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

II. Restoring 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

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Outline

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

II. Breaking U(1) symmetry ("trivial" for SU(2)) (last thursday)

Bogoliubov coupled-cluster method

[A. Signoracci, T. Duguet, G. Hagen, G. R. Jansen, in preparation (2014)]

[T. M. Henderson, G. E. Scuseria, J. Dukelsky, A. Signoracci, T. Duguet, PRC89, 054305 (2014)]

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

Angular-momentum-restored coupled-cluster formalism

[T. Duguet, to be published in J. Phys. G: Nucl. Part. Phys (2014) ; arXiv:1406.7183]

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 + … inter-nucleon interactions
- Solve A-body Schrödinger equation
- Thorough assessment of errors needed

High predictive power
Limited applicability domain

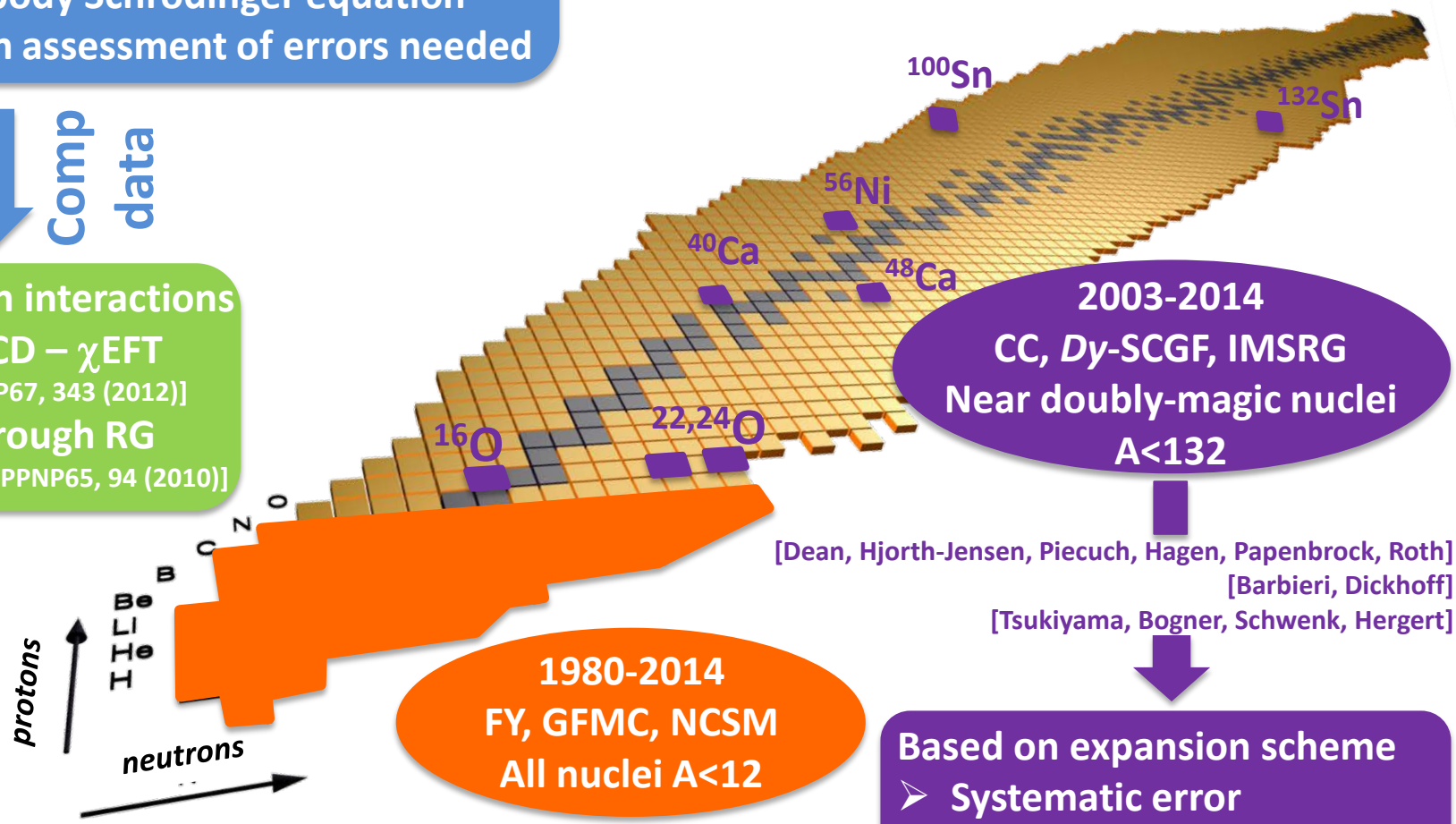
Input

Comp data

Inter-nucleon interactions
- Link to QCD – χEFT

[E. Epelbaum, PPNP67, 343 (2012)]
- Soften through RG

[S.K. Bogner *et al.*, PPNP65, 94 (2010)]



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

[Dean, Hjorth-Jensen, Piecuch, Hagen, Papenbrock, Roth]
[Barbieri, Dickhoff]
[Tsukiyama, Bogner, Schwenk, Hergert]

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

[Carlson, Pieper, Wiringa]
[Barrett, Vary, Navratil, Ormand]

