Development of Bogoliubov coupled cluster theory

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Motivation

- Ab-initio methods beyond the lightest nuclei
- Coupled cluster (CC) theory successfully implemented for ^{24}O, ^{40}Ca, etc.
  - Uses Slater determinant as reference state
  - Extends to doubly-closed subshell nuclei $\pm 1, \pm 2$ nucleons
  - Not suited to calculate truly open-shell nuclei
- Extend CC method to open-shell nuclei with Bogoliubov reference state (BCC)
  - Most important towards heavier nuclei
  - K. Emrich and J.G. Zabolitzky, Phys. Rev. B **30**, 2049 (1984)
  - W.A. Lahoz and R.F. Bishop, Z. Phys. B **73**, 363 (1988)
  - L.Z. Stolarczyk and H.J. Monkhorst, Mol. Phys. **108**, 3067 (2010)
- Same principle beyond the Gorkov-Green's extension of Dyson-SCGF methods
  - V. Soma, T. Duguet, and C. Barbieri, Phys. Rev. C **84**, 064317 (2011)
  - BCC is a computationally optimized alternative
  - Possibility to cross-check results beyond experimentally known region

Standard coupled cluster (CC) theory

- State of the art computational tool
  - Many-Body Methods in Chemistry and Physics, I. Shavitt and R.J. Bartlett
  - G. Hagen et al., Phys. Rev. C **82**, 034330 (2010)
- Exponential ansatz $|\Psi\rangle = e^{T}|\Phi\rangle$, where T is the cluster operator
- Cluster Operator $T = T_1 + T_2 + T_3 + \ldots$

$$T_1 = \sum_{ia} t_i^a a^\dagger i$$

$$T_2 = \frac{1}{(2!)^2} \sum_{ijab} t_{ij}^{ab} a^\dagger i b^\dagger j$$

- Physical wavefunction is built through np-nh excitations of Slater determinant $|\Phi\rangle$
- Approximate solution to Schrödinger equation by truncating T
- Typically use HF solution as reference state $|\Phi\rangle$
- Schrödinger equation with similarity-transformed Hamiltonian $\mathcal{H} = e^{-T} H e^{T}$

$$(H - E)e^{T}|\Phi\rangle = 0$$

$$(\mathcal{H} - E)|\Phi\rangle = 0$$

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CC formalism

- Baker-Campbell-Hausdorff expansion

$$\mathcal{H} = H + [H,T] + \frac{1}{2!}[[H,T],T] + \frac{1}{3!}[[[H,T],T],T] + \frac{1}{4!}[[[[H,T],T],T],T] + \dots$$

- Truncation to four T operators assuming two-body Hamiltonian
- Final expression of similarity-transformed Hamiltonian

$$\mathcal{H} = H + \left(HT\right)_C + \frac{1}{2!}\left(HTT\right)_C + \frac{1}{3!}\left(HTTT\right)_C + \frac{1}{4!}\left(HTTTT\right)_C = (He^T)_C$$

- Energy and amplitude equations

$$(\mathcal{H} - E)|\Phi\rangle = 0$$

1. Energy equation multiply on the left by $\langle\Phi|$
2. Amplitude equations multiply on the left by $\langle\Phi^{ab\dots}_{ij\dots}|$
   - Need as many amplitude equations as terms in cluster operator T
3. Assume intermediate normalization $\langle\Phi|\Psi\rangle = 1$

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Extension to (truly) open-shell nuclei

- Expansion techniques break down for calculations of (truly) open-shell nuclei
- Reference state explicitly breaking symmetry can account for superfluid nature
- Build CC techniques around Bogoliubov vacuum
- Difficulties
  - Quasiparticle basis- rewrite Hamiltonian normal-ordered wrt HFB vacuum
  - Diagrammatic techniques- rules (e.g. from Shavitt and Bartlett) need modification
  - Additional constraint equation- average particle number
  - Computational aspect- less expedient scaling

$$n_p^i n_h^j \text{ in CC} \rightarrow (n_p + n_h)^{i+j} \text{ in BCC}$$

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Bogoliubov algebra

- Bogoliubov transformation

$$c_l^\dagger = \sum_k U_{lk}^* \beta_k^\dagger + V_{lk} \beta_k \qquad c_l = \sum_k U_{lk} \beta_k + V_{lk}^* \beta_k^\dagger$$

