High-order resummation of Bogoliubov many-body perturbation theory

Pepijn DEMOL

Supervisors: Thomas DUGUET
Riccardo RAABE

Co-supervisor: Alexander TICHAI

ESNT workshop

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Rapid Communications | Editors' Suggestion

Improved many-body expansions from eigenvector continuation

P. Demol,[1] T. Duguet,[1,2] A. Ekström,[3] M. Frosini,[2] K. Hebeler,[4,5] S. König,[4,5,6] D. Lee,[7] A. Schwenk,[4,5,8] V. Somà,[2] and A. Tichai[9,8,4,5,*]

[1] *KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium*
[2] *IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*
[3] *Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden*
[4] *Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany*
[5] *ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*
[6] *Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA*
[7] *Facility for Rare Isotope Beams, Michigan State University, Michigan 48824, USA*
[8] *Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*
[9] *ESNT, IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*

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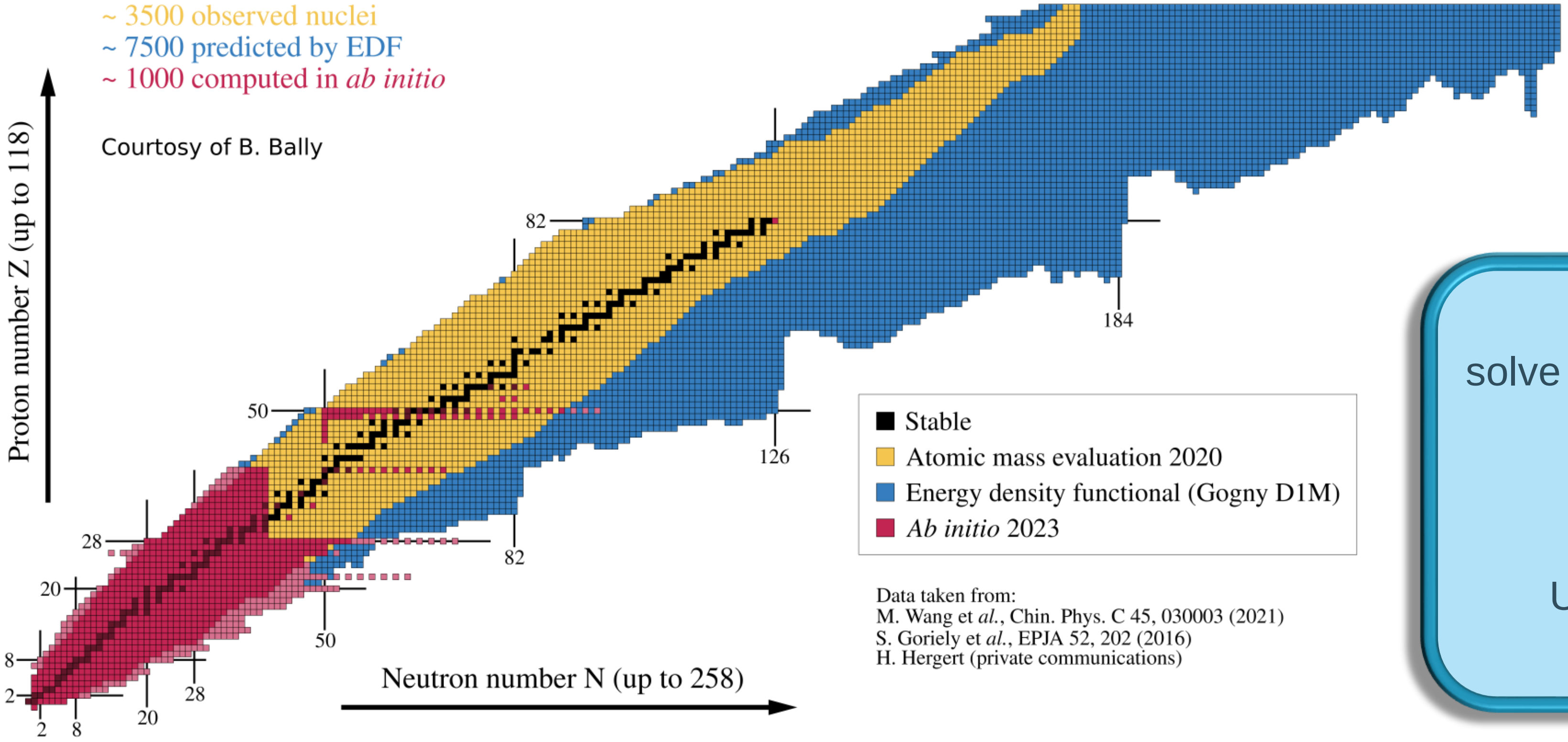
Ab initio approach to nuclear structure



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

$$H|\Psi_n^A\rangle = E_n^A|\Psi_n^A\rangle$$

Using controlled approximations
➔ systematically improvable

- Pushing *ab initio* requires computationally affordable many-body methods

➔ What about perturbation theory (PT)?

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Outline

- Perturbation theory and its potential pitfalls
- Closed-shell many-body perturbation theory (MBPT)
- Open-shell Bogoliubov many-body perturbation theory (BMBPT)
    - Bogoliubov states and Hartree-Fock-Bogoliubov (HFB)
    - Low-order results
    - High-order behaviour
- Resuming PT with eigenvector continuation (EC)

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“ The nuclear many-body problem is intrinsically non-perturbative. ”

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~~“ The nuclear many-body problem is intrinsically non-perturbative. ”~~

No meaning in absolute ➔ Perturbative with respect to what **starting point** ?

Partitioning: $H = H_0 + H_1$

Perturbation (H_1)

Unperturbed problem (H_0)

↳ solvable, i.e., $H_0|\Phi_n^{(0)}\rangle = E_n^{(0)}|\Phi_n^{(0)}\rangle$

“ Can one find an approriate H_0 such that the eigenstate of H can be obtained from a perturbative expansion in powers of H_1 ? ”

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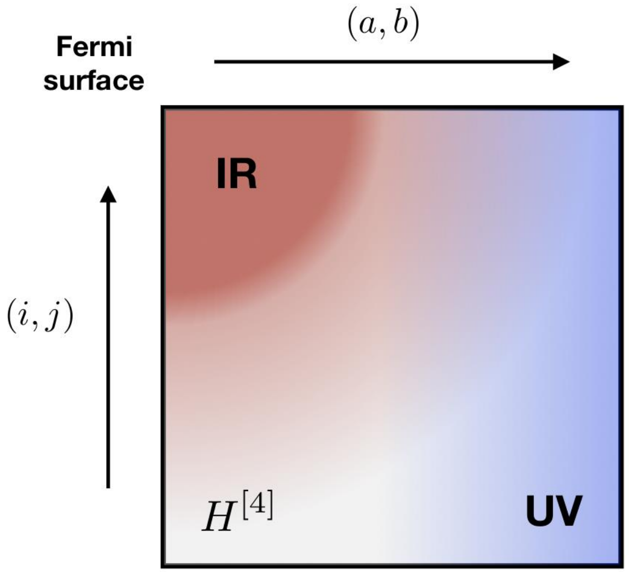
Two potential sources of non-perturbativeness



[1]

Infra-red (IR)

- Low energy ↔ long range
- Around Fermi surface
- Interaction: large scattering lengths

Ultra-violet (UV)

- High energy ↔ short range
- Low-to-high momentum coupling
- Interaction: hard core