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

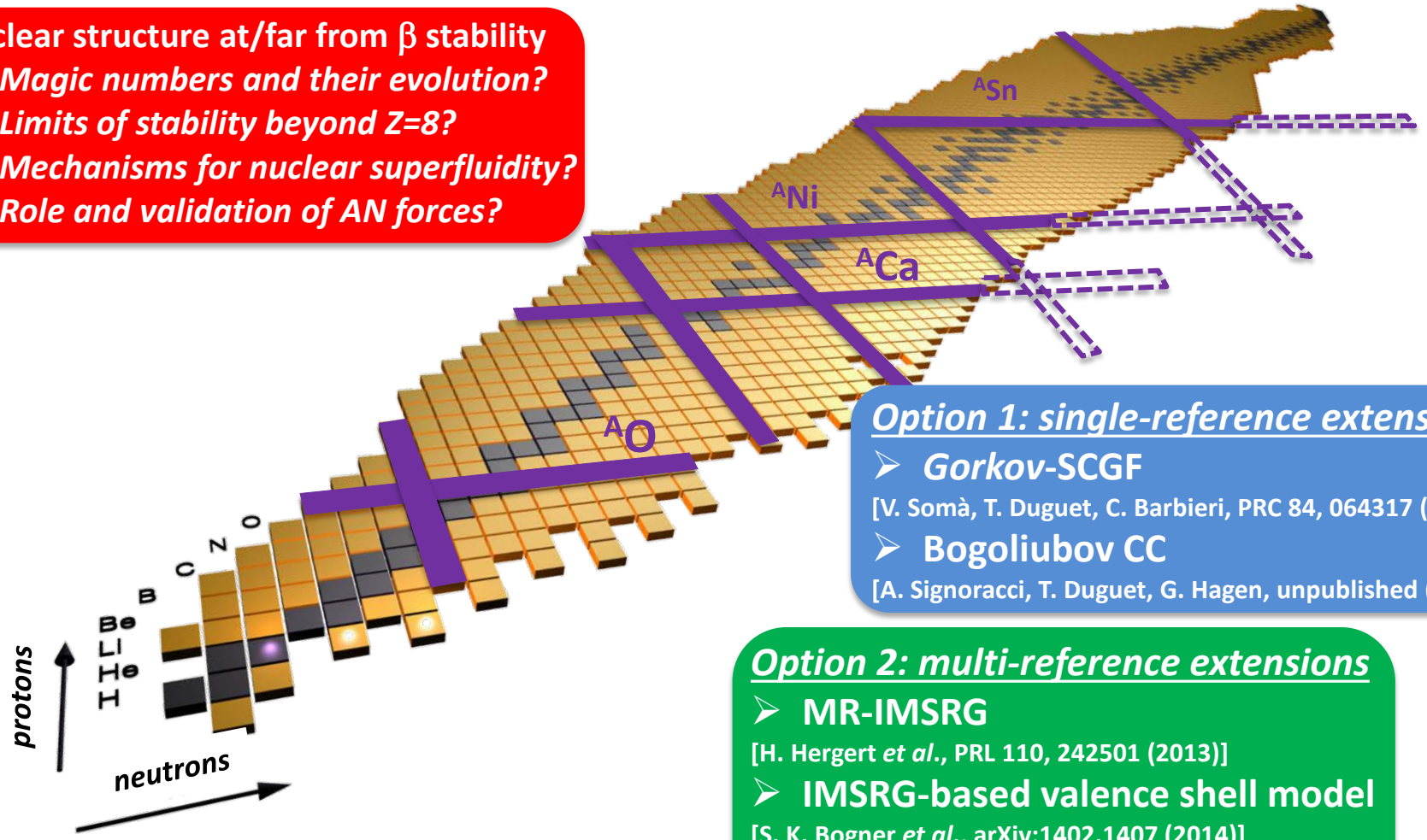
Towards ab-initio methods for open-shell nuclei

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

Target state — Wave operator — Reference state

$$|\Psi_0\rangle = \Omega_0 |\Phi_0\rangle$$

A-body ground state

Expand Ω_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

Breaks down for open-shell nuclei

Singly/doubly open shell

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

Contamination from other A / J^2 and M

ph degeneracy <-> Goldstone mode

Singly/doubly open shell

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

Multi-reference character

Finite inertia <-> *Resolve Goldstone mode*

Symmetry and symmetry breaking

Some symmetries of H

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

Dealt with by decoupling internal and CM motions

Symmetry breaking and associated physics

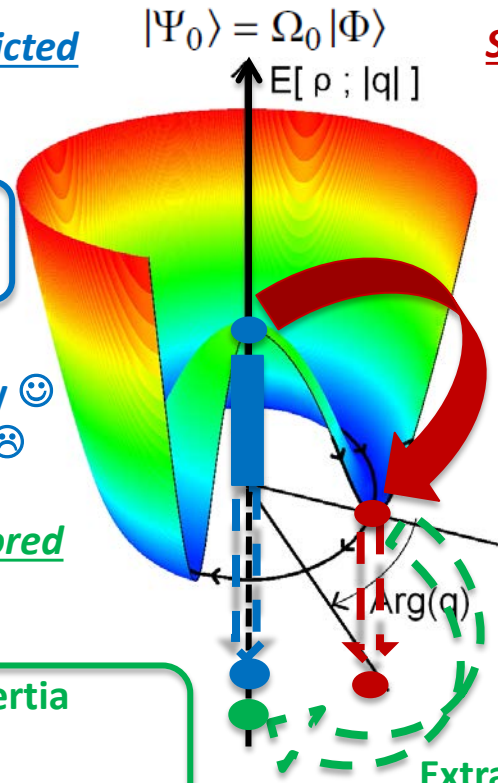
Correlations	ΔE	Excitation	Nuclei
Pairing	<2MeV	Gap	but doubly magic
Angular loc.	<20MeV	Rot. band	but singly magic

One way is to enforce the symmetry throughout the description

Another way is to let symmetry break in low order description

Symmetry restricted description

Symmetry breaking description



particle-hole (quasi)degeneracy

ph degeneracy <-> Goldstone mode

Good symmetry ☺
Hard to get ΔE ☹

Account of ΔE ☺

Symmetry restored description

Symmetry lost ☹
Fictitious in nuclei!

