Ab-initio coupled-cluster method for open-shell nuclei

I. Breaking symmetries

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I. Introduction: how does this fit with the rest?

II. Breaking $U(1)$ symmetry ("trivial" for $SU(2)$) (today)

Bogoliubov coupled-cluster method


III. Restoring $SU(2)$ or $U(1)$ symmetries (next thursday)

Angular-momentum-restored coupled-cluster formalism


Particle-number-restored Bogoliubov coupled-cluster formalism

[T. Duguet, in preparation (2014)]
Part I

Introduction
Non-perturbative \textit{ab-initio} many-body theories

\textit{Ab-initio} many-body theories
- Effective structure-less nucleons
- 2N + 3N + ... inter-nucleon interactions
- Solve A-body Schrödinger equation
- Thorough assessment of errors needed

Inter-nucleon interactions
- Link to QCD – \( \chi \)EFT
  [E. Epelbaum, PPNP67, 343 (2012)]
- Soften through RG
  [S.K. Bogner et al., PPNP65, 94 (2010)]

Input

High predictive power
Limited applicability domain

1980-2014
FY, GFMC, NCSM
All nuclei A<12

2003-2014
CC, Dy-SCGF, IMSRG
Near doubly-magic nuclei A<132

Based on expansion scheme
- Systematic error
- Cross-benchmarks needed

[Carlson, Pieper, Wiringa]
[Barrett, Vary, Navratil, Ormand]
Towards *ab-initio* methods for open-shell nuclei

**First objective:** generalize many-body methods to study complete isotopic/isotonic chains
- Go from a few 10s of nuclei to several 100s of nuclei

**Nuclear structure at/far from β stability**
- Magic numbers and their evolution?
- Limits of stability beyond Z=8?
- Mechanisms for nuclear superfluidity?
- Role and validation of AN forces?

**Option 1: single-reference extensions**
- **Gorkov-SCGF**
  [V. Somà, T. Duguet, C. Barbieri, PRC 84, 064317 (2011)]
- **Bogoliubov CC**
  [A. Signoracci, T. Duguet, G. Hagen, unpublished (2014)]

**Option 2: multi-reference extensions**
- **MR-IMSRG**
  [H. Hergert et al., PRL 110, 242501 (2013)]
- **IMSRG-based valence shell model**
  [S. K. Bogner et al., arXiv:1402.1407 (2014)]
- **CC-based valence shell model**
  [G. R. Jansen et al., arXiv:1402.2563 (2014)]
Breaking and restoring symmetries

Expansion around a single reference state

\[ |\Psi_0\rangle = \Omega_0 |\Phi_0\rangle \]

A-body ground state

\[ E_0 = \frac{\langle \Phi_0 | \hat{H} | \Psi_0 \rangle}{\langle \Phi_0 | \Psi_0 \rangle} \]

Ground-state energy

Target state \[ \rightarrow \] Wave operator \[ \rightarrow \] Reference state

Expand \( \Omega_0 \) such that \( E_0 \) is size extensive

Closed shell

RHF reference

conserves \( A, J^2, M \)

\( Dy-SCGF \)

CC

Breaks down for open-shell nuclei

Singly/doubly open shell

UHF(B) reference

\( \text{breaks} \ A / J^2 \ \text{and} \ M \)

Go-SCGF

Today BCC

Contamination from other \( A / J^2 \ \text{and} \ M \)

Singly/doubly open shell

UHF(B) manyfold

restores \( A / J^2 \ \text{and} \ M \)

AMR-CC & PNR-BCC

Next Thursday

Multi-reference character

Finite inertia

\( \leftrightarrow \)

Resolve Goldstone mode

Goldstone mode

\( ph \) degeneracy

\( \leftrightarrow \)
Bogoliubov coupled-cluster formalism
for singly open-shell nuclei

Hartree-Fock-Bogoliubov reference

Nuclear Hamiltonian

\[
H = \frac{1}{(1!)^2} \sum_{pq} t_{pq} c_p^\dagger c_q + \frac{1}{(2!)^2} \sum_{pqrs} v_{pqrs} c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{(3!)^2} \sum_{pqrsu} w_{pqrsu} c_p^\dagger c_q^\dagger c_r^\dagger c_s c_t c_s
\]

Bogoliubov transformation

\[
\beta_{\alpha}^\dagger = \sum_p U_{p\alpha} c_p + V_{p\alpha} c_p
\]

\[
\beta_{\alpha} = \sum_p U^*_{p\alpha} c_p + V^*_{p\alpha} c_p^\dagger
\]

