# Extending the reach of ab initio approaches using tensor factorization

**Lars Zurek**

with Thomas Duguet, Jean-Paul Ebran, and Mikael Frosini

ECT* next generation ab initio workshop, July 16, 2025

# Outline

- $H^{40}$ as driver of correlation energy and singular spectrum
- Need for cost reduction in BMBPT
- SVD-BMBPT

# $H^{40}$: driver of correlation energy

- This talk: Bogoliubov many-body perturbation theory, but ideas general

Duguet, Signoracci, JPG **44** (2016)
Tichai et al., PLB **786** (2018)
Arthuis et al., CPC **240** (2019)

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- Normal-order grand potential $\Omega = H - \lambda_A A$ and split

$$\Omega = \underbrace{\Omega^{00} + \Omega^{11}}_{\text{HFB}} + \underbrace{H^{22} + H^{31} + H^{13} + H^{40} + H^{04}}_{\text{via (perturbative) corrections}}$$

- Normal-ordered components

$$H^{40} = \frac{1}{4!} \sum_{k_1 \ldots k_4} H^{40}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4}$$

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- 3N interaction treated through rank reduction

Frosini et al., EPJA **57** (2021)

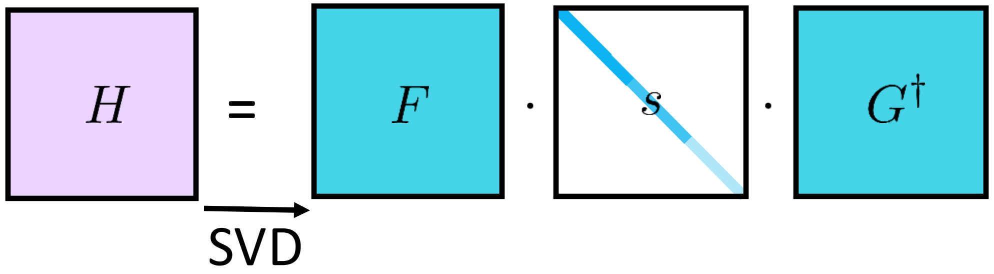
# $H^{40}$: driver of correlation energy

- First corrections to HFB ground state energy:

$$e^{(2)}_{\text{BMBPT}} = \frac{1}{4!} \sum_{k_1 \cdots k_4} \frac{H^{04}_{k_1 k_2 k_3 k_4} H^{40}_{k_1 k_2 k_3 k_4}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}} \qquad H^{04}_{k_1 k_2 k_3 k_4} = H^{40*}_{k_1 k_2 k_3 k_4}$$

$$e^{(3)}_{\text{BMBPT}} = \frac{1}{8} \sum_{k_1 \ldots k_6} \frac{H^{04}_{k_1 k_2 k_3 k_4} H^{22}_{k_3 k_4 k_5 k_6} H^{40}_{k_5 k_6 k_1 k_2}}{(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4})(E_{k_5} + E_{k_6} + E_{k_1} + E_{k_2})}$$

# Singular value decomposition



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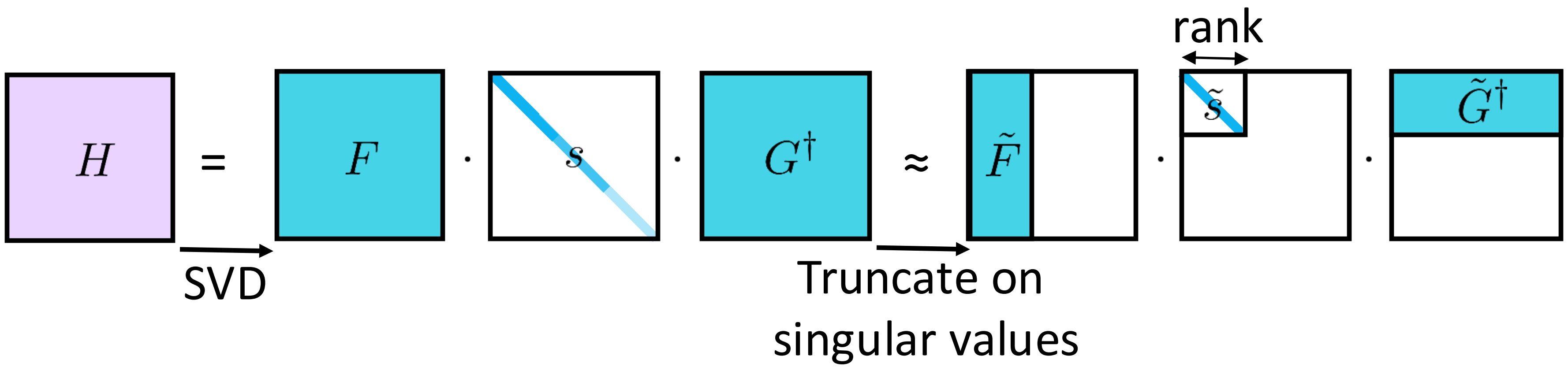

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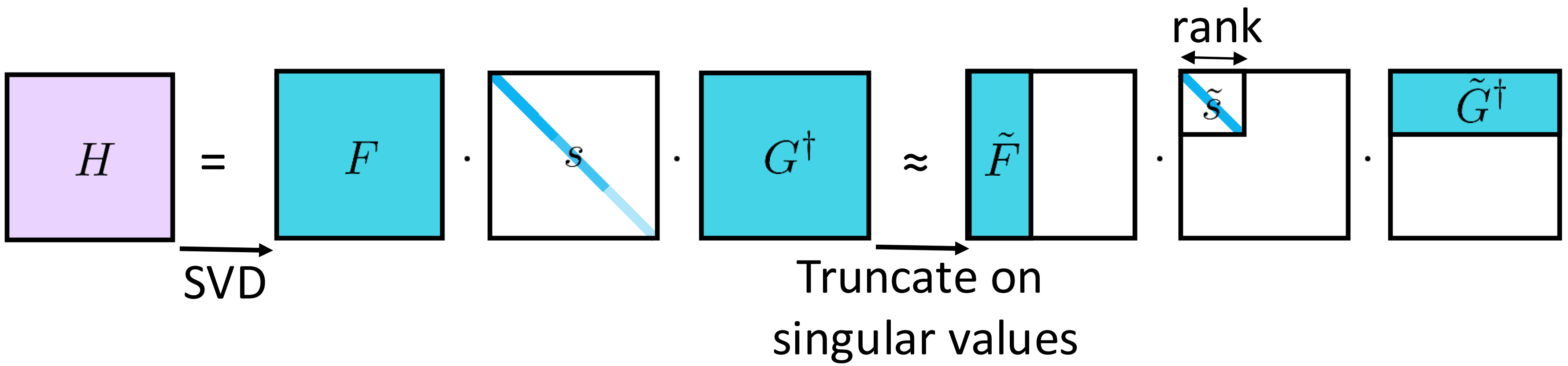
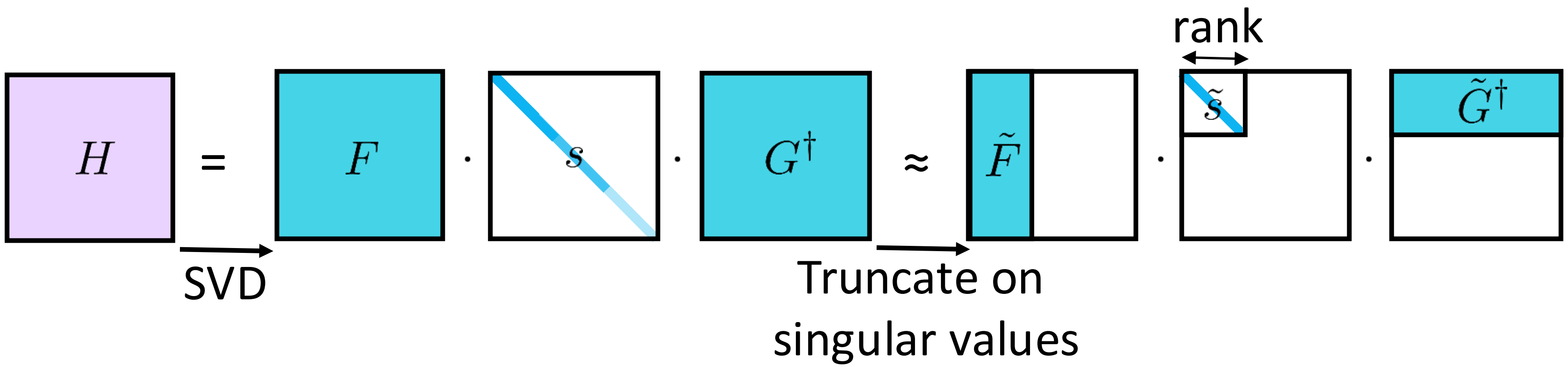
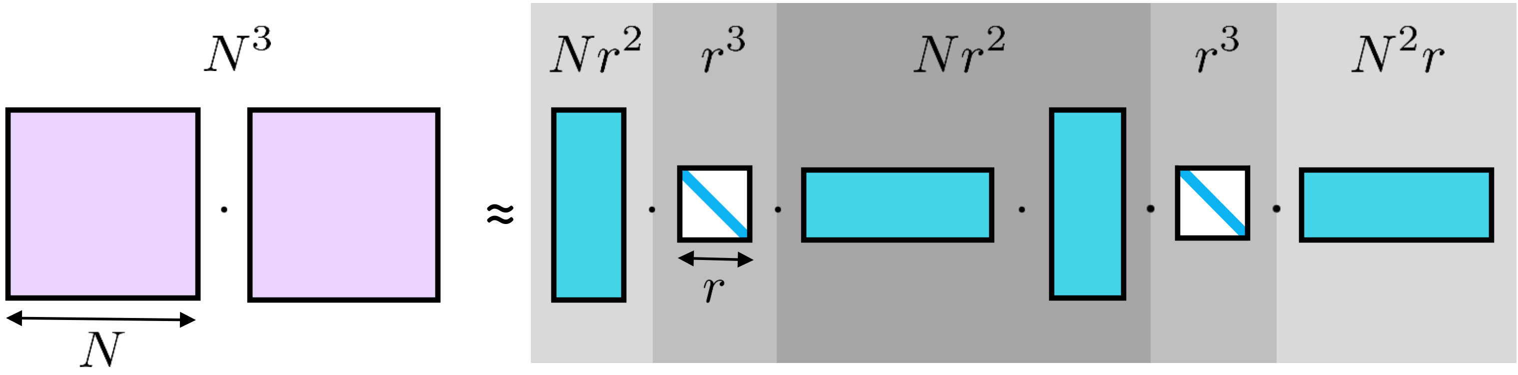



- Eckart-Young theorem: truncated SVD gives best possible rank-$r$ approximation of $H$ (measured in terms of Frobenius norm)

# Singular value decomposition




- Truncated SVD makes matrix products cheaper




- Contraction cost: $N^3 \to N^2 r$
- Maximal gain only when full matrices are never reconstructed

# $H^{40}$ singular spectrum

- Decompose $H^{40}$ using SVD

$$H^{40}_{k_1 k_2 k_3 k_4} = \sum_{\mu} F^{\mu}_{k_1 k_2} s_{\mu} G^{\mu}_{k_3 k_4}$$

form collective indices

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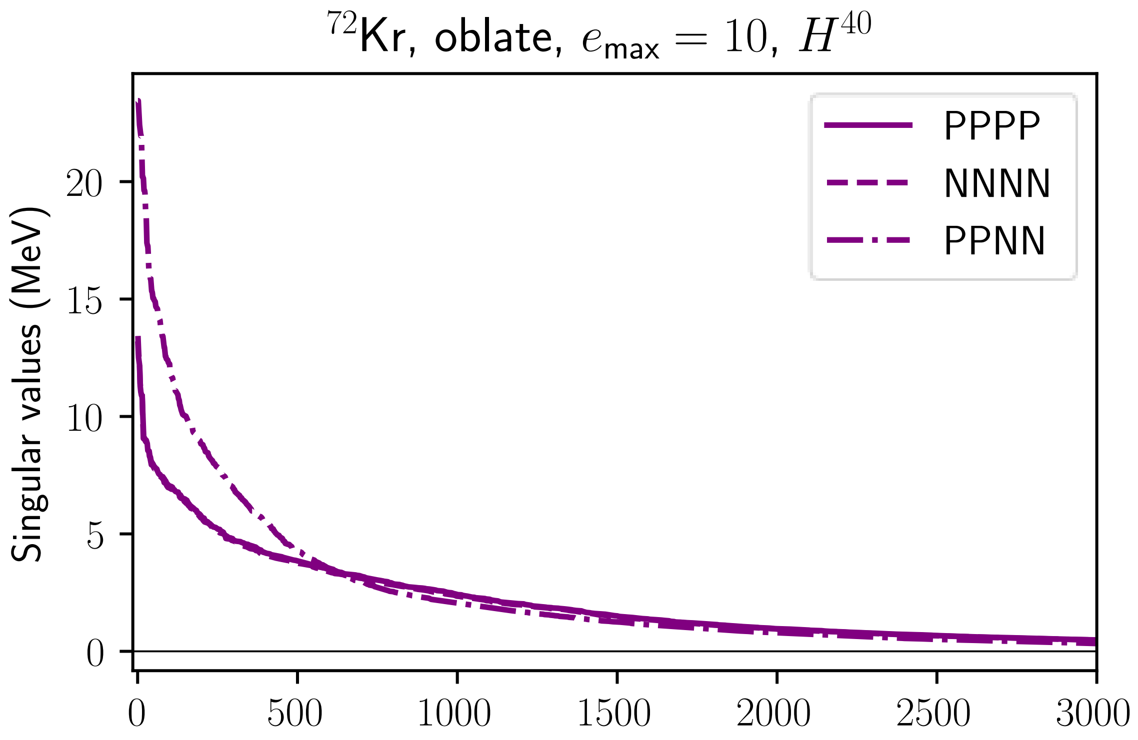


