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

II. Restoring symmetries

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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)) (last thursday)

Bogoliubov coupled-cluster method


III. Restoring SU(2) (today) and/or U(1) symmetries

Angular-momentum-restored coupled-cluster formalism


Particle-number-restored Bogoliubov coupled-cluster formalism

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

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

**High predictive power**
**Limited applicability domain**

#### Input
- **16O**
- **22,24O**
- **40Ca**
- **48Ca**
- **56Ni**
- **100Sn**
- **112Sn**

#### Comp data
- **2003-2014**
  - CC, Dy-SCGF, IMSRG
  - Near doubly-magic nuclei $A<132$

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

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

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

**2003-2014**
- [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  - [A. Signoracci, T. Duguet, G. Hagen, unpublished (2014)]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

**Target state**

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

A-body ground state

**Wave operator**

**Reference state**

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

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

Ground-state energy

**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
- BCC

**Singly/doubly open shell**

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

**Multi-reference character**

- Finite inertia
  - \( \leftrightarrow \)
- Resolve Goldstone mode

**Contamination**

from other \( A / J^2 \) and \( M \)

- \( \phi \) degeneracy
  - \( \leftrightarrow \)
- Goldstone mode
**Symmetry and symmetry breaking**

### Some symmetries of $H$

| Invariance     | Group         | $|\Psi^X>$ |
|----------------|---------------|-----------|
| Spatial trans. | $T(1)$        | $P$       |
| Gauge rot.     | $U(1)$        | $N,Z$     |
| Spatial rot.   | $SO(3)$       | $J,M$     |

### Correlations

<table>
<thead>
<tr>
<th>$\Delta E$</th>
<th>Excitation</th>
<th>Nuclei</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pairing</td>
<td>$&lt;2\text{MeV}$</td>
<td>Gap but doubly magic</td>
</tr>
<tr>
<td>Angular loc.</td>
<td>$&lt;20\text{MeV}$</td>
<td>Rot. band but singly magic</td>
</tr>
</tbody>
</table>

One way is to enforce the symmetry throughout the description. Another way is to let symmetry break in low order description.

### Restoration of symmetries

- $|\Psi^X>$
- $\Delta E$
- Spectro
- $N,Z \sim 1\text{MeV}$
- Pairing rot.
- $J,M \sim 2\text{MeV}$
- Rot. band

Crucial for specific observables.

### Symmetry breaking and associated physics

Symmetry restricted description

$$|\Psi_0\rangle = \Omega_0 |\Phi\rangle$$

$E[\rho ; |q|]$

Symmetry breaking description

- $\text{ph degeneracy} \iff \text{Goldstone mode}$
- Account of $\Delta E$
- Fictitious in nuclei!

Symmetry restored description

- Good symmetry
- Hard to get $\Delta E$

Symmetry lost

Extra $\Delta E$

Good symmetry

Finite inertia

$\iff$

Resolve Goldstone mode
Part II

Symmetry-restored coupled-cluster theory

Angular-momentum-restored coupled-cluster formalism

Particle-number-restored Bogoliubov coupled-cluster formalism
[T. Duguet, in preparation (2014)]
Account of single-reference CC method (1)

Nuclear Hamiltonian

\[ H = \sum_{\alpha \beta} t_{\alpha \beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha \beta \gamma \delta} v_{\alpha \beta \gamma \delta} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \]

Anti-symmetrized matrix elements

\[ \overline{v}_{\alpha \beta \gamma \delta} \equiv v_{\alpha \beta \gamma \delta} - v_{\alpha \beta \delta \gamma} \]

Wave-function ansatz

\[ |\Psi_0\rangle \equiv e^T |\Phi\rangle \]

Product state of reference

\[ |\Phi\rangle \equiv \prod_{i=1}^N a_i^\dagger |0\rangle \]

Cluster operator

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

\[ T_n \equiv \frac{1}{(n!)^2} \sum_{ijk \ldots abc} t_{ijk \ldots abc}^a b c \ldots a_k a_j a_i \]

N-tuple connected component

\[ T_1 |\Phi\rangle \rightarrow |\Phi_i^a\rangle \quad T_2 |\Phi\rangle \rightarrow |\Phi_{ij}^{ab}\rangle \]

Cluster operator

Norm kernel in intermediate normalization

\[ N(\infty, 0) \equiv \langle \Phi | \Psi_0 \rangle = 1 \quad \text{as} \quad \langle \Phi | T_n = 0 \]

