DE LA RECHERCHE À L'INDUSTRIE

Ab initio description of doubly open-shell nuclei via multi-reference expansion methods

DRF/IRFU/LENA

Mikael Frosini

Supervisors:

Thomas Duguet	CEA-DRF
Jean-Paul Ebran	CEA-DAM
Vittorio Somà	CEA-DRF

Colloque GANIL 2021

Context of this work

Ab initio microscopic description of nuclear structure

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD

Context of this work

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

Context of this work

***Ab initio* microscopic description of nuclear structure**

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

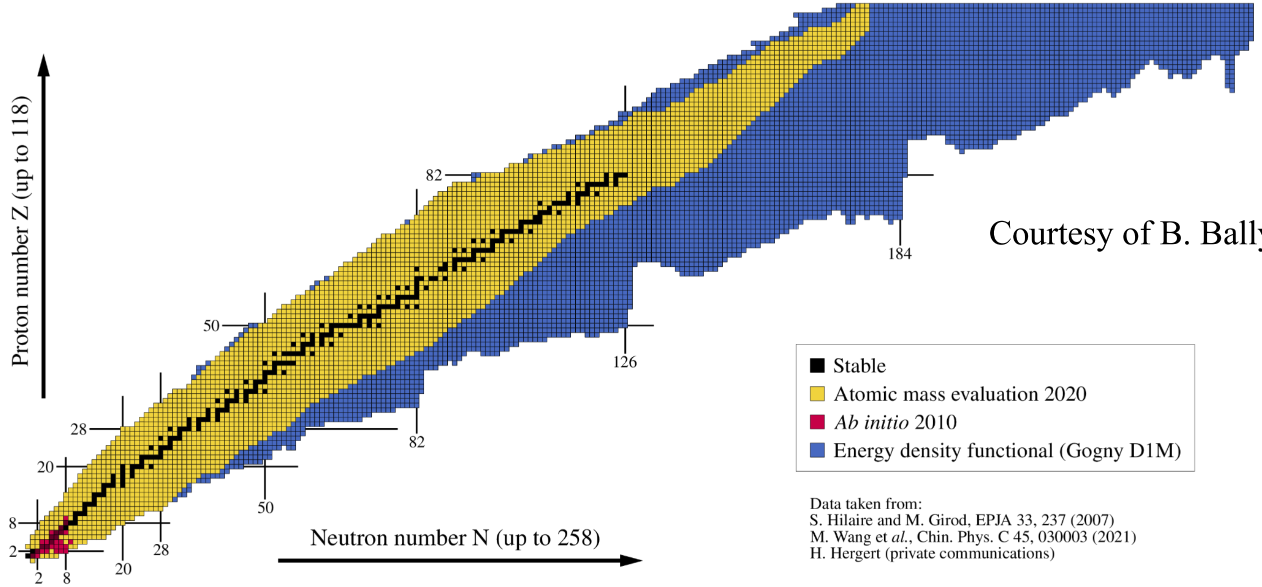
- Long term endeavor of *ab initio* **microscopic description**
    - **Consistency** (unified theoretical framework)
    - **Systematicity** (complete phenomenology)
    - **Accuracy & precision** (with respect to experiment)

Context of this work

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

- Long term endeavor of *ab initio* **microscopic description**
  - **Consistency** (unified theoretical framework)
  - **Systematicity** (complete phenomenology)
  - **Accuracy & precision** (with respect to experiment)

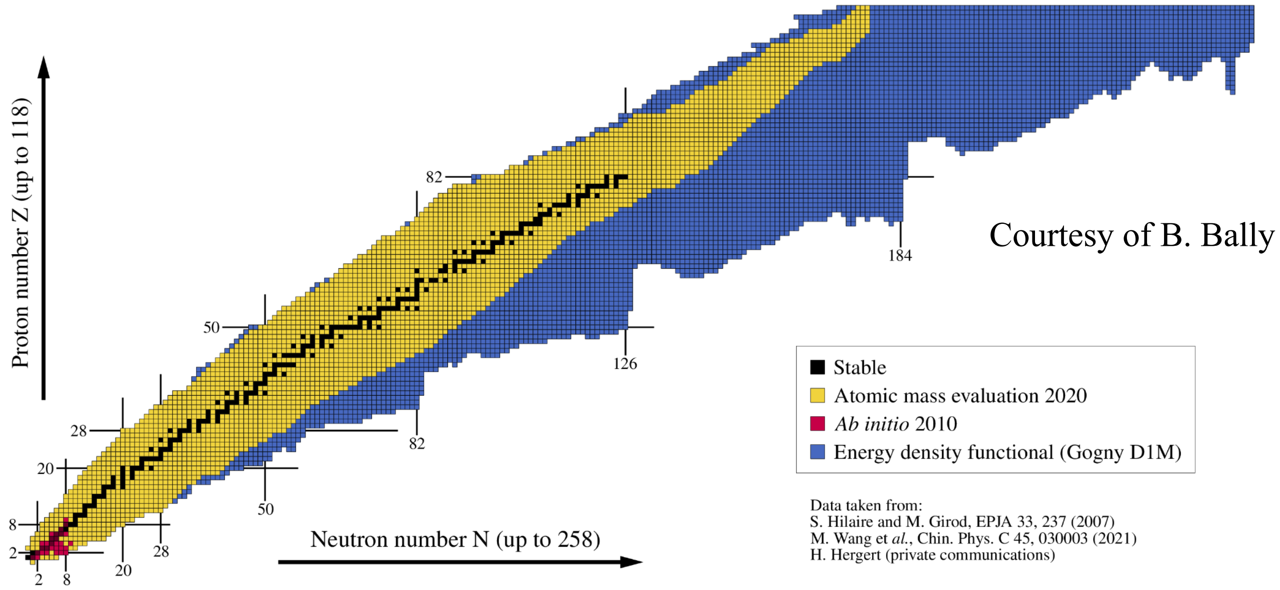


Courtesy of B. Bally

***Ab initio* microscopic description of nuclear structure**

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

- Long term endeavor of *ab initio* **microscopic description**
  - **Consistency** (unified theoretical framework)
  - **Systematicity** (complete phenomenology)
  - **Accuracy & precision** (with respect to experiment)



Light nuclei

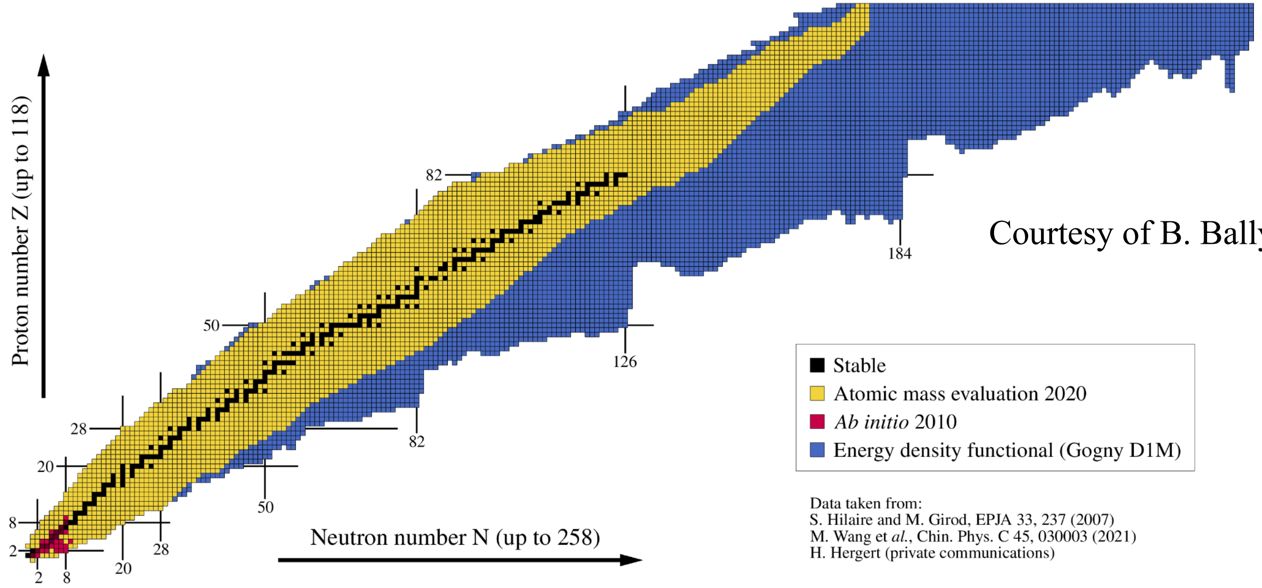
Quasi-exact methods

1990's
NCSM, MC

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

- Long term endeavor of *ab initio* **microscopic description**
  - **Consistency** (unified theoretical framework)
  - **Systematicity** (complete phenomenology)
  - **Accuracy & precision** (with respect to experiment)



Courtesy of B. Bally

Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
H. Hergert (private communications)

Light nuclei

Quasi-exact methods

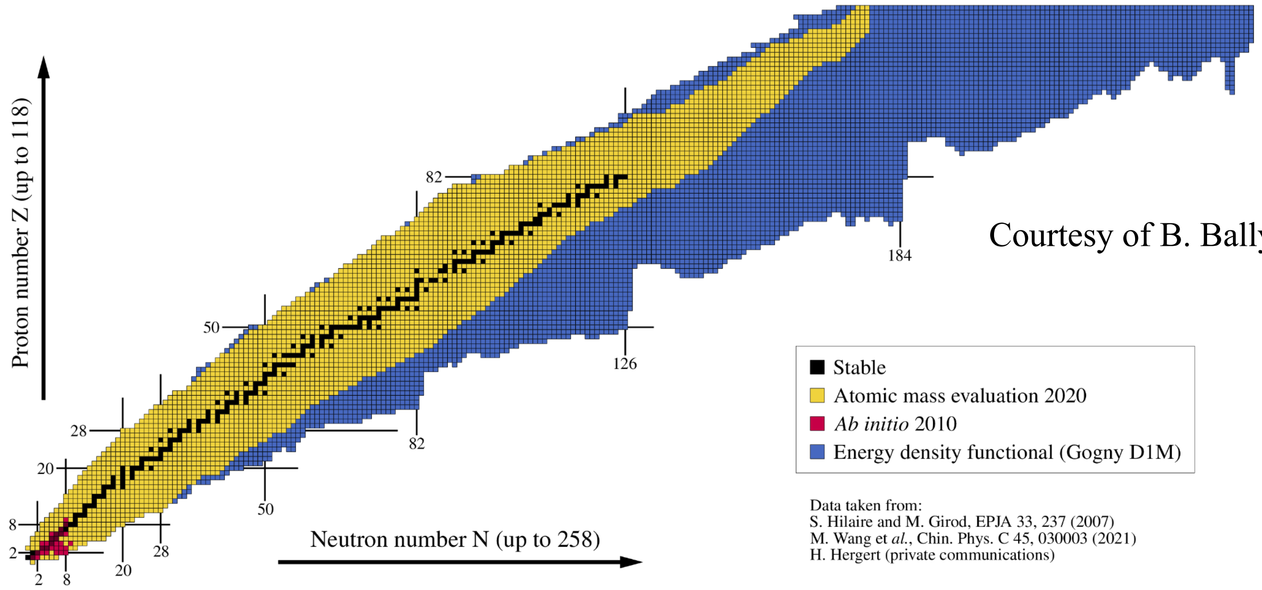
1990's
NCSM, MC

Exponential scaling

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

- Long term endeavor of *ab initio* **microscopic description**
  - **Consistency** (unified theoretical framework)
  - **Systematicity** (complete phenomenology)
  - **Accuracy & precision** (with respect to experiment)



Courtesy of B. Bally

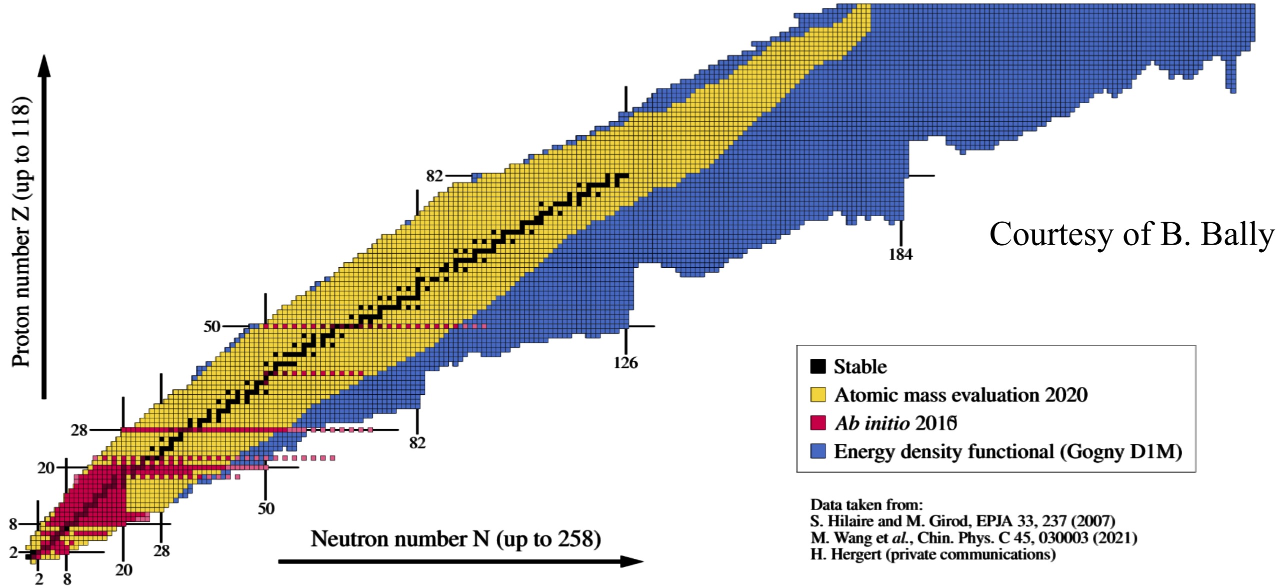
Light nuclei	1990's	
Quasi-exact methods	NCSM, MC	Exponential scaling

Closed shells	2000's	
Expansion methods Single-reference	MBPT, CC, SR-IMSRG, SCGF	Polynomial scaling

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

- Long term endeavor of *ab initio* **microscopic description**
  - **Consistency** (unified theoretical framework)
  - **Systematicity** (complete phenomenology)
  - **Accuracy & precision** (with respect to experiment)



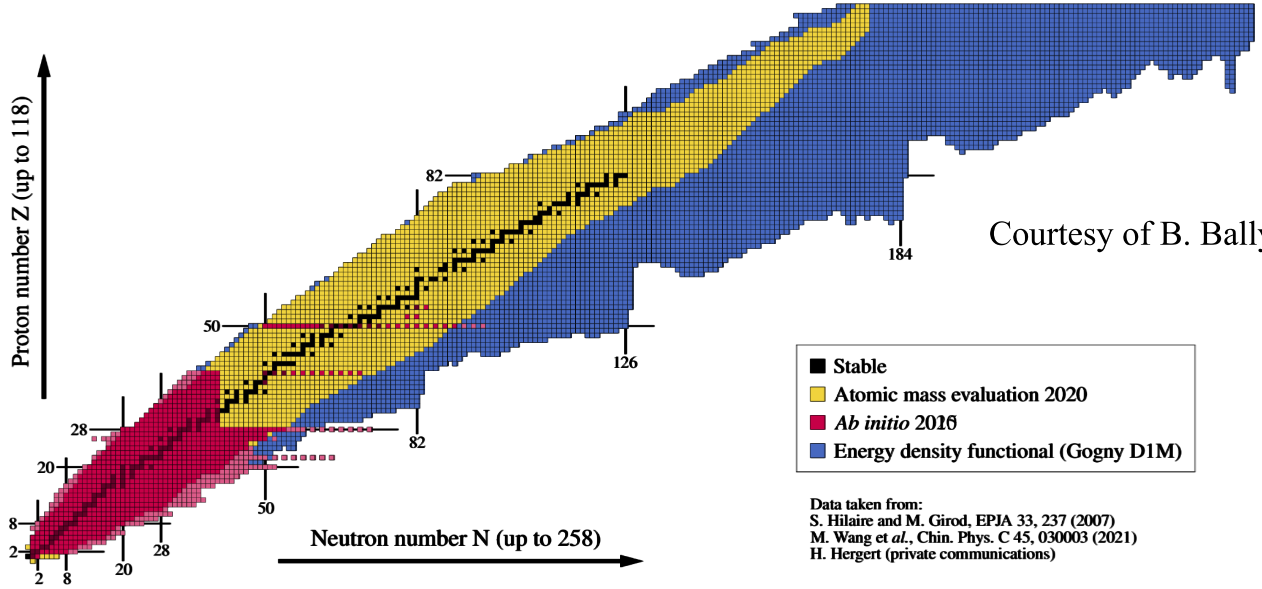
Courtesy of B. Bally

Light nuclei — **Quasi-exact methods**	**1990's** NCSM, MC		Exponential scaling
Closed shells — **Expansion methods Single-reference**	**2000's** MBPT, CC, SR-IMSRG, SCGF		Polynomial scaling
Singly open-shells — **Symmetry-breaking Multi-reference**	**2010's** BMBPT, BCC, *MR-IMSRG*, GSCGF		Polynomial scaling

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

- Long term endeavor of *ab initio* **microscopic description**
  - **Consistency** (unified theoretical framework)
  - **Systematicity** (complete phenomenology)
  - **Accuracy & precision** (with respect to experiment)



Courtesy of B. Bally

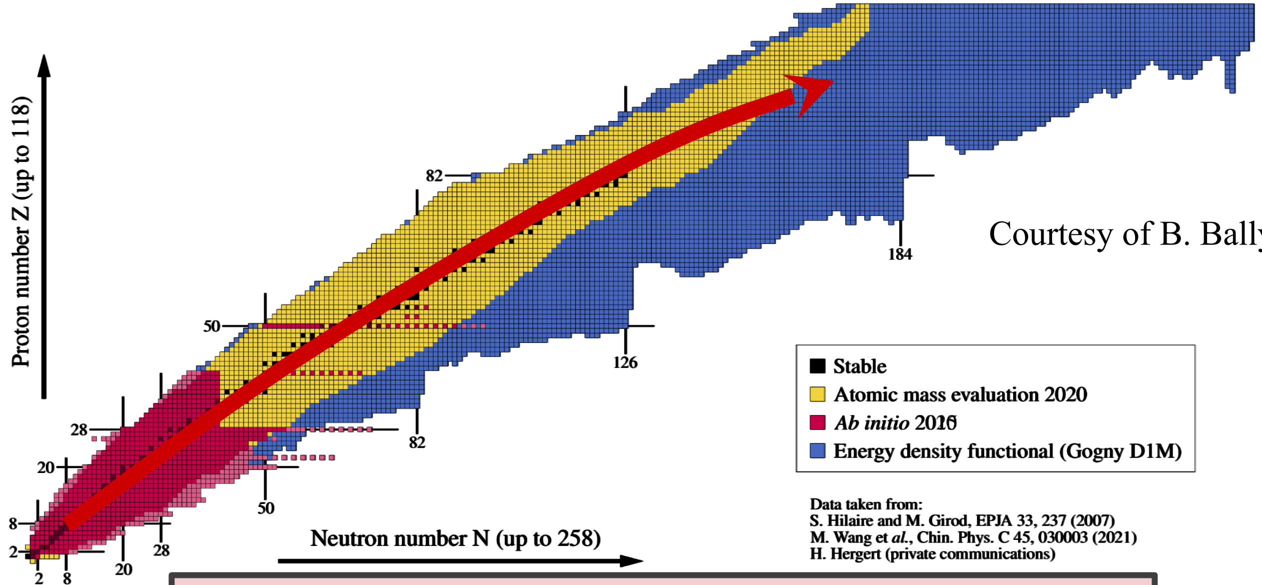
Light nuclei **Quasi-exact methods**	**1990's** NCSM, MC	Exponential scaling
Closed shells **Expansion methods** **Single-reference**	**2000's** MBPT, CC, SR-IMSRG, SCGF	Polynomial scaling
Singly open-shells **Symmetry-breaking** **Multi-reference**	**2010's** BMBPT, BCC, *MR-IMSRG*, GSCGF	Polynomial scaling
Doubly open-shells **Symmetry-breaking** **Multi-reference**	**2020-?** dBMBPT, dCC, *MR-IMSRG*	Polynomial scaling

Context of this work

Ab initio microscopic description of nuclear structure

1) A structure-less nucleons as degrees of freedom
2) Interaction systematically expanded (EFT) consistently with QCD
3) **Solve A-body Schrödinger equation to relevant accuracy**

- Long term endeavor of *ab initio* **microscopic description**
  - **Consistency** (unified theoretical framework)
  - **Systematicity** (complete phenomenology)
  - **Accuracy & precision** (with respect to experiment)



Courtesy of B. Bally

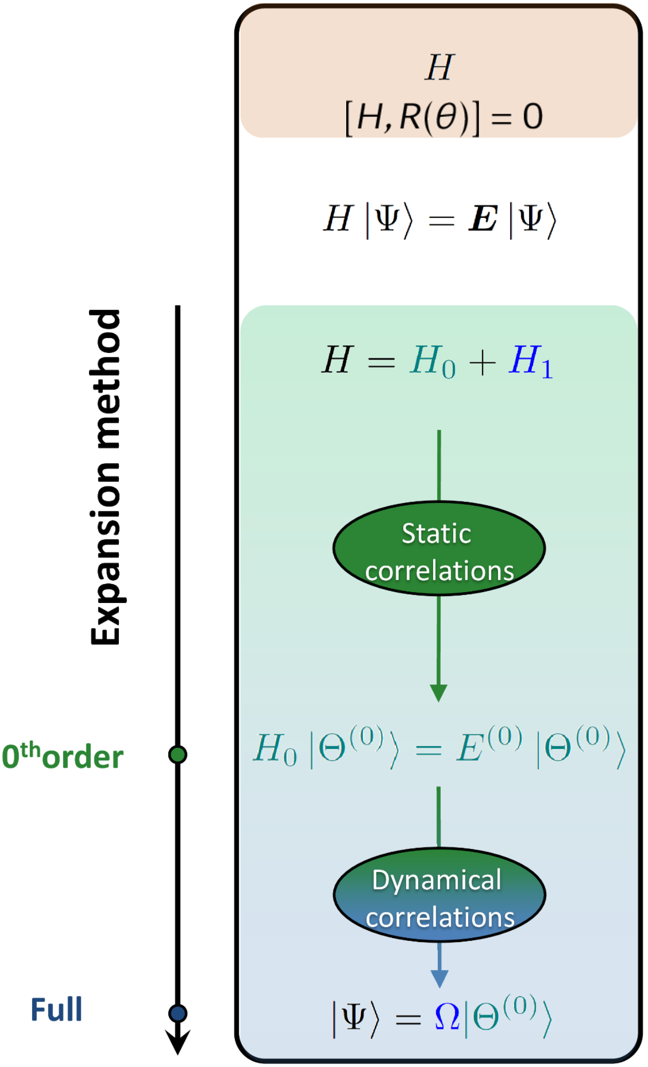
Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)
M. Wang et al., Chin. Phys. C 45, 030003 (2021)
H. Hergert (private communications)

Novel multi-reference expansion method

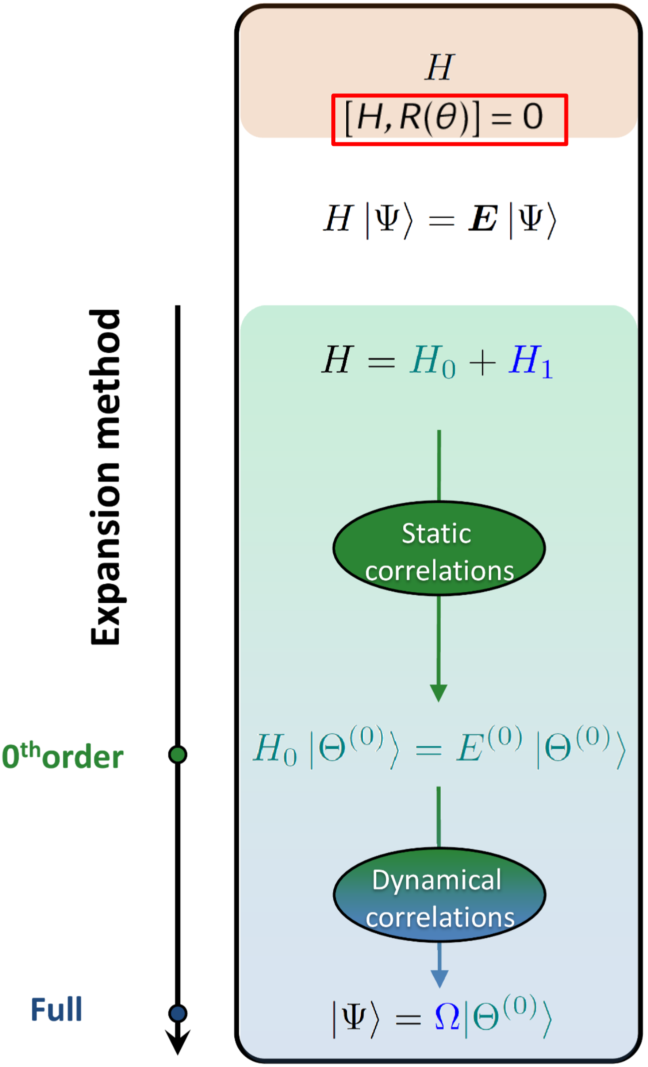
- **Polynomial**
- **Symmetry-conserving**
- **Doubly open-shell nuclei**
- **Ground and excited states**

Light nuclei — **Quasi-exact methods**	**1990's** NCSM, MC	Exponential scaling
Closed shells — **Expansion methods Single-reference**	**2000's** MBPT, CC, SR-IMSRG, SCGF	Polynomial scaling
Singly open-shells — **Symmetry-breaking Multi-reference**	**2010's** BMBPT, BCC, *MR-IMSRG*, GSCGF	Polynomial scaling
Doubly open-shells — **Symmetry-breaking Multi-reference**	**2020-?** dBMBPT, dCC, *MR-IMSRG*	Polynomial scaling