[1] A. Tichai et al., Front. Phys. 8:164 (2020)
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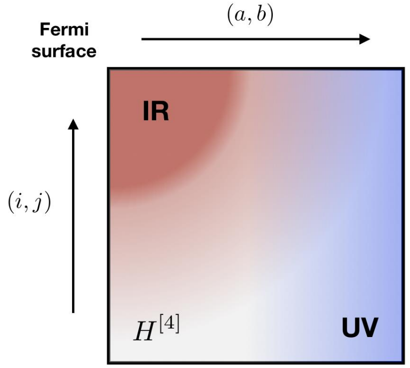

[1]

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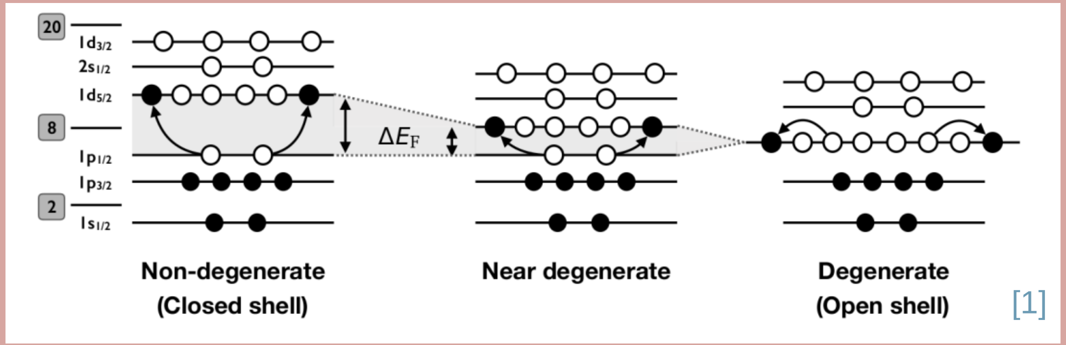
→ (Near) degenerate reference state



[1]

Alter H_0 to account for static corralations

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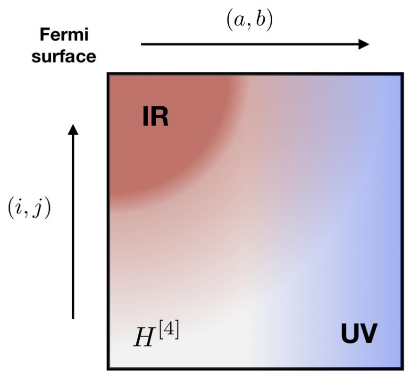

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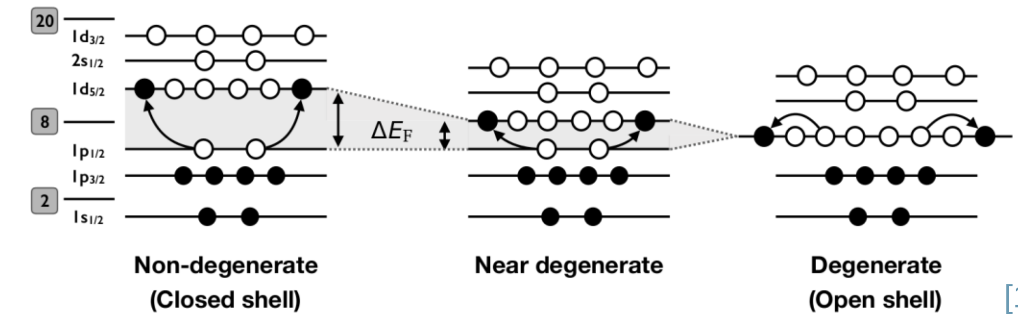

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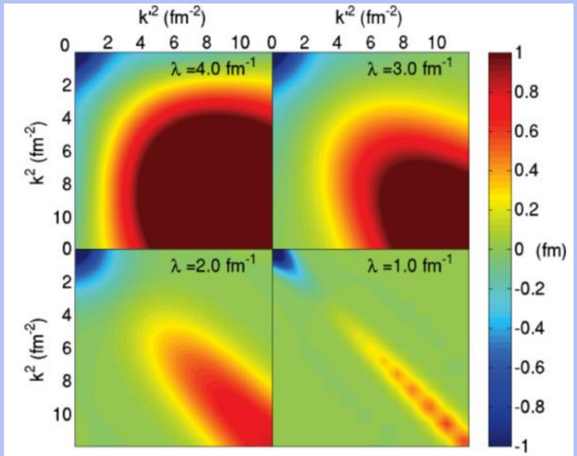

[2]

Tamed by preprocessing H ➔ SRG transformation

[1] A. Tichai et al., Front. Phys. 8:164 (2020)
[2] S. K. Bogner et al., Phys. Rev. C **75** (2007)

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Formal perturbation theory

- **Partitioning**

$$H = H_0 + H_1$$

↳ solvable, i.e., $H_0|\Phi_n^{(0)}\rangle = E_n^{(0)}|\Phi_n^{(0)}\rangle$

↳ Lowest: reference state $|\Phi\rangle$

- Perturbative expansion is a **powers series** in H_1

$$|\Psi\rangle = |\Phi\rangle + \sum_{k=1}^{\infty} \left(RH_1\right)^k |\Phi\rangle_\mathrm{C}$$

$$E = \langle\Phi|H|\Psi\rangle = \langle\Phi|H|\Phi\rangle + \sum_{k=1}^{\infty} \langle\Phi|H_1\left(RH_1\right)^k|\Phi\rangle_\mathrm{C}$$

where R is the **resolvent.** In Rayleigh-Schrödinger PT

$$R \equiv \sum_{n\neq 0} \frac{|\Phi_n^{(0)}\rangle\langle\Phi_n^{(0)}|}{E^{(0)} - E_n^{(0)}}$$

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MBPT formalism

- **Slater determinant** reference state

$$|\Phi\rangle \equiv \prod_i^A c_i^\dagger |0\rangle$$

- **Partitioning** of H in normal-order wrt. $|\Phi\rangle$

$$H_0 \equiv H^{0B} + \sum_p e_p : c_p^\dagger c_p :$$
$$H_1 \equiv H^{1B} - \sum_p e_p : c_p^\dagger c_p : + H^{2B}$$

- np-nh excitations of $|\Phi\rangle$ form **eigenbasis** of H_0

$$H_0 |\Phi_{ij\cdots}^{ab\cdots}\rangle = H^{0B} + (e_a + e_b + \cdots - e_i - e_j - \cdots)|\Phi_{ij\cdots}^{ab\cdots}\rangle$$

- E.g. MBPT **energy** correction at **second order**

$$E^{(2)} = -\sum_{ai} \frac{H_{ai} H_{ia}}{e_a - e_i} - \frac{1}{4} \sum_{abij} \frac{H_{abij} H_{ijab}}{e_a + e_b - e_i - e_j}$$