Finite inertia <-> ***Resolve Goldstone mode***

Extra ΔE ☺
Good symmetry ☺

Restoration of symmetries

$\|\Psi^x\rangle$	ΔE	Spectro
N,Z	~1MeV	Pairing rot.
J,M	~2MeV	Rot. band

Crucial for specific observables

Part II

Symmetry-restored coupled-cluster theory

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Account of single-reference CC method (1)

Nuclear Hamiltonian

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

Anti-symmetrized matrix elements

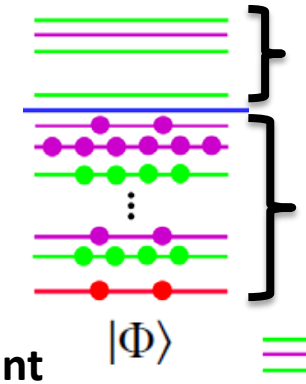
$$\bar{v}_{\alpha\beta\gamma\delta} \equiv v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$$

Wave-function ansatz

$$|\Psi_0\rangle \equiv e^T |\Phi\rangle$$

Product state of reference

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

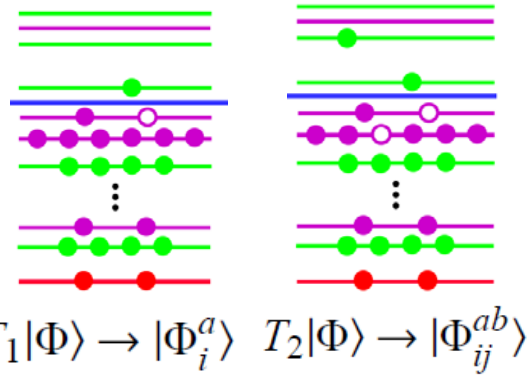


Cluster operator

$$T \equiv T_1 + T_2 + T_3 + \ldots$$

N-tuple connected component

$$T_n \equiv \frac{1}{(n!)^2} \sum_{ijk\ldots abc\ldots} t_{ijk\ldots}^{abc\ldots}\, a_a^\dagger a_b^\dagger a_c^\dagger \ldots a_k a_j a_i$$



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

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

xe^{-T}

$$\bar{H}|\Phi\rangle = E_0|\Phi\rangle$$

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

Similarity-transformed Hamiltonian

$$\bar{H} \equiv e^{-T} H e^{T}$$

Baker-Campbell-Hausdorff + Wick theorem

$$\bar{H} = H + (HT)_c + \frac{1}{2!}(HTT)_c + \frac{1}{3!}(HTTT)_c + \frac{1}{4!}(HTTTT)_c$$

Exponential naturally terminates

Energy equation

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

Disconnected parts canceled out a posteriori

Amplitude equation to determine T_n

$$\langle\Phi_{i\ldots}^{a\cdots}|(He^T)_c|\Phi\rangle = 0$$

Variant without xe^{-T} first

$$\langle\Phi|He^T|\Phi\rangle = E_0\langle\Phi|e^T|\Phi\rangle$$

$$\langle\Phi_{i\ldots}^{a\cdots}|He^T|\Phi\rangle = E_0\langle\Phi_{i\ldots}^{a\cdots}|e^T|\Phi\rangle$$

Define energy and norm kernels

$$H(\infty,0) = E_0 N(\infty,0)$$

$$H_{i\ldots}^{a\cdots}(\infty,0) = E_0 N_{i\ldots}^{a\cdots}(\infty,0)$$

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** $D^J_{MK}(\Omega) \equiv \langle \Psi^{JM}|R(\Omega)|\Psi^{J'K}\rangle \delta_{JJ'}$ **labeled by J and spanned by *M***

Wigner D functions

Eigen-states of H

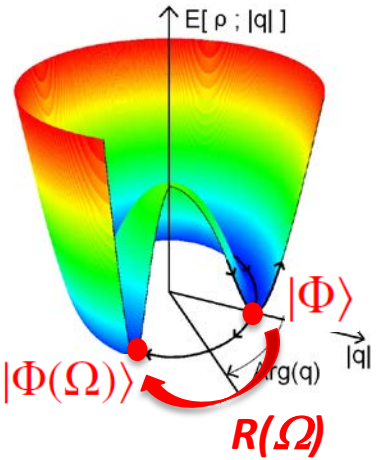
$[H, R(\Omega)] = 0$ **leads to** $H|\Psi^{JM}_\mu\rangle = E^J_\mu |\Psi^{JM}_\mu\rangle$

1) UHF reference state

$|\Phi\rangle$

2) Rotated reference state

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



Imaginary-time dependent scheme

Thouless transformation
Infinite sum of p-h excitations

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

Time-evolved state $|\Psi(\tau)\rangle \equiv \mathcal{U}(\tau)|\Phi\rangle$

Off-diagonal kernels

$$N(\tau,\Omega) \equiv \langle\Psi(\tau)|\mathbb{1}|\Phi(\Omega)\rangle$$
$$H(\tau,\Omega) \equiv \langle\Psi(\tau)|H|\Phi(\Omega)\rangle$$
$$J_i(\tau,\Omega) \equiv \langle\Psi(\tau)|J_i|\Phi(\Omega)\rangle$$
$$J^2(\tau,\Omega) \equiv \langle\Psi(\tau)|J^2|\Phi(\Omega)\rangle$$

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

Reduced kernel $\mathcal{O}(\tau,\Omega) \equiv O(\tau,\Omega)/N(\tau,0)$

Ground state and energy

$\lim_{\tau\to\infty}$

$|\Psi(\infty)\rangle = |\Psi^{J_0}_0\rangle$

$\mathcal{H}(\infty,\Omega) = E^{J_0}_0 \mathcal{N}(\infty,\Omega)$

-True for all Ω

-Usual sym. unrest. MB schemes (Ω = 0)

Intermediate normalization $\mathcal{N}(\tau,0) = 1$

Expand un-rotated energy kernel $\mathcal{H}(\infty,0) = E^{J_0}_0$

Master equations (2)

Expansion of rotated kernels over IRREPs of SU(2)

$$N(\infty,\Omega) = e^{-\tau E_0^{J_0}} \sum_{MK} \langle \Phi | \Psi_0^{J_0 M} \rangle \langle \Psi_0^{J_0 K} | \Phi \rangle D^{J_0}_{MK}(\Omega)$$

$$H(\infty,\Omega) = e^{-\tau E_0^{J_0}} E_0^{J_0} \sum_{MK} \langle \Phi | \Psi_0^{J_0 M} \rangle \langle \Psi_0^{J_0 K} | \Phi \rangle D^{J_0}_{MK}(\Omega)$$

