# *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)]*

# Part I

## *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

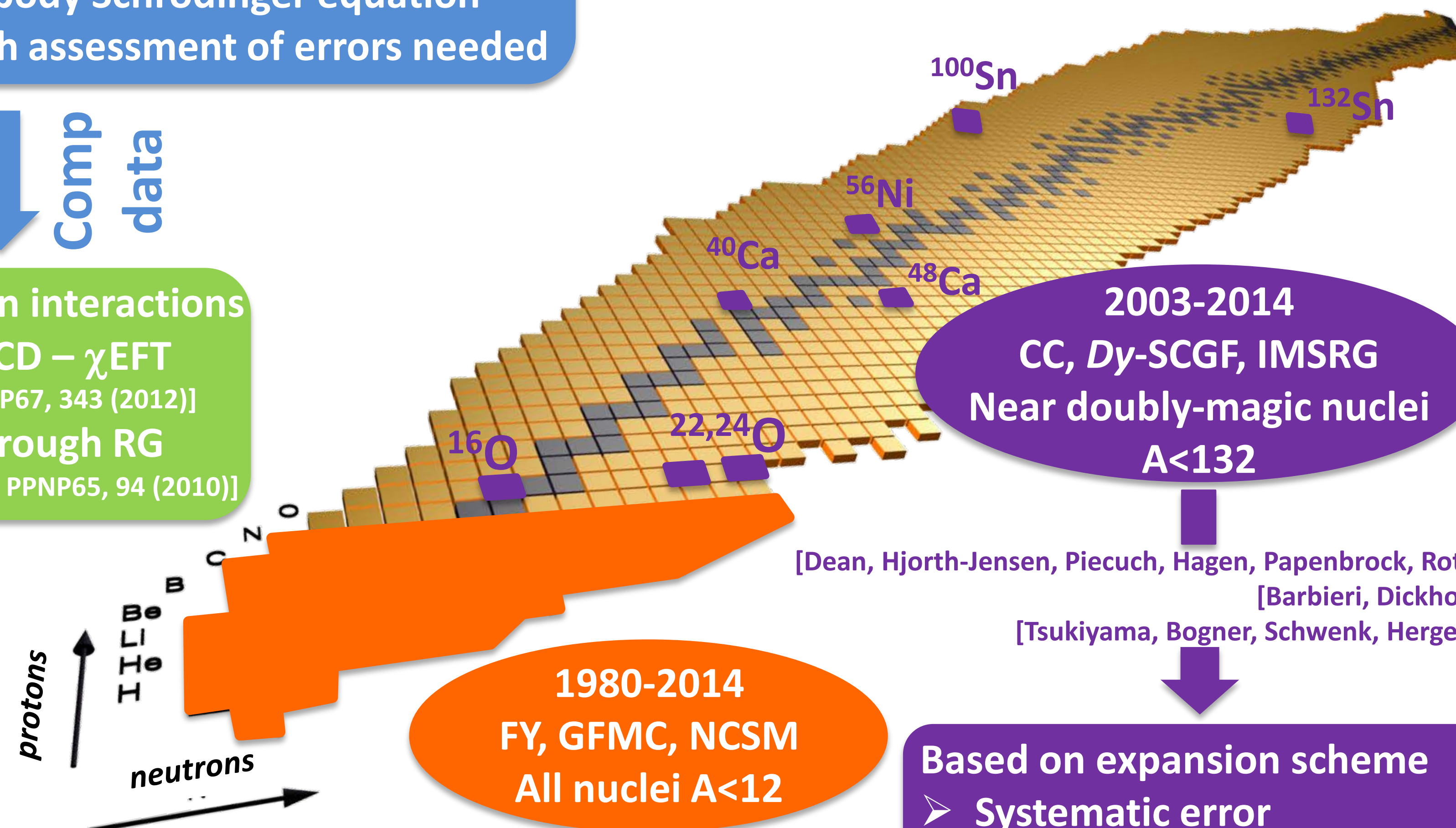
Input

Comp data

