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

I. Breaking symmetries

Thomas DUGUET

CEA, Service de Physique Nucléaire, Saclay, France
NSCL, Michigan State University, East Lansing, USA

NORDITA program on Computational Challenges in Nuclear and Many-Body Physics

Sept. 15th- Oct. 10th 2014, Stockholm
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)]
Introduction
**Non-perturbative *ab-initio* many-body theories**

*Ab-initio* many-body theories
- Effective structure-less nucleons
- $2N + 3N + \ldots$ 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**
- $16_8^O$
- $22,24_8^O$
- $40_{20}^{Ca}$
- $48_{20}^{Ca}$
- $56_2^{Ni}$

**Comp data**
- $100_{50}^{Sn}$
- $112_{50}^{Sn}$

**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]
[Dean, Hjorth-Jensen, Piecuch, Hagen, Papenbrock, Roth]
[Barbieri, Dickhoff]
[Tsukiyama, Bogner, Schwenk, Hergert]
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  [A. Signoracci, T. Duguet, G. Hagen, unpublished (2014)]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**
- **CC-based valence shell model**
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

\begin{align*}
\text{Wave operator} & \quad \Rightarrow \\
\text{Reference state} & \quad \Rightarrow
\end{align*}

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

Closed shell

- RHF reference
  - conserves \( A, J^2, M \)
  - Dy-SCGF CC

Singly/doubly open shell

- UHF(B) reference
  - breaks \( A / J^2 \) and \( M \)
  - Go-SCGF
  - Today BCC

- Contamination from other \( A / J^2 \) and \( M \)
  - ph degeneracy \(<\rightarrow\>
  - Goldstone mode

Singly/doubly open shell

- UHF(B) manyfold
  - restores \( A / J^2 \) and \( M \)
  - AMR-CC & PNR-BCC
  - Next thursday

Multi-reference character

- Finite inertia
  - \(<\rightarrow\>
  - Resolve Goldstone mode

Today

Next thursday
Bogoliubov coupled-cluster formalism
for singly open-shell nuclei

Hartree-Fock-Bogoliubov reference

Nuclear Hamiltonian

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

Bogoliubov transformation

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

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

Bogoliubov vacuum

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

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

Density matrices

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

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

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

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

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

Spectroscopic factors

\[
\beta_{\alpha}\beta_{\beta}^\dagger
\]

Binding energy

\[
E_0 = \frac{1}{2} \left[ \sum_{pq} t_{pq} \rho_{qp} - \sum_{\alpha} (E_{\alpha} - \lambda) \tilde{\delta}_{\alpha} \right] - \frac{1}{6} \left[ \sum_{pq} \Gamma_{pq}^3 \rho_{qp} + \Delta_{pq}^3 \kappa_{qp}^* \right]
\]

* m-scheme code
* Benchmarked against J-coupled
[V. Somà et al.]
Bogoliubov CC ansatz

Wave-function ansatz

\[ |\Psi\rangle \equiv e^{\mathcal{T}} |\Phi\rangle \]

Quasi-particle cluster operator

\[ \mathcal{T} \equiv \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \ldots \]

\[ [\mathcal{T}_n, \mathcal{T}_m] = 0 \]

Connected n-tuple excitation

\[ \mathcal{T}_1 \equiv \frac{1}{2!} \sum_{k_1 k_2} t_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \]

\[ \mathcal{T}_2 \equiv \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} t_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4} \]

Action of n-tuple excitation on the HFB vacuum

\[ |\Phi\rangle \]

\[ \mathcal{T}_1 |\Phi\rangle \rightarrow |\Phi^{\alpha\beta}\rangle \]

\[ \mathcal{T}_2 |\Phi\rangle \rightarrow |\Phi^{\alpha\beta\gamma\delta}\rangle \]

HFB vacuum

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

- Exponential generates connected + disconnected n-tuple excitations
- No distinction between particles and holes
- Fully anti-symmetric

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

Bogoliubov transformation + Wick’s theorem

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

\[ = \Omega^{00} + \frac{1}{1!} \sum_{k_1 k_2} \Omega^{11}_{k_1 k_2} \beta^{\dagger}_{k_1} \beta_{k_2} + \frac{1}{2!} \sum_{k_1 k_2} \left\{ \Omega^{20}_{k_1 k_2} \beta^{\dagger}_{k_1} \beta^{\dagger}_{k_2} + \Omega^{02}_{k_1 k_2} \beta_{k_2} \beta_{k_1} \right\} \]

\[ = E_{k_1} \delta_{k_1 k_2} \quad \text{with HFB reference state} \]

\[ + \frac{1}{(2!)^2} \sum_{k_1 k_2 k_3 k_4} \Omega^{22}_{k_1 k_2 k_3 k_4} \beta^{\dagger}_{k_1} \beta^{\dagger}_{k_2} \beta_{k_3} \beta_{k_4} \]

