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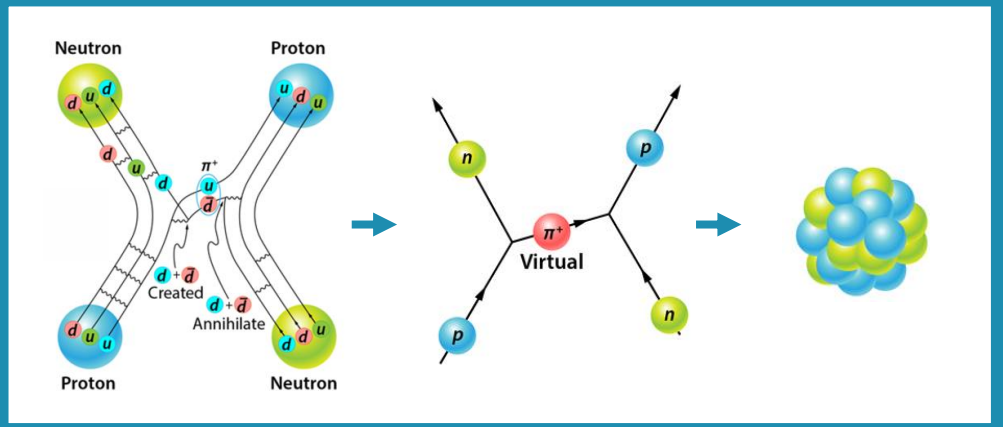
Bogoliubov Coupled Cluster theory for open-shell nuclei



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PhyNuBE school

08/12/2021

Outline

- “Ab initio” many-body approach to nuclear systems
- Open-shell frontier
- Bogoliubov coupled cluster (BCC) theory
- Scalability
- Results
- Outlook

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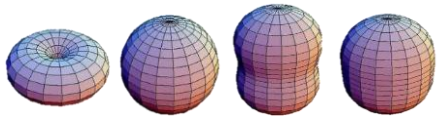
Huge diversity of nuclear phenomena

The atomic nucleus is a strongly correlated self-bound many-body quantum system and therefore intrinsically complex

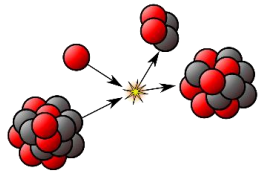
Ground-state properties:

Mass, binding energy, shape, moments, …



Nuclear reaction:

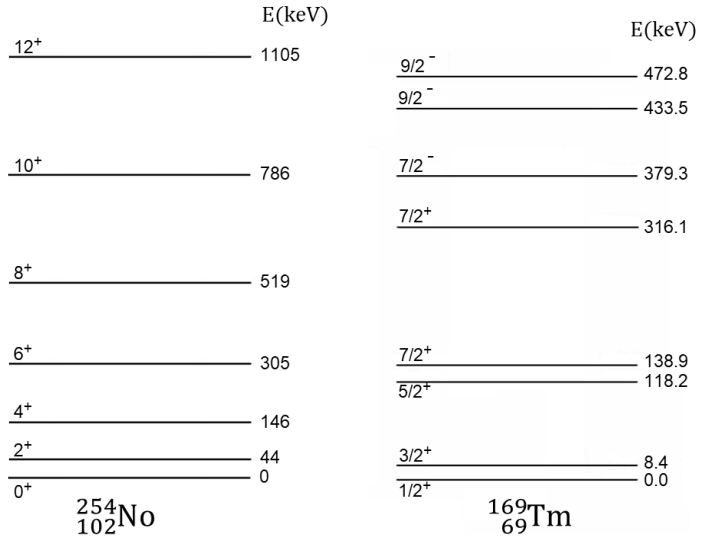
Fusion, knockout, transfer, …



Spectroscopy:

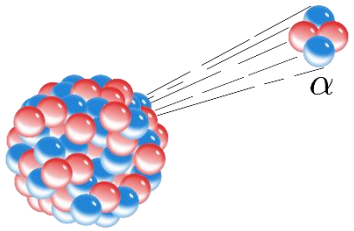
rotational & vibrational bands

Single-particle dominated excitations



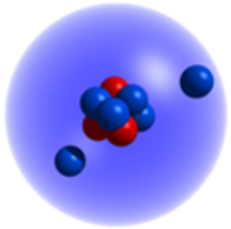
Radioactive decay:

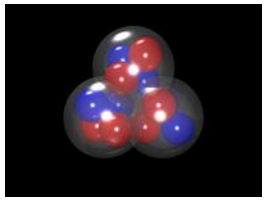
α, $\beta^{+/-}$, p, fission, …



Exotic structures:

Halo, clusters, …





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Huge diversity of nuclear phenomena

Many Models

- Examples
  - Liquid drop model
  - Rotational & vibrational models
  - Shell model
  - Nilsson model
  - …
- Short comings
  - Not straightforwardly improvable
  - No clear path to connect them

Effective Theories

- Resolves these short comings
  - Systematically improvable
  - Connections (reduction) possible