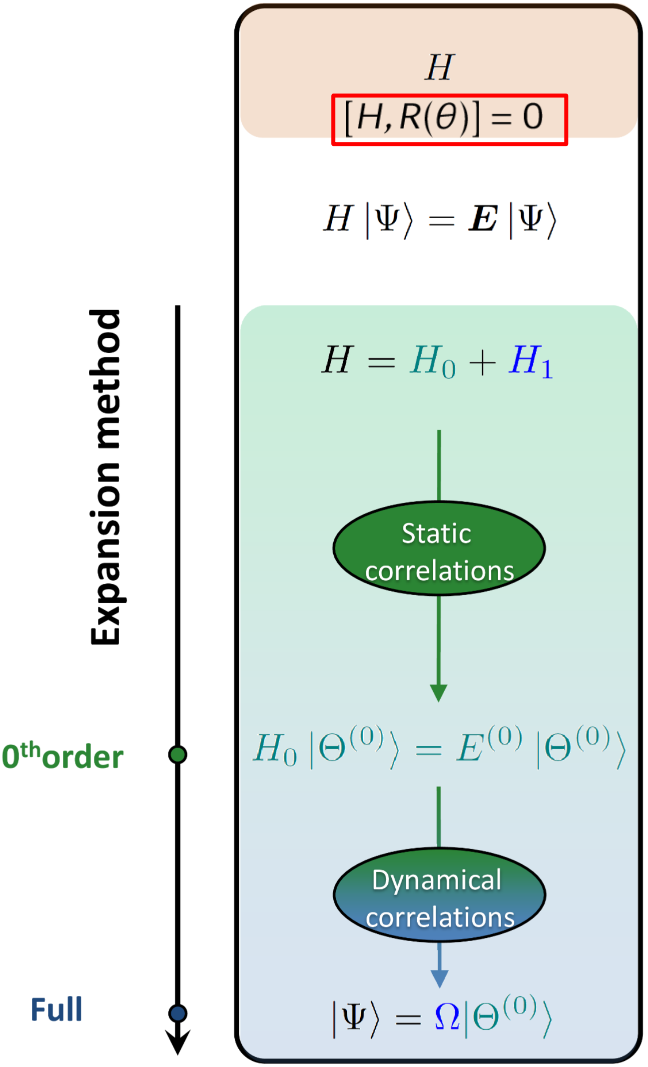
Expansion methods for open-shell nuclei



Expansion methods for open-shell nuclei



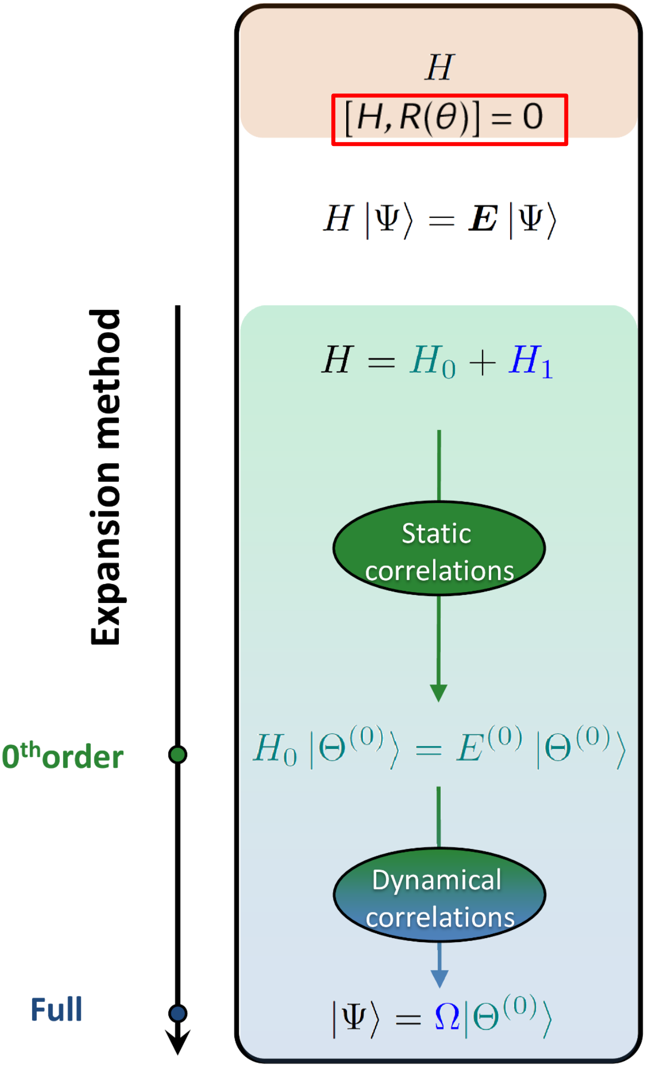
χ-EFT Hamiltonian



χ-EFT Hamiltonian

Secular equation

Expansion methods for open-shell nuclei

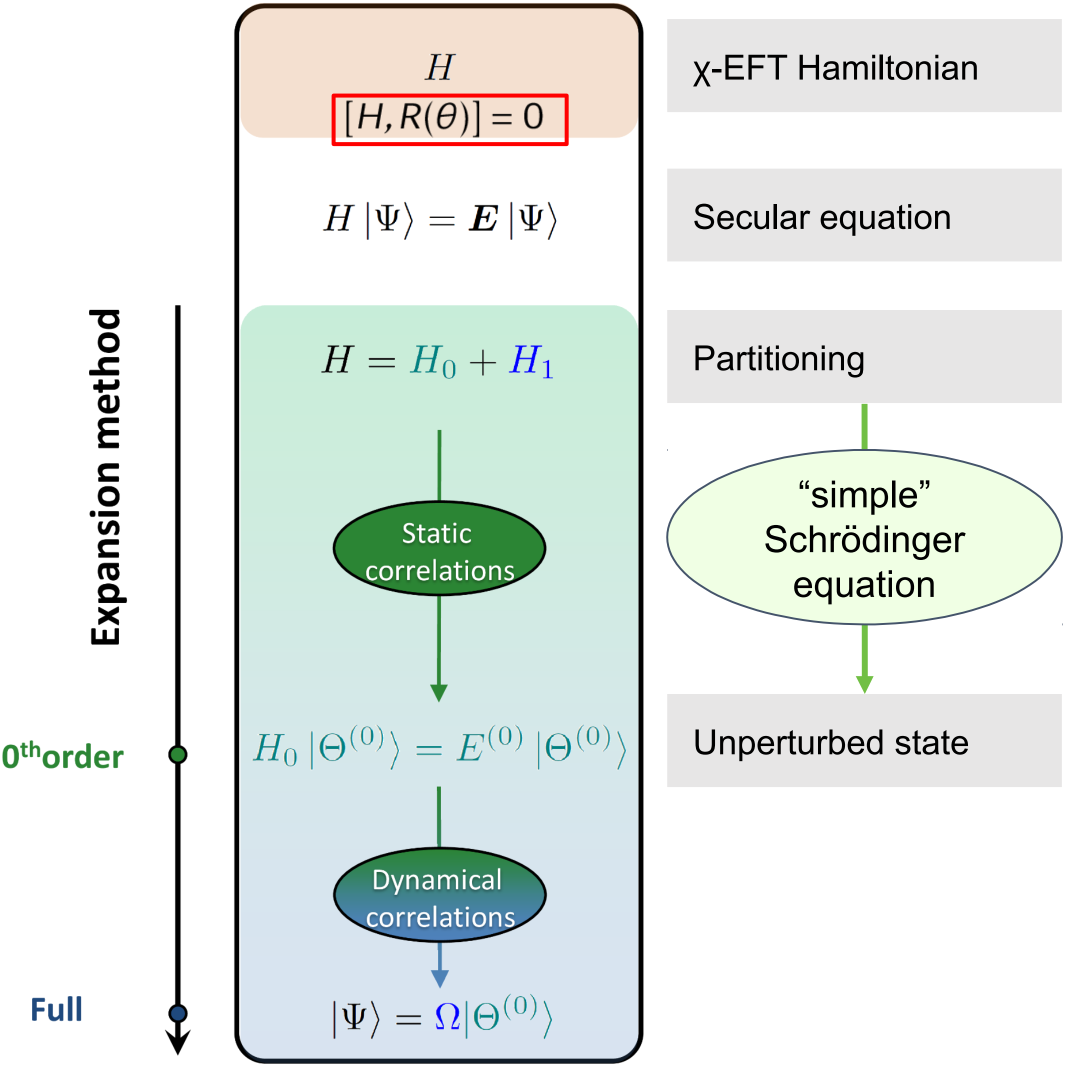


χ-EFT Hamiltonian

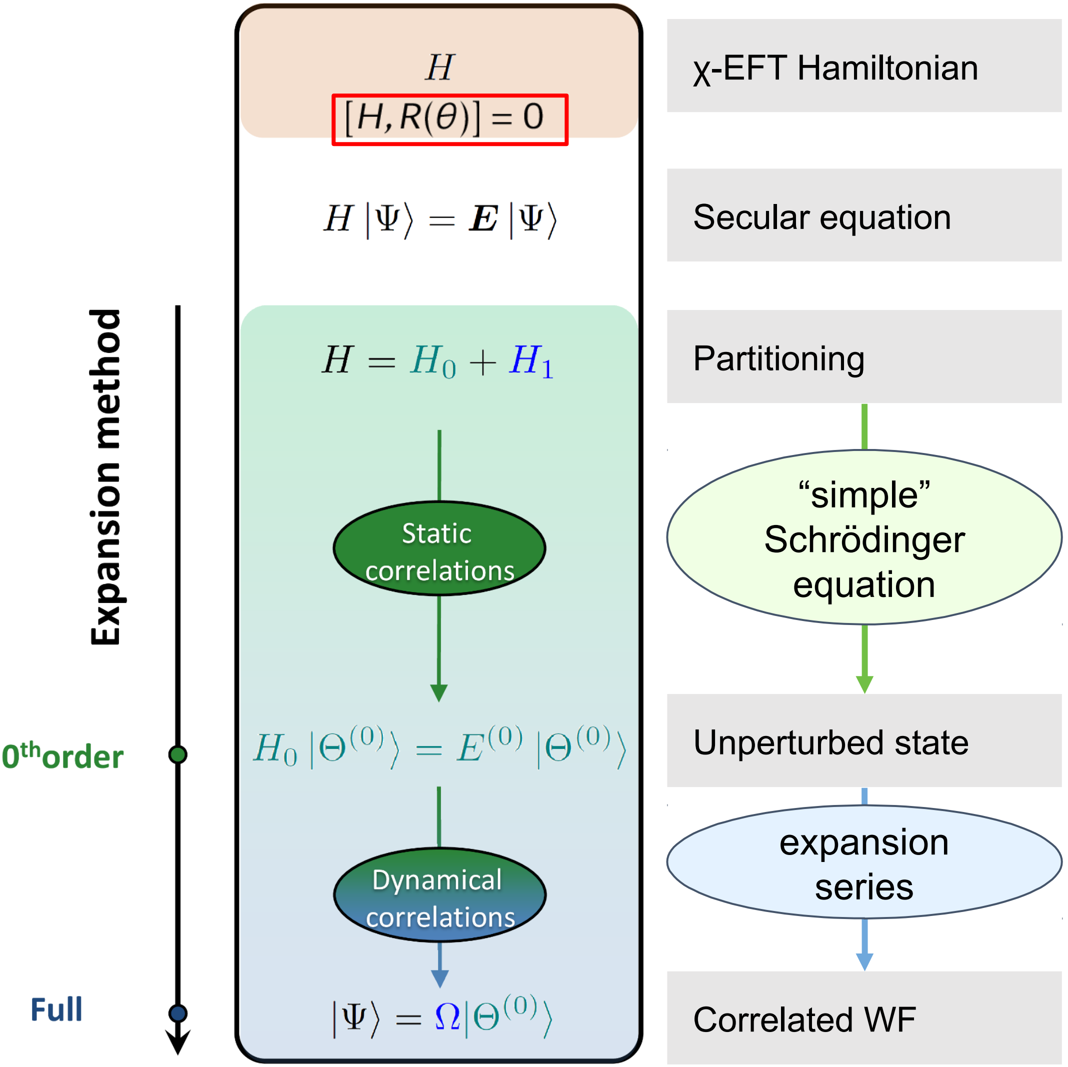
Secular equation

Partitioning

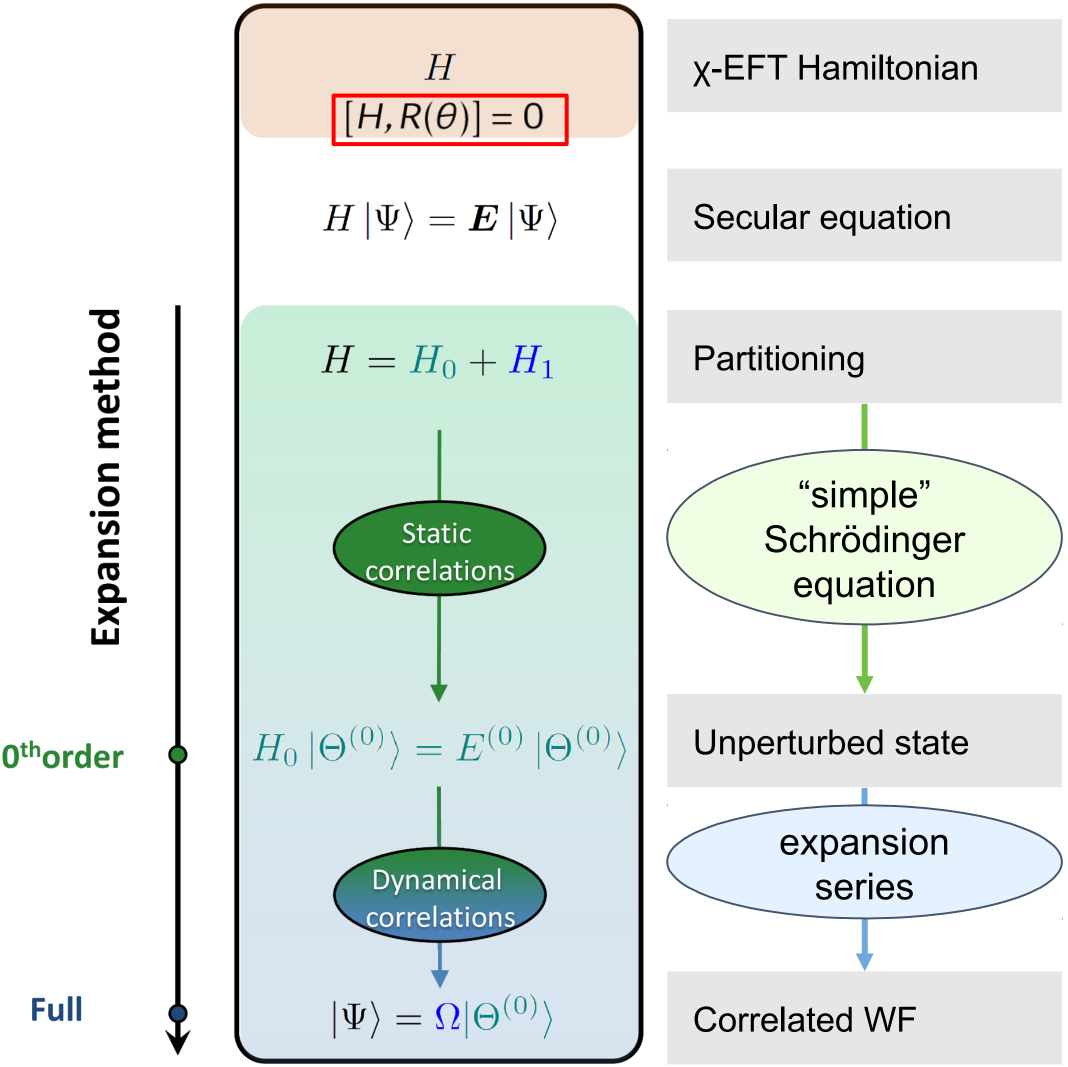
Expansion methods for open-shell nuclei



Expansion methods for open-shell nuclei



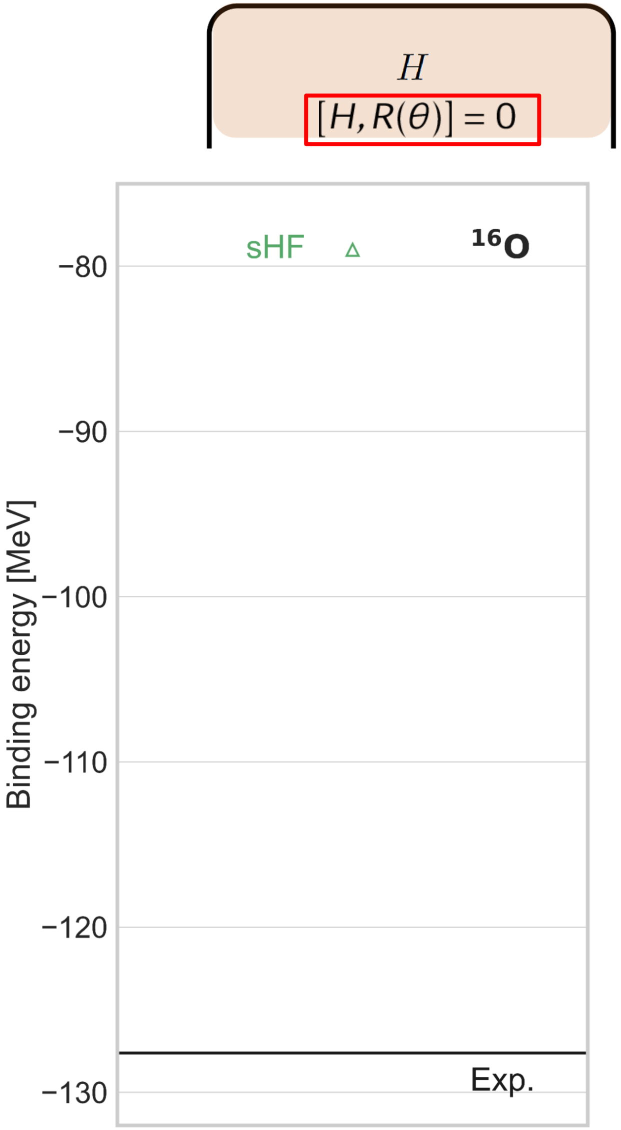
Expansion methods for open-shell nuclei

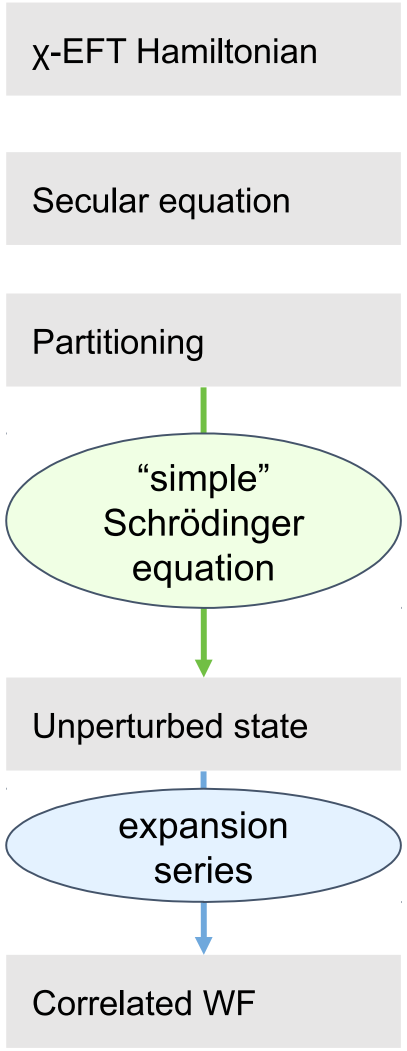


Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

Expansion methods for open-shell nuclei

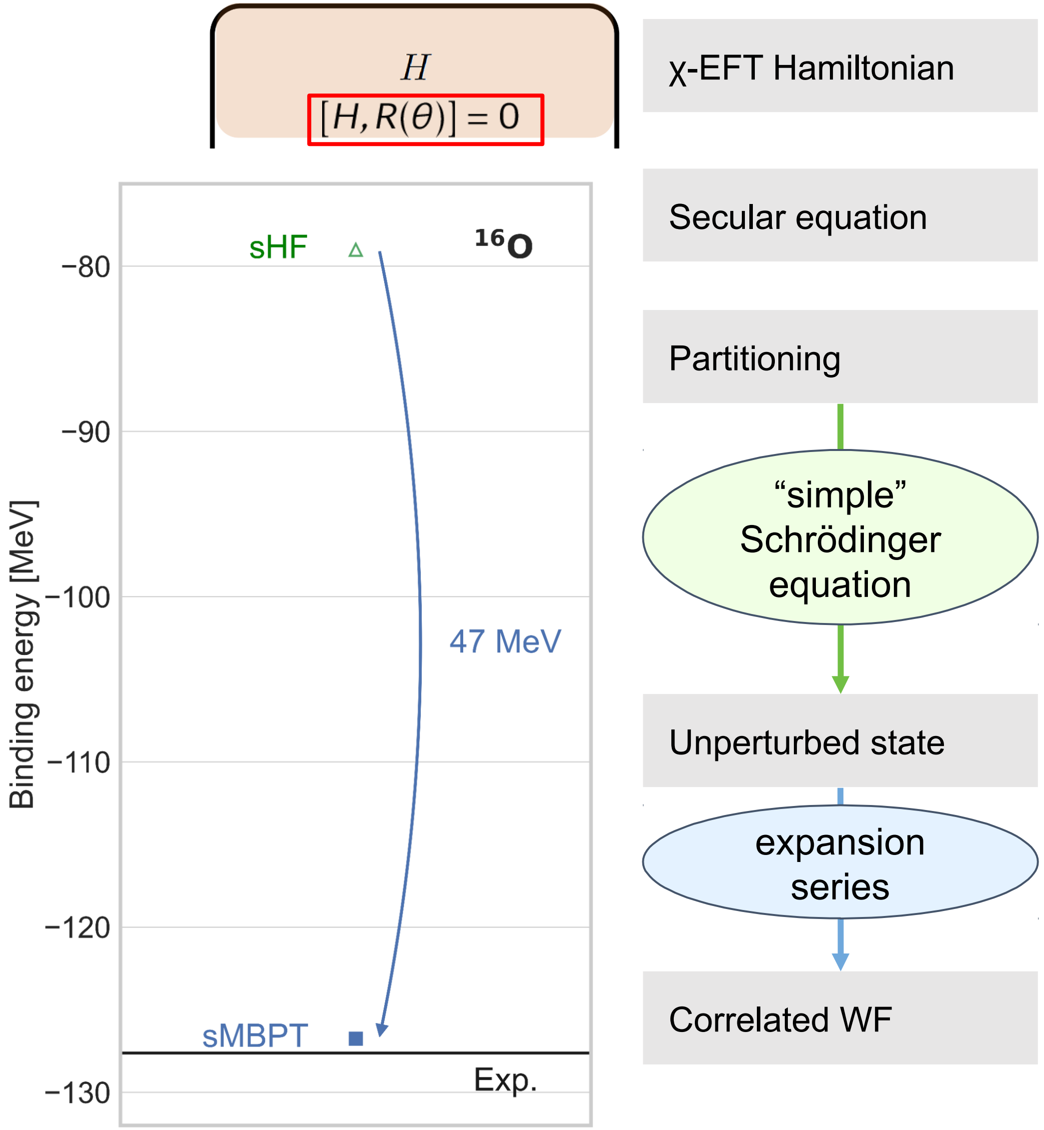




Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

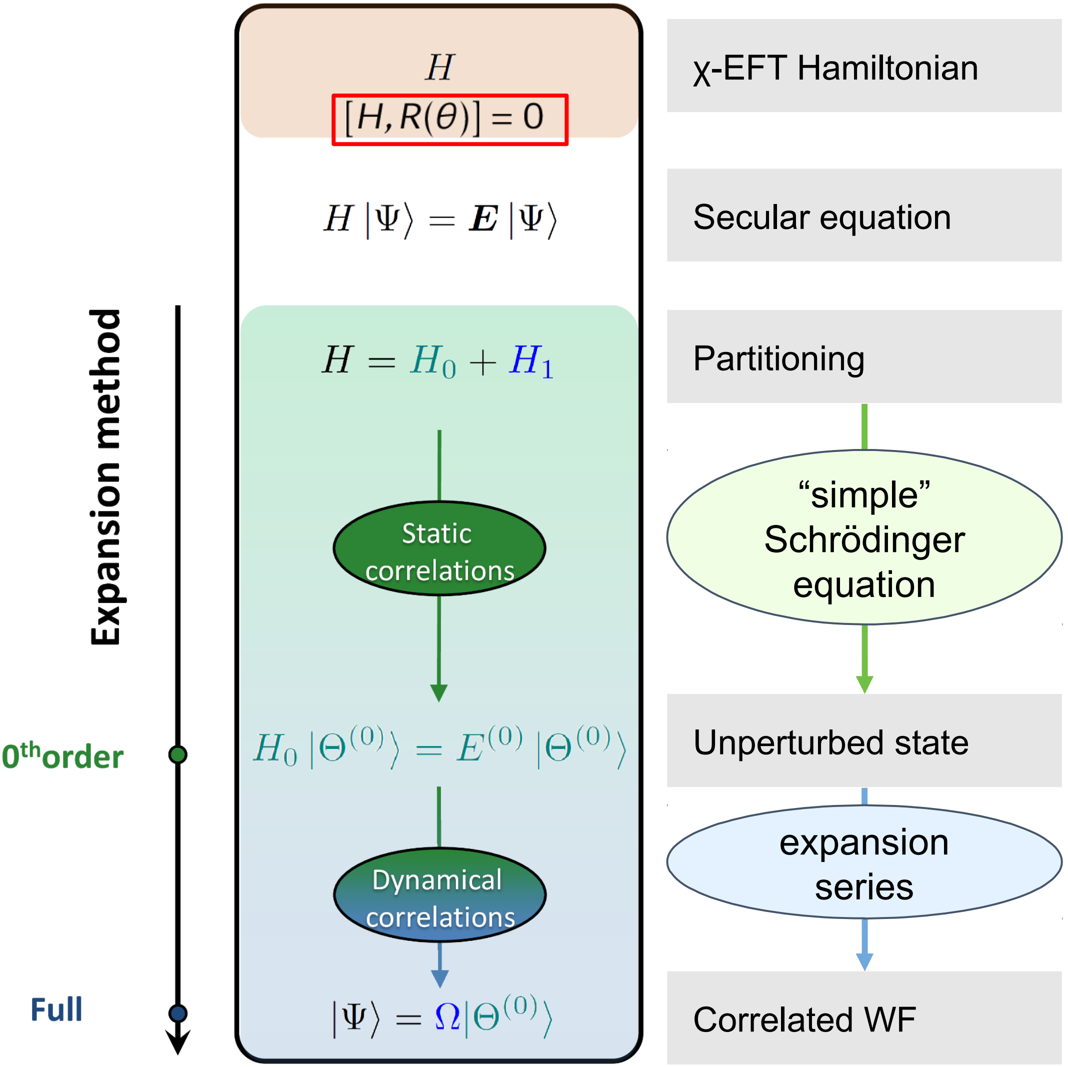
Expansion methods for open-shell nuclei



Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

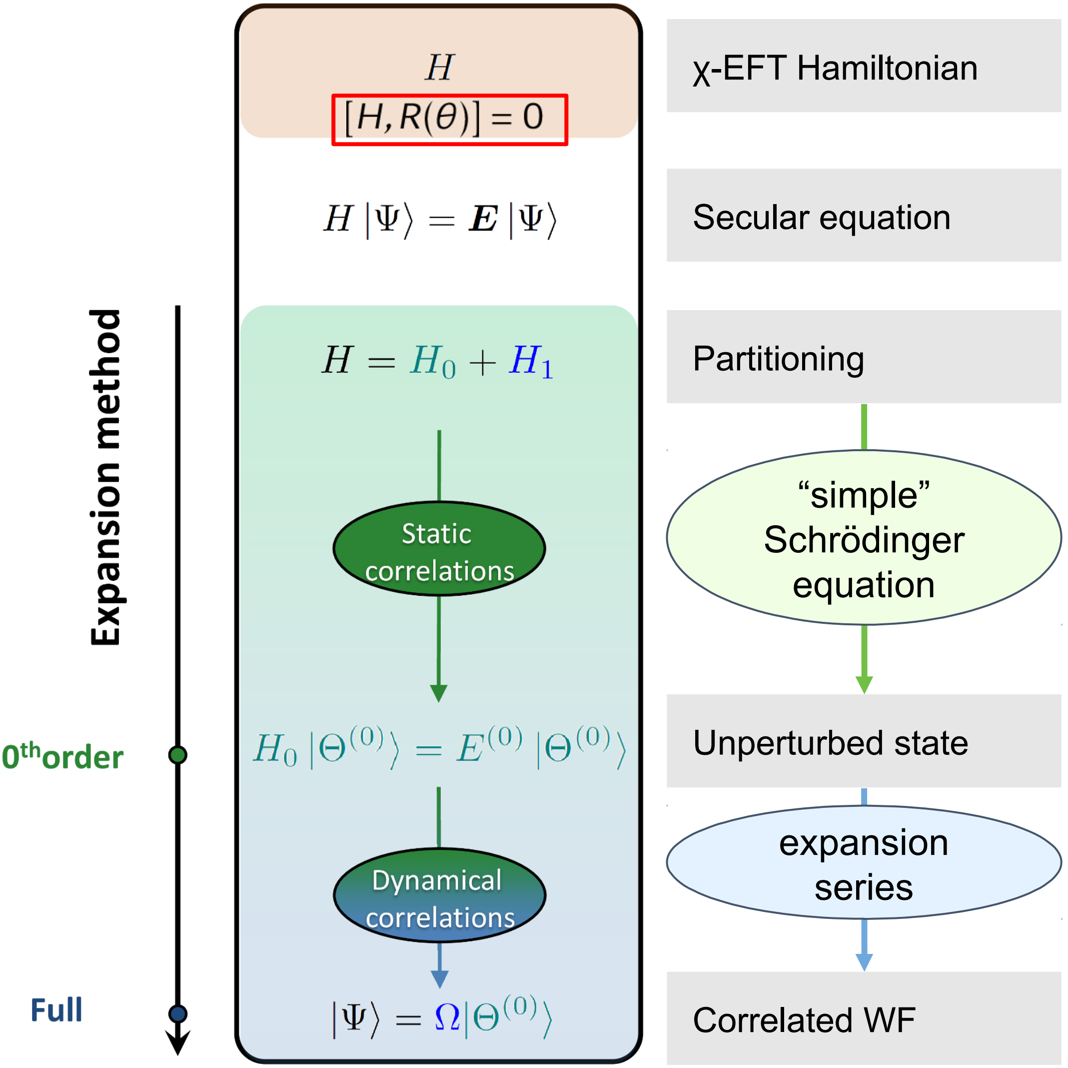
Expansion methods for open-shell nuclei



Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

Expansion methods for open-shell nuclei



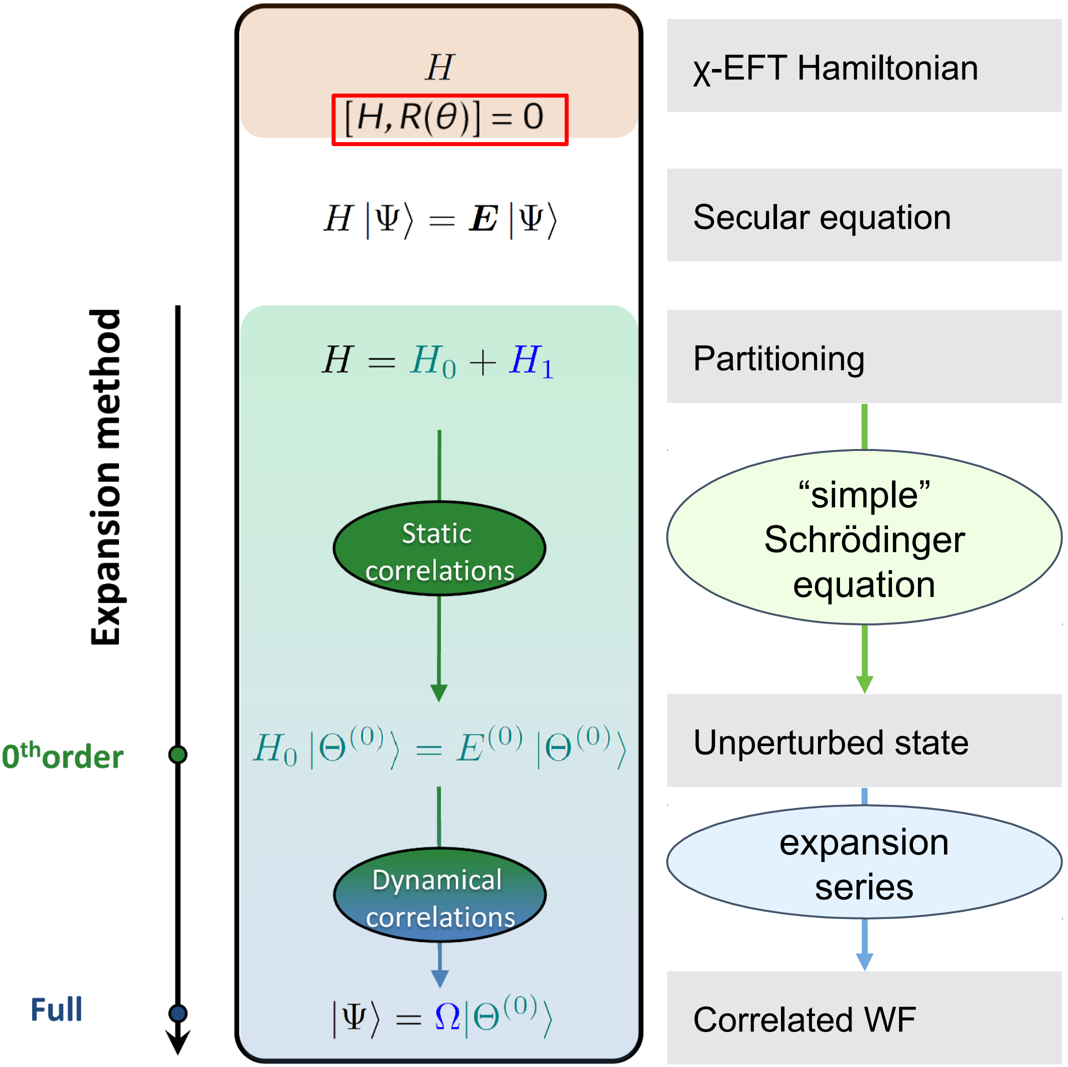
Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

Challenges in **open-shells**

- **Strongly correlated** systems
- Deformation, mp-mh → long range

Expansion methods for open-shell nuclei



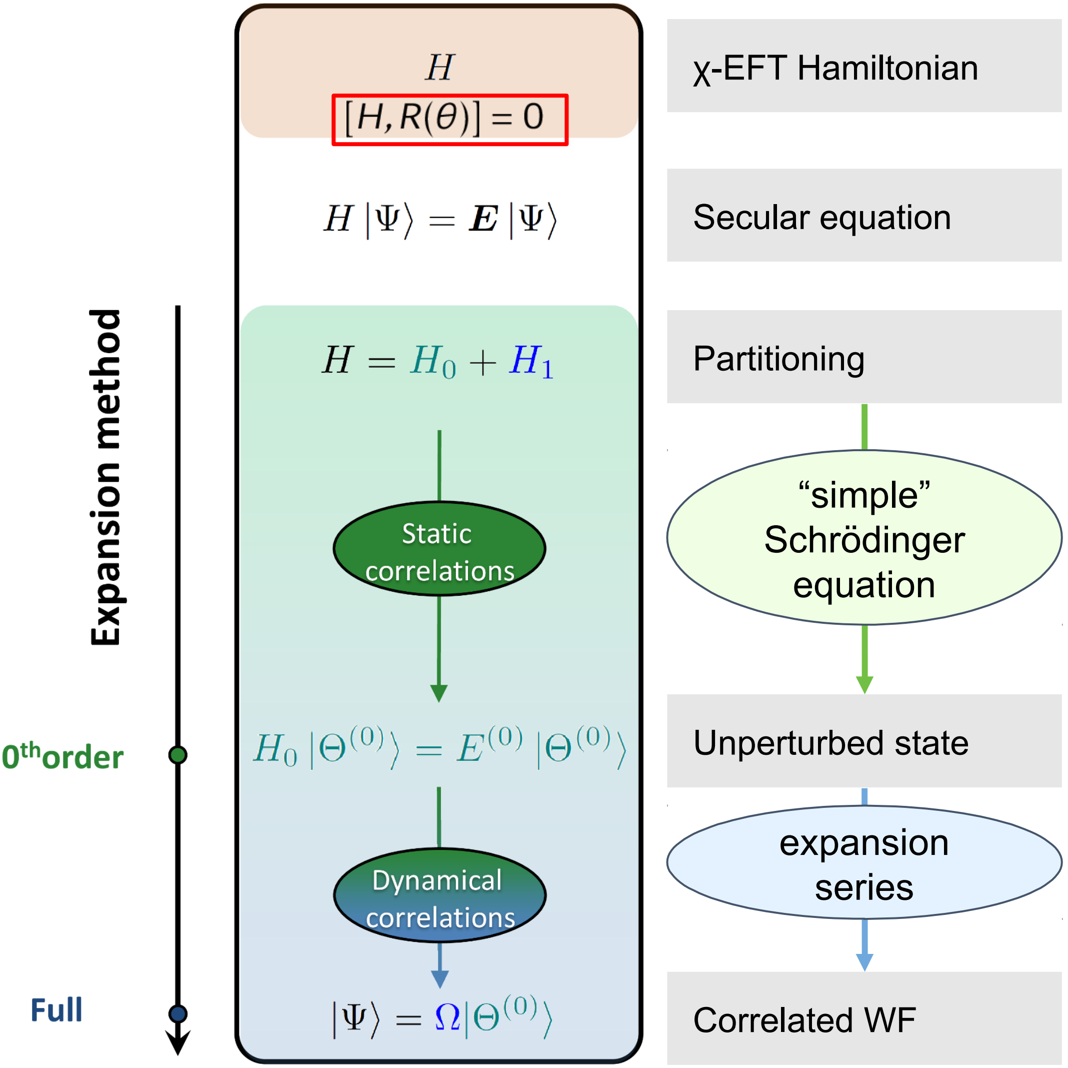
Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

