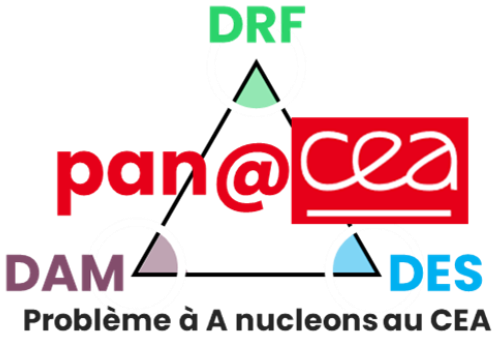


Extending the reach of nuclear ab initio calculations via dimensionality reduction techniques

Lars Zurek

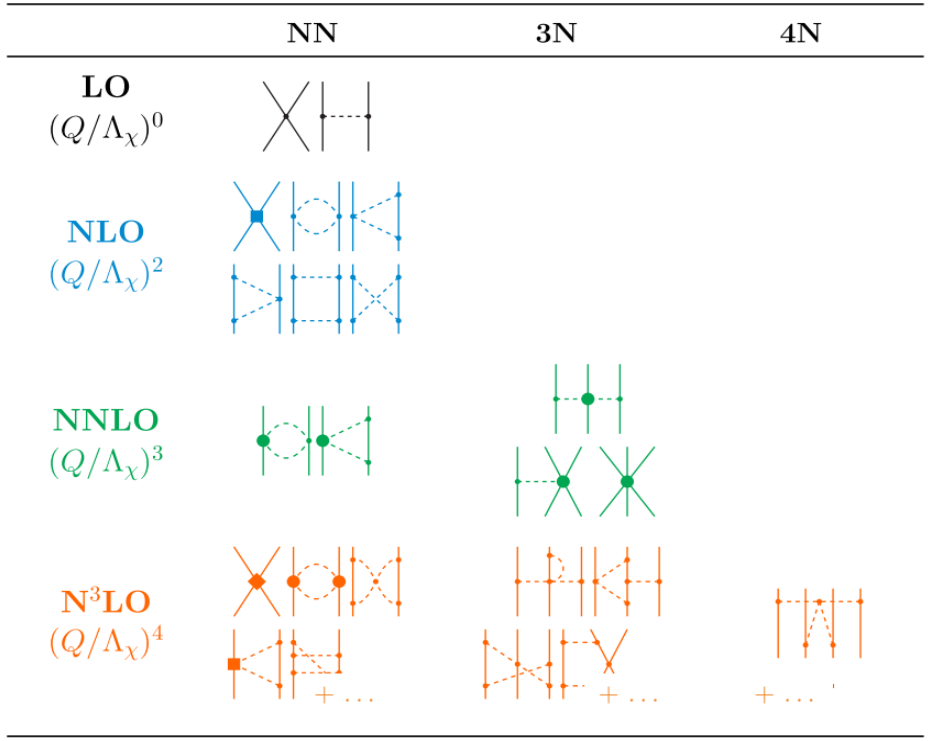
with Thomas Duguet, Jean-Paul Ebran, and Mikael Frosini

EuNPC, Caen, September 22, 2025

The nuclear ab initio approach

- Solve many-body Schrödinger equation for nuclear interactions from chiral effective field theory

- Rooted in quantum chromodynamics
- Systematically improvable
  - Uncertainty estimates “built-in”