Only non-zero ph matrix elements

Exponential generates connected + disconnected n-tuple excitations

Size extensive
Account of single-reference CC method (2)

Time-independent Schrödinger equation

\[ H |\Psi_0\rangle = E_0 |\Psi_0\rangle \]

\[ H |\Phi\rangle = E_0 |\Phi\rangle \]

\[ (He^T)_c |\Phi\rangle = E_0 |\Phi\rangle \]

Energy equation

\[ \langle \Phi |(He^T)_c |\Phi\rangle = E_0 \]

Amplitude equation to determine \( T_n \)

\[ \langle \Phi^{a\ldots} |(He^T)_c |\Phi\rangle = 0 \]

Similarity-transformed Hamiltonian

\[ \overline{H} = e^{-T} He^T \]

Baker-Campbell-Hausdorff + Wick theorem

\[ \overline{H} = H + (HT)_c + \frac{1}{2!}(HTT)_c + \frac{1}{3!}(HTTT)_c + \frac{1}{4!}(HTTTT)_c \]

Exponential naturally terminates

Variant without \( xe^{-T} \) first

\[ \langle \Phi |He^T |\Phi\rangle = E_0 \langle \Phi |e^T |\Phi\rangle \]

\[ \langle \Phi^{a\ldots} |He^T |\Phi\rangle = E_0 \langle \Phi^{a\ldots} |e^T |\Phi\rangle \]

Disconnected parts canceled out a posteriori

Define energy and norm kernels

\[ H(\infty, 0) = E_0 N(\infty, 0) \]

\[ H^{a\ldots}(\infty, 0) = E_0 N^{a\ldots}(\infty, 0) \]

Obtain algebraic expressions via Wick theorem

Approx <-> truncate \( T \) beyond a certain \( T_n \)

Exemple: retaining \( T_1 \) and \( T_2 \) defines CCSD
Master equations (1)

Symmetry group of $H$ includes $SU(2) = $ non abelian compact Lie group – Lie algebra $\{J_x, J_y, J_z\}$

$R(\alpha, \beta, \gamma) \equiv R(\Omega)$ and IRREPs are $D_{MK}^J(\Omega) \equiv \langle \Psi^J | R(\Omega) | \Psi^K \rangle \delta_{JJ'}$ labeled by $J$ and spanned by $M$

Eigen-states of $H$

$[H, R(\Omega)] = 0 \text{ leads to } H|\Psi^J_\mu\rangle = E^J_\mu |\Psi^J_\mu\rangle$

Imaginary-time dependent scheme

Evolution operator

$U(\tau) \equiv e^{-\tau H}$

Time-evolved state

$|\Psi(\tau)\rangle \equiv U(\tau)|\Phi\rangle$

$N(\tau, \Omega) \equiv \langle \Psi(\tau) | 1 | \Phi(\Omega) \rangle$

$H(\tau, \Omega) \equiv \langle \Psi(\tau) | H | \Phi(\Omega) \rangle$

$J_i(\tau, \Omega) \equiv \langle \Psi(\tau) | J_i | \Phi(\Omega) \rangle$

$J^2(\tau, \Omega) \equiv \langle \Psi(\tau) | J^2 | \Phi(\Omega) \rangle$

Dynamical equation

$H(\tau, \Omega) = -\partial_\tau N(\tau, \Omega)$

Reduced kernel

$O(\tau, \Omega) \equiv O(\tau, \Omega) / N(\tau, 0)$

1) UHF reference state

$|\Phi\rangle$

2) Rotated reference state

$|\Phi(\Omega)\rangle \equiv R(\Omega)|\Phi\rangle$

Thouless transformation

Infinite sum of $p$-$h$ excitations

Ground state and energy

$\lim_{\tau \to \infty} |\Psi(\infty)\rangle = |\Psi^J_0\rangle$

$H(\infty, \Omega) = E^J_0 N(\infty, \Omega)$

- True for all $\Omega$
- Usual sym. unrest. MB schemes ($\Omega = 0$)

Intermediate normalization

$N(\tau, 0) = 1$

Expand un-rotated energy kernel

$H(\infty, 0) = E^J_0$
Master equations (2)

Expansion of rotated kernels over IRREPs of SU(2)

\[ N(\infty, \Omega) = e^{-\tau E_0^J} \sum_{MK} \langle \Phi | \Psi_0^J M \rangle \langle \Psi_0^J K | \Phi \rangle D_{MK}^J(\Omega) \]

\[ H(\infty, \Omega) = e^{-\tau E_0^J} E_0^J \sum_{MK} \langle \Phi | \Psi_0^J M \rangle \langle \Psi_0^J K | \Phi \rangle D_{MK}^J(\Omega) \]

