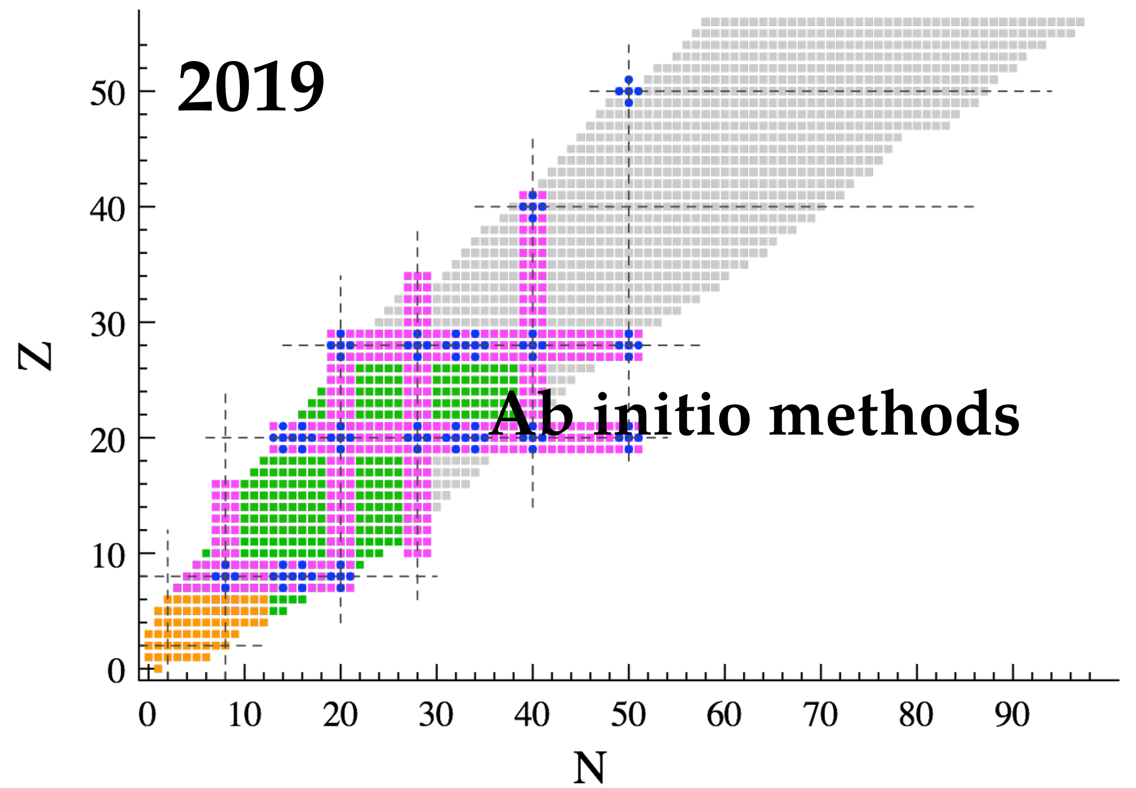
High-Order Many-Body Bogoliubov Perturbation Theory



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2019 in preparation

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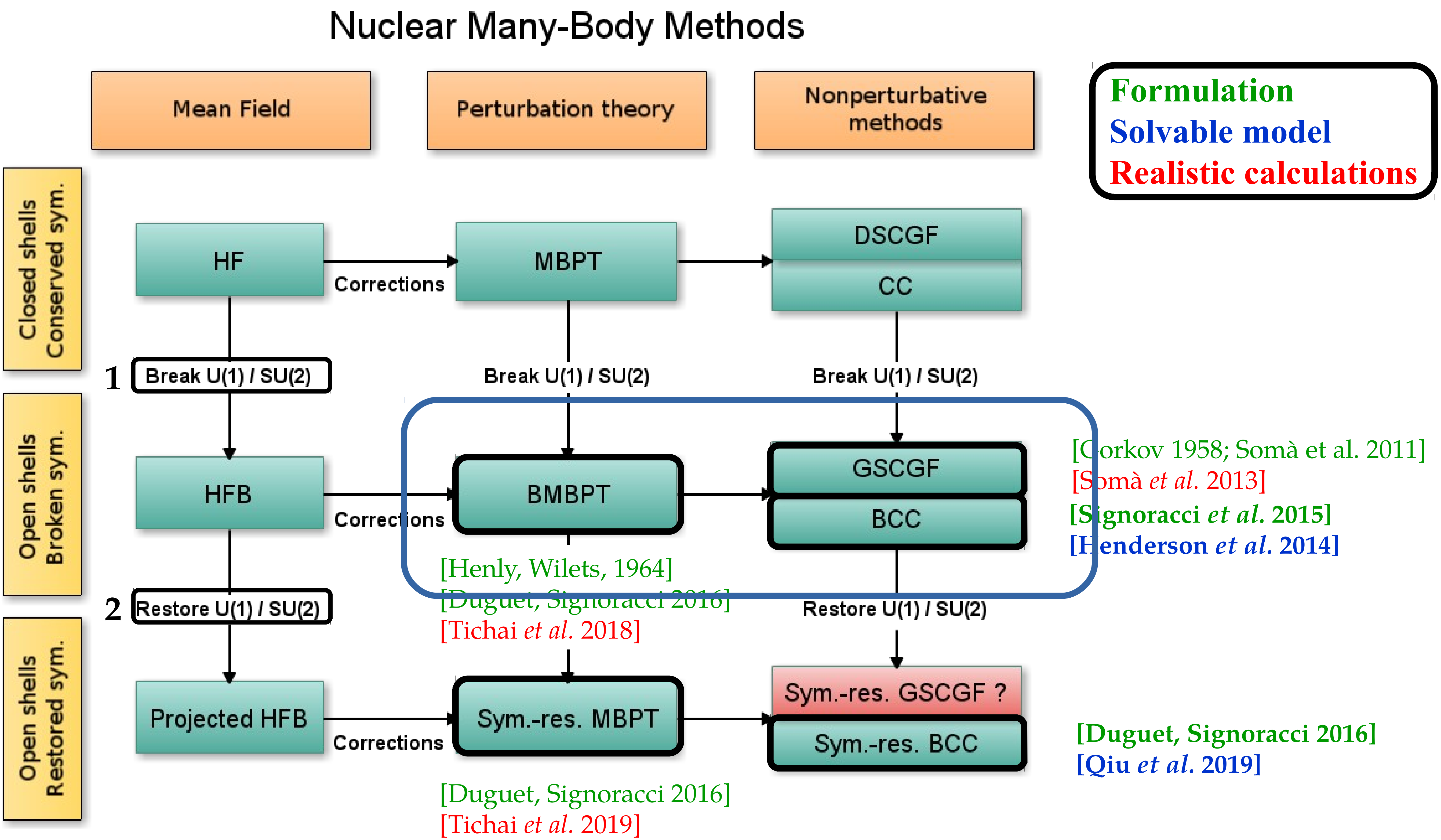
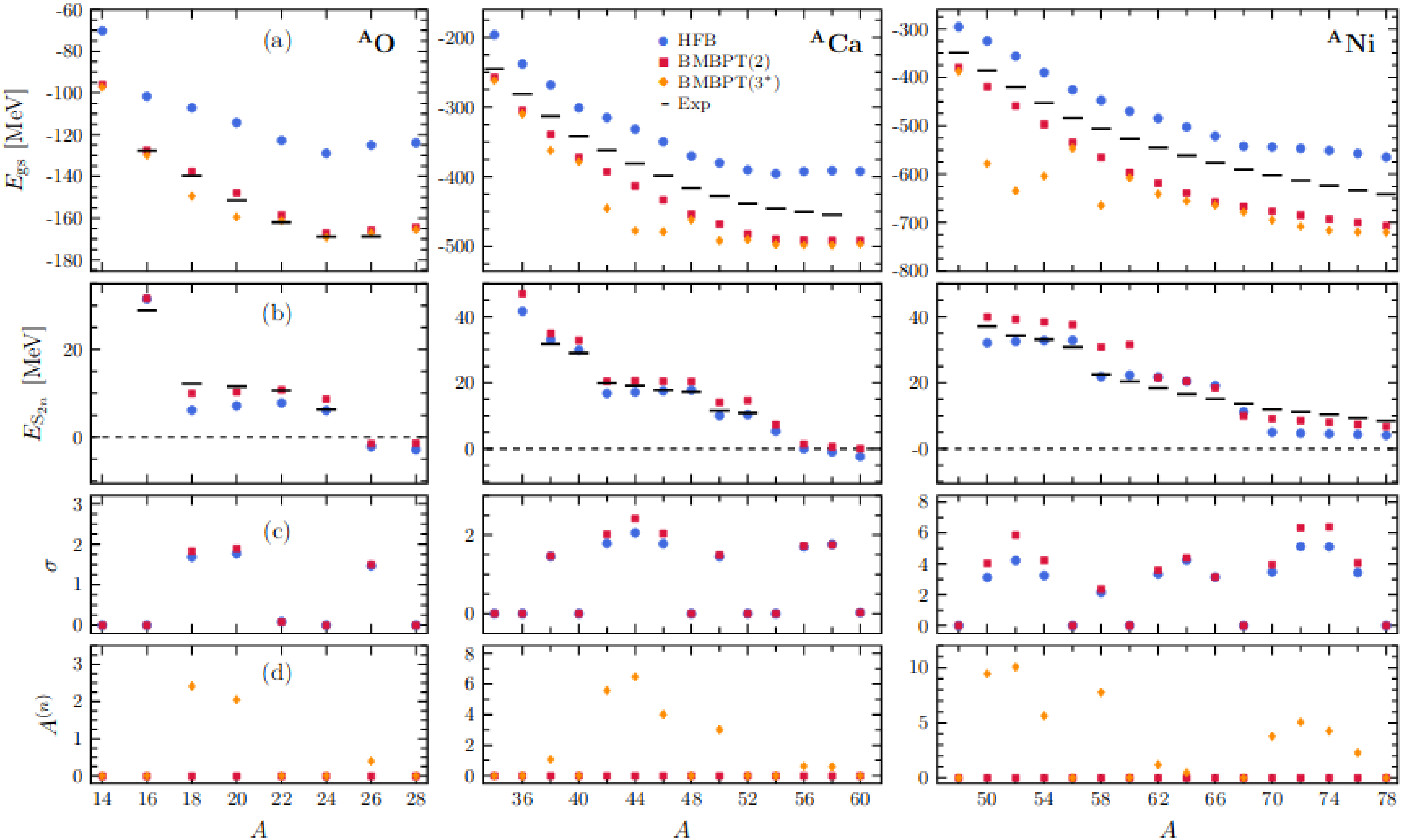
Single-reference expansion many-body methods and symmetries