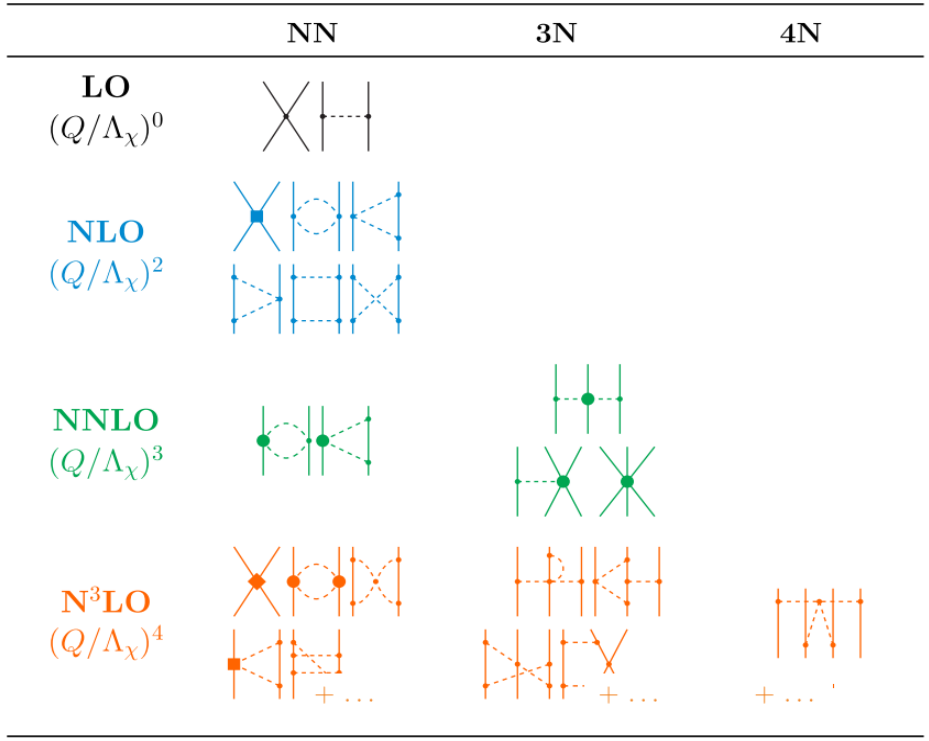
Hergert, Front. Phys. **8** (2020)

The nuclear ab initio approach

- Solve many-body Schrödinger equation for nuclear interactions from chiral effective field theory

- Rooted in quantum chromodynamics
- Systematically improvable
  - Uncertainty estimates “built-in”

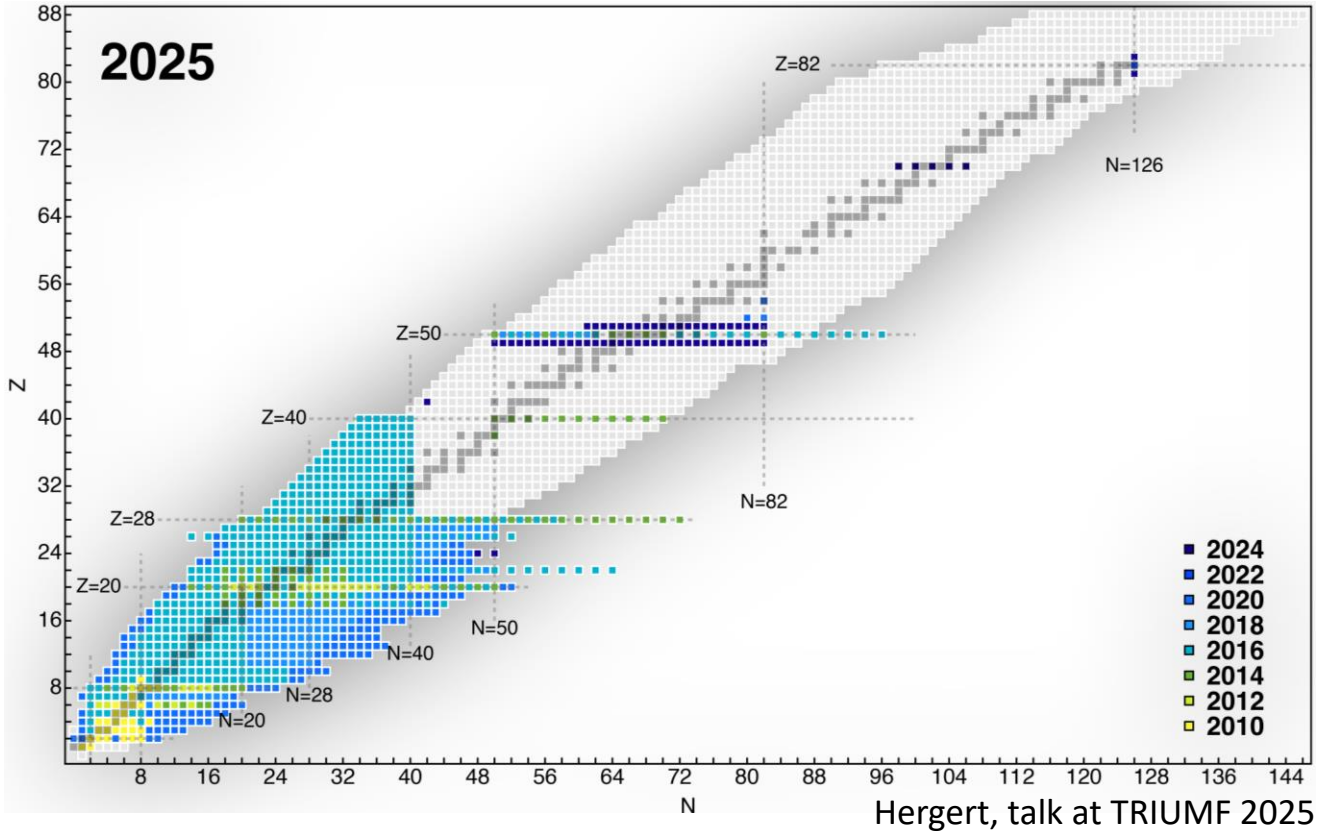
See talk of V. Somà tomorrow
14:00, Inspire 1