Time propagation selects the proper IRREP

\[ \mathcal{H}(\infty, \Omega) = E_0^J N(\infty, \Omega) \]

Straight ratio

IRREPs still mixed as \( \tau \to \infty \)

\[ \Rightarrow \]

The good symmetry is lost

Truncating kernels expanded around symmetry-breaking reference \( |\Phi\rangle \)

\[ N_{\text{approx}}(\infty, \Omega) \equiv \sum_J \sum_{MK} N_{MK}^J D_{MK}^J(\Omega) \]

\[ H_{\text{approx}}(\infty, \Omega) \equiv \sum_J \sum_{MK} E_{MK}^J N_{MK}^J D_{MK}^J(\Omega) \]

Symmetry-restored energy

\[ E_0^J = \frac{\sum_{MK} f_M^J f_K^J \int_{SU(2)} d\Omega D_{MK}^J(\Omega) \mathcal{H}(\infty, \Omega)}{\sum_{MK} f_M^J f_K^J \int_{SU(2)} d\Omega D_{MK}^J(\Omega) N(\infty, \Omega)} \]

Standard kernels \( D_{MK}^J(0) = \delta_{MK} \)

Symmetry-restored energy

\[ N_{\text{approx}}(\infty, 0) \equiv \sum_J \sum_M N_{MM}^J \]

\[ H_{\text{approx}}(\infty, 0) \equiv \sum_J \sum_M E_{MM}^J N_{MM}^J \]

Superfluous in exact limit but not after truncation

No fingerprint of mixing left to be used

Benefit of inserting rotation operator in kernels!
Angular-momentum-restored CC theory

Objectives: extend symmetry restoration techniques beyond PHF to any order in CC such that

1. It keeps the simplicity of a single-reference-like CC theory
2. It is valid for any symmetry (spontaneously) broken by the reference state
3. It is valid for any system, i.e. closed shell, near degenerate and open shell
4. It accesses not only the ground state but also the lowest state of each IRREP

1) Static correlations from integral over SU(2)
2) Dynamic correlations from CC expansions of kernels + consistent interference!

Technical points of importance

- Wick Theorem for off-diagonal matrix element $\langle \Phi|\ldots|\Phi(\Omega)\rangle$ of strings of operators
  [R. Balian. E. Brezin, NC 64, 37 (1969)]
- Care must be taken of both the rotated energy $H(\tau, \Omega)$ and norm $N(\tau, \Omega)$ kernels

Expansion and truncation must be consistent

Problematic to find a naturally terminating expansion

Does not stay normalized when $\Omega$ varies!
Many-body perturbation theory (1)

Symmetry-breaking unperturbed system

\[ H \equiv H_0 + H_1 \quad \text{where} \quad H_0 \equiv T + U = \sum_{\alpha} e_{\alpha} a_{\alpha}^\dagger a_{\alpha} \quad \text{Such that} \quad [H_0, R(\Omega)] \neq 0 \quad \text{and} \quad [H_1, R(\Omega)] \neq 0 \]

\[ H_0 |\Phi\rangle = \varepsilon_0 |\Phi\rangle \quad \text{with} \quad \varepsilon_0 = \sum_{i=1}^{N} e_i \]

\[ H_0 |\Phi_{ij...}^{ab...}\rangle = (\varepsilon_0 + \varepsilon_{ij...}^{ab...}) |\Phi_{ij...}^{ab...}\rangle \]

Rotated state

\[ |\Phi(\Omega)\rangle = \prod_{i=1}^{N} a_{i}^\dagger |0\rangle \quad \text{with} \quad a_{\alpha}^\dagger = \sum_{\beta} R_{\beta\alpha}(\Omega) a_{\beta}^\dagger \quad \text{and} \quad R_{\alpha\beta}(\Omega) \equiv \langle \alpha |R(\Omega)|\beta\rangle \]

\[ \langle \Phi|\Phi(\Omega)\rangle = \det M(\Omega) \quad \text{where} \quad M_{\alpha\beta}(\Omega) \equiv R_{\alpha\beta}(\Omega) \delta_{\alpha i} \delta_{\beta j} \]