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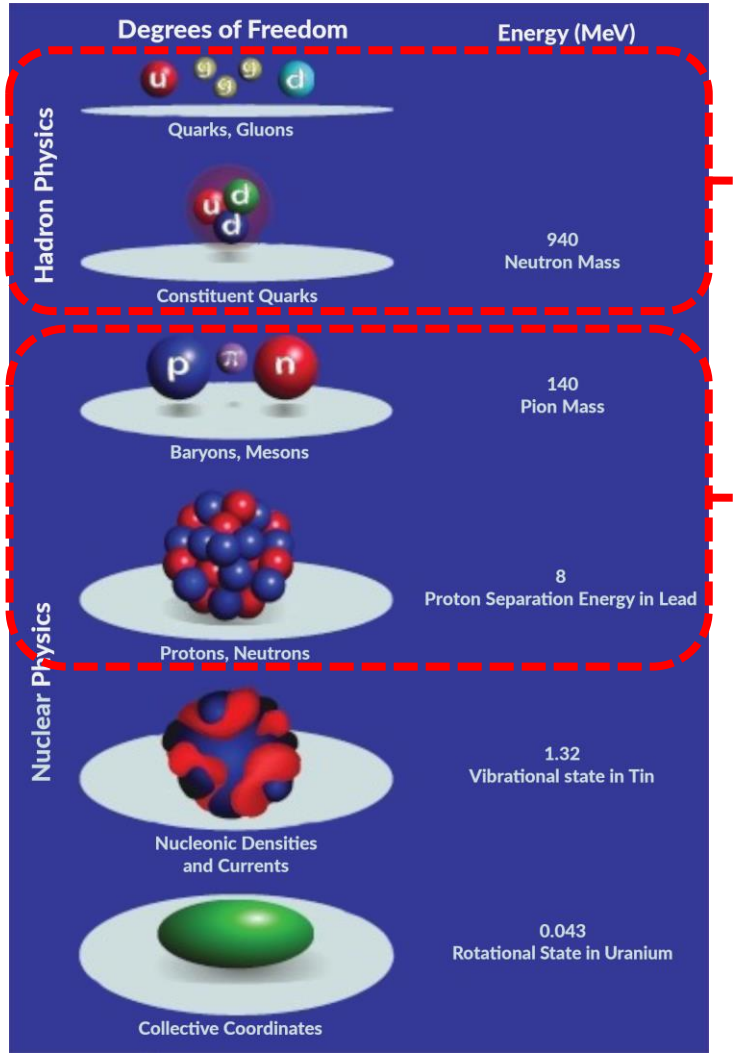
Effective field theory

Emergence of phenomena from effective description

More elementary description, reductionism



QCD

Chiral effective field theory (χ-EFT)

protons & neutrons as d.o.f.

Effective field theory (EFT)

1) Identifying appropriate degrees of freedom (d.o.f.)
2) ALL interactions complying with symmetries of underlying theory
3) Ordered in expansion governing hierarchy (power counting)
4) Fix low energy constants (LEC) from data (or underlying theory)

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Effective field theory

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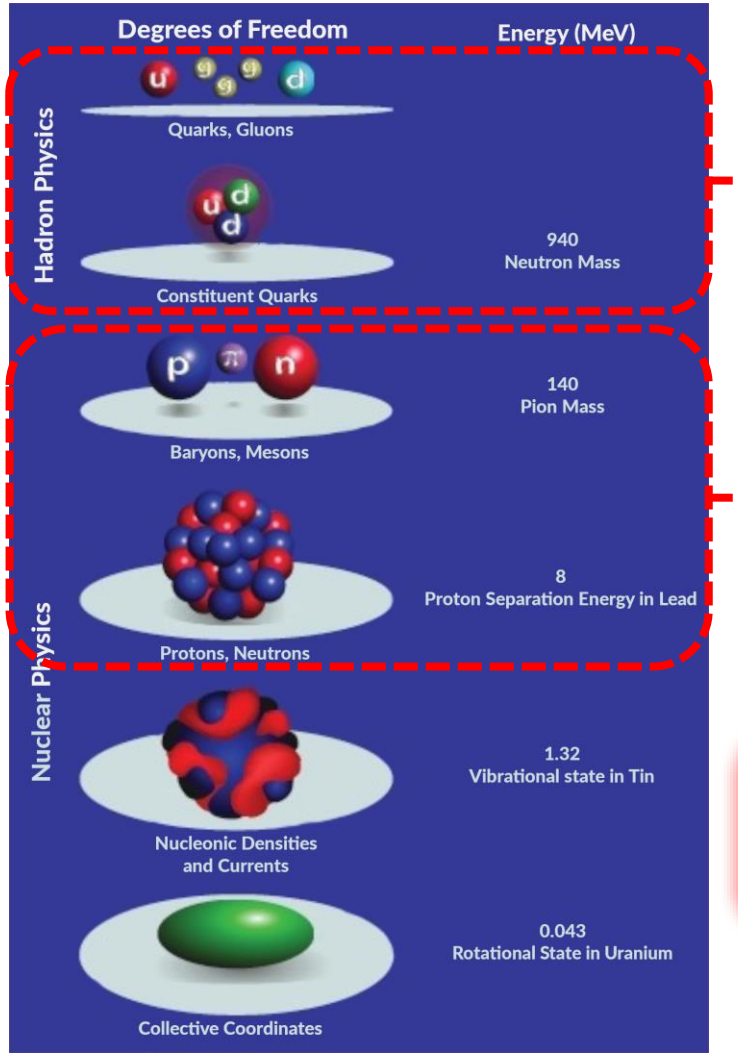

QCD

Chiral effective field theory (χ-EFT)

protons & neutrons as d.o.f.

***"Ab initio"* approach:**
Application of χ-EFT to describe the nucleus

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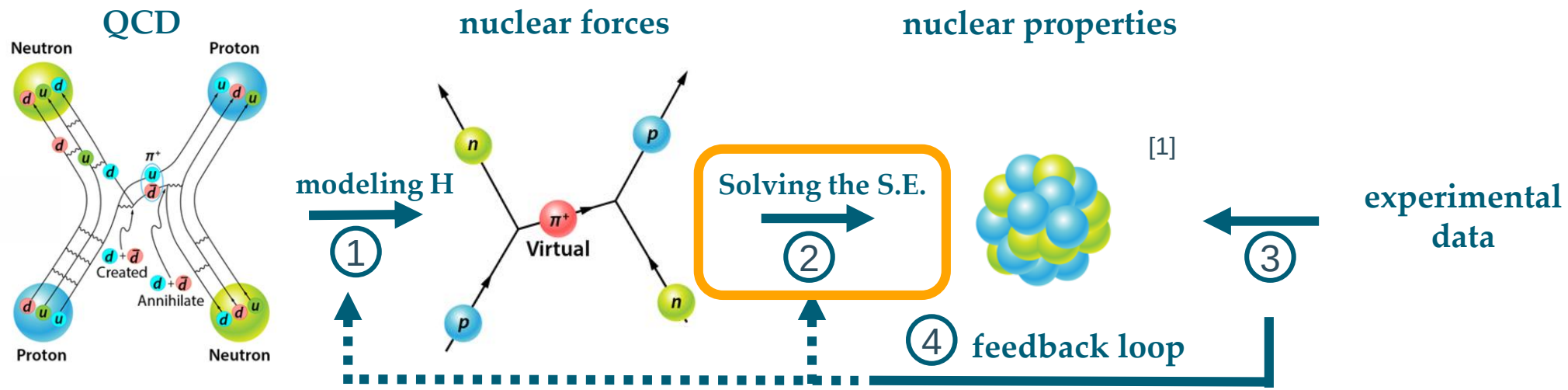
"*Ab initio*" approach to nuclear structure