- Here and in following:
  EM (1.8/2.0), $e_{3max}$ = 16, ω = 12 MeV

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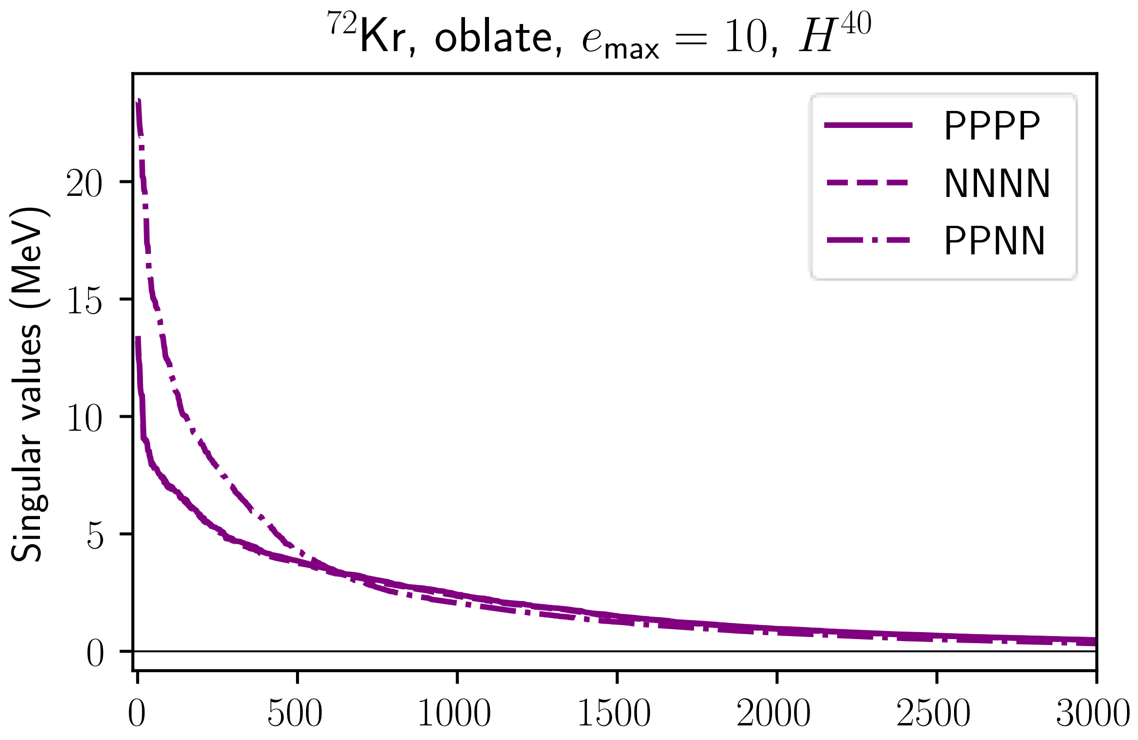
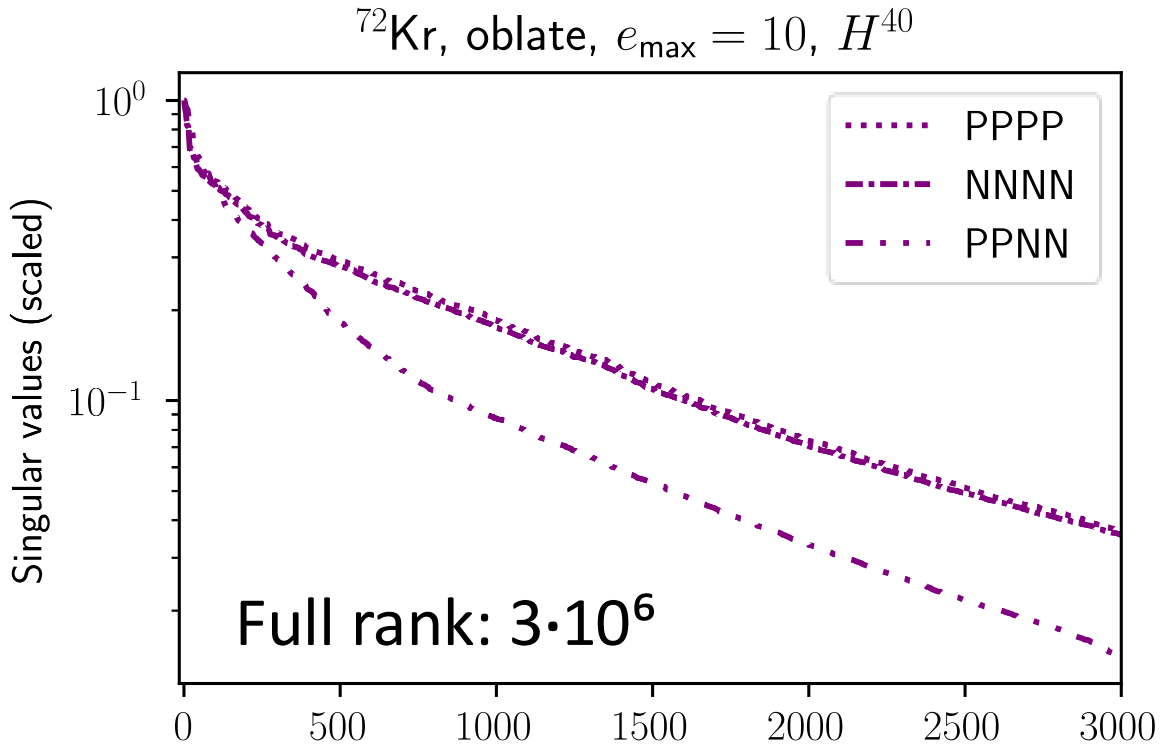
- Singular values fall off quickly
  → low-rank approximation possible



# $H^{40}$ singular spectrum

- Decompose $H^{40}$ using SVD

$$\underbrace{H^{40}_{k_1 k_2 k_3 k_4}} \approx \sum_{\mu=1}^{r} F^{\mu}_{k_1 k_2} s_\mu G^{\mu}_{k_3 k_4}$$

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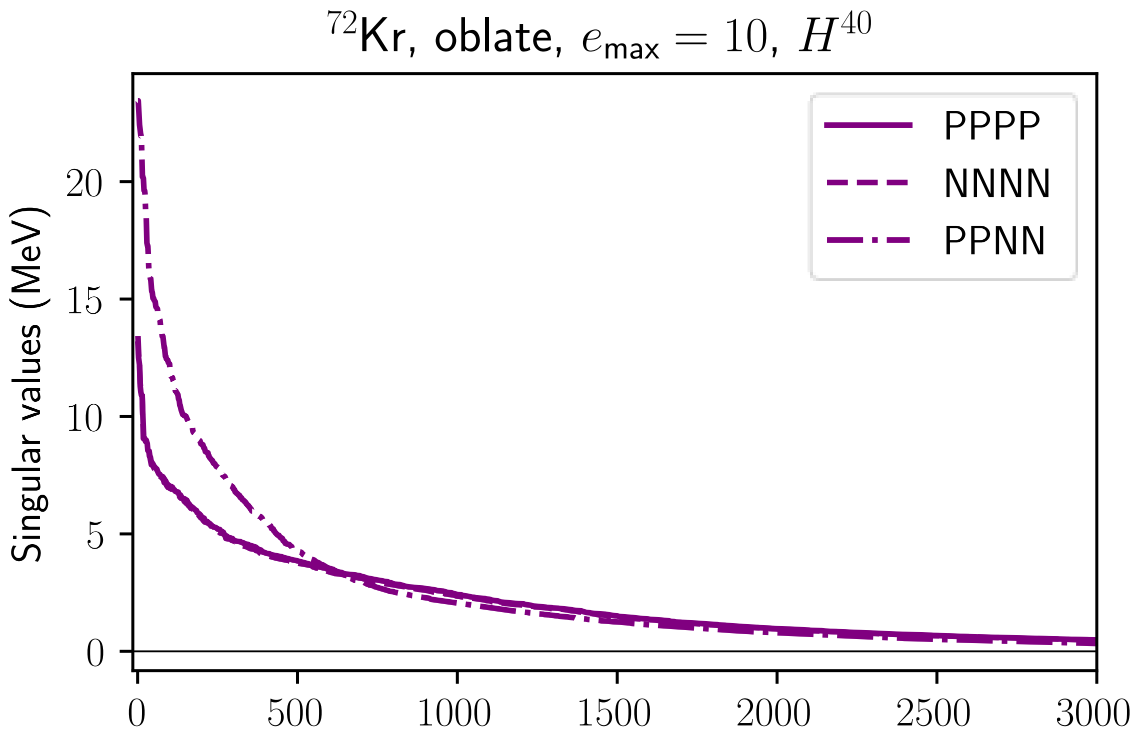
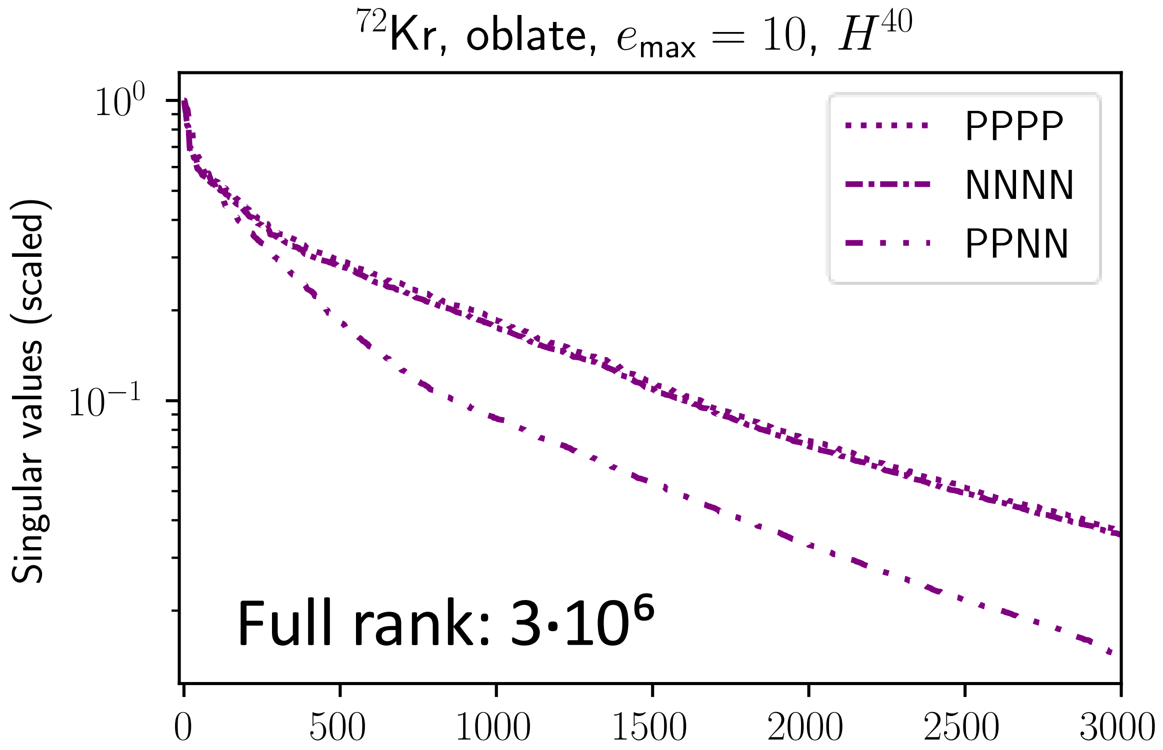
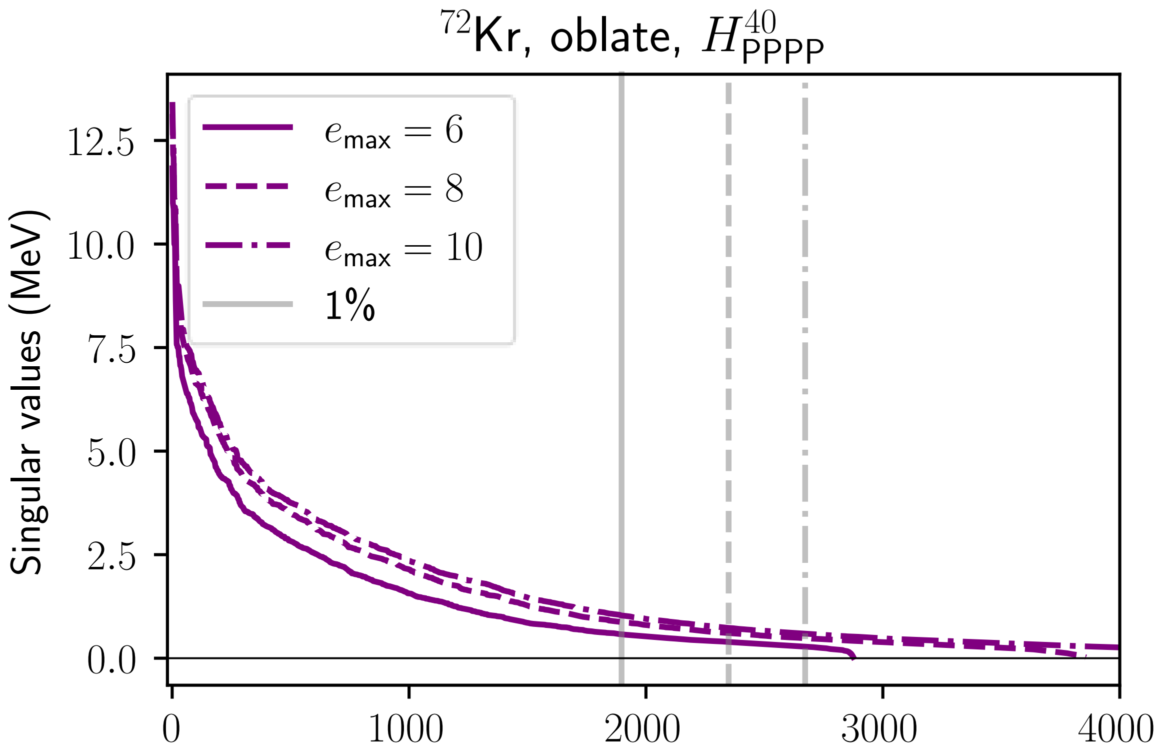