Time propagation selects the proper IRREP

Straight ratio

$$\mathcal{H}(\infty,\Omega) = E_0^{J_0} \mathcal{N}(\infty,\Omega)$$

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

$$N_{\text{approx}}(\infty,\Omega) \equiv \sum_J \sum_{MK} \mathcal{N}^J_{MK} D^J_{MK}(\Omega)$$

$$H_{\text{approx}}(\infty,\Omega) \equiv \sum_J \sum_{MK} \mathcal{E}^J_{MK} \mathcal{N}^J_{MK} D^J_{MK}(\Omega)$$

IRREPs still mixed as $\tau \to \infty$

<=>

The good symmetry is lost

Extract good IRREP

Orthogonality of IRREPs

Symmetry-restored energy

$$E_0^{J_0} = \frac{\sum_{MK} f_M^{J_0 *} f_K^{J_0} \int_{SU(2)} d\Omega \, D^{J_0 *}_{MK}(\Omega) \mathcal{H}(\infty,\Omega)}{\sum_{MK} f_M^{J_0 *} f_K^{J_0} \int_{SU(2)} d\Omega D^{J_0 *}_{MK}(\Omega) \mathcal{N}(\infty,\Omega)}$$

Standard kernels $D^J_{MK}(0) = \delta_{MK}$

$$N_{\text{approx}}(\infty,0) \equiv \sum_J \sum_M \mathcal{N}^J_{MM} \otimes$$

$$H_{\text{approx}}(\infty,0) \equiv \sum_J \sum_M \mathcal{E}^J_{MM} \mathcal{N}^J_{MM} \otimes$$

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 $\mathcal{H}(\tau,\Omega)$ *and* norm $\mathcal{N}(\tau,\Omega)$ kernels**

Expansion and truncation must be consistent

Problematic to find a naturally terminating expansion

Does not stay normalized when Ω varies!

Many-body perturbation theory (1)

Symmetry-breaking unperturbed system

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

$$\left.\begin{aligned} H_0 |\Phi\rangle &= \varepsilon_0 |\Phi\rangle \\ H_0 |\Phi_{ij\ldots}^{ab\ldots}\rangle &= (\varepsilon_0 + \varepsilon_{ij\ldots}^{ab\ldots}) |\Phi_{ij\ldots}^{ab\ldots}\rangle \end{aligned}\right\} \text{with} \left\{\begin{aligned} \varepsilon_0 &= \sum_{i=1}^{N} e_i \\ \varepsilon_{ij\ldots}^{ab\ldots} &= e_a + e_b + \ldots - e_i - e_j - \ldots \end{aligned}\right.$$

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

Ω-dependent part couples p and h spaces

$$\rho_{\alpha\beta}(\Omega) \equiv \frac{\langle \Phi | a_\beta^\dagger a_\alpha | \Phi(\Omega) \rangle}{\langle \Phi | \Phi(\Omega) \rangle} \longrightarrow \rho(\Omega) = \begin{pmatrix} 1^{hh} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ R(\Omega) M^{-1}(\Omega) & 0 \end{pmatrix} \equiv \rho(0) + \rho^{ph}(\Omega)$$

Density matrix of sym. unrest. reference state

Many-body perturbation theory (2)

Off-diagonal unperturbed propagator = basic contraction for Wick Theorem

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

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

Off diagonal Wick theorem
[R. Balian. E. Brezin, NC 64, 37 (1969)]

Rotated norm kernel

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

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

Rotated energy kernel

Factorization valid for any operator kernel $O(\tau,\Omega)$

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

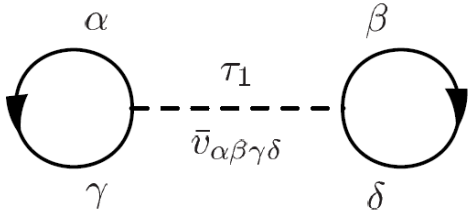
where $h(\tau,\Omega) \equiv t(\tau,\Omega)+v(\tau,\Omega) \equiv \sum_{n=0}^{\infty}\left[t^{(n)}(\tau,\Omega)+v^{(n)}(\tau,\Omega)\right]$

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

Many-body perturbation theory (3)

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

$$n_V^{(1)}(\tau,\Omega) = -\frac{1}{2}\sum_{\alpha\beta\gamma\delta}\int_0^\tau d\tau_1\, \bar{v}_{\alpha\beta\gamma\delta}\, G^0_{\gamma\alpha}(\tau_1,\tau_1;\Omega)\, G^0_{\delta\beta}(\tau_1,\tau_1;\Omega)$$



$$= -\frac{\tau}{2}\sum_{ij}\bar{v}_{ijij} \Big\} \; n_V^{(1)}(\tau,0)$$ ***= 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 Ω-dependent part***

Large τ limit

$$n(\tau,0) \underset{\tau\to\infty}{\longrightarrow} -\tau\Delta E_0^{J_0} + \ln\left[\sum_M |\langle\Phi|\Psi_0^{J_0M}\rangle|^2\right]$$

$$n(\tau,\Omega) - n(\tau,0) \underset{\tau\to\infty}{\longrightarrow} \aleph(\Omega)$$

$$\mathcal{N}(\infty,\Omega) = e^{\aleph(\Omega)}\langle\Phi|\Phi(\Omega)\rangle \equiv \mathcal{N}(\Omega)$$

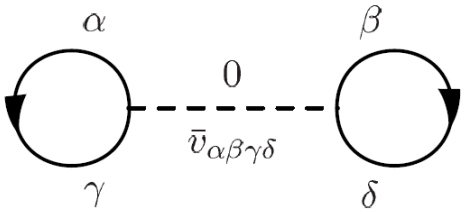
Goldstone linked-cluster based on UHF
->nice but not what we are after!

$$\Delta E_0^{J_0} = \langle\Phi|H_1\sum_{k=1}^{\infty}\left(\frac{1}{\varepsilon_0-H_0}H_1\right)^{k-1}|\Phi\rangle_c$$

Many-body perturbation theory (3)