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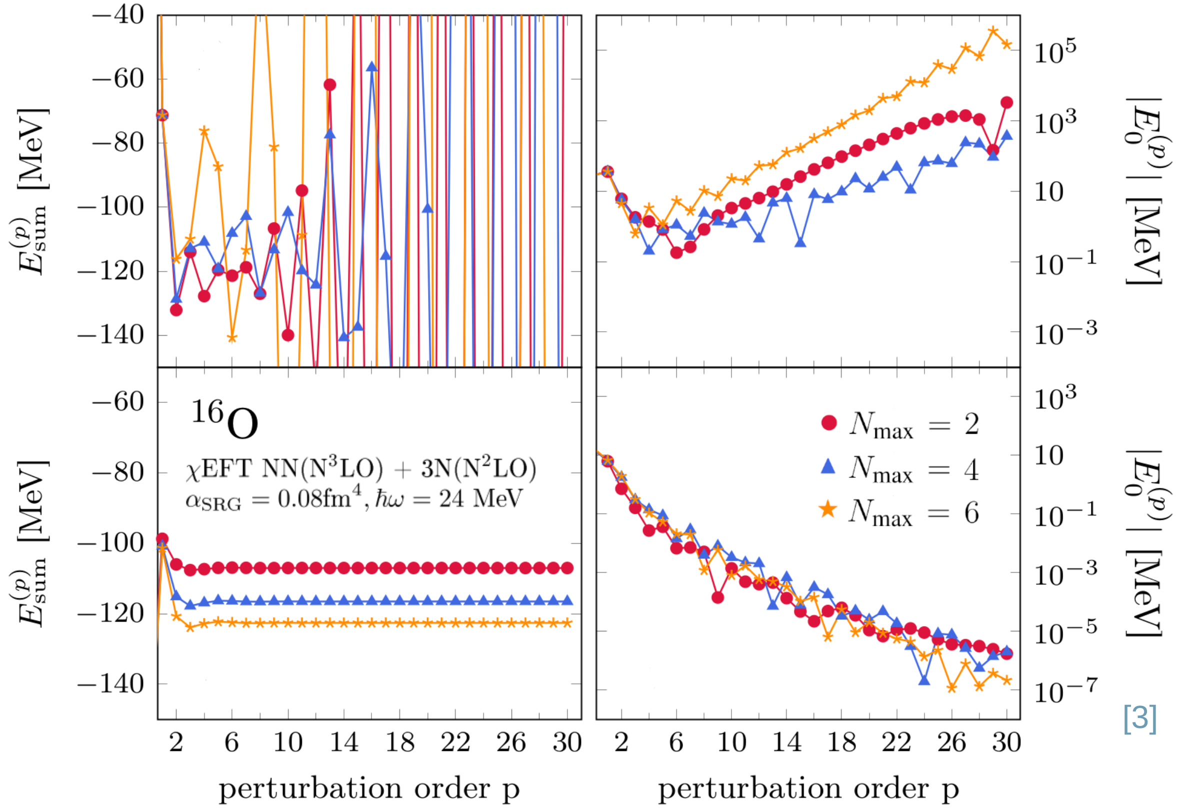
Convergence of MBPT: IR

- High-order obtained by iterative scheme restricted to small model space ➔ exact diagonalization (NCSM) feasible



→ H_0 = spherical harmonic oscillator

→ H_0 = Hartree-Fock

Adapting H_0 enabled to overcome IR divergence

[3] A. Tichai et al., Phys. Lett. B **765** (2016)

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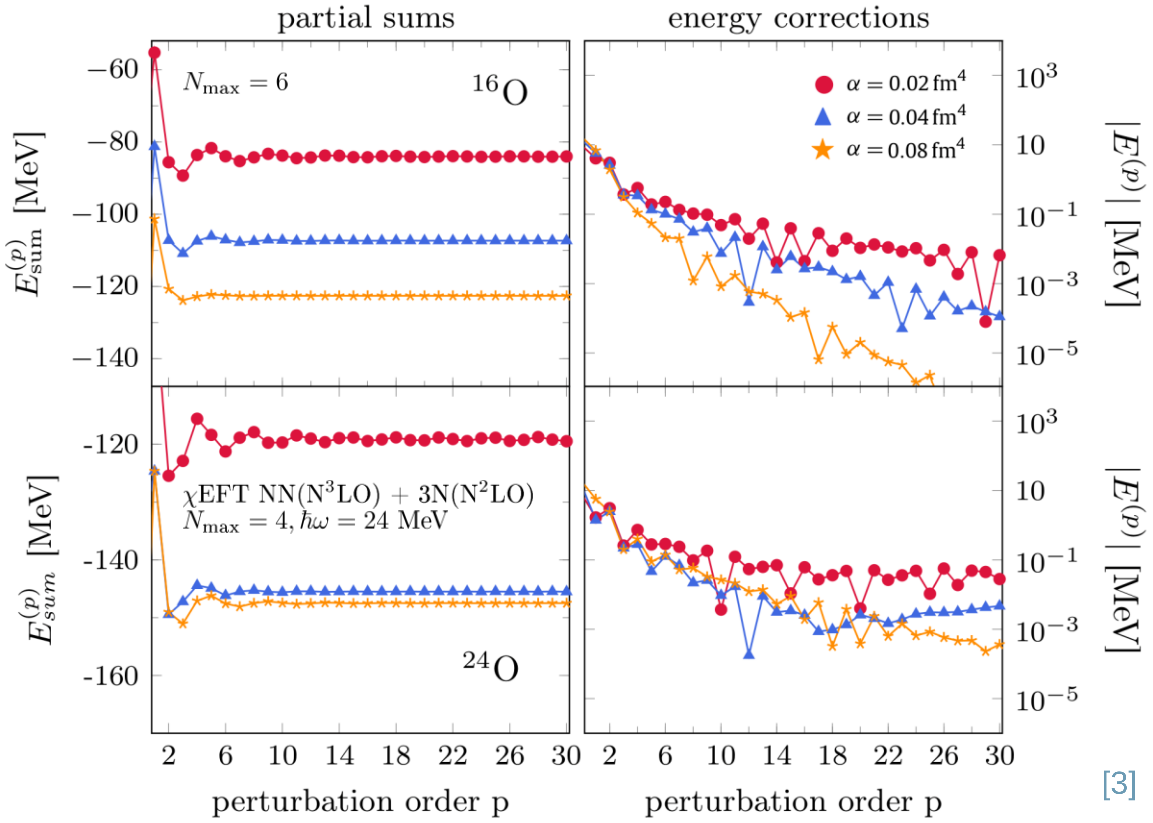
Convergence of MBPT: UV



[3]

- H_0 = Hartree-Fock

➔ Faster convergence for softer interactions

➔ Oscillatory behaviour for hard interactions

Optimized H_0 combined with sufficient SRG softening ➔ well-controlled PT for closed-shell nuclei

[3] A. Tichai et al., Phys. Lett. B **765** (2016)

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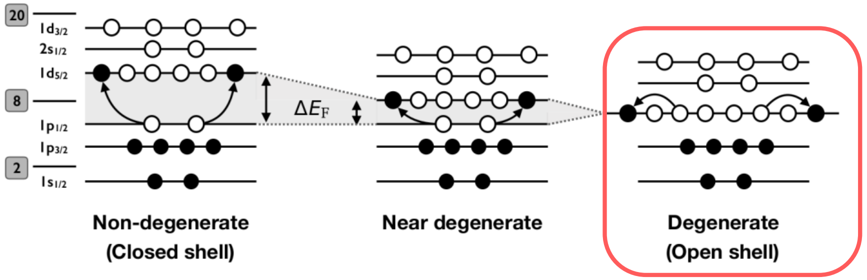
Extending MBPT for open-shell

- MBPT at second order

$$E^{(2)} = -\sum_{ai} \frac{H_{ai}H_{ia}}{e_a - e_i} - \frac{1}{4}\sum_{abij} \frac{H_{abij}H_{ijab}}{e_a + e_b - e_i - e_j}$$



[1]

$\rightarrow \; e_a \stackrel{!}{=} e_i$

- More general class of H_0 to lift degeneracy
  1. Multi-reference
     - Multi-configurational perturbation theory (MCPT) [4]
     - Projected generator coordinate method with PT (PGCM-PT) [5]
  2. Symmetry breaking
     - Singly-open shell: particle-number symmetry, U(1) ⟶ Bogoliubov vacuum state
     - Doubly-open shell: rotational symmetry, SU(2) ⟶ Deformed Slater determinant / Bogoliubov vacuum

[1] A. Tichai et al., Front. Phys. 8:164 (2020)
[4] Z. Rolik et al., J. Chem. Phys. 119 (2003)
[5] M. Frosini et al., Eur. Phys. J A 58 (2022)