Inter-nucleon interactions
- Link to QCD – $\chi$EFT

[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

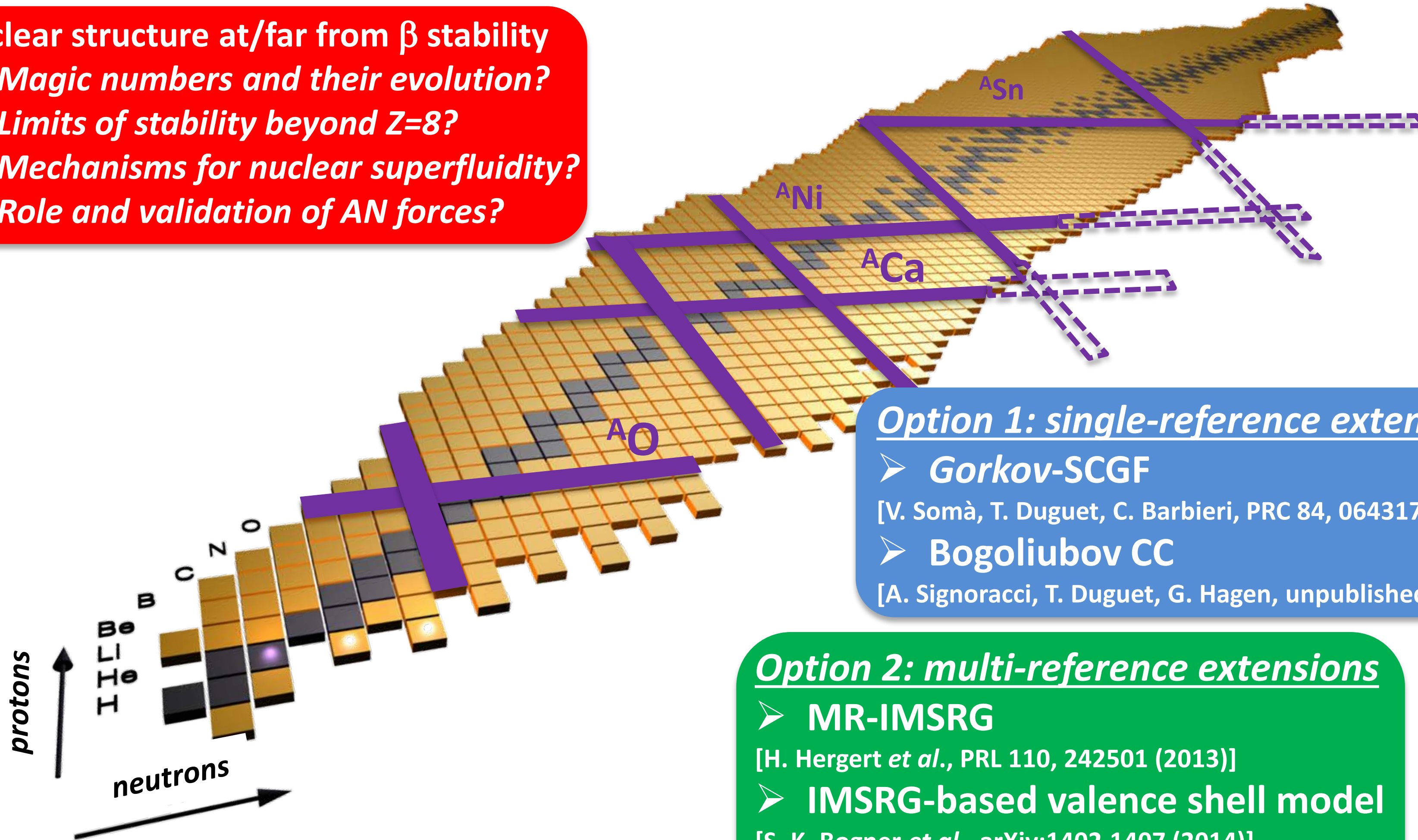
[Carlson, Pieper, Wiringa]
[Barrett, Vary, Navratil, Ormand]