Bogoliubov vacuum

\[
|\Phi\rangle \equiv C \prod_{\alpha} \beta_{\alpha} |0\rangle
\]

\[
\beta_k |\Phi\rangle = 0 \ \forall k
\]

Density matrices

\[
\rho_{qp} = \frac{\langle \Phi | c_p^\dagger c_q | \Phi \rangle}{\langle \Phi | \Phi \rangle}
\]

\[
\kappa_{qp} = \frac{\langle \Phi | c_p c_q | \Phi \rangle}{\langle \Phi | \Phi \rangle}
\]

Grand potential

\[
\Omega \equiv H - \lambda A
\]

Minimization under constraint

\[
\delta \frac{\langle \Phi | \Omega | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0 / \langle \Phi | A | \Phi \rangle = A
\]

HFB equation

\[
\begin{pmatrix}
 h & \Delta \\
 -\Delta^* & -h^*
\end{pmatrix}
\begin{pmatrix}
 U_k \\
 V_k
\end{pmatrix}
= E_k
\begin{pmatrix}
 U_k \\
 V_k
\end{pmatrix}
\]

Quasi-particle excitations

\[
|\Phi^{\alpha \beta \cdots}\rangle \equiv \beta_{\alpha}^\dagger \beta_{\beta}^\dagger \cdots |\Phi\rangle
\]

Spectroscopic factors

\[
\bar{\delta}_{\alpha} = \sum_l |V_{l\alpha}|^2
\]

Binding energy

\[
E_0 = -\frac{1}{2} \sum_{pq} t_{pq} \rho_{qp} - \sum_{\alpha} (E_{\alpha} - \lambda) \bar{\delta}_{\alpha}
\]

\[
-\frac{1}{6} \sum_{pq} \Gamma_{pq}^3 \rho_{qp} + \Delta_{pq}^{3N} \kappa_{qp}^*
\]

* m-scheme code
* Benchmarked against J-coupled

[V. Somà et al.]
Bogoliubov CC ansatz

Wave-function ansatz

\[ |\Psi\rangle \equiv e^T |\Phi\rangle \]

Quasi-particle cluster operator

\[ T \equiv T_1 + T_2 + T_3 + \ldots \]

\[ [T_n, T_m] = 0 \]

Connected n-tuple excitation

\[ T_1 \equiv \frac{1}{2!} \sum_{k_1 k_2} t_{k_1 k_2} \beta_{k_1} \beta_{k_2}^\dagger \]

\[ T_2 \equiv \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} t_{k_1 k_2 k_3 k_4} \beta_{k_1} \beta_{k_2} \beta_{k_3} \beta_{k_4}^\dagger \]

Action of n-tuple excitation on the HFB vacuum

\[ T_1 |\Phi\rangle \rightarrow |\Phi^{\alpha \beta}\rangle \]

\[ T_2 |\Phi\rangle \rightarrow |\Phi^{\alpha \beta \gamma \delta}\rangle \]

HFB vacuum

1) Handles Cooper instability = grasps key static correlations
2) Opens gap in excitations = makes dynamic correlations safe

- CC theory in qp basis with no breaking of U(1)
  [L. Stolarczyk, H. Monkhorst, MP108, 3067 (2010)]
- BCC theory restricted to BCS and simple geometry
  [K. Emrich, J. G. Zabolitzky, PRB30, 2049 (1984)]
  [W. A. Lahoz, R. F. Bishop, ZPB73, 363 (1988)]
Normal-ordered grand potential

\[ \Omega \equiv \Omega^{[0]} + \Omega^{[2]} + \Omega^{[4]} + \Omega^{[6]} \]

\[ = \Omega^{00} + \frac{1}{1!} \sum_{k_1k_2} \Omega^{11}_{k_1k_2} \beta^{\dagger}_{k_1} \beta_{k_2} = E_{k_1} \delta_{k_1k_2} \]

+ \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_2} \beta_{k_1} \right\} = 0

Each \( \Omega^{ij}_{k_1...k_1,k_{i+1}...k_{i+j}} \) is

* fully anti-symmetric
* expressed in terms of

\[ \begin{bmatrix}
  t_{pq} \\
  v_{pqrs} \\
  w_{pqrsstu}
\end{bmatrix} \begin{bmatrix}
  U_{pk} \\
  V_{pk}
\end{bmatrix} \]

Residual interaction

NO2B approximation

Very good in closed shell (1% error)

[S. Binder et al., PRC87 (2013) 021303]
Bogoliubov CC equations

Schrödinger equation

\[ \Omega |\Psi\rangle = \Omega_0 |\Psi\rangle \]

\[ \Omega |\Phi\rangle = \Omega_0 |\Phi\rangle \]

\[ (\Omega e^\mathcal{T})c |\Phi\rangle = \Omega_0 |\Phi\rangle \]