Assumptions

- Structure-less protons and neutrons as d.o.f.
  - All nucleons active (no inert core)
- Only elementary interactions between them
  - Sound connection to QCD
  - All possible interactions allowed by symmetry
  - Up to A-body forces (in principle)

***Ab initio* ("from scratch") scheme = solve A-body Schrödinger equation (S.E.)**

$$\hat{H}|\Psi_n^A\rangle = E_n^A|\Psi_n^A\rangle$$



[1]: APS/Alan Stonebraker

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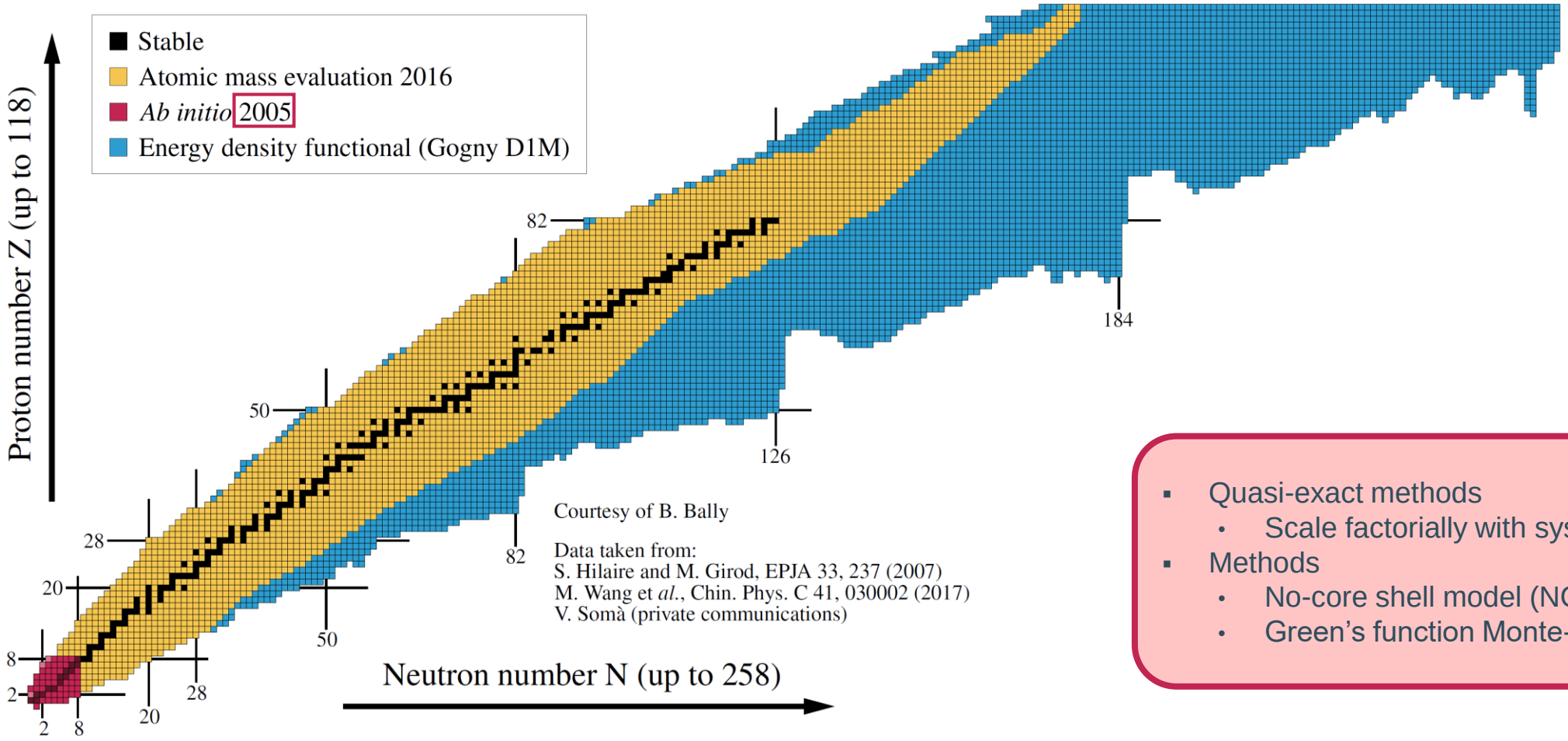
② Solving the Schrödinger equation



- Quasi-exact methods
  - Scale factorially with system size
- Methods
  - No-core shell model (NCSM)
  - Green's function Monte-Carlo (GFMC)