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 $\Omega_0$ 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<br>CC |

*Breaks down for open-shell nuclei*

**Singly/doubly open shell**

| UHF(B) reference |
|---|
| *breaks A / $J^2$ and M* |
| *Go*-SCGF<br>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*

ESNT

# 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 |

Dealt with by decoupling internal and CM motions

*Restoration of symmetries*

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

Crucial for specific observables

*Symmetry breaking and associated physics*

| Correlations | $\Delta$E | 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*

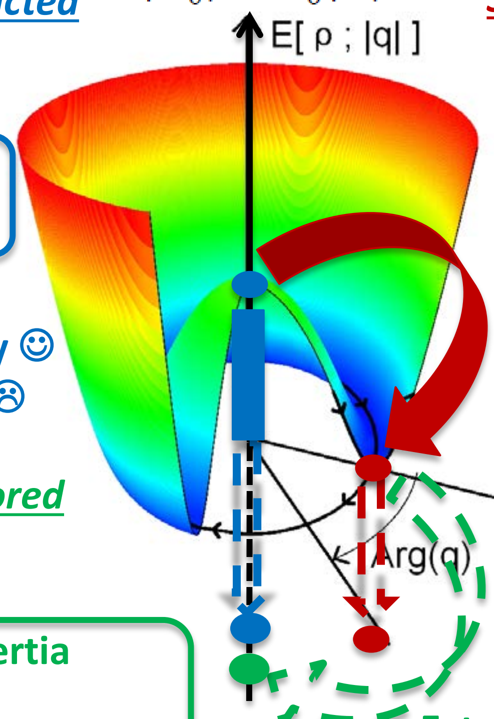
particle-hole (quasi)degeneracy

Good symmetry ☺
Hard to get $\Delta$E ☹

*Symmetry restored description*

Finite inertia
<->
*Resolve Goldstone mode*

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




*Symmetry breaking description*

ph degeneracy
<->
Goldstone mode

Account of $\Delta$E ☺

Symmetry lost ☹
*Fictitious in nuclei!*

Extra $\Delta$E ☺
Good symmetry ☺

# Part II

## *Symmetry-restored coupled-cluster theory*

**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)]

# Account of single-reference CC method (1)

**Nuclear Hamiltonian**

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

**Anti-symmetrized matrix elements**

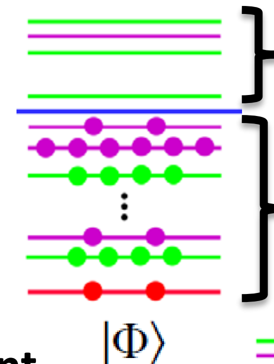
$$\bar{v}_{\alpha\beta\gamma\delta} \equiv v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}$$

**Wave-function ansatz**

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

**Product state of reference**

$$|\Phi\rangle \equiv \prod_{i=1}^{N} a^\dagger_i |0\rangle$$

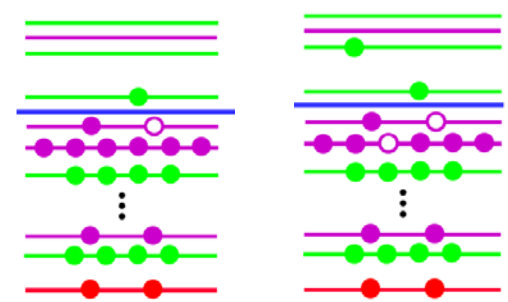



**Cluster operator**

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

**N-tuple connected component**

$$T_n \equiv \frac{1}{(n!)^2} \sum_{ijk\ldots abc\ldots} t^{abc\ldots}_{ijk\ldots}\, a^\dagger_a a^\dagger_b a^\dagger_c \ldots a_k a_j a_i$$




