

Resummation of Bogoliubov Many-Body Perturbation Theory using Eigenvector Continuation Techniques

And applications to doubly-open-shell nuclei

M. Frosini, P.Demol, A. Tichai, J.P. Ebran, V. Somà, T. Duguet

Progress in Ab Initio Techniques in Nuclear Physics, March 3-6, 2020, Vancouver

Perturbation Theory

Perturbation Theory

Many-body method

A. Tichai et al., arXiv:2001.10433 (2020)

- Least expensive method for nuclear structure
- Accurate low orders in open-shells

Perturbation Theory

Many-body method

A. Tichai et al., arXiv:2001.10433 (2020)

- Least expensive method for nuclear structure
- Accurate low orders in open-shells

Is PT converging? Not always!

- Possible to check in restricted model-spaces...
- ... but not in realistic calculations

Perturbation Theory

Many-body method

A. Tichai et al., arXiv:2001.10433 (2020)

- Least expensive method for nuclear structure
- Accurate low orders in open-shells

Is PT converging? Not always!

- · Possible to check in restricted model-spaces...
- ... but not in realistic calculations

Eigenvector Continuation

D. Frame et al., Phys. Rev. Lett. 121, 032501 (2018)

Perturbation Theory

 $H = H_0 + H_1$ $\mathcal{V} = |\Psi^{(0)}\rangle, \cdots, |\Psi^{(P)}\rangle$

Many-body method

A. Tichai et al., arXiv:2001.10433 (2020)

- Least expensive method for nuclear structure
- Accurate low orders in open-shells

Is PT converging? Not always!

- · Possible to check in restricted model-spaces...
- ... but not in realistic calculations

Eigenvector Continuation

D. Frame et al., Phys. Rev. Lett. 121, 032501 (2018)

Perturbation Theory

 $H = H_0 + H_1$ $\mathcal{V} = |\Psi^{(0)}\rangle, \cdots, |\Psi^{(P)}\rangle$

Many-body method

A. Tichai et al., arXiv:2001.10433 (2020)

- Least expensive method for nuclear structure
- Accurate low orders in open-shells

Is PT converging? Not always!

- · Possible to check in restricted model-spaces...
- ... but not in realistic calculations

Eigenvector Continuation

From perturbative to non-perturbative regime

$$x \sim 0$$
 $x = 1$

$$|\Psi^{EC}\rangle = \operatorname*{argmin}_{|\Psi\rangle\in \operatorname{span}\{\mathcal{V}\}} \frac{\langle \Psi|H|\Psi\rangle}{\langle \Psi|\Psi\rangle}$$

Perturbation Theory

 $H = H_0 + H_1$ $\mathcal{V} = |\Psi^{(0)}\rangle, \cdots, |\Psi^{(P)}\rangle$

Many-body method

A. Tichai et al., arXiv:2001.10433 (2020)

- Least expensive method for nuclear structure
- Accurate low orders in open-shells

Is PT converging? Not always!

- · Possible to check in restricted model-spaces...
- ... but not in realistic calculations

Eigenvector Continuation

D. Frame *et al.*, Phys. Rev. Lett. 121, 032501 (2018) ${igstar} H(x) = H_0 + x H_1$

From perturbative to non-perturbative regime

$$x \sim 0$$
 $x = 1$

$$|\Psi^{EC}
angle = \operatorname*{argmin}_{|\Psi
angle\in\operatorname{span}\{\mathcal{V}\}} rac{\langle\Psi|H|\Psi
angle}{\langle\Psi|\Psi
angle}$$

Properties

- Variational
- As expensive as PT

Perturbation Theory

 $H = H_0 + H_1$ $\mathcal{V} = |\Psi^{(0)}\rangle, \cdots, |\Psi^{(P)}\rangle$

Many-body method

A. Tichai et al., arXiv:2001.10433 (2020)

- Least expensive method for nuclear structure
- Accurate low orders in open-shells

Is PT converging? Not always!

