

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

I. Breaking symmetries

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Computational Challenges in Nuclear and Many-Body Physics



Sept. 15th- Oct. 10th 2014, Stockholm 1/19

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

II. Breaking $U(1)$ symmetry (“trivial” for $SU(2)$) (today)

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 $SU(2)$ or $U(1)$ symmetries (next thursday)

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

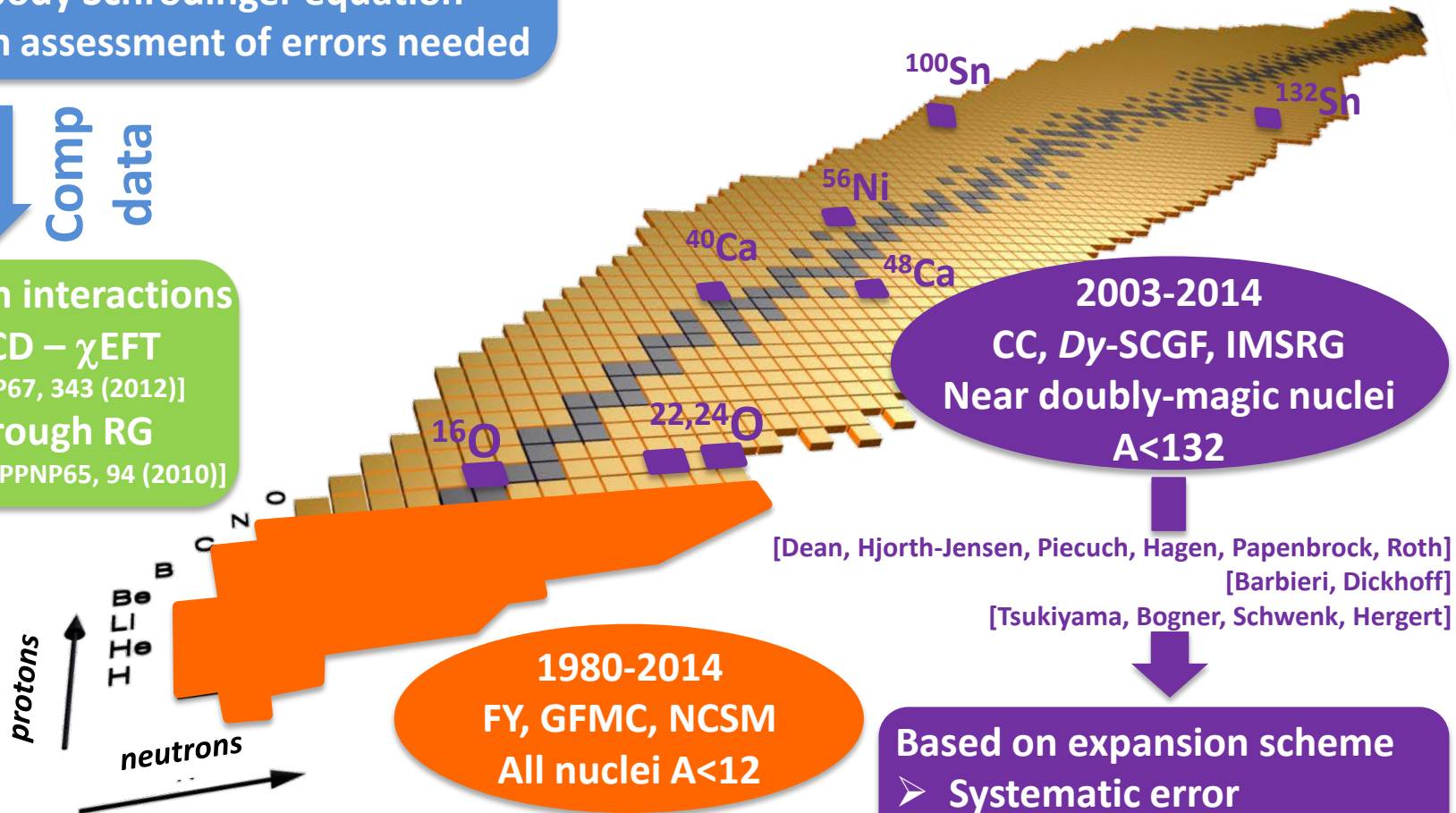
- Effective structure-less nucleons
- $2N + 3N + \dots$ inter-nucleon interactions
- Solve A -body Schrödinger equation
- Thorough assessment of errors needed

High predictive power
Limited applicability domain

↑ Input
↓ Comp data

Inter-nucleon interactions

- Link to QCD – χ 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
 $A < 132$