**Norm kernel in intermediate normalization**

Only non-zero ph matrix elements

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

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 $T_n$**

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

Obtain algebraic expressions via Wick theorem

Approx <-> truncate $T$ beyond a certain $T_n$

Exemple: retaining $T_1$ and $T_2$ defines CCSD

**Variant without $xe^{-T}$ first**

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

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

Define energy and norm kernels

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

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

ESNT

# 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

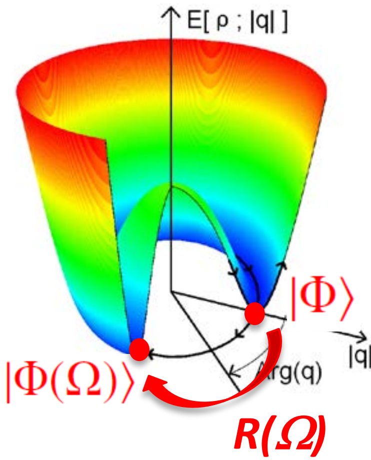
$[H, R(\Omega)] = 0$ leads to $H|\Psi^{JM}_\mu\rangle = E^J_\mu |\Psi^{JM}_\mu\rangle$

1) UHF reference state

$|\Phi\rangle$

2) Rotated reference state

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




Imaginary-time dependent scheme

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

*Thouless transformation*
*Infinite sum of p-h excitations*

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

Off-diagonal kernels

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

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 $\Omega$

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

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)**

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

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

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** $|\Phi\rangle$

$$N_{\text{approx}}(\infty,\Omega) \equiv \sum_J \sum_{MK} \mathcal{N}_{MK}^J\, D_{MK}^J(\Omega)$$

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

Extract good IRREP

Orthogonality of IRREPs

IRREPs still mixed as τ -> ∞

<=>

The good symmetry is lost

Symmetry-restored energy

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

*Superfluous in exact limit but not after truncation*

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

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

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

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 $\Omega$ varies!*

# Many-body perturbation theory (1)

**Symmetry-breaking unperturbed system**

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

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

**Rotated state**

$|\Phi(\Omega)\rangle = \prod_{i=1}^{N} a_{\bar{i}}^\dagger |0\rangle$ **with** $a_{\bar{\alpha}}^\dagger = \sum_\beta R_{\beta\alpha}(\Omega) a_\beta^\dagger$ **and** $R_{\alpha\beta}(\Omega) \equiv \langle \alpha | R(\Omega) | \beta \rangle$

$\langle \Phi | \Phi(\Omega) \rangle = \det M(\Omega)$ **where** $M_{\alpha\beta}(\Omega) \equiv R_{\alpha\beta}(\Omega) \delta_{\alpha i} \delta_{\beta j}$

**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**

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

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* $O(\tau,\Omega)$

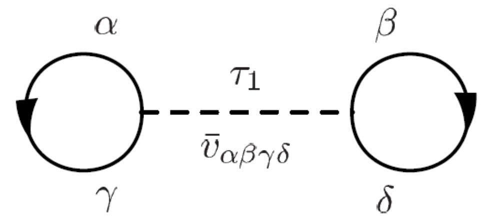
$$H(\tau,\Omega) = \langle\Phi|e^{-\tau H_0}\, T e^{-\int_0^\tau d\tau_1 H_1(\tau_1)}(T+V)|\Phi(\Omega)\rangle = h(\tau,\Omega)\,N(\tau,\Omega)$$

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 $O$

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

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




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

$n_V^{(1)}(\tau,0)$ ***= 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***

$$\begin{cases} n(\tau,0) \xrightarrow[\tau\to\infty]{} -\tau\Delta E_0^{J_0} + \ln\left[\sum_M |\langle\Phi|\Psi_0^{J_0M}\rangle|^2\right] \\ n(\tau,\Omega)-n(\tau,0) \xrightarrow[\tau\to\infty]{} \aleph(\Omega) \end{cases}$$

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

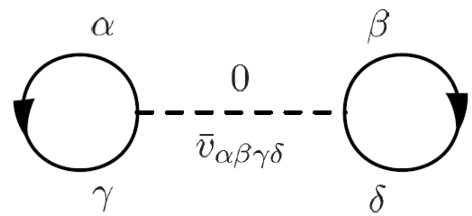
***Goldstone linked-cluster based on UHF***
***->nice but not what we are after!***