Challenges in **open-shells**

- **Strongly correlated** systems
- Deformation, mp-mh → long range

Expansion methods for open-shell nuclei



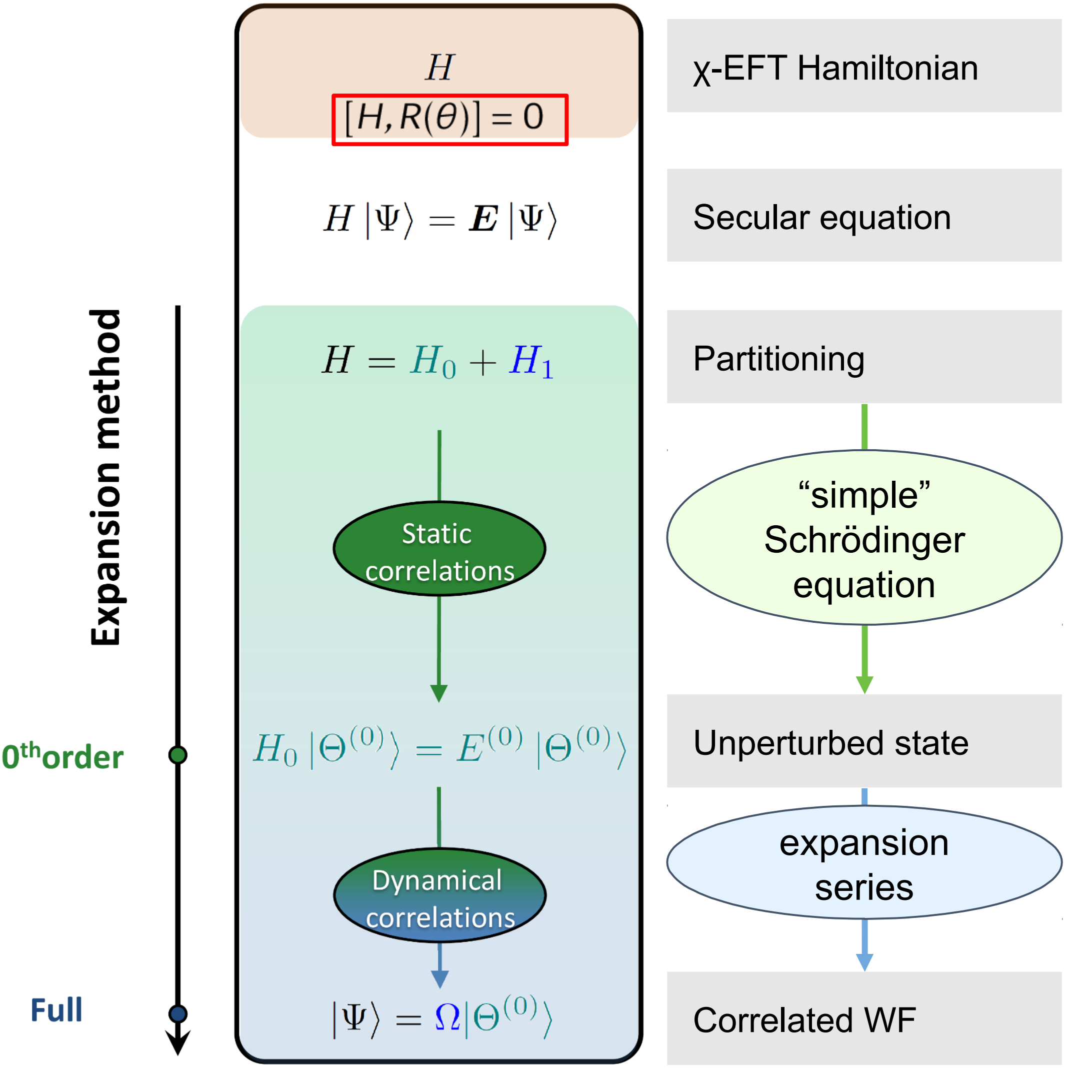
Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

Challenges in **open-shells**

- **Strongly correlated** systems
- Deformation, mp-mh → long range

Symmetric mean-field



Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

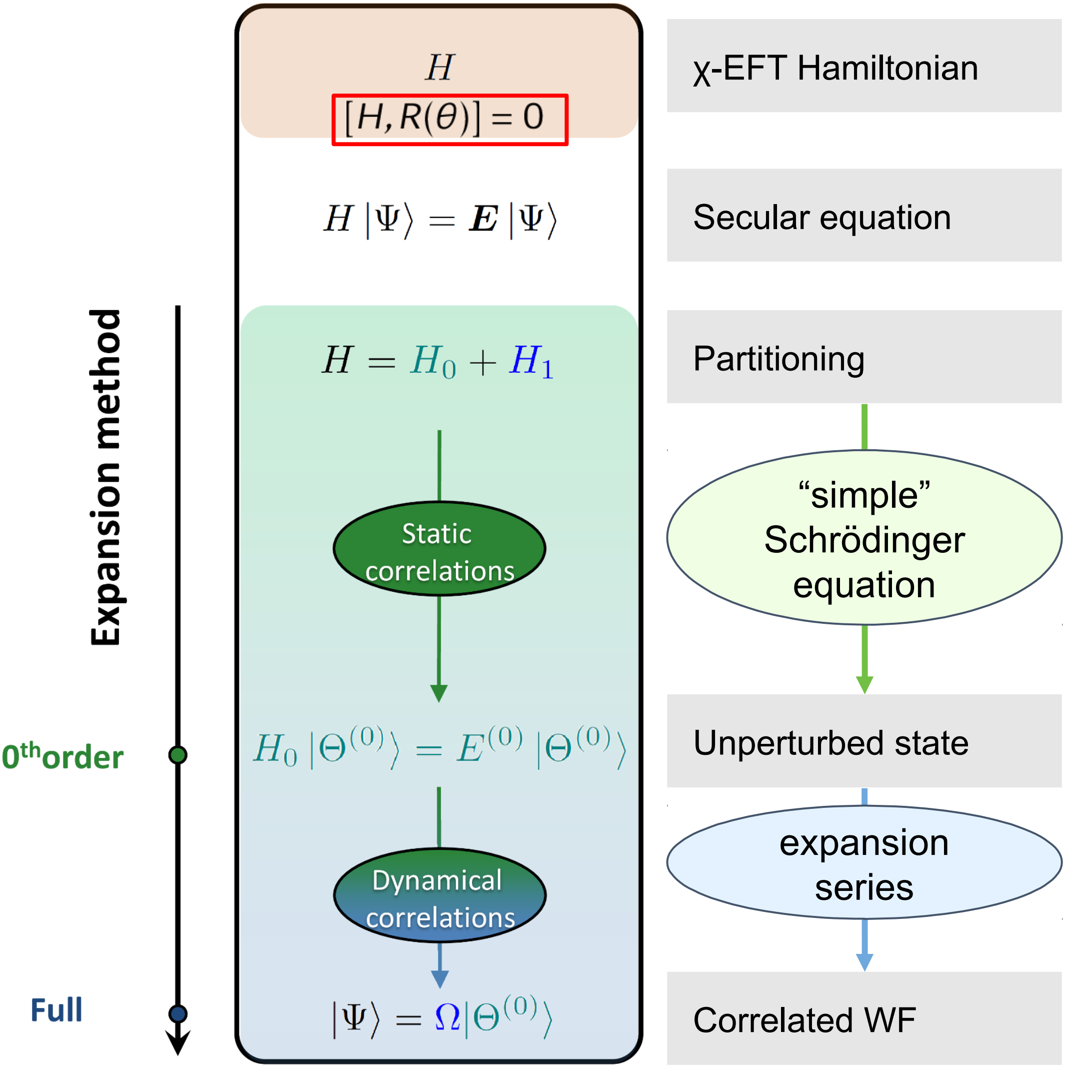
Challenges in **open-shells**

- **Strongly correlated** systems
- Deformation, mp-mh → long range

Symmetric mean-field

- Degeneracies, missing physics

Expansion methods for open-shell nuclei



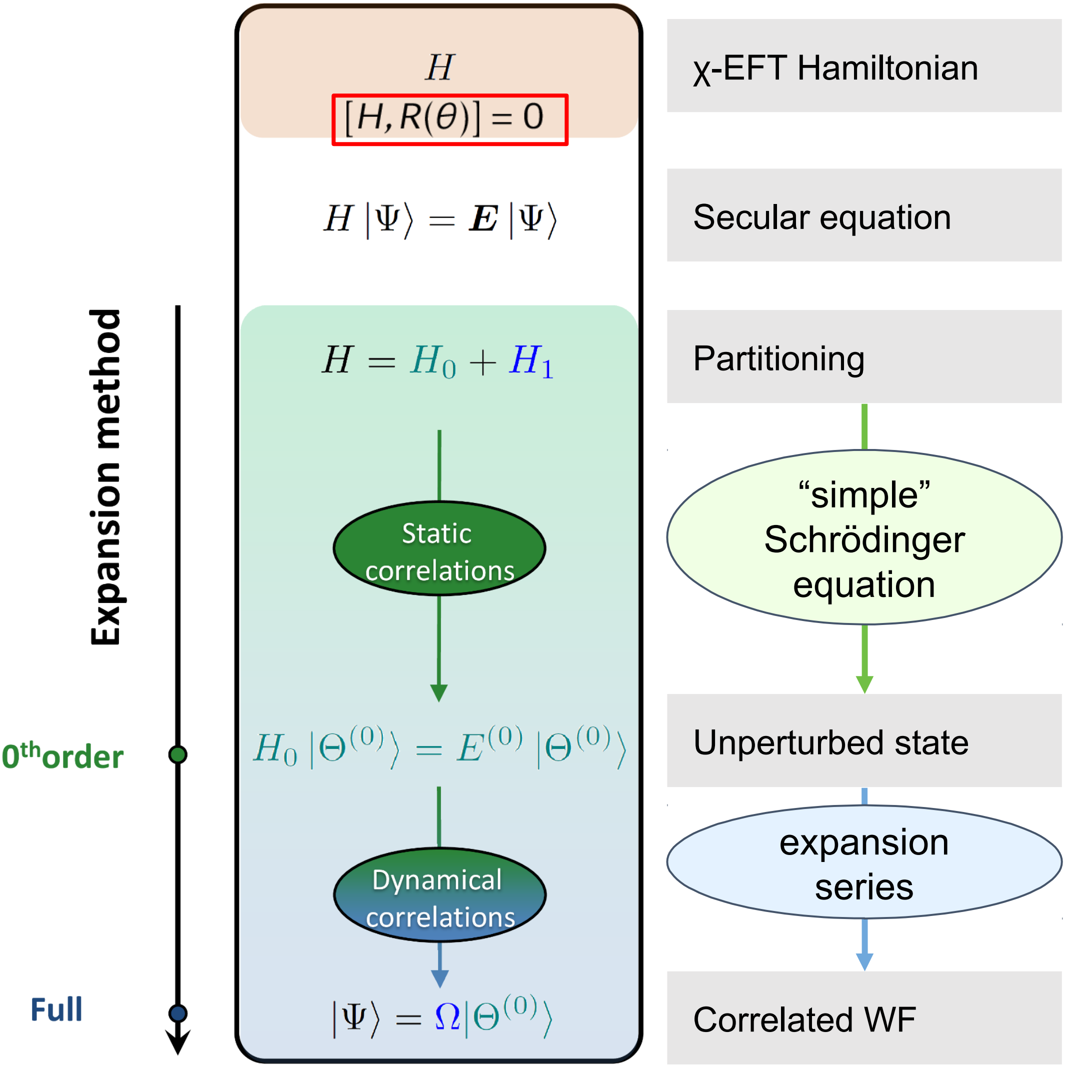
Resolution in **closed shell** systems
- **Weakly correlated** systems
- Symmetric mean-field methods

Challenges in **open-shells**
- **Strongly correlated** systems
- Deformation, mp-mh → long range

Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field

Expansion methods for open-shell nuclei



Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

Challenges in **open-shells**

- **Strongly correlated** systems
- Deformation, mp-mh → long range

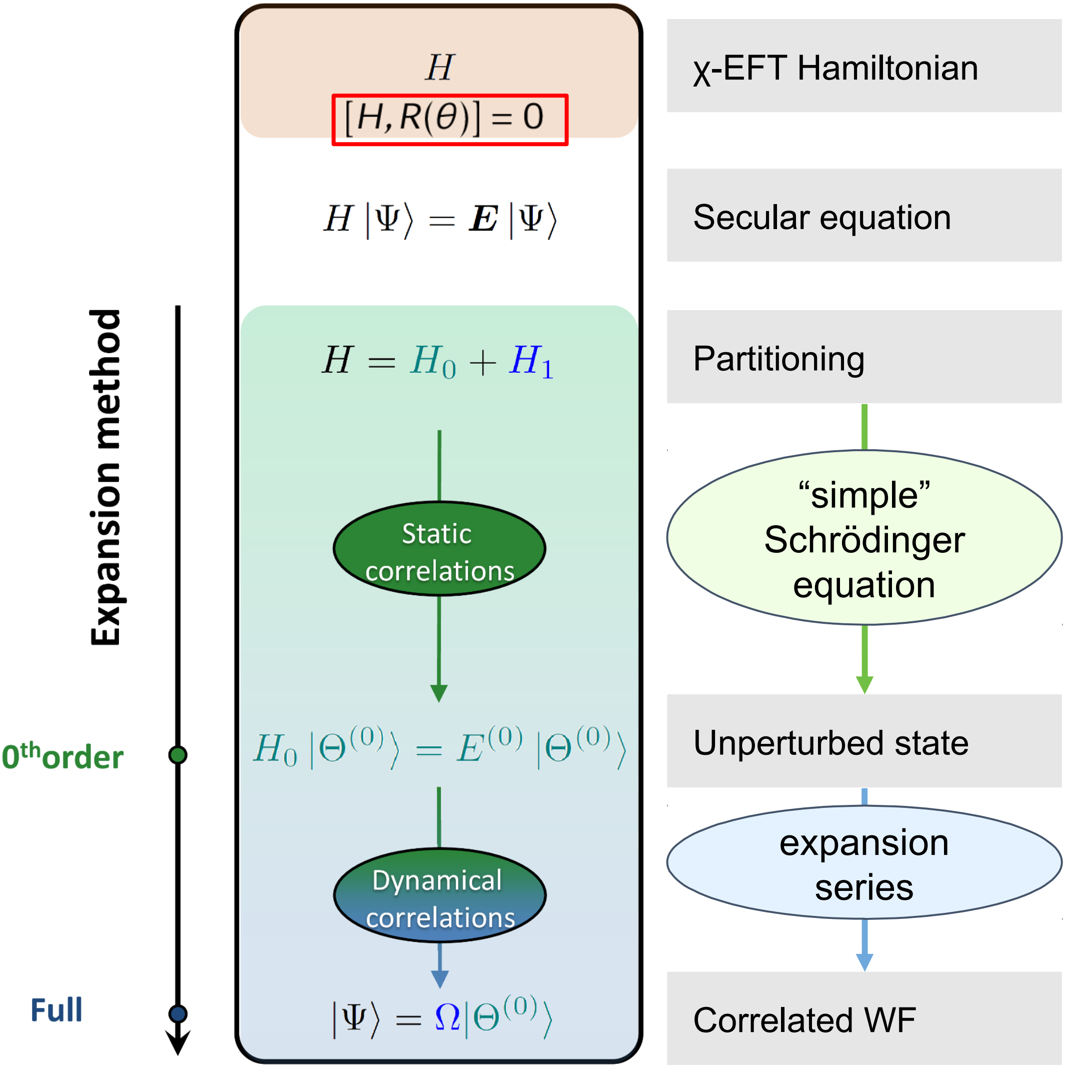
Symmetric mean-field

- Degeneracies, missing physics

Deformed mean-field

- Symmetry breaking expansion

Expansion methods for open-shell nuclei



Resolution in **closed shell** systems
- **Weakly correlated** systems
- Symmetric mean-field methods

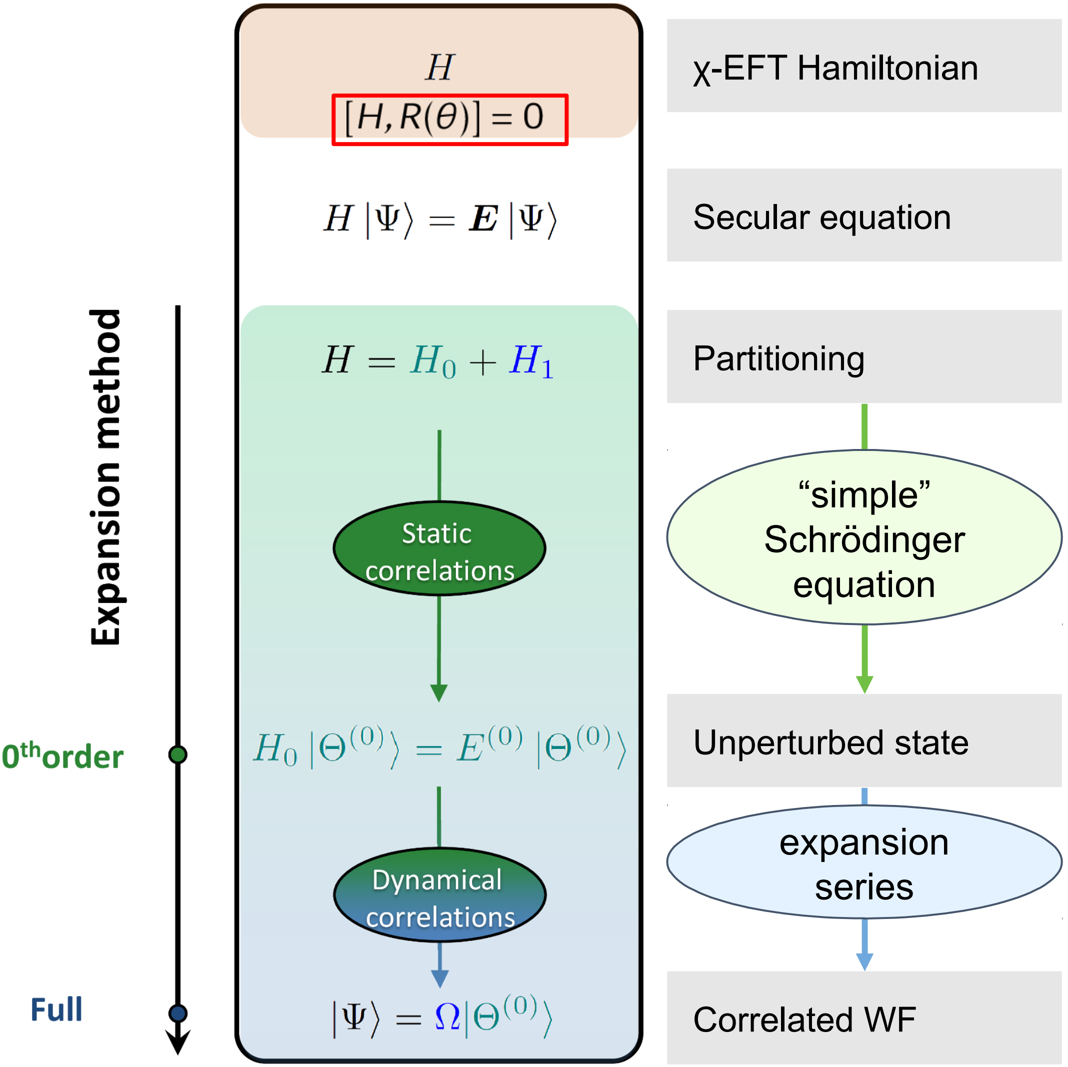
Challenges in **open-shells**
- **Strongly correlated** systems
- Deformation, mp-mh → long range

Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal

Expansion methods for open-shell nuclei



Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

Challenges in **open-shells**

- **Strongly correlated** systems
- Deformation, mp-mh → long range

Symmetric mean-field

- Degeneracies, missing physics

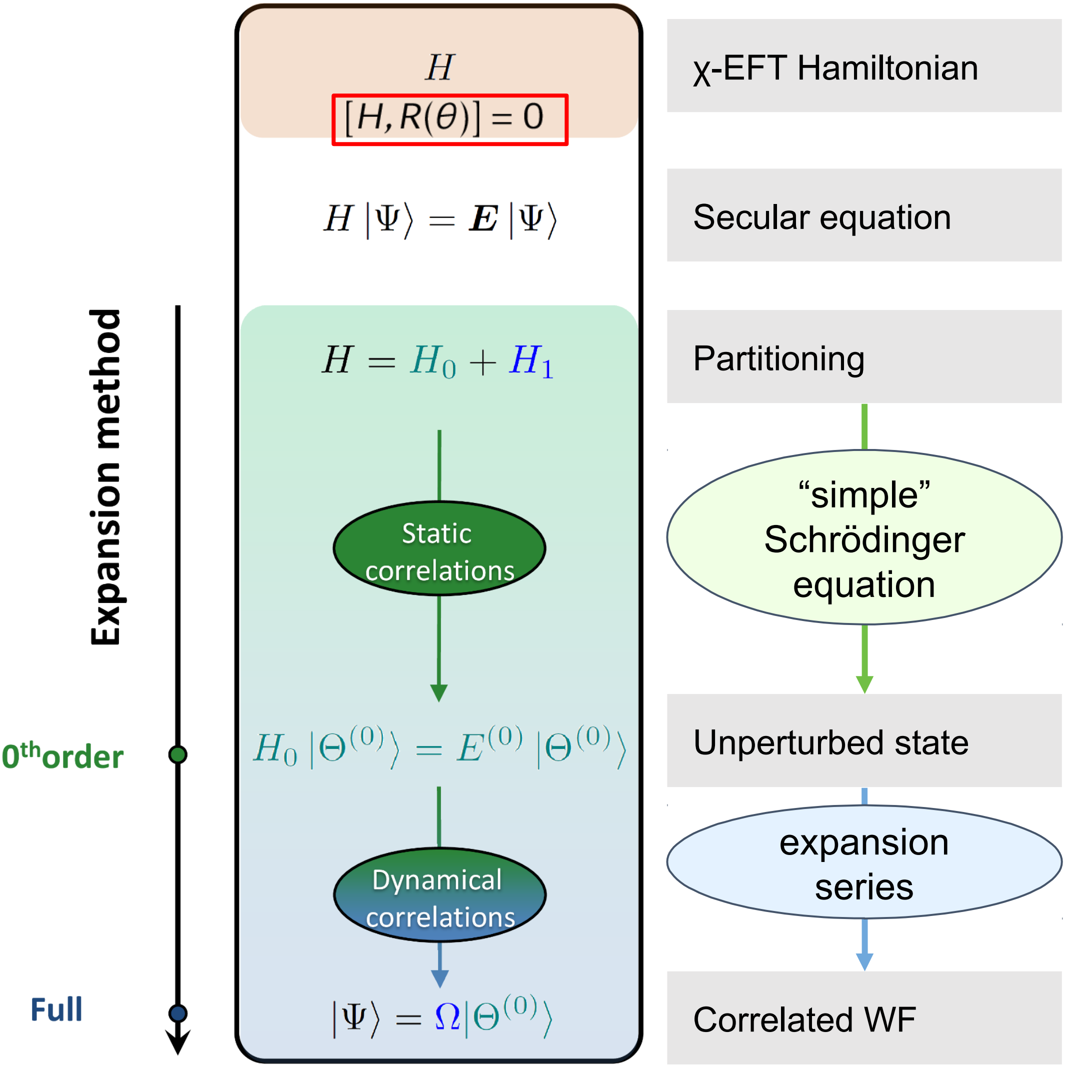
Deformed mean-field

- Symmetry breaking expansion

Multi-determinantal

- Hybrid scaling

Expansion methods for open-shell nuclei



Resolution in **closed shell** systems
- **Weakly correlated** systems
- Symmetric mean-field methods

Challenges in **open-shells**
- **Strongly correlated** systems
- Deformation, mp-mh → long range

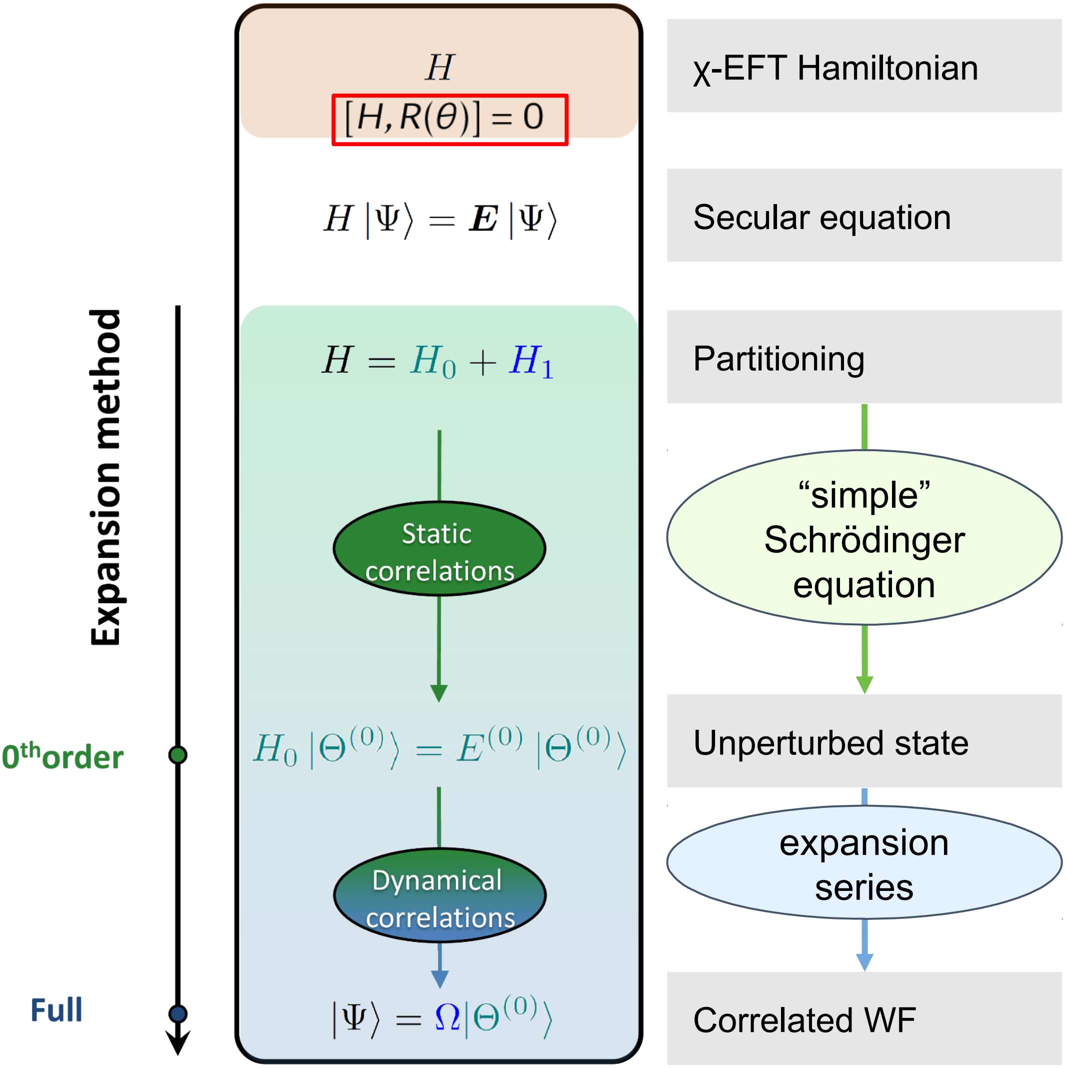
Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal
- Hybrid scaling

PGCM

Expansion methods for open-shell nuclei



Resolution in **closed shell** systems

- **Weakly correlated** systems
- Symmetric mean-field methods

Challenges in **open-shells**

- **Strongly correlated** systems
- Deformation, mp-mh → long range

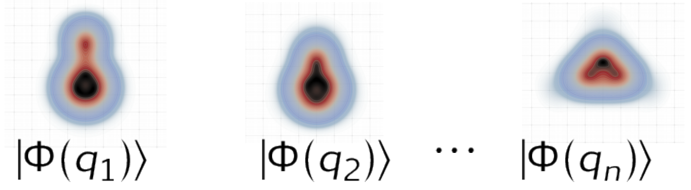
Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal
- Hybrid scaling

PGCM

Expansion methods for open-shell nuclei



H $[H, R(\theta)] = 0$	χ-EFT Hamiltonian
$H\,|\Psi\rangle = \boldsymbol{E}\,|\Psi\rangle$	Secular equation
$H = H_0 + H_1$	Partitioning
Static correlations	"simple" Schrödinger equation
$H_0\,|\Theta^{(0)}\rangle = E^{(0)}\,|\Theta^{(0)}\rangle$	Unperturbed state
Dynamical correlations	expansion series
$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$	Correlated WF

Expansion method: 0^{th} order → Full

Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal
- Hybrid scaling

PGCM

Expansion methods for open-shell nuclei

H

$[H, R(\theta)] = 0$

χ-EFT Hamiltonian

$H\,|\Psi\rangle = \boldsymbol{E}\,|\Psi\rangle$

Secular equation

$H = H_0 + H_1$

Partitioning

Static correlations

"simple" Schrödinger equation

Expansion method

0th order

$H_0\,|\Theta^{(0)}\rangle = E^{(0)}\,|\Theta^{(0)}\rangle$

Unperturbed state

Dynamical correlations

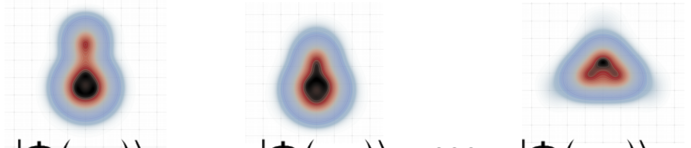
expansion series

Full

$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$

Correlated WF

Rotation physics



$|\Phi(q_1)\rangle$ $|\Phi(q_2)\rangle$ $\cdots$ $|\Phi(q_n)\rangle$

$P^{\tilde{\sigma}}|\Phi(q_1)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_2)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_n)\rangle$

Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal
- Hybrid scaling

PGCM

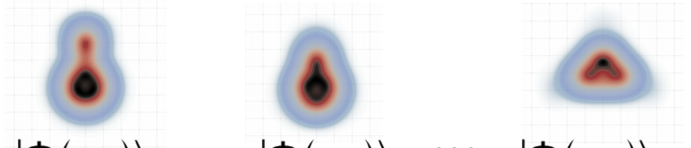
Expansion methods for open-shell nuclei

Expansion method

	H, $[H, R(\theta)] = 0$	χ-EFT Hamiltonian
	$H\,\lvert\Psi\rangle = \boldsymbol{E}\,\lvert\Psi\rangle$	Secular equation
	$H = H_0 + H_1$	Partitioning
	Static correlations	"simple" Schrödinger equation
0thorder	$H_0\,\lvert\Theta^{(0)}\rangle = E^{(0)}\,\lvert\Theta^{(0)}\rangle$	Unperturbed state
	Dynamical correlations	expansion series
Full	$\lvert\Psi\rangle = \Omega\lvert\Theta^{(0)}\rangle$	Correlated WF

Rotation physics

Vibration physics



$\lvert\Phi(q_1)\rangle$ $\lvert\Phi(q_2)\rangle$ $\cdots$ $\lvert\Phi(q_n)\rangle$

$P^{\tilde{\sigma}}\lvert\Phi(q_1)\rangle$ $P^{\tilde{\sigma}}\lvert\Phi(q_2)\rangle$ $P^{\tilde{\sigma}}\lvert\Phi(q_n)\rangle$

$$\lvert\Theta_\mu^{\tilde{\sigma}}\rangle \equiv \sum_q f_\mu^{\tilde{\sigma}}(q) P^{\tilde{\sigma}} \lvert\Phi(q)\rangle$$

Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal
- Hybrid scaling

PGCM

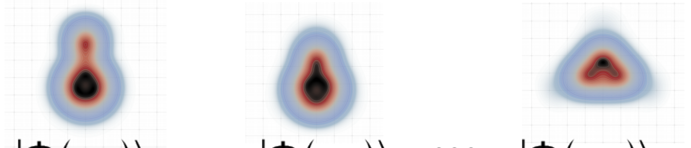
Expansion methods for open-shell nuclei

Expansion method

	H $[H, R(\theta)] = 0$	χ-EFT Hamiltonian
	$H \lvert\Psi\rangle = \boldsymbol{E} \lvert\Psi\rangle$	Secular equation
	$H = H_0 + H_1$	Partitioning
	Static correlations	"simple" Schrödinger equation
0th order	$H_0 \lvert\Theta^{(0)}\rangle = E^{(0)} \lvert\Theta^{(0)}\rangle$	Unperturbed state
	Dynamical correlations	expansion series
Full	$\lvert\Psi\rangle = \Omega \lvert\Theta^{(0)}\rangle$	Correlated WF

Rotation physics

Vibration physics



$|\Phi(q_1)\rangle \quad |\Phi(q_2)\rangle \quad \cdots \quad |\Phi(q_n)\rangle$

$P^{\tilde{\sigma}}|\Phi(q_1)\rangle \quad P^{\tilde{\sigma}}|\Phi(q_2)\rangle \quad P^{\tilde{\sigma}}|\Phi(q_n)\rangle$

$$|\Theta^{\tilde{\sigma}}_{\mu}\rangle \equiv \sum_q f^{\tilde{\sigma}}_{\mu}(q) P^{\tilde{\sigma}} |\Phi(q)\rangle$$

Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal
- Hybrid scaling

PGCM

Unperturbed state for open-shells
- **Long range collective** modes
  → Rotations, vibrations, pairing
- **Symmetry conserving** partitioning
- **Low dimensional** method

Expansion methods for open-shell nuclei

Expansion method

H

$[H, R(\theta)] = 0$

$H\,|\Psi\rangle = \boldsymbol{E}\,|\Psi\rangle$

$H = H_0 + H_1$

Static correlations

$H_0\,|\Theta^{(0)}\rangle = E^{(0)}\,|\Theta^{(0)}\rangle$

Dynamical correlations

$|\Psi\rangle = \Omega|\Theta^{(0)}\rangle$

0thorder

Full

χ-EFT Hamiltonian

Secular equation

Partitioning

"simple" Schrödinger equation

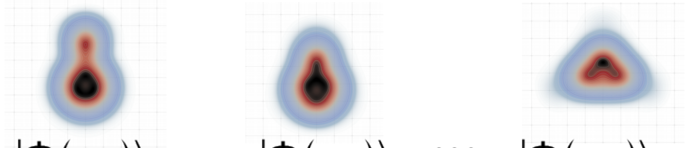
Unperturbed state

expansion series

Correlated WF

Rotation physics

Vibration physics



$|\Phi(q_1)\rangle$ $|\Phi(q_2)\rangle$ $\cdots$ $|\Phi(q_n)\rangle$

$P^{\tilde{\sigma}}|\Phi(q_1)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_2)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_n)\rangle$

$$|\Theta^{\tilde{\sigma}}_{\mu}\rangle \equiv \sum_q f^{\tilde{\sigma}}_{\mu}(q) P^{\tilde{\sigma}}|\Phi(q)\rangle$$

Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal
- Hybrid scaling

PGCM

Unperturbed state for open-shells
- **Long range collective** modes
  → Rotations, vibrations, pairing
- **Symmetry conserving** partitioning
- **Low dimensional** method

Multi-reference perturbation theory
- State specific
- Non orthogonal basis
- Large linear system

Expansion methods for open-shell nuclei

Expansion method

H

$[H, R(\theta)] = 0$

$H|\Psi\rangle = \boldsymbol{E}|\Psi\rangle$

$H = H_0 + H_1$

Static correlations

0thorder $\quad H_0|\Theta^{(0)}\rangle = E^{(0)}|\Theta^{(0)}\rangle$

Dynamical correlations

Full $\quad |\Psi\rangle = \Omega|\Theta^{(0)}\rangle$

χ-EFT Hamiltonian

Secular equation

Partitioning

"simple" Schrödinger equation

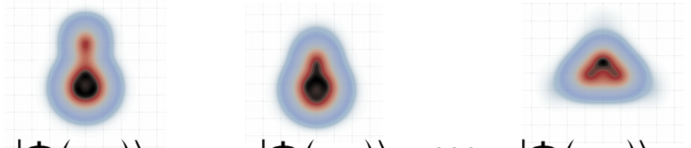
Unperturbed state

expansion series

Correlated WF

Rotation physics

Vibration physics



$|\Phi(q_1)\rangle \quad |\Phi(q_2)\rangle \quad \cdots \quad |\Phi(q_n)\rangle$

$P^{\tilde{\sigma}}|\Phi(q_1)\rangle \quad P^{\tilde{\sigma}}|\Phi(q_2)\rangle \quad P^{\tilde{\sigma}}|\Phi(q_n)\rangle$

$$|\Theta_\mu^{\tilde{\sigma}}\rangle \equiv \sum_q f_\mu^{\tilde{\sigma}}(q) P^{\tilde{\sigma}}|\Phi(q)\rangle$$

Symmetric mean-field
- Degeneracies, missing physics

Deformed mean-field
- Symmetry breaking expansion

Multi-determinantal
- Hybrid scaling

PGCM

Unperturbed state for open-shells
- **Long range collective** modes → Rotations, vibrations, pairing
- **Symmetry conserving** partitioning
- **Low dimensional** method

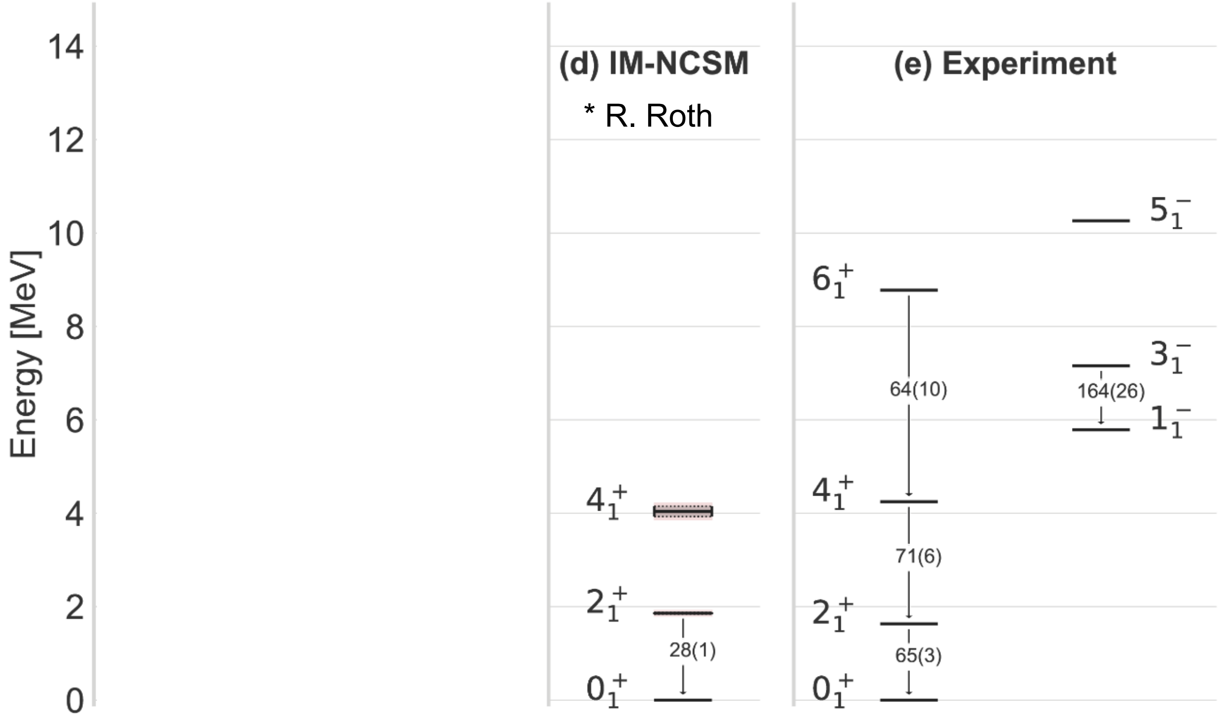
Multi-reference perturbation theory
- State specific
- Non orthogonal basis
- Large linear system

Symmetry conserving PT
Access to excited state
Formalism Inspired from QC
- [Burton20], [Tsuchimochi19]

Application to ^{20}Ne

Application to ^{20}Ne

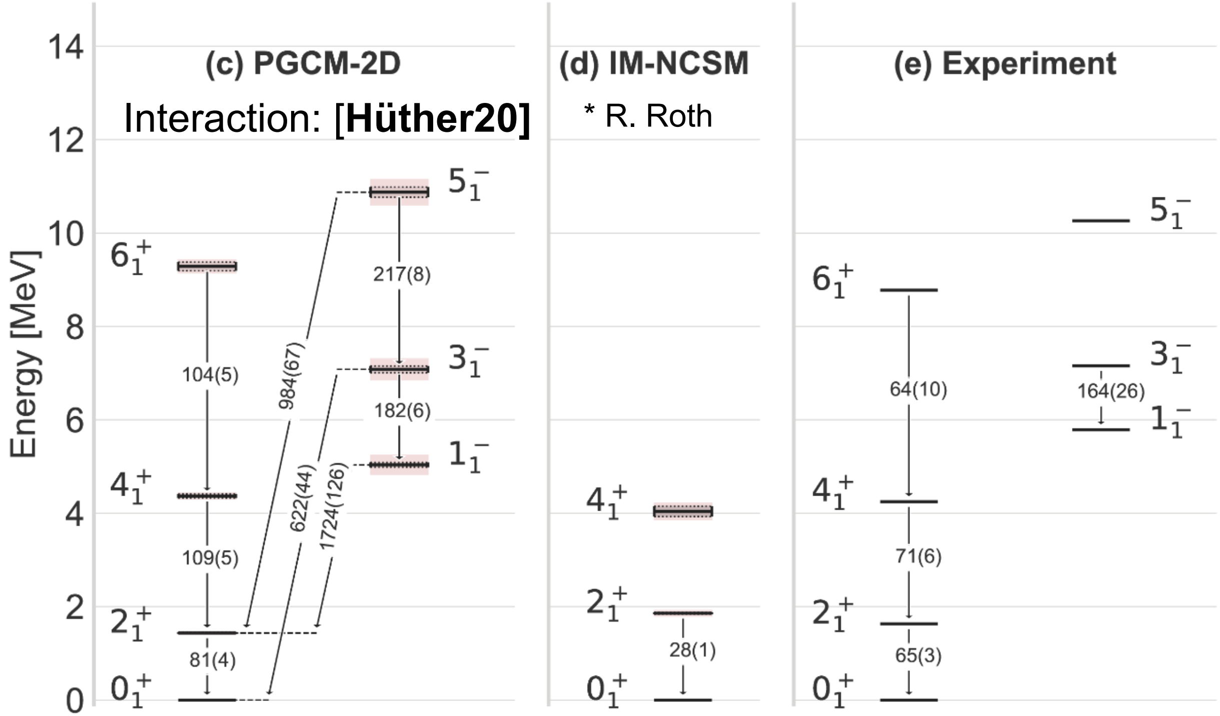
First order - PGCM



Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

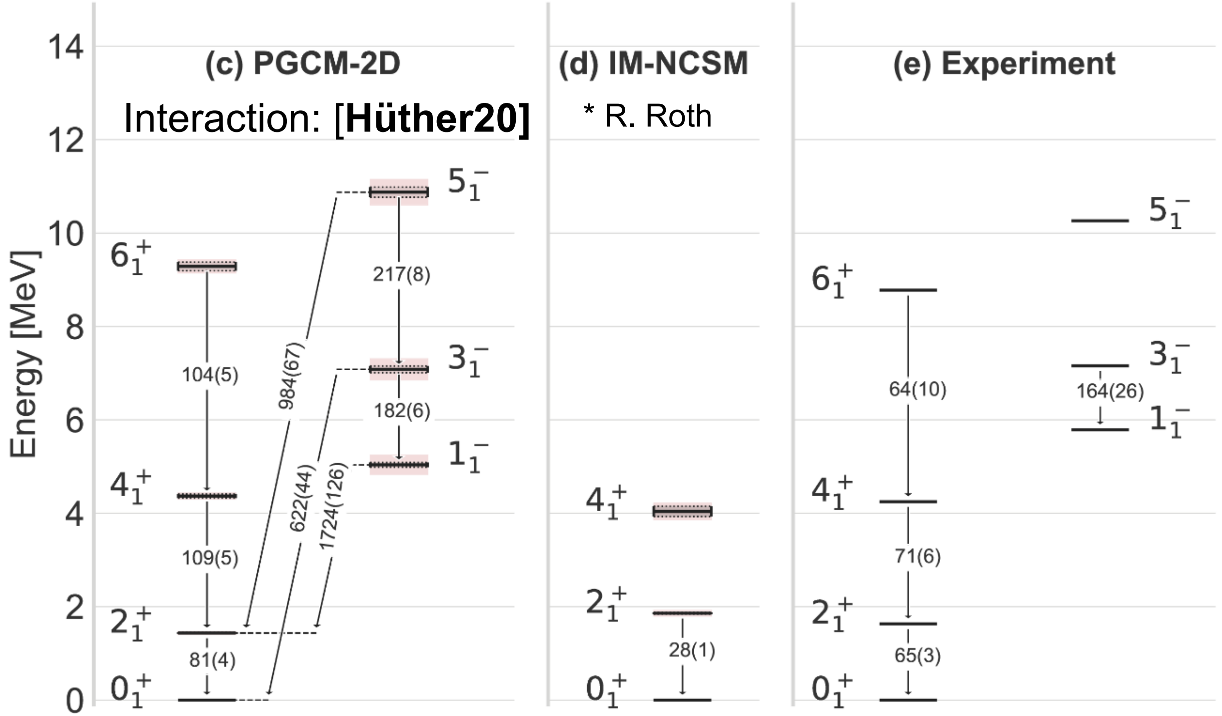
Application to ^{20}Ne

First order - PGCM



Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

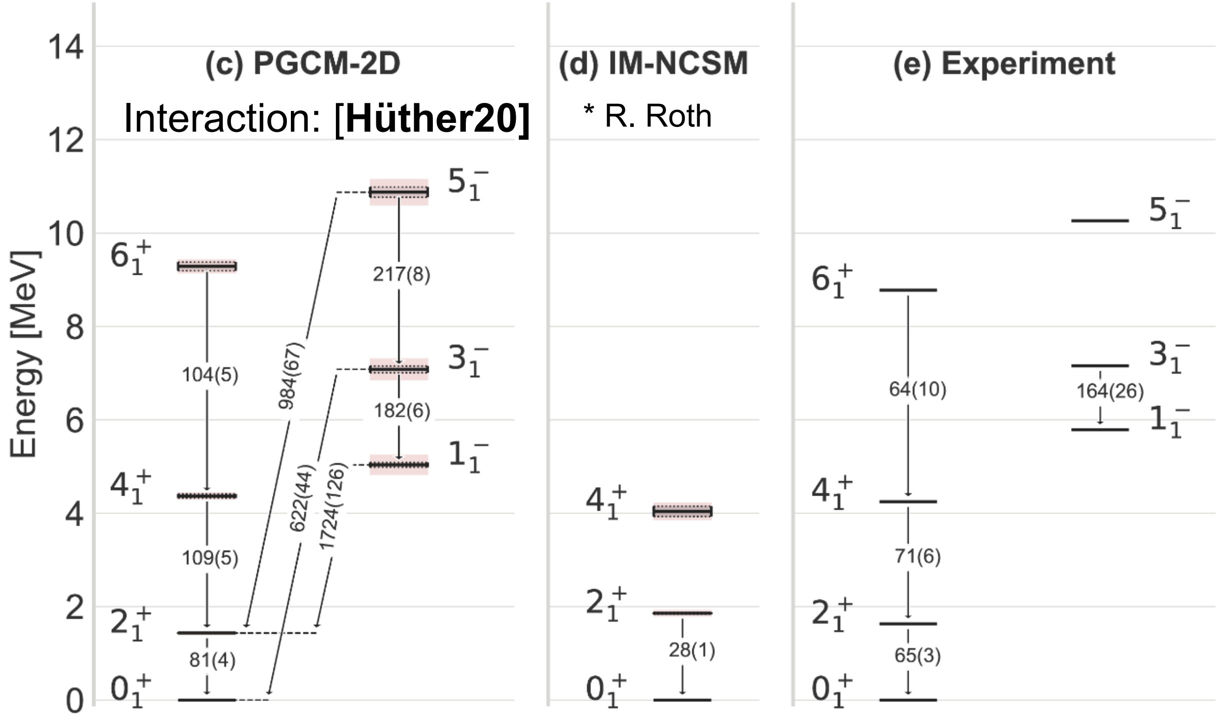
First order - PGCM



Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

First order - PGCM

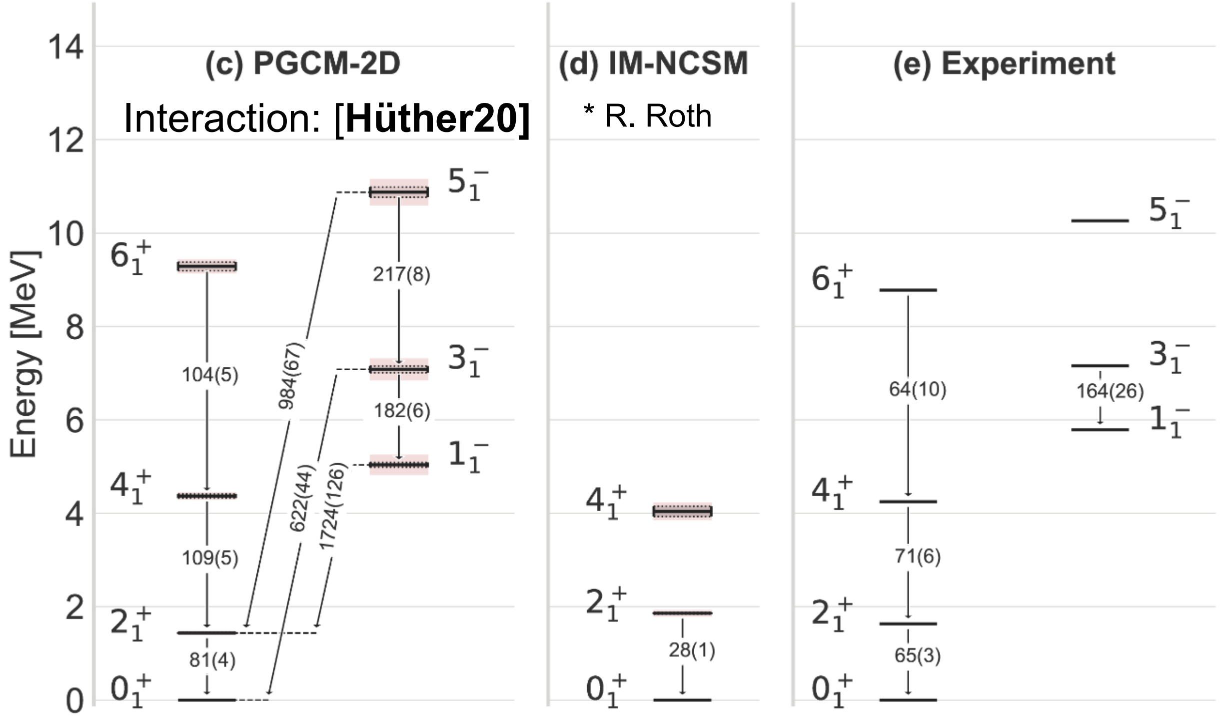


Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

First order - PGCM



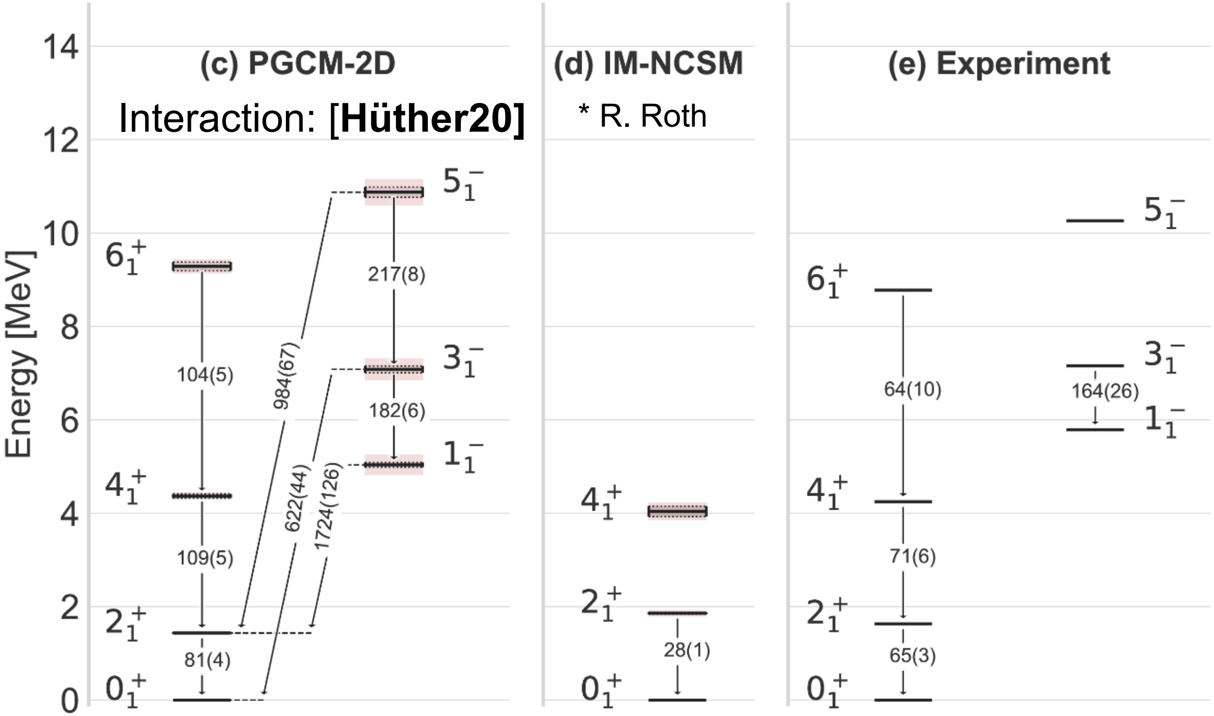
Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

Rich accessible phenomenology
→ Transition dens., pair transfers, etc.
→ Giant resonances (**A. Porro** poster)

First order - PGCM



Second order - PGCM-PT(2)

[Hergert21]

Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

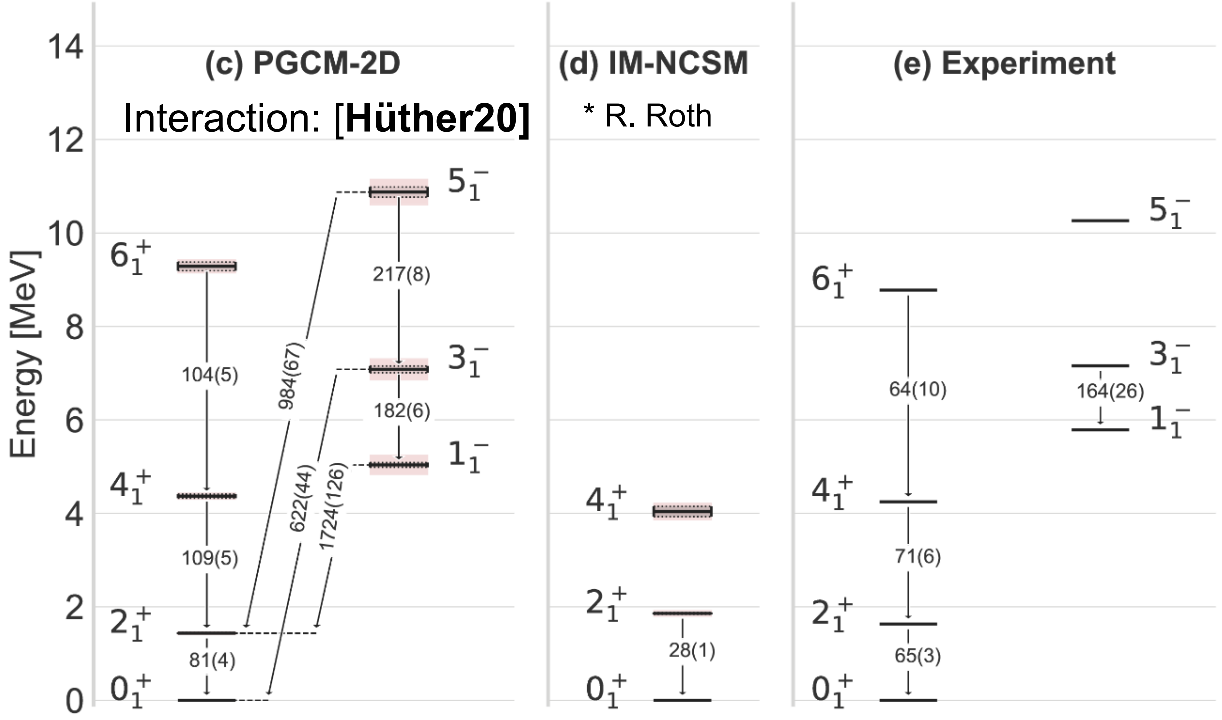
Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

Rich accessible phenomenology
→ Transition dens., pair transfers, etc.
→ Giant resonances (**A. Porro** poster)

Application to ^{20}Ne

First order - PGCM



Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

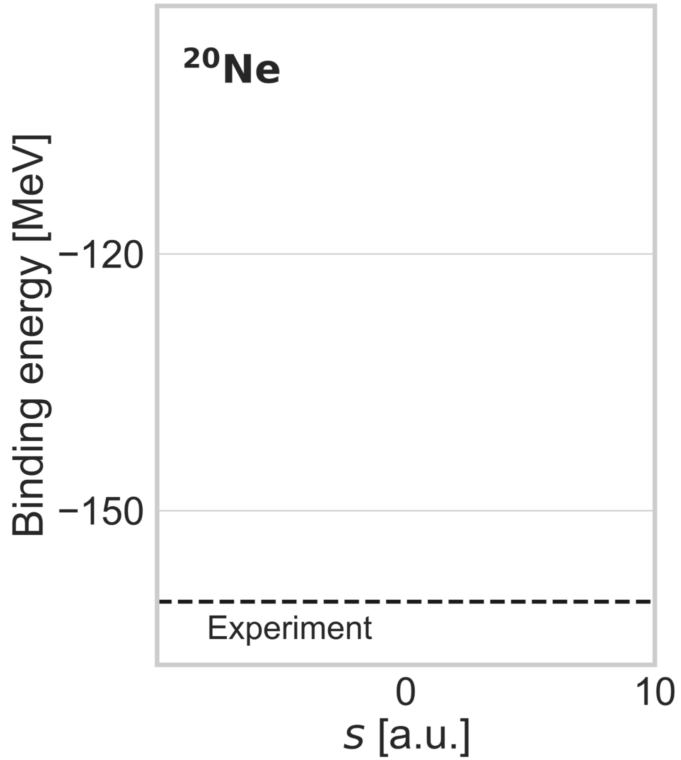
Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

Rich accessible phenomenology
→ Transition dens., pair transfers, etc.
→ Giant resonances (**A. Porro** poster)

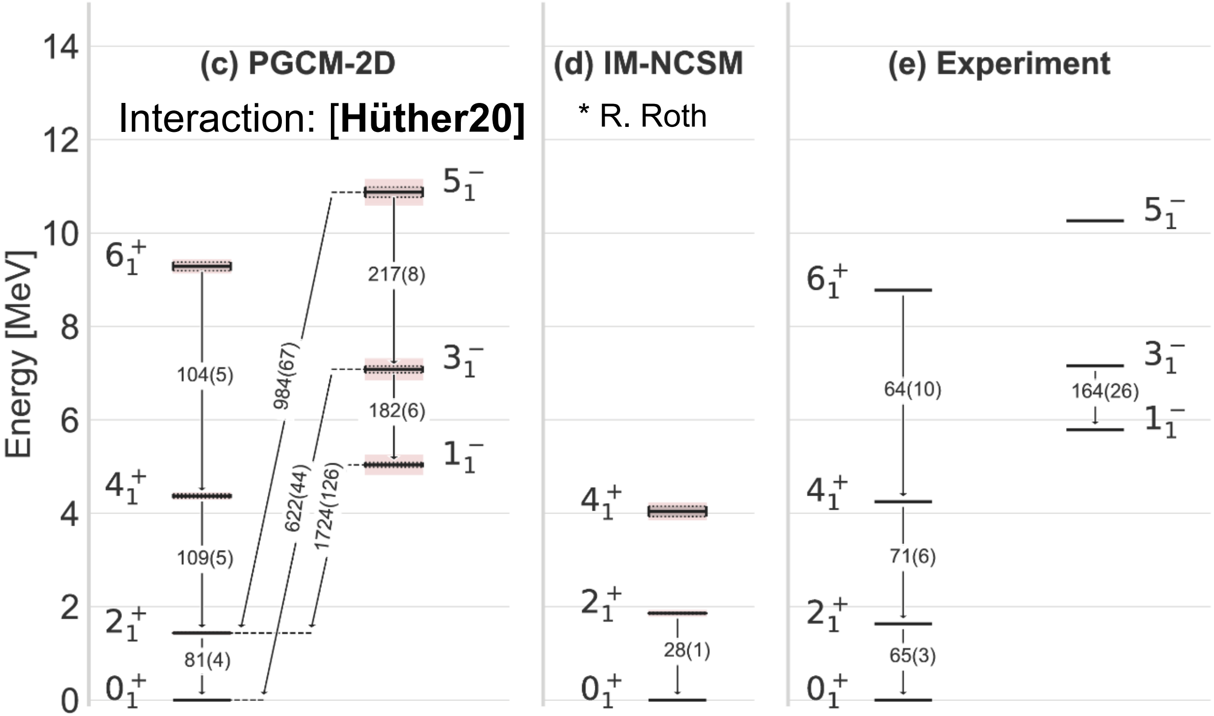
Second order - PGCM-PT(2)

