of **generalized m.e. scheme** for quasiparticle operators
- treat all $\Omega^{ij}$ components on same footing

‘*Ab initio* Bogoliubov coupled cluster theory for open-shell nuclei’

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- **angular-momentum coupling** w.r.t. extended scheme
computation of all normal-ordered $\Omega_{ij}$ components in \textit{spherical scheme}

$\Rightarrow$ basic ingredient of every $U(1)$-broken theory

second-order energy correction:

$$E^{(2)} = -\frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega_{k_1 k_2 k_3 k_4}^{40} \Omega_{k_1 k_2 k_3 k_4}^{04}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}$$

scaling increases significantly ($\approx 10.000$ for $^{16}$O):

HF-MBPT(2)$\sim n_p^2 n_h^2$ vs. BMBPT(2) $\sim N^4$

all diagrams up to third order implemented in \textit{J-coupled code}

implementation of all \textit{non-canonical diagrams}

$\Rightarrow$ test of Thouless theorem

consistent inclusion of three-body physics via NO2B approximation

fourth-order diagrams to be implemented soon
BMBPT – Status of Implementation

- computation of all normal-ordered $\Omega^{ij}$ components in **spherical scheme**
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Alexander Tichai – ESNT – March 02, 2018 – 7
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Hamiltonian

- use well-tested Hamiltonian from **chiral effective field theory**
  - NN @ N³LO with \( \Lambda_{2N} = 500 \) MeV
  - 3N @ N²LO with \( \Lambda_{3N} = 400 \) MeV

- additional **SRG transformation** for improving model-space convergence

- **soft interaction**: well suited for MBPT
  - HF-MBPT: A. Tichai, Langhammer, Binder, Roth PLB 756,10,283
  - NCSM-PT: A. Tichai, Gebrerufael, Vobig, Roth in prep.

- 3B physics via **NO2B approximation**

\[
V_{pqrs}^{2N} + \sum_{tu} V_{pqstu}^{3N} \rho_{tu} + \sum_{tu} V_{pqstu}^{3N} K_{tu}
\]

- auxiliary-state NO2B
- symmetry-breaking term

- Hamiltonian conserves particle number

\[
[H^{\text{NO2B}}, A] = 0
\]
Particle-Number Corrections

- monitoring the symmetry breaking of the **correlated state**
  - corrections to the particle-number expectation value
  - evaluation of particle-number variance

- **canonical HFB**: corrections to PN appear beyond second-order BMBPT

![Diagram with nodes and arrows representing the flow of calculations from initial HFB, through constrained HFB, normal ordering, BMBPT, to PN adjustment.](image-url)
Oxygen – Ground-State Energies

- $E_0$ [MeV]
- $E_{\text{corr}}$ [MeV]

$E^{(3)}$ is one order of magnitude smaller than $E^{(2)}$

- computational resources independent of system size
- error estimate on third-order correction: $\Delta E = \Delta A^{(3)} \cdot 8 \text{ MeV} / A \approx 5 \text{ MeV}$
- calculations of Ca, Ni and Sn chains coming soon

CPU workload:
10-20 CPU hours

consistent with different **non-perturbative** ab initio approaches

**comparable accuracy within 1-5 % of computing time**

**computational scaling is independent of system size**
very good agreement with state-of-the-art approaches
reproduction of experimentally observed shell gaps
particle-number breaking has little effect overall (already seen with GSCGF)
particle-number restoration could impact near magic number
Summary

- perturbation series is **rapidly convergent**
  
  ⇒ **use MBPT to solve many-body problem**

- open-shell many-body approaches require **more general reference states**
  - No-core shell model
  - Hartree-Fock-Bogoliubov
  - Generator-coordinate method
  - ...

- BMBPT provides promising alternative to state-of-the-art approaches
  
  ⇒ **open-shell nuclei from single-reference treatment**

- **excellent agreement** with competing many-body techniques
- algorithmically simple and computationally **very inexpensive**
- quasiparticle formulation enables treatment of **arbitrary mass numbers**
Outlook

**Symmetry-broken many-body perturbation theory ...**

- perform **survey calculations** and study systematics
- consider **higher orders** and other observables in BMBPT
  \[\Rightarrow\text{ automated diagram and code generation}\]
- implement iterative scheme for **particle-number adjustment**
- extension to other symmetries
- derivation of **EOM framework** for odd systems and excitation spectra

**... and beyond**

- **restoration** of broken symmetry
- account of **residual three-body interaction**
- investigate **non-perturbative** approaches
  \[\Rightarrow\text{ Bogoliubov coupled cluster}\]
Epilog

■ Thanks to my group
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    CEA DAM DIF, Arpajon, France
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    Michigan State University, USA
  • R. Roth
    Technische Universität Darmstadt, Germany