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

# Many-body perturbation theory (3)

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

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




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

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

$$+\frac{1}{2}\sum_{ijab}\bar{v}_{ijab}\,\rho^{ph}_{ai}(\Omega)\,\rho^{ph}_{bj}(\Omega)$$

*Genuinely $\Omega$-dependent part*

*Signals the symmetry breaking*

***Large $\tau$ limit*** $\quad h(\tau,\Omega) \xrightarrow[\tau\to\infty]{} h(\Omega) \quad \Big\} \quad \mathcal{H}(\infty,\Omega) = h(\Omega)\,\mathcal{N}(\Omega)$

**In the exact limit** $\quad \frac{\partial}{\partial\Omega}h(\Omega) = 0$

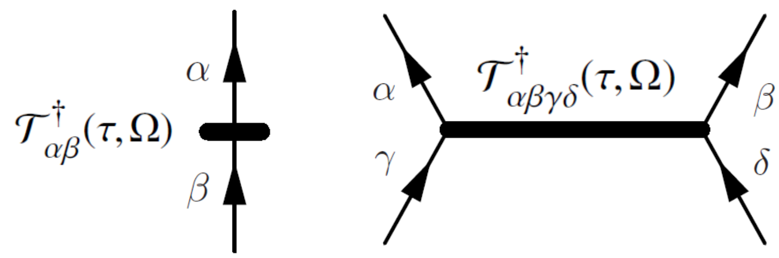
**After truncation** $\quad \frac{\partial}{\partial\Omega}h(\Omega) \neq 0$

# Coupled cluster theory (1) – energy kernel

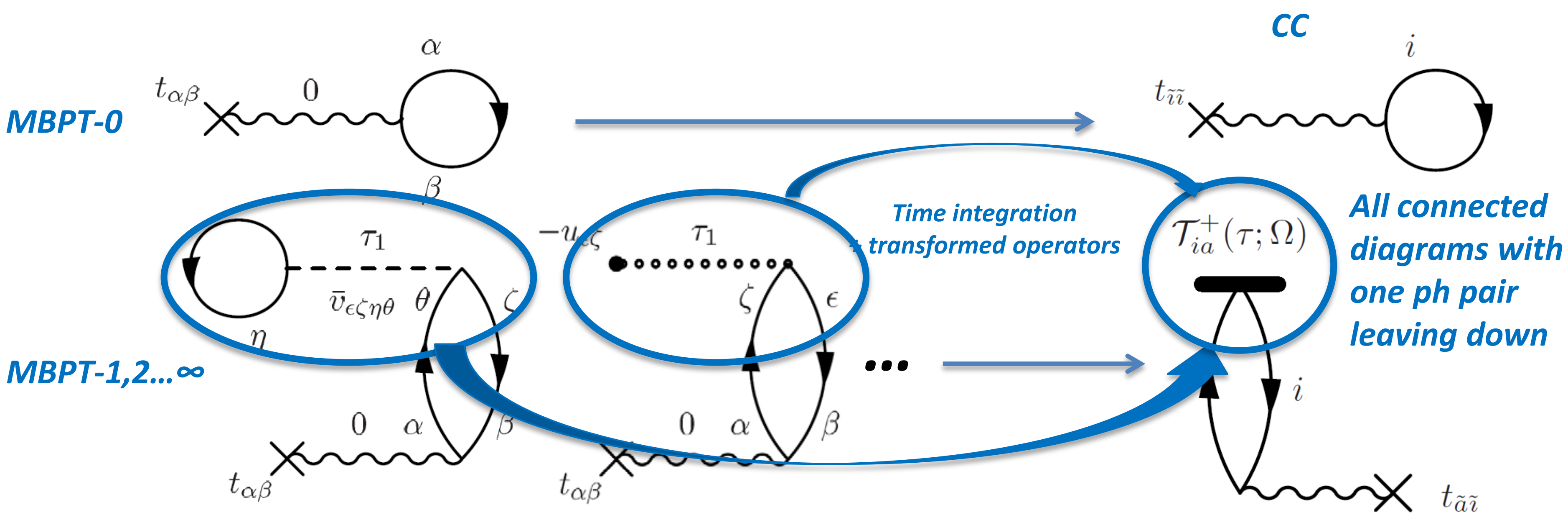
**β- and Ω-dependent cluster operators (or rather their hermitian conjuguate…)**