# $H^{40}$ singular spectrum

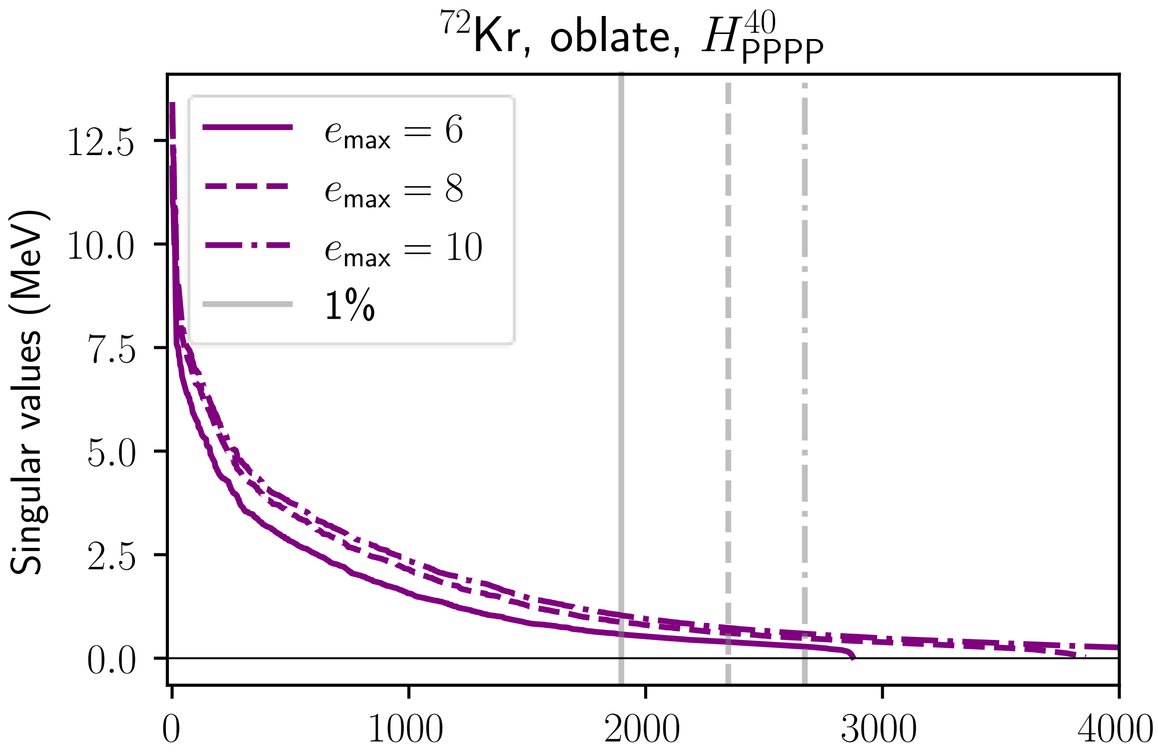
- Singular values converge with increasing $e_{max}$

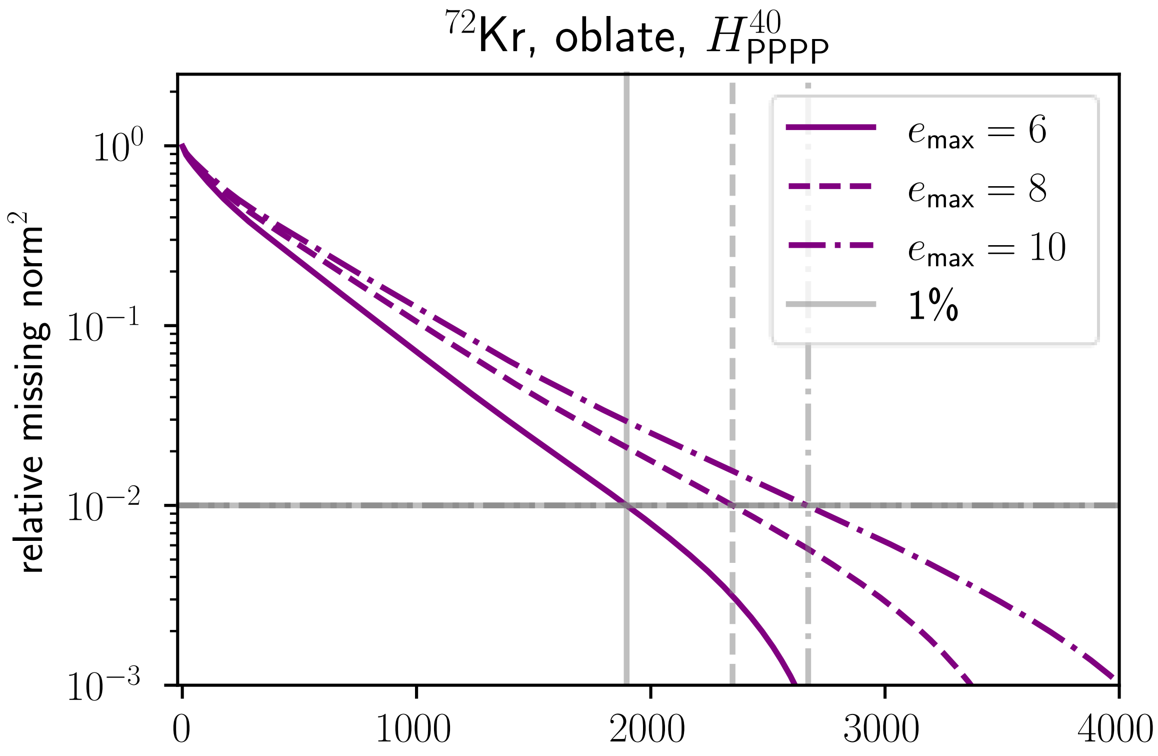


# $H^{40}$ singular spectrum

- Singular values converge with increasing $e_{max}$
- $H^{40}$ norm error strongly linked to BMBPT(2) accuracy

→ Need only $r$ ~ 2500 singular values to reach desired accuracy

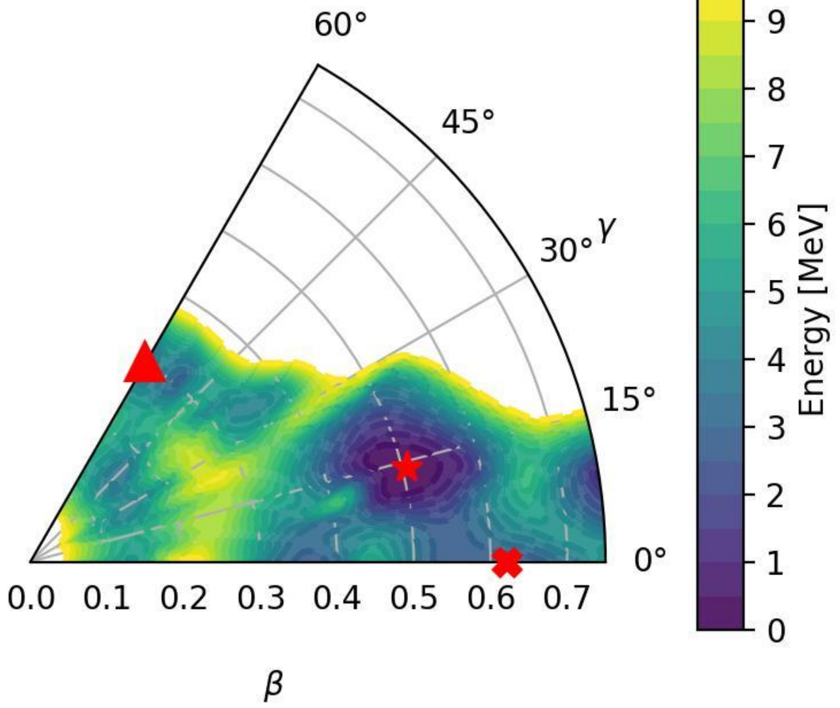


# $H^{40}$ singular spectrum

- Singular spectra very similar for HFB minima of different deformation

$^{72}$Kr, $e_{max}$ = 10



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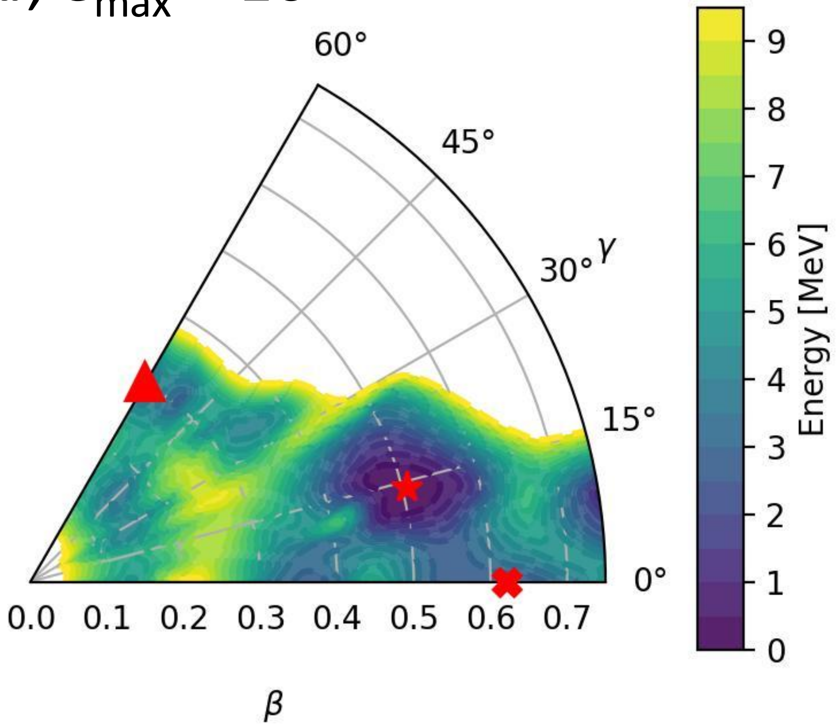
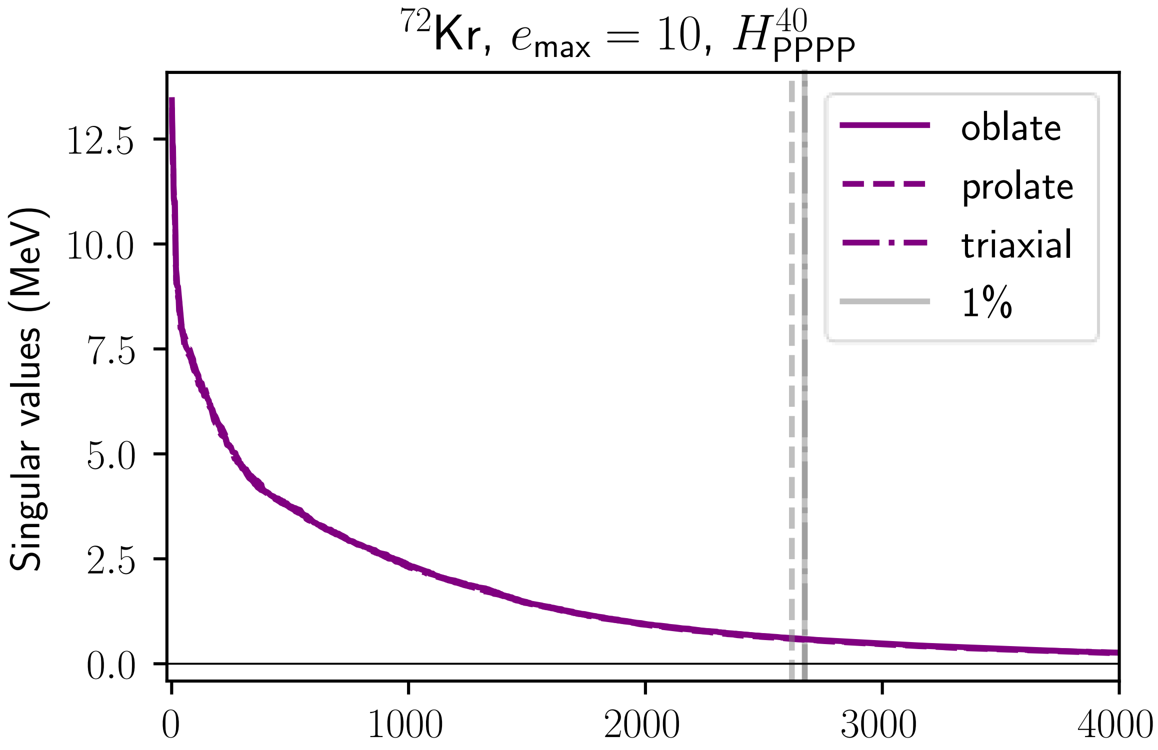
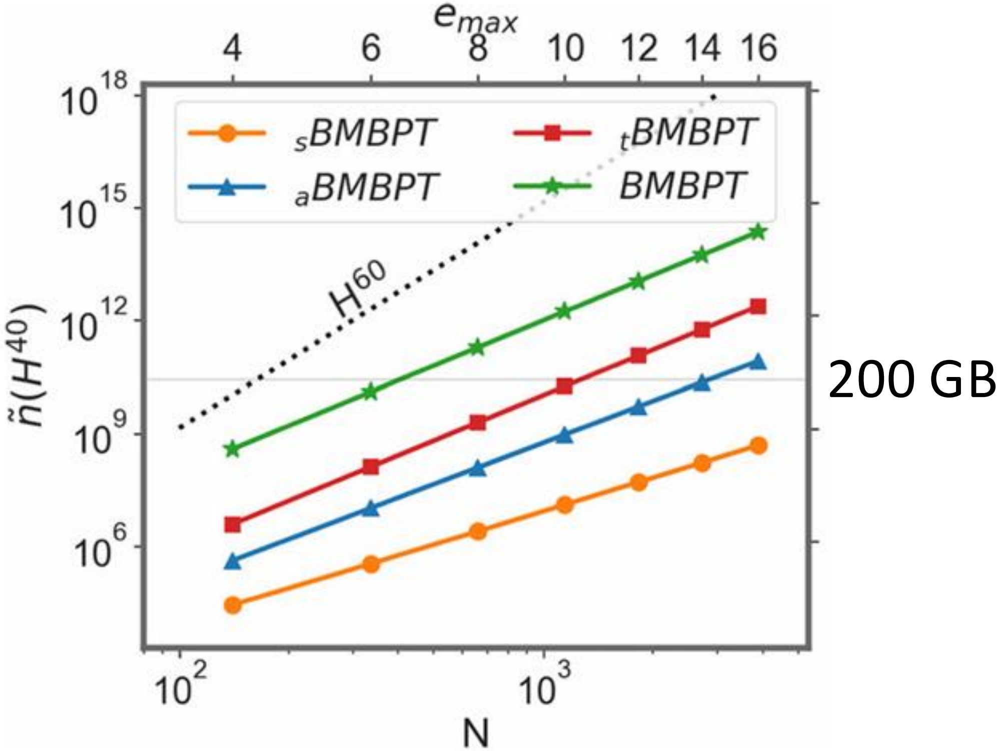