Non-hermitian similarity-transformed grand potential

\[ \bar{\Omega} \equiv e^{-\mathcal{T}} \Omega e^\mathcal{T} \]

Baker-Campbell-Hausdorff + Wick theorem

\[ \bar{\Omega} = \sum_{n=0}^{4} (\Omega \mathcal{T}^n)_c \]

Energy equation

\[ \langle \Phi | (\Omega e^\mathcal{T})c |\Phi\rangle = \Omega_0 \]

Amplitude equation to find \( \mathcal{T}_n \)

\[ \langle \Phi^{\alpha\beta...} | (\Omega e^\mathcal{T})c |\Phi\rangle_C = 0 \]

Truncate \( \mathcal{T} \) beyond a certain \( \mathcal{T}_n \)

Retaining \( \mathcal{T}_1 \) and \( \mathcal{T}_2 \) defines BCCSD

Infinite-order method

Efficient grasp of dynamic correlations

Size extensive

Expansion naturally terminates

+ equation to constrain \( \lambda \) / \[ \frac{\langle \Psi|A|\Psi\rangle}{\langle \Psi|\Psi\rangle} = A \]

BCC with Singles and Doubles

\[ \Omega_0 = \langle \Phi|\Omega (1 + \mathcal{T}_1 + \mathcal{T}_2 + \frac{1}{2}\mathcal{T}^2_1)|\Phi\rangle_C \]

\[ 0 = \langle \Phi^{\alpha\beta} |\Omega (1 + \mathcal{T}_1 + \frac{1}{2} \mathcal{T}^2_1 + \frac{1}{3!} \mathcal{T}^3_1 + \mathcal{T}_2 + \mathcal{T}_1 \mathcal{T}_2)|\Phi\rangle_C \]

\[ 0 = \langle \Phi^{\alpha\beta\gamma\delta} |\Omega (1 + \mathcal{T}_1 + \mathcal{T}_2 + \frac{1}{2} \mathcal{T}^2_1 + \frac{1}{2} \mathcal{T}^2_2 + \mathcal{T}_1 \mathcal{T}_2 + \frac{1}{3!} \mathcal{T}^3_1 + \frac{1}{4!} \mathcal{T}^4_1 + \frac{1}{2} \mathcal{T}^2_1 \mathcal{T}_2)|\Phi\rangle_C \]

Incorporates standard single-reference CC as a particular case
Diagrammatic and BCCSD equations (1)

Grand potential at normal-ordered two-body level

\[ \Omega^{[2]} = \]

\[ \Omega^{11} + \Omega^{20} + \Omega^{02} \]

\[ \Omega^{[4]} = \]

\[ \Omega^{22} + \Omega^{31} + \Omega^{13} + \Omega^{40} + \Omega^{04} \]

Cluster amplitudes at BCCSD level

- Generate all distinct connected diagrams
- Label external lines according to bra
- Sum over all internal lines
- Associate matrix elements to each vertex
  - \((n!)^{-1}\) factor for \(n\) equivalent internal lines
  - \((k!)^{-1}\) factor for \(k\) equivalent cluster vertices
  - \((-1)^n\) factor for \(n\) crossing lines
- Add permutation for inequivalent external lines
Diagrammatic and BCCSD equations (2)

Energy equation

\[ \Omega_0 = \langle \Phi | \Omega (\mathcal{T}_1 + \mathcal{T}_2 + \frac{1}{2} \mathcal{T}_1^2) | \Phi \rangle_C \]

Single amplitude equation

No distinction between particles and holes

Fewer diagrams than in CCSD

Similar for double amplitude equation

Can be extended to
(1) residual 3NF \( \Omega^{[6]} \)
(2) triples \( \mathcal{T}_3 \)

\[ 0 = \langle \Phi^{\alpha\beta} | \Omega (1 + \mathcal{T}_1 + \frac{1}{2} \mathcal{T}_1^2 + \frac{1}{3!} \mathcal{T}_1^3 + \mathcal{T}_2 + \mathcal{T}_1 \mathcal{T}_2) | \Phi \rangle_C \]
Part II.a.