[Hergert21]



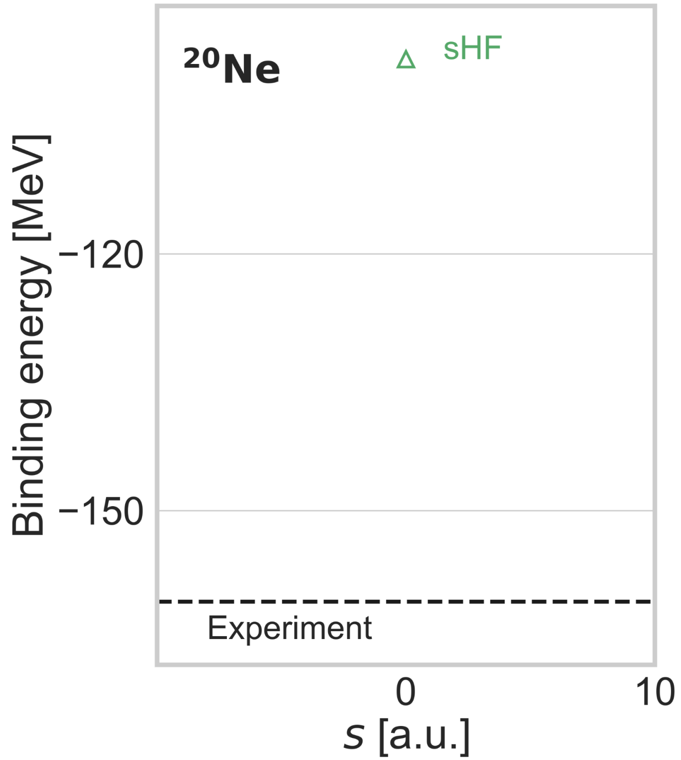
Application to ^{20}Ne

First order - PGCM



Second order - PGCM-PT(2)

[Hergert21]



Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

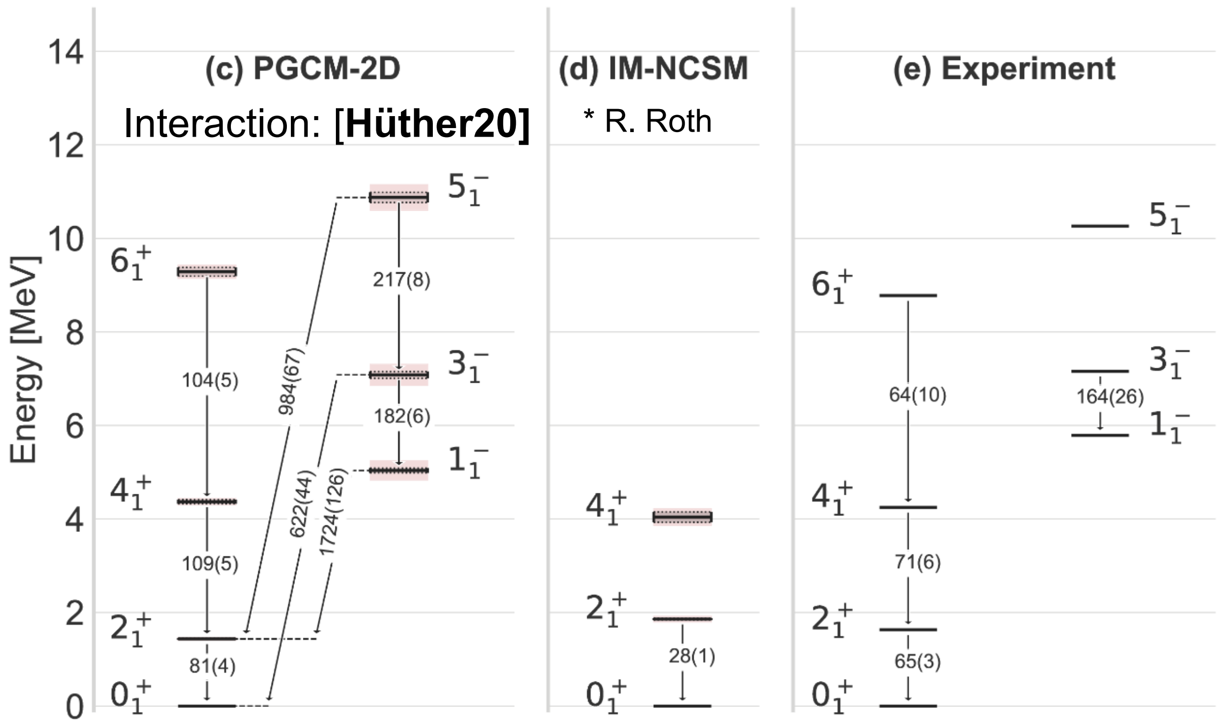
Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

Rich accessible phenomenology
→ Transition dens., pair transfers, etc.
→ Giant resonances (**A. Porro** poster)

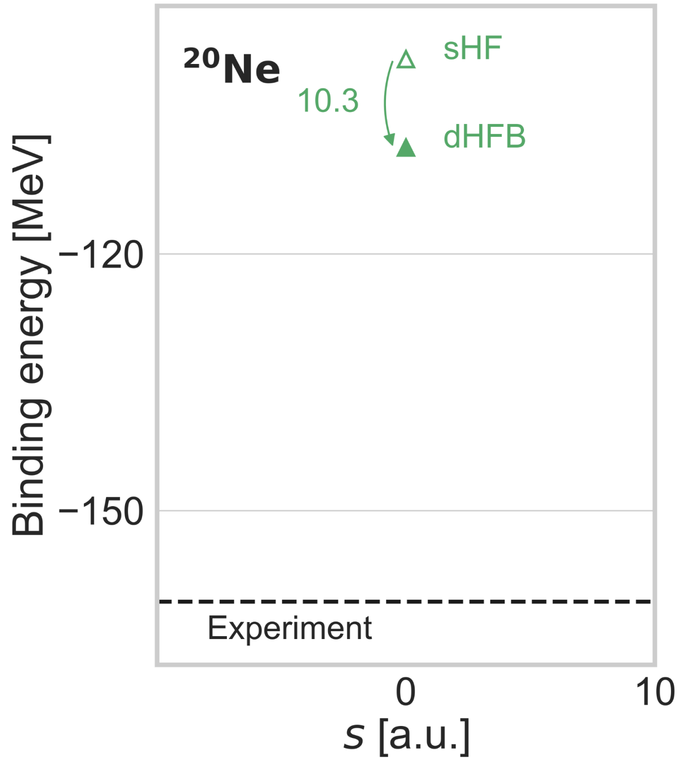
Application to ^{20}Ne

First order - PGCM



Second order - PGCM-PT(2)

[Hergert21]



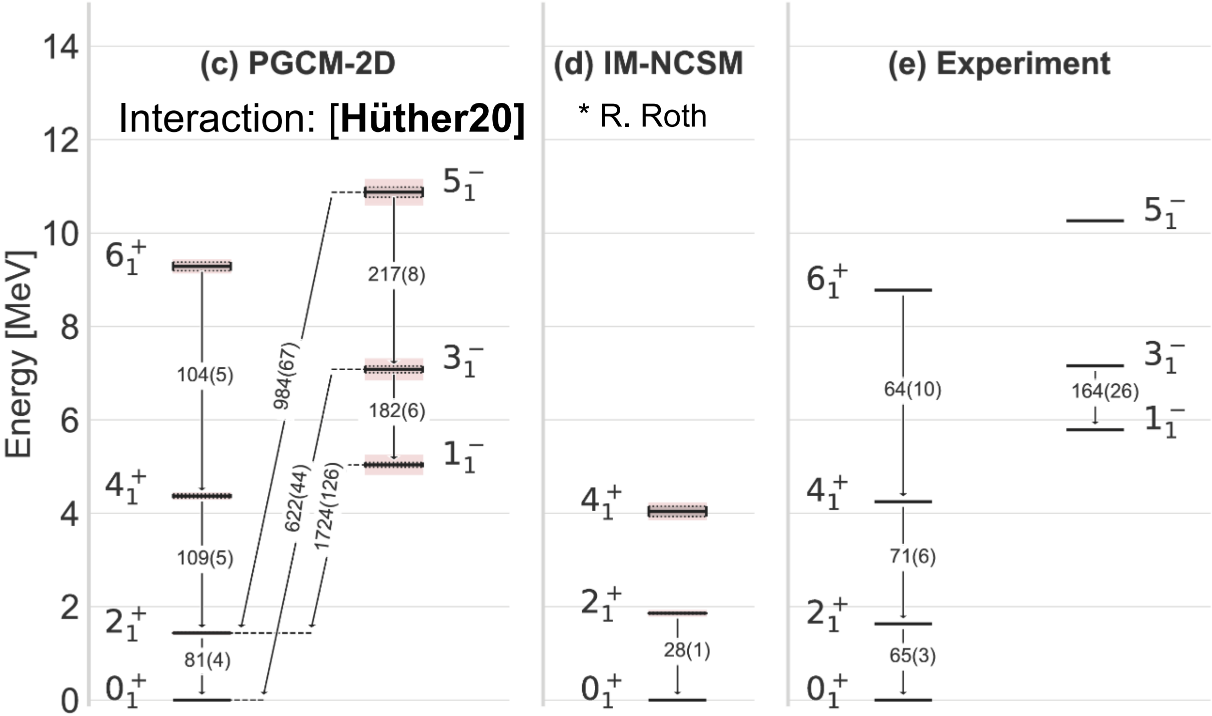
Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

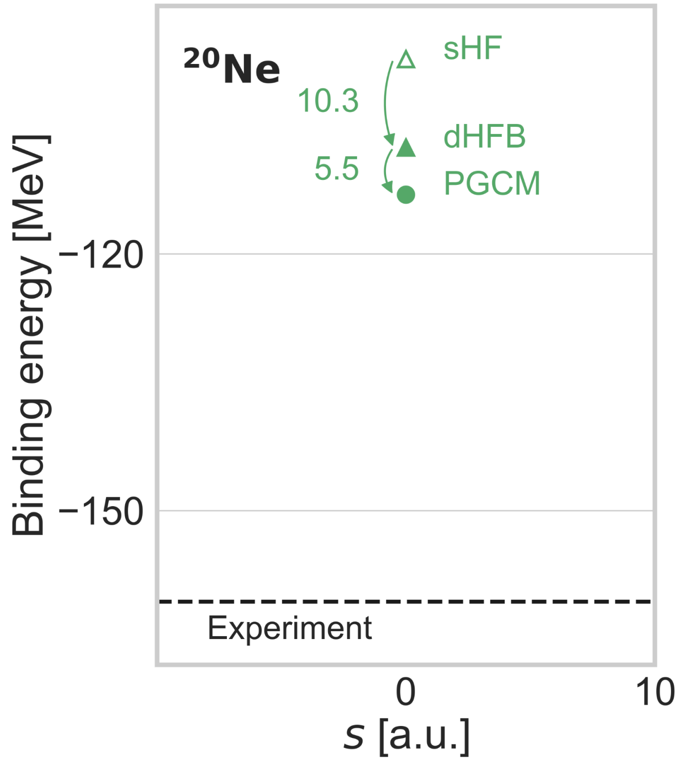
Rich accessible phenomenology
→ Transition dens., pair transfers, etc.
→ Giant resonances (**A. Porro** poster)

First order - PGCM



Second order - PGCM-PT(2)

[Hergert21]



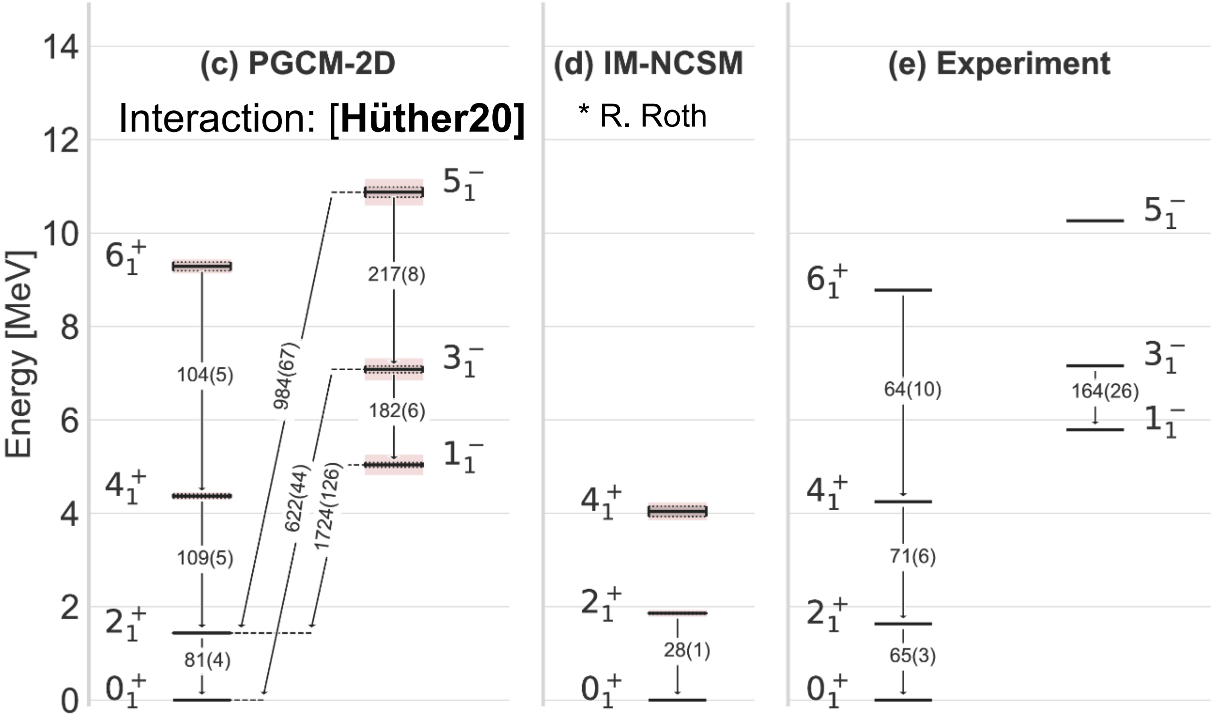
Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

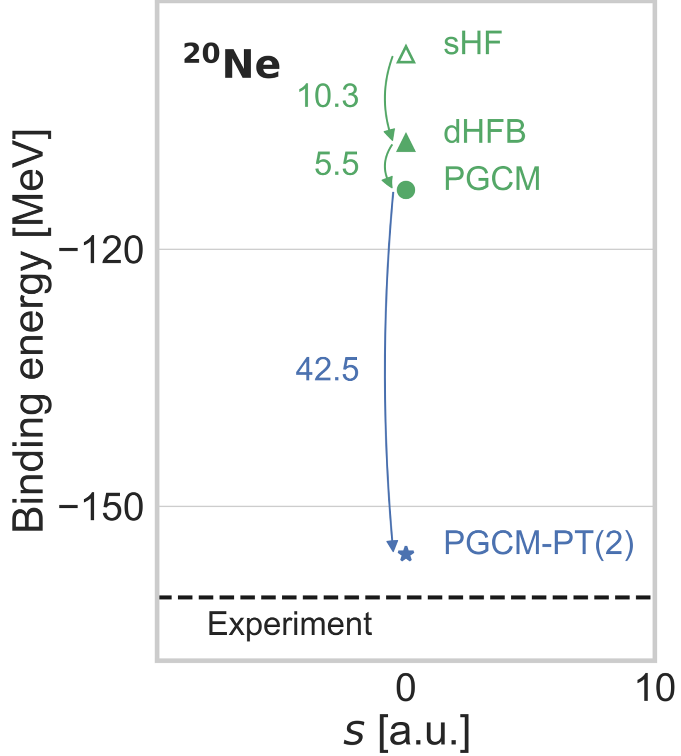
Rich accessible phenomenology
→ Transition dens., pair transfers, etc.
→ Giant resonances (**A. Porro** poster)

First order - PGCM



Second order - PGCM-PT(2)

[Hergert21]



Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

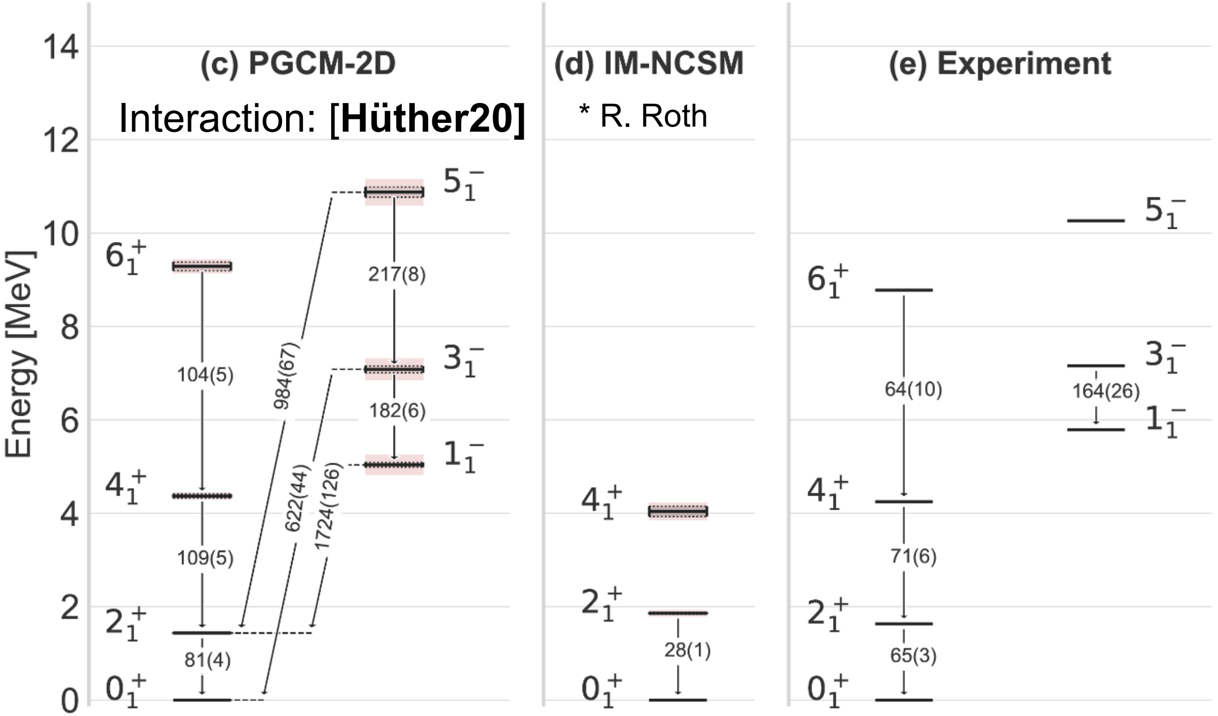
Investigation of correlations
- Dyn. corr. essential for description of BE
- Motivates theoretical modelling

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

Rich accessible phenomenology
→ Transition dens., pair transfers, etc.
→ Giant resonances (**A. Porro** poster)

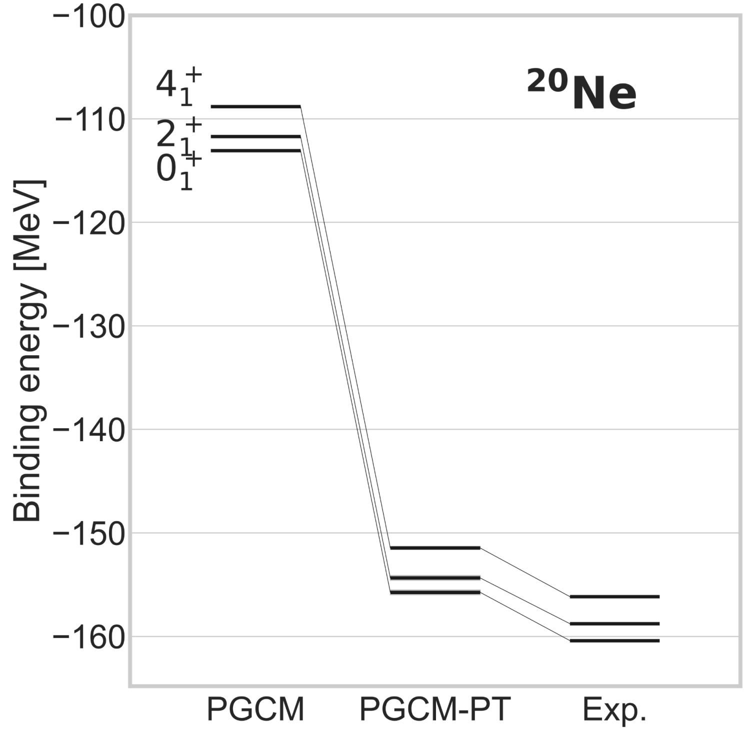
Application to ^{20}Ne

First order - PGCM



Second order - PGCM-PT(2)

[Hergert21]



Reference data
→ Experiment
→ Quasi-exact IM-NCSM [Roth21]

Good reproduction of **first bands**
- wrt. IM-NCSM and experiment
- within uncertainties?

Exaggerated collectivity
→ B(E2) off beyond uncertainties
→ Missing **dynamical correlations**

Rich accessible phenomenology
→ Transition dens., pair transfers, etc.
→ Giant resonances (**A. Porro** poster)

Collectivity
- Little correction expected
- Good account **static + dynamical**
- Small discrepancies
  - Lack of collective coordinates?

Conclusions & outlooks

- PGCM-PT formalism
  - New **multi-reference perturbation theory**
  - Applicable to
    - **Doubly open-shell** nuclei
    - Ground and **excited states**
- Correlations in nuclear structure calculations
  - Long range (**static**) vs. short range (**dynamical**) in first approximation
  - Convenient but **arbitrary boundary**
  - Optimal description of **collective modes via PGCM…**
  - … to be **enriched in perturbation**?
- Systematic uncertainties quantifications in *ab initio* methods
  - Mid-term goal of *ab initio* methods
  - Steady progress in the last few years
  - To be enriched in a systematic way

Thank you for your attention!

Thomas Duguet
Vittorio Somà
Andrea Porro

Jean-Paul Ebran
Yann Beaujeault-Taudiere

Benjamin Bally

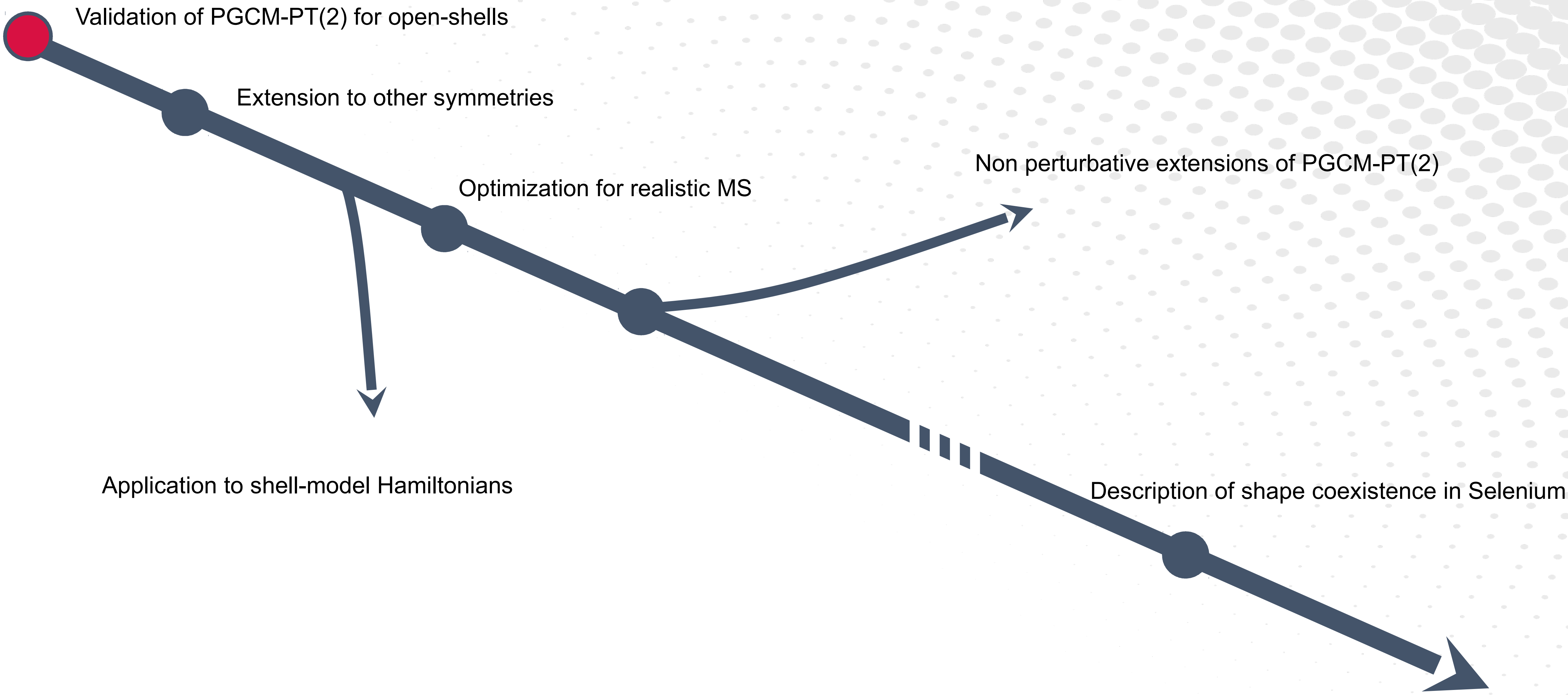
Heiko Hergert

Robert Roth
Alexander Tichai

Pepijn Demol

Backup slides

Outline of possible developments of PGCM-PT(2)



- [**Burton20**] *J. Chem. Theory Comput. 2020, 16, 9, 5586–5600* (2020)
- **[Tsuchimochi19]** *J. Chem. Theory Comput. 2019, 15, 12, 6688–6702* (2019)
- [**Hüther20]** *Physics Letters B Volume 808, 135651* (2020)
- [**Roth21**] IM-NSCM & FCI calculation, *private communication*
- **[Choi11]** *SIAM Journal on Scientific Computing, Volume 33, Issue 4, 1810-1836,* (2011)
- [**Hergert21**] MR-IMSRG evolved Hamiltonian files, *private communication*

Derivation and benchmarking

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level

- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3}$$

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3}$$

$$\longrightarrow$$

$$O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$ SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^{\Phi}] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$ SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$ SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

NO2B ⇔
Keep only k<3

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+ 0$$

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

NO2B ⇔
Keep only k<3

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+ 0$$

Three-body discarded beyond mean-field

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

NO2B ⇔
Keep only k<3

$$H^{\mathrm{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+0$$

Three-body discarded beyond mean-field

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

NO2B ⇔
Keep only k<3

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+0$$

Three-body discarded beyond mean-field

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

NO2B ⇔
Keep only k<3

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+0$$

Three-body discarded beyond mean-field

Playing with contractions

ρ

Derivation and benchmarking

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

NO2B ⇔
Keep only k<3

$$H^{\mathrm{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+0$$

Three-body discarded beyond mean-field

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

Playing with contractions

Arbitrary 1-body density matrixρ

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho] \equiv \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} ,$$

$$o^{a_1 \cdots a_n}_{b_1 \cdots b_n} = \sum_{l=n}^{N} \frac{(-1)^{l-n}}{(l-n)!} \left[\mathbf{o}^{(l)}[\rho] \cdot \rho^{\otimes (l-n)} \right]^{a_1 \cdots a_n}_{b_1 \cdots b_n} .$$

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+ 0$$

Three-body discarded beyond mean-field

NO2B ⇔
Keep only k<3

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

Playing with contractions

Arbitrary 1-body density matrix ρ

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho] \equiv \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} ,$$

$$o^{a_1 \cdots a_n}_{b_1 \cdots b_n} = \sum_{l=n}^{N} \frac{(-1)^{l-n}}{(l-n)!} \left[\mathbf{o}^{(l)}[\rho] \cdot \rho^{\otimes (l-n)} \right]^{a_1 \cdots a_n}_{b_1 \cdots b_n} .$$

Back and forth transformation
No Wick's theorem involved

ρ

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

$$H^{\mathrm{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+0$$

Three-body discarded beyond mean-field

NO2B ⇔
Keep only k<3

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

Playing with contractions

Arbitrary 1-body density matrix ρ

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho] \equiv \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} ,$$

$$o^{a_1 \cdots a_n}_{b_1 \cdots b_n} = \sum_{l=n}^{N} \frac{(-1)^{l-n}}{(l-n)!} \left[\mathbf{o}^{(l)}[\rho] \cdot \rho^{\otimes (l-n)} \right]^{a_1 \cdots a_n}_{b_1 \cdots b_n} .$$

Back and forth transformation
No Wick's theorem involved

Approximation

$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv \mathbf{o}^{(l)}[\rho] \text{ for } l \leq k,$$
$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv 0 \text{ for } l > k.$$

ρ

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

NO2B ⇔
Keep only k<3

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+ 0$$

Three-body discarded beyond mean-field

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

Playing with contractions

Arbitrary 1-body density matrix ρ

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho] \equiv \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} ,$$

$$o^{a_1 \cdots a_n}_{b_1 \cdots b_n} = \sum_{l=n}^{N} \frac{(-1)^{l-n}}{(l-n)!} \left[\mathbf{o}^{(l)}[\rho] \cdot \rho^{\otimes (l-n)} \right]^{a_1 \cdots a_n}_{b_1 \cdots b_n} .$$

Back and forth transformation
No Wick's theorem involved

Approximation

$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv \mathbf{o}^{(l)}[\rho] \text{ for } l \le k ,$$
$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv 0 \text{ for } l > k .$$

→ transformed back to sp basis

ρ

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+0$$

Three-body discarded beyond mean-field

NO2B ⇔
Keep only k<3

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

Playing with contractions

Arbitrary 1-body density matrix ρ

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho] \equiv \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} ,$$

$$o^{a_1 \cdots a_n}_{b_1 \cdots b_n} = \sum_{l=n}^{N} \frac{(-1)^{l-n}}{(l-n)!} \left[\mathbf{o}^{(l)}[\rho] \cdot \rho^{\otimes (l-n)} \right]^{a_1 \cdots a_n}_{b_1 \cdots b_n} .$$