# BMBPT(2) cost

- Necessary memory scales as $N^4$

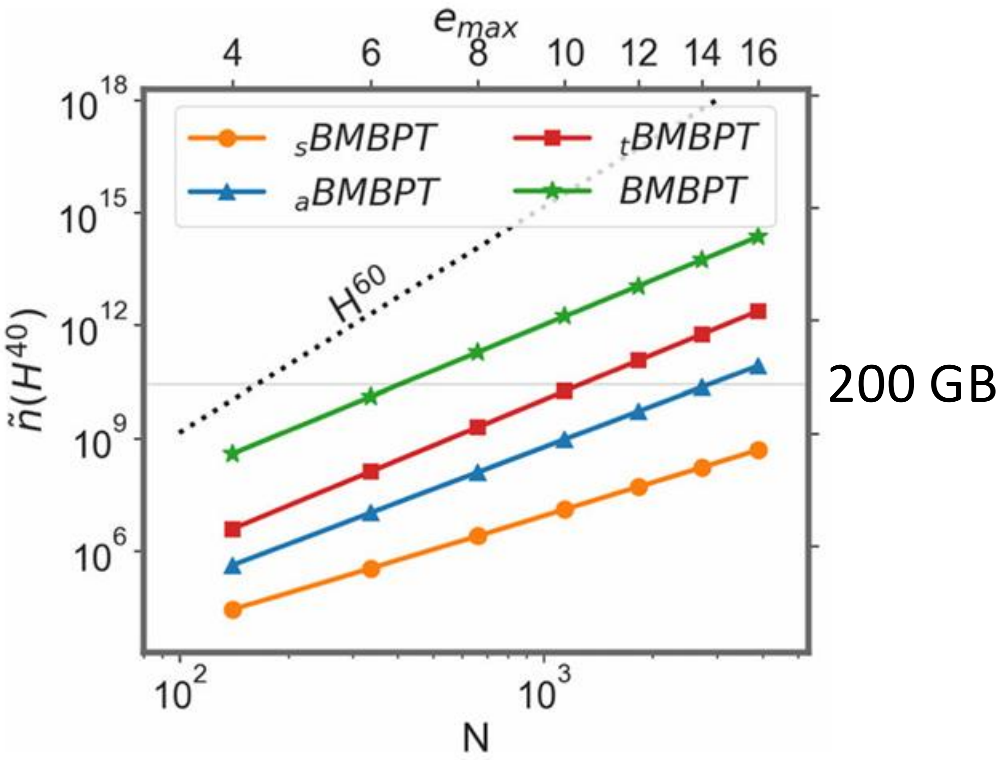



Frosini et al., EPJA **60** (2024)

# BMBPT(2) cost

- Necessary memory scales as $N^4$
- Construction of $H^{40}$ scales as $N^5$

$$H^{40}_{k_1k_2k_3k_4} = \sum_{\alpha\cdots\delta} H_{\alpha\beta\gamma\delta} U^*_{\alpha k_1} U^*_{\beta k_2} V^*_{\gamma k_3} V^*_{\delta k_4} +$$




Frosini et al., EPJA **60** (2024)

→ storage (and computation) cost needs to be reduced for heavy deformed calculations

# Required accuracy

- BMBPT as formal power series

$$E^{[P]} = \langle \Phi | H \sum_{p=0}^{P-1} (R_0\, \Omega_1^{(P)})^p | \Phi \rangle_c$$

Demol et al., EPJA **61** (2025)
Svensson et al., 2507.09079

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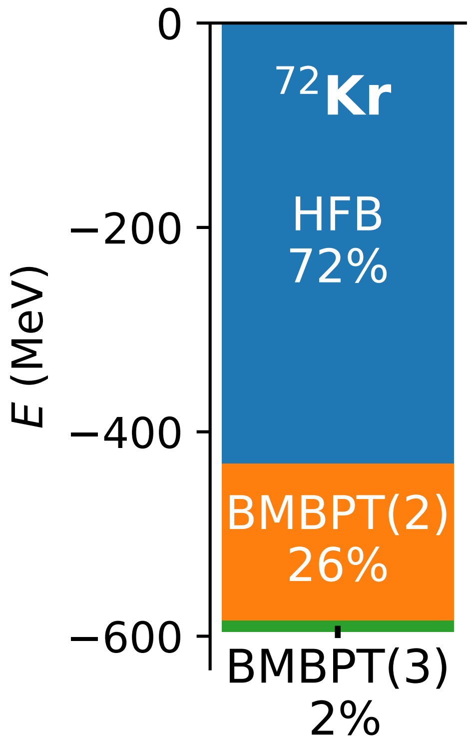
- Conservative estimate of missing next-order contribution

$$\left| e^{(4)}_{\mathrm{BMBPT}} \right| \sim \frac{1}{10} \left| e^{(3)}_{\mathrm{BMBPT}} \right| \sim \frac{1}{100} \left| e^{(2)}_{\mathrm{BMBPT}} \right|$$



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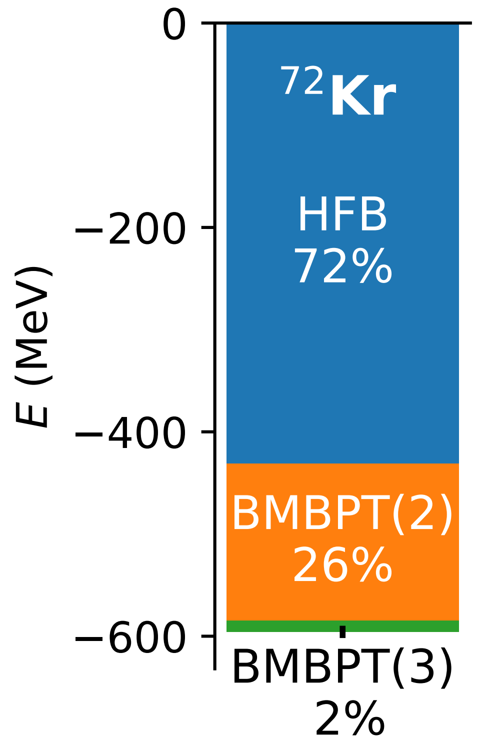
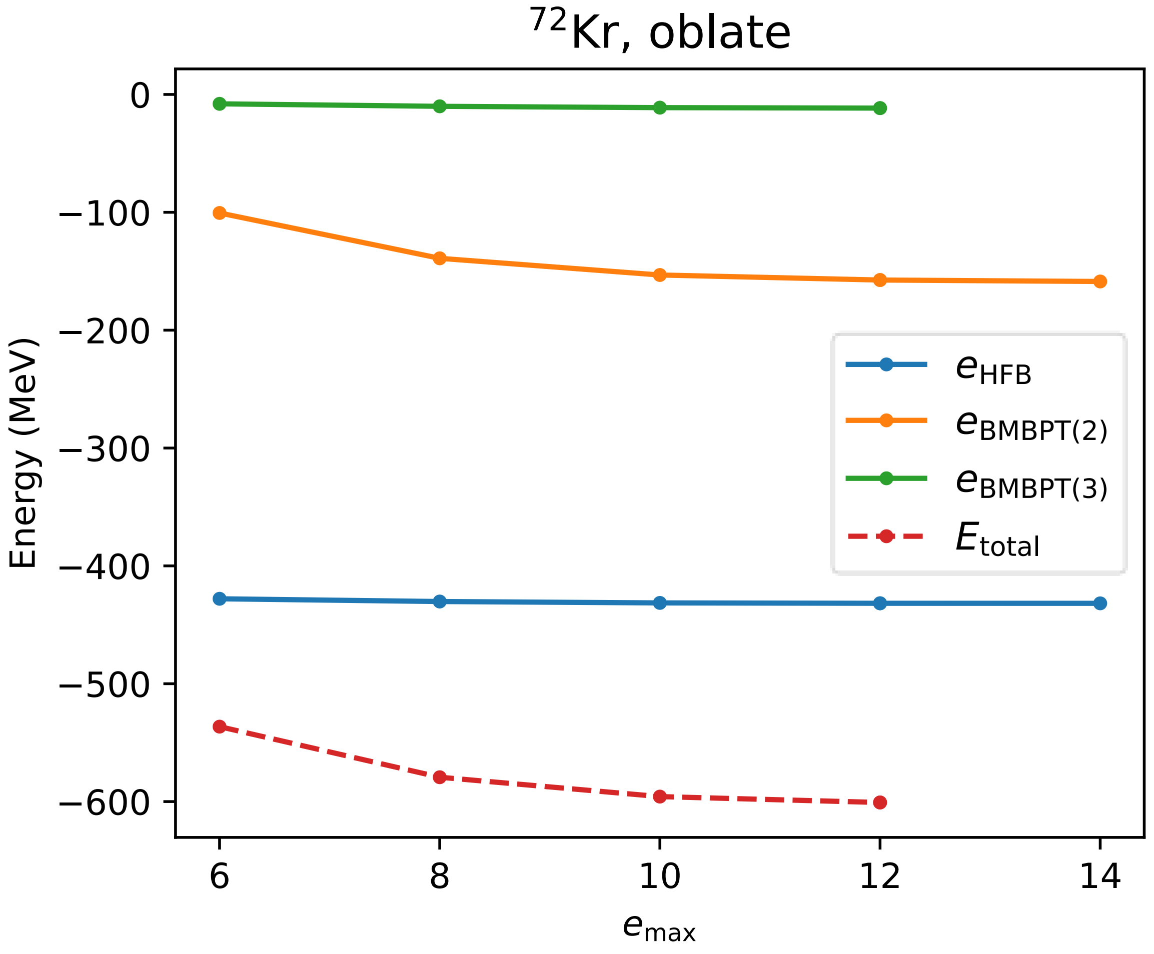
→ Defines calculation accuracy goal at BMBPT(3) level

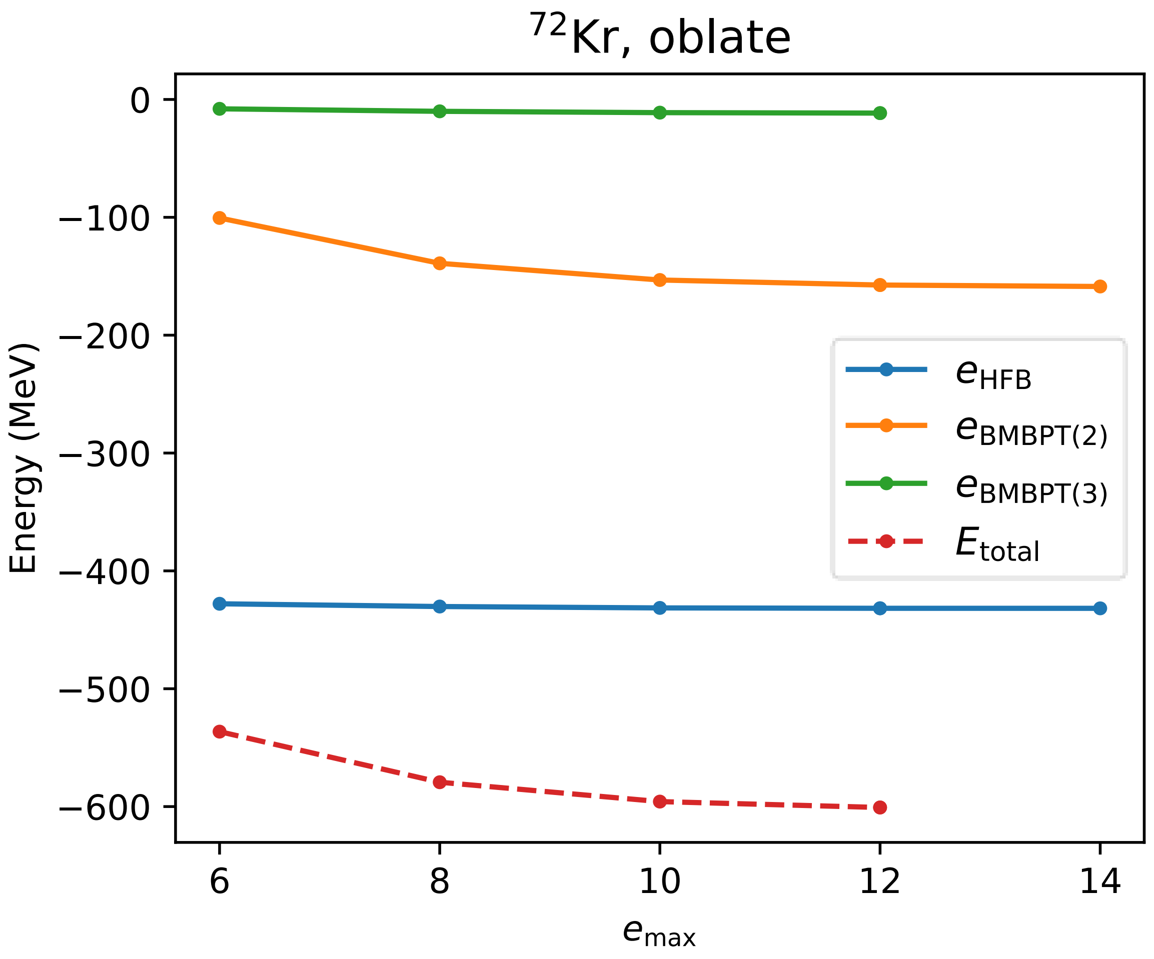


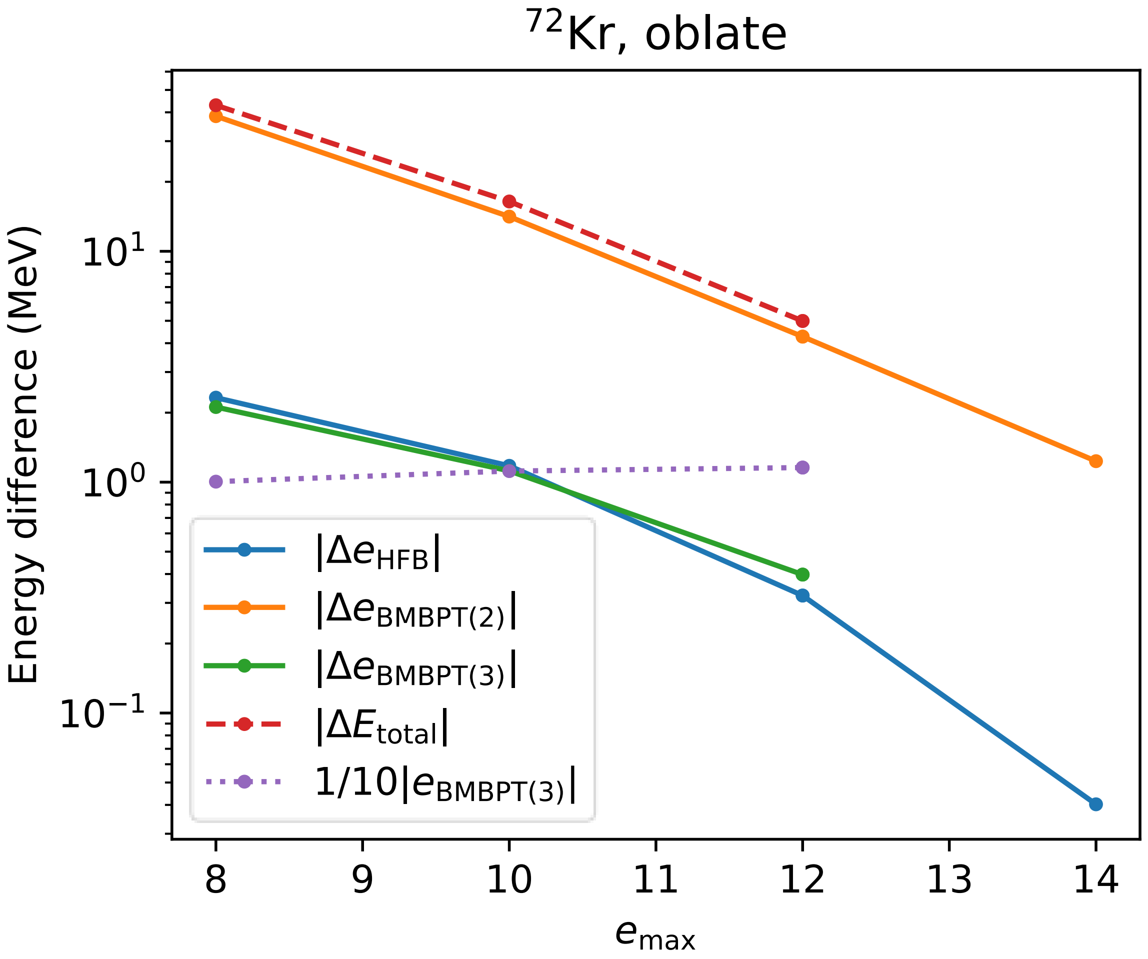
# Required accuracy: needed basis size



# Required accuracy: needed basis size

- Need $e_{max}$ ~ 14 for BMBPT(2), ~ 10 for BMBPT(3)