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

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




**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

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

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

*Cumbersome expressions*

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

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

**Transformed operators**

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

**Bi-orthogonal system**

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

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

*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**

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

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

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

## Dynamical amplitude equations

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

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

Imaginary-time-dependent equation of motion

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

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 $\mathcal{N}(\tau,\Omega)$ from MBPT***

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

**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**

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

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

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

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

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

***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***

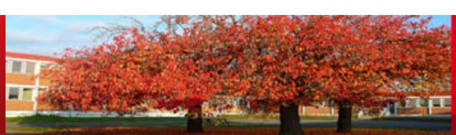
$$E_0^{J_0} = h(0)$$

***2. Projected Hartree Fock is recovered at lowest order***

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

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

**where** $$\begin{aligned} |\Phi_0^{JM}\rangle &\equiv \sum_K f_K^J P_{MK}^J |\Phi\rangle \\ P_{MK}^J &\equiv \frac{2J+1}{16\pi^2} \int_{D_{SU(2)}} d\Omega\, D_{MK}^{J*}(\Omega)\, R(\Omega) \end{aligned}$$



# 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 $\alpha, \beta, \gamma$
    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


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

# 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**

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

**Standard symmetry-unrestricted CC**

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

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

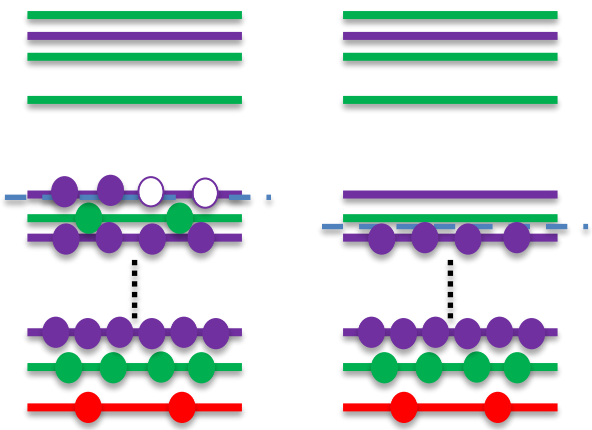
**No difference in exact limit/if conserved symmetry**

**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 $\Omega$ -> 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

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

Single reference / Non perturbative

**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)]

Single reference / Breaking symmetry

**MBPT and CC based on UHF**

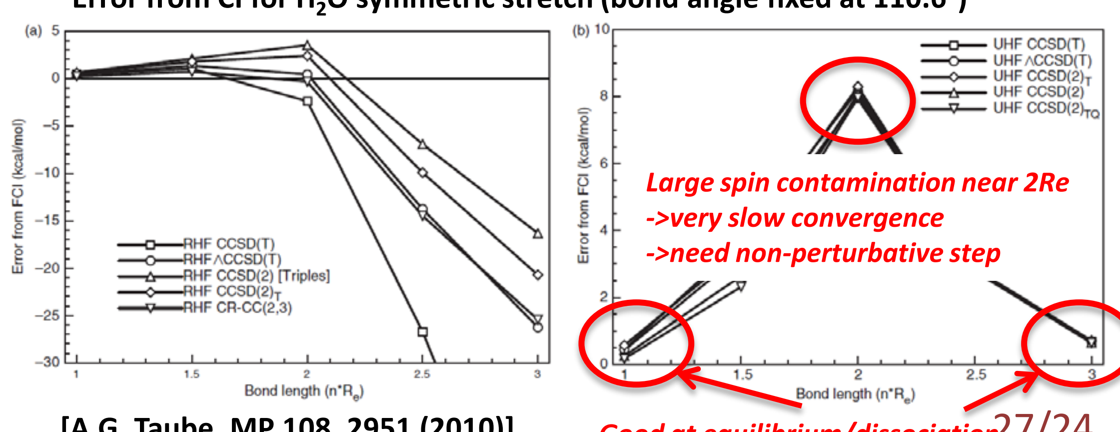
[R. J. Bartlett, ARPC 32, 359 (1981)]