Hergert, Front. Phys. **8** (2020)

The nuclear ab initio approach

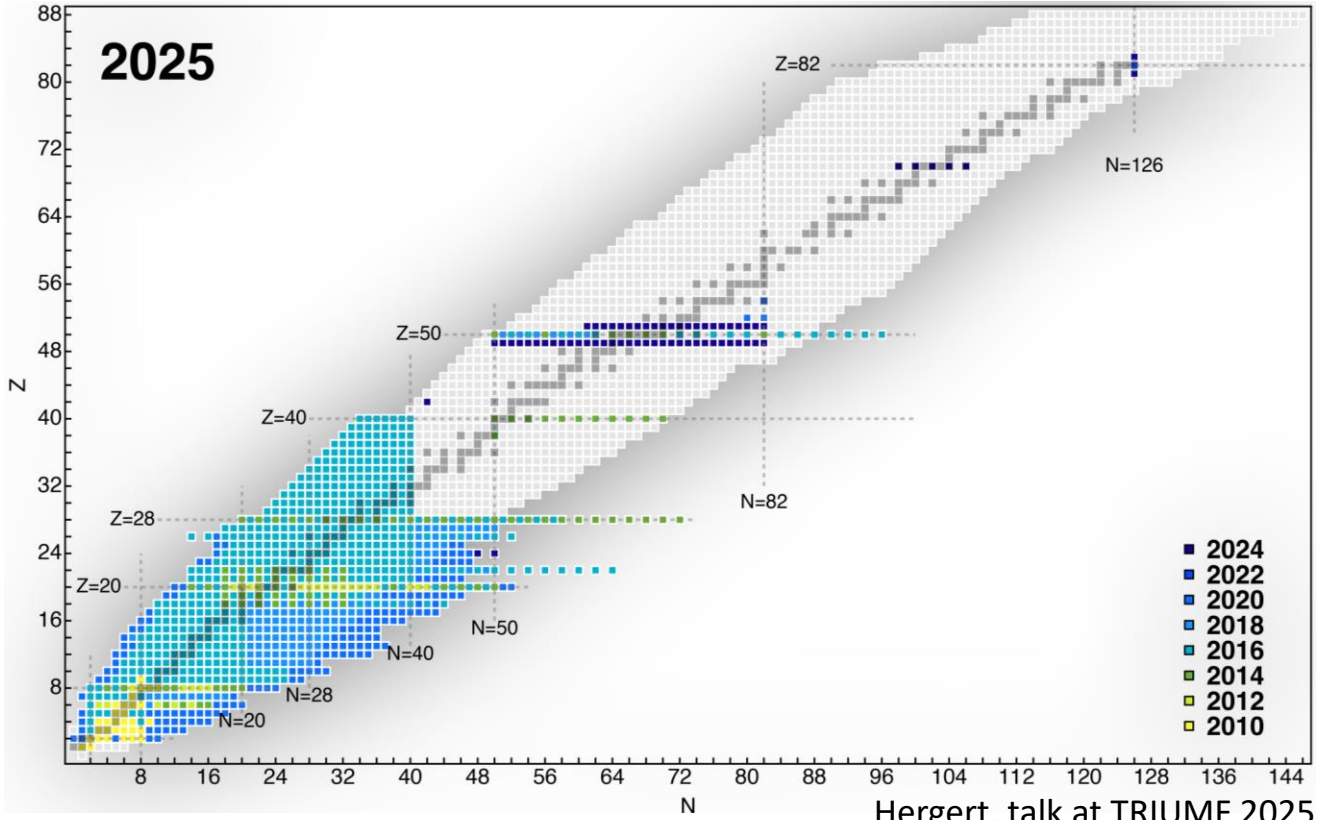
- “Exact” solution of many-body Schrödinger equation (by diagonalization) limited to lightest nuclei
- Instead: correlation expansion methods
  - Heavy nuclei
  - Open-shell nuclei
  - Precision calculations



