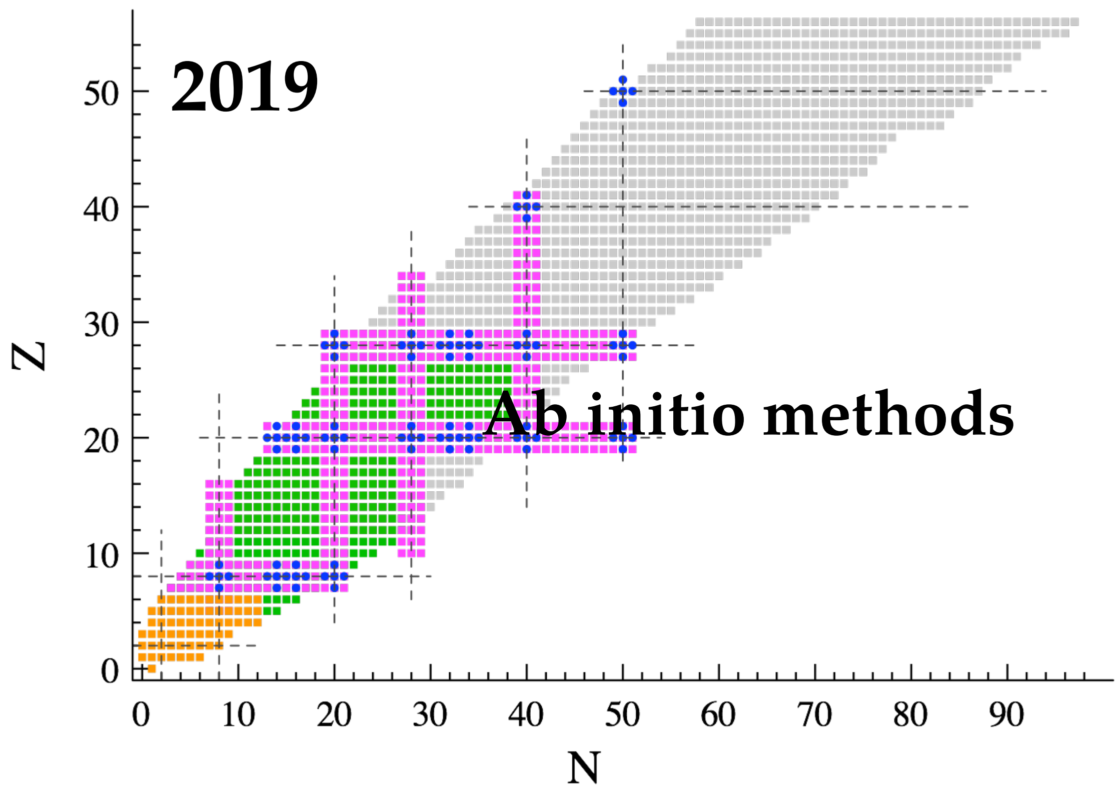
High-Order Many-Body Bogoliubov Perturbation Theory



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09/12/2019

P. Demol, M. Frosini, A. Tichai, J. Ripoche, V. Somà, T. Duguet 2019 in preparation

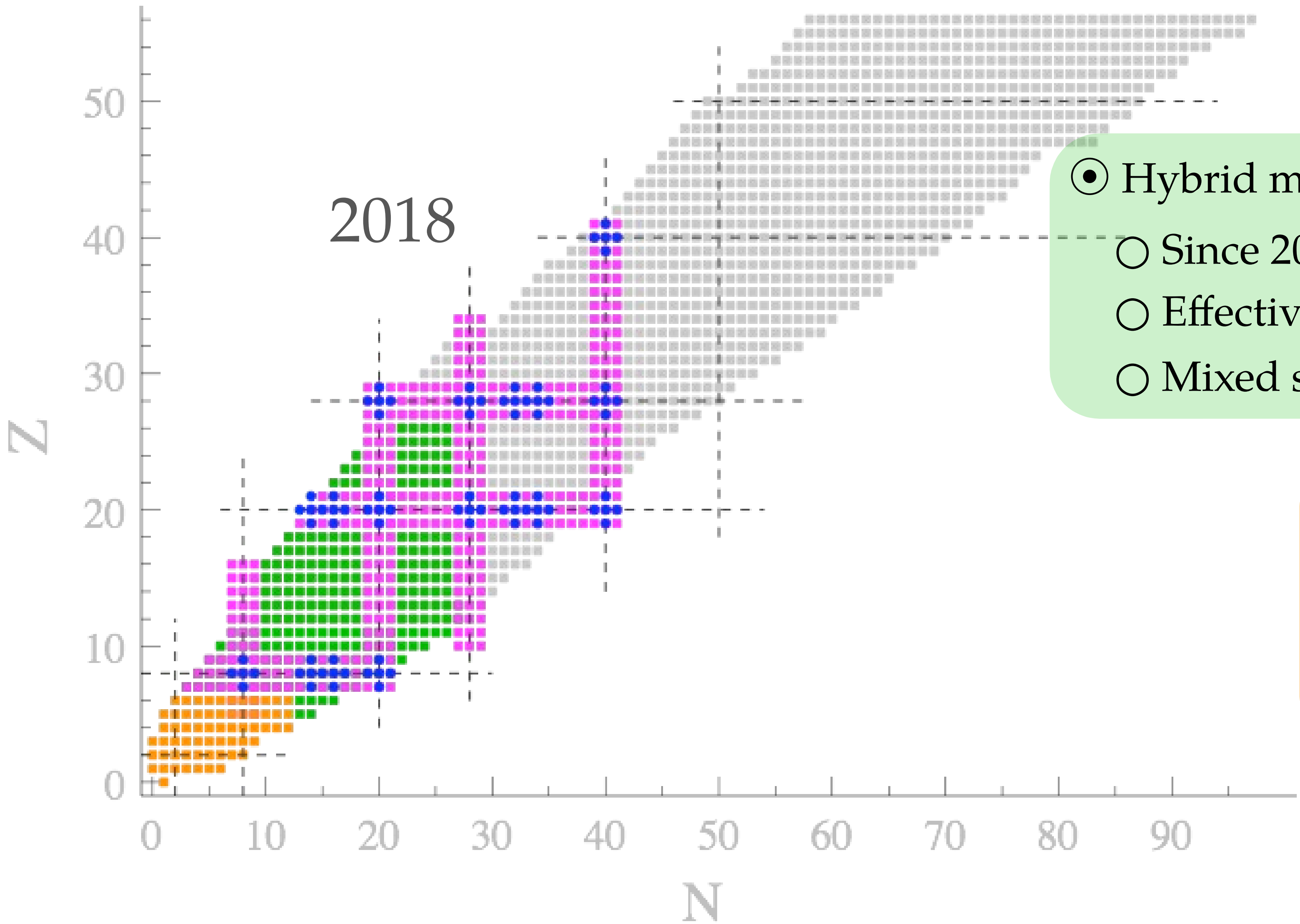
Contents

Contents

Ab initio nuclear chart

- Approximate methods for doubly closed-shells
  - Since 2000's
  - MBPT, SCGF, CC, IMSRG
  - Polynomial scaling