\[ + \frac{1}{3!} \sum_{k_1 k_2 k_3 k_4} \left\{ \Omega^{31}_{k_1 k_2 k_3 k_4} \beta^{\dagger}_{k_1} \beta^{\dagger}_{k_2} \beta^{\dagger}_{k_3} \beta_{k_4} + \Omega^{13}_{k_1 k_2 k_3 k_4} \beta^{\dagger}_{k_1} \beta_{k_4} \beta_{k_3} \beta_{k_2} \right\} \]

\[ + \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \left\{ \Omega^{40}_{k_1 k_2 k_3 k_4} \beta^{\dagger}_{k_1} \beta^{\dagger}_{k_2} \beta^{\dagger}_{k_3} \beta^{\dagger}_{k_4} + \Omega^{04}_{k_1 k_2 k_3 k_4} \beta_{k_4} \beta_{k_3} \beta_{k_2} \beta_{k_1} \right\} \]

\[ + \Omega^{[6]} \]

NO2B approximation

Very good in closed shell (1% error)

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

**Schrödinger equation**

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

\[xe^{-T} \quad \Omega |\Phi\rangle = \Omega_0 |\Phi\rangle\]

\[(\Omega e^T)_c |\Phi\rangle = \Omega_0 |\Phi\rangle\]

**Energy equation**

\[\langle \Phi | (\Omega e^T)_c |\Phi\rangle = \Omega_0\]

**Amplitude equation to find** \(T_n\)

\[\langle \Phi^{\alpha\beta\ldots} | (\Omega e^T)_c |\Phi\rangle_C = 0\]

**Non-hermitian similarity-transformed grand potential**

\[\widetilde{\Omega} \equiv e^{-T} \Omega e^T\]

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

Baker-Campbell-Hausdorff + Wick theorem

Size extensive

Expansion naturally terminates

**BCC with Singles and Doubles**

Incorporates standard single-reference CC as a particular case

**Equations to constrain** \(\lambda\)

\[\frac{\langle \Psi | A |\Psi\rangle}{\langle \Psi |\Psi\rangle} = A\]

**Infinite-order method**

Efficient grasp of dynamic correlations

Truncate \(T\) beyond a certain \(T_n\)

Retaining \(T_1\) and \(T_2\) defines BCCSD

\[
\begin{align*}
\Omega_0 &= \langle \Phi | \Omega (1 + T_1 + T_2 + \frac{1}{2} T_1^2) |\Phi\rangle_C \\
0 &= \langle \Phi^{\alpha\beta} | \Omega (1 + T_1 + \frac{1}{2} T_1^2 + \frac{1}{3!} T_1^3 + T_2 + T_1 T_2) |\Phi\rangle_C \\
0 &= \langle \Phi^{\alpha\beta\gamma\delta} | \Omega (1 + T_1 + T_2 + \frac{1}{2} T_1^2 + \frac{1}{2} T_2^2 \\
&\quad + T_1 T_2 + \frac{1}{3!} T_1^3 + \frac{1}{4} T_1^4 + \frac{1}{2} T_1^2 T_2) |\Phi\rangle_C
\end{align*}
\]
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 \( \Omega_0^{[6]} \)
(2) triples \( \mathcal{T}_3 \)
Pairing Hamiltonian from BCCD

Set up

**Attractive pairing grand potential**

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

**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**

\[ \varepsilon_p = p \Delta \varepsilon \]

**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 (√)
- 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
- BCCD

**Look for highly accurate many-body methods that**

- Scale polynomial with system size
- Can be applied to more realistic Hamiltonians

**What about BCCD?**

- 100 levels
- Half filling
- \( \Delta \varepsilon = 300 \text{ keV} \)
- \( G_c/\Delta \varepsilon = 0.18 \)

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

- 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

- 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 $^{16}$O

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

$^{18}$Ne, $^{18}$O + 2 nucleons
$^{20}$Mg, $^{20}$O + 4 nucleons

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

Infrared extrapolation from $\hbar w=50,53,55,58$MeV

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

where

$b = \sqrt{\hbar/(M\omega)}$

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

Extends SR-CC to genuinely open-shells!
- Scales as $(n_h+n_p)^6$
- $\sim 1.5$ MeV > 2PA-EOM-CCSD in $^{18}$O and $^{18}$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)

Double amplitude equation

\[ 0 = \langle \Phi | (1 + T_1 + T_2 + \frac{1}{2} T_1^2 + \frac{1}{2} T_2^2 + \frac{1}{4} T_1 T_2 + \frac{1}{4} T_1^2 T_2 + \frac{1}{4} T_2^2 T_1 + \frac{1}{16} T_1^2 T_2^2) | \psi \rangle \]