**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)]

# AMR-CC scheme in one slide

**Kernels**

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

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

**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 $\Omega$

**Norm kernel**

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

**connected kernels of Lie algebra operators**

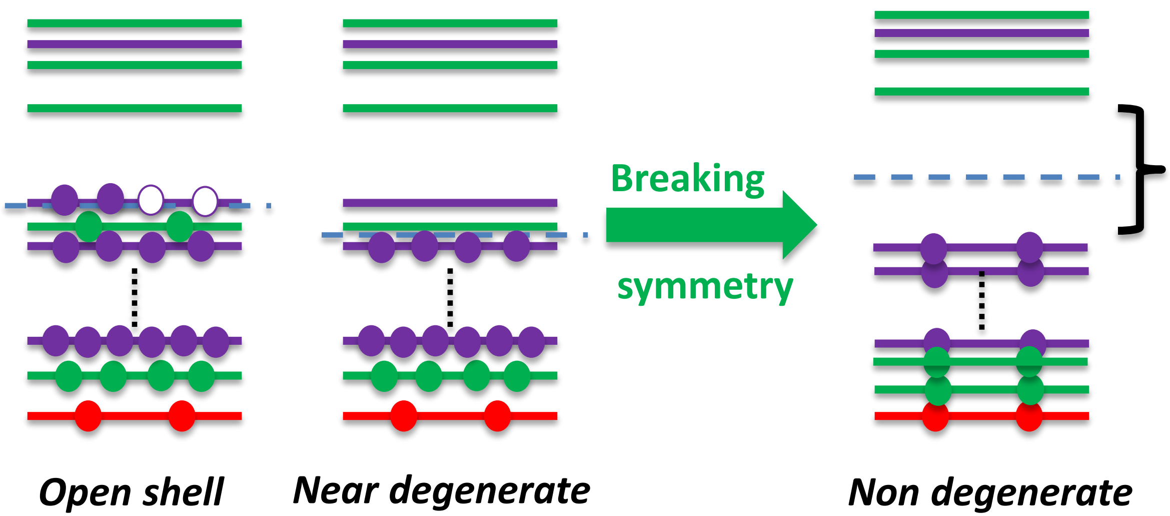
***Solve in stationary limit at $\tau=\infty$***

**Recovers single-reference CC at $\Omega = 0$**
**Recovers Projected HF at lowest order**

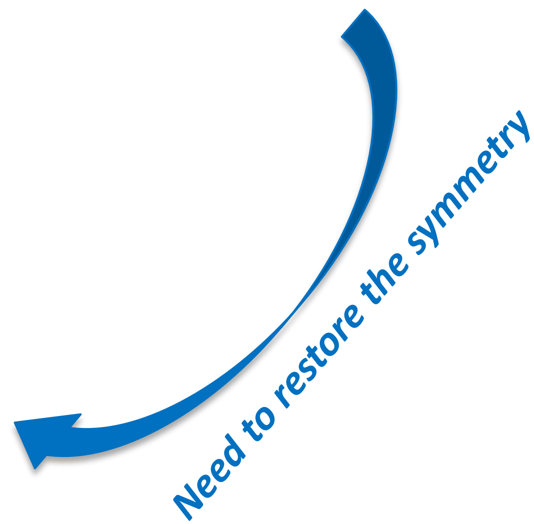
**Set of SR-CC calculations for $N_{sym}$~$(10)^{angle}$ values of $\Omega$**