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

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

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

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

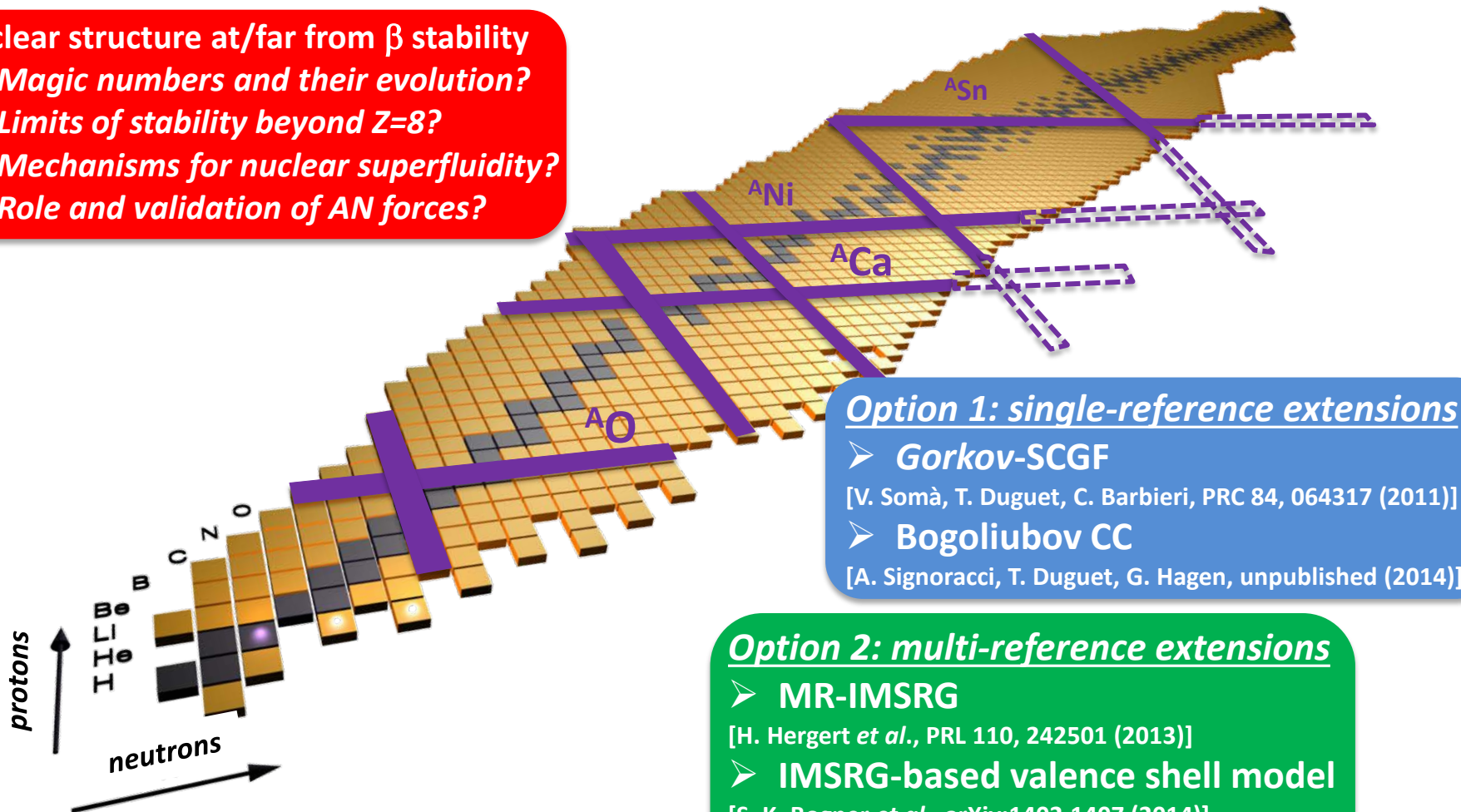
Towards *ab-initio* methods for open-shell nuclei

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

Expand Ω_0 such that



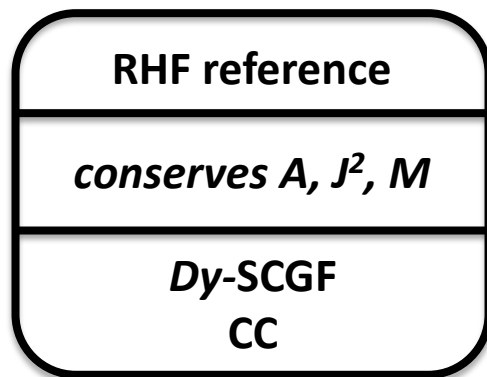
E_0 is size extensive

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

Ground-state energy

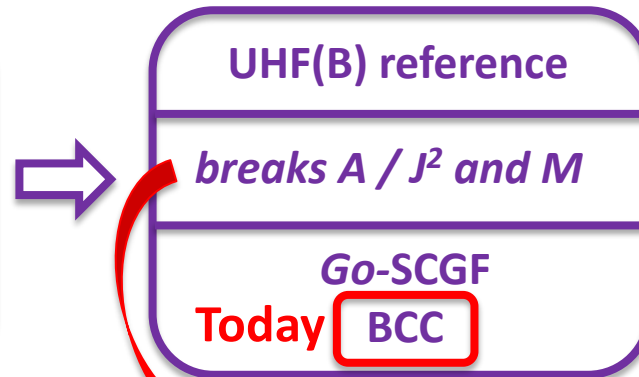
$|\Psi_0\rangle = \Omega_0 |\Phi_0\rangle$
A-body ground state

