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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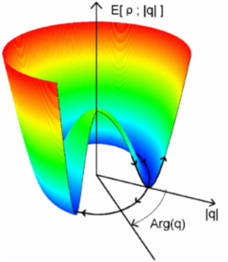
CEA - Saclay

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**

$\Rightarrow$ **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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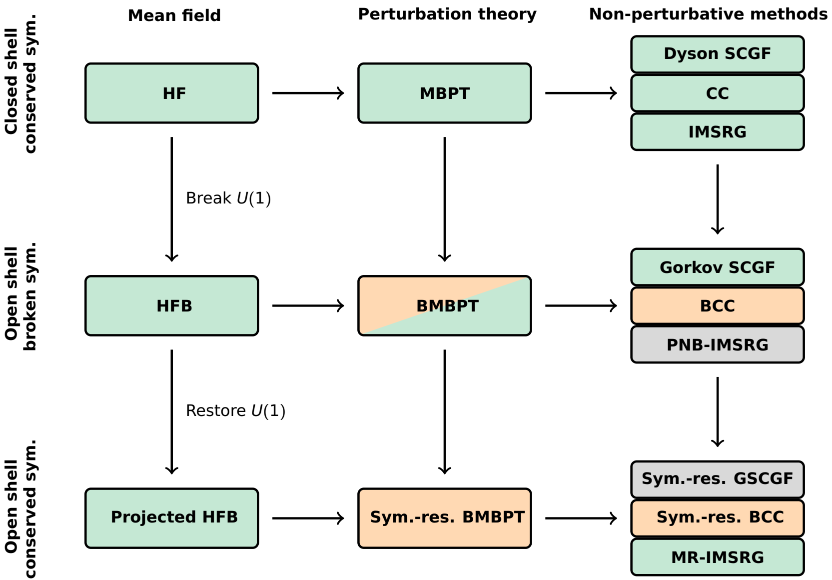
Novel approach:
Combine symmetry breaking
with perturbation theory:
Bogoliubov MBPT

Single-Reference Many-Body Theory



BMBPT – Basic Principles

- 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

$U(1)$: **global gauge symmetry** $\Leftrightarrow$ **pairing correlations**
$SU(2)$: angular-momentum symmetry $\Leftrightarrow$ quadrupolar correlations

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

$$\beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p \qquad \beta_k = \sum_p U_{pk}^\star c_p + V_{pk}^\star c_p^\dagger$$

- 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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BMBPT – Time-Dependent Formalism

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

$$\mathcal{U}(\tau) = e^{-\tau\Omega}$$

- definition of **partitioning** $\Omega = \Omega_0 + \Omega_1$ fixes the unperturbed system
- derive perturbation expansion for $\mathcal{U}(\tau)$

$$\mathcal{U}(\tau) = \exp(-\tau\Omega_0) T \exp(-\int_0^\tau dt\, \Omega_1(t))$$

- introduction of **unperturbed propagators**

$$\mathbf{G}^0 = \begin{pmatrix} G^{+-(0)} & G^{--(0)} \\ G^{++(0)} & G^{-+(0)} \end{pmatrix}, \qquad G^{+-(0)}_{k_1k_2}(\tau_1,\tau_2) = \frac{\langle\Phi|\mathrm{T}[\beta^\dagger_{k_1}(\tau_1)\beta_{k_2}(\tau_2)]|\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

- ground-state observables obtained by expanding **operator kernels**

$$O = \lim_{\tau\to\infty} \langle\Phi|e^{-\tau\Omega_0}\, \mathrm{T} e^{-\int_0^\tau \mathrm{d}t\Omega_1(t)} O|\Phi\rangle$$

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- 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

$\Rightarrow$ **public code available in near future**

P. Arthuis, T. Duguet, A. Tichai, R.-D. Lasseri, J.-P. Ebran, in prep. (2018)

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

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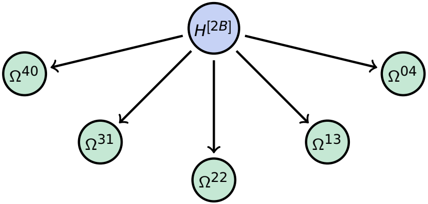
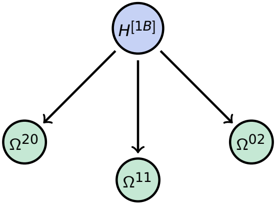