- Approximate methods for singly open-shell
  - Since 2010's
  - BMBPT, GGF, BCC, MR-IMSRG, MCPT
  - Polynomial scaling



- Hybrid methods (ab initio shell model)
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- “Exact” methods
  - Since 1980's
  - Monte Carlo, CI, FY…
  - Factorial scaling

Single-reference expansion many-body methods

Many-body problem

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

A-Body Hamiltonian
$H = T + V^{2N} + V^{3N} + \cdots + V^{AN}$

A-Body wave-function
5 variables, A nucleons

U(1) Symmetry

$$[H, A] = 0$$

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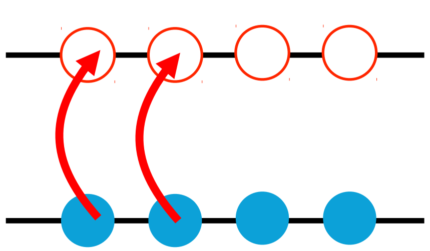
$$[H, A] = 0$$

Symmetry conserving expansion

$H = H_0 + H_1$ such that $[H_0, A] = 0$, $[H_1, A] = 0$

⇒ Full $|\Psi_n^A\rangle$ as perturbed eigenstate.

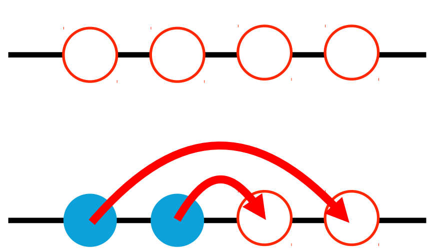
Closed-shell



Non-degenerate

Good starting point

Open-shell



Degenerate

Improper starting point

Single-reference expansion many-body methods

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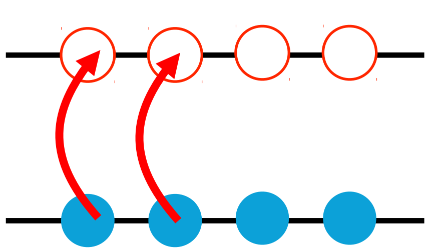

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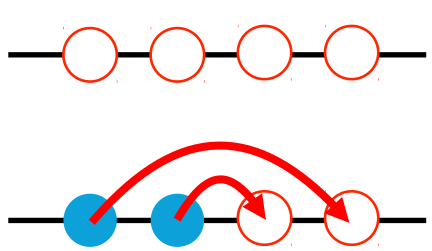