Closed shell



Breaks down for open-shell nuclei

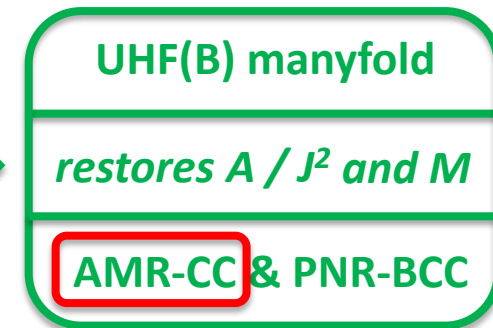
Singly/doubly open shell



Contamination from other A / J^2 and M

ph degeneracy
 $\leftrightarrow$
Goldstone mode

Singly/doubly open shell



Next thursday
Multi-reference character

Finite inertia
 $\leftrightarrow$
Resolve Goldstone mode

Bogoliubov coupled-cluster formalism for singly open-shell nuclei

[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)]

Hartree-Fock-Bogoliubov reference

Nuclear Hamiltonian

$$\begin{aligned}
 H \equiv & \frac{1}{(1!)^2} \sum_{pq} t_{pq} c_p^\dagger c_q \\
 & + \frac{1}{(2!)^2} \sum_{pqrs} \bar{v}_{pqrs} c_p^\dagger c_q^\dagger c_s c_r \\
 & + \frac{1}{(3!)^2} \sum_{pqrst} \bar{w}_{pqrst} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s
 \end{aligned}$$

Bogoliubov transformation

$$\begin{aligned}
 \beta_\alpha^\dagger &= \sum_p U_{p\alpha} c_p^\dagger + V_{p\alpha} c_p \\
 \beta_\alpha &= \sum_p U_{p\alpha}^* c_p + V_{p\alpha}^* c_p^\dagger
 \end{aligned}$$

**Breaks U(1) symmetry
associated with good A**

Bogoliubov vacuum

$$|\Phi\rangle \equiv C \prod_\alpha \beta_\alpha |0\rangle$$

$$\beta_k |\Phi\rangle = 0 \quad \forall k$$

Density matrices

$$\rho_{qp} \equiv \frac{\langle \Phi | c_p^\dagger c_q | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

$$\kappa_{qp} \equiv \frac{\langle \Phi | c_p c_q | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

Grand potential

$$\Omega \equiv H - \lambda A$$

Minimization under constraint

$$\delta \frac{\langle \Phi | \Omega | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0 \quad / \quad \langle \Phi | A | \Phi \rangle = A$$



HFB equation

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

Quasi-particle excitations

$$|\Phi^{\alpha\beta\dots}\rangle \equiv \beta_\alpha^\dagger \beta_\beta^\dagger \dots |\Phi\rangle$$

Spectroscopic factors

$$\mathfrak{S}_\alpha^- = \sum_l |V_{l\alpha}|^2$$

Binding energy

$$\begin{aligned}
 \mathcal{E}_0 = & +\frac{1}{2} \left[\sum_{pq} t_{pq} \rho_{qp} - \sum_\alpha (E_\alpha - \lambda) \mathfrak{S}_\alpha^- \right] \\
 & - \frac{1}{6} \left[\sum_{pq} \Gamma_{pq}^{3N} \rho_{qp} + \Delta_{pq}^{3N} \kappa_{qp}^* \right]
 \end{aligned}$$

***m-scheme code**

***Benchmarked against J-coupled
[V. Somà et al.]**

Bogoliubov CC ansatz

Wave-function ansatz

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

Quasi-particle cluster operator

$$\mathcal{T} \equiv \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \dots$$

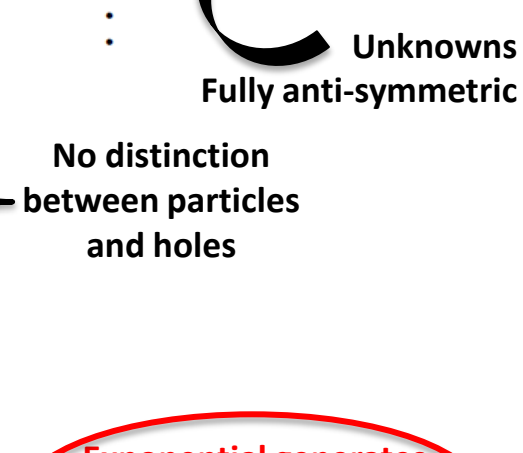
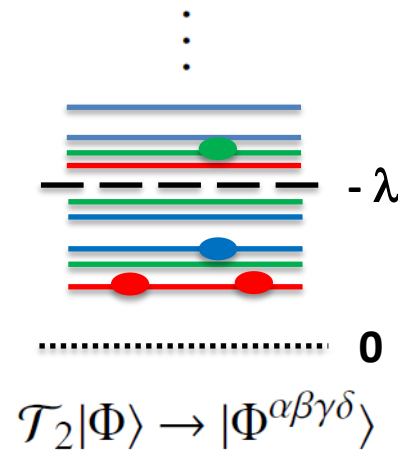
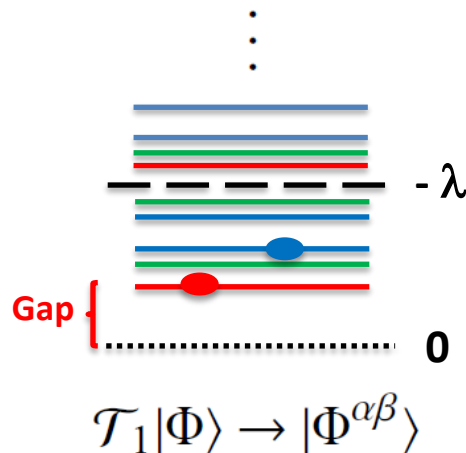
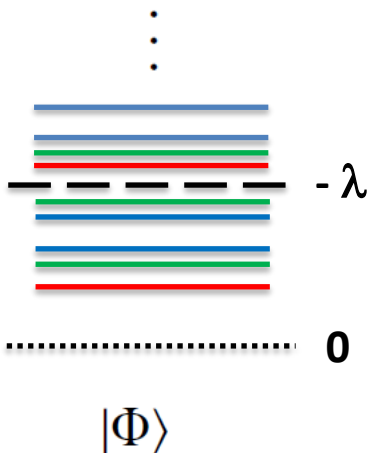
$$[\mathcal{T}_n, \mathcal{T}_m] = 0$$