Off diagonal unperturbed one-body density matrix \( \Omega \)-dependent part couples p and h spaces

\[ \rho_{\alpha\beta}(\Omega) = \frac{\langle \Phi|a_{\beta}^\dagger a_{\alpha}|\Phi(\Omega)\rangle}{\langle \Phi|\Phi(\Omega)\rangle} \]

\[ \rho(\Omega) = \begin{pmatrix} 1^{hh} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ R(\Omega)M^{-1}(\Omega) & 0 \end{pmatrix} \equiv \rho(0) + \rho^{ph}(\Omega) \]

Density matrix of sym. unrest. reference state
Many-body perturbation theory (2)

Off-diagonal unperturbed propagator = basic contraction for Wick Theorem

\[
G^0_{\alpha\beta}(\tau_1, \tau_2; \Omega) \equiv \frac{\langle \Phi | T[a_\alpha(\tau_1)a_\beta(\tau_2)]|\Phi(\Omega)\rangle}{\langle \Phi|\Phi(\Omega)\rangle} = G^0_{\alpha\alpha}(\tau_1 - \tau_2)\delta_{\alpha\beta} + G^{ph}_{\alpha\beta}(\tau_1, \tau_2)\rho^{ph}_{\alpha\beta}(\Omega)
\]

Evolution operator \( \mathcal{U}(\tau) \)

Rotated norm kernel

\[
N(\tau, \Omega) = \langle \Phi | e^{-\tau H_0} T e^{-\int_0^\tau d\tau_1 H_1(\tau_1)} |\Phi(\Omega)\rangle = e^{-\tau \varepsilon_0 + n(\tau, \Omega)} \langle \Phi |\Phi(\Omega)\rangle
\]

where \( n(\tau, \Omega) \equiv \sum_{k=1}^{\infty} n^{(k)}(\tau, \Omega) \) = connected vacuum-to-vacuum diagrams

Rotated energy kernel

\[
H(\tau, \Omega) = \langle \Phi | e^{-\tau H_0} T e^{-\int_0^\tau d\tau_1 H_1(\tau_1)} (T + V) |\Phi(\Omega)\rangle = h(\tau, \Omega) N(\tau, \Omega)
\]

where \( h(\tau, \Omega) \equiv t(\tau, \Omega) + v(\tau, \Omega) \equiv \sum_{n=0}^{\infty} \left[ t^{(n)}(\tau, \Omega) + v^{(n)}(\tau, \Omega) \right] \)

and \( o(\tau, \Omega) = \) vacuum-to-vacuum diagrams linked to \( O \)

[R. Balian. E. Brezin, NC 64, 37 (1969)]
Many-body perturbation theory (3)

Connected vacuum-to-vacuum norm diagrams – Example at first order

\[ n_{V}^{(1)}(\tau, \Omega) = -\frac{1}{2} \sum_{\alpha\beta\gamma\delta} \int_{0}^{\tau} d\tau_{1} \, \bar{v}_{\alpha\beta\gamma\delta} \, G^{0}_{\gamma\alpha}(\tau_{1}, \tau_{1}; \Omega) \, G^{0}_{\delta\beta}(\tau_{1}, \tau_{1}; \Omega) \]

\[ = -\frac{\tau}{2} \sum_{ij} \bar{v}_{ijij} \]

\[ n_{V}^{(1)}(\tau, 0) = \text{standard sym. unrest. contribution} \]

\[ - \sum_{ija} \frac{\bar{v}_{ijaj}}{e_{a} - e_{i}} \rho^{ph}_{ai}(\Omega) \left( 1 - e^{-\tau(e_{a} - e_{i})} \right) \]

\[ - \frac{1}{2} \sum_{ijab} \frac{\bar{v}_{ijab}}{e_{a} + e_{b} - e_{i} - e_{j}} \left( 1 - e^{-\tau(e_{a} + e_{b} - e_{i} - e_{j})} \right) \rho^{ph}_{ai}(\Omega) \rho^{ph}_{bj}(\Omega) \]

Genuinely \( \Omega \)-dependent part

Large \( \tau \) limit

\[ n(\tau, 0) \xrightarrow{\tau \to \infty} -\tau \Delta E_{0}^{J_0} + \ln \left[ \sum_{M} |\langle \Phi|\Psi_{0}^{J_0M} \rangle|^{2} \right] \]

\[ N(\infty, \Omega) = e^{N(\Omega)} \left| \langle \Phi|\Phi(\Omega) \rangle \right| \]

Goldstone linked-cluster based on UHF

- nice but not what we are after!

\[ \Delta E_{0}^{J_0} = \langle \Phi|H_{1} \sum_{k=1}^{\infty} \left( \frac{1}{\varepsilon_{0} - H_{0}} \right)^{k-1} |\Phi\rangle \]
Many-body perturbation theory (3)