Back and forth transformation
No Wick's theorem involved

Approximation

$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv \mathbf{o}^{(l)}[\rho] \text{ for } l \leq k,$$
$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv 0 \text{ for } l > k.$$

→ transformed back to sp basis

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

Specific case of the interaction

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

NO2B ⇔
Keep only k<3

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+0$$

Three-body discarded beyond mean-field

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

Playing with contractions

Arbitrary 1-body density matrix ρ

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho] \equiv \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} ,$$

$$o^{a_1 \cdots a_n}_{b_1 \cdots b_n} = \sum_{l=n}^{N} \frac{(-1)^{l-n}}{(l-n)!} \left[\mathbf{o}^{(l)}[\rho] \cdot \rho^{\otimes (l-n)} \right]^{a_1 \cdots a_n}_{b_1 \cdots b_n} .$$

Back and forth transformation
No Wick's theorem involved

Approximation

$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv \mathbf{o}^{(l)}[\rho] \text{ for } l \leq k ,$$
$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv 0 \text{ for } l > k .$$

→ transformed back to sp basis

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

Specific case of the interaction

$$\bar{h}^{(0)}[\rho] \equiv \frac{1}{3!} w^{(3)} \cdot \rho^{\otimes(3)} ,$$
$$\bar{h}^{(1)}[\rho] \equiv t^{(1)} - \frac{1}{2!} w^{(3)} \cdot \rho^{\otimes(2)} ,$$
$$\bar{h}^{(2)}[\rho] \equiv v^{(2)} + w^{(3)} \cdot \rho ,$$

ρ

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions

BMF : **NO2B** approximation

Expansive storage + runtime

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

Normal ordering wrt. $|\Phi\rangle$SD

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho^\Phi] = \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} .$$

Tensor product

$$H^{\text{NO2B}}[\rho^\Phi] \equiv t \cdot \rho^\Phi + \frac{1}{2!} v \cdot \rho^\Phi \cdot \rho^\Phi + \frac{1}{3!} w \cdot \rho^\Phi \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ t + v \cdot \rho^\Phi + \frac{1}{2!} w \cdot \rho^\Phi \cdot \rho^\Phi$$
$$+ v \cdot + w \cdot \rho^\Phi$$
$$+ 0$$

Three-body discarded beyond mean-field

NO2B ⇔
Keep only k<3

Limits of NO2B

In open-shells
- **Expansive** calculations
- **SB** Hamiltonians
- Intricate workarounds

In medium interactions

Involve **only 1-body** density matrices
Symmetric truncated operator
SP basis → **start other calculations**

Playing with contractions

Arbitrary 1-body density matrix ρ

$$\mathbf{o}^{a_1 \cdots a_k}_{b_1 \cdots b_k}[\rho] \equiv \sum_{n=k}^{N} \frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k} ,$$

$$o^{a_1 \cdots a_n}_{b_1 \cdots b_n} = \sum_{l=n}^{N} \frac{(-1)^{l-n}}{(l-n)!} \left[\mathbf{o}^{(l)}[\rho] \cdot \rho^{\otimes (l-n)} \right]^{a_1 \cdots a_n}_{b_1 \cdots b_n} .$$

Back and forth transformation
No Wick's theorem involved

Approximation

$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv \mathbf{o}^{(l)}[\rho] \text{ for } l \leq k ,$$
$$\bar{\mathbf{o}}^{(l)}[\rho] \equiv 0 \text{ for } l > k .$$

→ transformed back to sp basis

Specific case of the interaction

$$\bar{h}^{(0)}[\rho] \equiv \frac{1}{3!} w^{(3)} \cdot \rho^{\otimes (3)} ,$$
$$\bar{h}^{(1)}[\rho] \equiv t^{(1)} - \frac{1}{2!} w^{(3)} \cdot \rho^{\otimes (2)} ,$$
$$\bar{h}^{(2)}[\rho] \equiv v^{(2)} + w^{(3)} \cdot \rho ,$$

Simple and cheap
Same symmetries as ρ
Reduces to NO2B in closed shells
Generalizable to n > 3

Expansive storage + runtime

Higher rank nuclear forces

1N and 2N **always treated** explicitly
3N (4N) **manageable** at HF(B) level
- Low complexity
- Symmetry reductions
BMF : **NO2B** approximation

$$O \equiv \frac{1}{(1!)^2} o^{a_1}_{b_1} C^{a_1}_{b_1} + \frac{1}{(2!)^2} o^{a_1 a_2}_{b_1 b_2} C^{a_1 a_2}_{b_1 b_2} + \frac{1}{(3!)^2} o^{a_1 a_2 a_3}_{b_1 b_2 b_3} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \longrightarrow O = \frac{1}{(1!)^2} \mathbf{o}^{a_1}_{b_1} : C^{a_1}_{b_1} : + \frac{1}{(2!)^2} \mathbf{o}^{a_1 a_2}_{b_1 b_2} : C^{a_1 a_2}_{b_1 b_2} : + \frac{1}{(3!)^2} \mathbf{o}^{a_1 a_2 a_3}_{b_1 b_2 b_3} : C^{a_1 a_2 a_3}_{b_1 b_2 b_3} :$$

$$\frac{1}{(n-k)!} \left[o^{(n)} \cdot \rho^{\Phi \otimes (n-k)} \right]^{a_1 \cdots a_k}_{b_1 \cdots b_k}$$

Tensor product

- Benchmark
  - Model spaces, densities, methods, observables
- Low error at converged e_{3max}
  - < 3% on all observables
  - Independent wrt. trial density
  - Applicable to all methods
- Drawbacks
  - Dependent on deformation
  - 3% errors
  - Same as state of the art
- Perspectives
  - Comparison with generalised Wick theorem
  - Use EDF trial density matrices for heavier systems

Limits of NO2

In open-shells
- **Expansive** calculatio
- **SB** Hamiltonians
- Intricate workaround

...ond mean-field

...ion

...rmed back to sp basis

In medium interac

Involve **only 1-body** density
Symmetric truncated opera
SP basis → **start other calculations**

No Wick's theorem involved

$$\bar{h}^{(1)}[\rho] \equiv t^{(1)} - \frac{1}{2!} w^{(3)} \cdot \rho^{\otimes(2)},$$
$$\bar{h}^{(2)}[\rho] \equiv v^{(2)} + w^{(3)} \cdot \rho,$$

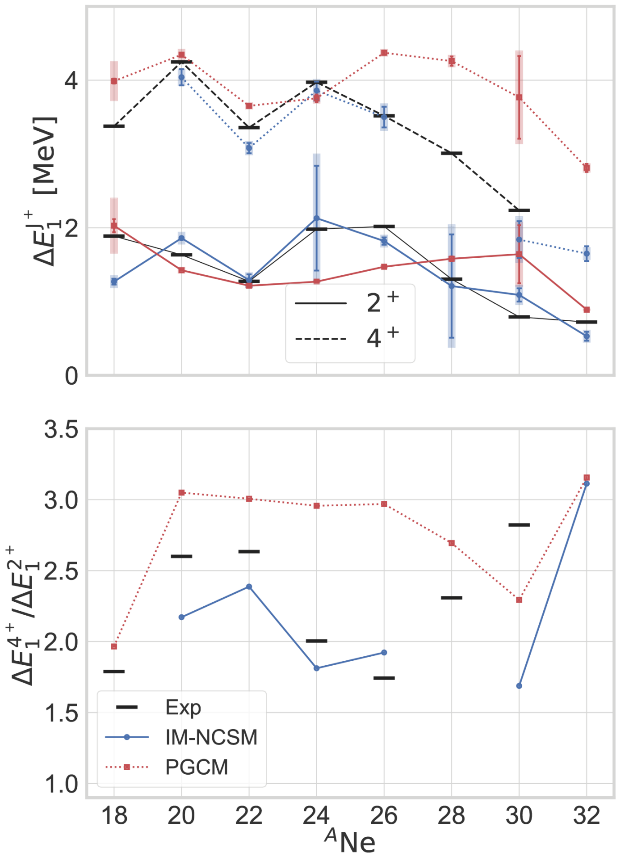
... interaction

... cheap
...metries as ρ
Reduces to NO2B in closed shells
Generalizable to n > 3

Systematics in the Neon chain

Systematics in the Neon chain

2^+ and 4^+ excitation energies

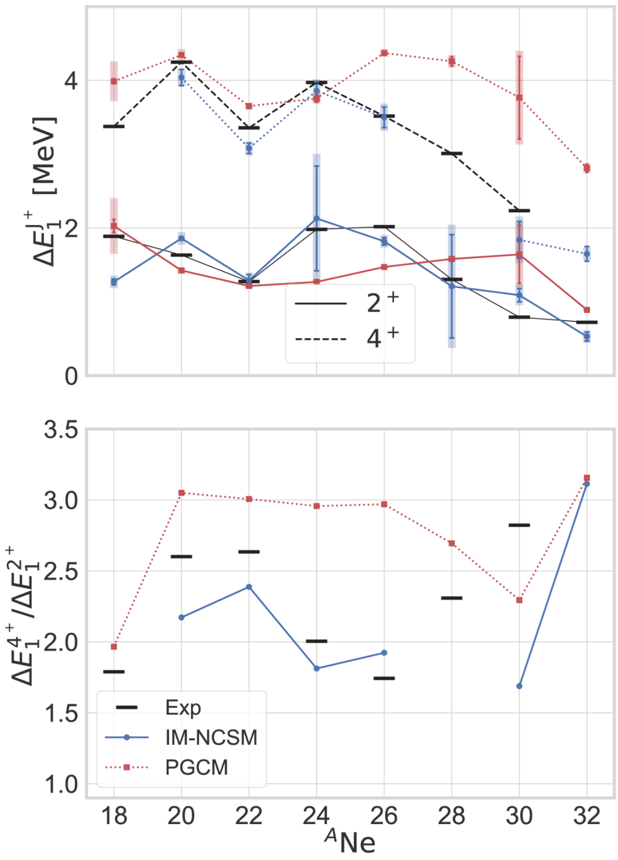


Good account of $^{18\text{-}24}$Ne
Missing physics for $^{26\text{-}30}$Ne

- **Dynamical correlations**
- Static correlations?

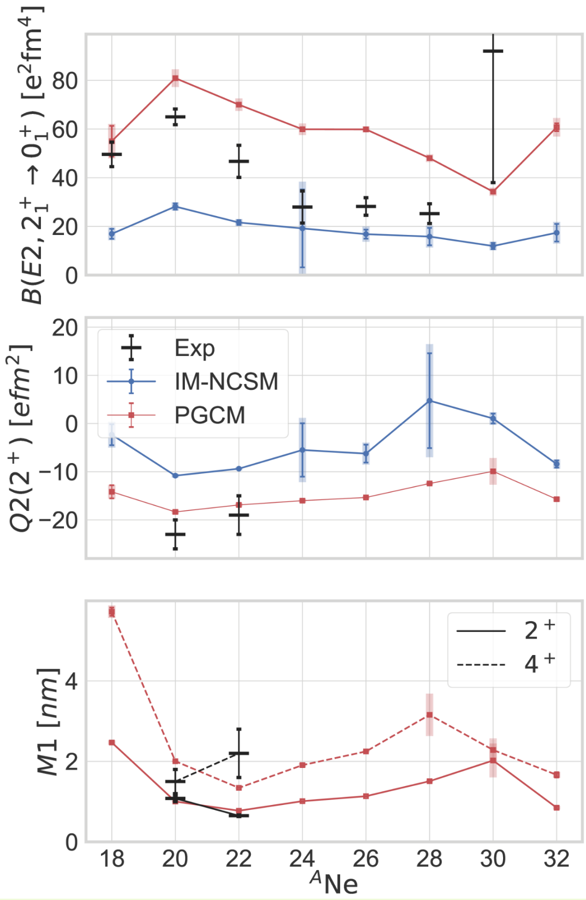
Systematics in the Neon chain

2⁺ and 4⁺ excitation energies



Good account of $^{18-24}$Ne
Missing physics for $^{26-30}$Ne
- **Dynamical correlations**
- Static correlations?

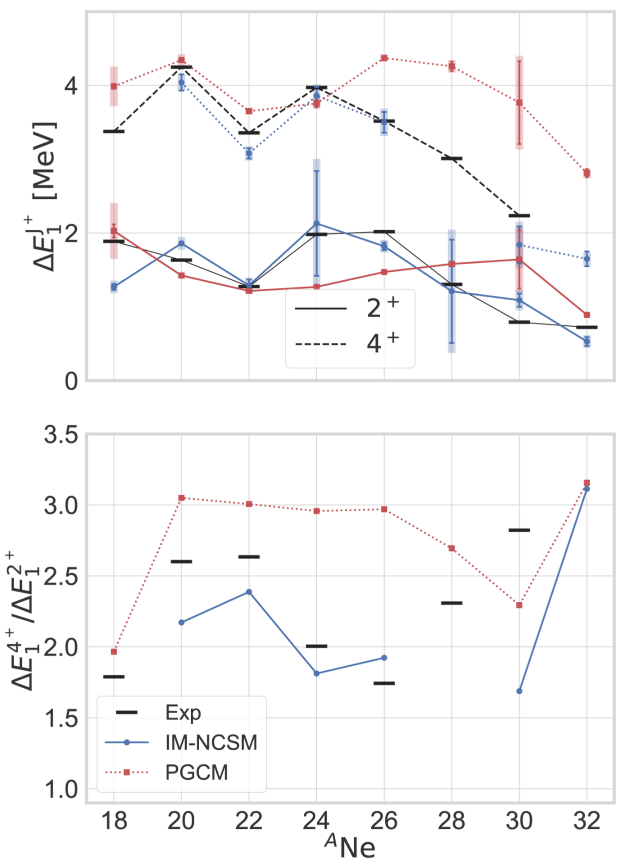
2⁺ and 4⁺ EM moments and transitions



Collectivity trend correctly described
Exaggerated → **Missing dynamical**?
Wrong trend for ^{30}Ne…
- Can we explain it?

Systematics in the Neon chain

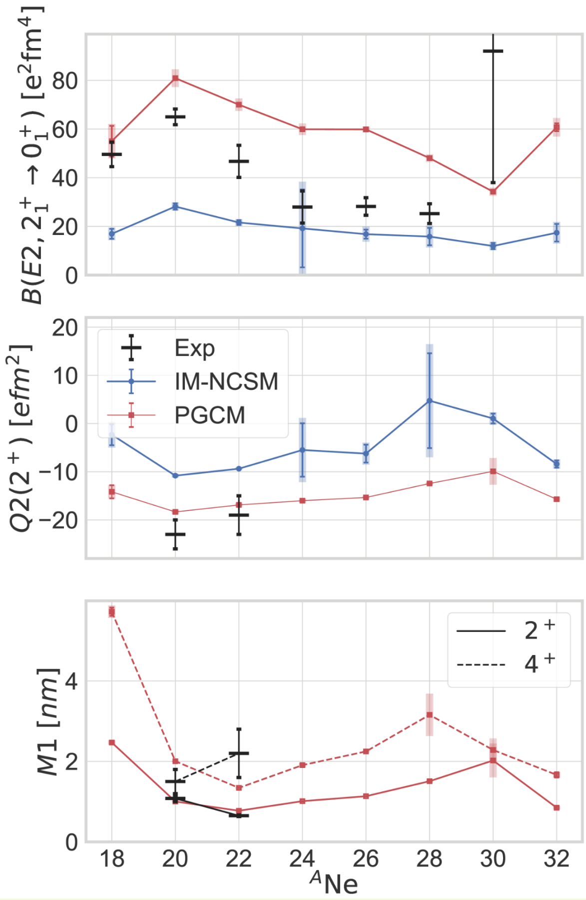
2+ and 4+ excitation energies



Good account of $^{18-24}$Ne
Missing physics for $^{26-30}$Ne

- **Dynamical correlations**
- Static correlations?

2+ and 4+ EM moments and transitions



Collectivity trend correctly described
Exaggerated → **Missing dynamical**?
Wrong trend for ^{30}Ne…

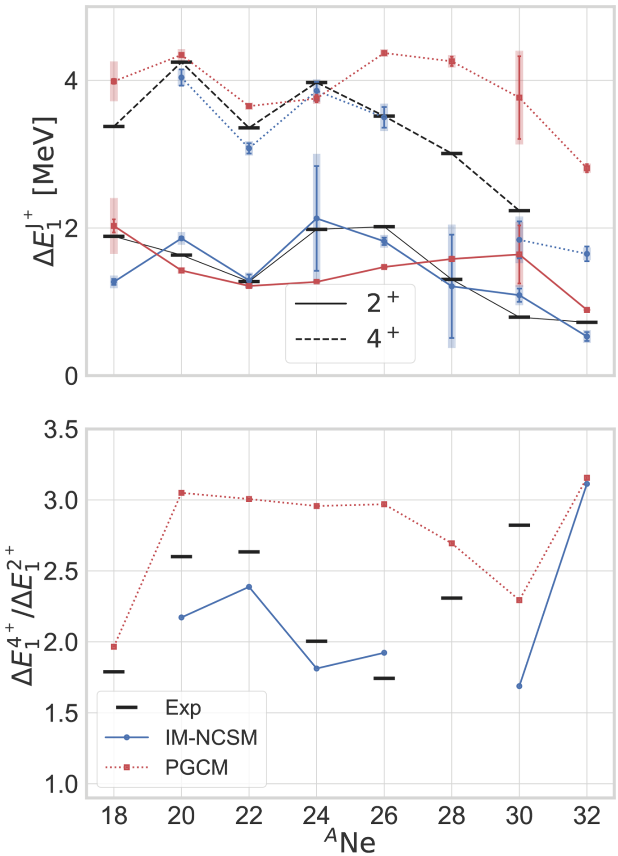
- Can we explain it?

Special case of ^{30}Ne

- **Island of inversion**
- Difficult for all methods

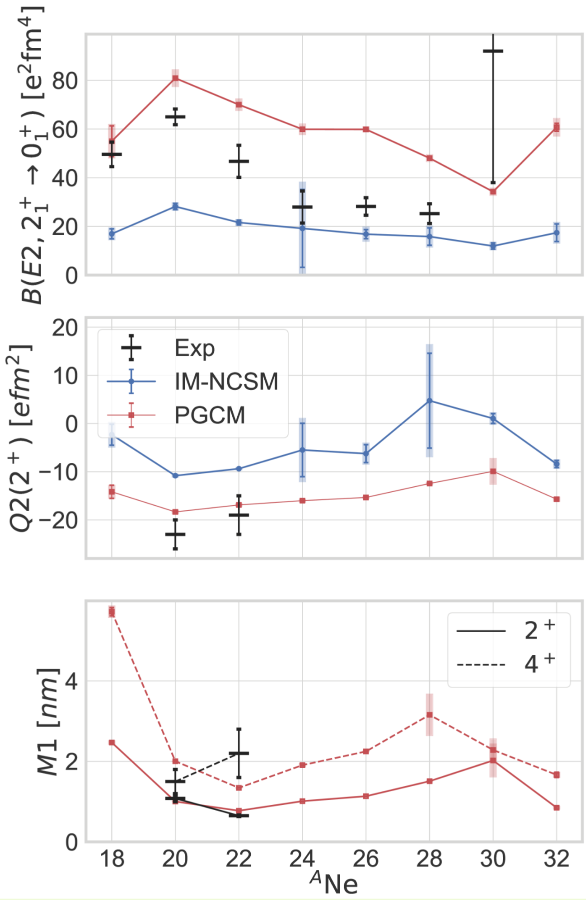
Systematics in the Neon chain

2+ and 4+ excitation energies



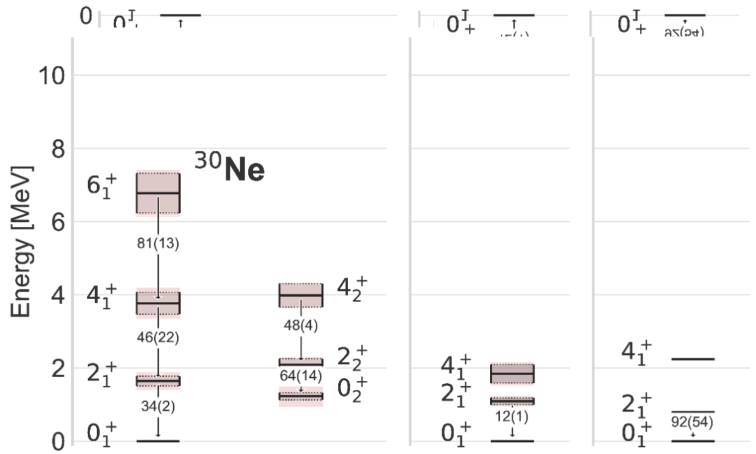
Good account of $^{18-24}$Ne
Missing physics for $^{26-30}$Ne
- **Dynamical correlations**
- Static correlations?

2+ and 4+ EM moments and transitions



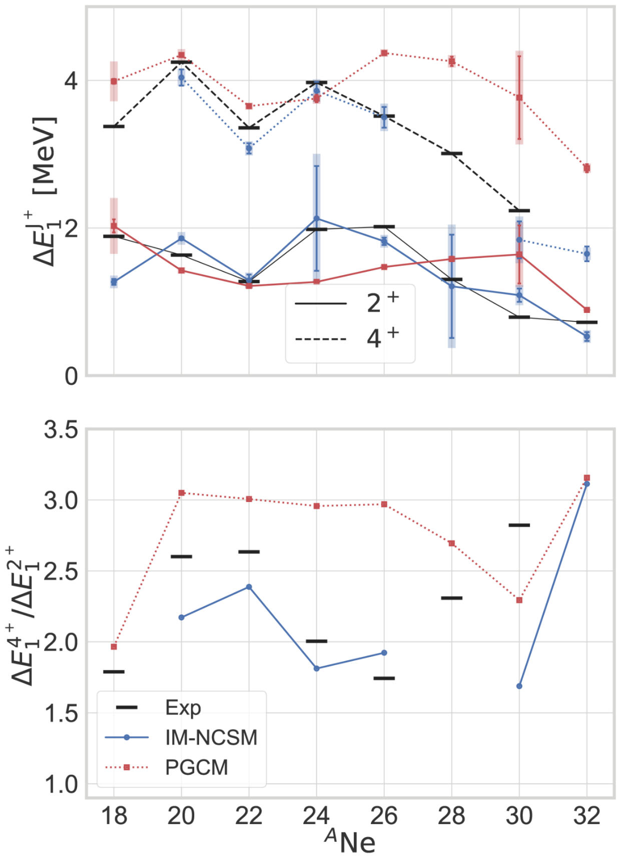
Collectivity trend correctly described
Exaggerated → **Missing dynamical**?
Wrong trend for ^{30}Ne…
- Can we explain it?

Special case of ^{30}Ne
- **Island of inversion**
- Difficult for all methods



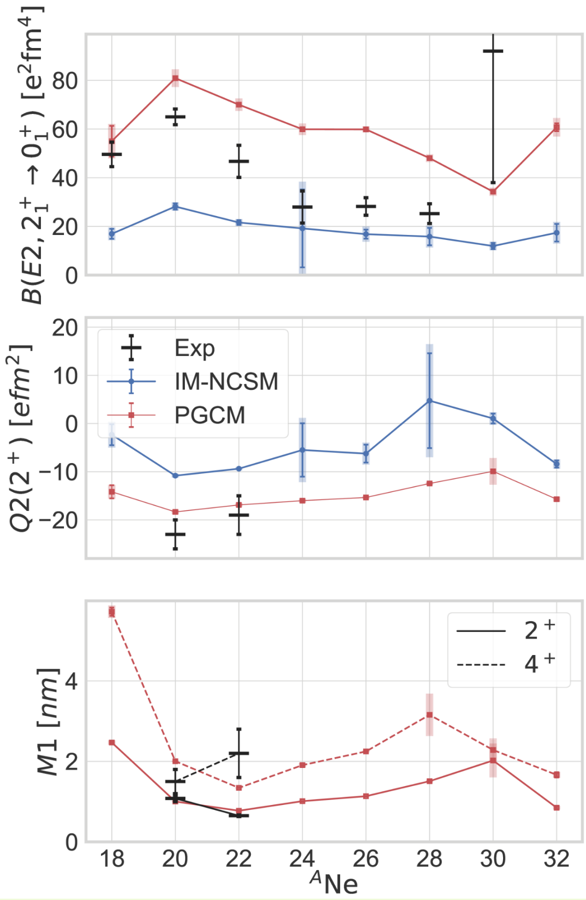
Systematics in the Neon chain

2⁺ and 4⁺ excitation energies



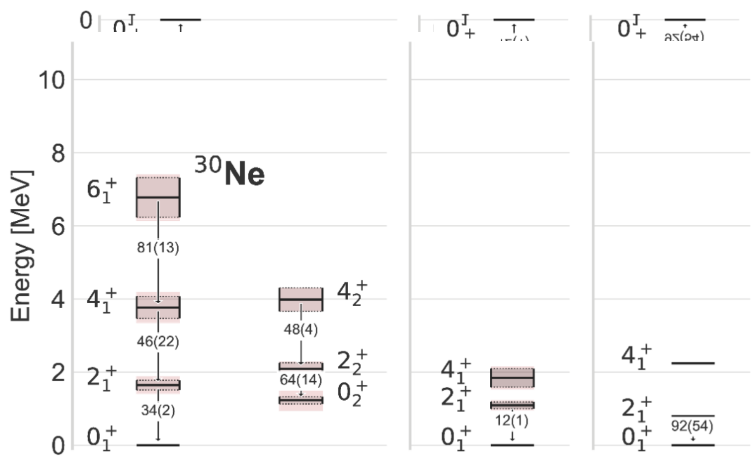
Good account of $^{18-24}$Ne
Missing physics for $^{26-30}$Ne
- **Dynamical correlations**
- Static correlations?

2⁺ and 4⁺ EM moments and transitions



Collectivity trend correctly described
Exaggerated → **Missing dynamical**?
Wrong trend for ^{30}Ne…
- Can we explain it?

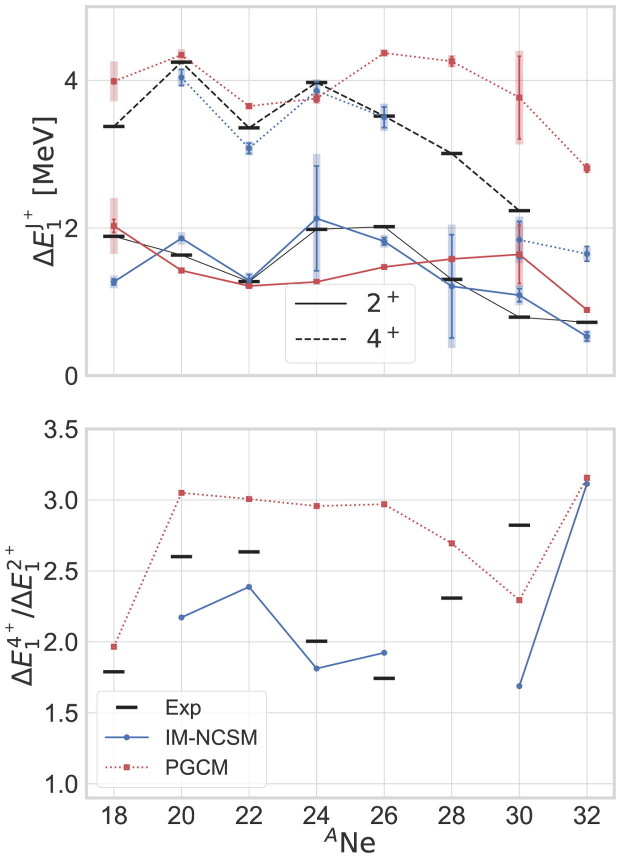
Special case of ^{30}Ne
- **Island of inversion**
- Difficult for all methods



IM-NCSM: misses rotational character
PGCM second band more rotational

Systematics in the Neon chain

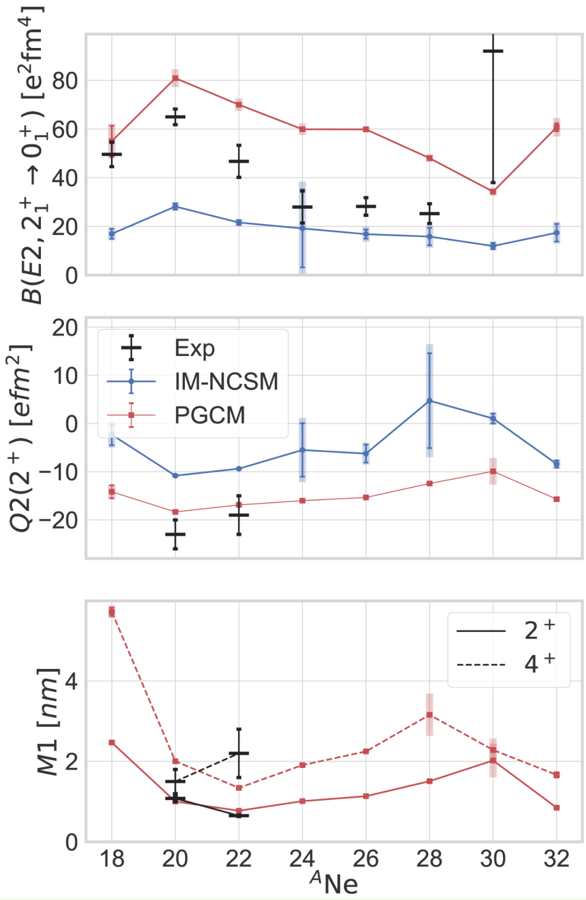
2^+ and 4^+ excitation energies



Good account of $^{18-24}$Ne
Missing physics for $^{26-30}$Ne

- **Dynamical correlations**
- Static correlations?

2^+ and 4^+ EM moments and transitions

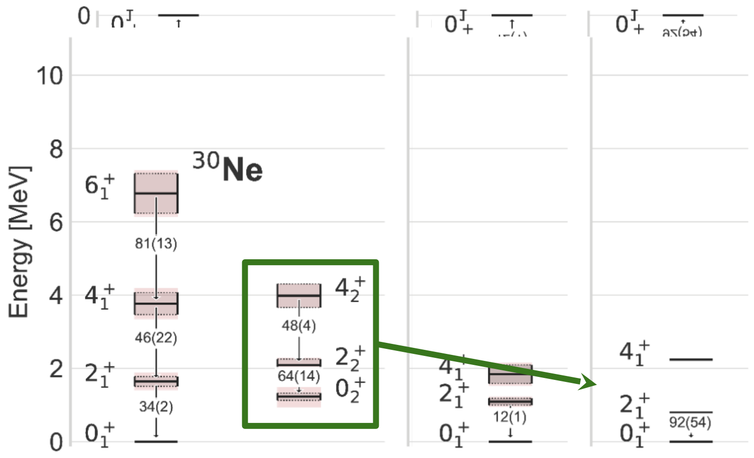


Collectivity trend correctly described
Exaggerated → **Missing dynamical**?
Wrong trend for ^{30}Ne…

- Can we explain it?