Particle number corrections in BMBPT

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



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

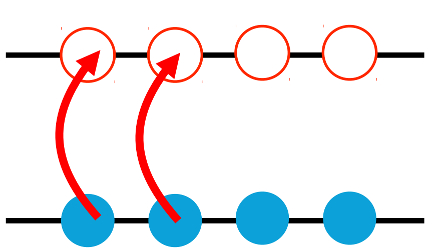
$$[H, A] = 0$$

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.

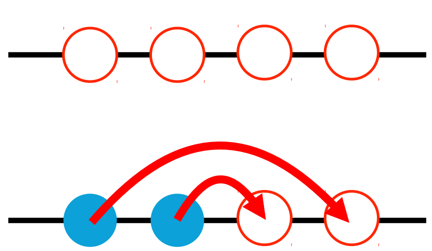
Closed-shell



Non-degenerate

Good starting point

Open-shell



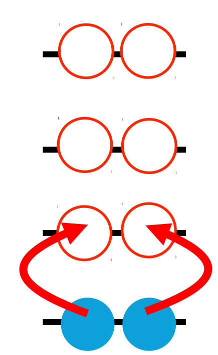
Degenerate

Improper starting point

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

High order constrained BMBPT

Constrained BMBPT

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

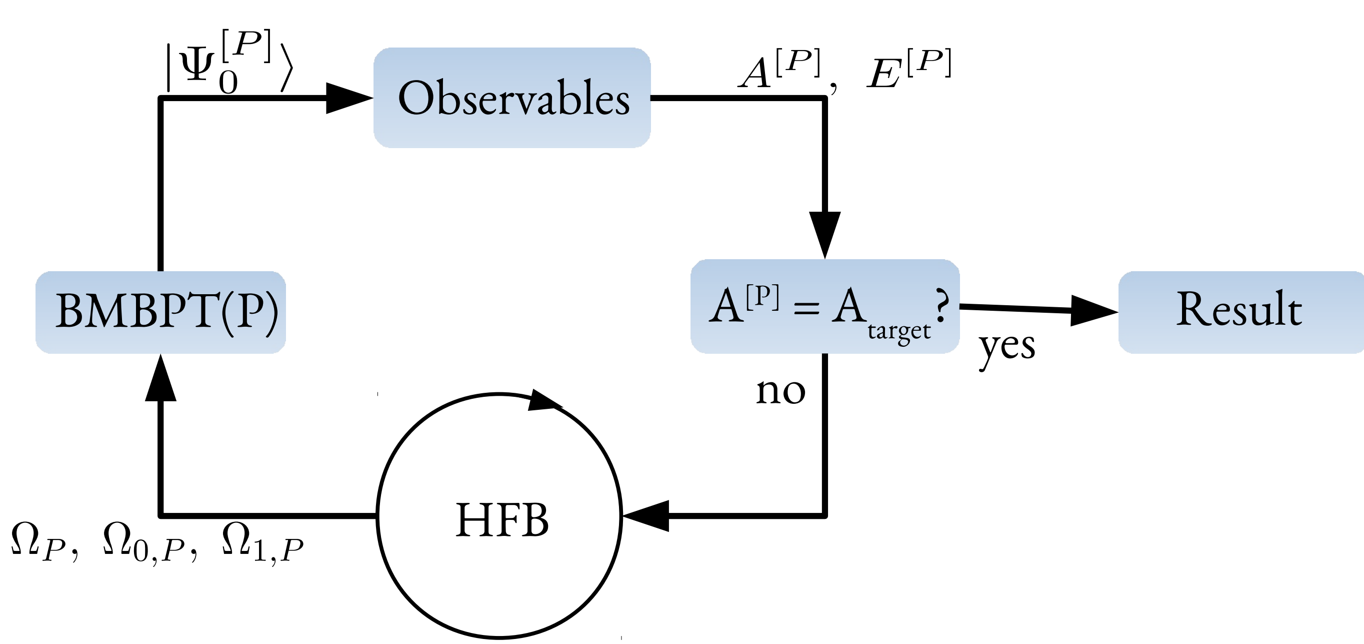
Workaround

- Numerically costly.
- *A posteriori* correction.