Connected vacuum-to-vacuum energy diagrams – example at zero order

\[ v^{(0)}(\tau, \Omega) = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \tilde{v}_{\alpha\beta\gamma\delta} G^0_{\gamma\alpha}(0, 0; \Omega) G^0_{\delta\beta}(0, 0; \Omega) \]

\[ = \frac{1}{2} \sum_{ij} \tilde{v}_{ijij} v^{(0)}(\tau, 0) = \text{standard sym. unrest. contribution} \]

\[ + \sum_{ijc} \tilde{v}_{ijcj} \rho^{ph}_{ci}(\Omega) \]

\[ + \frac{1}{2} \sum_{ijab} \tilde{v}_{ijab} \rho^{ph}_{ai}(\Omega) \rho^{ph}_{bj}(\Omega) \]

Genuinely \(\Omega\)-dependent part

Large \(\tau\) limit

\[ h(\tau, \Omega) \xrightarrow{\tau \to \infty} h(\Omega) \]

\[ \mathcal{H}(\infty, \Omega) = h(\Omega) N(\Omega) \]

Signals the symmetry breaking

In the exact limit

\[ \frac{\partial}{\partial \Omega} h(\Omega) = 0 \]

After truncation

\[ \frac{\partial}{\partial \Omega} h(\Omega) \neq 0 \]
Coupled cluster theory (1) – energy kernel

\( \mathcal{T}^\dagger_1(\tau, \Omega) \equiv \frac{1}{(1!)^2} \sum_{ia} \mathcal{T}^\dagger_{ia}(\tau, \Omega) a_i^\dagger a_a \)

\( \mathcal{T}^\dagger_2(\tau, \Omega) \equiv \frac{1}{(2!)^2} \sum_{ijab} \mathcal{T}^\dagger_{ijab}(\tau, \Omega) a_i^\dagger a_j^\dagger a_b a_a \)

\( \mathcal{T}_{\alpha\beta}(\tau, \Omega) \)

Kinetic energy kernel = connected diagrams linked to \( T(0) \)

MBPT-0

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0
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MBPT-1,2...∞

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0
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Similar for the potential energy kernel

All connected diagrams with one ph pair leaving down

Time integration + transformed operators

Coupled cluster theory (2) – energy kernel

Algebraic expressions

1) Same formal structure as in standard CC
2) Natural termination of an exponential
3) No use of Baker-Campbell-Hausdorff
4) Expand with off diagonal Wick theorem

\[ t(\tau, \Omega) = \langle \Phi | T + T_1^\dagger(\tau, \Omega) T | \Phi(\Omega) \rangle \langle \Phi | \Phi(\Omega) \rangle^{-1} \]

\[ = \sum_i t_{\pi i}(\Omega) + \sum_{ia} T_{ia}^\dagger(\tau, \Omega) t_{\alpha i}(\Omega) \]

\[ v(\tau, \Omega) = \langle \Phi | V + T_1^\dagger(\tau, \Omega) V + T_2^\dagger(\tau, \Omega) V + \frac{1}{2} T_1^\dagger(\tau, \Omega) V | \Phi(\Omega) \rangle \langle \Phi | \Phi(\Omega) \rangle^{-1} \]

\[ = \frac{1}{2} \sum_{ij} \bar{v}_{ijij}(\Omega) + \sum_{ija} T_{ija}^\dagger(\tau, \Omega) \bar{v}_{aaji}(\Omega) + \frac{1}{4} \sum_{ijab} T_{ijab}^\dagger(\tau, \Omega) \bar{v}_{aibi}(\Omega) + \sum_{ijab} T_{ia}^\dagger(\tau, \Omega) T_{jib}^\dagger(\tau, \Omega) \bar{v}_{aibi}(\Omega) \]

Transformed operators

- Exact same expressions as in standard CC
- Same CPU cost at a given truncation level

Bi-orthogonal system

\[ |\tilde{\alpha}\rangle \equiv D(\Omega)|\alpha\rangle \]

\[ \langle \tilde{\alpha}| \equiv \langle \alpha|D^{-1}(\Omega) \]

\[ D(\Omega) \equiv 1 + \rho^{ph}(\Omega) \]

CC expansion of the off diagonal energy kernel

\[ h(\tau, \Omega) = \frac{\langle \Phi | e^{T^\dagger(\tau, \Omega)} H | \Phi(\Omega) \rangle_c}{\langle \Phi | \Phi(\Omega) \rangle} = \langle \Phi | e^{T^\dagger(\tau, \Omega)} \tilde{H}(\Omega) | \Phi \rangle_c \]