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Bogoliubov vacuum state

- Quasi-particle operators defined via unitary **Bogoliubov transformation**

$$\beta_k = \sum_p U^*_{pk} c_p + V^*_{pk} c^\dagger_p$$

- **Bogoliubov vacuum**

$$|\Phi\rangle \equiv \mathcal{C} \prod_k \beta_k |0\rangle$$

- Breaks particle-number symmetry

$$\hat{A}|\Phi\rangle \neq A|\Phi\rangle$$

- **Grand potential operator** Ω normal ordered wrt. $|\Phi\rangle$

$$\Omega \equiv H - \lambda A = \Omega^{00} + \Omega^{20} + \Omega^{11} + \Omega^{02} + \Omega^{40} + \Omega^{31} + \cdots + \Omega^{60} + \cdots$$

where e.g.

$$\Omega^{31} \equiv \frac{1}{3!\ 1!} \sum_{k_1 k_2 k_3 k_4} \Omega^{31}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta_{k_4}$$

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Hartree-Fock-Bogoliubov

- **Hartree-Fock-Bogoliubov** extends HF and minimizes energy over manifold of Bogoliubov states
- Minimization under **constraint** of $\langle \Phi | A | \Phi \rangle = A_0$

$$\frac{\delta}{\delta|\Phi\rangle}\left(\frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} - \lambda\frac{\langle\Phi|(A-A_0)|\Phi\rangle}{\langle\Phi|\Phi\rangle}\right) = 0$$

- Boils down to self-consistent diagonalization of HFB Hamiltonian matrix

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

HF field

pairing field

Quasi-particle energies: $E_k \geq \Delta_F > 0$

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Bogoliubov many-body perturbation theory [6,7]

- **Partitioning**

$$\Omega_0 \equiv \Omega^{00} + \sum_k E_k \beta_k^\dagger \beta_k$$

$$\Omega_1 \equiv \Omega^{20} + (\Omega^{11} - \sum_k E_k \beta_k^\dagger \beta_k) + \Omega^{02} + \Omega^{40} + \Omega^{31} + \cdots$$

- 2n-quasiparticle excitations of $|\Phi\rangle$ form **eigenbasis** of Ω_0

$$\Omega_0 |\Phi^{k_1 k_2 \cdots}\rangle = \Omega^{00} + (E_{k_1} + E_{k_2} + \cdots)|\Phi^{k_1 k_2 \cdots}\rangle$$

- E.g. **BMBPT** at second order

$$E^{(2)} = -\frac{1}{2} \sum_{k_1 k_2} \frac{\Omega^{20}_{k_1 k_2} \Omega^{02}_{k_1 k_2}}{\boxed{E_{k_1} + E_{k_2}}} - \frac{1}{24} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{04}_{k_1 k_2 k_3 k_4}}{\boxed{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}} \longrightarrow > 0$$

- Perturbative expansion under **constraint** $\langle A \rangle = A_0$ at each order
  - Similar in spirit to MBPT-based orbital-dependent DFT [8]
  - Different strategies to implement this constraint, e.g. redefinition of $|\Phi\rangle$ and/or λ at each order in PT [9,10]
  - No correction at BMBPT(2) when using HFB reference state

[6] T.Duguet, A.Signoracci, J. Phys. G: Nucl. Part. Phys. **44** (2016)
[7] P. Arthuis et al., Comput. Phys. Commun. 240 (2019)
[8] R.J. Furnstahl, in: A. Schwenk, J. Polonyi (Eds), Springer Berlin Heidelberg (2012) pp. 133–191
[9] PD et al., Ann. Phys. (N Y) 424 (2021)
[10] PD, A.Tichai, T. Duguet (2023), to be submitted

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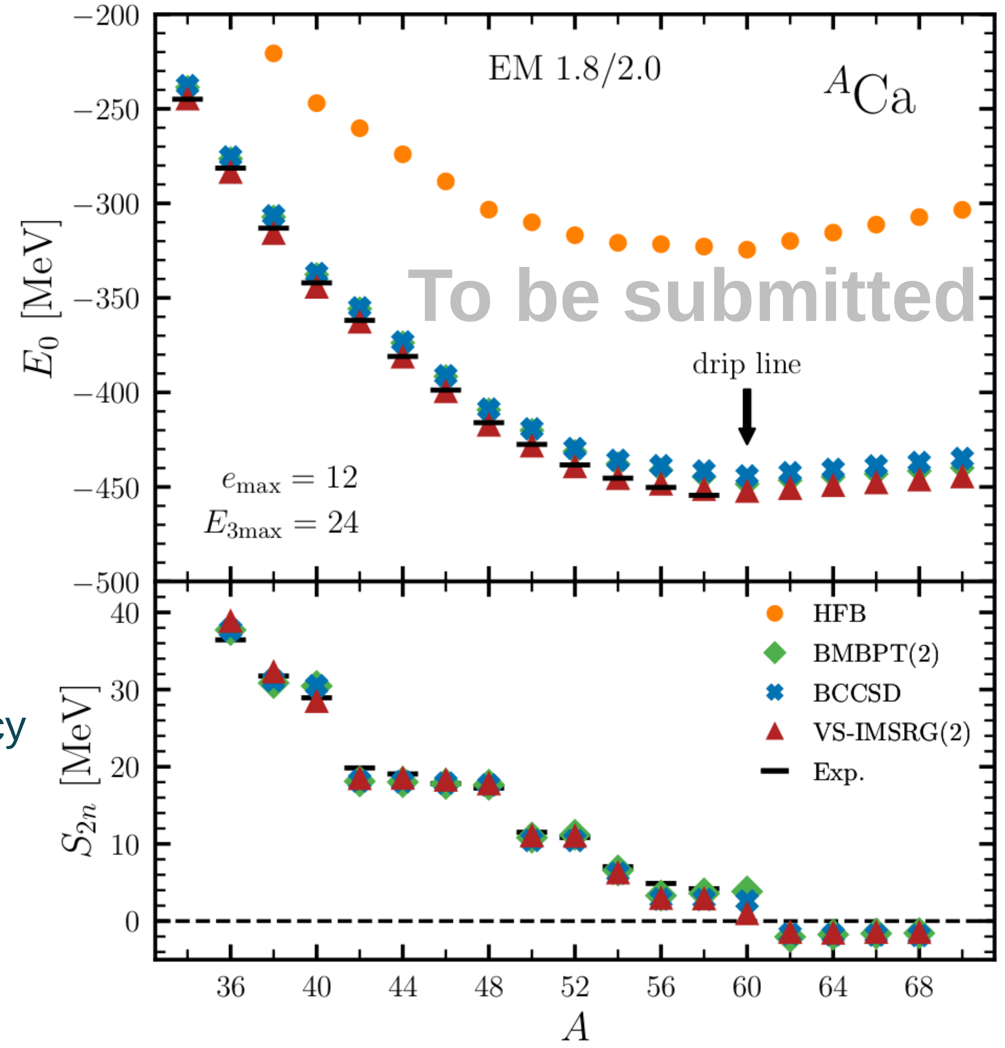
Low-order BMBPT results

- BMBPT(2) compared to non-perturbative many-body methods
  - VS-IMSRG(2)
  - **BCCSD**
- BMBPT(2) in very good agreement at fraction of the cost
- Low-order BMBPT great workhorse for sufficiently soft interactions
- BCC promising new method for harder interaction & higher accuracy



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[11] A. Tichai, PD, T. Duguet (2023) to be submitted