Toward high orders

- Series behavior?
- Particle number asymptotic restoration?
- Check low orders

Order P constraint



Why?
Truncated expansions → Wrong average particle number.

Intrisincally iterative

Particle number adjusted at each working order P.

Truncation

$\mathcal{H}^1$ e_{max} 2, 4, 6

$\mathcal{H}^N$ 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

Bogoliubov reference state

Bogoliubov transformation

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

$$\beta^\dagger_k = \sum_p U_{pk}\, c^\dagger_p + V_{pk}\, c_p$$

$$\mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \text{ unitary, i.e. } \begin{array}{l} \{\beta_k, \beta_{k'}\} = 0 \\ \{\beta^\dagger_k, \beta^\dagger_{k'}\} = 0 \\ \{\beta_k, \beta^\dagger_{k'}\} = \delta_{kk'} \end{array}$$

Bogoliubov state

$$|\Phi\rangle \equiv C \prod_k \beta_k |0\rangle$$

$$\underbrace{\beta_k\, |\Phi\rangle = 0 \ \ \forall k}$$

Vacuum state
Reduces to SD in H_A if V=0

Breaks U(1) symmetry

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

Quasi-particle excitations

$$|\Phi^{\alpha\beta\ldots}\rangle \equiv \beta^\dagger_\alpha \beta^\dagger_\beta \ldots |\Phi\rangle$$

$\underbrace{\text{Orthonormal basis of Fock space}}$

Reduces to npnh excit. in H_A if V=0

Ritz variational problem with a Bogoliubov ansatz

$$\Omega = H - \lambda A$$

Minimize $\dfrac{\langle\Phi|\Omega|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \Omega^{00}$ while keeping

1) the Bogoliubov transformation unitary
2) particle number fixed on average

HFB eigenvalue equation

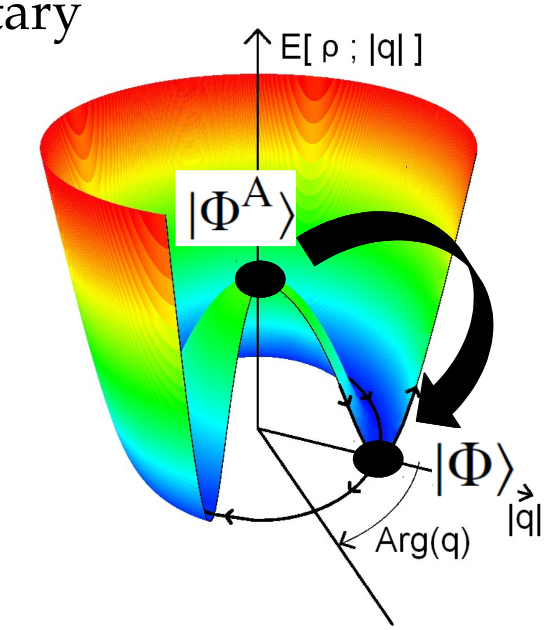
$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \underbrace{\begin{pmatrix} U_k \\ V_k \end{pmatrix}} = \underbrace{E_k} \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

with

$$h_{pq} \equiv \langle\Phi|\{[c_p, \Omega], c^\dagger_q\}|\Phi\rangle$$

$$\Delta_{pq} \equiv \langle\Phi|\{[c_p, \Omega], c_q\}|\Phi\rangle$$

Fully characterize $|\Phi\rangle$ Quasi-particle energies > 0



Time independent (un)constrained BMBPT

Splitting and basis

$$\Omega_P \equiv \Omega_{0,P} + \Omega_{1,P} \qquad |\Phi_P^{k_1 k_2 \cdots}\rangle \equiv \beta^\dagger_{k_1}\beta^\dagger_{k_2}\cdots|\Phi_P\rangle$$

$$\Omega_{0,P}|\Phi^{k_1 k_2\cdots}\rangle = (\Omega^{00,P} + E_{k_1,P} + E_{k_2,P} + \cdots)|\Phi^{k_1 k_2\cdots}\rangle$$

Auxiliary problem

$$\Omega_P(x) \equiv \Omega_{0,P} + x\Omega_{1,P}, \;\; x \in [0,1]$$

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

$$\lim_{x\to 1} |\Psi_n(x)\rangle = |\Psi_n^{\mathrm{A}}\rangle$$

$$\lim_{x\to 1} \tilde{\mathcal{E}}_n(x) = \mathcal{E}_n^{\mathrm{A}}$$

Perturbative expansion

$$|\Psi_{n,P}(x)\rangle \equiv |\Phi^{(0)}_{n,P}\rangle + x\,|\Phi^{(1)}_{n,P}\rangle + x^2\,|\Phi^{(2)}_{n,P}\rangle + ... = |\Phi^{(0)}_{n,P}\rangle + \sum_{p\geq 1} x^p\,|\Phi^{(p)}_{n,P}\rangle$$

$$\tilde{\mathcal{E}}_{n,P}(x) \equiv \tilde{\mathcal{E}}^{(0)}_{n,P} + x\,\tilde{\mathcal{E}}^{(1)}_{n,P} + x^2\,\tilde{\mathcal{E}}^{(2)}_{n,P} + \cdots = \tilde{\mathcal{E}}^{(0)}_{n,P} + \sum_{p\geq 1} x^p\,\tilde{\mathcal{E}}^{(p)}_{n,P}$$

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

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

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

Linked diagrams contributing to the wave-function
Computationally: Matrix-Vector product
Visited configuration space increasing at each order

Order-P approximation

$$|\Psi_n^{[P]}(x)\rangle \equiv |\Phi^{(0)}_{n,0}\rangle + \sum_{p\geq 1}^{P} x^p\,|\Phi^{(p)}_{n,0}\rangle$$

$$|\Psi_{n,P}^{[P]}(x)\rangle \equiv |\Phi^{(0)}_{n,P}\rangle + \sum_{p=1}^{P} x^p\,|\Phi^{(p)}_{n,P}\rangle$$

Two subcases considered:

Unconstrained:
- Constrained at HFB level
- A_{HFB} matches A
- Series

Constrained:
- Constrained at working order P
- $A^{[P]}$ matches A
- Iterative process (root finding)
- Vacuum, splitting, expansion P-dependent
- Sequence of partial sums