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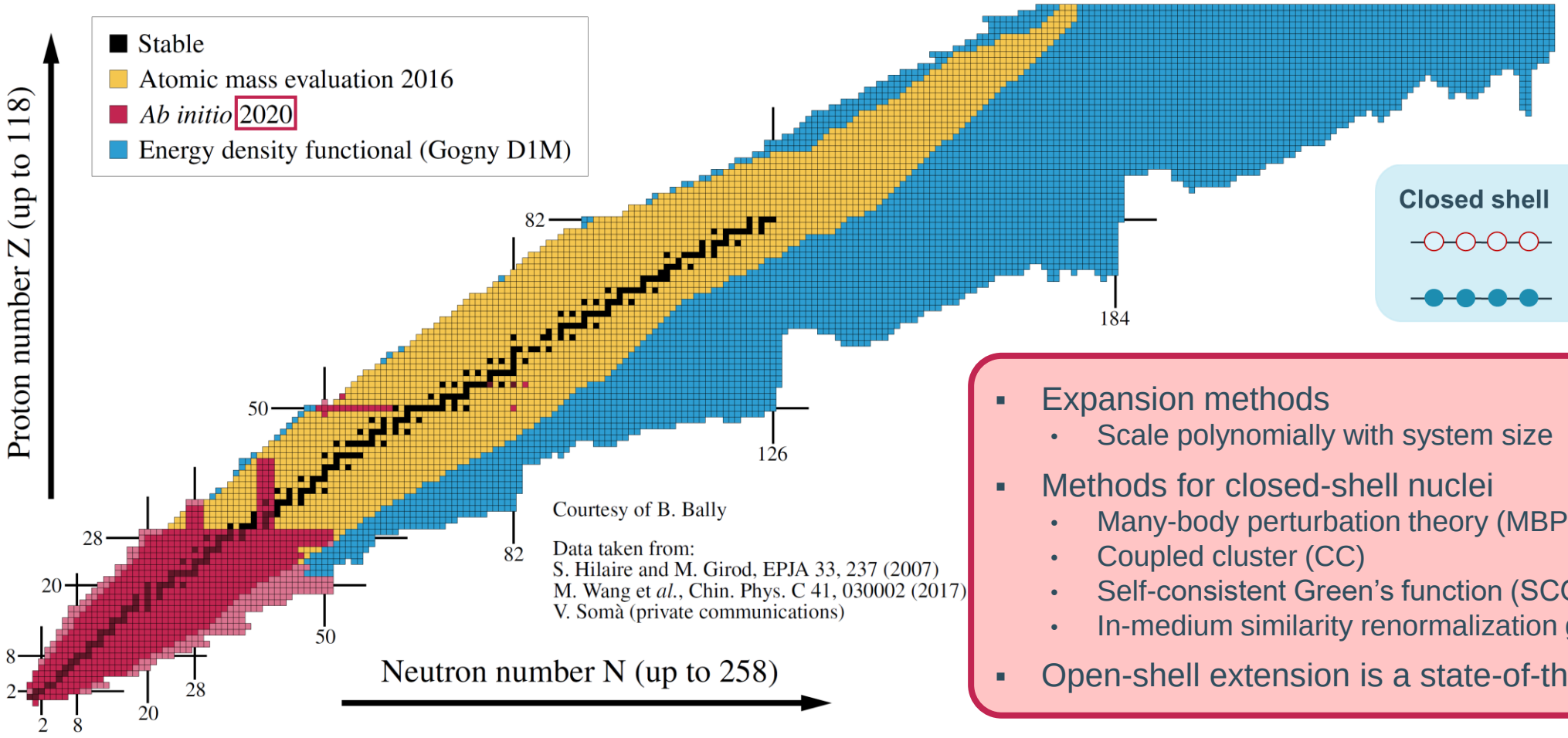

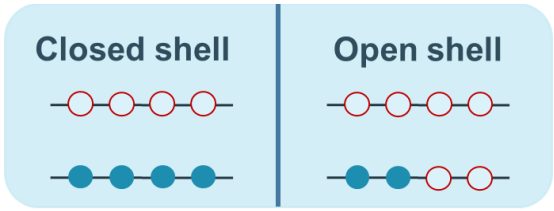

- Expansion methods
  - Scale polynomially with system size
- Methods for closed-shell nuclei
  - Many-body perturbation theory (MBPT)
  - Coupled cluster (CC)
  - Self-consistent Green's function (SCGF)
  - In-medium similarity renormalization group (IMSRG)
- Open-shell extension is a state-of-the-art challenge

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Open-shell systems

Beyond mean field

Expansion method: $\hat{H} = \hat{H}_0 + \hat{H}_1$

Mean field method:
Hartree-Fock-Bogoliubov (HFB)

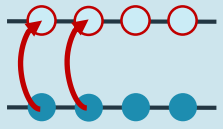
GS: $|\Phi\rangle$

$$\begin{cases} \hat{H}_0|\Phi_n\rangle = E_n^{(0)}|\Phi_n\rangle \\ |\Psi_n^A\rangle = \hat{\mathcal{W}}|\Phi_n\rangle \end{cases}$$

Symmetry conserving:

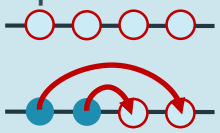
$$[\hat{H}_0, \hat{A}] = 0$$
$$[\hat{H}_1, \hat{A}] = 0$$

closed shell



non-degenerate
good starting point

open shell



degenerate
IR divergence

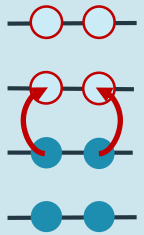
Bogoliubov transformation

Solved IR divergence

Symmetry breaking:

$$[\hat{H}_0, \hat{A}] \neq 0$$
$$[\hat{H}_1, \hat{A}] \neq 0$$

open → closed shell



non-degenerate
good starting point
pairing incorporated

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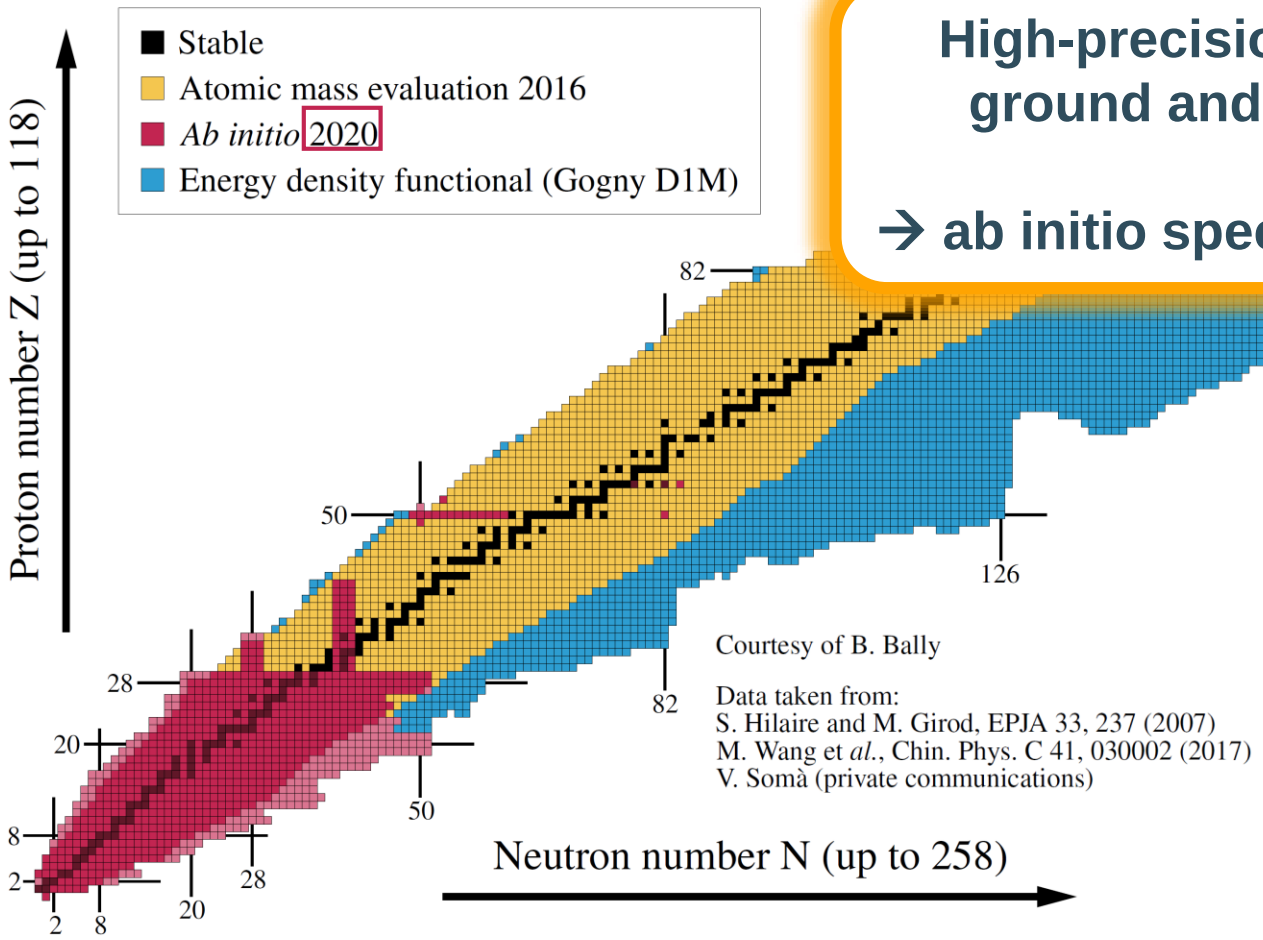
② Solving the Schrödinger equation



High-precision non-perturbative many-body method for ground and excited states of singly open-shell nuclei

→ ab initio spectroscopy along complete semi-magic chains

- Particle-number symmetry-breaking extensions

		Formalized	Implemented	
perturbative ←	BMBPT	✓	✓	[2]
non-perturbative ←	(EOM-)BCC	(✘) ✓	(✘) ✘	[3]
non-perturbative ←	GSCGF	✓	✓	[4]

[2] A.Tichai, P.Arthuis, T. Duguet et al. *Phys. Lett.* **B 786** 195 (2018)
[3] A.Signoracci, T. Duguet et al. *Phys. Rev. C* **91** 064320 (2015)
[4] V. Somà, T. Duguet, C. Barbieri, *Phys. Rev. C* **84** 064317 (2011)

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Bogoliubov Coupled Cluster

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Mean field method: Hartree-Fock-Bogoliubov (HFB)

GS: $|\Phi\rangle$

$$\begin{cases} \hat{H}_0|\Phi_n\rangle = E_n^{(0)}|\Phi_n\rangle \\ |\Psi_n^A\rangle = \hat{\mathcal{W}}|\Phi_n\rangle \end{cases}$$

BCC → $|\Psi_0^A\rangle = e^{\hat{\mathcal{T}}}|\Phi\rangle$

EOM-BCC → $|\Psi_n^A\rangle = \hat{\mathcal{R}}_n|\Psi_0^A\rangle$

$|\Psi_n^{A\pm1}\rangle = \hat{\mathcal{R}}_n^{\pm1}|\Psi_0^A\rangle$

Quasi-particle cluster operator

$$\hat{\mathcal{T}} \equiv \hat{\mathcal{T}}_1 + \hat{\mathcal{T}}_2 + \hat{\mathcal{T}}_3 + \cdots$$

BCCSD

- Singles → $\hat{\mathcal{T}}_1 \equiv \frac{1}{2!}\sum_{k_1k_2} t_{k_1k_2}\beta_{k_1}^\dagger\beta_{k_2}^\dagger$
- Doubles → $\hat{\mathcal{T}}_2 \equiv \frac{1}{4!}\sum_{k_1k_2k_3k_4} t_{k_1k_2k_3k_4}\beta_{k_1}^\dagger\beta_{k_2}^\dagger\beta_{k_3}^\dagger\beta_{k_4}^\dagger$
- Triples → $\hat{\mathcal{T}}_3 \equiv \frac{1}{6!}\sum_{k_1k_2k_3k_4k_5k_6} t_{k_1k_2k_3k_4k_5k_6}\beta_{k_1}^\dagger\beta_{k_2}^\dagger\beta_{k_3}^\dagger\beta_{k_4}^\dagger\beta_{k_5}^\dagger\beta_{k_6}^\dagger$

excitation amplitudes

$\hat{A}|\Psi_0\rangle \equiv \hat{A}\left(e^{\hat{\mathcal{T}}_1+\hat{\mathcal{T}}_2}|\Phi\rangle\right) \neq \mathrm{A}|\Psi_0\rangle$ → Monitor and constrain $\langle A\rangle$

Quasi-particle creation operators

unitary mix of ordinary particle creation and annihilation operators $\{c_p^\dagger, c_p\}$

$$\beta_k^\dagger \equiv \sum_p U_{pk}c_p^\dagger + V_{pk}c_p$$

$$\beta_k \equiv \sum_p U_{pk}^* c_p + V_{pk}^* c_p^\dagger$$

Solutions of a set of non-linear algebraic equations which can be solved iteratively