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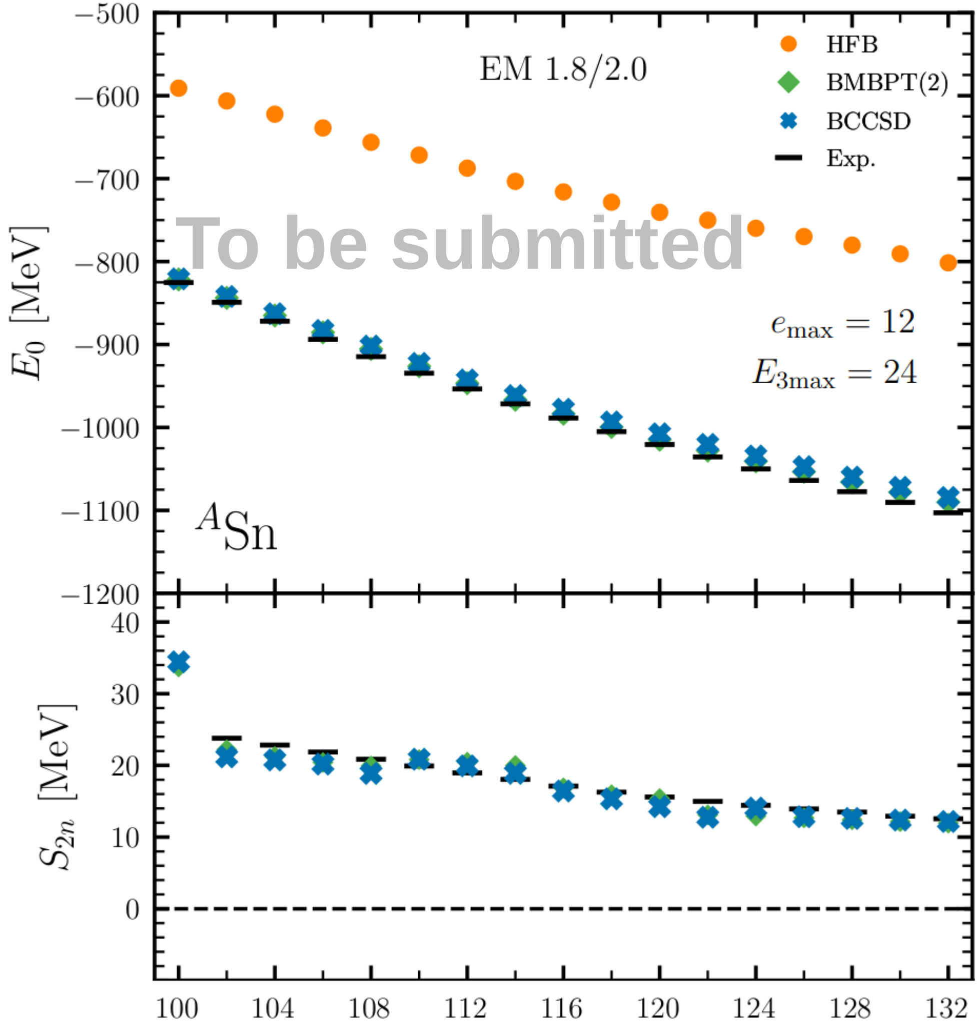

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High-order BMBPT

- Investigate high-order behaviour in small model space
  → allowing exact diagonalization (BCI)

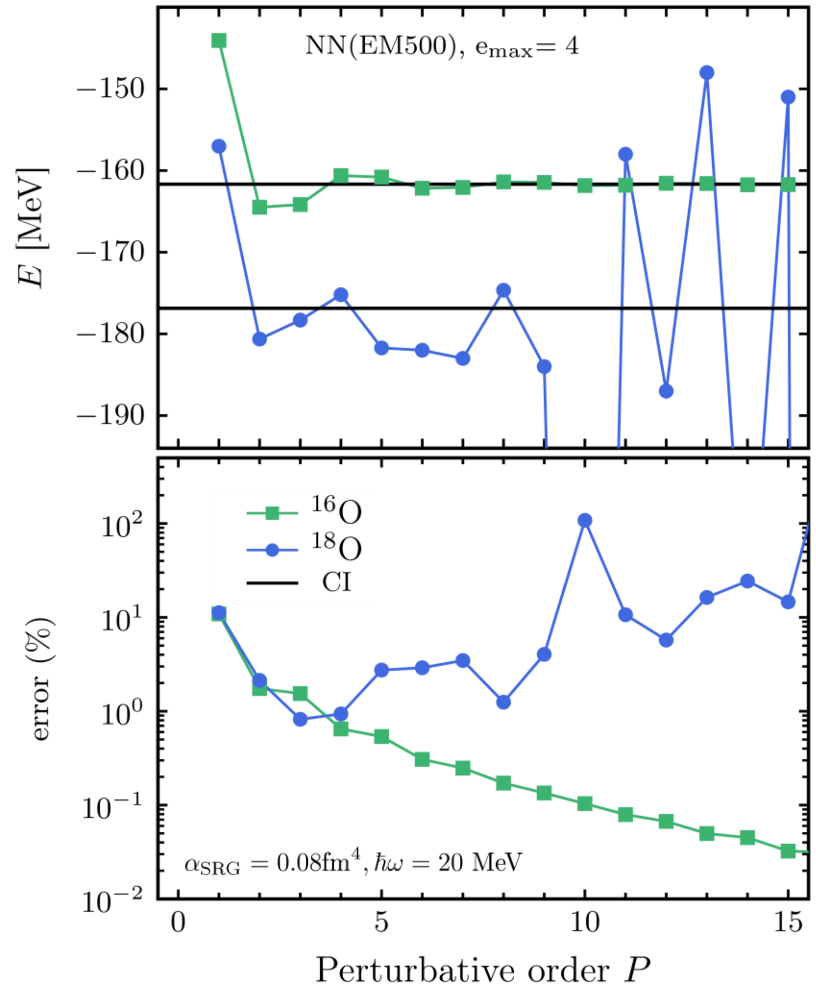
- Use all tricks of closed-shell MBPT
  - SRG-softening to tackle UV
  - HFB partitioning to treat IR

- Particle number constrained at each order

- Closed shell (BMBPT → MBPT) convergent behaviour

- Open shell, Taylor series diverges

- First idea, Padé resummation



[9]

[9] PD et al., Ann. Phys. (N Y) 424 (2021)