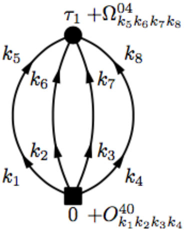
BMBPT – Status of Implementation

- computation of all normal-ordered Ω^{ij} components in **spherical scheme**

  ⇒ **basic ingredient of every $U(1)$-broken theory**

- second-order energy correction:

$$E^{(2)} = -\frac{1}{4!}\sum_{k_1k_2k_3k_4}\frac{\Omega^{40}_{k_1k_2k_3k_4}\,\Omega^{04}_{k_1k_2k_3k_4}}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$



- 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 **J-coupled code**
- implementation of all **non-canonical diagrams**

  ⇒ **test of Thouless theorem**

- consistent inclusion of three-body physics via NO2B approximation
- **fourth-order diagrams** to be implemented soon

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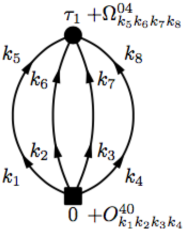

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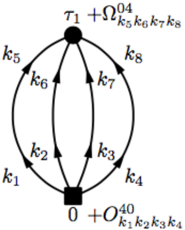

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Hamiltonian

- use well-tested Hamiltonian from **chiral effective field theory**
  - NN @ N^3LO with $\Lambda_{2N} = 500\,\text{MeV}$
  - 3N @ N^2LO with $\Lambda_{3N} = 400\,\text{MeV}$
- additional **SRG transformation** for improving model-space convergence
- **soft interaction**: well suited for MBPT

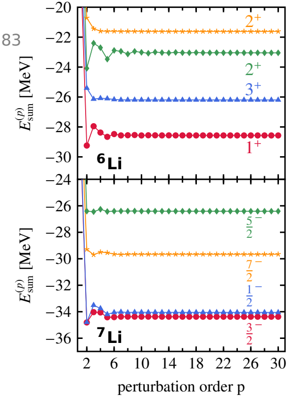
  HF-MBPT: A. Tichai, Langhammer, Binder, Roth PLB 756,10,283

  NCSM-PT: A. Tichai, Gebrerufael, Vobig, Roth in prep.
- 3B physics via **NO2B approximation**

$$\underbrace{V^{2N}_{pqrs} + \sum_{tu} V^{3N}_{pqtsu}\rho_{ut}}_{\text{auxiliary-state NO2B}} + \underbrace{\cancel{\sum_{tu} V^{3N}_{pqrstu}\kappa_{tu}}}_{\text{symmetry-breaking term}}$$