Special case of ^{30}Ne

- **Island of inversion**
- Difficult for all methods



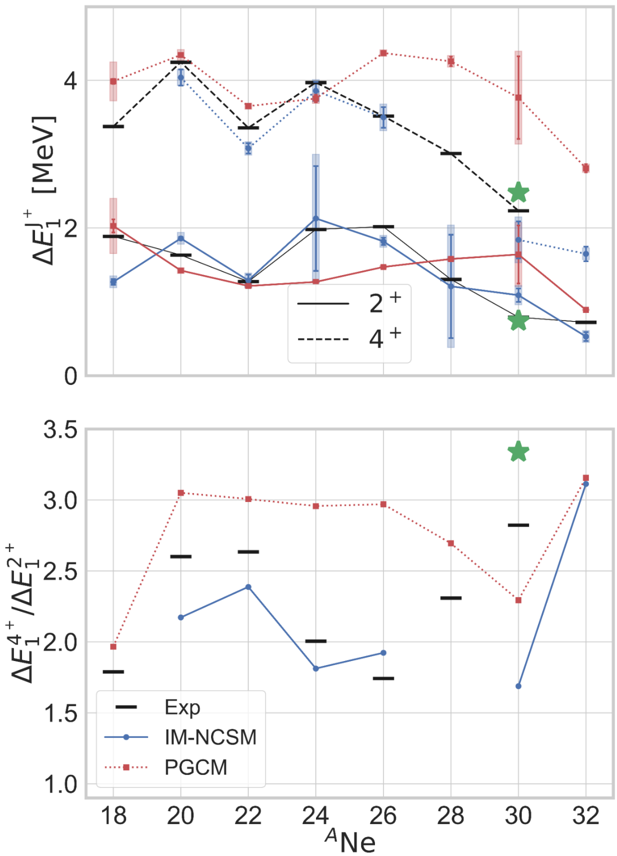
IM-NCSM: misses rotational character
PGCM second band more rotational

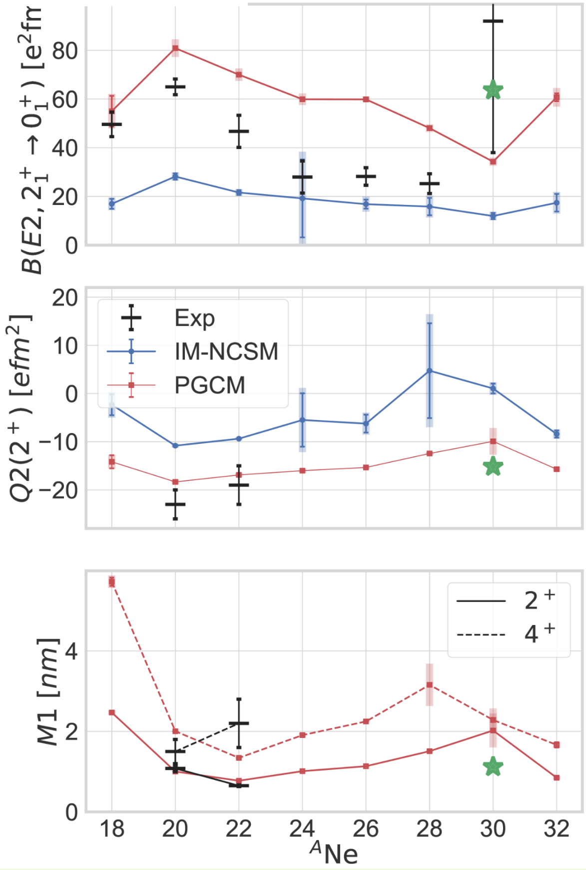
Systematics in the Neon chain

2⁺ and 4⁺ excitation energies

2⁺ and 4⁺ EM moments and transitions

★ PGCM ^{30}Ne Intruder band

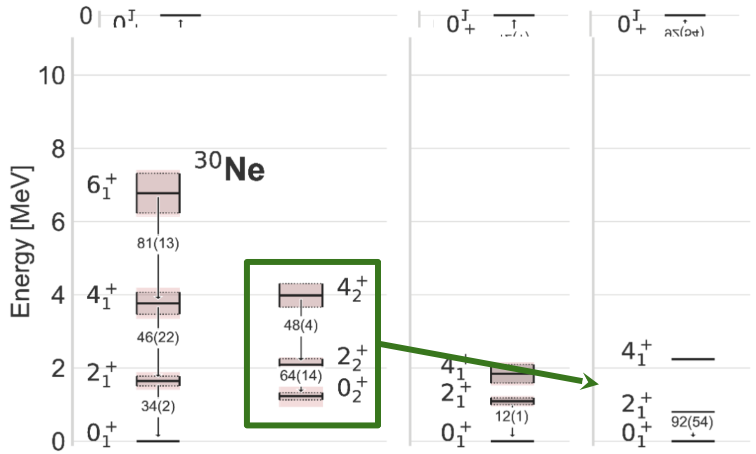




Good account of $^{18-24}$Ne
Missing physics for $^{26-30}$Ne
- **Dynamical correlations**
- Static correlations?

Collectivity trend correctly described
Exaggerated → **Missing dynamical**?
Wrong trend for ^{30}Ne…
- Can we explain it?

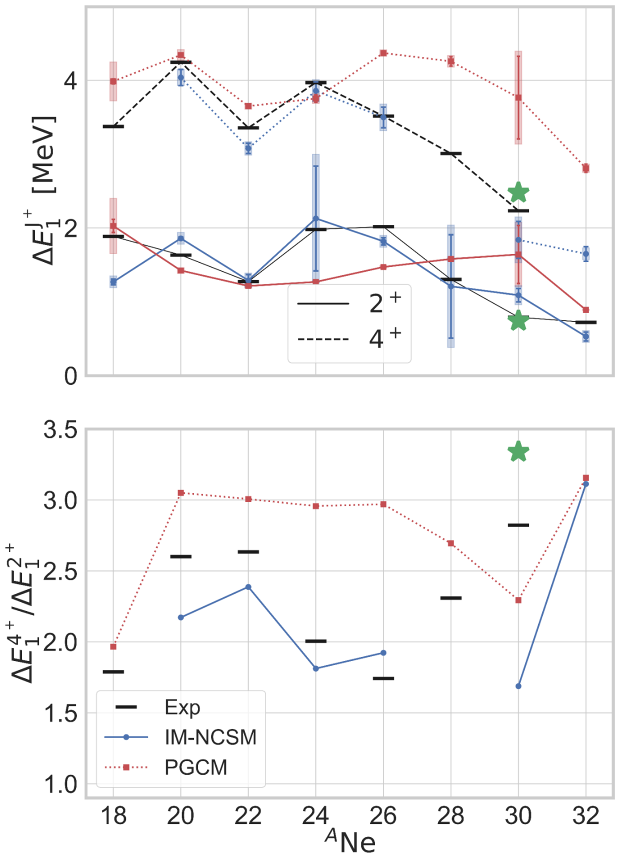
Special case of ^{30}Ne
- **Island of inversion**
- Difficult for all methods

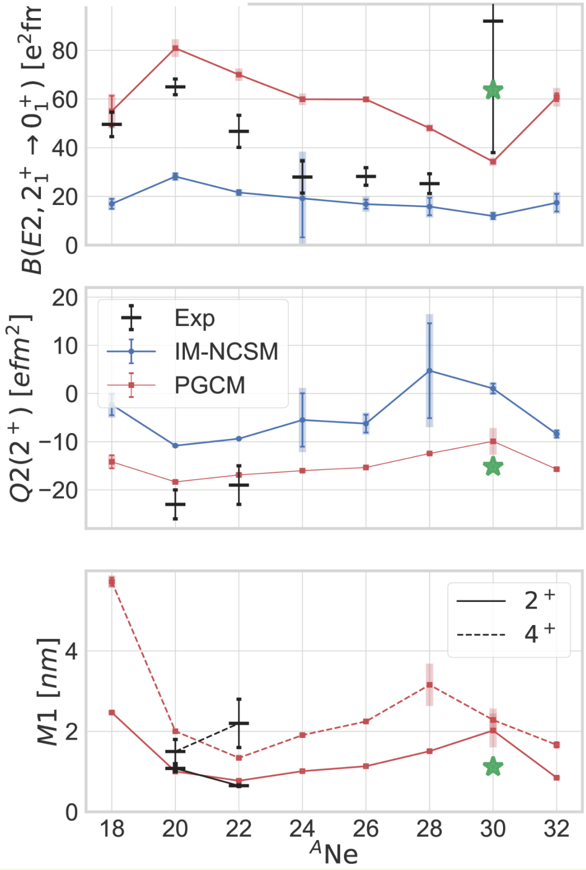


IM-NCSM: misses rotational character
PGCM second band more rotational

2⁺ and 4⁺ excitation energies **2⁺ and 4⁺ EM moments and transitions**

★ PGCM [30]Ne Intruder band

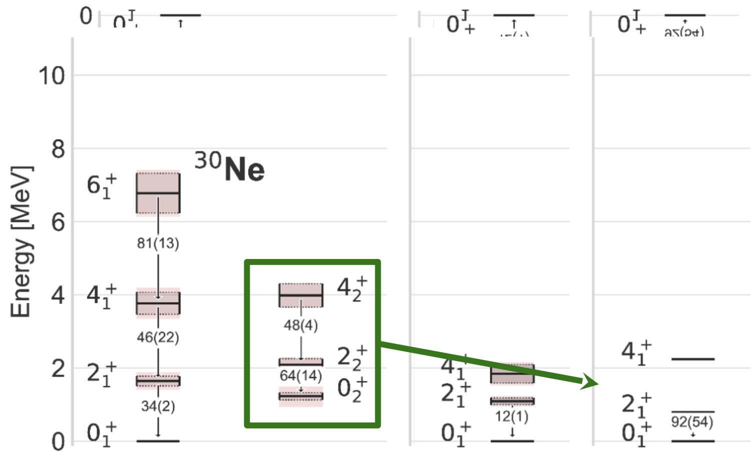




Good account of [18-24]Ne
Missing physics for [26-30]Ne
- **Dynamical correlations**
- Static correlations?

Collectivity trend correctly described
Exaggerated → **Missing dynamical**?
Wrong trend for [30]Ne…
- Can we explain it?

Special case of [30]Ne
- **Island of inversion**
- Difficult for all methods

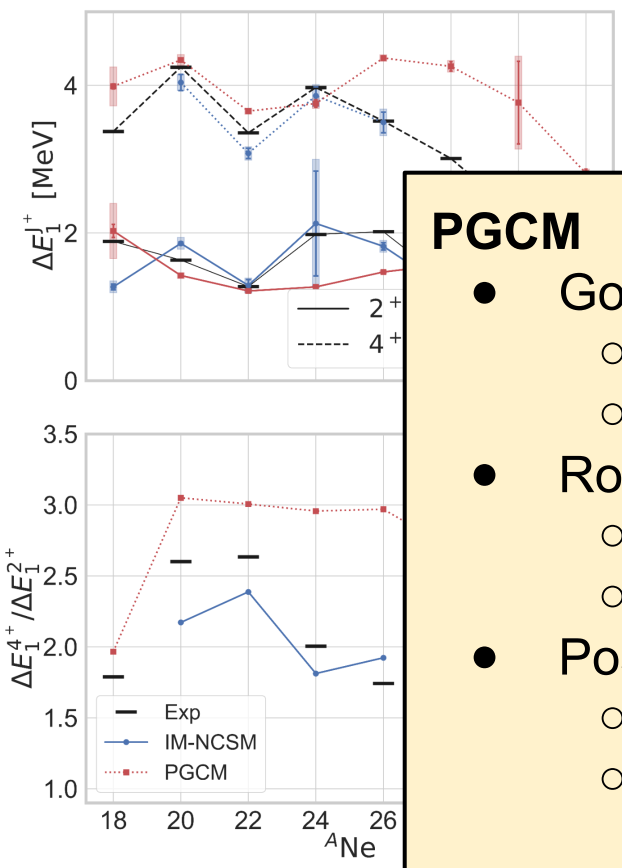


IM-NCSM: misses rotational character
PGCM second band more rotational

How to lower the intruder band?

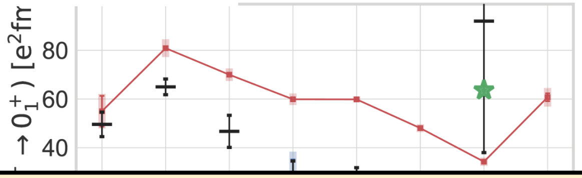
Systematics in the Neon chain

2^+ and 4^+ excitation energies

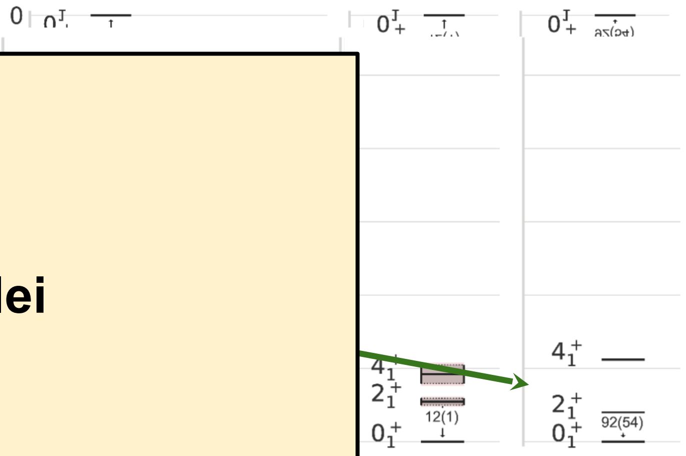


2^+ and 4^+ EM moments and transitions

★ **PGCM ^{30}Ne Intruder band**



Special case of ^{30}Ne
- **Island of inversion**
- Difficult for all methods



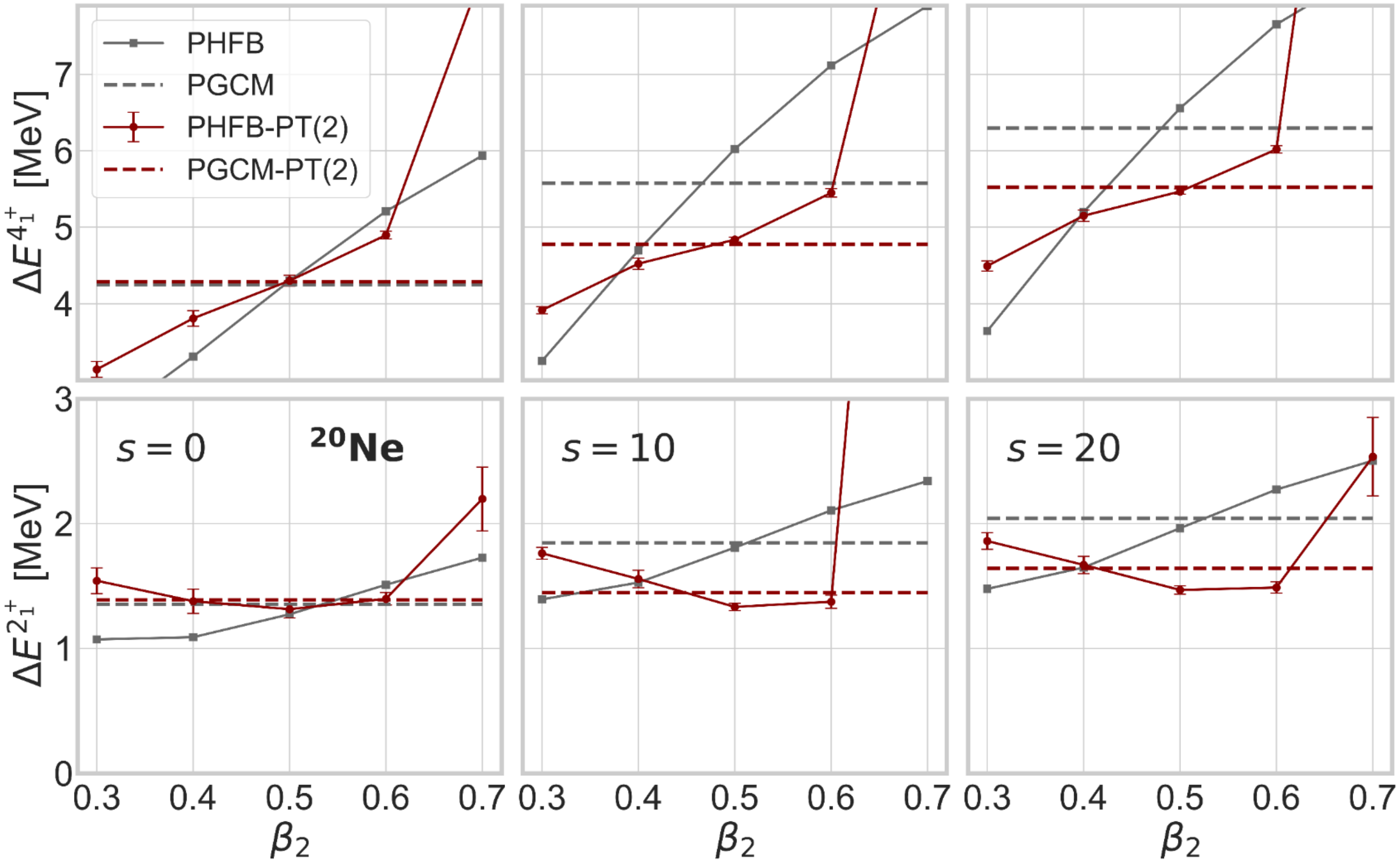
PGCM
- Good **overall agreement** with experiment
  - Spectra, moments and transitions
  - Working best for **standard rotational nuclei**
- Room for improvement
  - **Island of inversion**
  - Missing fd-fp cross-shell correlations in ^{30}Ne
- Possible improvements
  - Enlarge set of collective coordinates
  - **Add elementary excitations**
    - Perturbatively (PGCM-PT next)
    - **Into PGCM ansatz**

Good account of $^{18-24}$Ne
Missing physics for $^{26-30}$Ne
- **Dynamical correlations**
- Static correlations?

described
Exaggerated → **Missing dynamical**?
Wrong trend for ^{30}Ne…
- Can we explain it?

otational character
more rotational

How to lower the intruder band?


PHFB
PGCM
PHFB-PT(2)
PGCM-PT(2)
$\Delta E^{4_1^+}$ [MeV]
$\Delta E^{2_1^+}$ [MeV]
$s = 0$
^{20}Ne
$s = 10$
$s = 20$
β_2
0.3 0.4 0.5 0.6 0.7
0 1 2 3 4 5 6 7

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^{\dagger}(s) H U(s)\,, \quad s \to \infty$$

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^{\dagger}(s) H U(s)\,, \quad s \to \infty$$

Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

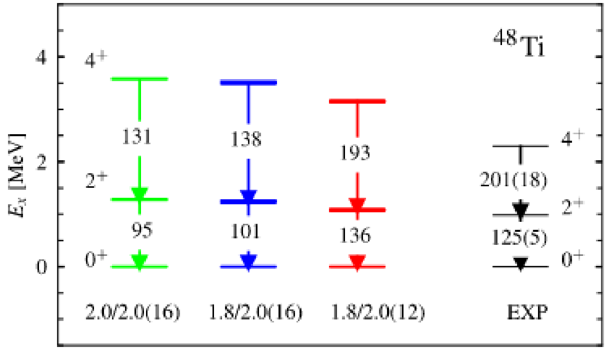
$$H(s) = U^{\dagger}(s) H U(s)\,, \quad s \to \infty$$

Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

Ab Initio **Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca**

J. M. Yao,[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,∥] and H. Hergert[1,4,¶]



Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^{\dagger}(s) H U(s)\,, \quad s \to \infty$$

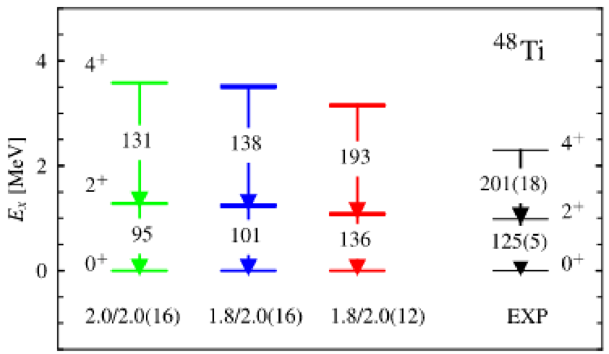
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

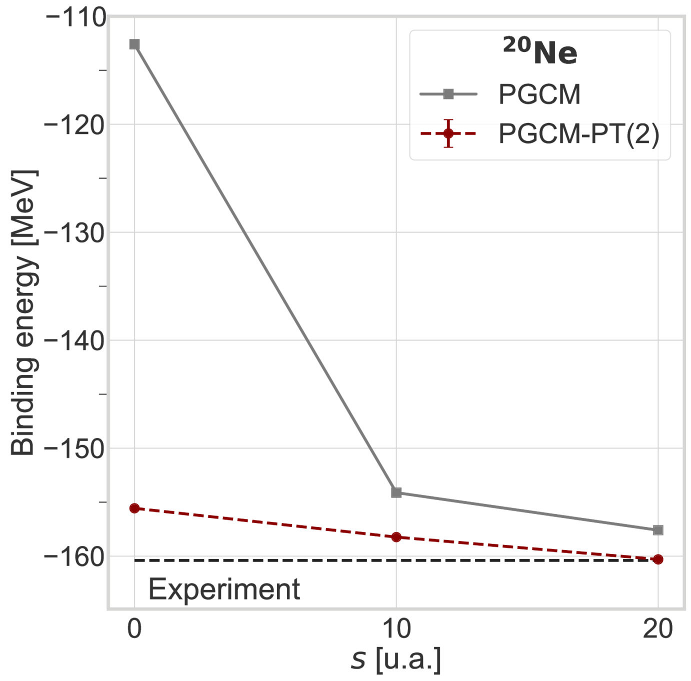
PGCM + MR-IMSRG [Yao20]

- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

***Ab Initio* Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca**

J. M. Yao,[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,∥] and H. Hergert[1,4,¶]





PGCM with 5 points
3 flow values s = 0, 10, 20

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^\dagger(s) H U(s)\,, \quad s \to \infty$$

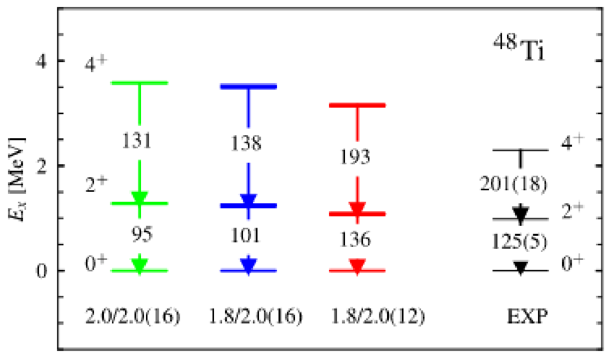
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

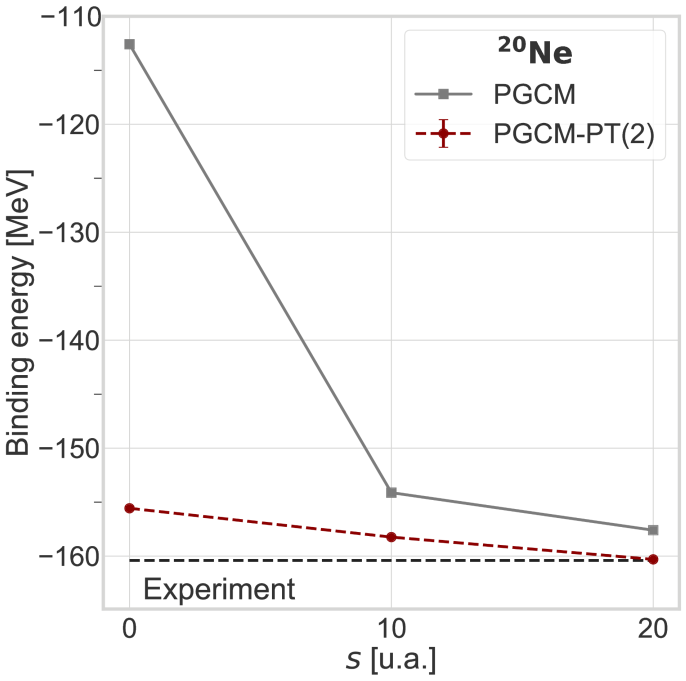
PGCM + MR-IMSRG [Yao20]

- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

Ab Initio Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca

J. M. Yao,[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,‖] and H. Hergert[1,4,¶]





PGCM with 5 points
3 flow values s = 0, 10, 20

PGCM-PT(2) **always correcting**

- **2 MeV** at s=20
- **Approximate decoupling** of $|\Theta^{(0)}\rangle$

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

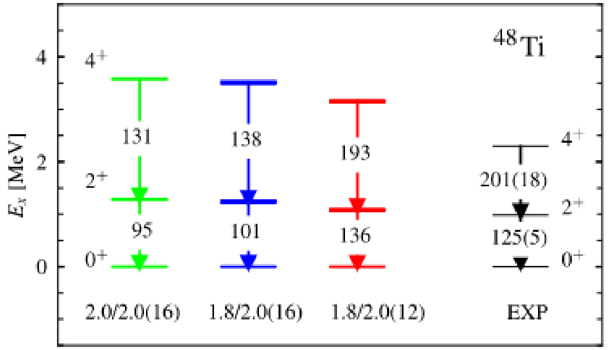
$$H(s) = U^{\dagger}(s) H U(s)\,, \quad s \to \infty$$

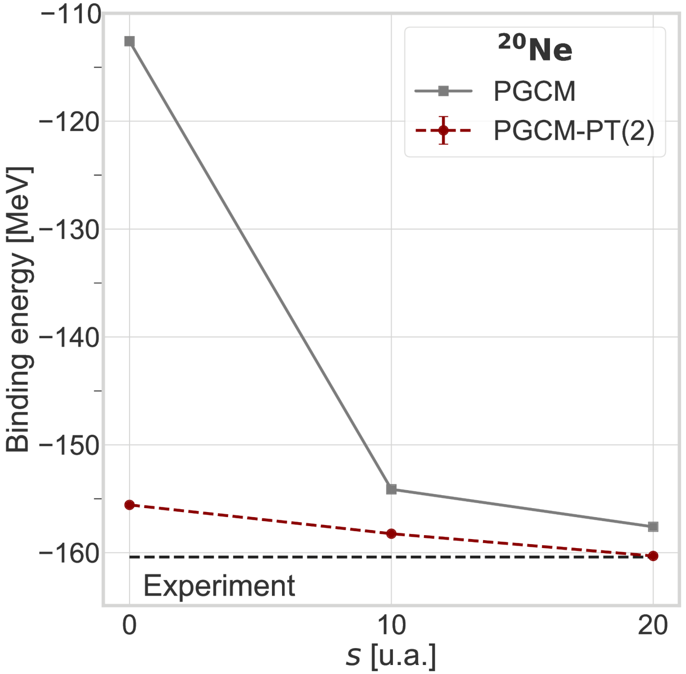
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

Ab Initio **Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca**

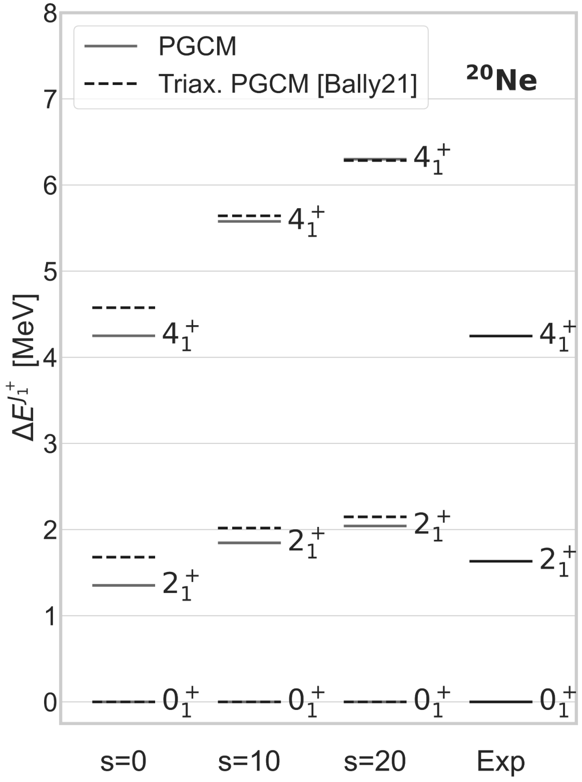
J. M. Yao[1,*] B. Bally,[2,†] J. Engel[2,‡] R. Wirth[1,§] T. R. Rodríguez[3,∥] and H. Hergert[1,4,¶]





PGCM with 5 points
3 flow values s = 0, 10, 20

PGCM-PT(2) **always correcting**
- **2 MeV** at s=20
- **Approximate decoupling** of $|\Theta^{(0)}\rangle$



Effect of flow evolution on PGCM spectra
- **Systematic band dilatation**
- **Not corrected** with **triaxiality**

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

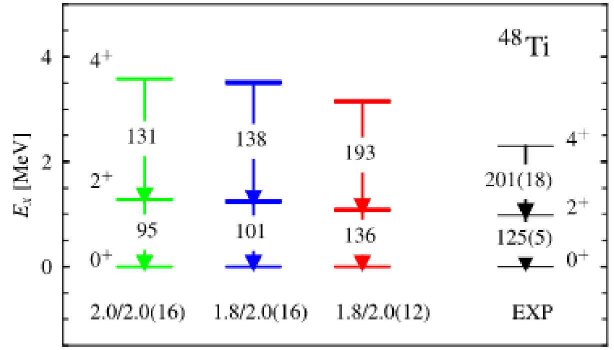
$$H(s) = U^\dagger(s) H U(s)\,,\quad s \to \infty$$

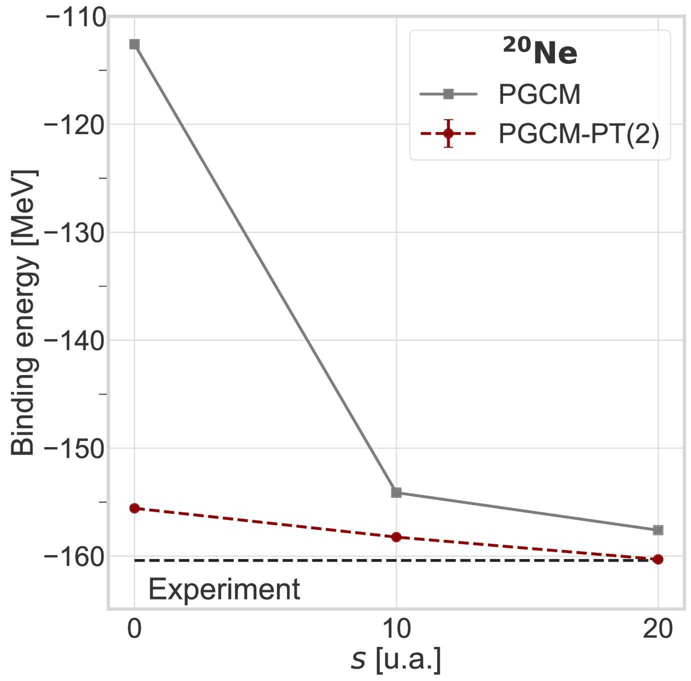
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