Evaluation of observables

Observable O

$\cancel{[O,H]=0}$

$$O|\Psi_n^A\rangle = \mathcal{O}_n|\Psi_n^A\rangle$$

$$\begin{cases} \mathcal{O}_n & = & \langle\Phi_n|O|\Psi_n^A\rangle \\ \mathcal{O}_n & = & \dfrac{\langle\Psi_n^A|O|\Psi_n^A\rangle}{\langle\Psi_n^A|\Psi_n^A\rangle} \end{cases}$$

$$O = \Omega,\ \ \Omega(x),\ \ H,\ \ A,\ \ A^2$$

$$|\Psi_n^A\rangle \to |\Psi_n^{[P]}\rangle, |\Psi_{n,P}^{[P]}\rangle$$

Projective approach

$$\begin{aligned} \mathcal{O}_{n,P}^{[P]}(x) &\equiv \mathrm{Re}\frac{\langle\Phi_{n,P}^{(0)}|O|\Psi_{n,P}^{[P]}(x)\rangle}{\langle\Phi_{n,P}^{(0)}|\Psi_{n,P}^{(P)}(x)\rangle} \\ &= \sum_{p=0}^{P} x^p \langle\Phi_{n,P}^{(0)}|O|\Phi_{n,P}^{(p)}\rangle \end{aligned}$$

Expectation value approach

$$\begin{aligned} \langle O\rangle_{n,P}^{[P]}(x) &\equiv \frac{\langle\Psi_{n,P}^{[P]}(x)|O|\Psi_{n,P}^{[P]}(x)\rangle}{\langle\Psi_{n,P}^{[P]}(x)|\Psi_{n,P}^{[P]}(x)\rangle} \\ &= \frac{\sum_{pq=0}^{P} x^{p+q}\langle\Phi_{n,P}^{(p)}|O|\Phi_{n,P}^{(q)}\rangle}{\sum_{rs=0}^{P} x^{r+s}\langle\Phi_{n,P}^{(r)}|\Phi_{n,P}^{(s)}\rangle} \end{aligned}$$

- Partial sum of series.
- Visits smaller configuration space than the wave-function.
- Traditionally used in realistic calculations.
- Matches eigenvalue for eigenvectors.

- Rational fraction.
- Visits same configuration space as the wave-function
- Computationally expansive in realistic calculations.
- Bounded from below.

Summary

Operator	Eigenvalue	Projective	Pade resummation	Eigenvector Continuation	Exact Diagonalization
Ω	$\mathcal{E}_n^A$	$\mathcal{E}_{n,P}^{[P]}$			$\mathcal{E}_{n,P,ex}$
A	$\mathcal{A}_n^A$	$\mathcal{A}_{n,P}^{[P]}$			$\mathcal{A}_{n,P,ex}$
H	E_n^A	$E_{n,P}^{[P]}$			$E_{n,P,ex}$
$(A-\mathcal{A})^2$	$\Delta\mathcal{A}_n^A(=0)$	$\Delta\mathcal{A}_{n,P}^{[P]}$			$\Delta\mathcal{A}_{n,P,ex}$
$(A-\mathcal{A})^2/\mathcal{A}_0$	$\rho^2_{\mathcal{A}n}(=0)$	$\rho^{2\ [P]}_{\mathcal{A}n,P}$			$\rho^2_{\mathcal{A}n,ex,P}$

Lower index P removed in case of unconstrained BMBPT

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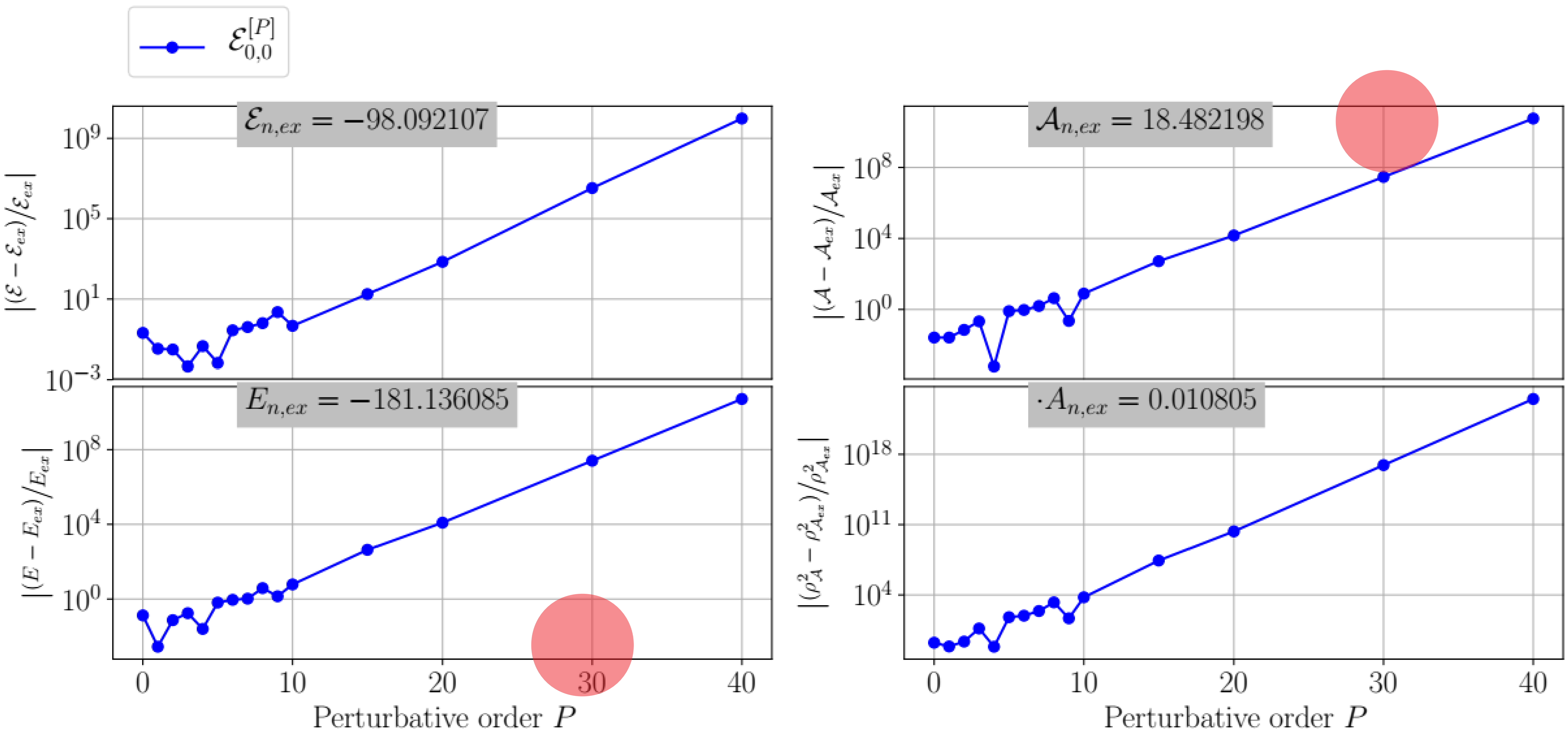
O18, Emax 4, SDT + IT