Hergert, talk at TRIUMF 2025

Ab initio challenges

- “Exact” solution of many-body Schrödinger equation (by diagonalization) limited to lightest nuclei
- Instead: correlation expansion methods
  - Heavy nuclei
  - Open-shell nuclei
  - Precision calculations
- But: current ab initio calculations cannot do all three at the same time



Hergert, talk at TRIUMF 2025

Dimensionality reduction

- Different strategies to reduce computational burden
- Using a better single-particle basis: approximate natural orbitals

  Tichai et al., PRC **99** (2019)
  Scalesi et al., EPJA **61** (2025)

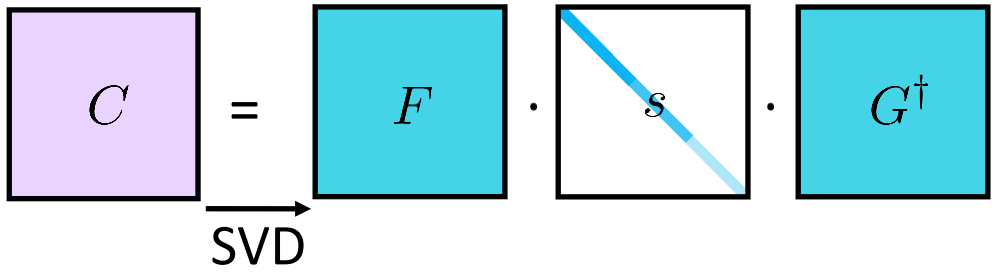
- Eliminate irrelevant matrix elements by importance truncation

  Roth et al., PRL **99** (2007)
  Porro et al., EPJA **57** (2021)

