Bogoliubov Many-Body Perturbation Theory for Open-Shell Nuclei

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Nuclear theory for nuclear experiments
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Outline

- On *ab initio* methods

- Why a symmetry-breaking perturbation theory?

- Bogoliubov Many-Body Perturbation Theory
  - Diagrammatic BMBPT formalism
  - First applications to ground-state energies of $^{A}$O, $^{A}$Ca, $^{A}$Ni

- Conclusion and perspectives
• **Introduction on *ab initio* methods**

• Why a symmetry-breaking perturbation theory?

• **Bogoliubov Many-Body Perturbation Theory**
  - Diagrammatic BMBPT formalism
  - First applications to ground-state energies of $^4$O, $^4$Ca, $^5$Ni

• **Conclusion and perspectives**
The nucleus as a problem

Diversity of phenomena

- Ground-state properties (mass, ...)
- Excited states properties (vibrational bands, ...)
- Decay modes (strong, EW)
- Reaction properties (scattering, fusion...)

A complex interaction

- Emerging from QCD
- Non-perturbative character
- Three-, four-, etc., forces to be included

Complex many-body problem

- Mesoscopic system
- Importance of finite-size effects
- Various excitation modes at similar energy

[B. Bally, private communication (2018)]
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Nuclear theory as a problem

Quantum many-body methods

• SM, EDFs not systematically improvable
• Ab initio limited by factorial/exponential scaling

Breakthrough in the past 15 years
• Ab initio expansion methods scaling polynomially
• Hamiltonian modeling from chiral EFT
• Preprocessing of the Hamiltonian
• Novel / hybrid approaches developed

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[B. Bally, private communication (2018)]
"Exact" ab initio methods

- Since the 80’s
- GFMC, NCSM, FY

Courtesy of V. Soma, T. Duguet
Ab initio methods

Access to closed-shell nuclei

- Since the 2000's
- DSCGF, CC, IMSRG

Courtesy of V. Soma, T. Duguet
Access to open-shell nuclei

- Since the 2010's
- GSCGF, BCC, MR-IMSRG

Courtesy of V. Soma, T. Duguet
Ab initio methods

Ab initio shell model

- Since 2014
- Effective interaction via CC, IMSRG, NCSM, MBPT
Ab initio many-body scheme

\[ H |\psi_A^k \rangle = E_k^A |\psi_A^k \rangle \]

- \( H \): A-body Hamiltonian
- \( |\psi_A^k \rangle \): A-body wave function

Definitions
- Nucleons as point-like degrees of freedom
- Active in full A-body Hilbert space
- Elementary interactions
- Solve A-body Schrödinger equation (SE)
- Thorough estimate of error

1. Modeling
2. SE
3. Data
4. Feedback

- Form of the Hamiltonian?
- Link to QCD?
- 3-body, ..., up to A-body forces?
- Accuracy of the SE solving?
- Doable for nuclei up to A \( \sim 300 \)?
- Need more effective approaches?
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- **Definitions**
  - Nucleons as point-like degrees of freedom
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- **Schrödinger equation**
  - Accuracy of the SE solving?
  - Doable for nuclei up to \( A \sim 300 \)?
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- **Modeling** → **SE** → **Data**
  - \( H \)
  - \( E^A_k, J, B(E\lambda) \... \)
  - Feedback
Hamiltonians for \textit{ab initio} methods

Chiral EFT Hamiltonians: A link to QCD [EM, ..]

- $H$ from chiral Effective Field Theory
  - Link to QCD through its symmetries
  - Natural hierarchy of terms (inc. 3-, 4NF, ...)
  - Systematically improvable

- $N$-body force fitted to $N$-body sector

- Game changer but overbinds for $A \gtrsim 20$

[Lapoux et al., 2016]
Hamiltonians for *ab initio* methods

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### Departure from strict *ab initio* approach [NNLOsat, ...]
- Attempt at better reproducing experimental data
- Keep chiral EFT approach
- Fit not only in $N$-body sector for $N$-body force
- Good reproduction of Ca isotopes, radii...
Ab initio and observables

Even-even binding energies

- Diff. methods, consistent results
- Reproduction of drip-line
**Ab initio and observables**

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**Neighbouring nuclei**

- Specificity of SCGF
- Nice and consistent results
**Ab initio and observables**

### Even-even binding energies

- **Diff. methods, consistent results**
- **Reproduction of drip-line**

![Even-even binding energies graph]