# 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



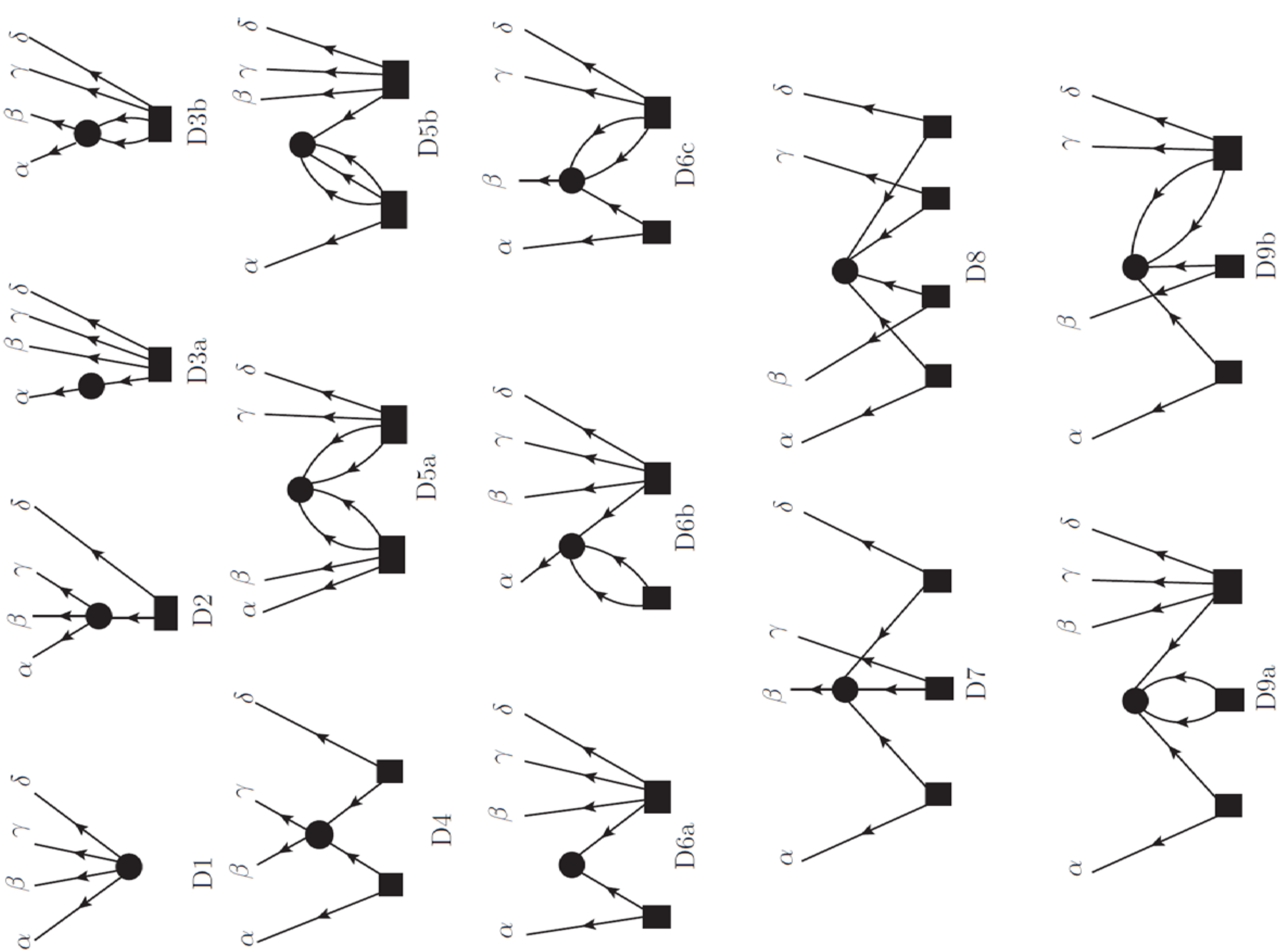

**Lowdin operator in low-order MBPT based on UHF**

[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**




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