- Bogoliubov vacuum $|\Phi\rangle \equiv \mathcal{C} \prod_j \beta_j |0\rangle$
- Natural extension from particle-hole language
- Simplifies some aspects of standard CC theory
- Rewrite Hamiltonian, i.e. normal order with respect to $|\Phi\rangle$
  - Derived including three-body interactions (to include implicit two-body component)

$$\begin{aligned} H &= H^{00} + H^{11} + H^{20} + H^{02} + \dots \\ &= \tilde{H}^{00} + \sum_{k_1 k_2} \tilde{H}^{11}_{k_1 k_2} \beta^\dagger_{k_1} \beta_{k_2} + \frac{1}{2!} \sum_{k_1 k_2} \left\{ \tilde{H}^{20}_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2} + \tilde{H}^{02}_{k_1 k_2} \beta_{k_2} \beta_{k_1} \right\} + \dots \end{aligned}$$

Each matrix element can be written as a function of NN, NNN, U, V

Bogoliubov coupled cluster theory

- Hamiltonian replaced by grand canonical potential $\Omega = H - \lambda N$
- Solution for nucleus with N_0 particles given by

$$\Omega|\Psi\rangle = \Omega_0|\Psi\rangle$$

- Constraint equation $N_0 = \frac{\langle\Psi|N|\Psi\rangle}{\langle\Psi|\Psi\rangle}$
- Exponential ansatz $|\Psi\rangle = e^{\mathcal{T}}|\Phi\rangle$
- Quasiparticle cluster operator $\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \dots$

$$\mathcal{T}_1 = \frac{1}{2!}\sum_{k_1 k_2} \tilde{\mathbf{t}}_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2}$$

$$\mathcal{T}_2 = \frac{1}{4!}\sum_{k_1 k_2 k_3 k_4} \tilde{\mathbf{t}}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4}$$

- Similarity transformed grand canonical potential $\bar{\Omega}$

Extension of standard coupled cluster theory

- Motivated by procedure in standard coupled cluster theory
  - Produce eigenvalue equation $\bar{\Omega}|\Phi\rangle = \Omega_0|\Phi\rangle$
  - Utilize Baker-Campbell-Hausdorff expansion
  - Truncate to four $\mathcal{T}$ operators (six with explicit three-body contribution)
  - Limit to connected terms only
  - Only quasiparticle creation operators in $\mathcal{T} \to \Omega$ to the left

$$\bar{\Omega} = \Omega + \left(\Omega\mathcal{T}\right)_C + \frac{1}{2!}\left(\Omega\mathcal{T}\mathcal{T}\right)_C + \frac{1}{3!}\left(\Omega\mathcal{T}\mathcal{T}\mathcal{T}\right)_C + \frac{1}{4!}\left(\Omega\mathcal{T}\mathcal{T}\mathcal{T}\mathcal{T}\right)_C = (\Omega e^{\mathcal{T}})_C$$

- Subtract reference energy for convenience $\Omega_N = \Omega - \langle\Phi|\Omega|\Phi\rangle$
- Produce energy and amplitude equations

$$\langle\Phi|\bar{\Omega}_N|\Phi\rangle_C = \Delta\Omega_0$$
$$\langle\Phi^{\alpha\beta\cdots}|\bar{\Omega}_N|\Phi\rangle_C = 0$$

- Solve under constraint of average particle number

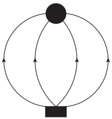
$$N_0 = \frac{\langle\Phi|e^{\mathcal{T}^\dagger} N e^{\mathcal{T}}|\Phi\rangle}{\langle\Phi|e^{\mathcal{T}^\dagger} e^{\mathcal{T}}|\Phi\rangle} = \langle\Phi|e^{\mathcal{T}^\dagger} N e^{\mathcal{T}}|\Phi\rangle_C$$