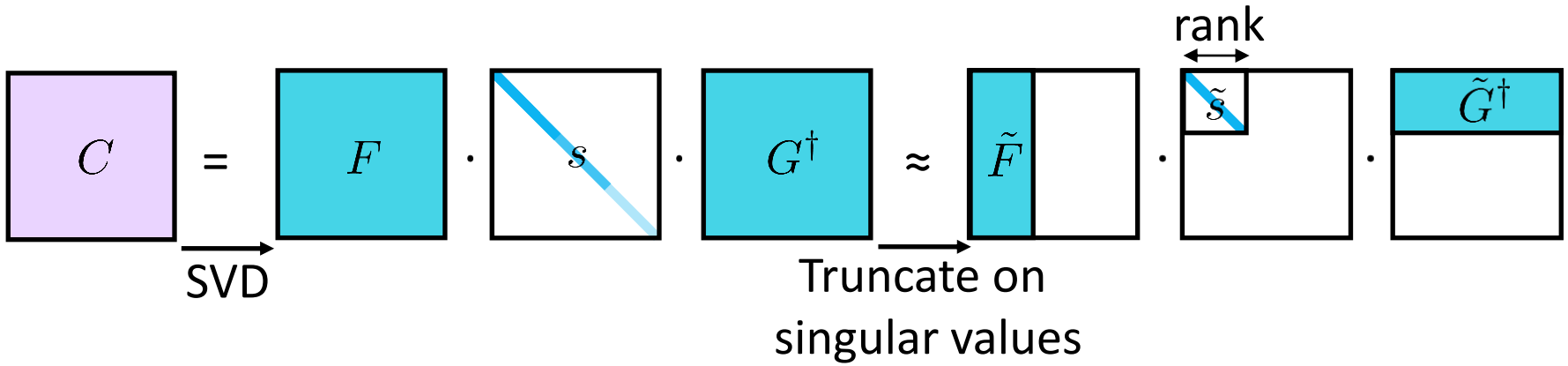
- Replace tensors by multiple smaller ones via tensor factorization

  Frosini et al., EPJA **60** (2024)
  Tichai et al., PRR **6** (2024)