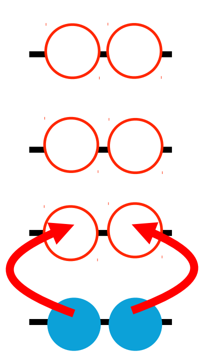
Degenerate

Improper starting point

Symmetry breaking expansion

$H = H'_0 + H'_1$ such that $[H'_0, A] \neq 0$, $[H'_1, A] \neq 0$

Open-shell



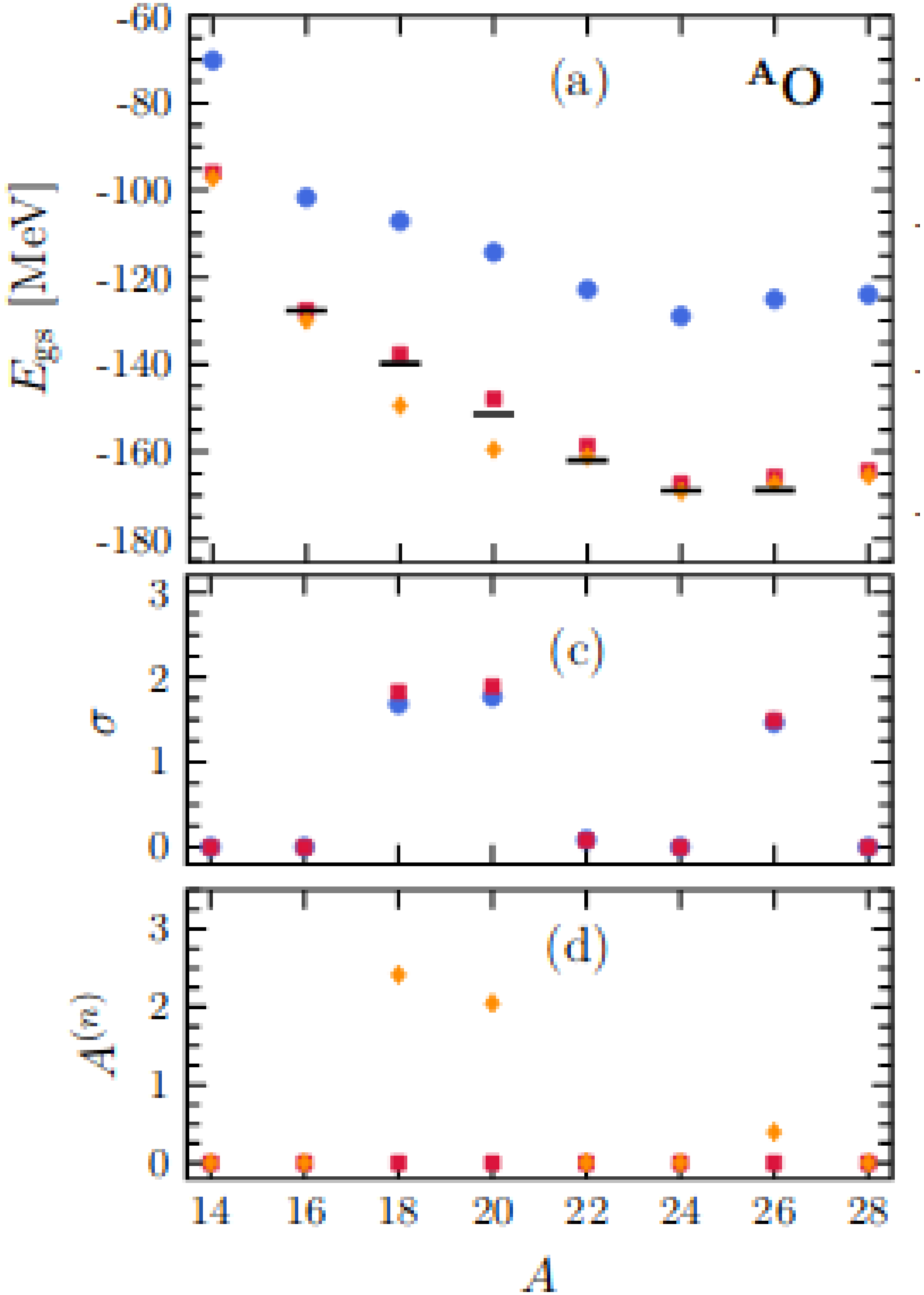
Non-degenerate

Proper starting point

- Static / dynamical correlations
- Polynomial cost at given order
- Truncated expansions break symmetry

A. Tichai, P. Arthuis *et al.* Phys.Lett. B786 (2018) 195-200 arXiv:1806.10931

Particle number corrections in BMBPT



HFB
2nd order
3rd order

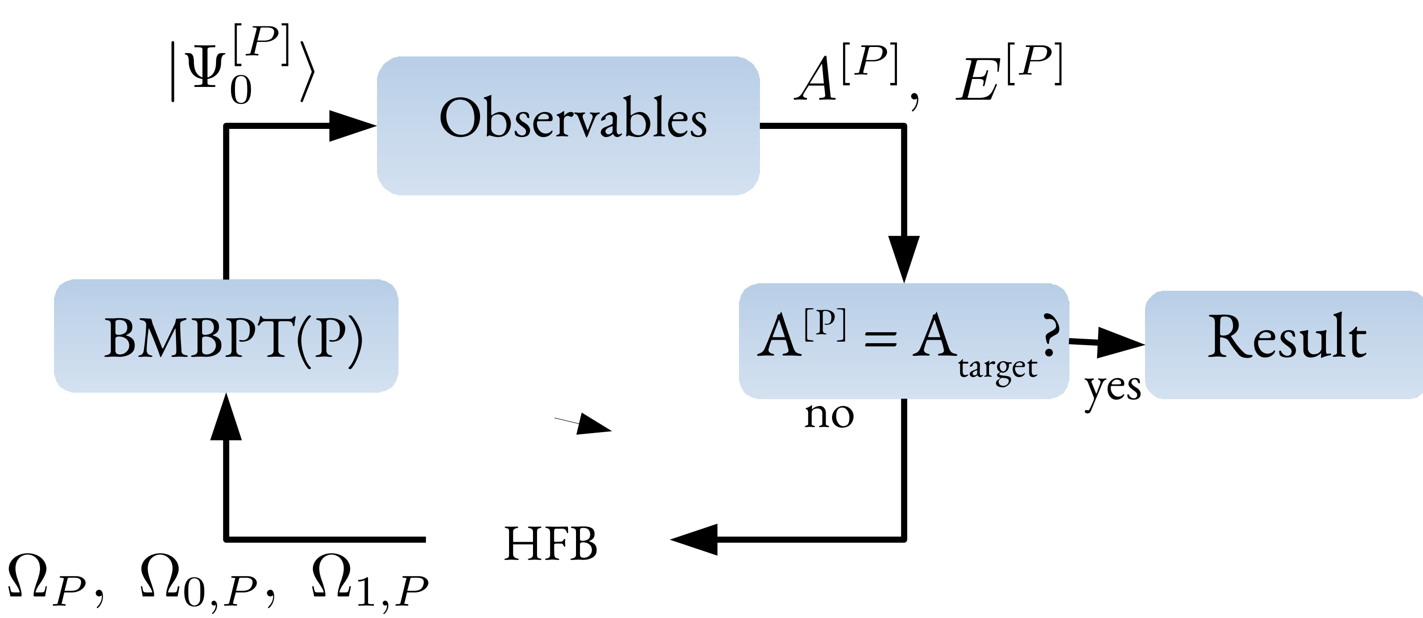
High order constrained BMBPT

Constrained BMBPT
- Constrain average A at each order P.
- Convergence?

Workaround
- Numerically costly.
- *A posteriori* correction.

Toward high orders
- Series behavior? => resummation
- Particle number asymptotic restoration?
- Check low orders

Order P constraint



Intrisincally iterative

Particle number adjusted at each working order P.

Truncation

$\mathcal{H}^1$ $\mathcal{H}^N$

e_{max} 2, 4, 6 SD(T)(Q)

Building CI Matrix.

Toy Model / Proof of principle

Realistic interaction

Far from model space convergence

CI truncation contamination at high order

More informations than standard MBPT

Contents

Time independent (un)constrained BMBPT

$$\{a, a^\dagger\} \to \{\beta, \beta^\dagger\}$$

$$|\Phi_P^{k_1 k_2 \cdots}\rangle \equiv \beta_{k_1}^\dagger \beta_{k_2}^\dagger \cdots |\Phi_P\rangle$$

$$H \to \Omega_P \equiv H - \lambda_P A$$

$$\Omega_P \equiv \Omega_{0,P} + \Omega_{1,P}$$

$$\Omega_P(x) \equiv \Omega_{0,P} + x\Omega_{1,P}$$

$$x \in [0, 1]$$

$$\Omega_P(x)|\Psi_{n,P}(x)\rangle = \tilde{\mathcal{E}}_{n,P}(x)|\Psi_{n,P}(x)\rangle$$

Time independent (un)constrained BMBPT

$$\{a, a^\dagger\} \rightarrow \{\beta, \beta^\dagger\}$$

$$|\Phi_P^{k_1 k_2 \cdots}\rangle \equiv \beta_{k_1}^\dagger \beta_{k_2}^\dagger \cdots |\Phi_P\rangle$$