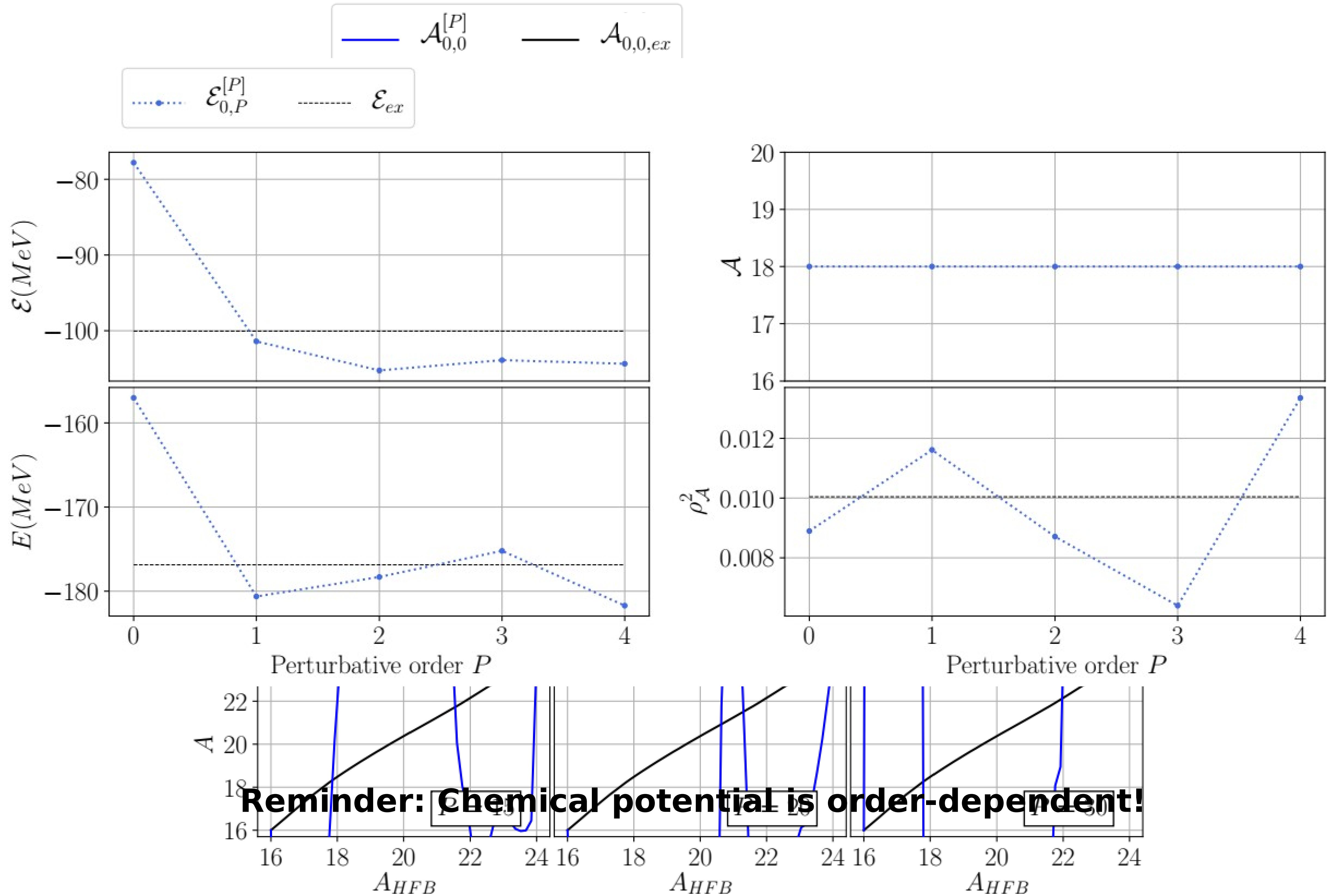
First results of unconstrained BMBPT



See A. Tichai talk

Maybe constraining would help?

Constrained BMBPT Taylor series



Reminder: Chemical potential is order-dependent!

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?**

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

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

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.

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 $|\Phi_n^{(0)}\rangle, \cdots, |\Phi_n^{(P)}\rangle$

$$\begin{aligned} \boldsymbol{\Omega}_{ij,P} &\equiv \langle \Phi_{n,P}^{(i)} | \Omega | \Phi_{n,P}^{(j)} \rangle \\ \boldsymbol{N}_{ij,P} &\equiv \langle \Phi_{n,P}^{(i)} | \Phi_{n,P}^{(j)} \rangle. \end{aligned} \quad \xrightarrow[\textbf{Eigenvalue Problem}]{\textbf{Generalized}} \quad \boxed{\boldsymbol{\Omega} X = \lambda \boldsymbol{N} X.}$$

$\mathcal{K}_n^P \equiv \mathrm{Vect}\{\Omega^p |\Phi_n\rangle,\ p \leq P\}$ Diagonalization on Krylov space: similar to Lanczos algorithm

Ground state

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

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

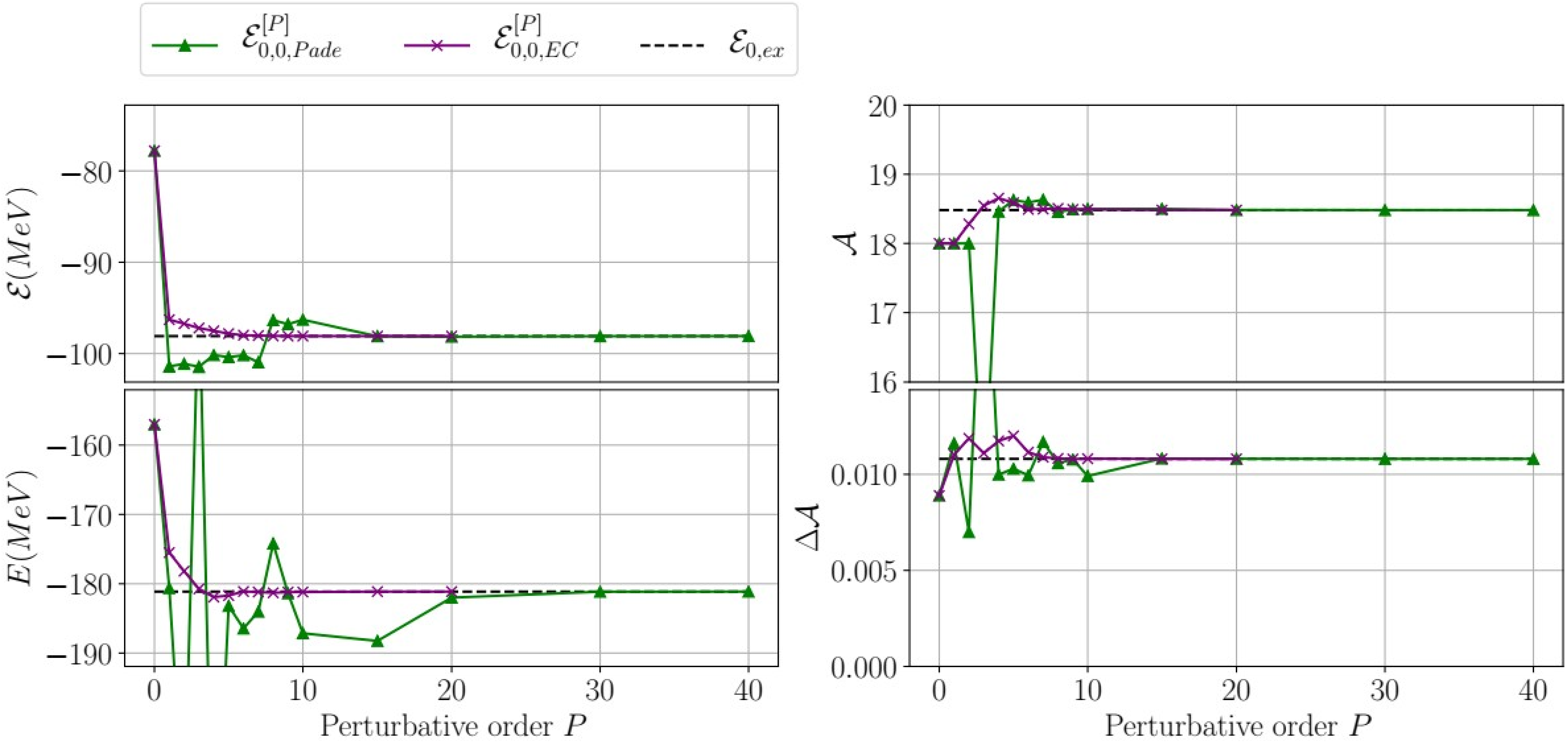
- No need of computing the vectors explicitly
- Increases complexity
- Valid also at low orders
- Variational: improves at each iteration