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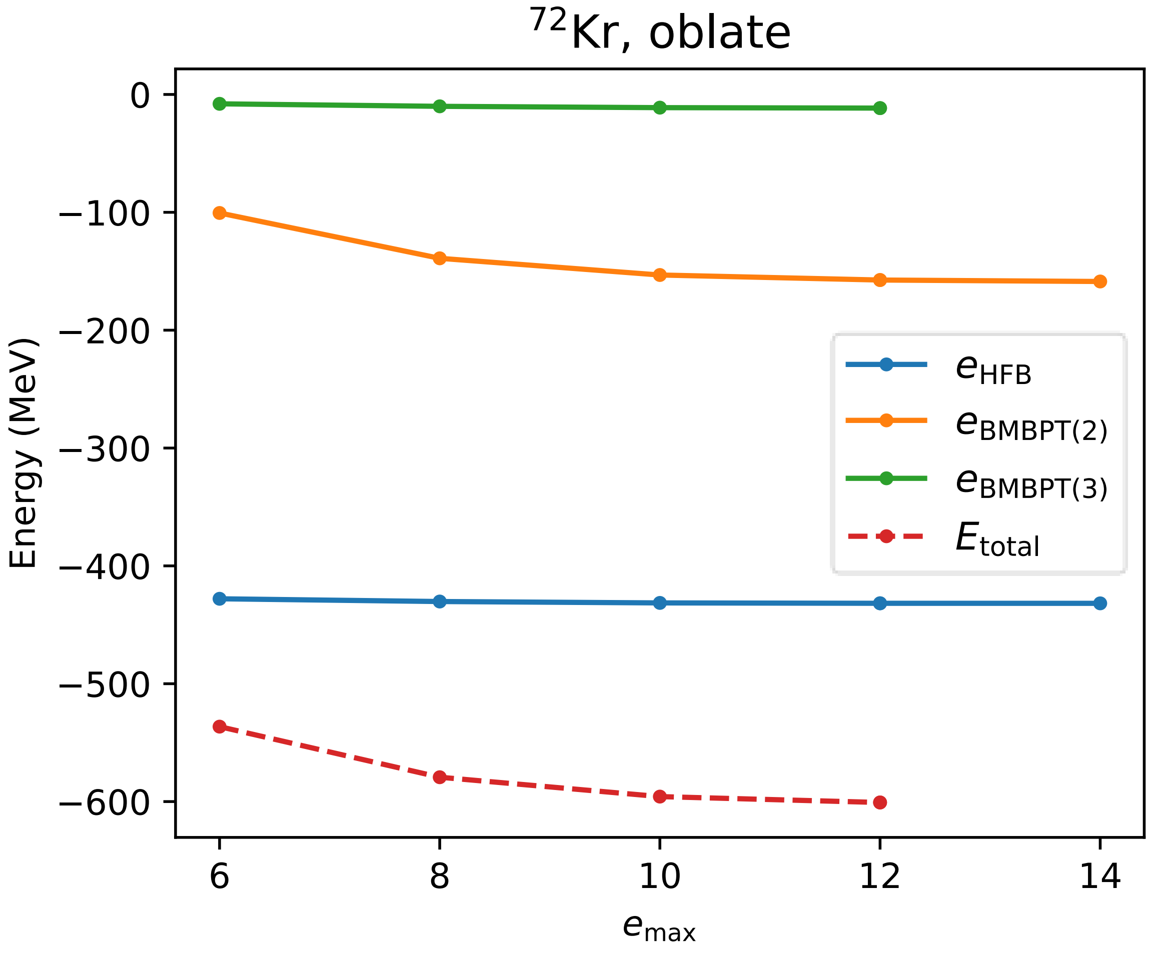
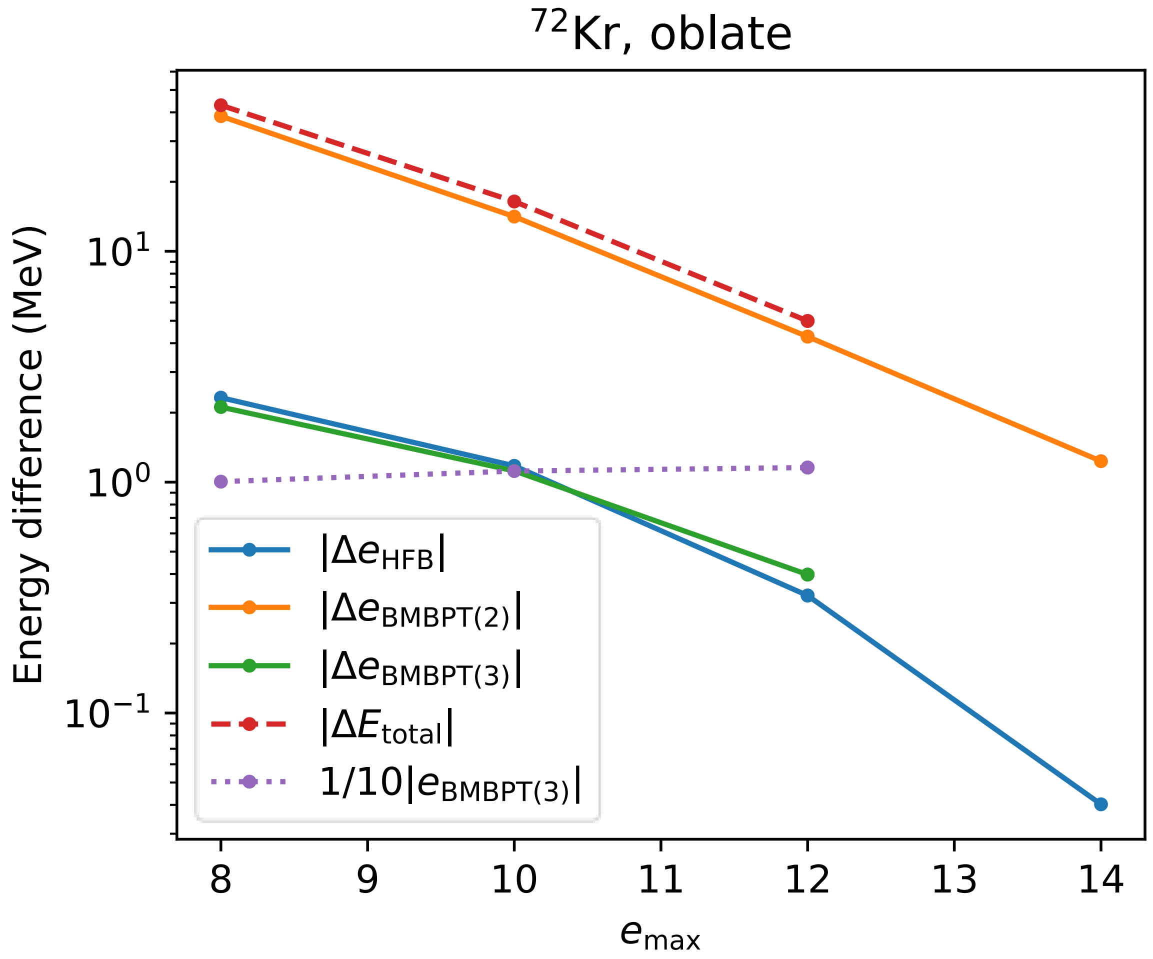



- Computed with SVD-BMBPT

# Randomized SVD

Halko et al., SIREV **53** (2011)
Martinsson, Tropp, ActaNum **403** (2020)

- Lanczos-type algorithm to find largest singular values
- Number of necessary singular values determined on the fly using stochastic estimator of decomposition quality
  Tropp, Webber, 2306.12418 (2023)
- Based on matrix-vector products

# Implicit product

Frosini et al., EPJA **60** (2024)

- To circumvent $N^5$ construction and $N^4$ storage of $H^{40}_{k_1k_2k_3k_4}$ consider instead only "matrix-vector" products

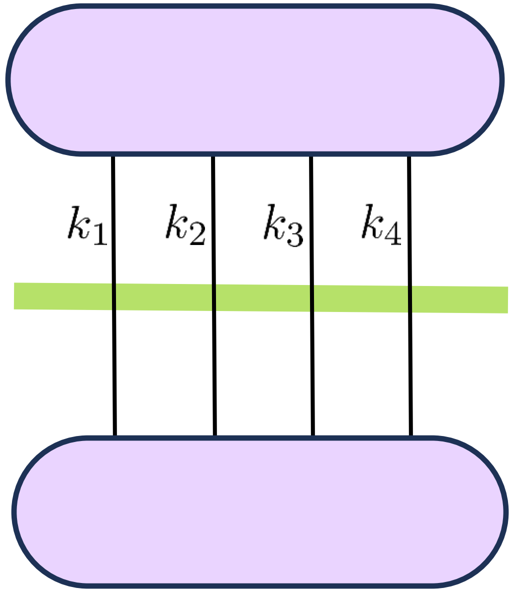
$$\sum_{k_3k_4} H^{40}_{\underline{k_1k_2}\,\underline{k_3k_4}} X^{02}_{\underline{k_3k_4}}$$

- Implicit FAM-like products    Carlsson et al., PRC **86** (2012)
    1. transform $X^{02}$ to underlying spherical HO basis
    2. calculate product in that basis
    3. transform back

→ cost of one implicit product: $N^{4-\delta}$

# BMBPT(2)

$$e^{(2)}_{\text{BMBPT}} = \frac{1}{4!} \sum_{k_1 \cdots k_4} \frac{H^{04}_{k_1 k_2 k_3 k_4} H^{40}_{k_1 k_2 k_3 k_4}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}$$



# SVD-BMBPT(2)

Frosini et al., EPJA **60** (2024)

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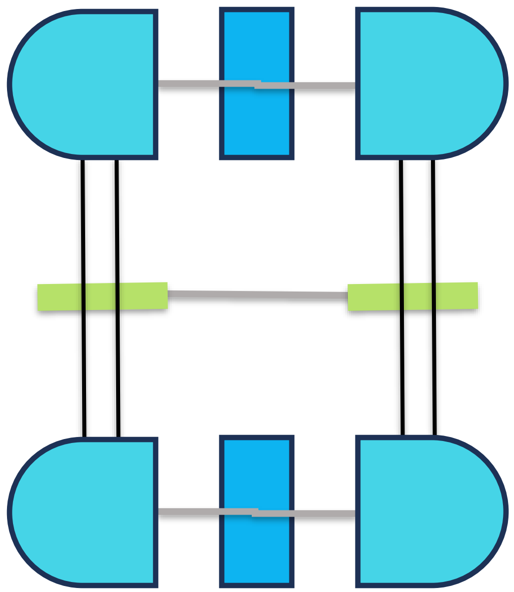
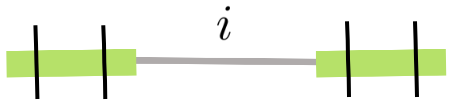


- For denominators:
  discretized inverse Laplace transform Braess, Hackbusch, IMAJNA **25** (2005)

$$\frac{1}{(E_{k_1}+E_{k_2})+(E_{k_3}+E_{k_4})} = \sum_{i=1}^{n_d\sim 10} d^{i}_{k_1k_2} d^{i}_{k_3k_4}$$



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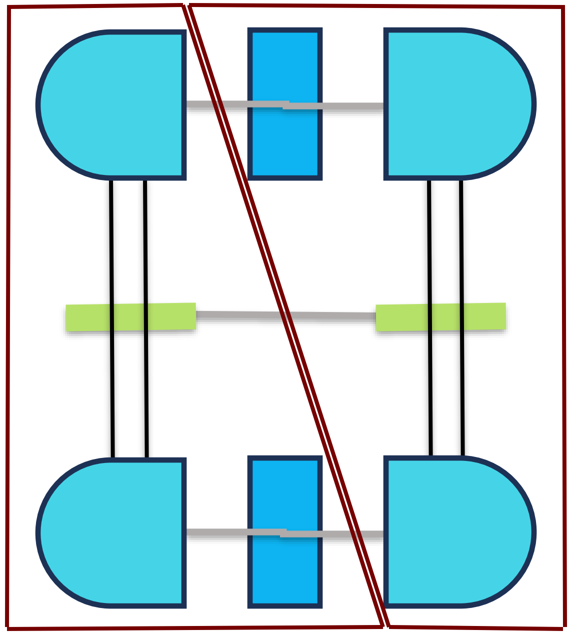

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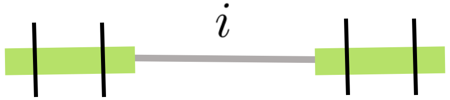