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$$\Omega_P \equiv \Omega_{0,P} + \Omega_{1,P}$$

$$\Omega_P(x) \equiv \Omega_{0,P} + x\Omega_{1,P}$$

$$x \in [0, 1]$$

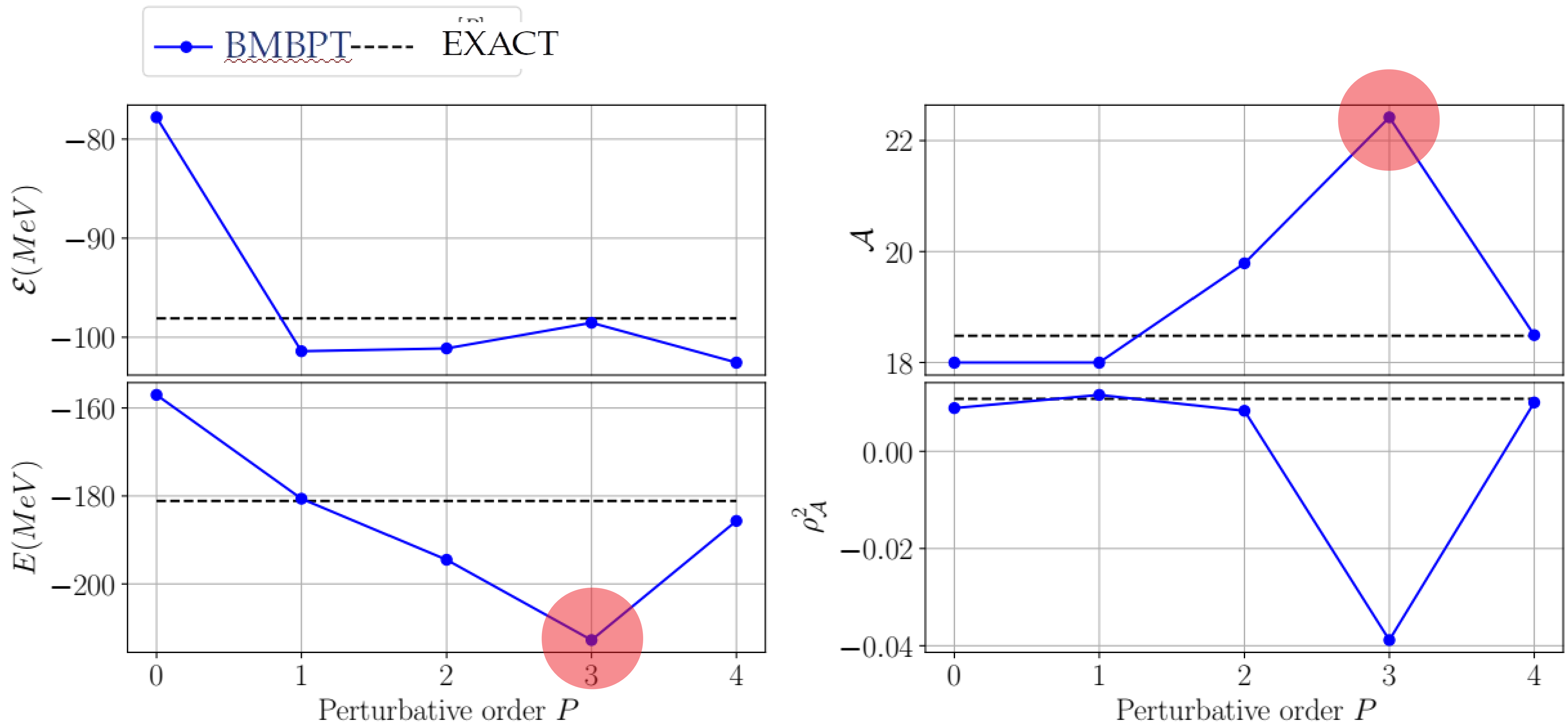
$$\langle \Phi_n | \Phi_n^{(p)} \rangle \equiv \delta_{np}$$

$$\tilde{\mathcal{E}}_{n,P}^{(p)} = \langle \Phi_{n,P}^{(0)} | \Omega_{1,P} | \Phi_{n,P}^{(p-1)} \rangle$$