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

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



$$= +\frac{1}{2}\sum_{ij} \bar{v}_{ijij} \Big\} \quad v^{(0)}(\tau,0)$$ ***= standard sym. unrest. contribution***

$$+\sum_{ijc} \bar{v}_{ijcj}\,\rho^{ph}_{ci}(\Omega)$$

$$+\frac{1}{2}\sum_{ijab} \bar{v}_{ijab}\,\rho^{ph}_{ai}(\Omega)\,\rho^{ph}_{bj}(\Omega) \Big\}$$ ***Genuinely Ω-dependent part***

Large τ limit $h(\tau,\Omega) \underset{\tau\to\infty}{\longrightarrow} h(\Omega) \Big\} \quad \mathcal{H}(\infty,\Omega) = h(\Omega)\,\mathcal{N}(\Omega)$

Signals the symmetry breaking

In the exact limit $\dfrac{\partial}{\partial\Omega} h(\Omega) = 0$

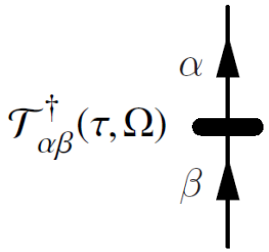
After truncation $\dfrac{\partial}{\partial\Omega} h(\Omega) \neq 0$

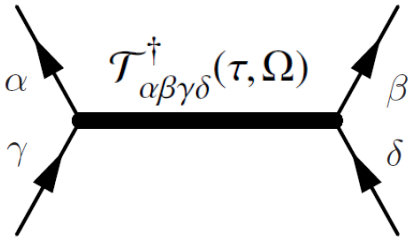
Coupled cluster theory (1) – energy kernel

β- and Ω-dependent cluster operators (or rather their hermitian conjuguate…)

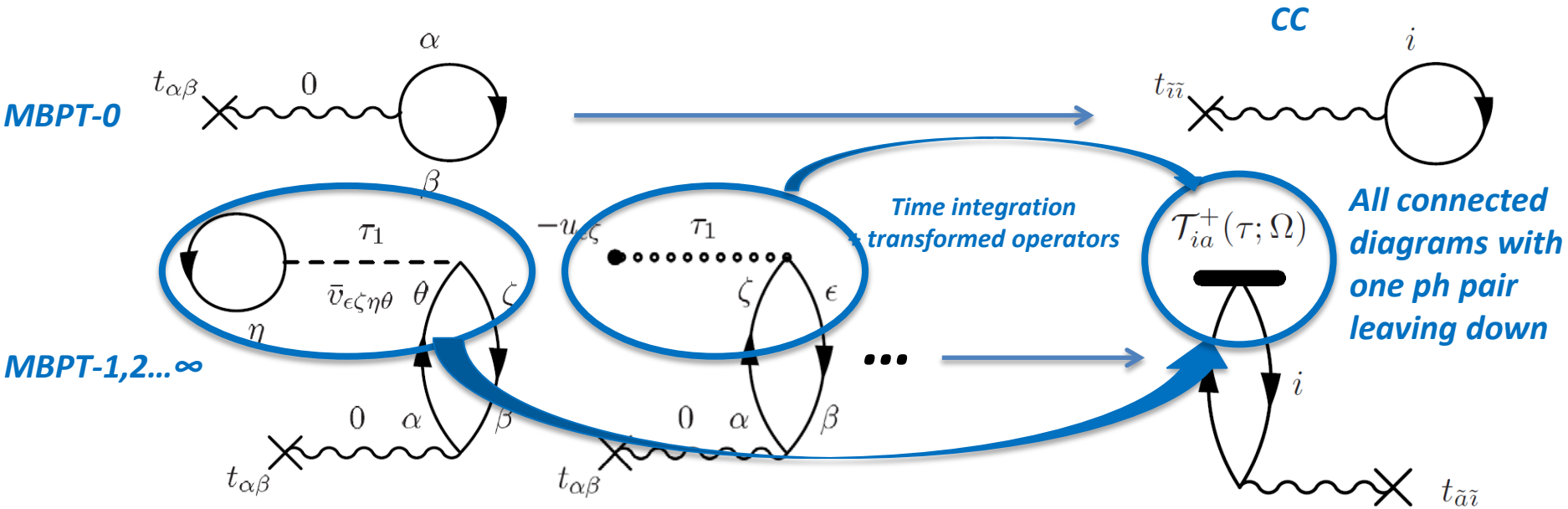
$$\mathcal{T}_1^\dagger(\tau,\Omega) \equiv \frac{1}{(1!)^2}\sum_{ia}\mathcal{T}_{ia}^\dagger(\tau,\Omega)\,a_i^\dagger\,a_a$$

$$\mathcal{T}_2^\dagger(\tau,\Omega) \equiv \frac{1}{(2!)^2}\sum_{ijab}\mathcal{T}_{ijab}^\dagger(\tau,\Omega)\,a_i^\dagger\,a_j^\dagger\,a_b\,a_a$$





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



Similar for the potential energy kernel

Coupled cluster theory (2) – energy kernel

Algebraic expressions

1) Cluster operators contracted with T/V
2) No contraction within cluster operator
3) No contraction among cluster operators

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

Cumbersome expressions

$$t(\tau,\Omega) = \langle\Phi|T + \mathcal{T}_1^\dagger(\tau,\Omega)\,T|\Phi(\Omega)\rangle_c \langle\Phi|\Phi(\Omega)\rangle^{-1}$$

$$= \sum_i t_{\tilde{i}\tilde{i}}(\Omega) + \sum_{ia} \mathcal{T}_{ia}^\dagger(\tau,\Omega)\, t_{\tilde{a}\tilde{i}}(\Omega)$$

$$v(\tau,\Omega) = \langle\Phi|V + \mathcal{T}_1^\dagger(\tau,\Omega)\,V + \mathcal{T}_2^\dagger(\tau,\Omega)\,V + \tfrac{1}{2}\mathcal{T}_1^{\dagger 2}(\tau,\Omega)\,V|\Phi(\Omega)\rangle_c \langle\Phi|\Phi(\Omega)\rangle^{-1}$$

$$= \tfrac{1}{2}\sum_{ij} \bar{v}_{\tilde{i}\tilde{j}\tilde{i}\tilde{j}}(\Omega) + \sum_{ija} \mathcal{T}_{ia}^\dagger(\tau,\Omega)\,\bar{v}_{\tilde{a}\tilde{j}\tilde{i}\tilde{j}}(\Omega) + \tfrac{1}{4}\sum_{ijab} \mathcal{T}_{ijab}^\dagger(\tau,\Omega)\,\bar{v}_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}}(\Omega) + \sum_{ijab} \mathcal{T}_{ia}^\dagger(\tau,\Omega)\,\mathcal{T}_{jb}^\dagger(\tau,\Omega)\,\bar{v}_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}}(\Omega)$$