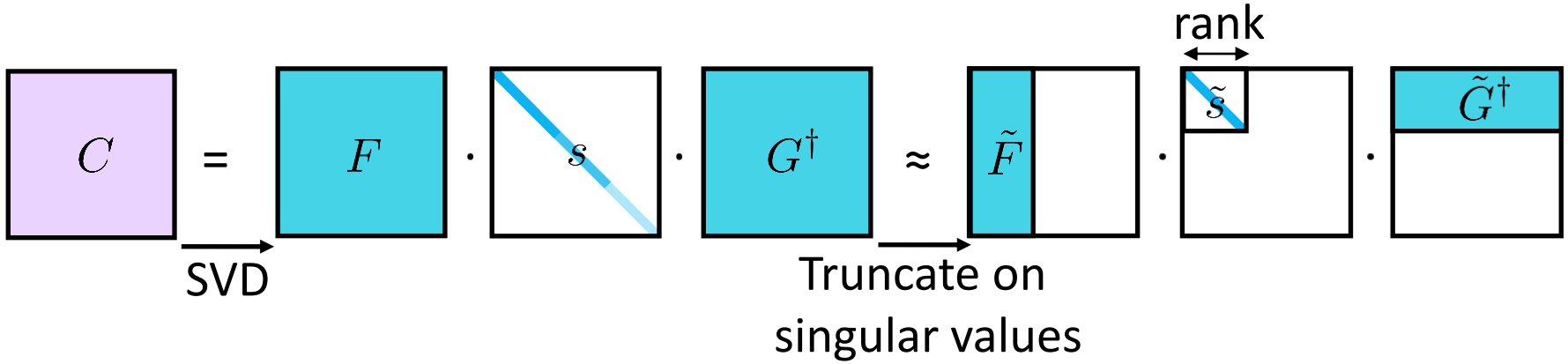
Singular value decomposition



Singular value decomposition

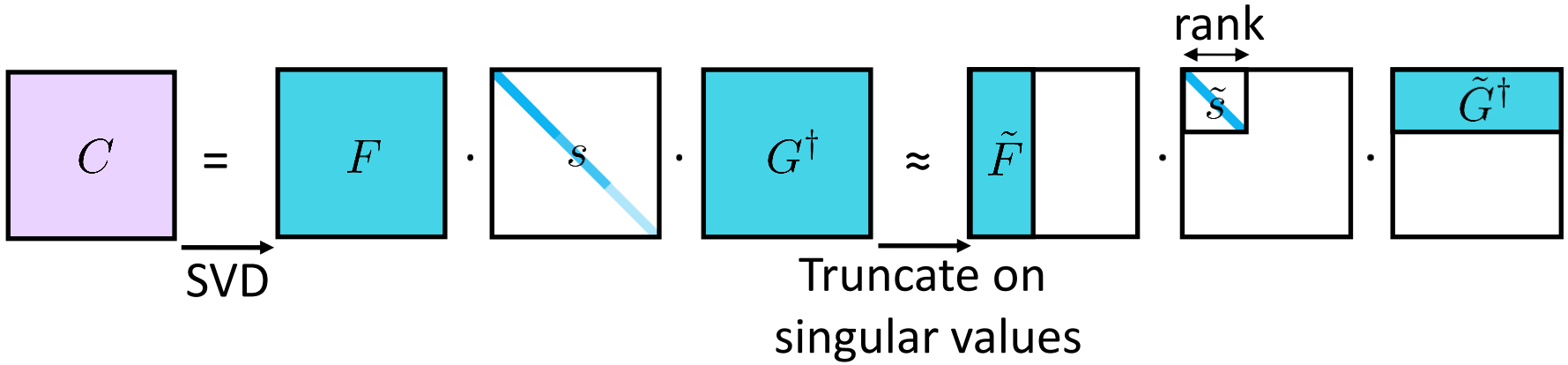


Singular value decomposition



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

Singular value decomposition



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

- Large computational benefits possible if small ranks can be used
- Maximal gain only when full matrices are never reconstructed

Bogoliubov many-body perturbation theory

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

- Split nuclear Hamiltonian: $H = \underbrace{H^{00} + H^{11}}_{\text{Exact (HFB)}} + \underbrace{H^{22} + H^{31} + H^{13} + H^{40} + H^{04}}_{\text{via perturbative corrections}}$

- 3N interaction treated through rank reduction Frosini et al., EPJA **57** (2021)

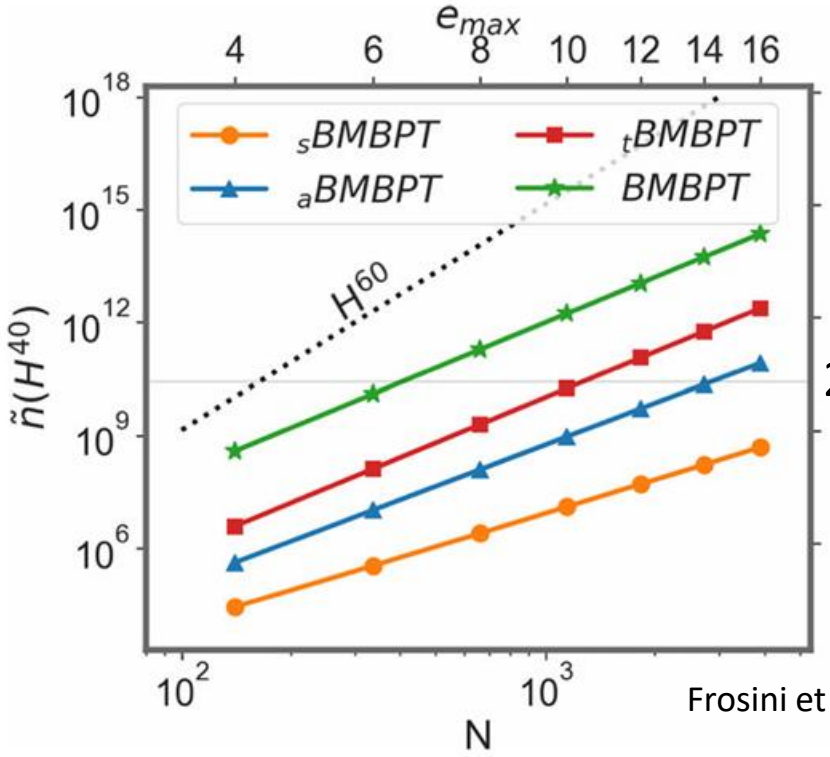
Bogoliubov many-body perturbation theory