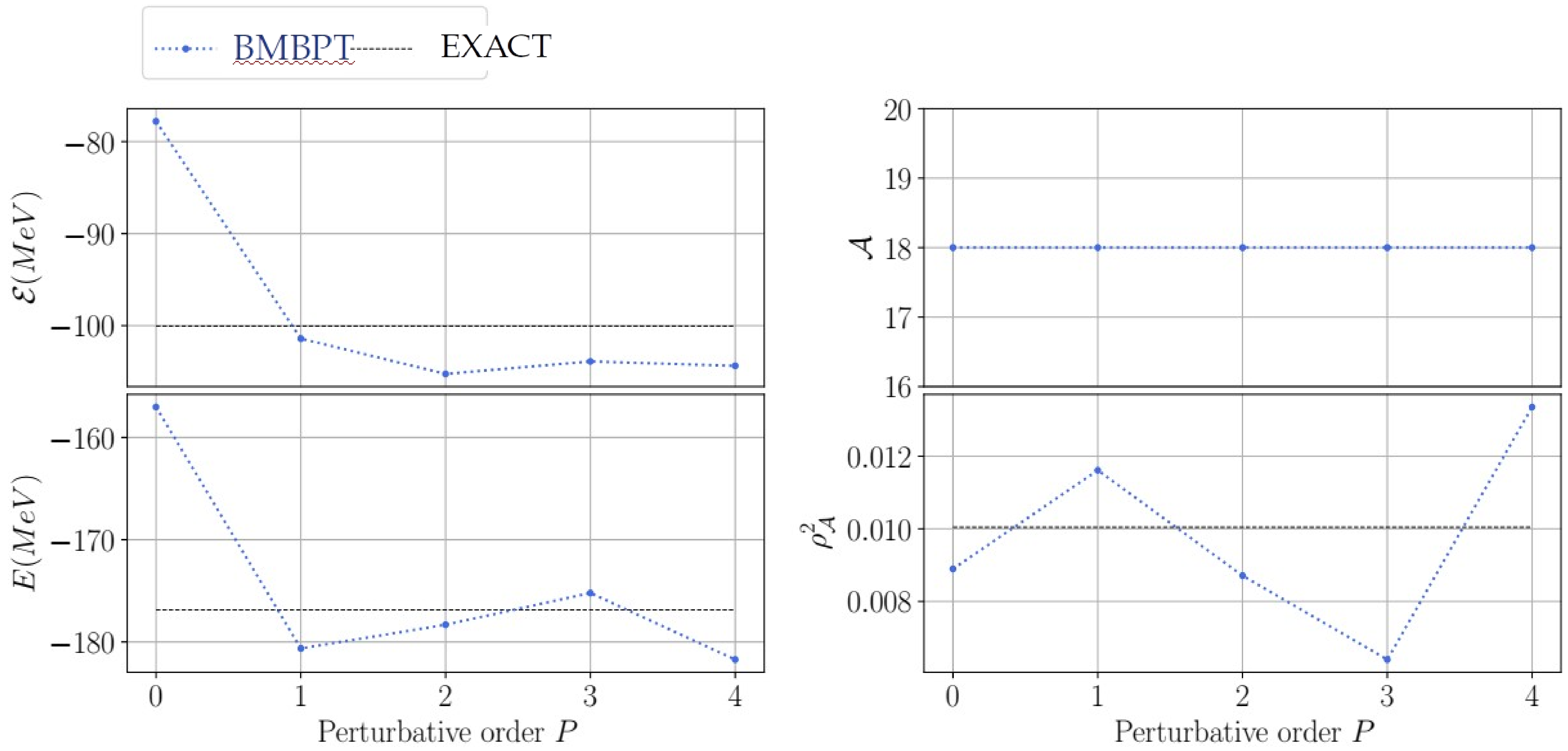
$$|\Phi_{n,P}^{(p)}\rangle = \left(\Omega_P^{00} + \sum_{k \in n} E_k - \Omega_{0,P} \right)^{-1} \left[\Omega_{1,P} |\Phi_{n,P}^{(p-1)}\rangle - \sum_{1 \leq j \leq p} \tilde{\mathcal{E}}_{n,P}^{(j)} \Phi_{n,P}^{(p-j)} \rangle \right]$$