Need equations for the CC amplitudes
N-tuples off-diagonal norm and energy kernels

\[ N_{ij\ldots}^{ab\ldots}(\tau, \Omega) \equiv \langle \Psi(\tau) | A_{ij\ldots}^{ab\ldots} | \Phi(\Omega) \rangle \]

where \( A_{ij\ldots}^{ab\ldots} \equiv a_i^\dagger a_i a_b^\dagger a_j \ldots \)

\[ H_{ij\ldots}^{ab\ldots}(\tau, \Omega) \equiv \langle \Psi(\tau) | HA_{ij\ldots}^{ab\ldots} | \Phi(\Omega) \rangle \]

Dynamical amplitude equations

1) Perform MBPT expansion
2) Recast in terms of cluster operators
3) Remove disconnected terms involving \( A_{ij\ldots}^{ab\ldots} \)
4) Recast in terms of transformed operators

\[ H_{ij\ldots}^{ab\ldots}(\tau, \Omega) = -\partial_\tau N_{ij\ldots}^{ab\ldots}(\tau, \Omega) \]

Imaginary-time-dependent equation of motion

\[ \langle \Phi | e^{T(\tau, \Omega)} \hat{H}(\Omega) | \Phi_{ij\ldots}^{ab\ldots} \rangle_c = -\partial_\tau T_{ij\ldots}^{ab\ldots}(\tau, \Omega) \]

1) CC scheme for transformed cluster amplitudes
3) Amplitude equations formally identical to those in standard CC
5) Transformed amplitudes reduce to bare ones for \( \Omega = 0 \); i.e. standard CC

Note: one eventually solves in the stationary limit, i.e. at \( \tau = \infty \)
Coupled cluster theory (4) – norm

No direct naturally terminating expansion of $N(\tau, \Omega)$ from MBPT

Solution to this key problem comes from

- Coupled ODEs satisfied by Wigner D functions
  [D. A. Varshalovich et al., Quantum Theory of Angular Momentum, 1988]
- Expansion of $J_i(\tau, \Omega)$ over Wigner D functions
- Factorization of connected kernels $j_i(\tau, \Omega)$

\[
\frac{\partial}{\partial \alpha} N(\tau, \Omega) + \frac{i}{\hbar} j_z(\tau, \Omega) N(\tau, \Omega) = 0
\]
\[
\frac{\partial}{\partial \beta} N(\tau, \Omega) - \frac{i}{\hbar} \left[ \sin \alpha j_x(\tau, \Omega) - \cos \alpha j_y(\tau, \Omega) \right] N(\tau, \Omega) = 0
\]
\[
\frac{\partial}{\partial \gamma} N(\tau, \Omega) + \frac{i}{\hbar} \left[ \sin \beta \cos \alpha j_x(\tau, \Omega) + \sin \beta \sin \alpha j_y(\tau, \Omega) + \cos \beta j_z(\tau, \Omega) \right] N(\tau, \Omega) = 0
\]

This rational ensures that the symmetry is exactly restored at any truncation order of $j_i(\tau, \Omega)$

\[
\frac{\int_{SU(2)} d\Omega D^{J*}_{MK}(\Omega) J_z(\tau, \Omega)}{\int_{SU(2)} d\Omega D^{J*}_{MK}(\Omega) N(\tau, \Omega)} = M\hbar
\]
\[
\frac{\sum_{MK} f_{MK}^J f_{MK}^J \int_{SU(2)} d\Omega D^{J*}_{MK}(\Omega) J^2(\tau, \Omega)}{\sum_{MK} f_{MK}^J f_{MK}^J \int_{SU(2)} d\Omega D^{J*}_{MK}(\Omega) N(\tau, \Omega)} = J(J + 1)\hbar^2
\]
\[
\int_{SU(2)} d\Omega D^{J*}_{MK}(\Omega) \left[ \sin \beta \cos \alpha J_x(\tau, \Omega) + \sin \beta \sin \alpha J_y(\tau, \Omega) + \cos \beta J_z(\tau, \Omega) \right] = K\hbar
\]

Note: Extends to any CC order a known result of projected HF
  e.g. [K. Enami et al., PRC59 (1999) 135]
Important limits