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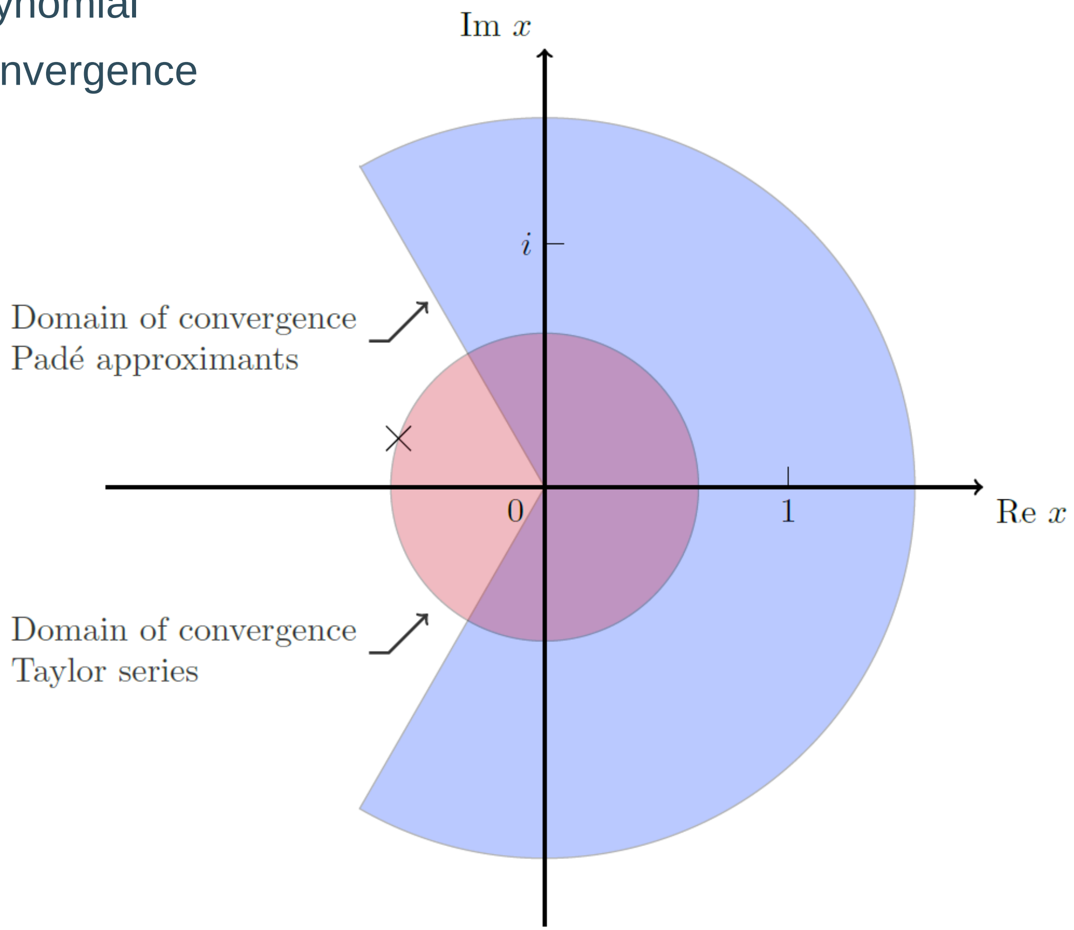
Padé resummation

- Based on rational function approximation instead of simple polynomial
- Can incorporate poles in complex plane → larger domain of convergence

Taylor: $$f(x) = \sum_{i=0}^{P} c_i x^i + O(x^{P+1})$$

Padé: $$f(x) = \frac{\sum_{i=1}^{M} p_i x^i}{1 + \sum_{i=1}^{N} q_i x^i} + O(x^{M+N})$$



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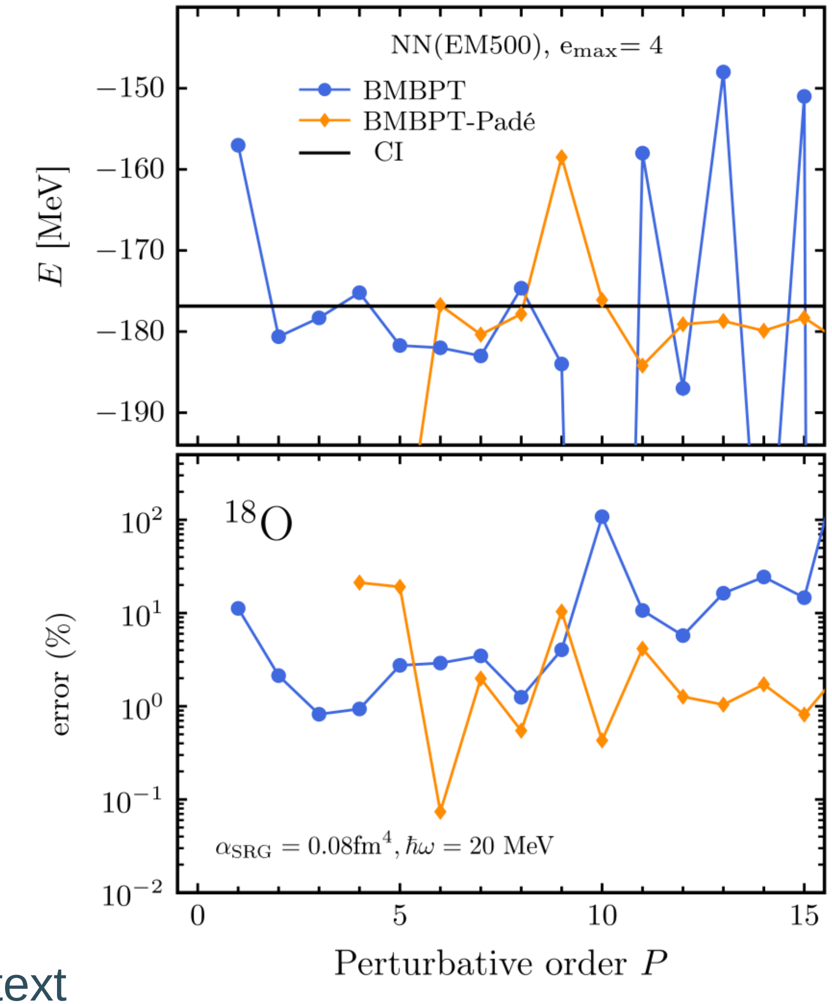
Padé resummation

- Padé approximants show erratic behavior
  - Due to particle number constraint
  - Eventually do approach the exact limit when $P \sim 30$
  - Rely on some a priori analytic knowledge of underlying expansion



[9]

➔ Padé resummation not reliably applicable in this BMBPT context

[9] PD et al., Ann. Phys. (N Y) 424 (2021)

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Resumming PT with EC [12,13]

- Parameter-dependent partitioning

$$H(c) \equiv H_0 + c\,H_1$$

- There exists a regime $0 \leq c \leq c_e < 1$ where solving the many-body problem is easier than at $c = 1$
- The eigenvectors of $H(c)$ visit a low-dimensional subspace when varying c

1) Solve for N_{EC} auxiliary states (training points) $|\Psi(c_i)\rangle, i = 0, \ldots, N_{\mathrm{EC}}$ associated with $H(c_i), c_i \in [0, c_e]$

2) Construct and compute eigenstates of $N_{\mathrm{EC}} \times N_{\mathrm{EC}}$ matrix $\langle\Psi(c_j)|H(1)|\Psi(c_i)\rangle$

- State associated to $H(c_i)$ at order P in PT

$$|\Psi_P(c_i)\rangle \equiv \sum_{p=0}^{P} {c_i}^p |\Phi^{(p)}\rangle$$

[12] D. Frame et al., Phys. Rev. Lett. **121** (2018)
[13] PD et al., Phys. Rev. C **101** (2020)

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Resumming PT with EC

- State associated to $H(c_i)$ at order P in PT

$$|\Psi_P(c_i)\rangle \equiv \sum_{p=0}^{P} {c_i}^p |\Phi^{(p)}\rangle$$

- Linear transformation

$$\begin{pmatrix} |\Psi_P(c_1)\rangle \\ |\Psi_P(c_2)\rangle \\ \vdots \\ |\Psi_P(c_{N_{\mathrm{EC}}})\rangle \end{pmatrix} = \begin{pmatrix} 1 & c_1 & c_1^2 & \cdots & c_1^P \\ 1 & c_2 & c_2^2 & \cdots & c_2^P \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & c_{N_{\mathrm{EC}}} & c_{N_{\mathrm{EC}}}^2 & \cdots & c_{N_{\mathrm{EC}}}^P \end{pmatrix} \begin{pmatrix} |\Phi^{(0)}\rangle \\ |\Phi^{(1)}\rangle \\ |\Phi^{(2)}\rangle \\ \vdots \\ |\Phi^{(P)}\rangle \end{pmatrix}$$

$$\mathrm{span}\{|\Psi_P(c_i)\rangle; i = 1, \cdots, N_{\mathrm{EC}}\} = \mathrm{span}\{|\Phi^{(p)}\rangle; p = 0, \cdots, P\}$$