Connected n-tuple excitation

$$\mathcal{T}_1 \equiv \frac{1}{2!} \sum_{k_1 k_2} t_{k_1 k_2} \beta_{k_1}^\dagger \beta_{k_2}^\dagger$$

$$\mathcal{T}_2 \equiv \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} t_{k_1 k_2 k_3 k_4} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3}^\dagger \beta_{k_4}^\dagger$$

Action of n-tuple excitation on the HFB vacuum



Exponential generates connected + disconnected n-tuple excitations

HFB vacuum

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

- CC theory in qp basis with no breaking of U(1)
[L. Stolarczyk, H. Monkhorst, MP108, 3067 (2010)]
- BCC theory restricted to BCS and simple geometry
[K. Emrich, J. G. Zabolitzky, PRB30, 2049 (1984)]
[W. A. Lahoz, R. F. Bishop, ZPB73, 363 (1988)]

Normal-ordered grand potential

Bogoliubov transformation + Wick's theorem

Each $\Omega_{k_1 \dots k_i k_{i+1} \dots k_{i+j}}^{ij}$ is

*fully anti-symmetric

*expressed in terms of

$$\begin{bmatrix} t_{pq} \\ \bar{v}_{pqrs} \\ w_{pqrstuv} \end{bmatrix} \begin{bmatrix} U_{pk} \\ V_{pk} \end{bmatrix}$$

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

$$= \Omega^{00} + \frac{1}{1!} \sum_{k_1 k_2} \Omega_{k_1 k_2}^{11} \beta_{k_1}^\dagger \beta_{k_2} \quad \xrightarrow{\text{with HFB reference state}} \quad = E_{k_1} \delta_{k_1 k_2}$$

$$+ \frac{1}{2!} \sum_{k_1 k_2} \left\{ \Omega_{k_1 k_2}^{20} \beta_{k_1}^\dagger \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_2}^\dagger + \Omega_{k_1 k_2}^{02} \beta_{k_1} \beta_{k_1} \beta_{k_2} \beta_{k_2} \right\} = 0$$

Residual interaction

$$+ \frac{1}{(2!)^2} \sum_{k_1 k_2 k_3 k_4} \Omega_{k_1 k_2 k_3 k_4}^{22} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3} \beta_{k_4}$$

$$+ \frac{1}{3!} \sum_{k_1 k_2 k_3 k_4} \left\{ \Omega_{k_1 k_2 k_3 k_4}^{31} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3}^\dagger \beta_{k_4} + \Omega_{k_1 k_2 k_3 k_4}^{13} \beta_{k_1} \beta_{k_2} \beta_{k_3} \beta_{k_4} \right\}$$

$$+ \frac{1}{4!} \sum_{k_1 k_2 k_3 k_4} \left\{ \Omega_{k_1 k_2 k_3 k_4}^{40} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3}^\dagger \beta_{k_4}^\dagger + \Omega_{k_1 k_2 k_3 k_4}^{04} \beta_{k_1} \beta_{k_2} \beta_{k_3} \beta_{k_4} \right\}$$

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

➔ NO2B approximation

Very good in closed shell (1% error)

[S. Binder *et al.*, PRC87 (2013) 021303]

Bogoliubov CC equations

Schrödinger equation

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

$$xe^{-\mathcal{T}} \rightarrow \bar{\Omega}|\Phi\rangle = \Omega_0|\Phi\rangle$$

$$(\Omega e^{\mathcal{T}})_c |\Phi\rangle = \Omega_0|\Phi\rangle$$

Energy equation

$$\langle\Phi|(\Omega e^{\mathcal{T}})_c|\Phi\rangle = \Omega_0$$

Amplitude equation to find $\mathcal{T}_n$

$$\langle\Phi^{\alpha\beta\dots}|(\Omega e^{\mathcal{T}})_c|\Phi\rangle_c = 0$$

Truncate $\mathcal{T}$ beyond a certain $\mathcal{T}_n$

Retaining $\mathcal{T}_1$ and $\mathcal{T}_2$ defines BCCSD

Infinite-order method

Efficient grasp of dynamic correlations

Non-hermitian similarity-transformed grand potential

$$\bar{\Omega} \equiv e^{-\mathcal{T}} \Omega e^{\mathcal{T}}$$

Baker-Campbell-Hausdorff + Wick theorem

$$\bar{\Omega} = \sum_{n=0}^4 (\Omega \mathcal{T}^n)_c$$

Expansion naturally terminates

Size extensive

+ equation to constrain λ / $\frac{\langle\Psi|A|\Psi\rangle}{\langle\Psi|\Psi\rangle} = A$