Transformed operators

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

Bi-orthogonal system

$$|\tilde{\alpha}\rangle \equiv D(\Omega)|\alpha\rangle \qquad \langle\tilde{\alpha}| \equiv \langle\alpha|D^{-1}(\Omega)$$

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

$$\tilde{O}(\Omega) \equiv \left(\frac{1}{n!}\right)^2 \sum_{\alpha\ldots\beta\gamma\ldots\delta} O_{\tilde{\alpha}\ldots\tilde{\beta}\tilde{\gamma}\ldots\tilde{\delta}}(\Omega)\, a_\alpha^\dagger \ldots a_\beta^\dagger a_\delta \ldots a_\gamma$$

Need equations for the CC amplitudes

CC expansion of the off diagonal energy kernel

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

Coupled cluster theory (3) – amplitudes

N-tuples off-diagonal norm and energy kernels

$$N^{ab\cdots}_{ij\cdots}(\tau,\Omega) \equiv \langle \Psi(\tau)|A^{ab\cdots}_{ij\cdots}|\Phi(\Omega)\rangle$$

$$H^{ab\cdots}_{ij\cdots}(\tau,\Omega) \equiv \langle \Psi(\tau)|HA^{ab\cdots}_{ij\cdots}|\Phi(\Omega)\rangle$$

where $A^{ab\cdots}_{ij\cdots} \equiv a^\dagger_a a_i a^\dagger_b a_j \ldots$

Dynamical amplitude equations

1) Perform MBPT expansion
2) Recast in terms of cluster operators
3) Remove disconnected terms involving $A^{ab\cdots}_{ij\cdots}$
4) Recast in terms of transformed operators

$$H^{ab\cdots}_{ij\cdots}(\tau,\Omega) = -\partial_\tau N^{ab\cdots}_{ij\cdots}(\tau,\Omega)$$

Imaginary-time-dependent equation of motion

$$\langle \Phi|e^{\mathcal{T}^\dagger(\tau,\Omega)}\tilde{H}(\Omega)|\Phi^{ab\cdots}_{ij\cdots}\rangle_c = -\cancel{\partial_\tau \mathcal{T}^\dagger_{ij\cdots ab\cdots}}(\tau,\Omega)$$

Naturally terminating

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

$$N(\tau,\Omega) = e^{-\tau\varepsilon_0 + n(\tau,\Omega)} \langle \Phi | \Phi(\Omega) \rangle$$

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 $j_i(\tau,\Omega)$**

Display naturally terminating CC expansions

Initial condition

$$\mathcal{N}(\tau,0) = 1$$

Coupled ODEs

$$\frac{\partial}{\partial\alpha}\mathcal{N}(\tau,\Omega) + \frac{i}{\hbar} j_z(\tau,\Omega)\,\mathcal{N}(\tau,\Omega) = 0$$

$$\frac{\partial}{\partial\beta}\mathcal{N}(\tau,\Omega) - \frac{i}{\hbar}\Big[\sin\alpha\, j_x(\tau,\Omega) - \cos\alpha\, j_y(\tau,\Omega)\Big]\mathcal{N}(\tau,\Omega) = 0$$

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

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

$$\frac{\int_{SU(2)} d\Omega\, D^{J\,*}_{MK}(\Omega)\,\mathcal{J}_z(\tau,\Omega)}{\int_{SU(2)} d\Omega\, D^{J\,*}_{MK}(\Omega)\,\mathcal{N}(\tau,\Omega)} = M\hbar$$

$$\frac{\sum_{MK} f^{J\,*}_M f^J_K \int_{D_{SU(2)}} d\Omega\, D^{J\,*}_{MK}(\Omega)\,\mathcal{J}^2(\tau,\Omega)}{\sum_{MK} f^{J\,*}_M f^J_K \int_{D_{SU(2)}} d\Omega\, D^{J\,*}_{MK}(\Omega)\,\mathcal{N}(\tau,\Omega)} = J(J+1)\hbar^2$$

$$\frac{\int_{SU(2)} d\Omega\, D^{J\,*}_{MK}(\Omega)\Big[\sin\beta\cos\alpha\,\mathcal{J}_x(\tau,\Omega) + \sin\beta\sin\alpha\,\mathcal{J}_y(\tau,\Omega) + \cos\beta\,\mathcal{J}_z(\tau,\Omega)\Big]}{\int_{SU(2)} d\Omega\, D^{J\,*}_{MK}(\Omega)\,\mathcal{N}(\tau,\Omega)} = K\hbar$$

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

$$E_0^J = \frac{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D_{MK}^{J*}(\Omega)\, h(\Omega)\, \mathcal{N}(\Omega)}{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D_{MK}^{J*}(\Omega)\, \mathcal{N}(\Omega)}$$

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

$$E_0^{J_0} = h(0)$$

2. Projected Hartree Fock is recovered at lowest order

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

$$\Rightarrow \quad E_0^{J(0)} = \frac{\langle\Phi_0^{JM}|H|\Phi_0^{JM}\rangle}{\langle\Phi_0^{JM}|\Phi_0^{JM}\rangle}$$

where $|\Phi_0^{JM}\rangle \equiv \sum_K f_K^J P_{MK}^J |\Phi\rangle$

$$P_{MK}^J \equiv \frac{2J+1}{16\pi^2} \int_{D_{SU(2)}} d\Omega\, D_{MK}^{J*}(\Omega)\, R(\Omega)$$