Symmetry-restored energy

$$E^J_0 = \frac{\sum_{MK} f^J_M f^J_K \int_{SU(2)} d\Omega \  D^J_{MK} (\Omega) h(\Omega) \ N(\Omega)}{\sum_{MK} f^J_M f^J_K \int_{SU(2)} d\Omega \  D^J_{MK} (\Omega) \ N(\Omega)}$$

1. Standard SR-CC is recovered at \( \Omega = 0 \) or if \( |\Phi\rangle \) does not break the symmetry

$$E^J_0 = h(0)$$

2. Projected Hartree Fock is recovered at lowest order

\[ h^{(0)}(\tau, \Omega) = \frac{\langle \Phi | H | \Phi(\Omega) \rangle}{\langle \Phi | \Phi(\Omega) \rangle} \]
\[ j_i^{(0)}(\tau, \Omega) = \langle \Phi | J_i | \Phi(\Omega) \rangle \]
\[ N^{(0)}(\tau, \Omega) = \langle \Phi | \Phi(\Omega) \rangle \]

$$E^{J(0)}_0 = \frac{\langle \Phi^{JM}_0 | H | \Phi^{JM}_0 \rangle}{\langle \Phi^{JM}_0 | \Phi^{JM}_0 \rangle}$$

where

$$|\Phi^{JM}_0\rangle \equiv \sum_K f^K J_P^{J} P^{J}_{MK} |\Phi\rangle$$

$$P^{J}_{MK} \equiv \frac{2J + 1}{16\pi^2} \int_{D_{SU(2)}} d\Omega D^{J*}_{MK}(\Omega) R(\Omega)$$
1) Solve unrestricted HF equations to generate $|\Phi\rangle$

2) Discretize the integration domain of the Euler angles $\Omega = \alpha, \beta, \gamma$

3) For each combination of $\alpha, \beta, \gamma$
   
   1) Compute matrices $R_{\alpha\beta}(\Omega)$ and $\rho^{ph}_{\alpha\alpha}(\Omega)$ in the HF single-particle basis
   
   2) Build the system of bi-orthogonal bases
   
   3) Transform the matrix elements of $T$ and $V$ in the bi-orthogonal system
   
   4) Initiate $T_n^{(1)}(\Omega)$ and run the SR-CC code using the matrix elements of $\tilde{T}(\Omega)$ and $\tilde{V}(\Omega)$
   
   5) At convergence compute and store $h(\Omega), j_i(\Omega)$ and $j^2(\Omega)$

4) Using the $j_i(\Omega)$ and $N(0) = 1$, solve the coupled ODEs that determine $N(\Omega)$

5) Calculate the yrast energies $E_0^J$ and check that $J^2$ is indeed exactly restored

\[
E_0^J = \frac{\sum_{MK} f_M^J f_K^J \int_{SU(2)} d\Omega \, D_{MK}^J(\Omega) \, h(\Omega) \, N(\Omega)}{\sum_{MK} f_M^J f_K^J \int_{SU(2)} d\Omega \, D_{MK}^J(\Omega) \, N(\Omega)}
\]
Conclusions and perspectives

- First consistent symmetry-restoration scheme within CC theory
- Main features
  - Applies to any symmetry
  - Applies to any system
  - Reduces to standard SR-CC if symmetry is not broken
  - Reduces to Projected Hartree Fock at lowest order
  - Features naturally terminating expansion of energy and norm kernels
  - Accesses yrast spectroscopy
  - Denotes a multi-reference scheme amenable to parallelization

Future

- Particle-number Bogoliubov CC formalism
- Implement for (doubly) open-shell nuclei
Complementary slides
Summary

Symmetry restored for ground-state energy

\[ E_0^{J_0} = \frac{\sum_{MK} f_M^{J_0} f_K^{J_0} \int_{SU(2)} d\Omega \ D_{MK}^{J_0}(\Omega) \ h(\Omega) \ N(\Omega)}{\sum_{MK} f_M^{J_0} f_K^{J_0} \int_{SU(2)} d\Omega \ D_{MK}^{J_0}(\Omega) \ N(\Omega)} \]

Consistent SR-CC-like terminating expansions

Standard symmetry-unrestricted CC

\[ E_0^{J_0} = h(0) \]

From linked/connected kernels of SU(2) Lie algebra

No difference in exact limit/if conserved symmetry

Final remarks
1) Numerical procedure to integrate over SU(2) routinely applied in MR-EDF
2) Reduces to standard CC if the reference state does not break the symmetry
3) Reduces to Projected Hartree Fock at lowest order
4) Accesses yrast spectroscopy by restoring on \( J \neq J_0 \)
5) Truncates consistently energy and Lie algebra kernels at a given n-tuple order
6) Set of single-reference-like CC calculations at various \( \Omega \) -> amenable to parallelization
7) Captures consistently static and dynamic correlations along with their interference
Issues with near degenerate systems