BCC with Singles and Doubles

$$\Omega_0 = \langle\Phi|\Omega(1 + \mathcal{T}_1 + \mathcal{T}_2 + \frac{1}{2}\mathcal{T}_1^2)|\Phi\rangle_c$$

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

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

Incorporates standard single-reference CC as a particular case 11/19

Diagrammatic and BCCSD equations (1)

Grand potential at normal-ordered two-body level

$$\Omega^{[2]} = \Omega^{11} + \Omega^{20} + \Omega^{02}$$

$$\Omega^{[4]} = \Omega^{22} + \Omega^{31} + \Omega^{13} + \Omega^{40} + \Omega^{04}$$

Cluster amplitudes at BCCSD level



- Generate all distinct connected diagrams
- Label external lines according to bra
- Sum over all internal lines
- Associate matrix elements to each vertex
 - $(n!)^{-1}$ factor for n equivalent internal lines
 - $(k!)^{-1}$ factor for k equivalent cluster vertices
 - $(-1)^n$ factor for n crossing lines
- Add permutation for inequivalent external lines

Diagrammatic and BCCSD equations (2)

Energy equation

$$\Omega_0 = \langle \Phi | \Omega (\mathcal{T}_1 + \mathcal{T}_2 + \frac{1}{2} \mathcal{T}_1^2) | \Phi \rangle_C$$



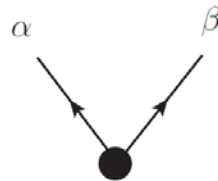
Single amplitude equation

No distinction between particles and holes

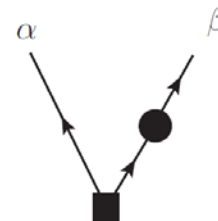


Fewer diagrams than in CCSD

Similar for double amplitude equation



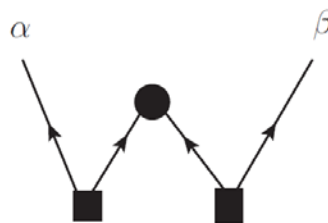
S1



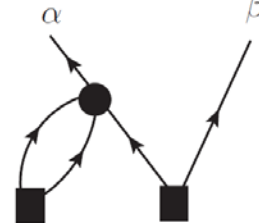
S2a



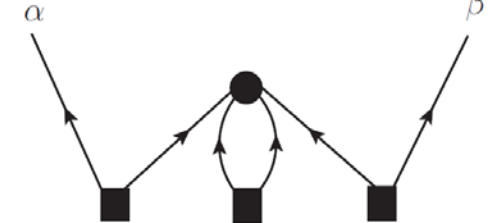
S2b



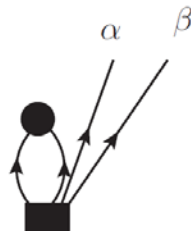
S3a



S3b



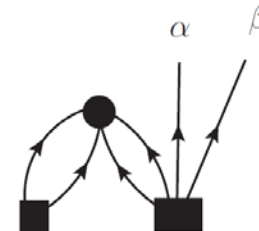
S4



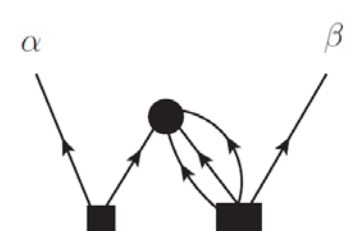
S5a



S5b



S6a



S6b

Can be extended to
(1) residual 3NF $\Omega^{[6]}$
(2) triples $\mathcal{T}_3$

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

Pairing Hamiltonian from BCCD

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

Attractive pairing grand potential

$$\Omega = \sum_p (\epsilon_p - \lambda) N_p - G \sum_{pq} P_p^\dagger P_q$$

Doubly-degenerate picket fence model $\epsilon_p = p \Delta \epsilon$
Model for, e.g., deformed nuclei

Pair operators

$$\begin{aligned} N_p &= a_{p\uparrow}^\dagger a_{p\uparrow} + a_{p\downarrow}^\dagger a_{p\downarrow} \\ P_p^\dagger &= a_{p\uparrow}^\dagger a_{p\downarrow}^\dagger \end{aligned}$$

SU(2) algebra

$$\begin{aligned} [P_p, P_q^\dagger] &= +\delta_{pq} (1 - N_p) \\ [N_p, P_q] &= -2\delta_{pq} P_p \\ [N_p, P_q^\dagger] &= +2\delta_{pq} P_p^\dagger \end{aligned}$$