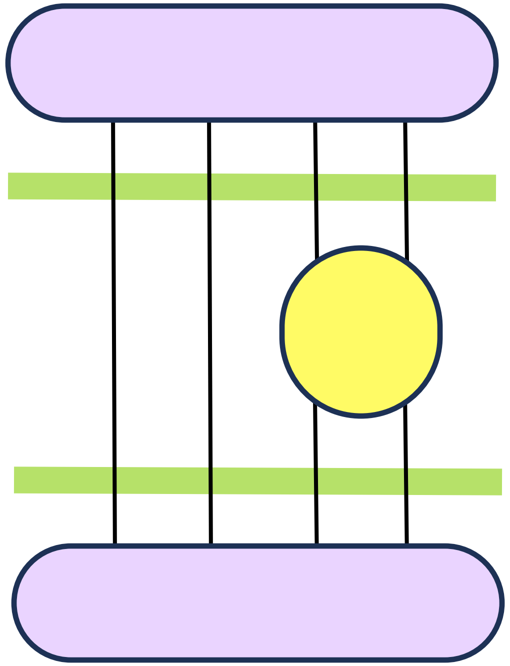

- Form intermediates by doing expensive sums first

# BMBPT(3)

- Next correction to HFB ground state energy:

$$e^{(3)}_{\text{BMBPT}} = \frac{1}{8} \sum_{k_1 \dots k_6} \frac{H^{04}_{k_1 k_2 k_3 k_4} H^{22}_{k_3 k_4 k_5 k_6} H^{40}_{k_5 k_6 k_1 k_2}}{(E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4})(E_{k_5} + E_{k_6} + E_{k_1} + E_{k_2})}$$

- Evaluation of energy scales as $N^6$



# BMBPT(3)

$$-C^{40}_{k_5 k_6 k_1 k_2}(2)$$

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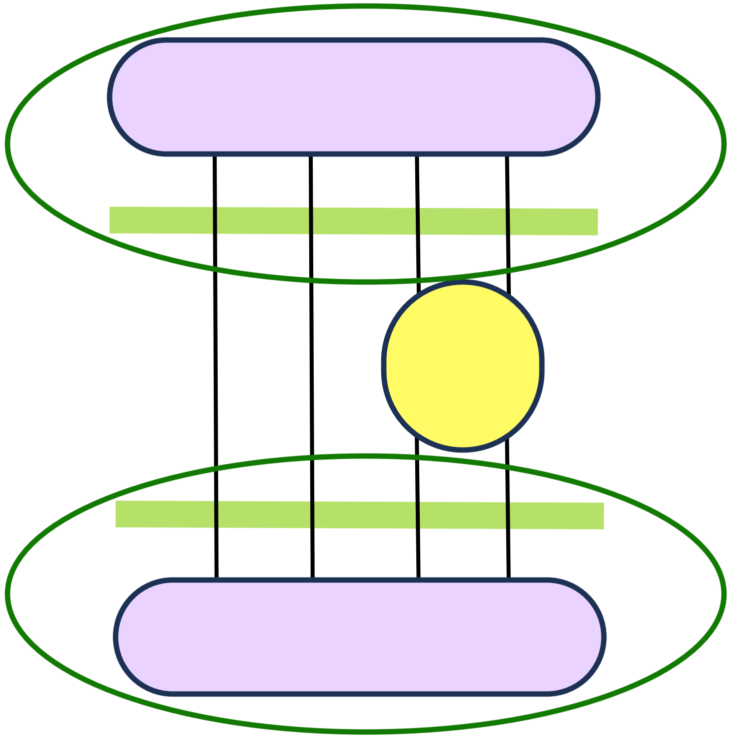
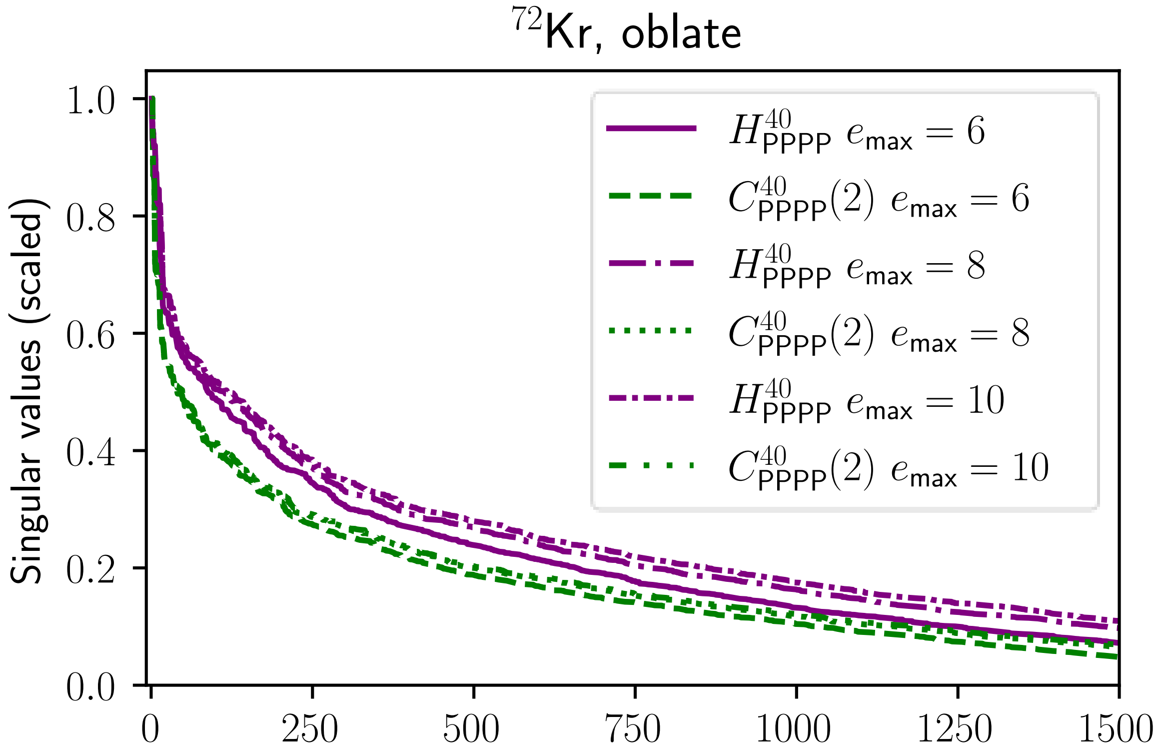


# Singular spectrum

- $C^{40}(2)$ initially falls off a bit faster than $H^{40}$



# Singular spectrum

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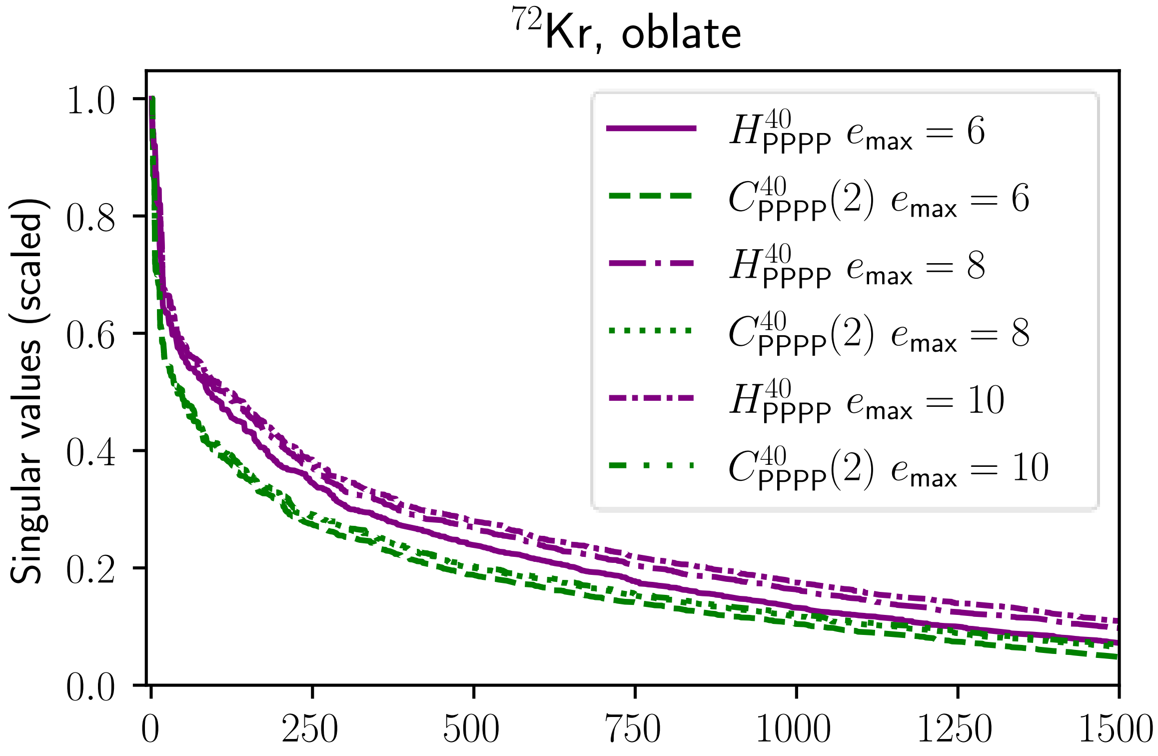
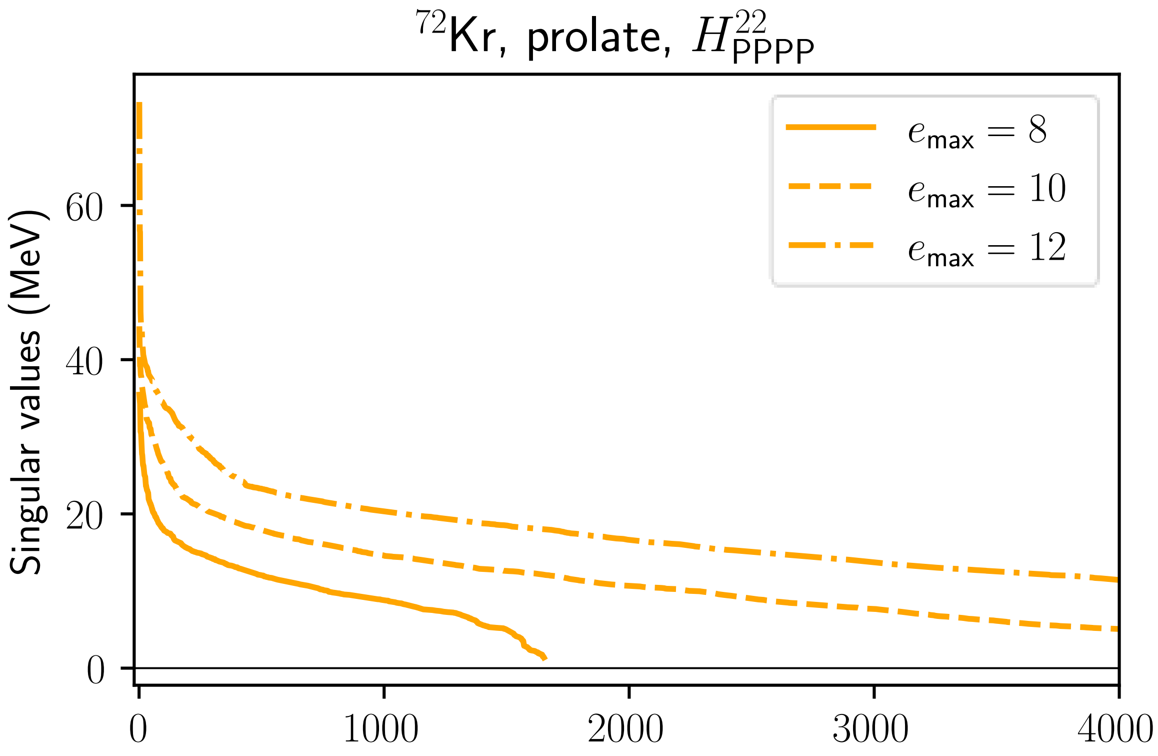
- $H^{22}$ does not converge with increasing $e_{max}$

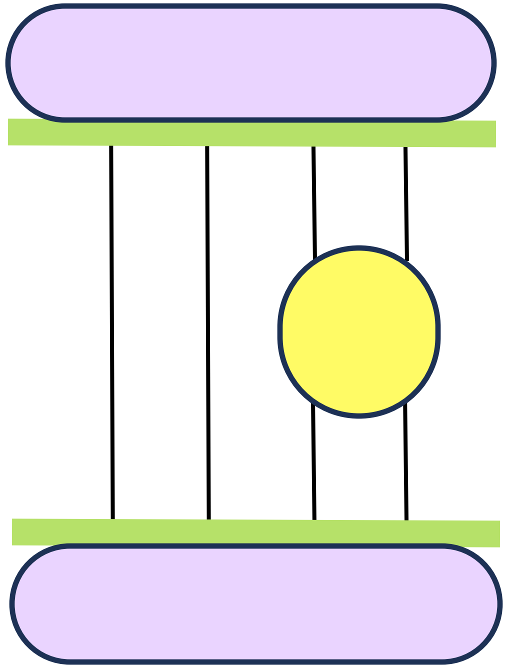


# SVD-BMBPT(3)

- Project $H^{22}$ to both sides on subspace spanned $C^{40}(2)$ by singular vectors

$$s'_{\mu\nu} = \sum_{k_1 \dots k_4} F^{\mu *}_{k_1 k_2} H^{22}_{k_1 k_2 k_3 k_4} F^{\nu}_{k_3 k_4}$$



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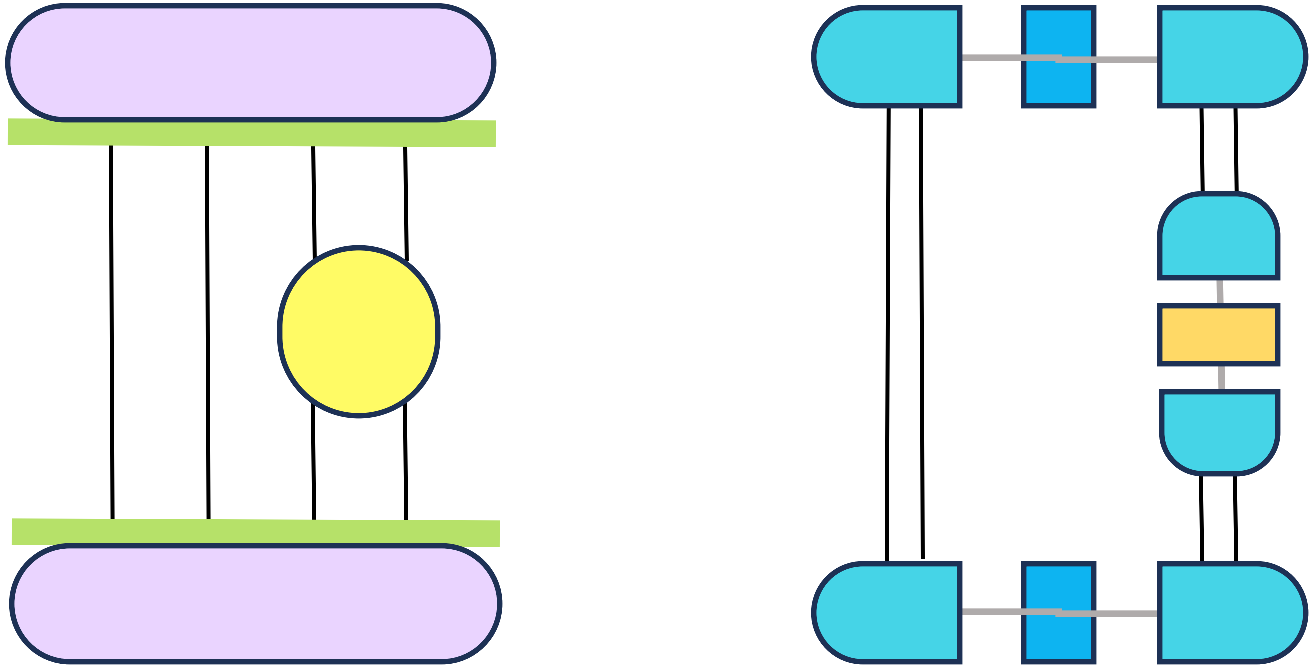