- Construct and compute eigenstates $(P+1) \times (P+1)$ matrix $\langle \Phi^{(p)} | H | \Phi^{(q)} \rangle$

↳ Access to excited states[14] → Talk by Margarida tomorrow

[14] M. Companys Franzke, Phys. Lett. B 830 (2022)

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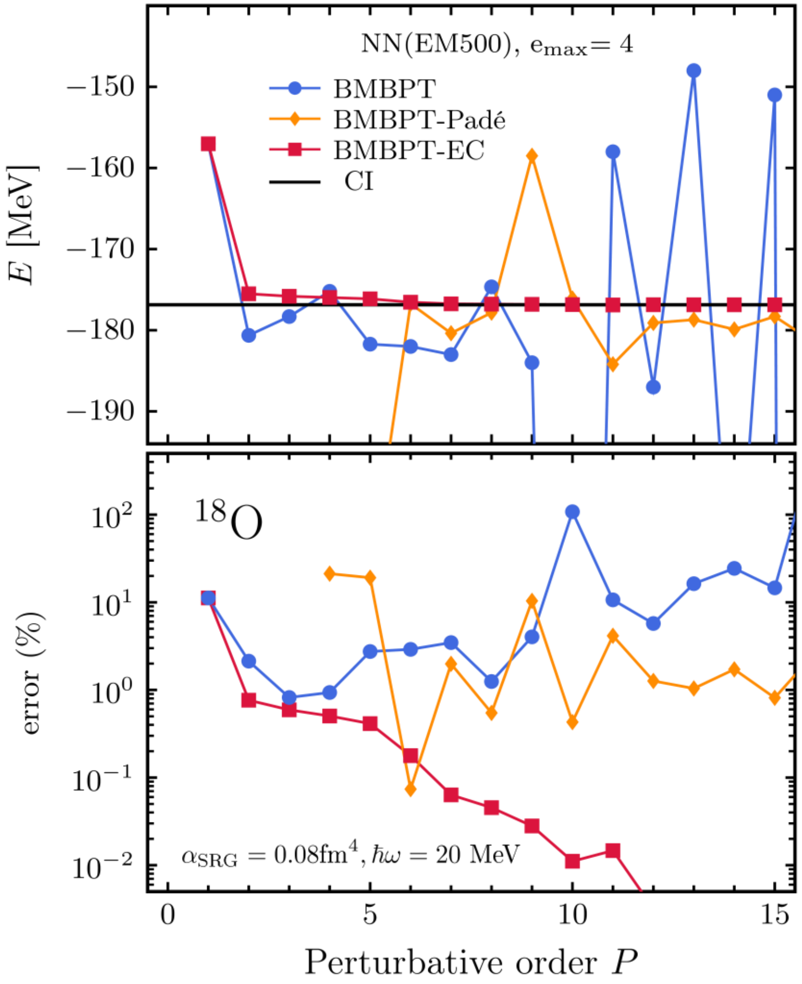
EC-resumed BMBPT

- EC yields rapidly convergent BMBPT expansion
- EC is variational ➔ monotonic convergence from above

➔ Does EC improve also closed-shell MBPT?



[9,13]

[9] PD et al., Ann. Phys. (N Y) 424 (2021)
[13] PD et al., Phys. Rev. C **101** (2020)

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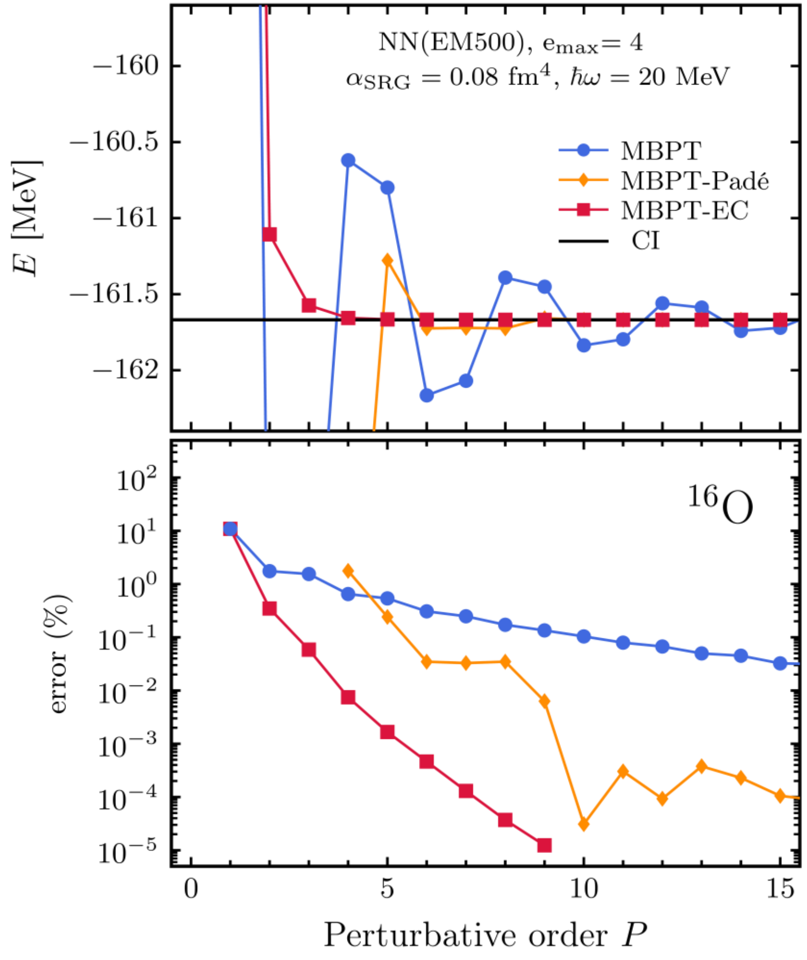
EC-resumed closed-shell MBPT

- Note: very different scale !
- EC accelerates convergence significantly, outperforming Padé

➔ Is EC capable resumming divergent closed-shell MBPT?



[9]

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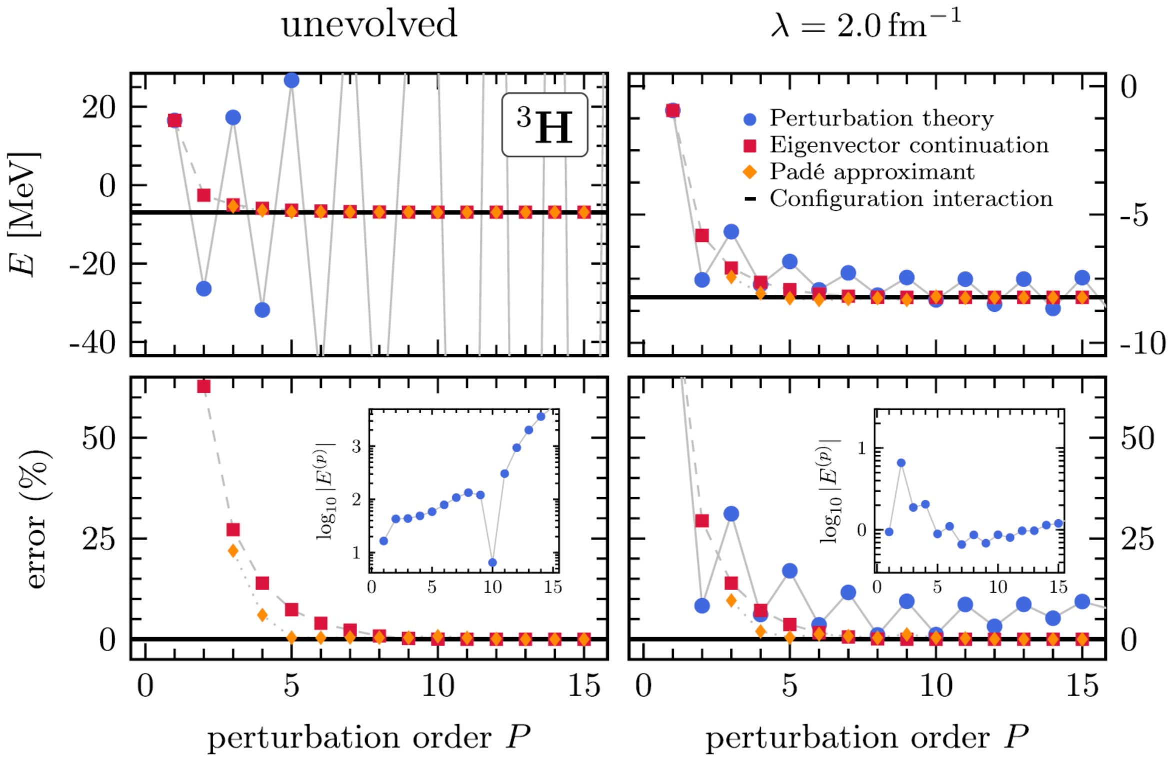
EC-resumed MBPT: ^{3}H