Exact ground-state energy

- Diagonalization within seniority-0 subspace

[A. Volya, B.A. Brown, W. Zelevinsky, PLB509, 37 (2001)]

- Richardson solution

[R.W. Richardson, PL3, 277 (1963), PR141 (1966)]

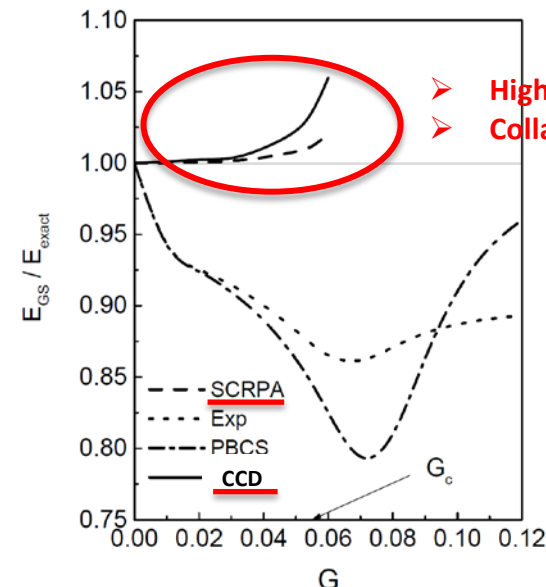
- *Cheaper than full diagonalization ($\sqrt{\quad}$)
- *Still scales exponentially
- > Limited to ~40 levels at half filling

Look for highly accurate many-body methods that

- scale polynomial with system size
- can be applied to more realistic Hamiltonians

Typical approximate methods

- BCS and projected BCS (before variation)
- Coupled cluster theory with doubles
- Self-consistent RPA



- High accuracy in normal phase
- Collapse near superfluid transition

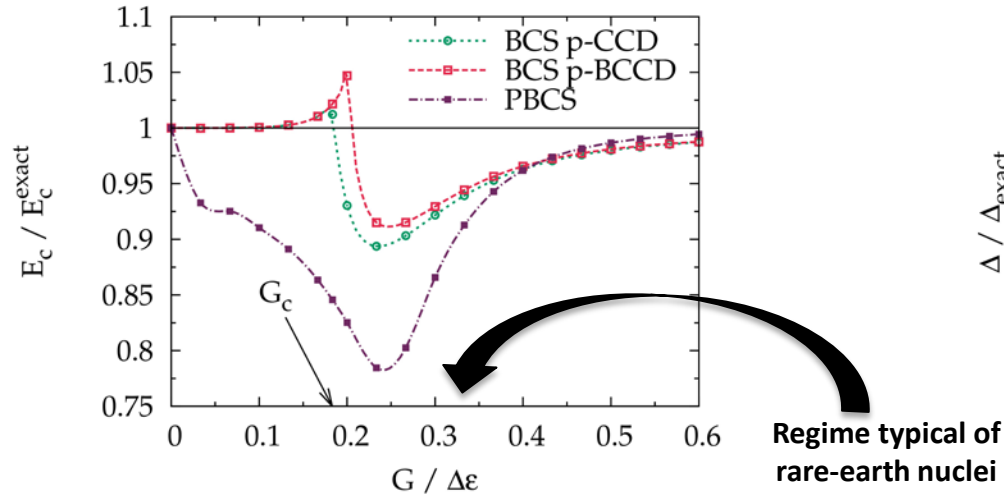
What about BCCD?

- *100 levels
- *Half filling
- * $\Delta \epsilon = 300 \text{ keV}$
- * $G_c / \Delta \epsilon = 0.18$

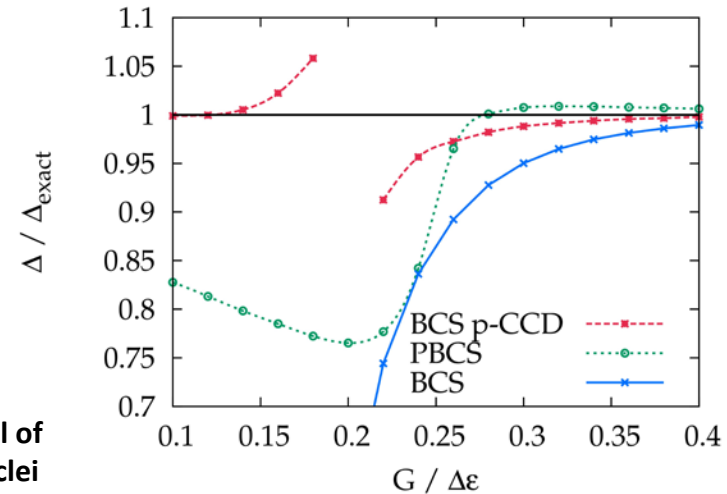
[J. Dukelsky et al., NPA714, 63 (2003)]

Results for 100 levels at half filling

Correlation energy



Pairing “gap”