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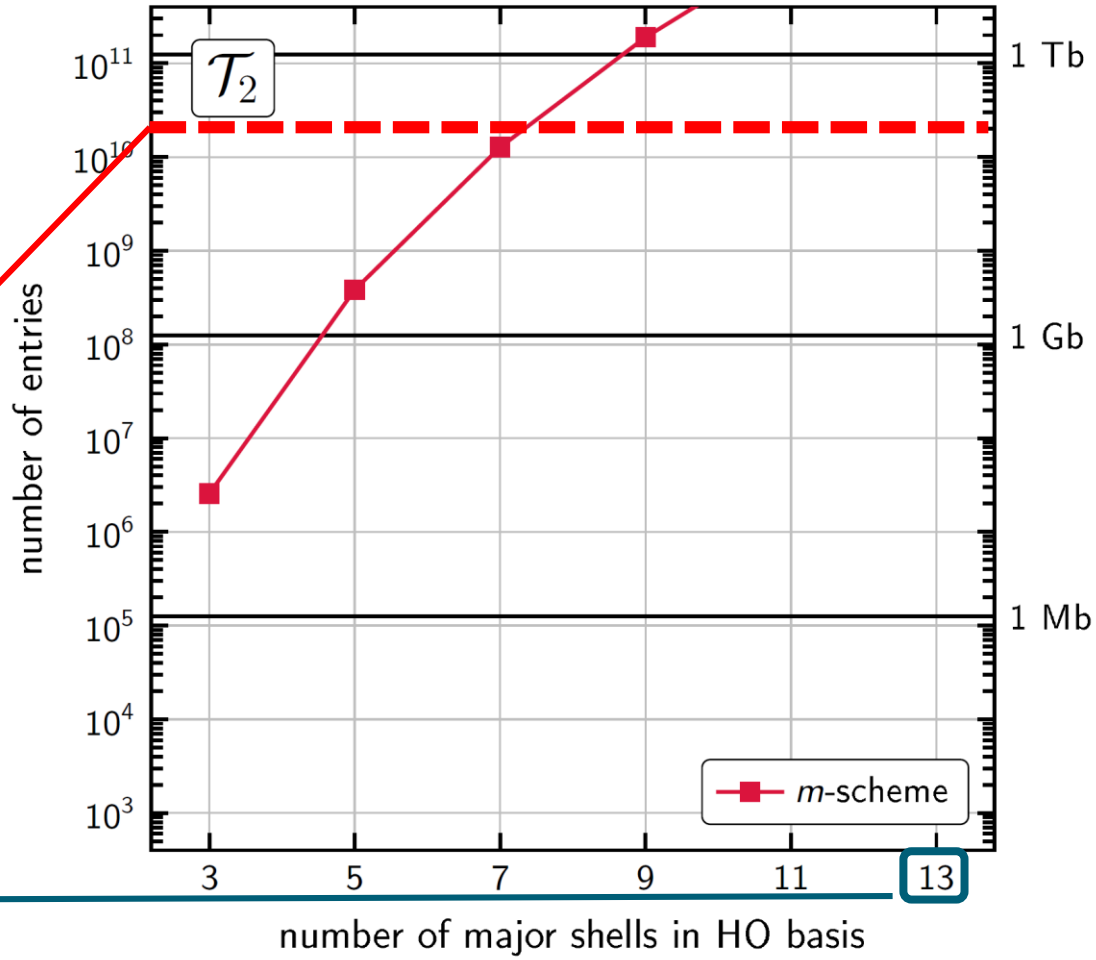
Scalability

m-scheme BCC

- Direct implementation of the BCC equations

✕ not scalable to large model spaces

Computational wall: ≈ 200Gb of RAM



Model space size required for high-precision calculations

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Scalability

m-scheme BCC

- Direct implementation of the BCC equations

✗ not scalable to large model spaces

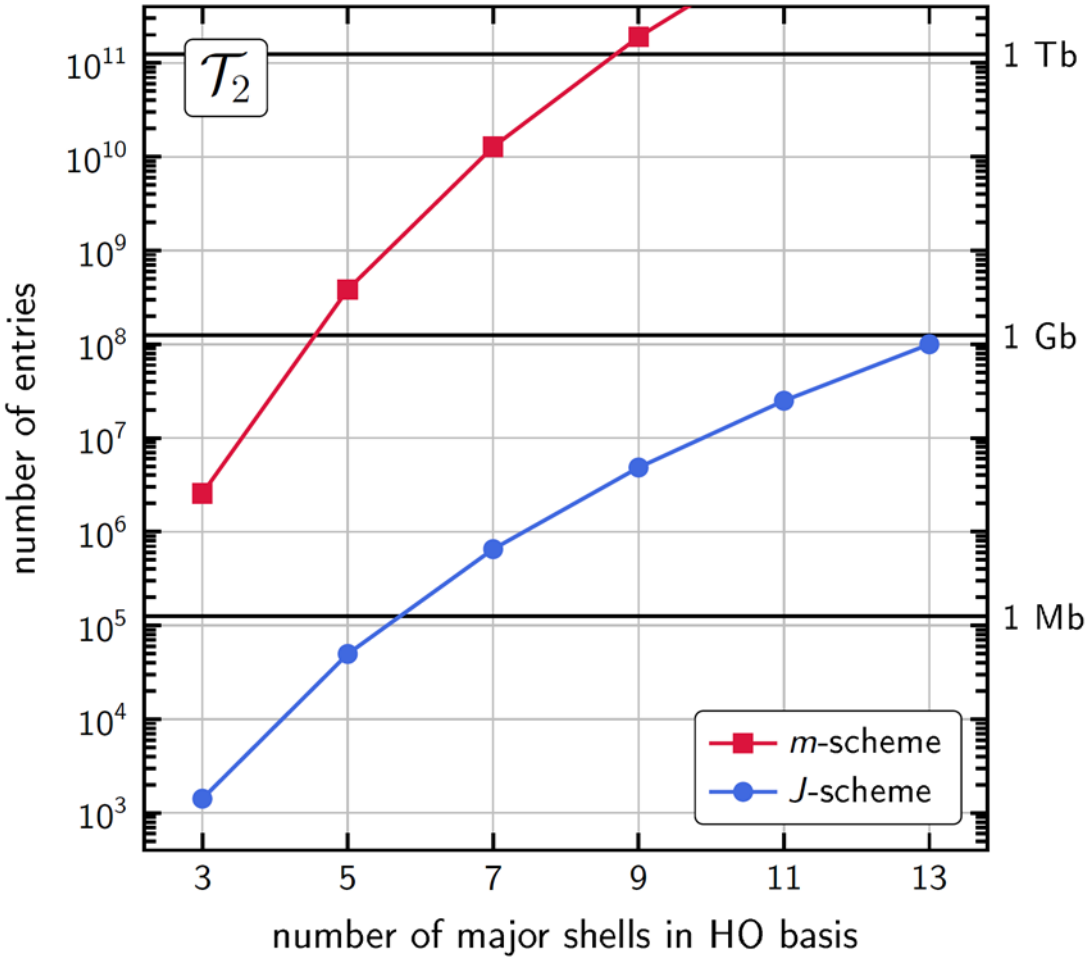
Angular momentum coupling (AMC)