Contents

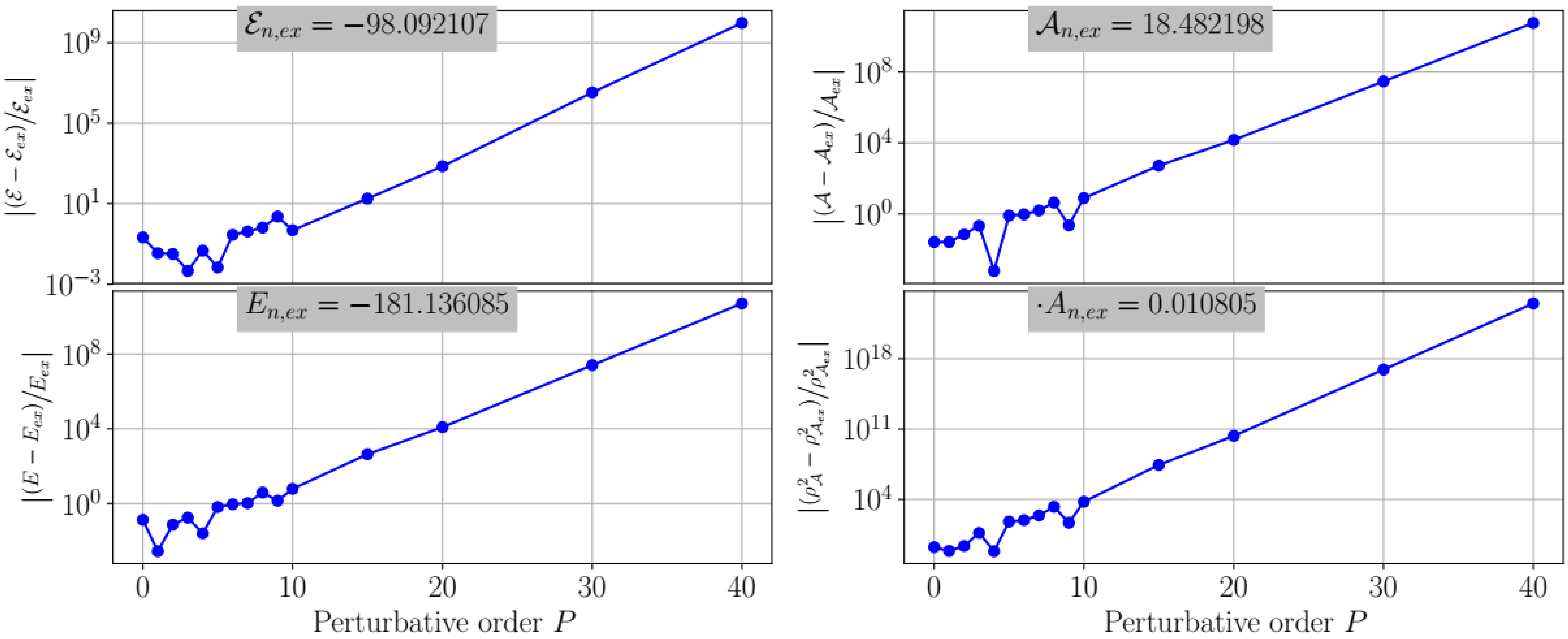
First results of unconstrained BMBPT



Constrained BMBPT Taylor series

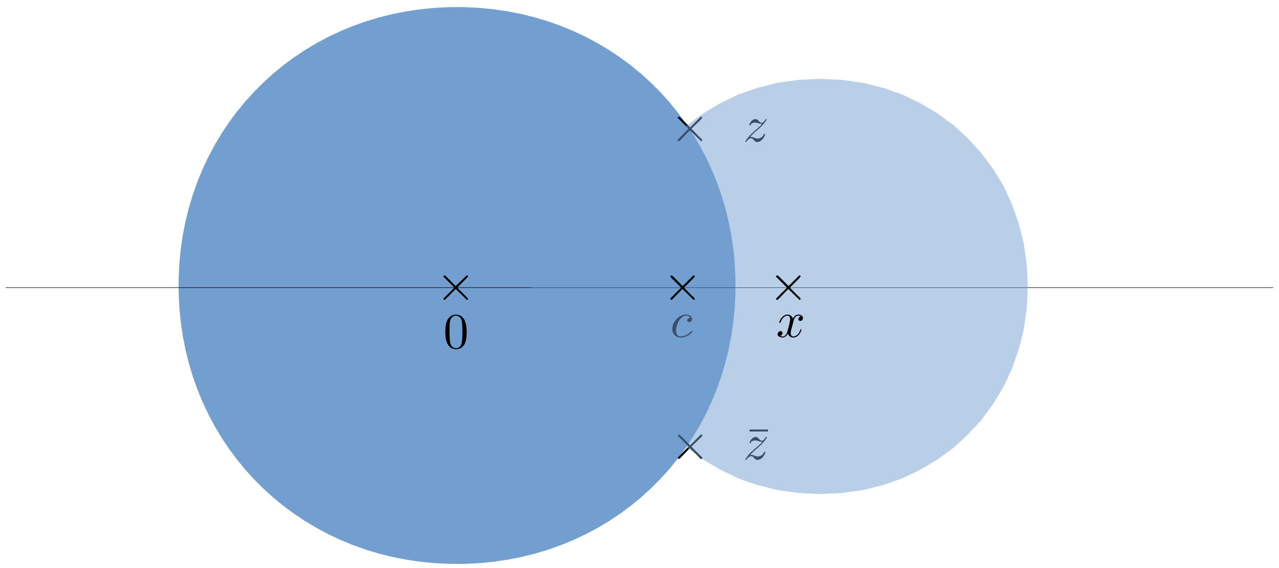


But series are diverging...



Analytic continuation

Dillon Frame et al. Phys. Rev. Lett 121.3 (2018) arXiv: 1711.07090



$$|\Psi(c)\rangle = \sum_n \frac{c^n}{n!}|\Psi^{(n)}(0)\rangle$$

$$|\Psi(x)\rangle = \sum_m \frac{(x-c)^m}{m!}|\Psi^{(m)}(x)\rangle$$

$$|\Psi(x)\rangle = \sum_{nm} \frac{(x-c)^m c^n}{n!m!}|\Psi^{(m+n)}(0)\rangle$$

Eigen-vector continuation

D. K. Frame et al. Phys. Rev. Lett 121.3 (2018) arXiv: 1711.07090

$|\Psi_n^{[P]}(x)\rangle$ visits a small space and is converging for small x $\quad 0 < x_0 < \cdots < x_P \ll 1$

Extrapolate $|\Psi_n^{[P]}\rangle$ **by diagonalizing** Ω **on** $|\Psi_n^{[P]}(x_0)\rangle, \cdots, |\Psi_n^{[P]}(x_P)\rangle$ or equivalently on $|\Phi_n^{(0)}\rangle, \cdots, |\Phi_n^{(P)}\rangle$

$$\mathbf{\Omega}_{ij,P} \equiv \langle \Phi_{n,P}^{(i)} | \Omega | \Phi_{n,P}^{(j)} \rangle$$
$$\boldsymbol{N}_{ij,P} \equiv \langle \Phi_{n,P}^{(i)} | \Phi_{n,P}^{(j)} \rangle.$$

Generalized Eigenvalue Problem

$$\mathbf{\Omega} X = \lambda \boldsymbol{N} X.$$

Ground state

$$|\bar{\Psi}_{0,P,EC}^{[P]}(x)\rangle \equiv \text{argmin}_{|\Psi\rangle \in \mathcal{K}_0^P} \frac{\langle \Psi | \Omega_P | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

P-order approx. of Ω ground state connected to $|\Phi_0\rangle$

Excited states

Not done here but reachable too.