Algorithm

Steps to follow on the basis of a symmetry-unrestricted (e.g. m scheme) SR-CC code

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 α, β, γ
    1) Compute matrices $R_{\alpha\beta}(\Omega)$ and $\rho^{ph}_{ai}(\Omega)$ 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 $\mathcal{T}_n^{\dagger(1)}(\Omega)$ 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 $\mathcal{N}(0) = 1$, solve the coupled ODEs that determine $\mathcal{N}(\Omega)$
5) Calculate the yrast energies E_0^J and check that J^2 is indeed exactly restored

$$E_0^J = \frac{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D_{MK}^{J*}(\Omega)\, h(\Omega)\, \mathcal{N}(\Omega)}{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D_{MK}^{J*}(\Omega)\, \mathcal{N}(\Omega)}$$

Conclusions and perspectives

Conclusions

- 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

Appendix

Complementary slides

Summary

Symmetry restored for ground-state energy

Consistent SR-CC-like terminating expansions

$$E_0^{J_0} = \frac{\sum_{MK} f_M^{J_0 *} f_K^{J_0} \int_{SU(2)} d\Omega \, D_{MK}^{J_0 *}(\Omega) \, h(\Omega) \, \mathcal{N}(\Omega)}{\sum_{MK} f_M^{J_0 *} f_K^{J_0} \int_{SU(2)} d\Omega \, D_{MK}^{J_0 *}(\Omega) \, \mathcal{N}(\Omega)}$$

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

Standard symmetry-unrestricted CC

$$E_0^{J_0} = h(0)$$

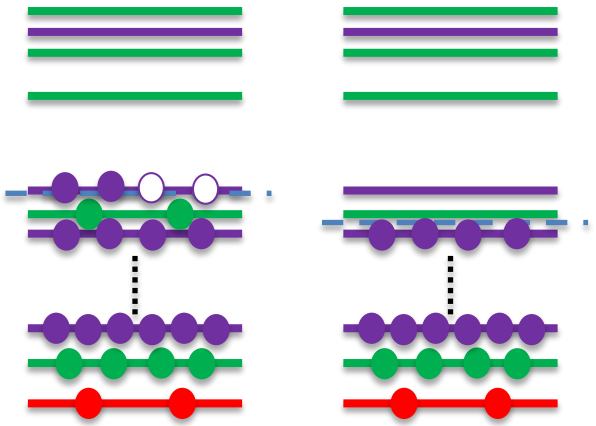
No difference in exact limit/if conserved symmetry

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 Ω -> amenable to *parallelization***
7) **Captures consistently static and dynamic correlations along with their interference**

Issues with near degenerate systems

Problematic reference states



Open shell *Near degenerate*

Multi reference

MR-MBPT
MR-CC
MR-IMSRG

Single reference
Perturbative

Single reference
Non perturbative

Single reference
Breaking symmetry

MBPT fails because of $e_a - e_i \to 0$

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)]

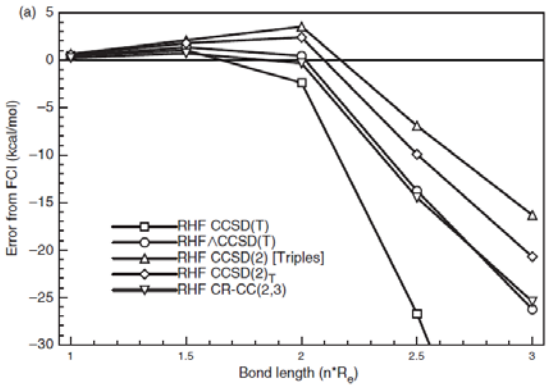
-EOM-CC for states near closed shell reference
[J.F. Stanton, R. J. Bartlett, JCP 98, 7029 (1993)]
[G. Jansen *et al.*, PRC 83, 054306 (2011)]

-Spin-adapted CC theory for high spin states
[M. Heckert *et al.*, JCP 124, 124105 (2006)]

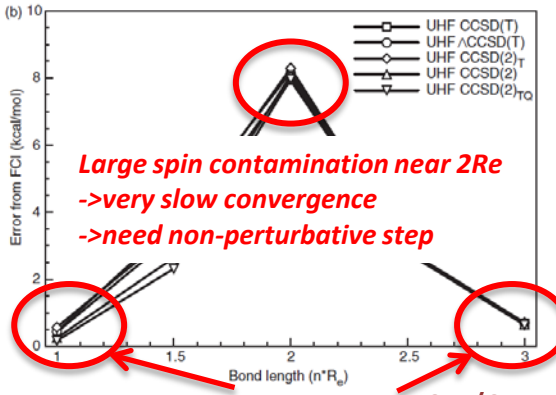
MBPT and CC based on UHF
[R. J. Bartlett, ARPC 32, 359 (1981)]

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_2O symmetric stretch (bond angle fixed at 110.6°)



[A.G. Taube, MP 108, 2951 (2010)]



Good at equilibrium/dissociation

AMR-CC scheme in one slide

Kernels

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

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

Symmetry-restored energy

$$E_0^J = \frac{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D_{MK}^{J*}(\Omega)\, h(\Omega)\, \mathcal{N}(\Omega)}{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D_{MK}^{J*}(\Omega)\, \mathcal{N}(\Omega)}$$

Coupled cluster imaginary-time-dependent scheme

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

N-tuply excited energy kernels

$$h_{ij\ldots}^{ab\ldots}(\tau,\Omega) = \langle\Phi|e^{\mathcal{T}^\dagger(\tau,\Omega)}\tilde{H}(\Omega)|\Phi_{ij\ldots}^{ab\ldots}\rangle_c$$

$$h_{ij\ldots}^{ab\ldots}(\tau,\Omega) = -\partial_\tau \mathcal{T}_{ij\ldots ab\ldots}^\dagger$$