**Neighbouring nuclei**

- **Specificity of SCGF**
- **Nice and consistent results**

![Neighbouring nuclei graph]

### Excitation spectra

- **Hybrid shell-model IM-SRG**
- **Closer to experiment than SM**

![Excitation spectra graph]
Ab initio and observables

Even-even binding energies
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Neighbouring nuclei
- Specificity of SCGF
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Excitation spectra
- Hybrid shell-model IM-SRG
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Charge and nucleon radii
- Use of NNLOsat for experimental accuracy
- Pre- & post-diction of exp. properties
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"Exact" methods (80's)
- GFMC, NCSM, FY

Closed-shell methods (00's)
- DSCGF, CC, IMSRG

Open-shell methods (10's)
- GSCGF, BCC, MR-IMSRG

Ab initio shell model (2014)
- EL via CC, IMSRG, NCSM...

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**Ab initio** shell model (2014)
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- Closed-shell MBPT shown to compete with non-perturbative methods [Tichai *et al.* 2016]

Access open-shell nuclei through SR perturbative expansion method?
- Precise enough at (relatively) low order
- Low computational cost

Courtesy of V. Soma, T. Duguet
SR expansion methods vs \((U(1))\) symmetry

Operators of interest

- Nuclear Hamiltonian: \(H = T + V + W\)
- Particle number operator: \(A\)
- Grand potential: \(\Omega = H - \lambda A\)

A-body eigenvalue problem

\[
H|\psi_k^{A}\rangle = E_k^{A}|\psi_k^{A}\rangle
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**Particle number conserving**

- Split \(H: H = H_0 + H_1\)
- \([A, H_0] = 0\)
- Introduce reference state
  \[
  |\psi_0^A\rangle = U^A(\infty)|\Phi^A\rangle
  \]
- Wave operator to be expanded
- Reference state solution of the SE
  \[
  H_0|\Phi^A\rangle = E_0^A|\Phi^A\rangle
  \]
- Symmetry-conserving method
  - Slater determinant reference state
Expansion methods and degenerate systems

- Basic idea: collect dynamical correlations through ph excitations
- Open-shell nuclei are degenerate w.r.t. ph excitations

 Expansion breakdown signals non-dynamical correlations (superfluidity, ...)

![Diagram showing closed-shell and open-shell configurations](image)
Expansion methods and degenerate systems

- Basic idea: collect dynamical correlations through ph excitations
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Expansion breakdown signals non-dynamical correlations (superfluidity, ...)

- Various possible approaches
  - High-order non-pertubative method (if near-degenerate)
  - Multi-reference/configuration method (MR-MBPT, MR-CC, MR-IMSRG, MCPT)
  - Use a symmetry-breaking reference state

Lift the degeneracy
Expansion methods and degenerate systems

- Basic idea: collect dynamical correlations through ph excitations
- Open-shell nuclei are degenerate w.r.t. ph excitations

\[ \Psi \rightarrow \Psi_{n+1} \rightarrow \Psi_{n+2} \rightarrow \cdots \]

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\[ \Psi_{\text{Degenerate Slater}} \rightarrow \Psi_{\text{Bogoliubov vacuum}} \]

Symmetries to be restored eventually
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  Wave operator to be expanded
  Reference state solution of the SE
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  \(\Rightarrow\) Slater determinant reference state

**Particle number breaking**
- Split \(\Omega\): \(\Omega = \Omega_0 + \Omega_1\)
  \([A, \Omega_0] \neq 0\)
- Introduce reference state
  \(|\psi_0^A\rangle = U(\infty) |\Phi\rangle\)
  Wave operator to be expanded
  Reference state solution of the SE
  \(\Omega_0 |\Phi\rangle = E_0 |\Phi\rangle\)
- Symmetry-breaking method
  \(\Rightarrow\) Bogoliubov reference state
The BMBPT project

Particle-number-projected BMBPT formalism

Exact diagrammatic expansion with symmetry breaking and restoration


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
• Introduction on *ab initio* methods

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• **Bogoliubov Many-Body Perturbation Theory**
  ◦ Diagrammatic BMBPT formalism
  ◦ First applications to ground-state energies of $^A\text{O}$, $^A\text{Ca}$, $^A\text{Ni}$