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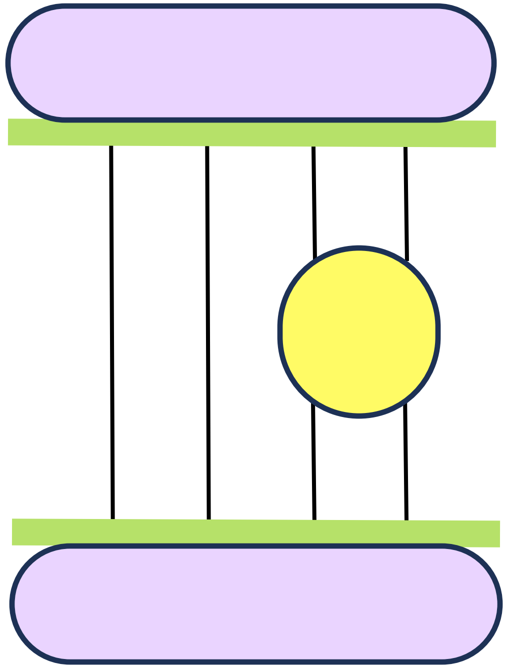
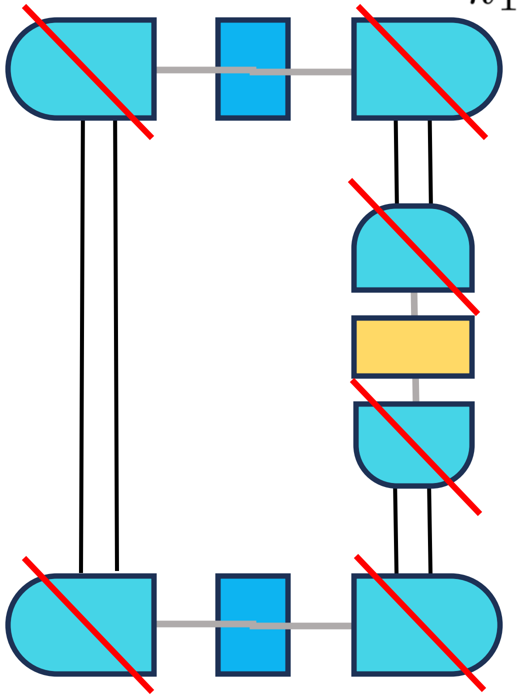
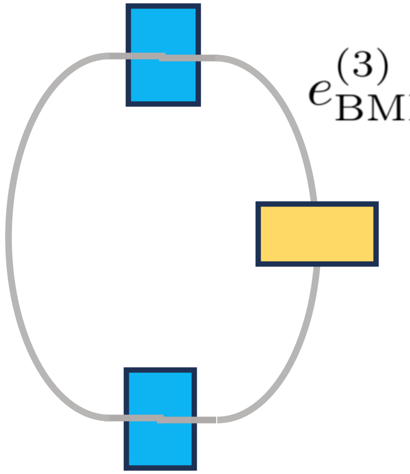
- Singular vectors form unitary matrices $\sum_{k_1 k_2} F^{\mu *}_{k_1 k_2} F^{\nu}_{k_1 k_2} = \delta_{\mu\nu}$



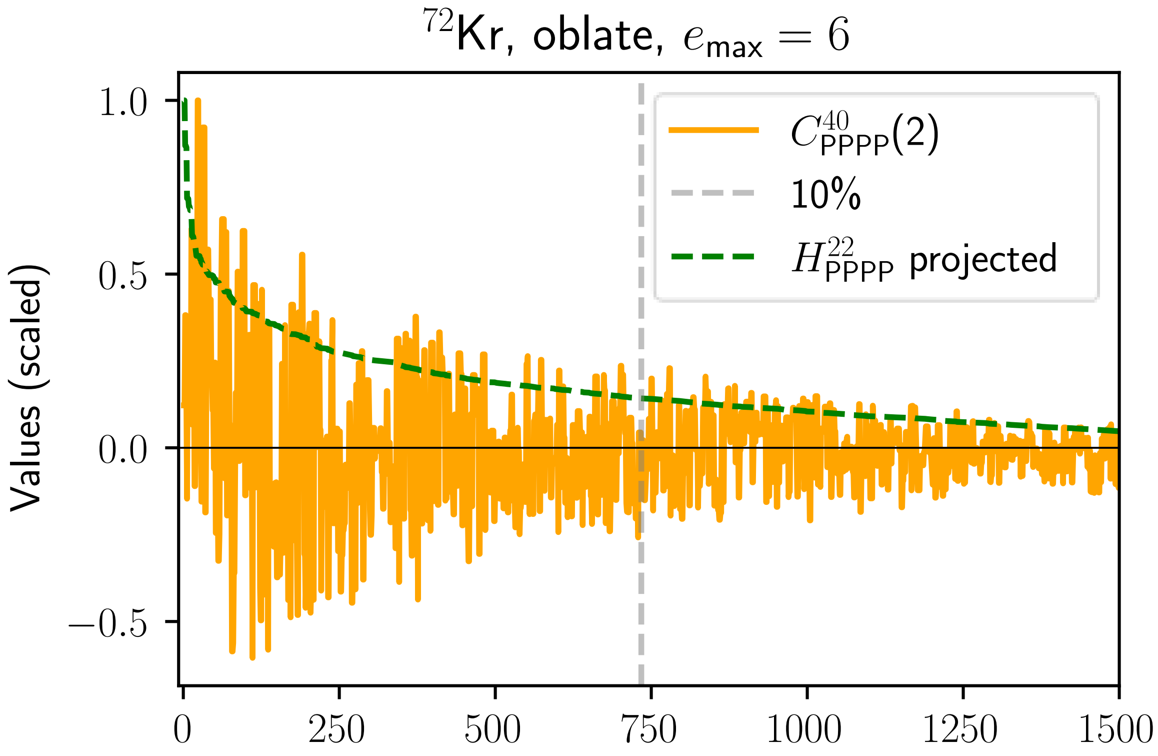




$$e^{(3)}_{\mathrm{BMBPT}} = \frac{1}{8} \sum_{\mu} s^2_{\mu} s'_{\mu\mu}$$

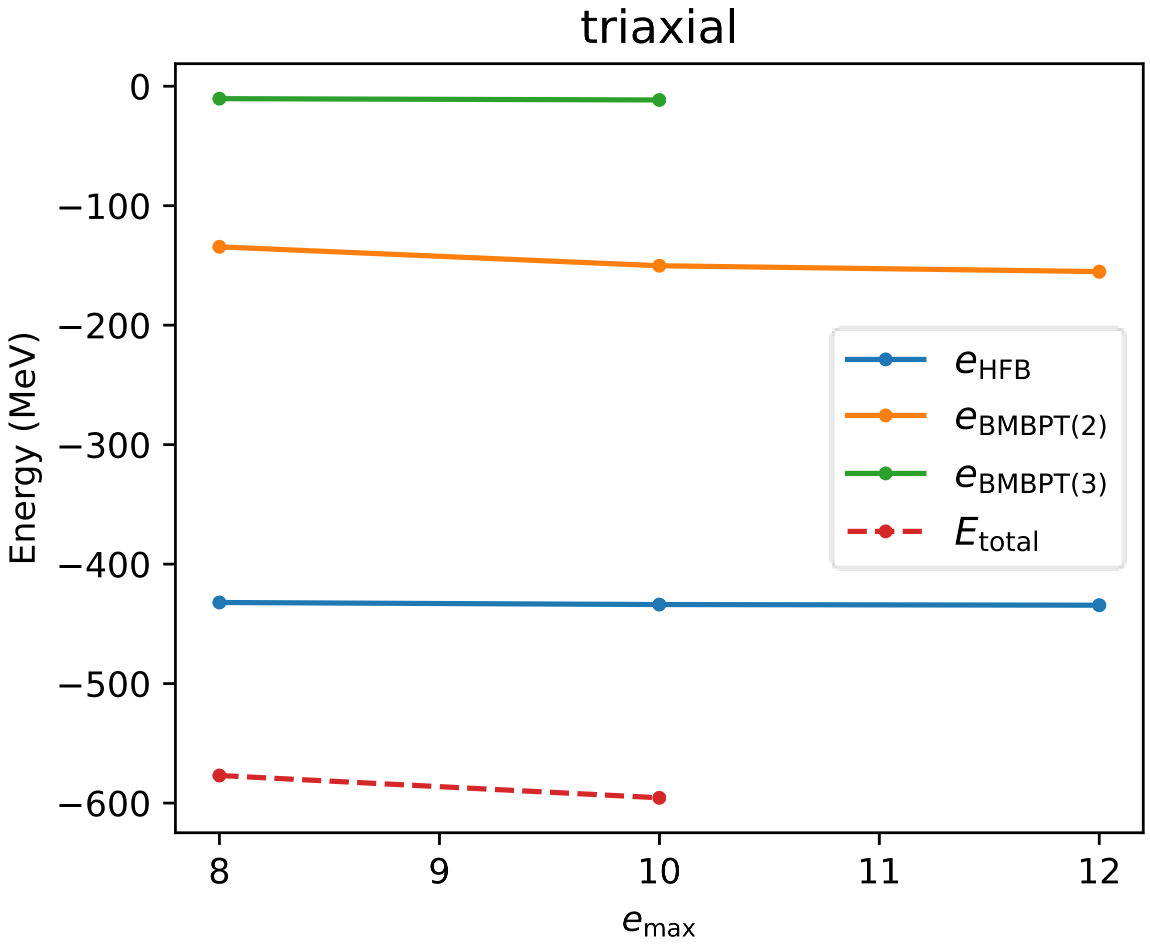
# $H^{40}$ singular spectrum

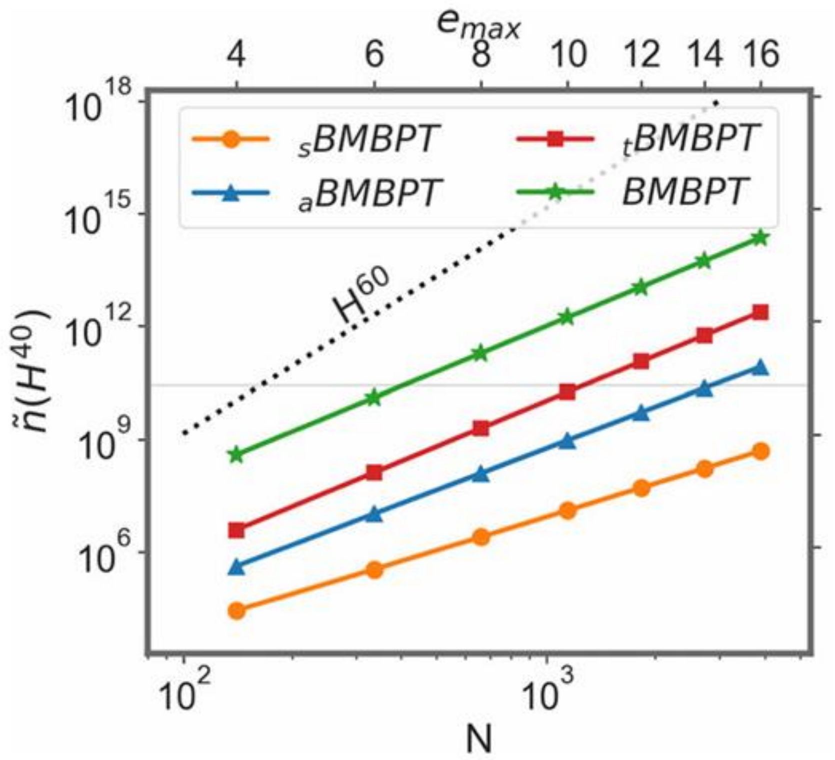
- $H^{22}$ projected on subspace spanned $C^{40}(2)$ by singular vectors falls off



# Summary

- Tensor factorization allows to make computationally unfeasible calculations tractable




Frosini et al., EPJA **60** (2024)