Operator in bi-orthogonal system

$$\begin{aligned} |\tilde{\alpha}\rangle &\equiv D(\Omega)|\alpha\rangle \\ \langle\tilde{\alpha}| &\equiv \langle\alpha|D^{-1}(\Omega) \end{aligned}$$

for each rotation angle Ω

Norm kernel

$$\frac{\partial}{\partial\alpha}\mathcal{N}(\tau,\Omega) + \frac{i}{\hbar} j_z(\tau,\Omega)\,\mathcal{N}(\tau,\Omega) = 0$$

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

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

connected kernels of Lie algebra operators

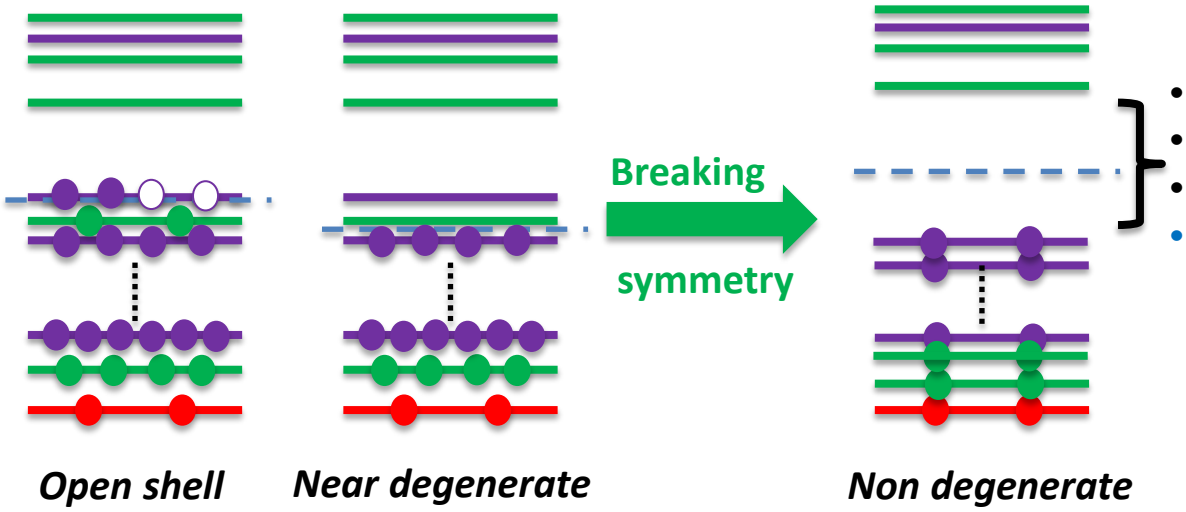
Solve in stationary limit at $\tau=\infty$

Recovers single-reference CC at Ω = 0
Recovers Projected HF at lowest order

Set of SR-CC calculations for N_{sym}~$(10)^{angle}$ values of Ω

Symmetry breaking reference state

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



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

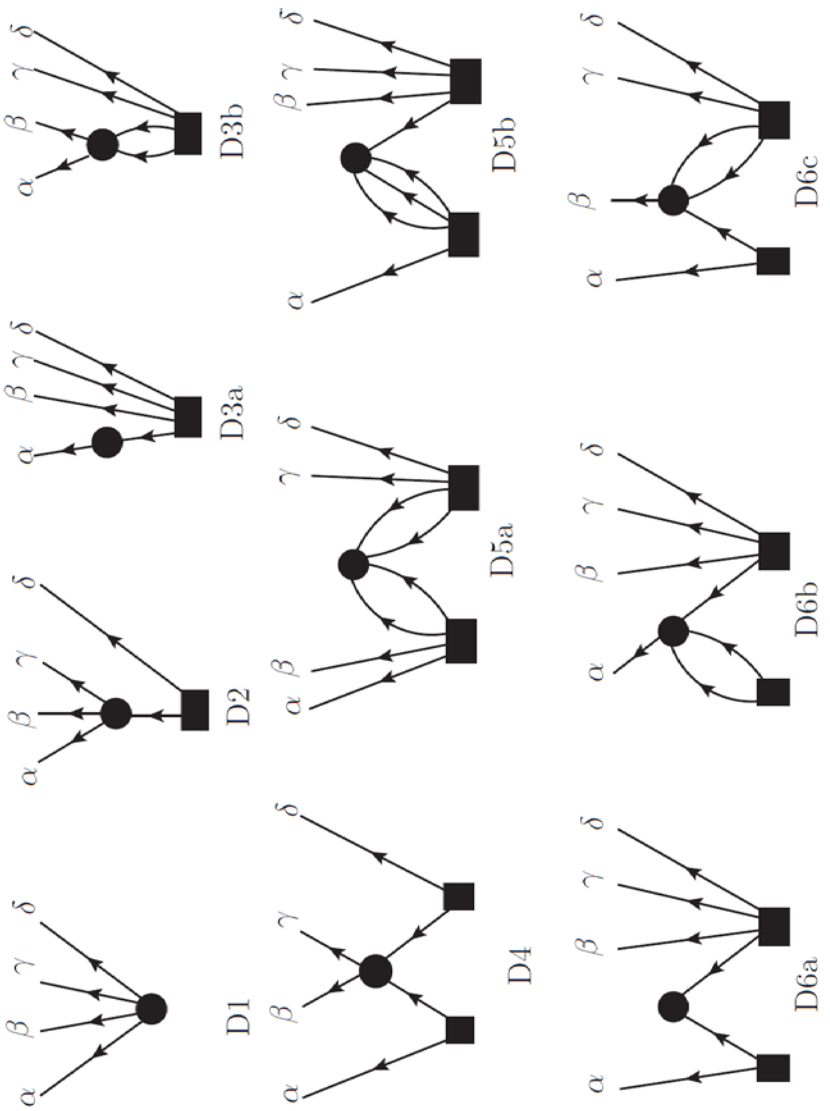
Lowdin operator in low-order MBPT based on UHF
[P.-O. Lowdin, PR 97, 1509 (1955)]
[H.B. Schlegel, JCP 92, 3075 (1988)]
[P.J. Knowles, N.C. Hardy, JCP 88, 6991 (1988)]

Need to restore the symmetry

No generic and consistent symmetry broken & restored CC theory…

Diagrammatic and BCCSD equations (3)

Double amplitude equation



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