Summary

Operator	Eigenvalue	Projective	Pade resummation	Eigenvector Continuation	Exact
Ω	$\mathcal{E}_n^A$	$\mathcal{E}_{n,P}^{[P]}$	$\mathcal{E}_{n,P,Pade}^{[P]}$	$\mathcal{E}_{n,P,EC}^{[P]}$	$\mathcal{E}_{n,P,ex}$
A	$\mathcal{A}_n^A$	$\mathcal{A}_{n,P}^{[P]}$	$\mathcal{A}_{n,P,Pade}^{[P]}$	$\mathcal{A}_{n,P,EC}^{[P]}$	$\mathcal{A}_{n,P,ex}$
H	E_n^A	$E_{n,P}^{[P]}$	$E_{n,P,Pade}^{[P]}$	$E_{n,P,EC}^{[P]}$	$E_{n,P,ex}^{[P]}$
$(A-\mathcal{A})^2$	$\Delta\mathcal{A}_n^A(=0)$	$\Delta\mathcal{A}_{n,P}^{[P]}$	$\Delta\mathcal{A}_{n,P,Pade}^{[P]}$	$\Delta\mathcal{A}_{n,P,EC}^{[P]}$	$\Delta\mathcal{A}_{n,P,ex}^{[P]}$
$(A-\mathcal{A})^2/\mathcal{A}_0$	$\rho^2_{\mathcal{A}n}(=0)$	$\rho^{2\ [P]}_{\mathcal{A}n,P}$	$\rho^{2\ [P]}_{\mathcal{A}n,P,Pade}$	$\rho^{2\ [P]}_{\mathcal{A}n,P,EC}$	$\rho^2_{\mathcal{A}n,ex,P}$

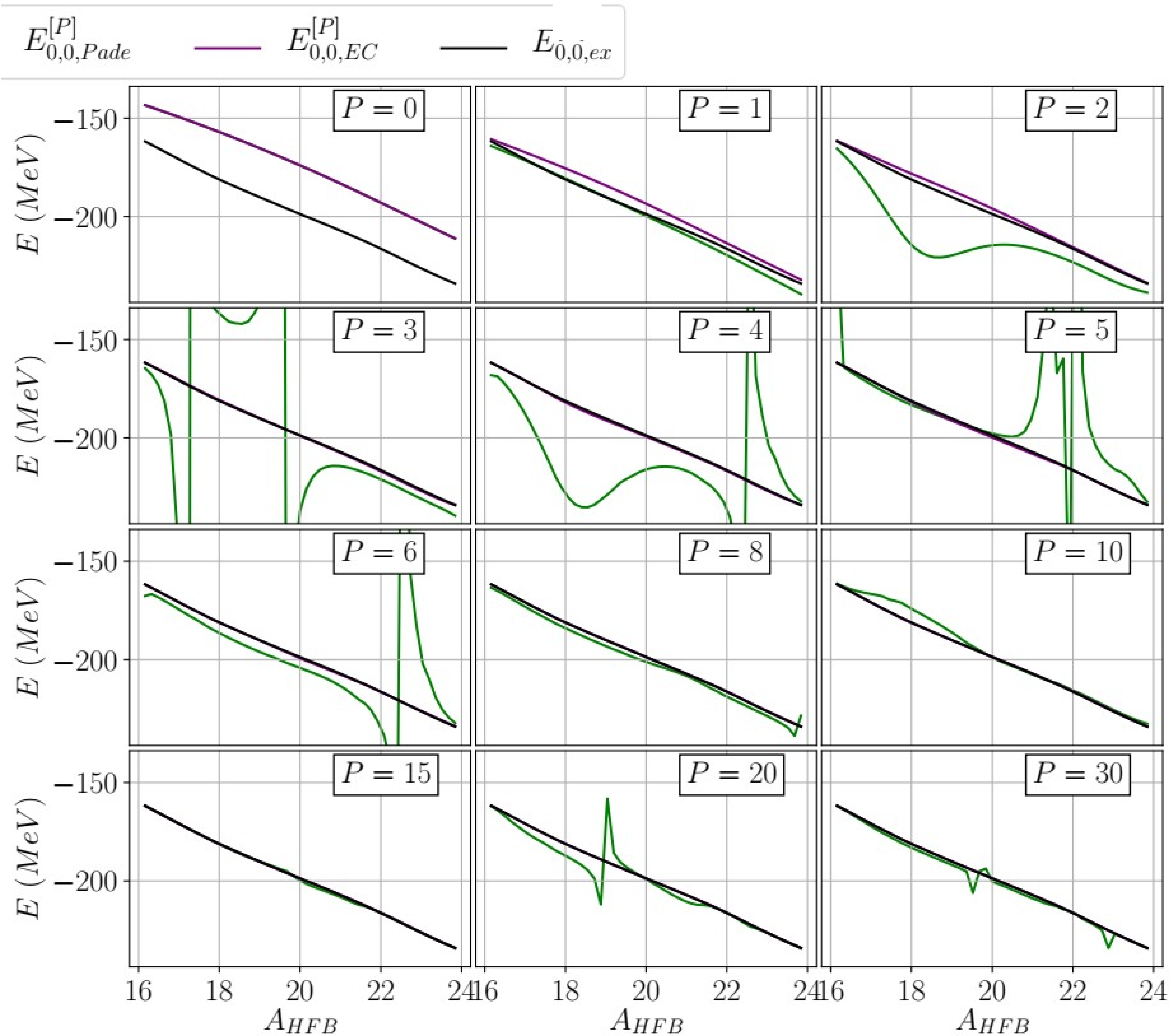
Lower indice P removed in case of unconstrained BMBPT