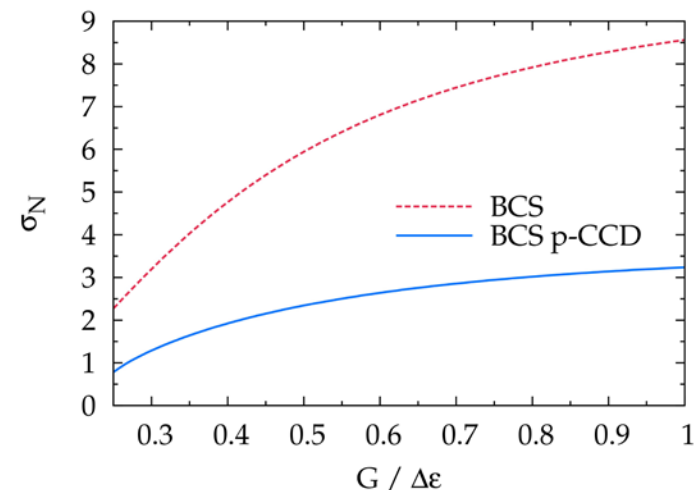


$$\Delta_c = G \sum_p \left[\langle \Psi | p^\dagger p | \Psi \rangle - \frac{1}{4} \langle \Psi | N_p | \Psi \rangle^2 \right]$$

- High accuracy in normal & superfluid phases
- Superior to PBCS in regime of interest
- Superiority improves with system size
- Doubles reduce symmetry breaking vs BCS
- Conclusions valid away from half filling
- Symmetry restoration crucial near closed shell

[PNR Bogoliubov CC theory, T. Duguet, in preparation (2014)]

Variance in A



Triples correction will further improve



Phase transition wrongly of first order
Second-order character recovered from singles

Test calculations of semi-magic $N/Z=8$ nuclei

Set up

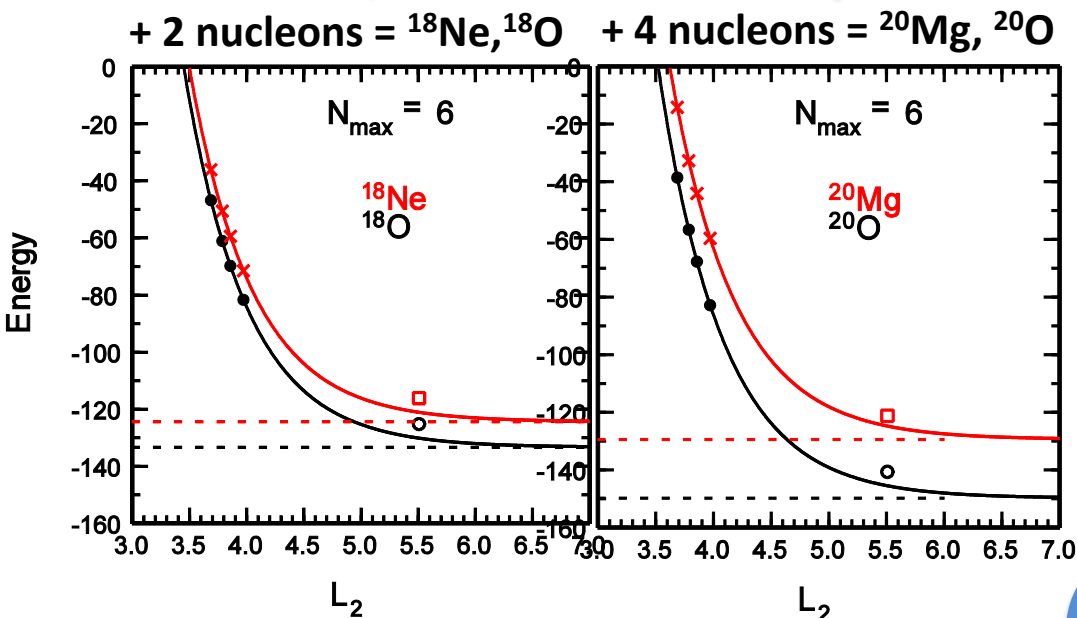
- NNLO_{opt} 2NF ($\Lambda = 500 \text{ MeV/c}$)
[A. Ekstrom *et al.*, PRL110, 192502 (2013)]
- No 3NF yet
- HO basis
 - $N_{\text{max}} = 6$
 - $hw = 26$ and $50, 53, 55, 58 \text{ MeV}$
- m-scheme code

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

Accessible via 2PA-EOM-CCSD
[G. Jansen *et al.*, PRC83 (2011) 054306]
3p-1h on top of ^{16}O

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

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



Nucleus	E_{min}	$E_{N_{\text{max}}=6}^{\text{CCSD}}$	E_{∞}	$E_{N_{\text{max}}=12}^{\text{CCSD}}$
^{16}O	-119.211	-119.211	-124.905	-123.453
^{18}O	-125.2	-126.476	-133.284	-132.990
^{20}O	-140.672	n/a	-149.788	n/a
^{18}Ne	-116.141	-117.927	-124.351	-124.850
^{20}Mg	-121.186	n/a	-129.410	n/a

Infrared extrapolation from $hw=50,53,55,58\text{MeV}$

[R. Furnstahl *et al.*, (2014) arXiv:1408.0252]

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

where

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

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

Extends SR-CC to genuinely open-shells!