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

- Split nuclear Hamiltonian: $H = \underbrace{H^{00} + H^{11}}_{\text{Exact (HFB)}} + \underbrace{H^{22} + H^{31} + H^{13} + H^{40} + H^{04}}_{\text{via perturbative corrections}}$

- 3N interaction treated through rank reduction Frosini et al., EPJA **57** (2021)

- First correction to HFB ground state energy requires $H^{40}_{k_1 k_2 k_3 k_4}$



200 GB

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

Randomized SVD

Halko et al., SIREV **53** (2011)
Martinsson, Tropp, ActaNum **403** (2020)
Tropp, Webber, 2306.12418 (2023)

- Decompose H^{40} despite it being too big for memory

- 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 construction and storage of $H^{40}_{k_1 k_2 k_3 k_4}$ consider instead only "matrix-vector" products

$$\sum_{k_3 k_4} H^{40}_{k_1 k_2 k_3 k_4} X^{02}_{k_3 k_4}$$

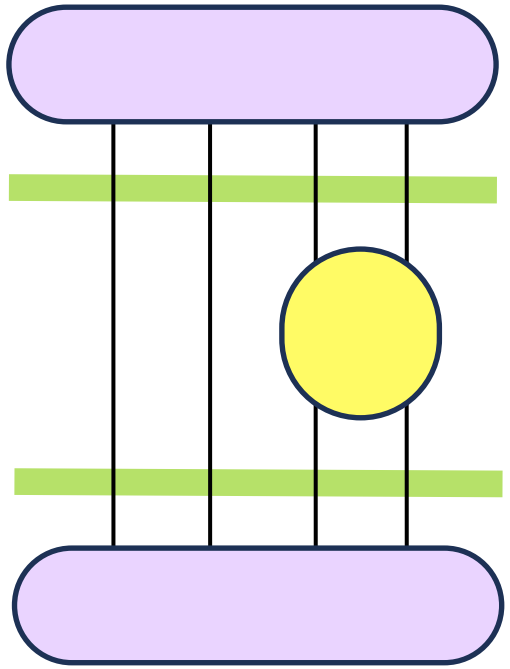
- Efficient implicit FAM-like products Carlsson et al., PRC **86** (2012)
  1. transform X^{02} to underlying spherical HO basis
  2. calculate product in that basis
  3. transform back

BMBPT(3)

- Next correction to HFB ground state energy:

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

- Evaluation of energy scales as N^6

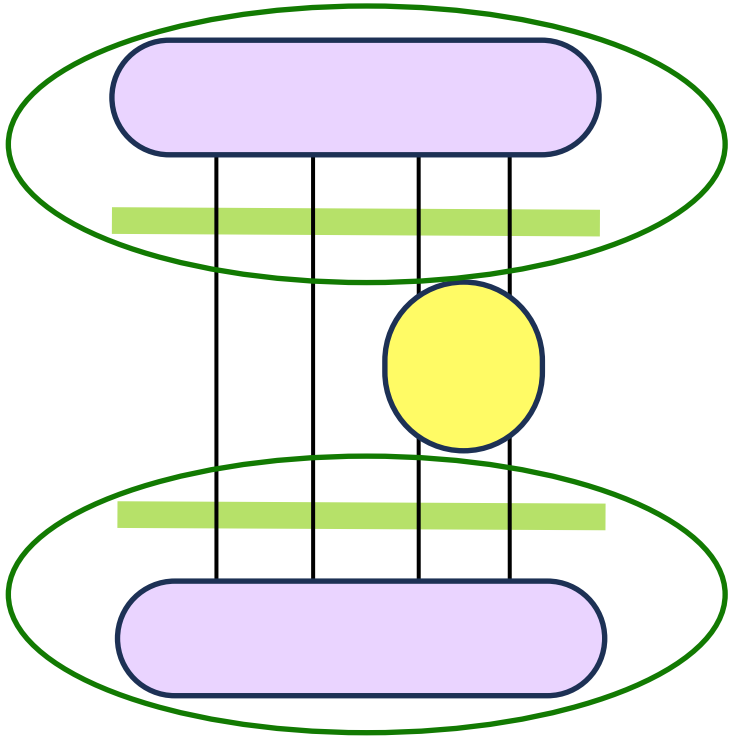


BMBPT(3)