Resummed observables in unconstrained BMBPT

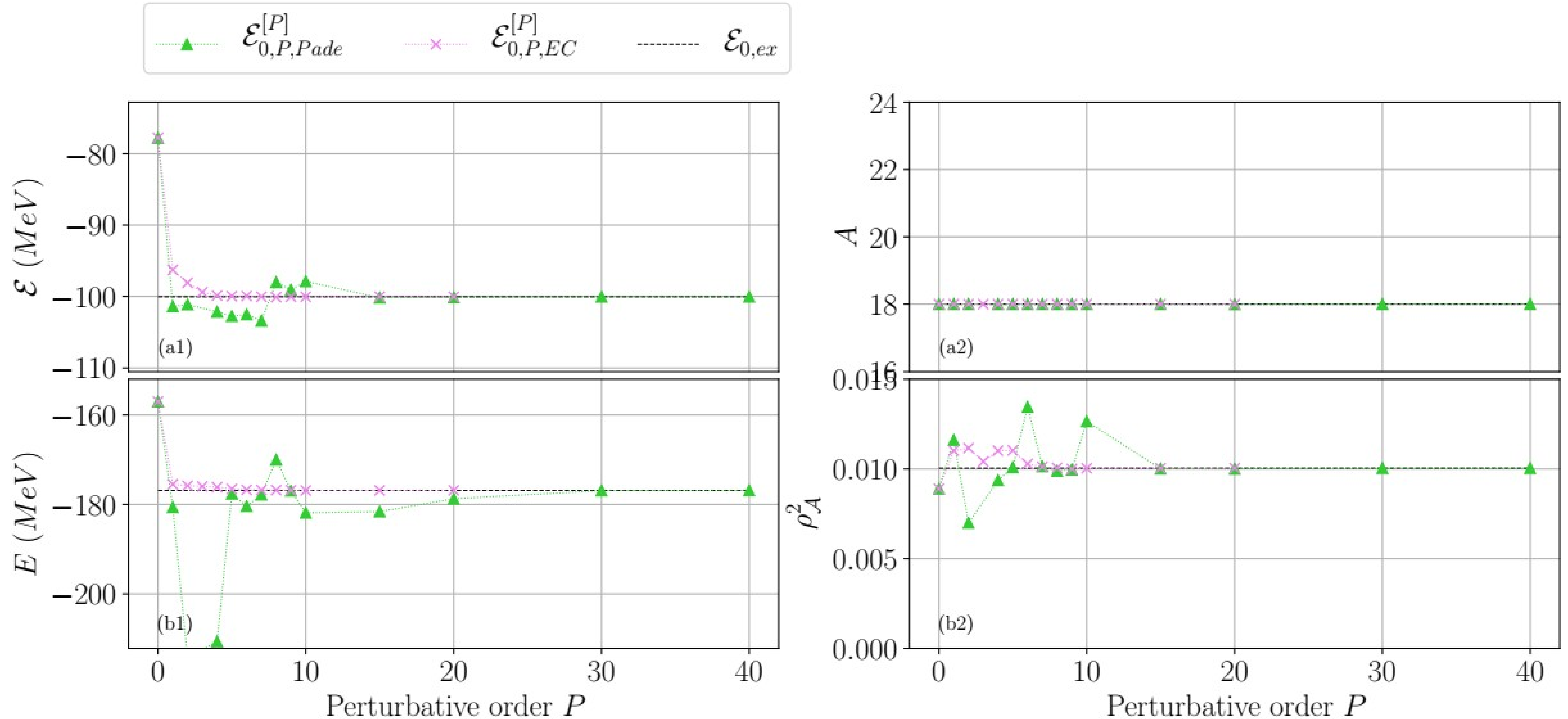


Still wrong particle number even in the limit...

Resummed observables wrt. HFB



Constrained BMBPT



A posteriori correction

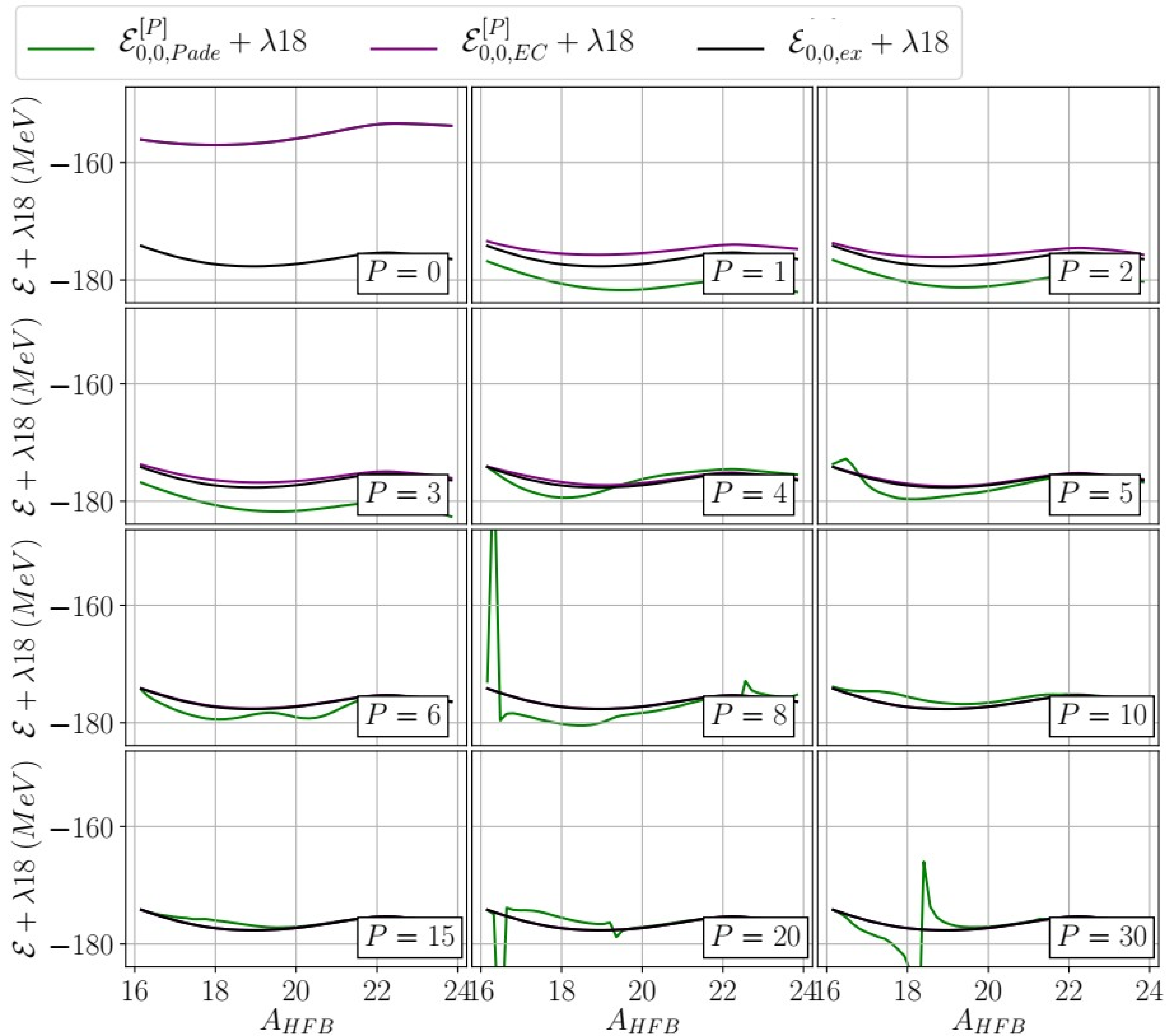
Goal : Correct for the discrepancy in average neutron / proton number without constraining at order P > 0