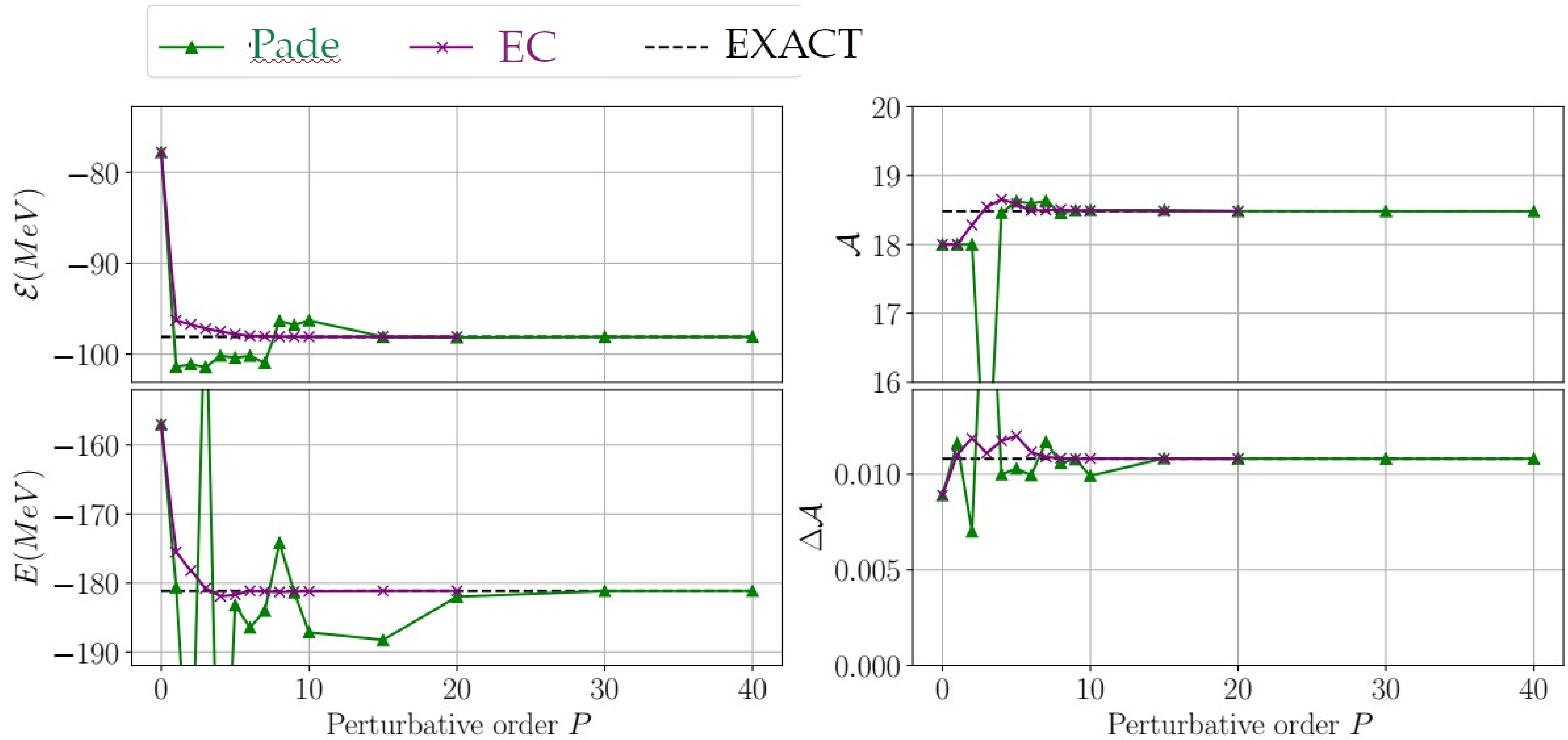
Observables

$$\mathcal{O}_{n,P,EC}^{[P]} \equiv \frac{\langle \Phi_n | O | \Psi_{n,P,EC}^{[P]} \rangle}{\langle \Phi_n | \Psi_{n,P,EC}^{[P]} \rangle}$$

Remarks

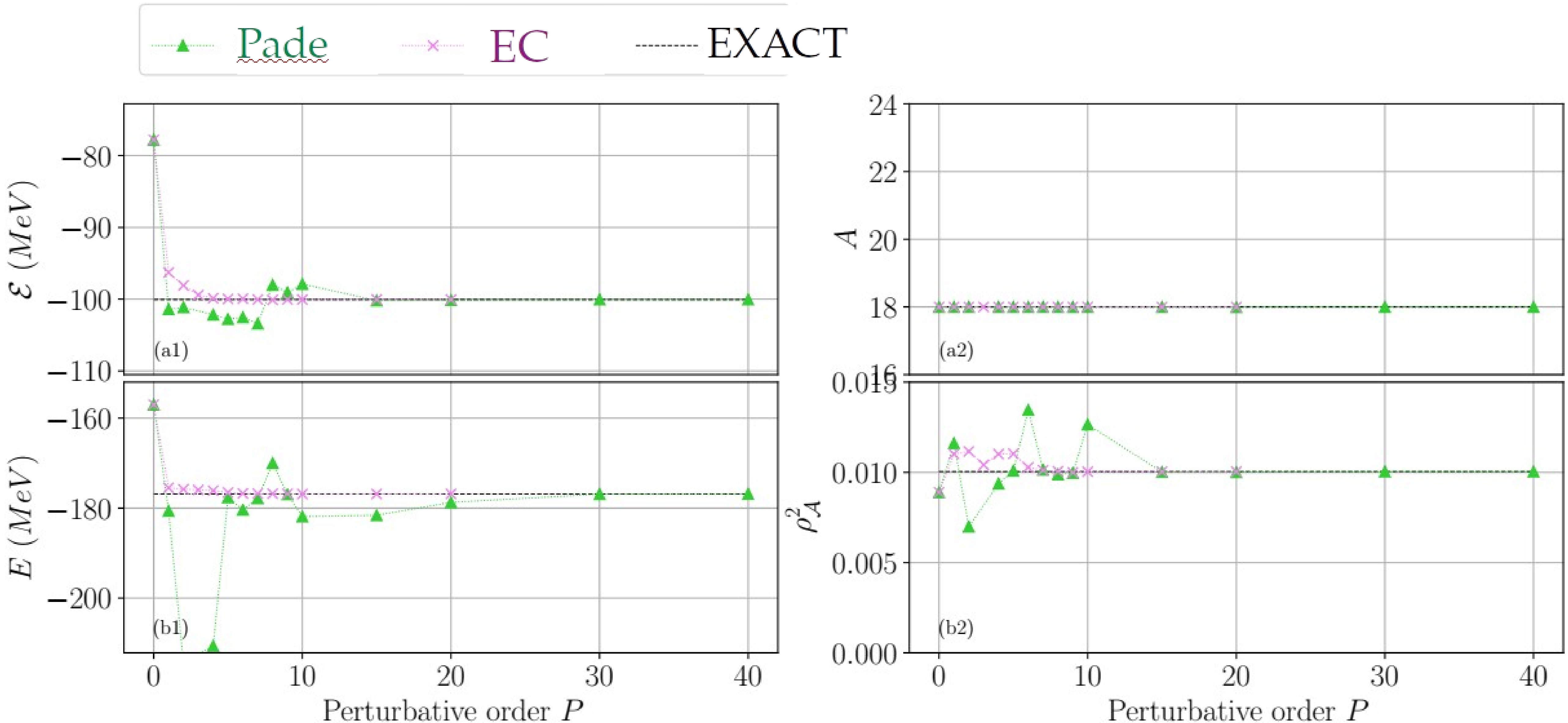
- No need of computing the vectors explicitly
- Increases complexity
- Valid also at low orders
- Variational: improves at each iteration

Resummed observables in unconstrained BMBPT



Still wrong particle number even in the limit...

Constrained BMBPT



A posteriori correction

Goal : Correct for the discrepancy in average neutron / proton number without constraining at order P > 0