Problematic reference states

- Near degenerate
- Open shell

High-order CC based on RHF or ROHF
- CCSDT or CR-CC(2,3) for single bond breaking
  [J. Noga, R.J. Bartlett, JCP 86, 7041 (1987)]
  [P. Piecuch, M. Wloch, JCP 123, 224105 (2005)]
- CCSDTQ or CR-CC(2,4) for double bond breaking
  [J. Olsen et al., JCP 104, 8007 (1996)]
- EOM-CC for states near closed shell reference
  [J.F. Stanton, R. J. Bartlett, JCP 98, 7029 (1993)]
  [G. Jansen et al., PRC 83, 054306 (2011)]
- Spin-adapted CC theory for high spin states
  [M. Heckert et al., JCP 124, 124105 (2006)]

MBPT and CC based on UHF
[R. J. Bartlett, ARPC 32, 359 (1981)]
CC and SCGF based on HFB
[V. Somà, T. Duguet, C. Barbieri, PRC 84, 064317 (2011)]
[A. Signoracci, T. Duguet, G. Hagen, to be published (2014)]

Error from CI for H$_2$O symmetric stretch (bond angle fixed at 110.6°)

Large spin contamination near 2Re
->very slow convergence
->need non-perturbative step

Good at equilibrium/dissociation

Error from CI (a) and FCI (b) scaling

[A.G. Taube, MP 108, 2951 (2010)]
AMR-CC scheme in one slide

Kernels

\[ O(\tau, \Omega) = o(\tau, \Omega)N(\tau, \Omega) \text{ with } O = H, J^2, J_z \]

\[ H(\tau, \Omega) = -\partial_\tau N(\tau, \Omega) \]

Symmetry-restored energy

\[ E_0^J = \frac{\sum_{MK} f^J_M f^J_K \int_{SU(2)} d\Omega \; D^J_{MK}(\Omega) h(\Omega) N(\Omega)}{\sum_{MK} f^J_M f^J_K \int_{SU(2)} d\Omega \; D^J_{MK}(\Omega) N(\Omega)} \]

Coupled cluster imaginary-time-dependent scheme

Connected and naturally terminating expansions of off-diagonal energy and norm kernels

N-tuply excited energy kernels

\[ h_{ij...}^{ab...}(\tau, \Omega) = \langle \Phi | e^{\mathcal{T}^+(\tau, \Omega)} \tilde{H}(\Omega) | \Phi_{ij...}^{ab...} \rangle \]

\[ h_{ij...}^{ab...}(\tau, \Omega) = -\partial_\tau \mathcal{T}_{ij...ab...}^+ \]

Operator in bi-orthogonal system

\[ | \tilde{\alpha} \rangle \equiv D(\Omega) | \alpha \rangle \]

\[ \langle \tilde{\alpha} | \equiv \langle \alpha | D^{-1}(\Omega) \]

for each rotation angle \( \Omega \)

Solve in stationary limit at \( \tau = \infty \)

Recovers single-reference CC at \( \Omega = 0 \)

Recovers Projected HF at lowest order

Set of SR-CC calculations for \( N_{sym} \sim (10) \) angle values of \( \Omega \)

Connected kernels of Lie algebra operators
Symmetry breaking reference state

Purpose of symmetry breaking reference state $|\Phi\rangle$

- Opens the gap at $\varepsilon_F$
- Non degenerate reference
- Diagrammatic methods well behaved
- Incorporates non-perturbative physics

Open shell

Near degenerate

Non degenerate

Lowdin operator in low-order MBPT based on UHF

[P.-O. Lowdin, PR 97, 1509 (1955)]
[H.B. Schlegel, JCP 92, 3075 (1988)]
[P.J. Knowles, N.C. Hardy, JCP 88, 6991 (1988)]

No generic and consistent symmetry broken & restored CC theory...
Diagrammatic and BCCSD equations (3)

Double amplitude equation

\[
0 = \langle \Phi^\alpha \beta \gamma \delta | \Omega (1 + T_1 + T_2 + \frac{1}{2} T_1^2 + \frac{1}{2} T_2^2 + T_1 T_2 + \frac{1}{3!} T_1^3 + \frac{1}{4!} T_1^4 + \frac{1}{2} T_1^2 T_2) | \Phi \rangle_C
\]