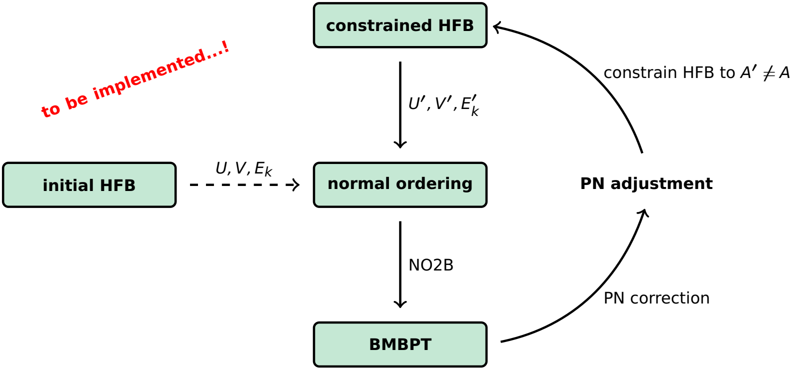
- Hamiltonian conserves particle number

$$[H^{\text{NO2B}}, A] = 0$$

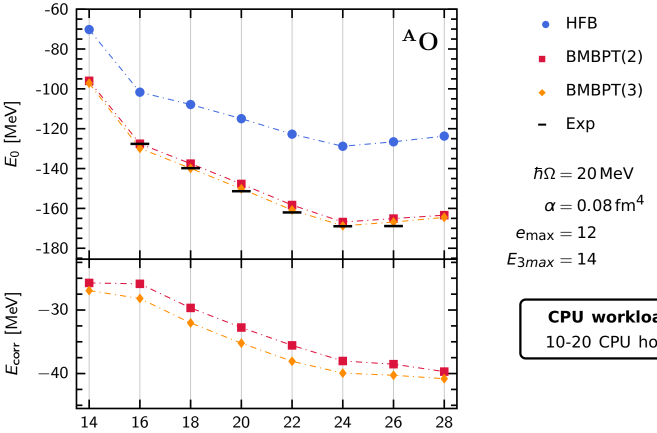


Particle-Number Corrections

- 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



Oxygen – Ground-State Energies



$\hbar\Omega = 20\,\text{MeV}$

$\alpha = 0.08\,\text{fm}^4$

$e_{\text{max}} = 12$

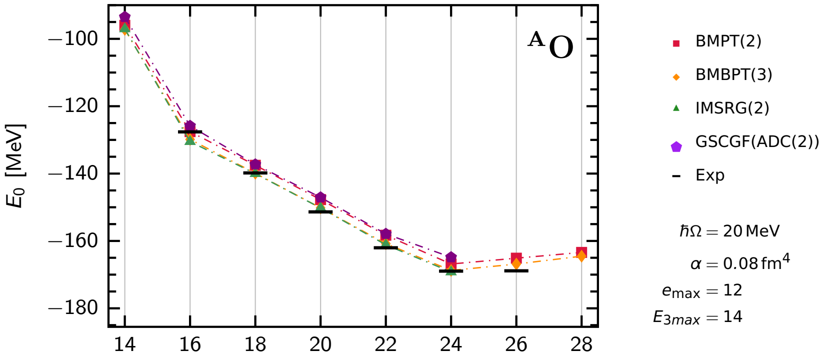
$E_{3max} = 14$

CPU workload:
10-20 CPU hours

P. Arthuis, A. Tichai, H. Hergert, R. Roth, T. Duguet, (2018), in prep.

- $E^{(3)}$ is one order of magnitude smaller than $E^{(2)}$
- computational resources **independent of system size**
- **error estimate** on third-order correction: $\Delta E = \Delta A^{(3)} \cdot 8\,\text{MeV}/A \approx 5$ MeV
- calculations of **Ca, Ni and Sn chains** coming soon

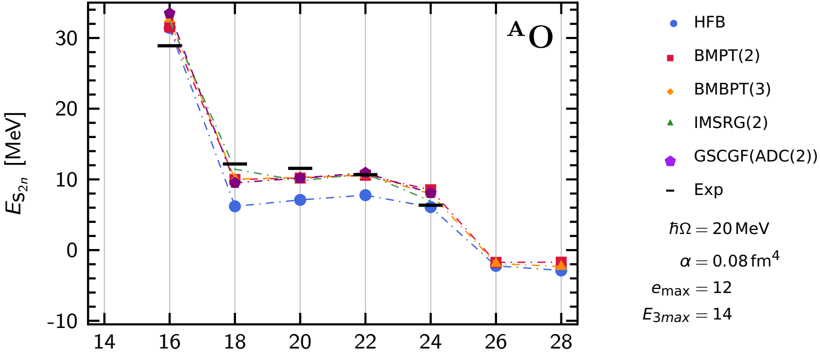
Oxygen – Comparison with other Methods



P. Arthuis, A. Tichai, H. Hergert, R. Roth, T. Duguet, (2018), in prep.

- consistent with different **non-perturbative** ab initio approaches
- comparable accuracy within **1-5 % of computing time**
- computational scaling is **independent of system size**

Oxygen – Two-Neutron Separation Energies



P. Arthuis, A.Tichai, H. Hergert, R. Roth, T. Duguet, (2018), in prep.

- **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

$\Rightarrow$ **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

$\Rightarrow$ **Bogoliubov coupled cluster**

Epilog

- **Thanks to my group**
  - P. Arthuis, M. Drissi, T. Duguet, V. Somà
    CEA, Saclay, France
- **Thanks to our collaborators**
  - J.-P. Ebran, J. Ripoche
    CEA DAM DIF, Arpajon, France
  - H. Hergert
    Michigan State University, USA
  - R. Roth
    Technische Universität Darmstadt, Germany

COMPUTING TIME