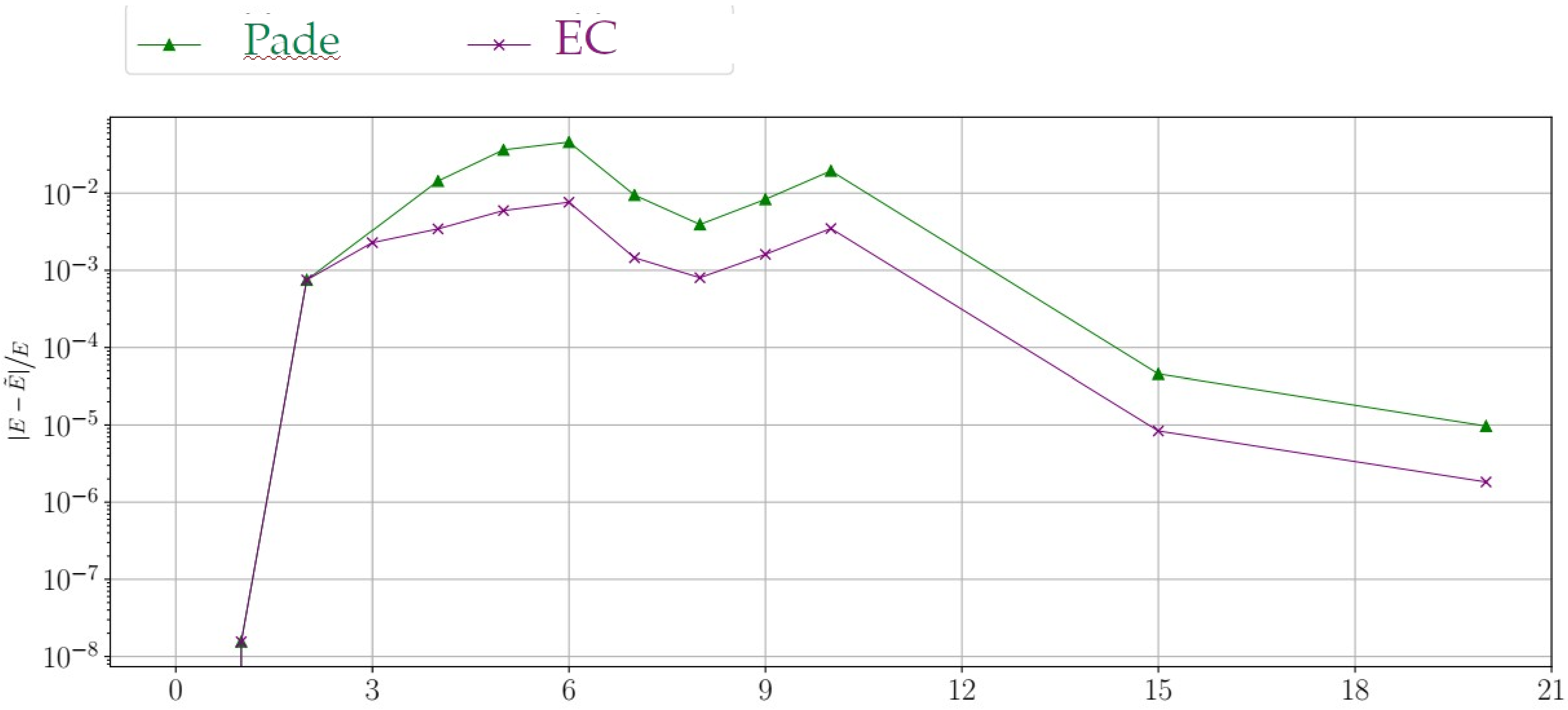
$$E_0^{[P]}\Big|_{A_0} = \mathcal{E}_0^{[P]} + \lambda A_0.$$

$$E_0^{[P]}\Big|_{A_0+\delta A} \approx E_0^{[P]}\Big|_{A_0} + \lambda \delta A$$

$$\tilde{E}_0^{P}\Big|_{A} \equiv E_0^{[P]}\Big|_{A^{[P]}} + \lambda \left(A - A^{[P]}\right) = \mathcal{E}_0^{[P]}\Big|_{A^{[P]}} + \lambda A$$

- No additional work (only one vacuum).
- Valid for small corrections.
- Apply to all computation methods of observables.
- Already used at order 3 in realistic calculations.

Comparison with constrained BMBPT



Perturbative order P

Contents

Conclusion

Accurate results at low order

- Standard projective approach accurate (divergence at high order).
- Significant contamination to A appear early.

***A posteriori* corrections**

- Accurate workaround to constrained BMBPT.
- No additional cost.

Resummation techniques

- Pade does not help at low order.
- Eigenvector continuation: promising result
- What about computational cost?
- Increases convergence rate.

Particle number restoration

- Need commutation between A and H…
- … seem to appear at larger configuration space.
- SDT(Q)(P) : higher order in PT with full operator.
- Underlines the need for projection techniques.

Thanks for your attention

- **Pepijn Demol**
- **Julien Ripoche**
- **Alexander Tichai**
- **Thomas Duguet**
- **Vittorio Somà**

Resummation of projective observables using Pade approximants

$\mathrm{O}^{[P]}_{n,P}(x) = \sum_{p=0}^{P} x^p \langle \Phi^{(0)}_{n,P} | O | \Phi^{(p)}_{n,P} \rangle$ **How to deal with divergent partial sums at x=1?**

$\mathcal{O}(x) (= \sum o_i x^i)$

$$\mathcal{O}[M/N](x) = \frac{\sum_{i=1}^{M} a_i x^i}{1 + \sum_{i=1}^{N} b_i x^i} \text{ so that } \left.\frac{\mathrm{d}^k \mathcal{O}\,[M/N]}{\mathrm{d}x^k}\right|_{x=0} = \left.\frac{\mathrm{d}^k \mathcal{O}}{\mathrm{d}x^k}\right|_{x=0} \ \forall\ 0 \le k \le M+N.$$

$$\mathcal{O}\,[M/N]\,(x) \equiv \frac{\begin{vmatrix} o_{M-N+1} & o_{M-N+2} & \cdots & o_{M+1} \\ o_{M-N+2} & o_{M-N+3} & \cdots & o_{M+2} \\ \vdots & \vdots & \ddots & \vdots \\ o_M & o_{M+1} & \cdots & o_{M+N} \\ \sum_{i=0}^{M-N} o_i x^{N+i} & \sum_{i=0}^{M-N+1} o_i x^{N+i-1} & \cdots & \sum_{i=0}^{M} o_i x^i \end{vmatrix}}{\begin{vmatrix} o_{M-N+1} & o_{M-N+2} & \cdots & o_{M+1} \\ o_{M-N+2} & o_{M-N+3} & \cdots & o_{M+2} \\ \vdots & \vdots & \ddots & \vdots \\ o_M & o_{M+1} & \cdots & o_{M+N} \\ x^N & x^{N-1} & \cdots & 1 \end{vmatrix}}.$$

Unconstrained: resummation of the projective truncated series.

Constrained: resummation of the partial sum at each order.

Remarks:

- Captures poles in the complex plane.
- Efficient at high order only: instabilities.
- No extra work: post-treatment only.

Importance truncation

A. Tichai, J. Ripoche, T. Duguet arXiv:1902.09043

P=2