Current status

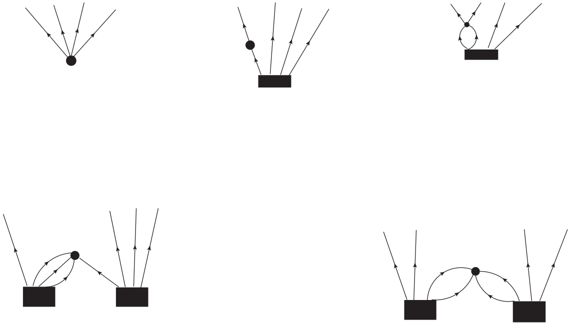
- Formalism
  - Derivation of BCCSD complete (too complex to show on slides)
  - Evaluated in 3 ways- algebraic (by hand), symbolic (J. Sadoudi), diagrammatic
  - Can recover standard CCSD in Slater determinant limit
    - Produce more general extended coupled cluster method in straightforward limit
  - BCCSDT derivation completed using symbolic method (J. Sadoudi)
- Implementation
  - Utilize *NN* interactions from chiral potential (+RG)
  - Bogoliubov vacuum from solution of HFB equations
    - *m*-scheme version nearly complete
    - Utilizes symmetry properties (subblock matrices in most reduced form)
  - BCCS derived and coded in *m*-scheme with intermediates
    - Extension to BCCSD necessary and upcoming
  - Allocated time on supercomputing machines for calculations
- Illustration using BCCD
  - Truncation to $\mathcal{T} = \mathcal{T}_2$
  - Should include most important effects at lowest order (two-body potential?)
  - Singles contribution corresponds to Thouless theorem; HFB solution used
  - Not recommended for real implementation- BCCSD required

Bogoliubov coupled cluster theory with doubles (BCCD): diagrammatic

Energy term



Amplitude terms



Bogoliubov coupled cluster with doubles (BCCD): algebraic

- Energy equation

$$\Delta\Omega_0^{BCCD} = \langle\Phi|\bar{\Omega}_N|\Phi\rangle_C = \langle\Phi|\Omega_N \mathcal{T}_2|\Phi\rangle$$

- With fully antisymmetrized matrix elements of grand canonical potential
  - $\tilde{\Omega}^{ij}_{k_1\ldots k_i k_{i+1}\ldots k_{i+j}} = (-1)^{\sigma(P)}\Omega^{ij}_{P(k_1\ldots k_i|k_{i+1}\ldots k_{i+j})}$
  - $\sigma(P)$ refers to the signature of the permutation P
  - $P(\ldots|\ldots)$ denotes separation between quasiparticles and quasiholes

$$\Delta\Omega_0^{BCCD} = \frac{1}{(4!)^2}\sum_{\substack{k_1k_2k_3k_4\\ k_1'k_2'k_3'k_4'}}\langle\Phi|\tilde{\Omega}^{04}_{k_1k_2k_3k_4}\beta_{k_1}\beta_{k_2}\beta_{k_3}\beta_{k_4}\tilde{\mathbf{t}}_{k_1'k_2'k_3'k_4'}\beta^\dagger_{k_1'}\beta^\dagger_{k_2'}\beta^\dagger_{k_3'}\beta^\dagger_{k_4'}|\Phi\rangle$$

- Full solution

$$\Delta\Omega_0^{BCCD} = \frac{1}{4!}\sum_{k_1k_2k_3k_4}\tilde{\Omega}^{04}_{k_1k_2k_3k_4}\tilde{\mathbf{t}}_{k_1k_2k_3k_4}$$

- Find quasiparticle amplitudes from amplitude equation

$$0 = \langle\Phi^{\alpha\beta\gamma\delta}|\bar{\Omega}_N|\Phi\rangle_C = \langle\Phi^{\alpha\beta\gamma\delta}|\Omega^{40}|\Phi\rangle + \langle\Phi^{\alpha\beta\gamma\delta}|\Omega\mathcal{T}_2|\Phi\rangle_C + \frac{1}{2}\langle\Phi^{\alpha\beta\gamma\delta}|\Omega\mathcal{T}_2^2|\Phi\rangle_C$$