J-scheme BCC

- Exploit shared rotational symmetry of $\hat{H}$ and computational basis
- Spherical BCC equations much more involved
- Assisted with automated AMC tools [5]

✓ Resolves scalability problem

- Benchmarked w.r.t. m-scheme code (small model spaces)



[5] A. Tichai et al., *Eur. Phys. J. A* **56** 10 272 (2020)

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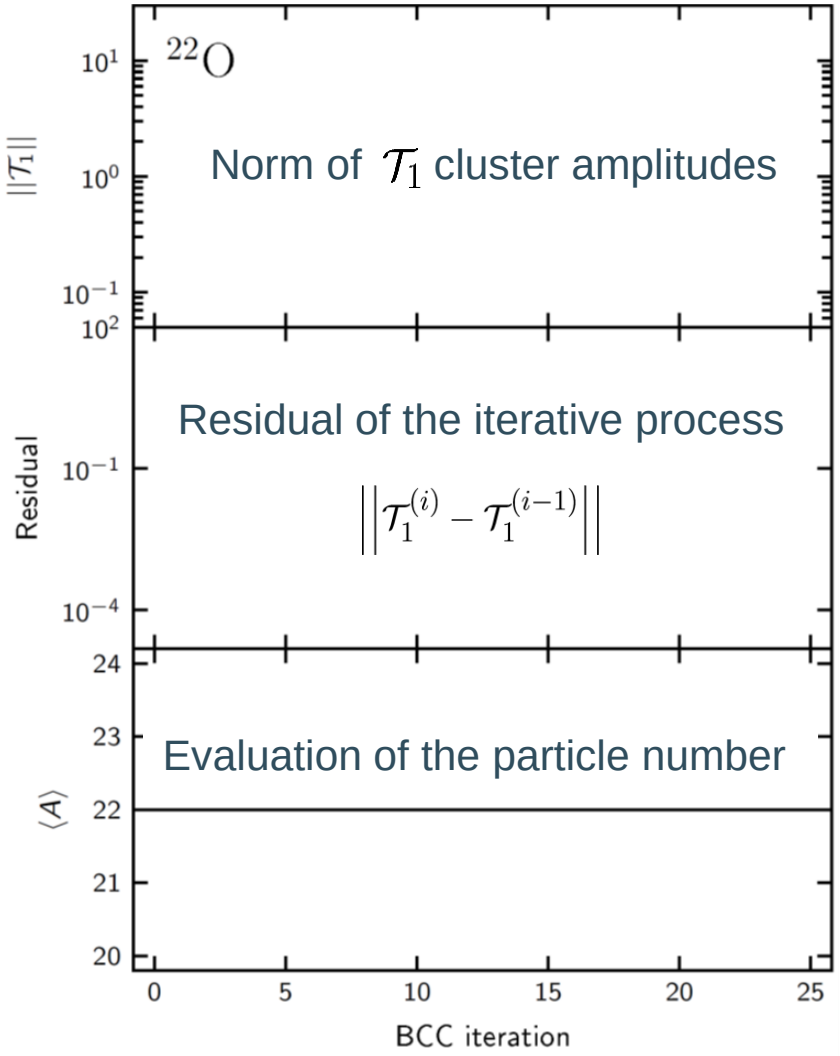
Results

- m-scheme BCCSD
- Ground-state ^{22}O
- 5 major shells in computational basis



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m-scheme BCCSD ^{22}O

Initial results
- ✗ Iterative process diverges

↓ Enforce convergence with mixing techniques ↓

Simple mixing
- ✓ Resolves divergence
- ✓ In agreement with results in *Signorracci et al.* [3]
- ✗ Convergence is very slow