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

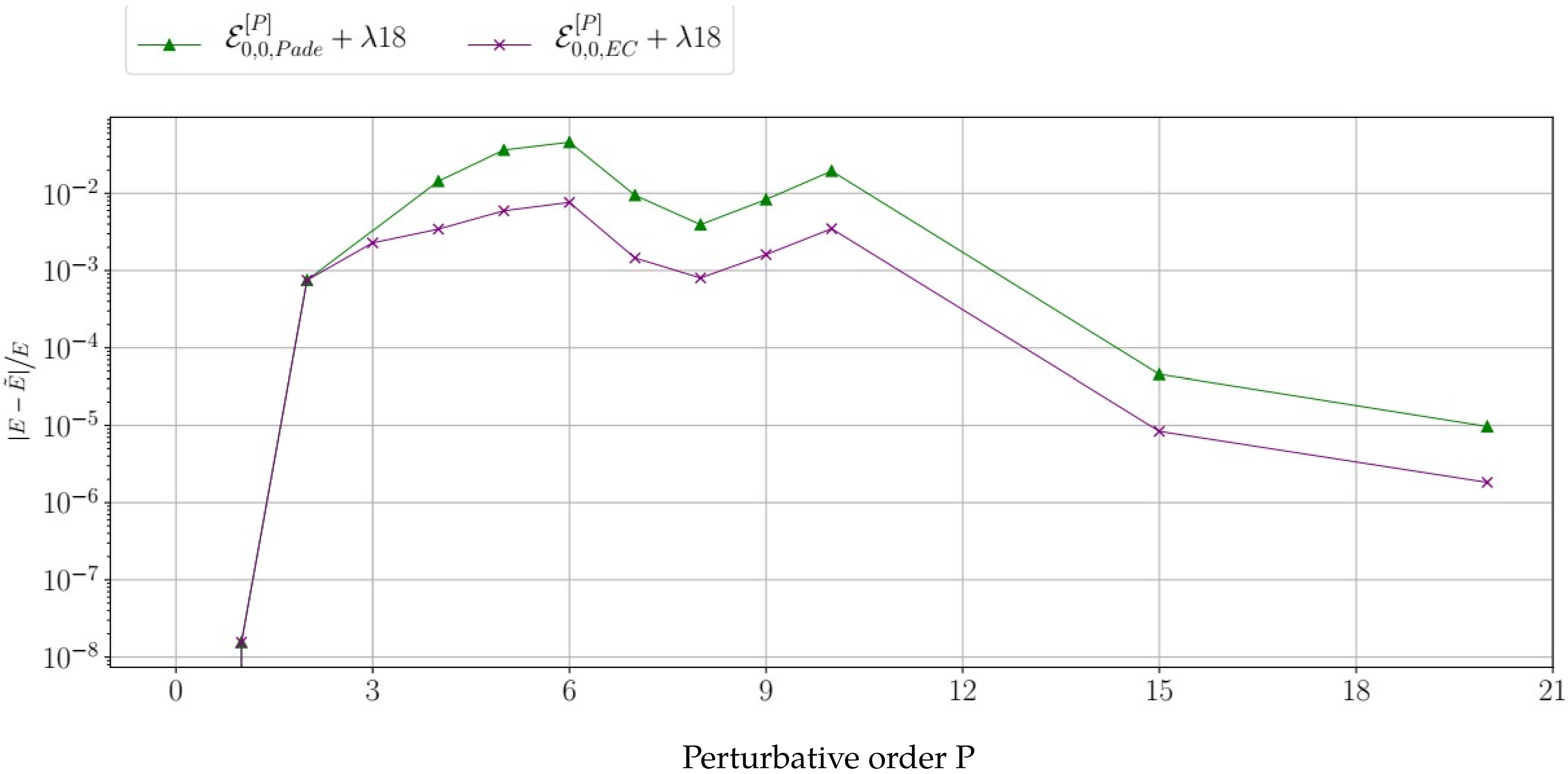
$$\tilde{E}_0^{P}\Big|_{A} \equiv E_0^{[P]}\Big|_{A^{[P]}} + \lambda\left(A - A^{[P]}\right) = \mathcal{E}_0^{[P]}\Big|_{A^{[P]}} + \lambda A$$

- 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.

A posteriori correction vs. HFB vacuum



Comparison with constrained BMBPT



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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

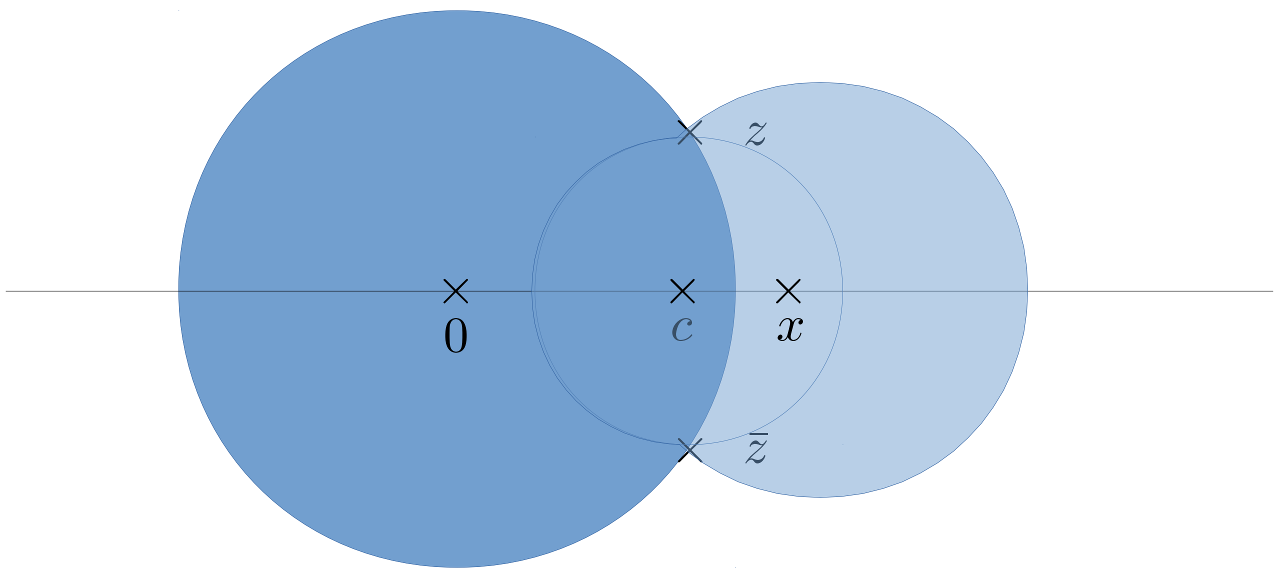
- Need commutation between A and H…
- … seem to appear at larger configuration space.
- SDT(Q)(P) : higher order in PT with full operator.
- Underlines the need for projection techniques.

Thank you!

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

Analytic continuation

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



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

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

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

Importance truncation

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

P=2