Ab Initio Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca

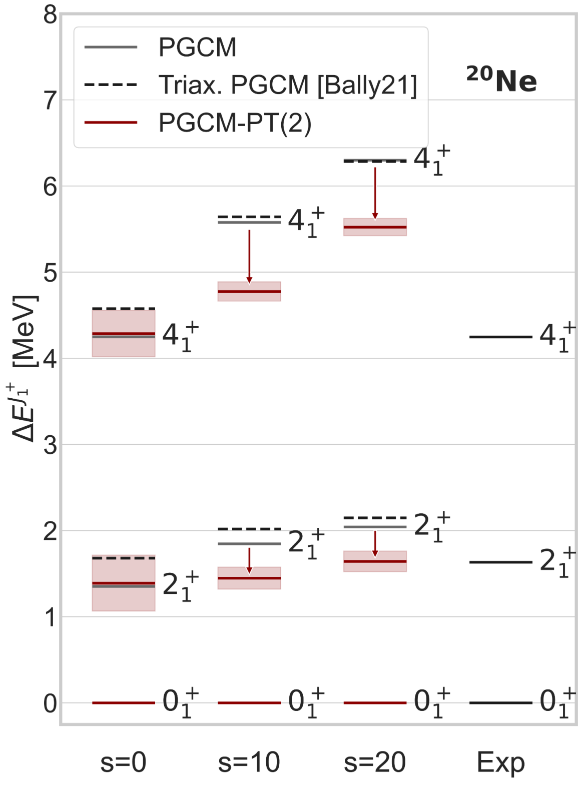
J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodríguez, and H. Hergert





PGCM with 5 points
3 flow values s = 0, 10, 20

PGCM-PT(2) **always correcting**
- **2 MeV** at s=20
- **Approximate decoupling** of $|\Theta^{(0)}\rangle$



Effect of flow evolution on PGCM spectra
- **Systematic band dilatation**
- **Not corrected** with **triaxiality**

Coherently corrected via PGCM-PT(2)
- **Reshuffling** of correlations
- Dynamical correlations needed

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^\dagger(s) H U(s)\,, \quad s \to \infty$$

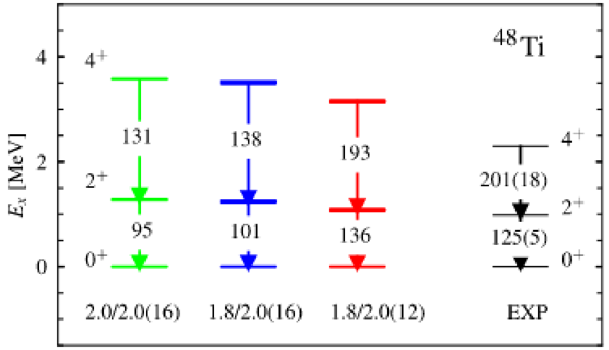
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]

- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

***Ab Initio* Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca**

J. M. Yao,[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,‖] and H. Hergert[1,4,¶]



Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^{\dagger}(s) H U(s)\,, \quad s \to \infty$$

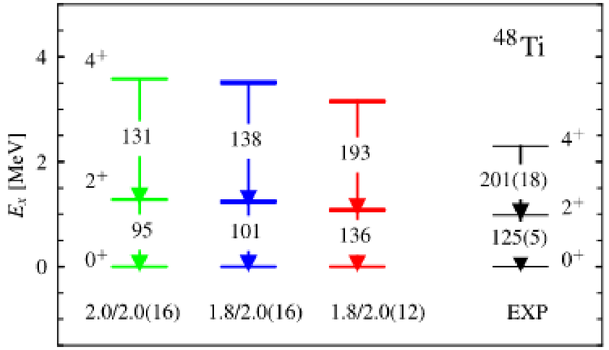
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]

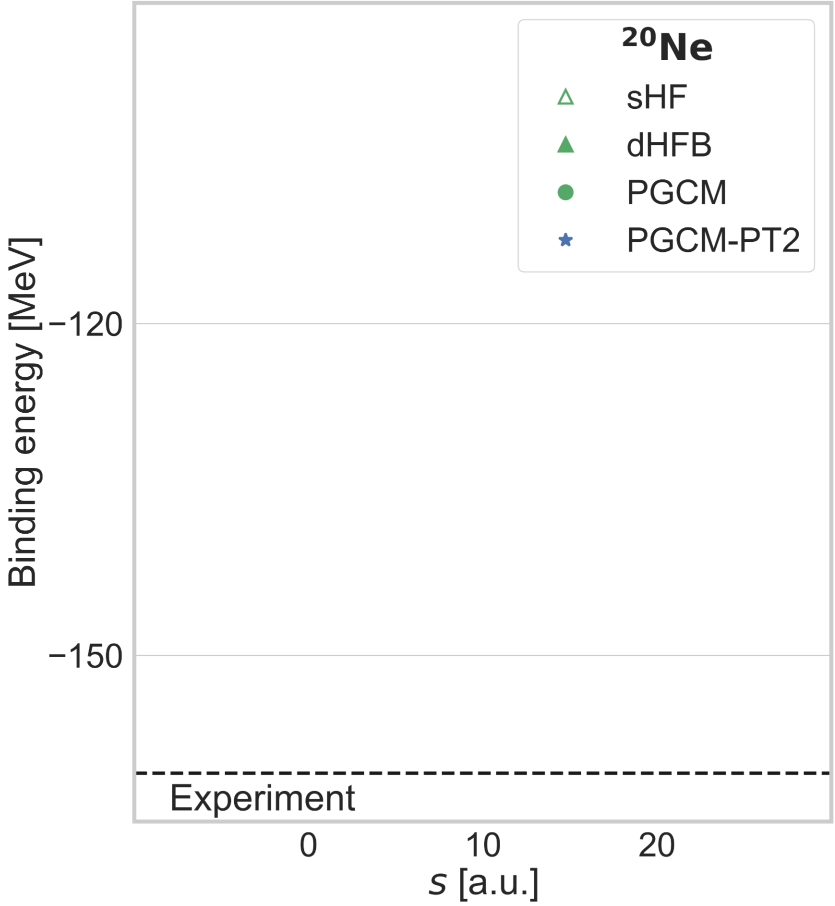
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

***Ab Initio* Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca**

J. M. Yao,[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,∥] and H. Hergert[1,4,¶]



Reshuffling of correlations



Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^{\dagger}(s) H U(s)\,, \quad s \to \infty$$

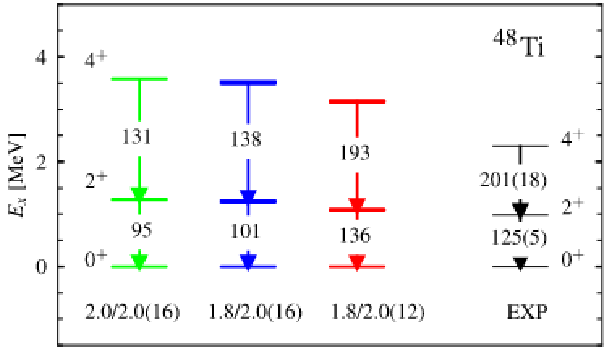
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]

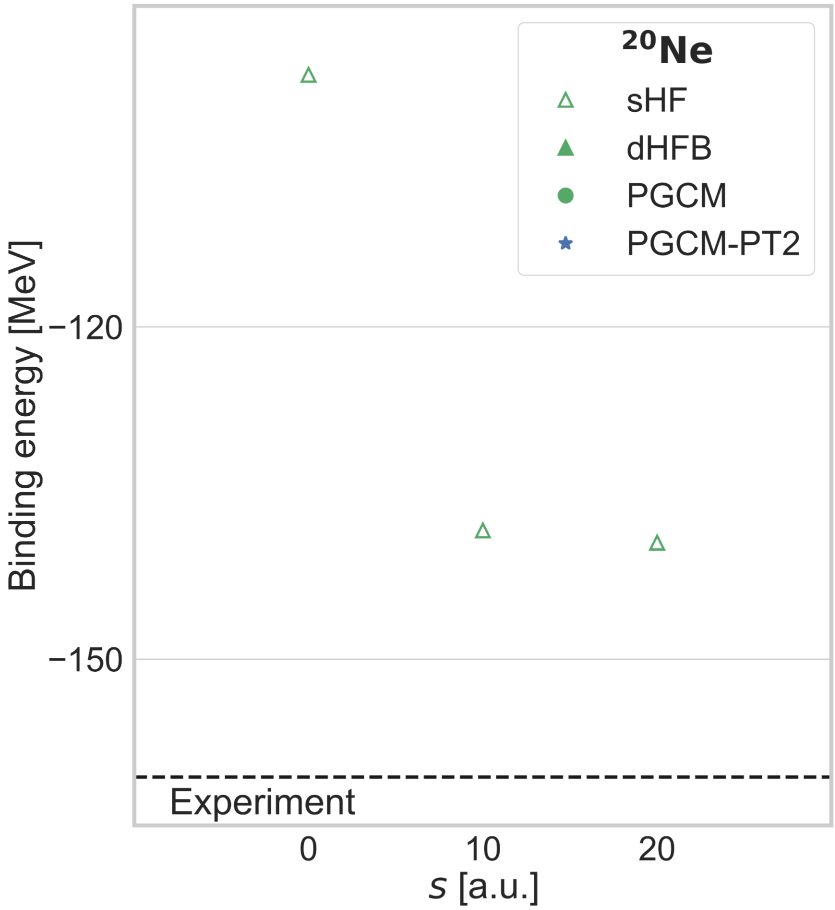
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

Ab Initio **Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of** ^{48}**Ca**

J. M. Yao[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,‖] and H. Hergert[1,4,¶]



Reshuffling of correlations



MR-IMSRG preprocessing
→ Lowers sHF starting point

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^{\dagger}(s) H U(s) \,, \quad s \to \infty$$

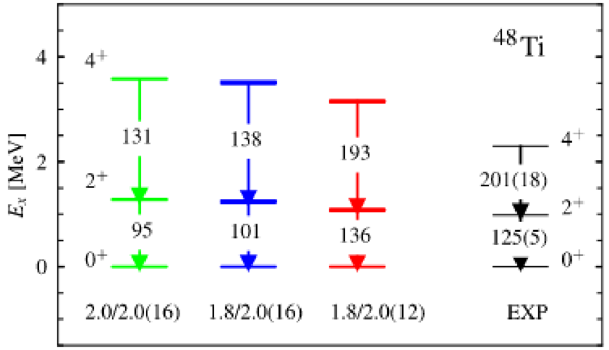
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]

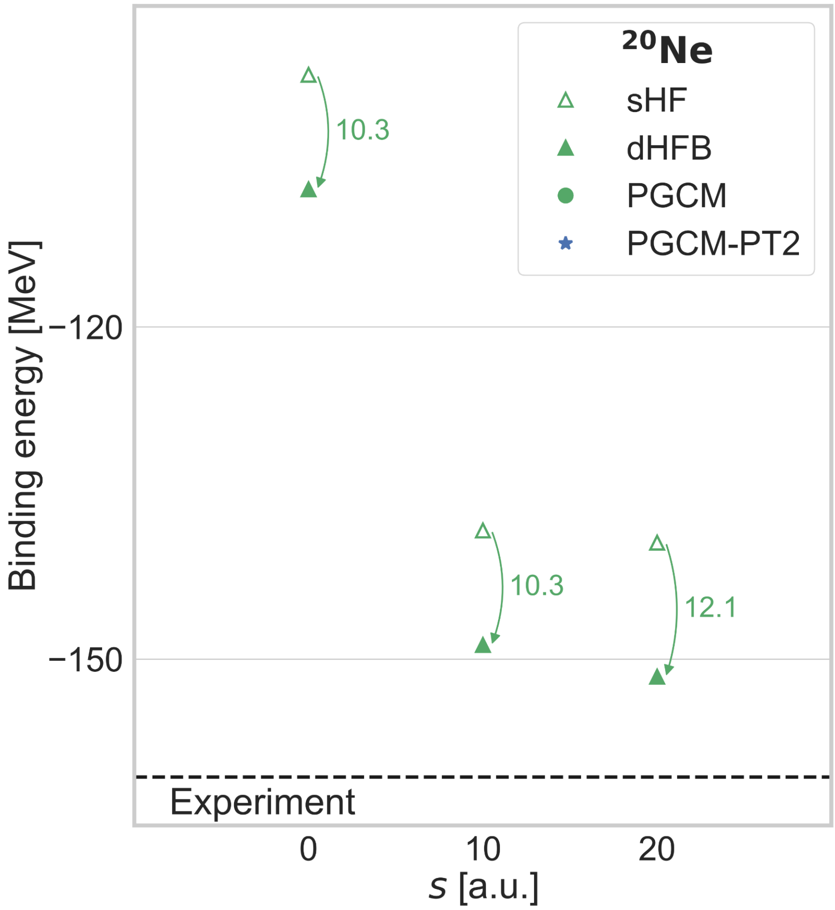
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

***Ab Initio* Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca**

J. M. Yao[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,∥] and H. Hergert[1,4,¶]



Reshuffling of correlations



MR-IMSRG preprocessing
→ Lowers sHF starting point

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^{\dagger}(s) H U(s)\,, \quad s \to \infty$$

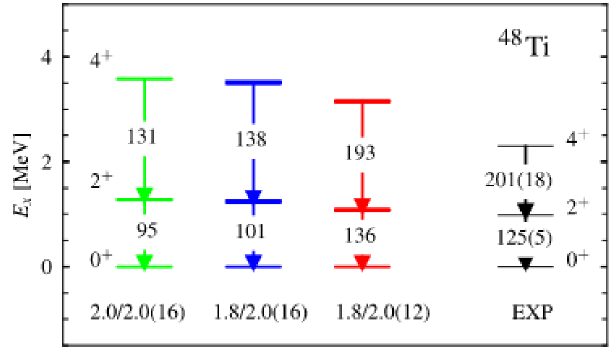
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]

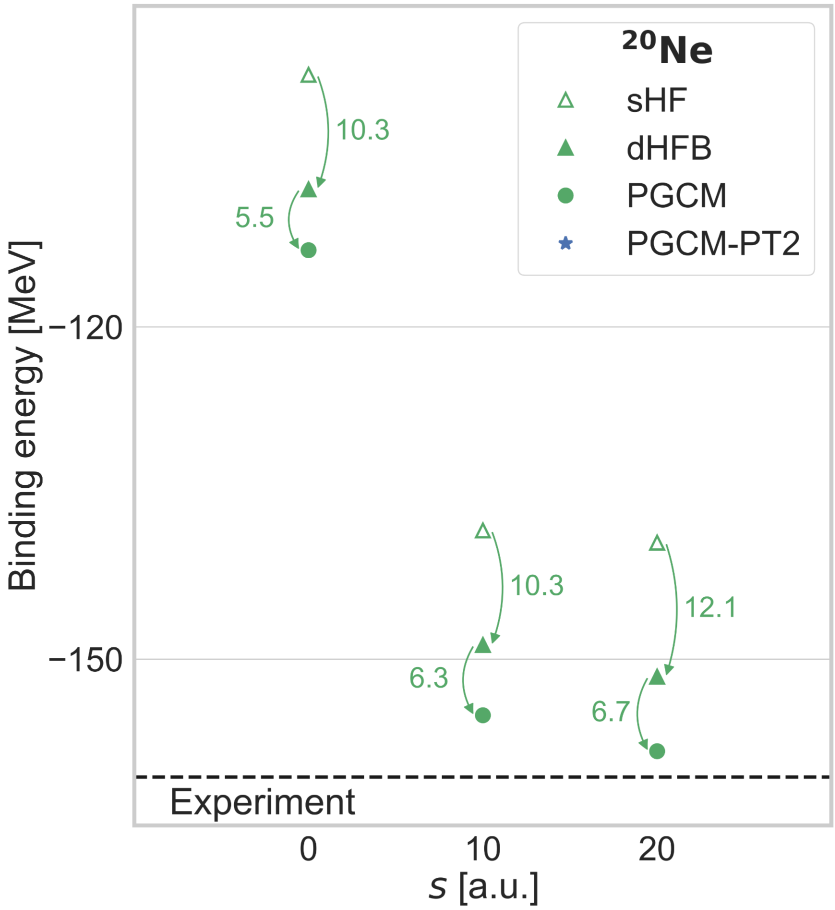
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

***Ab Initio* Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca**

J. M. Yao[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,||] and H. Hergert[1,4,¶]



Reshuffling of correlations



MR-IMSRG preprocessing
→ Lowers sHF starting point

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

$$H(s) = U^{\dagger}(s) H U(s)\,,\quad s \to \infty$$

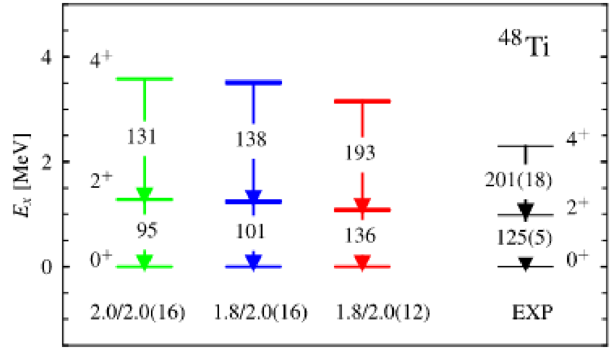
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]

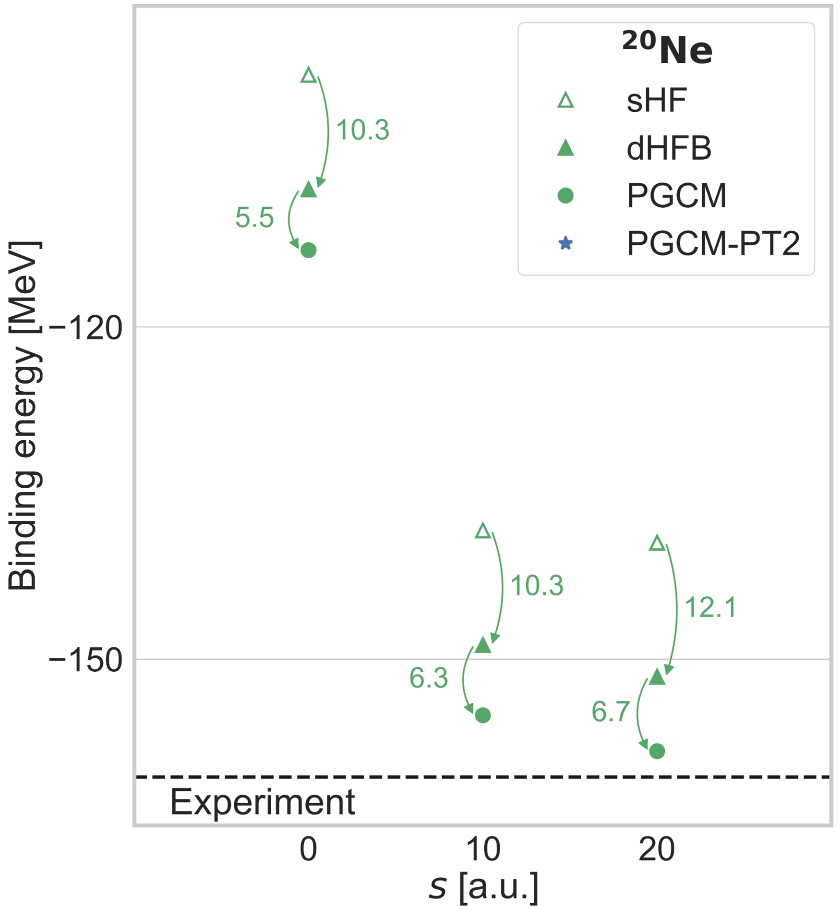
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

Ab Initio **Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca**

J. M. Yao[1,*] B. Bally,[2,†] J. Engel,[2,‡] R. Wirth,[1,§] T. R. Rodríguez,[3,∥] and H. Hergert[1,4,¶]



Reshuffling of correlations



MR-IMSRG preprocessing
→ Lowers sHF starting point

→ **Enhances** static correlations
- Symmetry breaking
- Symmetry restoration

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

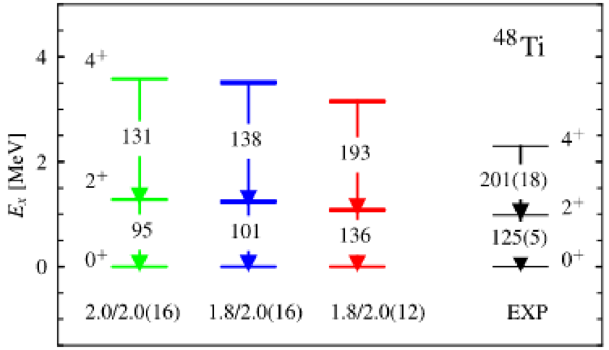
$$H(s) = U^\dagger(s) H U(s)\,, \quad s \to \infty$$

Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

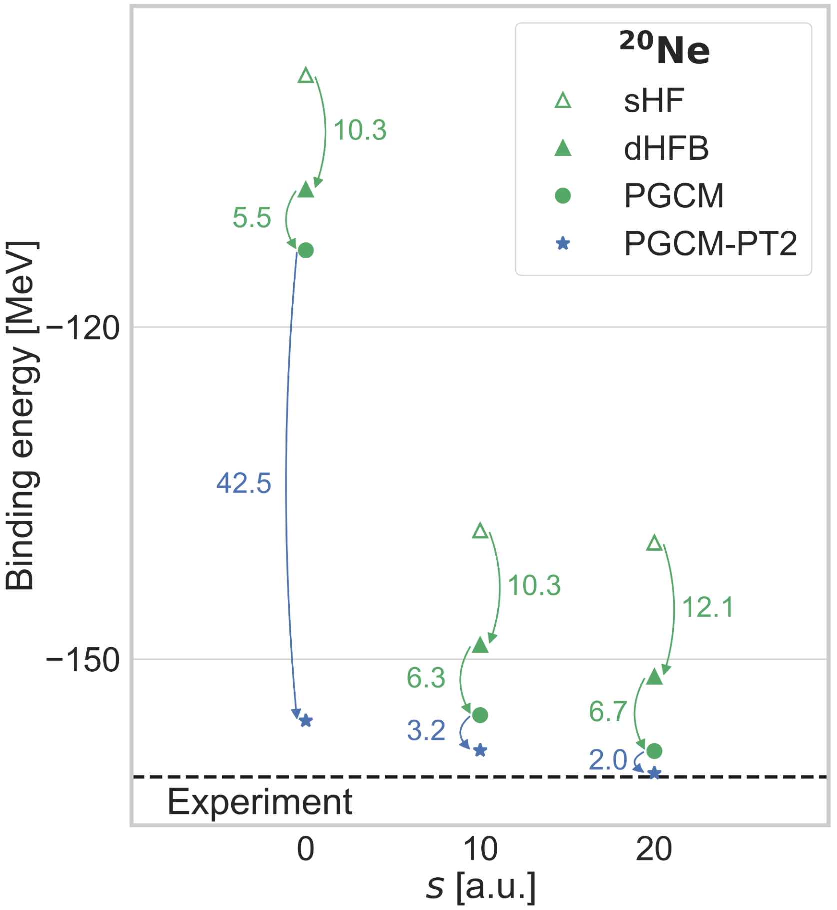
PGCM + MR-IMSRG [Yao20]
- Already existing
- Encouraging results
- **Improved by PGCM-PT?**

Ab Initio Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca

J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodríguez, and H. Hergert



Reshuffling of correlations



MR-IMSRG preprocessing
→ Lowers sHF starting point

→ **Enhances** static correlations
- Symmetry breaking
- Symmetry restoration

→ **Tames down** dynamical corr.
- But still needed (1.25 %)

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

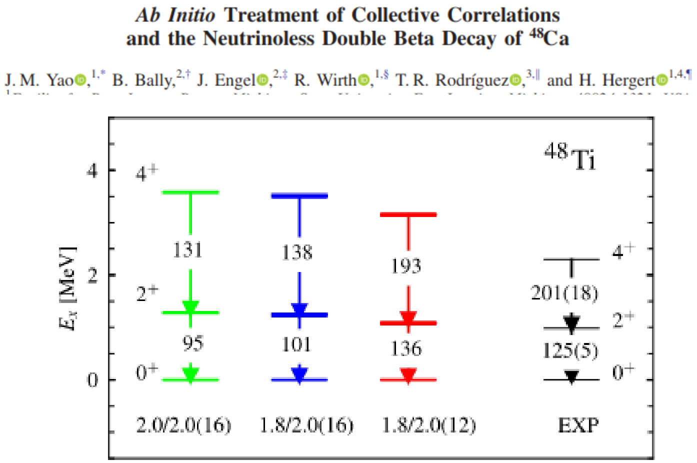
Nucleus-dependent preprocessing of H

$$H(s) = U^\dagger(s) H U(s), \quad s \to \infty$$

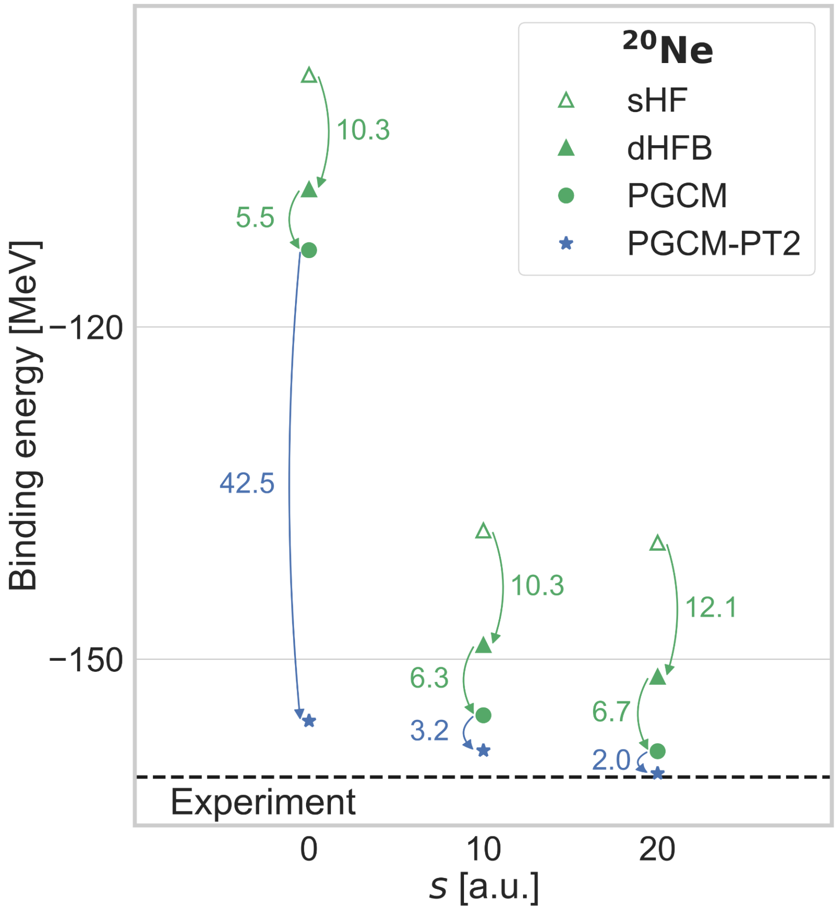
Decouples $|\Theta^{(0)}\rangle$ from $\mathcal{Q}$ space
-- Approaches ground state of $H(s \to \infty)$
Recasting dynamical corr. into H(s)

PGCM + MR-IMSRG [Yao20]

- Already existing
- Encouraging results
- **Improved by PGCM-PT?**



Reshuffling of correlations



MR-IMSRG preprocessing
→ Lowers sHF starting point

→ **Enhances** static correlations
- Symmetry breaking
- Symmetry restoration

→ **Tames down** dynamical corr.
- But still needed (1.25 %)

MR-IMSRG
→ **More perturbative** problem
→ Grasps **high-lying correlations**
→ **Smaller model space for PT**?
Necessary **posterior correction**
- **Optimal combination?**

Combining PGCM-PT(2) with MR-IMSRG preprocessed Hamiltonians

MR-IMSRG [Hergert16]

Nucleus-dependent preprocessing of H

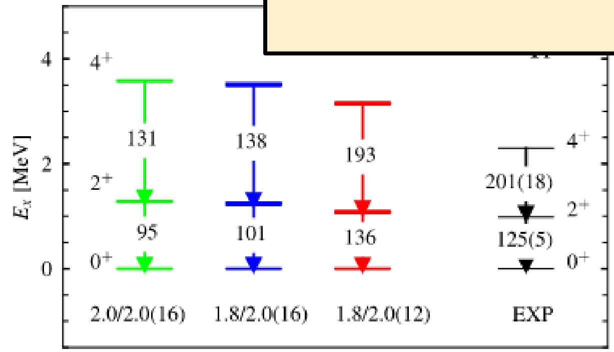
$H(s) = U^{\dagger}$

Decouples $|\Theta^{(0}$
-- Approaches g
Recasting dyna

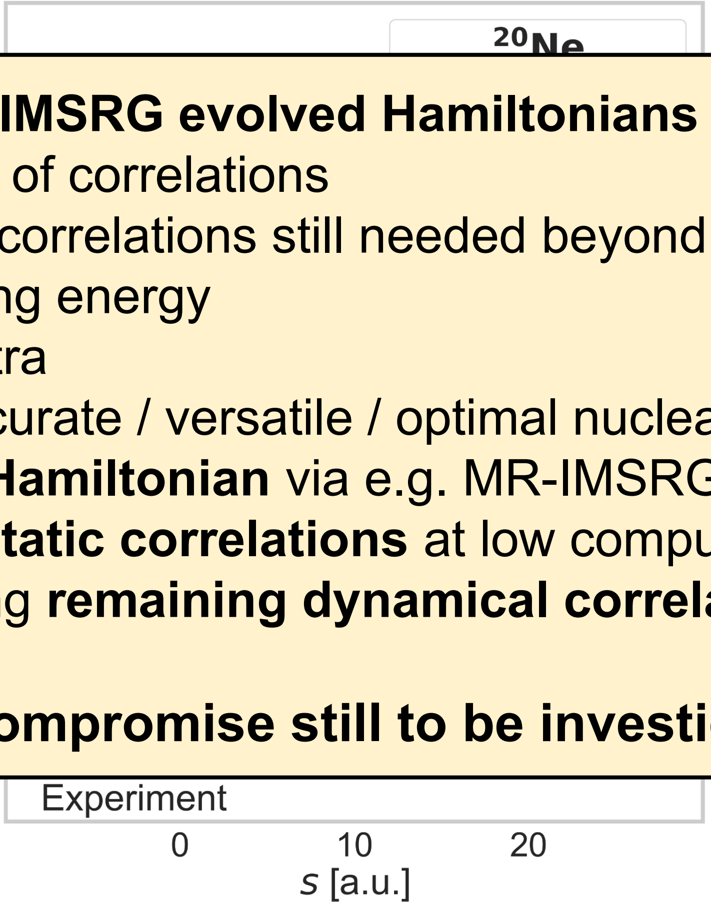
PGCM + MR-IM
- Already ex
- Encouragi
- **Improved**

Ab Initio Treatmen
and the Neutrinoless

J. M. Yao,[1,*] B. Bally,[2,†] J. Engel,[2,‡] R.



Reshuffling of correlations



MR-IMSRG preprocessing

ons

corr.
%)

em
ations
r PT?
tion
- Optimal combination?

- PGCM-PT(2) with **MR-IMSRG evolved Hamiltonians**
  - Reshuffling of correlations
  - Dynamical correlations still needed beyond PGCM
    - Binding energy
    - Spectra
- Three levers for an accurate / versatile / optimal nuclear structure description
  a. **Preprocessing of Hamiltonian** via e.g. MR-IMSRG
  b. PGCM to **capture static correlations** at low computational cost
  c. PGCM-PT(2) to bring **remaining dynamical correlations**

Optimal compromise still to be investigated