- Possible to check in restricted model-spaces...
- ... but not in realistic calculations

Eigenvector Continuation

D. Frame *et al.*, Phys. Rev. Lett. 121, 032501 (2018) ${igsar} H(x) = H_0 + x H_1$

From perturbative to non-perturbative regime

$$x \sim 0$$
 $x = 1$

$$\Psi^{EC} \rangle = \operatorname*{argmin}_{|\Psi\rangle \in \operatorname{span}\{\mathcal{V}\}} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Properties

- Variational
- As expensive as PT

Accuracy? Convergence rate?

Towards high orders

P. Demol et al., arXiv:1911.12578 (2019)

• Small one-body basis (emax 4)

- Small configuration space (up to triples)
- Comparison with exact diagonalisation (BCI)

P. Demol et al., arXiv:2002.02724 (2020)

Towards high orders

P. Demol et al., arXiv:1911.12578 (2019)

P. Demol et al., arXiv:2002.02724 (2020)

• Small one-body basis (emax 4)

- Small configuration space (up to triples)
- Comparison with exact diagonalisation (BCI)



Towards high orders

• Small one-body basis (emax 4)

- Small configuration space (up to triples)
- Comparison with exact diagonalisation (BCI)



Results

- BMBPT(2,3) withing few % of BCI
- But eventually diverges
- Exponential convergence of EC
- EC accurate wrt. Truncated BCI

P. Demol et al., arXiv:1911.12578 (2019)

P. Demol et al., arXiv:2002.02724 (2020)

Towards high orders

Small one-body basis (emax 4)

- Small configuration space (up to triples)
- Comparison with exact diagonalisation (BCI)



Results

- BMBPT(2,3) withing few % of BCI
- But eventually diverges
- Exponential convergence of EC
- EC accurate wrt. Truncated BCI

Realistic calculations?

P. Demol et al., arXiv:1911.12578 (2019)

P. Demol et al., arXiv:2002.02724 (2020)

EC built on top of PT

- EC(2,3) from singles and doubles
- NO2B approximation
- Realistic model spaces

EC built on top of PT

- EC(2,3) from singles and doubles
- NO2B approximation
- Realistic model spaces

Reference state

- Symmetry-broken HFB
 - Axially deformed
 - Parity-breaking

EC built on top of PT

- EC(2,3) from singles and doubles
- NO2B approximation
- Realistic model spaces

Reference state

- Symmetry-broken HFB
 - Axially deformed
 - Parity-breaking



EC built on top of PT

- EC(2,3) from singles and doubles
- NO2B approximation
- Realistic model spaces

Reference state

- Symmetry-broken HFB
 - Axially deformed
 - Parity-breaking

On the poster

- Oxygen chain for comparison
- Discussion on the results



- Variational
- Applicable to all observables (e.g. densities)

- Variational
- Applicable to all observables (e.g. densities)



- Variational
- Applicable to all observables (e.g. densities)





- Variational
- Applicable to all observables (e.g. densities)





Thanks for your attention

Hope to see you at the poster session!

References

Improved many-body expansions from eigenvector continuation arXiv:1911.12578 (2019)

P. Demol, T. Duguet, A. Ekström, M. Frosini, K. Hebeler, S. König, D. Lee, A. Schwenk, V. Somà, and A. Tichai

Bogoliubov many-body perturbation theory under constraint

arXiv:2002.02724 (2020)

P. Demol, M. Frosini, A. Tichai V. Somà, and T. Duguet

Acknowledgments



KU LEUVEN



Jean-Paul Ebran

Alexander Tichai

- Raphael Lasseri
- Vittorio Somà

Pepijn Demol



- TECHNISCHE UNIVERSITÄT DARMSTADT
- Robert Roth

- Andrea Porro
- Lorenzo Contessi
- Franscesco Raimondi
- Julien Ripoche
- Heiko Hergert
- Benjamin Bally
- Pierre Arthuis







UNIVERSITY OF