BCCD- amplitude equation

$$
\begin{aligned}
0 = \tilde{\Omega}^{40}_{\alpha\beta\gamma\delta} &+ \sum_{k_1}\Big[\tilde{\Omega}^{11}_{\alpha k_1}\tilde{\mathbf{t}}_{k_1\beta\gamma\delta} + \tilde{\Omega}^{11}_{\beta k_1}\tilde{\mathbf{t}}_{\alpha k_1\gamma\delta} + \tilde{\Omega}^{11}_{\gamma k_1}\tilde{\mathbf{t}}_{\alpha\beta k_1\delta} + \tilde{\Omega}^{11}_{\delta k_1}\tilde{\mathbf{t}}_{\alpha\beta\gamma k_1}\Big] \\
&+ \frac{1}{2}\sum_{k_1 k_2}\Big[\tilde{\Omega}^{22}_{\alpha\beta k_1 k_2}\tilde{\mathbf{t}}_{k_1 k_2\gamma\delta} + \tilde{\Omega}^{22}_{\alpha\gamma k_1 k_2}\tilde{\mathbf{t}}_{k_1 k_2\delta\beta} + \tilde{\Omega}^{22}_{\alpha\delta k_1 k_2}\tilde{\mathbf{t}}_{k_1 k_2\beta\gamma} \\
&\qquad + \tilde{\Omega}^{22}_{\beta\gamma k_1 k_2}\tilde{\mathbf{t}}_{k_1 k_2\alpha\delta} + \tilde{\Omega}^{22}_{\beta\delta k_1 k_2}\tilde{\mathbf{t}}_{k_1 k_2\gamma\alpha} + \tilde{\Omega}^{22}_{\gamma\delta k_1 k_2}\tilde{\mathbf{t}}_{k_1 k_2\alpha\beta}\Big] \\
&+ \frac{1}{12}\sum_{k_1 k_2 k_3 k_4}\tilde{\Omega}^{04}_{k_1 k_2 k_3 k_4}\Big[2(\tilde{\mathbf{t}}_{\alpha k_1 k_2 k_3}\tilde{\mathbf{t}}_{k_4\beta\gamma\delta} + \tilde{\mathbf{t}}_{\beta k_1 k_2 k_3}\tilde{\mathbf{t}}_{\alpha k_4\gamma\delta} \\
&\qquad + \tilde{\mathbf{t}}_{\gamma k_1 k_2 k_3}\tilde{\mathbf{t}}_{\alpha\beta k_4\delta} + \tilde{\mathbf{t}}_{\delta k_1 k_2 k_3}\tilde{\mathbf{t}}_{\alpha\beta\gamma k_4}) \\
&\qquad + 3(\tilde{\mathbf{t}}_{k_1 k_2\alpha\beta}\tilde{\mathbf{t}}_{k_3 k_4\gamma\delta} + \tilde{\mathbf{t}}_{k_1 k_2\alpha\gamma}\tilde{\mathbf{t}}_{k_3 k_4\delta\beta} + \tilde{\mathbf{t}}_{k_1 k_2\alpha\delta}\tilde{\mathbf{t}}_{k_3 k_4\beta\gamma})\Big]
\end{aligned}
$$

- Also need constraint equation for average particle number
- Solve system of equations iteratively
- Update Lagrange parameter each iteration

Conclusions/Outlook

- Conclusions
  - BCC derived in various truncation schemes in general indices
  - Diagrammatic technique developed, reproduces algebraic result
  - Motivated procedure, displayed illustrative BCCD
  - Maintain single-reference nature, even for open-shell
- Future steps
  - First and foremost, finalize HFB and BCCS codes to demonstrate convergence
  - Implement BCCSD in *m*-scheme
  - Calculate realistic closed-shell nuclei to compare/benchmark standard CC results
  - Calculate open-shell nuclei to benchmark in-medium SRG/Gorkov-Green's function
  - Include three-body forces at least at normal-ordered two-body level
  - Implement equation-of-motion BCC, projection, etc.