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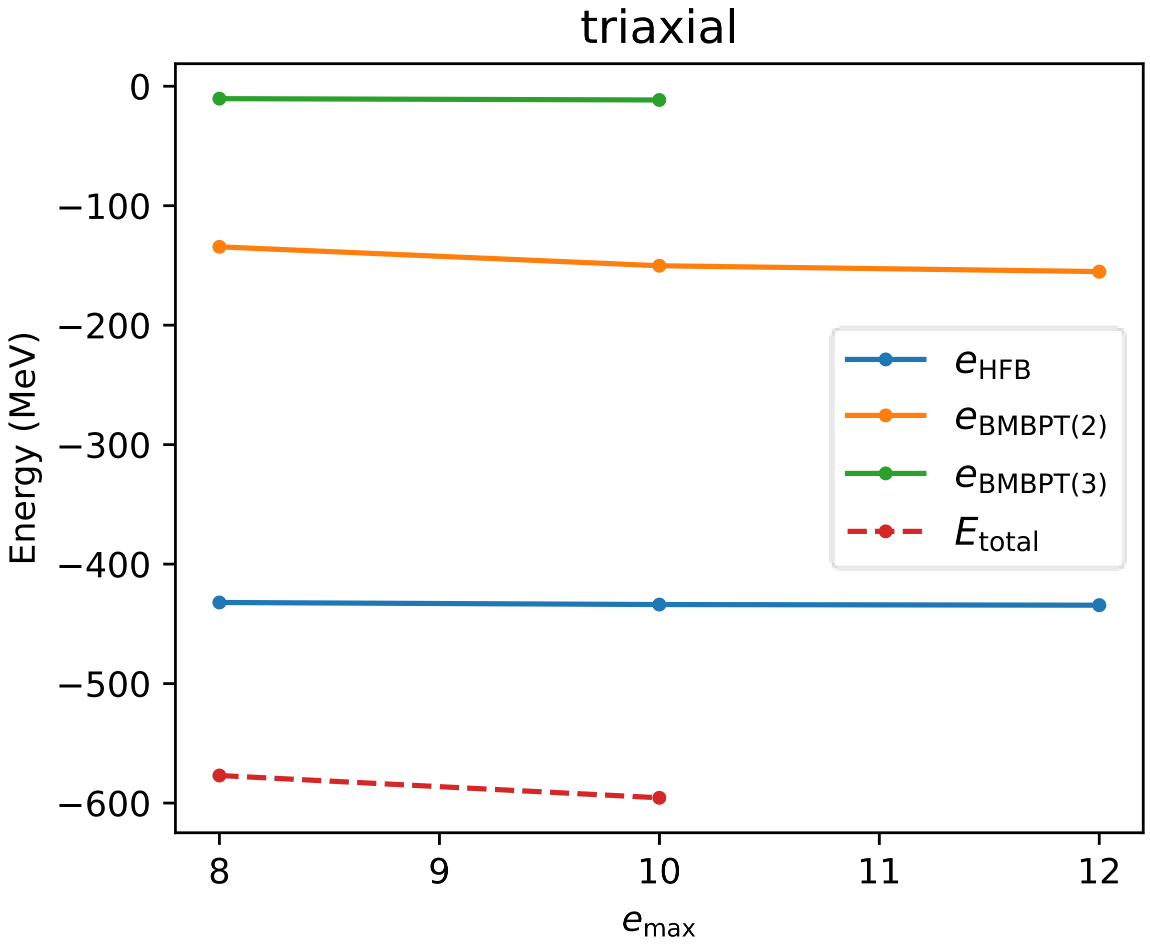


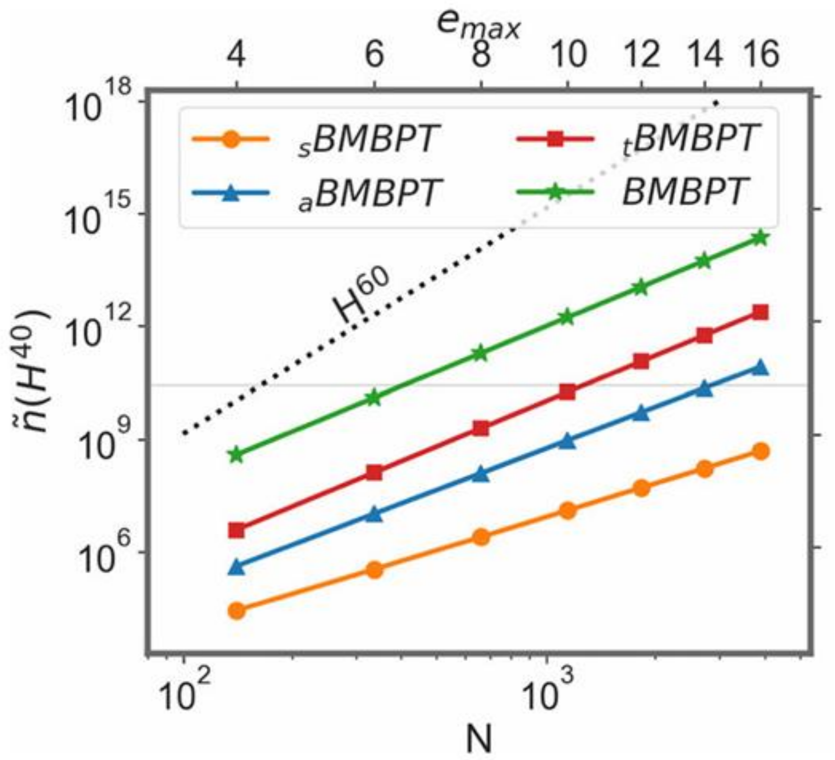


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larger $e_{max}$ requires preparing talk earlier

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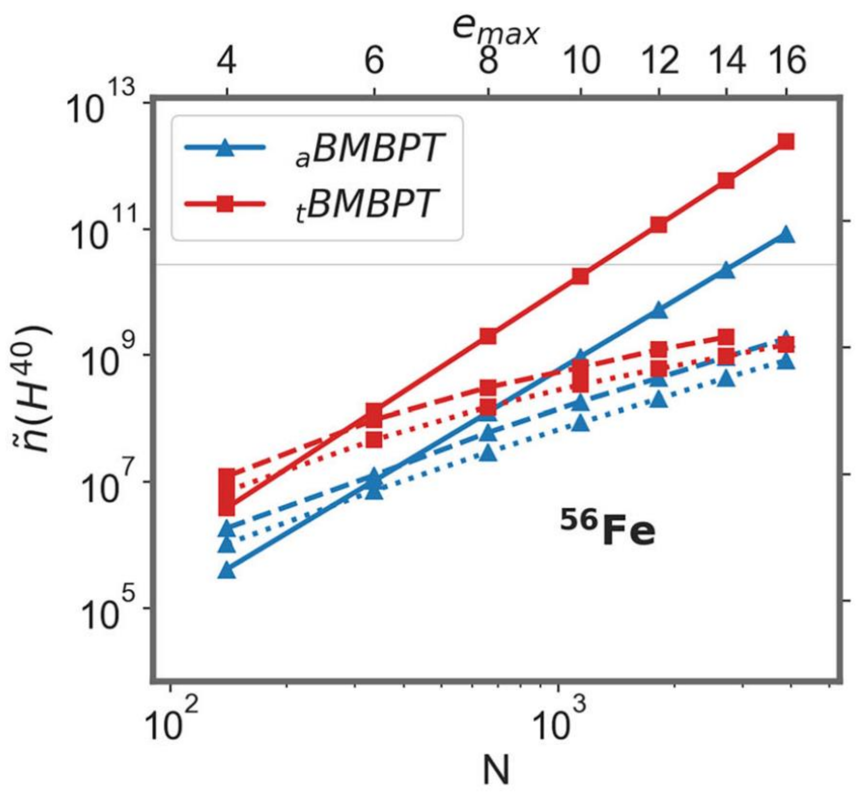


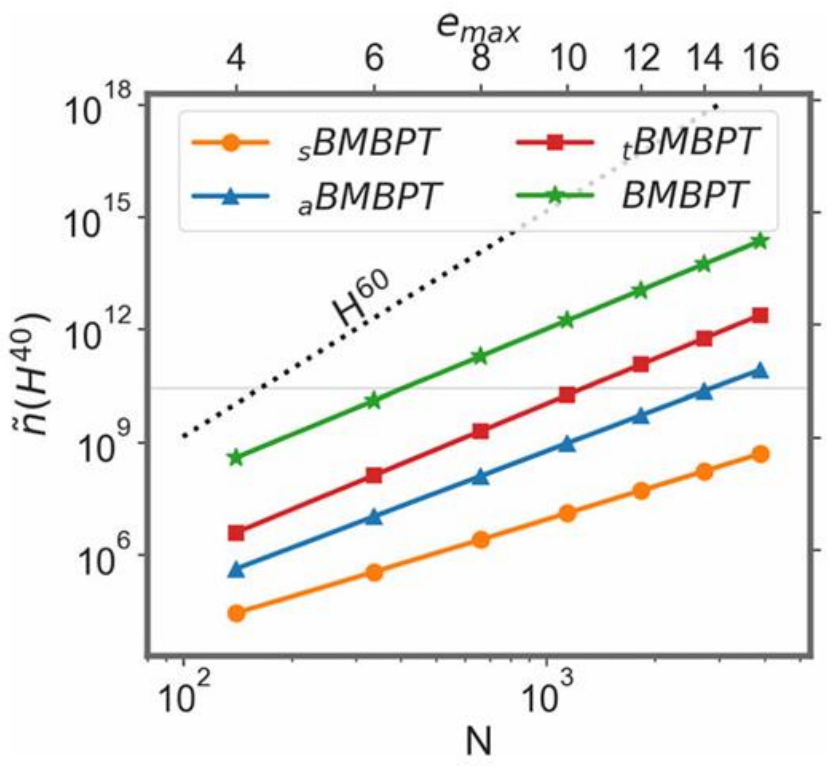


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- Tensor factorization allows to make computationally unfeasible calculations tractable
- Low-rank structure of $H^{40}$ allows for efficient evaluation of correlation energy (at least) in BMBPT(2, 3)
- SVD-BMBPT is subspace-projected BMBPT (apparently with a good subspace)

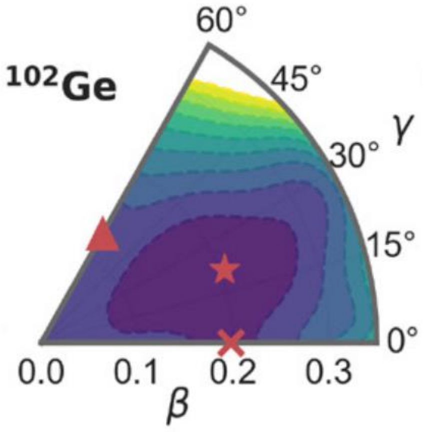
# Summary

- Tensor factorization allows to make computationally unfeasible calculations tractable
- Low-rank structure of $H^{40}$ allows for efficient evaluation of correlation energy (at least) in BMBPT(2, 3)
- SVD-BMBPT is subspace-projected BMBPT (apparently with a good subspace)
- Memory usage: $\mathcal{O}(rN^2) \ll \mathcal{O}(N^4)$
- CPU time: $\mathcal{O}(rN^{4-\delta}) \ll \mathcal{O}(N^5, N^6)$

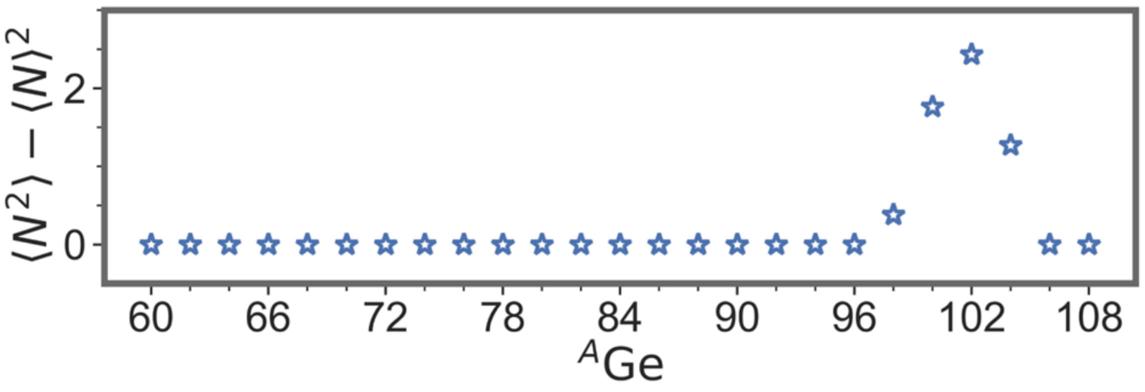
# Outlook

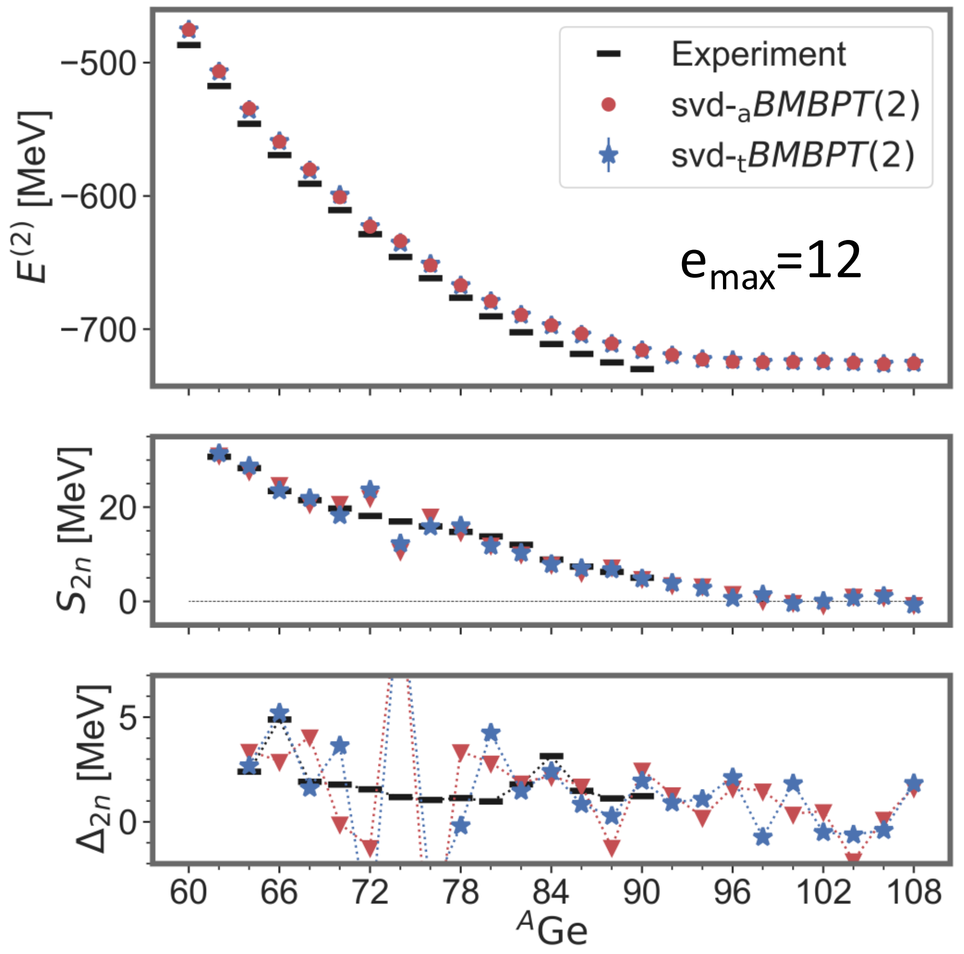
- Particle number constraint at BMBPT(3) level

Demol et al., AOP **424** (2021)
Demol et al., EPJA **61** (2025)




Frosini et al., EPJ Conf **302** (2024)



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Tropp, Webber, 2306.12418 (2023)

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## Thanks for your attention

and to
Thomas Duguet, Jean-Paul Ebran, and Mikael Frosini