[9]

- HO partitioning
- No SRG softening (left panels)

➔ EC is able to overcome both IR and UV sources of divergence

➔ Padé performs as well as EC

[9] PD et al., Ann. Phys. (N Y) 424 (2021)

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Conclusion

- Perturbative expansions may face IR and UV sources of divergence
- Closed-shell MBPT
  - IR tackled by using the HF reference state
  - UV treated by SRG softening
  - EC overcomes both UV & IR and delivers rapid convergence
- Open-shell BMBPT
  - Low-orders give reliable results
  - High-orders diverge, even with SRG & HFB tricks
  - EC elegantly achieves convergence
- Outlook
  - EC for excited states → talk by Margarida
  - EC-BMBPT in realistic model spaces?
    - All tools available

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KU LEUVEN
Research Foundation Flanders
Opening new horizons

Collaborators

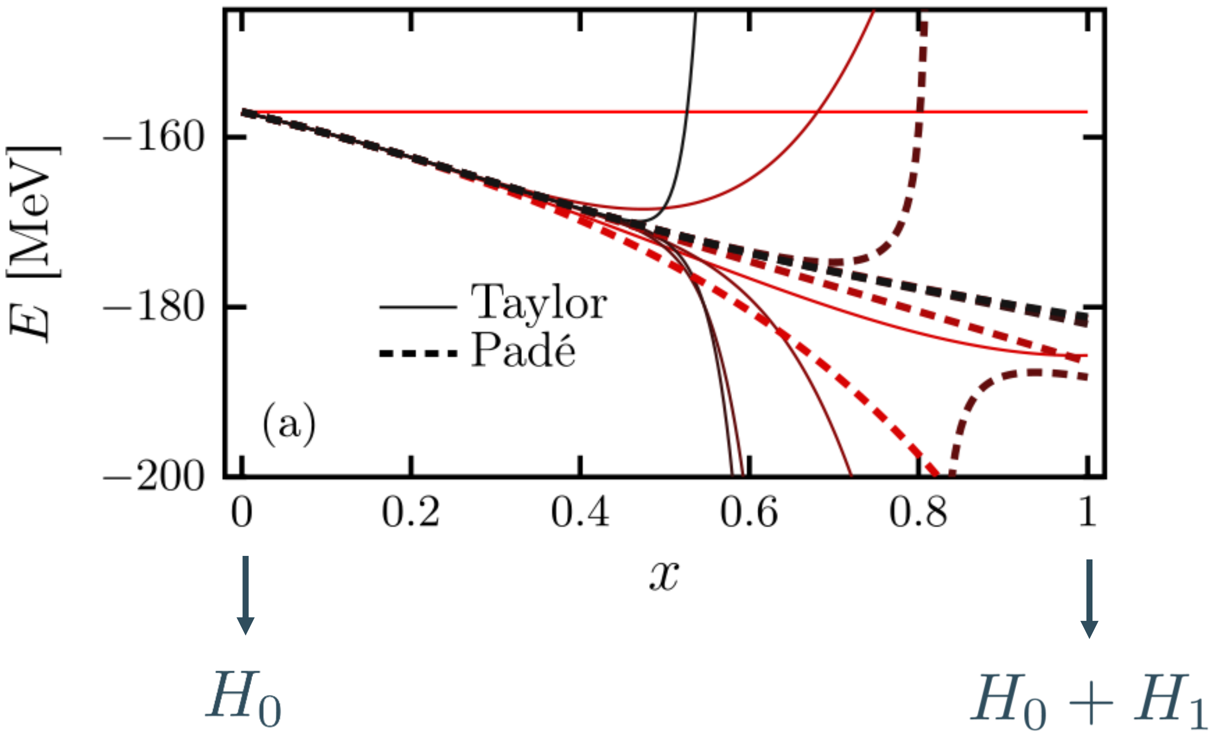
T. Duguet
R. Raabe

T. Duguet
J.-P. Ebran
M. Frosini
A. Porro
A. Roux
A. Scalesi
V. Somà

G. Hagen

R. Roth
A. Tichai

Padé approximants



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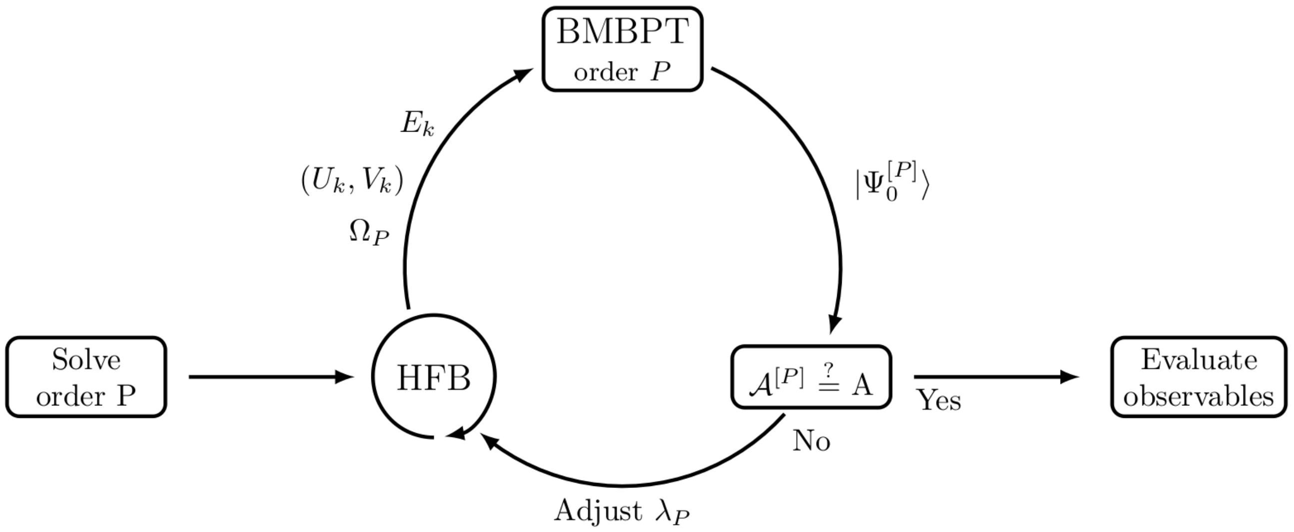
Particle number constraint

- Method used in this study: counteract particle-number shift by compansating with the reference state



- Other strategies are possible → PD, T. Duguet, A. Tichai (2023), to be submitted

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