↓ Convergence acceleration method ↓

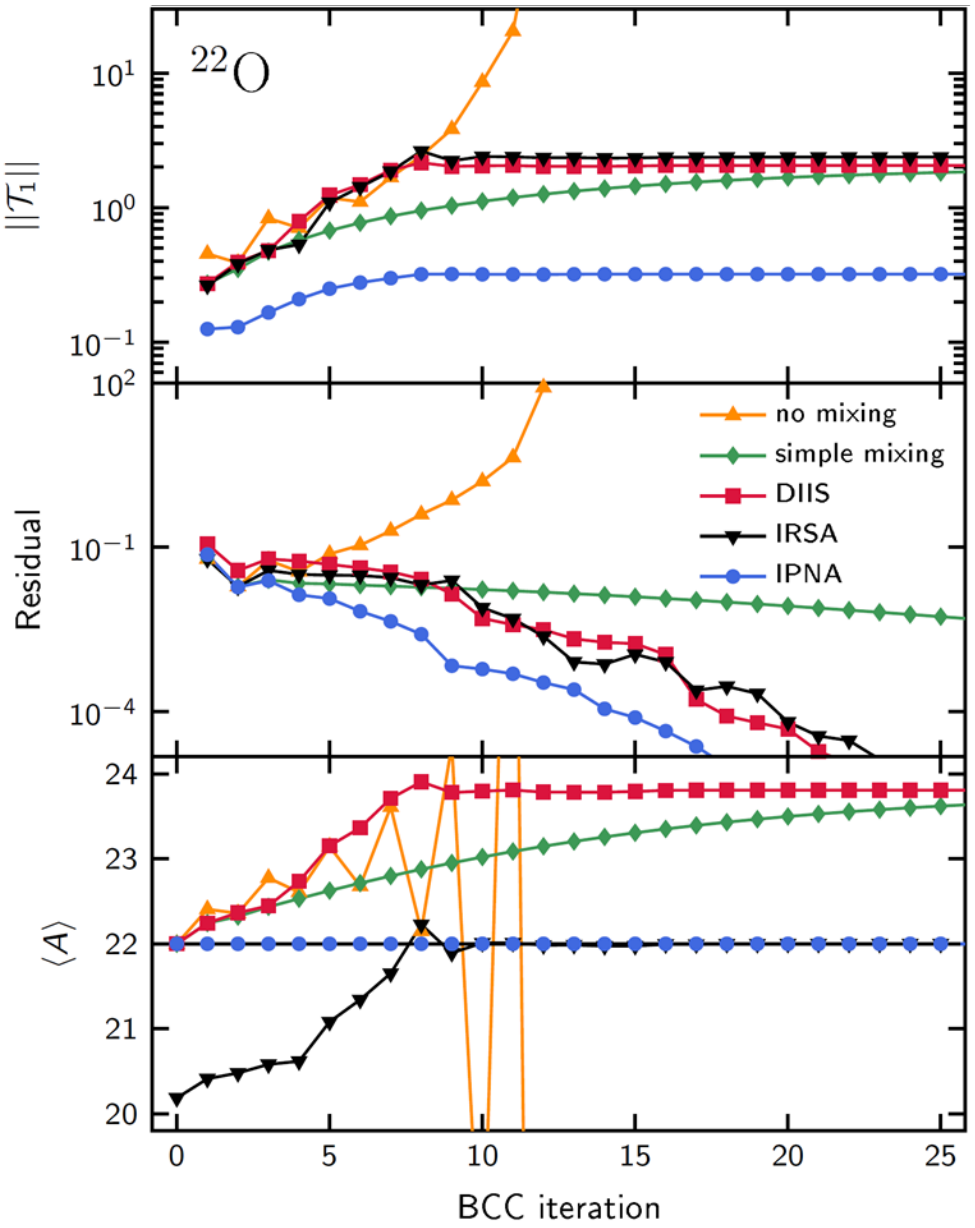
Direct Inversion of the Iterative Subspace (DIIS)
- ✓ Much faster convergence
- ✗ Average particle number has shifted

↓ particle number adjustment proposed in [3] ↓

Iterative reference state adjustment (IRSA)
- ✓ BCC solution correct particle number on average
- ✗ Suitable reference state does not always exist
- ✗ Computationally very intensive

↓ Novel particle number adjustment ↓

Internal particle number adjustment (IPNA)
- ✓ particle number constrained in each BCC iteration
- ✓ BCC converges even faster
- ✓ Cluster amplitudes are reduced



[3] A.Signoracci, T. Duguet et al. *Phys. Rev. C* **91** 064320 (2015)

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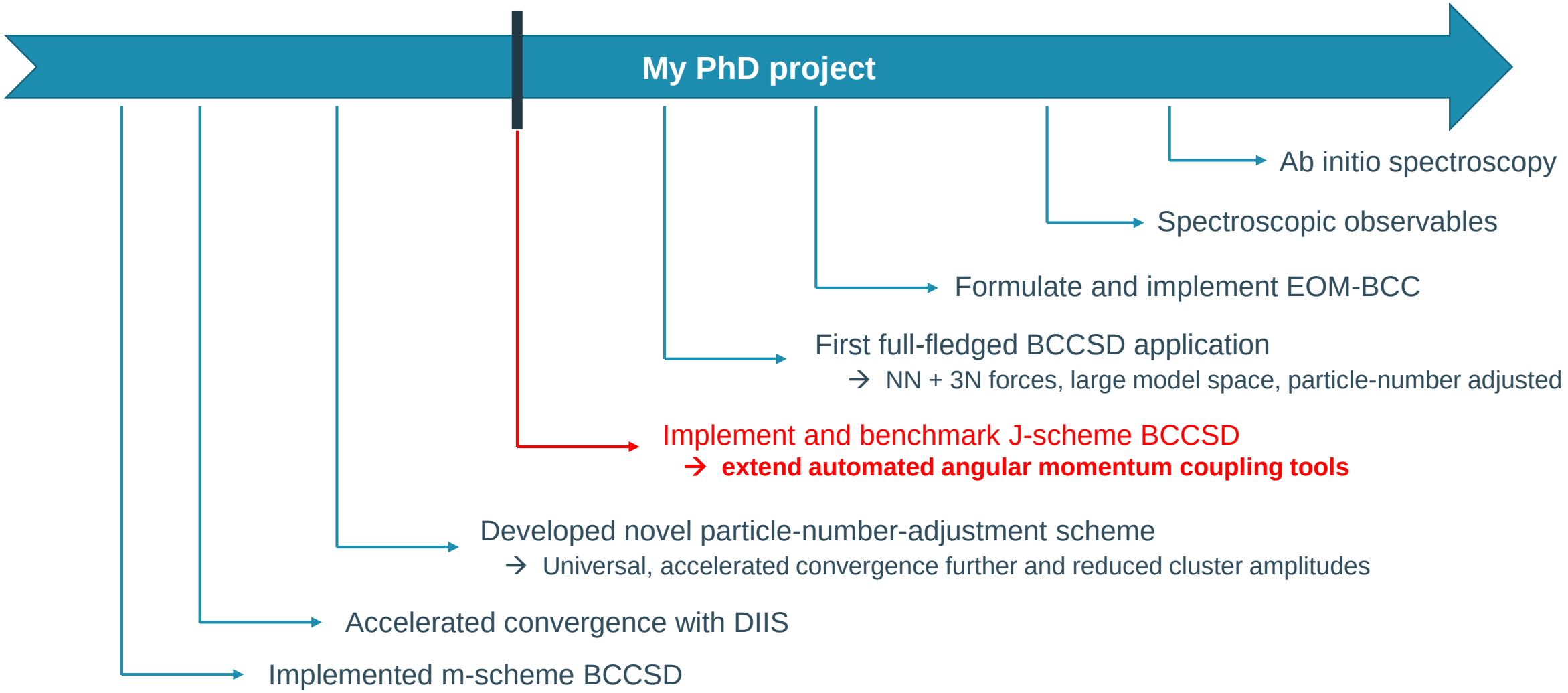

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