• Conclusion and perspectives
Bogoliubov reference state

Bogoliubov vacuum $|\Phi\rangle$: $\beta_k |\Phi\rangle = 0 \forall k$

$$\beta_k = \sum_p U^*_p c_p + V^*_p c_p^\dagger$$

$$\beta_k^\dagger = \sum_p U_p c_p^\dagger + V_p c_p$$

Particle-number breaking

$A|\Phi\rangle \neq A|\Phi\rangle$

Breaks $U(1)$ symmetry
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Grand potential $\Omega$ in qp basis, normal-ordered w.r.t. $|\Phi\rangle$

$$\Omega = \Omega^{00} + \frac{1}{1!} \sum_{k_1k_2} \Omega^{11}_{k_1k_2} \beta^\dagger_{k_1} \beta_{k_2} + \frac{1}{2!} \sum_{k_1k_2} \left\{ \Omega^{20}_{k_1k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2} + \Omega^{02}_{k_1k_2} \beta_{k_1} \beta_{k_2} \right\}$$

$$+ \frac{1}{(2!)^2} \sum_{k_1k_2k_3k_4} \Omega^{22}_{k_1k_2k_3k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta_{k_3} \beta_{k_4}$$

$$+ \frac{1}{3!} \sum_{k_1k_2k_3k_4} \left\{ \Omega^{31}_{k_1k_2k_3k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta_{k_4} + \Omega^{13}_{k_1k_2k_3k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta_{k_4} \right\}$$

$$+ \frac{1}{4!} \sum_{k_1k_2k_3k_4} \left\{ \Omega^{40}_{k_1k_2k_3k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4} + \Omega^{04}_{k_1k_2k_3k_4} \beta_{k_1} \beta_{k_2} \beta_{k_3} \beta_{k_4} \right\} + \ldots$$
Grand potential partitioning

\[ \Omega_0 = \Omega^{00} + \tilde{\Omega}^{11} = \Omega^{00} + \sum_k E_k \beta_k^\dagger \beta_k \]

\[ \Omega_1 = \tilde{\Omega}^{11} + \Omega^{20} + \Omega^{02} + \Omega^{[4]} + \Omega^{[6]} \]
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**Time-evolved state**

\[ |\psi(\tau)\rangle \equiv U(\tau)|\Phi\rangle \]

\[ = e^{-\tau \Omega_0} T e^{-\int_0^\tau d\tau \Omega_1(\tau)} |\Phi\rangle \]
Time-dependent BMBPT

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Ground state energy of an open-shell nucleus

\[ E^A_0 - \lambda A = \langle \Psi^A_0 | \Omega | \Phi \rangle_c = \lim_{\tau \to \infty} \langle \Phi | T e^{-\int_0^\tau d\tau \Omega_1(\tau)} \Omega | \Phi \rangle_c \]
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### Propagators

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

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

**Perturbative expansion of g.s. energy**
\[ E^A_0 - \lambda A = \langle \Phi | \left\{ \Omega(0) - \int_0^\infty d\tau_1 T [\Omega_1(\tau_1) \Omega(0)] \right. \]
\[ + \frac{1}{2!} \int_0^\infty d\tau_1 d\tau_2 T [\Omega_1(\tau_1) \Omega_1(\tau_2) \Omega(0)] \]
\[ + \ldots \} |\Phi\rangle_c \]
Building blocks of the diagrammatic

Normal-ordered form of $\Omega$ with respect to $|\Phi\rangle$

$$\Omega = \Omega^{00} + \Omega^{11} + \Omega^{02} + \Omega^{20} + \Omega^{13} + \Omega^{04} + \Omega^{22} + \Omega^{31} + \Omega^{40} + \ldots$$
Building blocks of the diagrammatic

Normal-ordered form of $\Omega$ with respect to $|\Phi\rangle$

$$\Omega = \Omega^{00} + \Omega^{11} + \Omega^{20} + \Omega^{02} + \Omega^{22} + \Omega^{31} + \Omega^{13} + \Omega^{40} + \Omega^{04} + \ldots$$

Diagonal propagators

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

$$(k_1 \tau_1)$$

$$(k_2 \tau_2)$$
Diagrammatic rules for observable $E_0^A - \lambda A$

Diagrams of observables from building blocks

I. Topological rules

- No external legs
- No oriented loop between vertices
- No self-contraction
- Propagators go out of the $\Omega$ vertex at time 0
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II. Algebraic rules
- Vertex, propagators labelling
- Sign factor for crossing lines
- Symmetry factor for equivalent lines, vertex exchange
- Sum over all q.p. states, integrate over all time labels
Derivation of a second-order diagram

\[ \tau_2 - \bar{\Omega}_{k_9k_{10}} \]

\[ + \Omega_{k_5k_6k_7k_8}^0 \]

\[ + \Omega_{k_1k_2k_3k_4}^4 \]

\[ 0 + \Omega_{k_1k_2k_3k_4}^{10} \]