- Scales as $(n_h + n_p)^6$
- ~1.5 MeV > 2PA-EOM-CCSD in ^{18}O and ^{18}Mg
- Critical to restore A near closed shell
- Storage of $\mathcal{T}_2$ in m scheme beyond $N_{\text{max}} = 8$?
- More involved distribution of $\mathcal{T}_2$
- Use SVD
- [T. Kinoshita *et al.*, JCP 119 (2003) 7756]
- Code in J-coupled scheme

Conclusions

- Development of Bogoliubov CC theory for genuinely open-shell nuclei
- Parallel effort to Gorkov-SCGF and MR-IMSRG
- m-scheme implementation at the singles and doubles level
 - *First proof-of-principle results*
 - *Allows for the treatment of doubly-open-shell systems*
 - *Currently limited to $N_{max} = 8$ due to storage scheme*

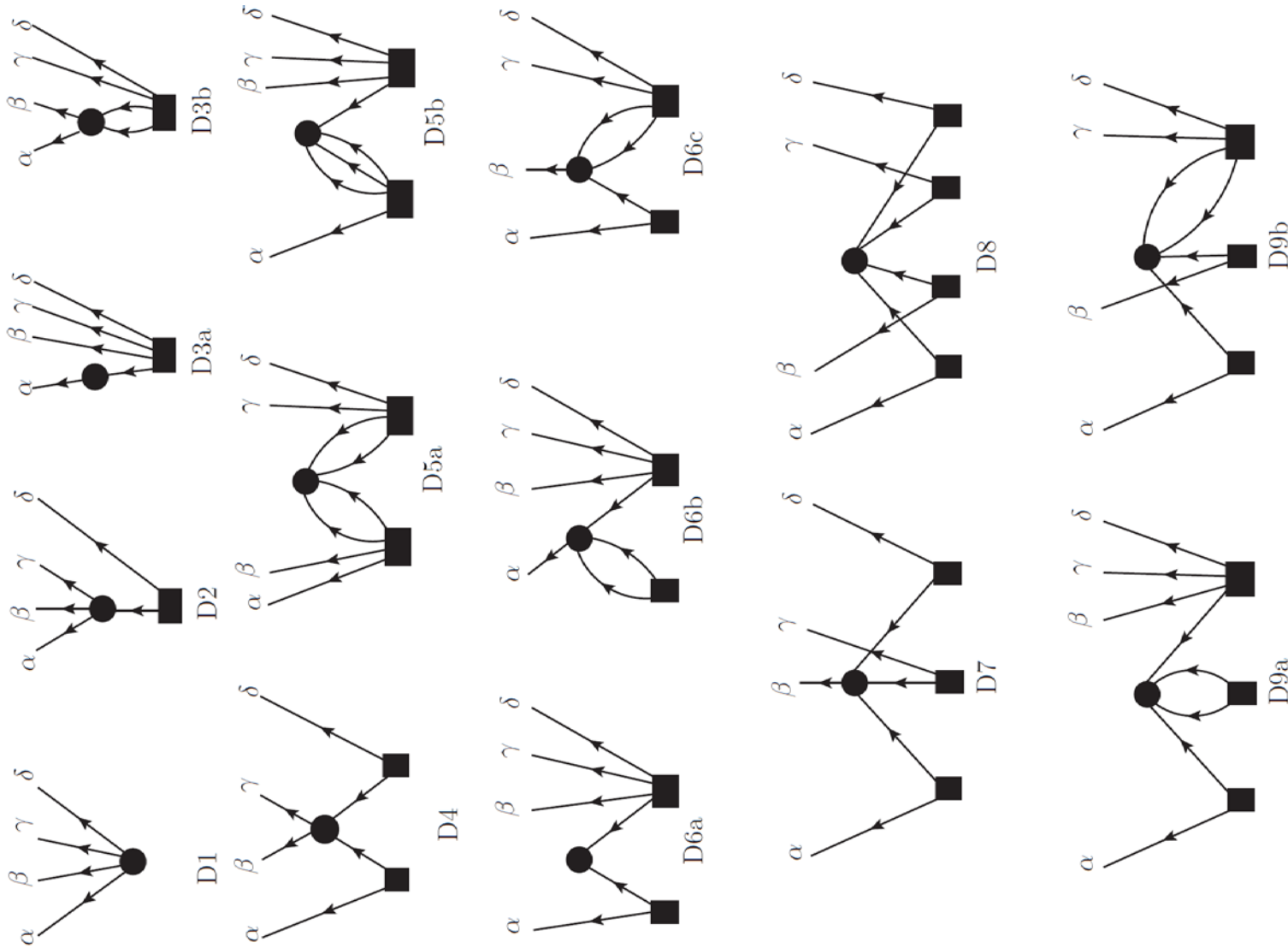
Future

- Develop option(s) to go to larger bases
- Implementation of 3NF at normal-ordered two-body level
- Extend to Equation-Of-Motion Bogoliubov CC theory
- Wealth of potential applications
 - *Problems of experimental interest*
 - *Cross-benchmarking with Gorkov-SCGF and MR-IMSRG*
- Symmetry-restored Bogoliubov CC theory and applications

Complementary slides

Diagrammatic and BCCSD equations (3)

Double amplitude equation



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