Pairing Hamiltonian from BCCD

Set up

Attractive pairing grand potential

\[ \Omega = \sum_p (\epsilon_p - \lambda) N_p - G \sum_{pq} P^+_p P_q \]

Pair operators

\[ N_p = a^+_p a^+_p + a^+_p a^+_p \]

\[ P^+_p = a^+_p a^+_p \]

SU(2) algebra

\[ [P_p, P^+_q] = \delta_{pq} (1 - N_p) \]

\[ [N_p, P_q] = -2 \delta_{pq} P_p \]

\[ [N_p, P^+_q] = 2 \delta_{pq} P^+_p \]

Doubly-degenerate picket fence model

\[ \epsilon_p = p \Delta \epsilon \]

Model for, e.g., deformed nuclei

Exact ground-state energy

- Diagonalization within seniority-0 subspace
  [A. Volya, B.A. Brown, W. Zelevinsky, PLB509, 37 (2001)]

- Richardson solution
  [R.W. Richardson, PL3, 277 (1963), PR141 (1966)]

* Cheaper than full diagonalization (\[ \sqrt{\text{ }} \])
* Still scales exponentially
  -> Limited to ~40 levels at half filling

Typical approximate methods

- BCS and projected BCS (before variation)
- Coupled cluster theory with doubles
- Self-consistent RPA

[J. Dukelsky et al., NPA714, 63 (2003)]

What about BCCD?

* 100 levels
* Half filling
* \[ \Delta \epsilon = 300 \text{keV} \]
* \[ G_c / \Delta \epsilon = 0.18 \]

Look for highly accurate many-body methods that
- Scale polynomial with system size
- Can be applied to more realistic Hamiltonians

High accuracy in normal phase
Collapse near superfluid transition
Results for 100 levels at half filling

Correlation energy

- High accuracy in normal & superfluid phases
- Superior to PBCS in regime of interest
- Superiority improves with system size
- Doubles reduce symmetry breaking vs BCS
- Conclusions valid away from half filling
- Symmetry restoration crucial near closed shell

[PNR Bogoliubov CC theory, T. Duguet, in preparation (2014)]

Pairing “gap”

Variance in A

Triples correction will further improve

Phase transition wrongly of first order
Second-order character recovered from singles
Test calculations of semi-magic $N/Z=8$ nuclei

Set up

- $\text{NNLO}_{\text{opt}}$ 2NF ($\Lambda = 500$ MeV/c)
  [A. Ekstrom et al., PRL110, 192502 (2013)]
- No 3NF yet
- HO basis
  - $N_{\text{max}} = 6$
  - $hw = 26$ and $50,53,55,58$ MeV
- m-scheme code

**Ground-state binding energy**

Accessible via 2PA-EOM-CCSD  
[G. Jansen et al., PRC83 (2011) 054306]  
3p-1h on top of $^{16}\text{O}$

Only accessible via BCCSD  
(can do any number of valence nucleons)

**BCCSD = CCSD to the ev level in doubly closed-shell $^{16}\text{O}$**

Infrared extrapolation from $h\omega=50,53,55,58\text{MeV}$  

$E(L) = E_\infty + A_\infty e^{-2k_\infty L}$  
where

$b = \sqrt{\hbar/(M\omega)}$  
$L = \sqrt{2(N + 3/2 + 2)b}$

**Extends SR-CC to genuinely open-shells!**

- Scales as $(n_h+n_p)^6$
- $\sim 1.5\text{ MeV} > 2\text{PA-EOM-CCSD in }^{18}\text{O and }^{18}\text{Mg}$
- Critical to restore $A$ near closed shell
- Storage of $T_2$ in $m$ scheme beyond $N_{\text{max}} = 8$?
- More involved distribution of $T_2$
- Use SVD
  [T. Kinoshita et al., JCP 119 (2003) 7756]
- Code in J-coupled scheme
Conclusions and perspectives

Conclusions

- Development of Bogoliubov CC theory for genuinely open-shell nuclei
- Parallel effort to Gorkov-SCGF and MR-IMSRG
- m-scheme implementation at the singles and doubles level
  - First proof-of-principle results
  - Allows for the treatment of doubly-open-shell systems
  - Currently limited to $N_{\text{max}} = 8$ due to storage scheme

Future

- Develop option(s) to go to larger bases
- Implementation of 3NF at normal-ordered two-body level
- Extend to Equation-Of-Motion Bogoliubov CC theory
- Wealth of potential applications
  - Problems of experimental interest
  - Cross-benchmarking with Gorkov-SCGF and MR-IMSRG
- Symmetry-restored Bogoliubov CC theory and applications
Appendix

Complementary slides
Diagrammatic and BCCSD equations (3)

\[ 0 = \langle \Phi | \Phi(1 + T_1 + T_2 + \frac{1}{2} T_2^2 + \frac{1}{4} T_1^2 T_2 + \frac{1}{4} T_1^4 + \frac{1}{4} T_1^4 T_2) | \Phi \rangle. \]