Time-dependent and time-integrated expressions:

\[ \text{PE2.6} = -\frac{1}{3!} \sum_{k_1k_2k_3k_4k_8} \Omega_{k_1k_2k_3k_4}^4 \Omega_{k_1k_2k_3k_8}^0 \bar{\Omega}_{k_8k_4}^{11} \int_0^\infty d\tau_1 d\tau_2 \theta(\tau_1 - \tau_2) e^{-\tau_1(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_8})} e^{\tau_2(E_{k_8} - E_{k_4})} \]

\[ = -\frac{1}{3!} \sum_{k_1k_2k_3k_4k_8} \Omega_{k_1k_2k_3k_4}^4 \Omega_{k_1k_2k_3k_8}^0 \bar{\Omega}_{k_8k_4}^{11} \frac{1}{(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}) (E_{k_1} + E_{k_2} + E_{k_3} + E_{k_8})} \]

Convention

Order \( p \)

\[ \uparrow \]

Order \( p + 1 \) in standard counting
Low-order diagrams in NO2B approximation

Zeroth-order diagram

- PE0.1

First-order diagrams

- PE1.1
- PE1.2
Low-order diagrams in NO2B approximation

Zeroth-order diagram

PE0.1

First-order diagrams

PE1.1
PE1.2

Second-order diagrams

PE2.1
PE2.2
PE2.3
PE2.4
PE2.5
PE2.6
PE2.7
PE2.8

Numerical implementation

• Zeroth-, first- and second-order diagrams
• No particle number constraint at second order yet
• Chiral EFT Hamiltonian: 2NF (N3LO), 3NF (N2LO)
• SRG-evolved (\(\alpha = 0.08\) fm\(^4\))
• NO2B approximation

Basis parameters

\(\hbar \Omega = 20\) MeV
\(e_{\text{max}} = 12\)
\(E_{3\text{max}} = 14\)

Higher-order diagrams and expressions generated automatically

[PA, Duguet, Tichai, Lasseri, Ebran, 1809.01187 (accepted in CPC)]
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    [Tichai, Arthuis, Duguet, Hergert, Somà, Roth, Phys. Lett. B 786 (2018)]

- Conclusion and perspectives
Closed-shell results agree with established HF-MBPT

- $E^{(2*)}$ one order of magnitude smaller than $E^{(1)}$
  - First indication of convergence

- Reproduction of experimentally observed shell gaps
- Second-order without particle number adjustment so far
- Ni chain shows similar results
Very good agreement with non-perturbative approaches ($\leq 2\%$)
- Agree with exact results for O
- Consistent with other methods for Ca

Effects of particle-number breaking
- Little overall effect (similar to GGF)
- Particle-number restoration could impact near magic numbers
Numerical scaling

- Two orders of magnitude cheaper than non-perturbative \textit{ab initio} methods
  - Best accuracy/cost ratio
- Method of interest for large-scale \textit{ab initio} calculations
  - Test of newly developed chiral H
  - Systematic prediction/post-diction of nuclear properties
Outline

• Introduction on *ab initio* methods

• Why a symmetry-breaking perturbation theory?

• Bogoliubov Many-Body Perturbation Theory
  ◇ Diagrammatic BMBPT formalism
  ◇ First applications to ground-state energies of $^A$O, $^A$Ca, $^A$Ni

• Conclusion and perspectives
Conclusion

Rapid extension of *ab initio* methods

- Up to Ni (Sn) isotopes
- Good agreement between very different approaches
- Better Hamiltonians needed for improved accuracy

Numerical implementation of BMBPT(1) and BMBPT(2*)

- Very low-cost correlated method
- Competes with non-perturbative *ab initio* methods

BMBPT diagrams generated and evaluated automatically

- Fast and error-safe
- Open-source code available
Perspectives

Extend the scope of BMBPT

- New observables
- Excited states and transitions
- Symmetry restoration

Interplay with other developments

- Automated generation for PBMBT, GSCGF
- Shared numerical developments with BCC
- Numerical implementation

Further extension of *ab initio* methods

- Hybridation of methods
- Automated tools for new formalisms / higher order
- Need for new techniques to overcome computational limitations
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Thank you for your attention!