- Next correction to HFB ground state energy:

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

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



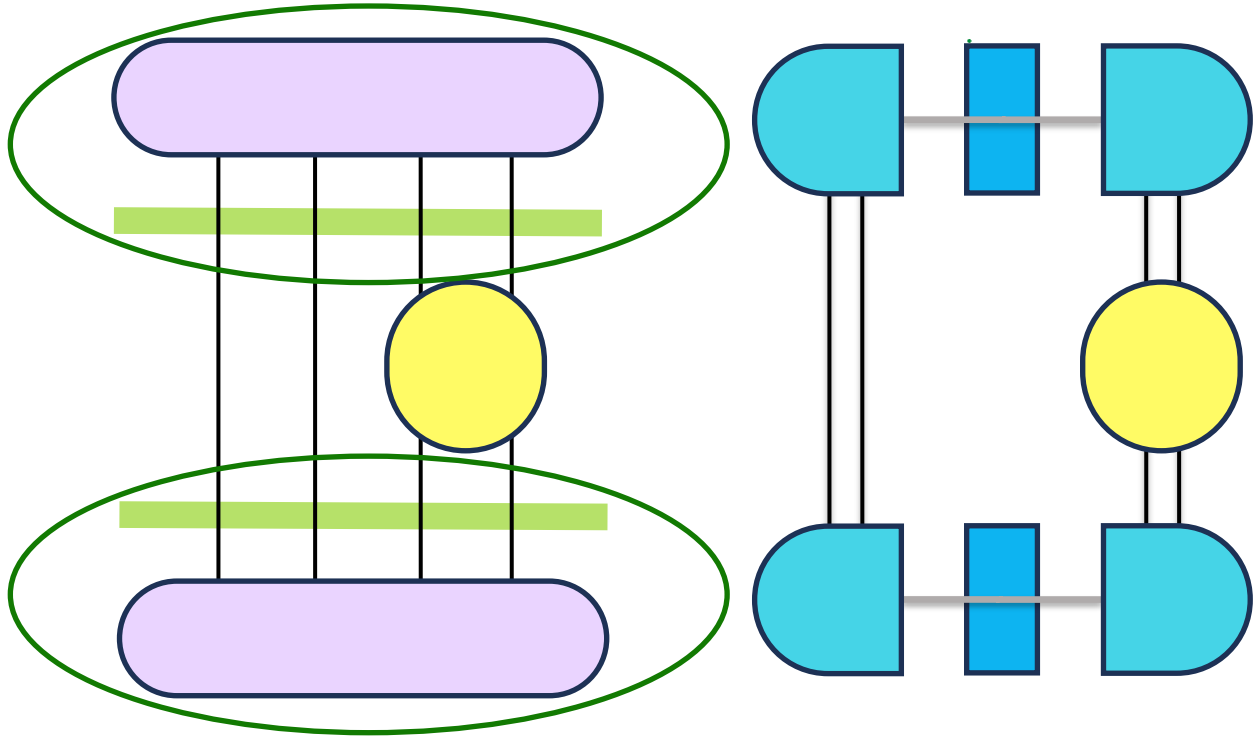
BMBPT(3)

- Next correction to HFB ground state energy:

$$e^{(3)}_{\mathrm{BMBPT}} = \frac{1}{8}\sum_{k_1\ldots k_6}\frac{H^{04}_{k_1k_2k_3k_4}H^{22}_{k_3k_4k_5k_6}H^{40}_{k_5k_6k_1k_2}}{(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})(E_{k_5}+E_{k_6}+E_{k_1}+E_{k_2})}$$

$$= -C^{40}_{k_5k_6k_1k_2}(2)$$

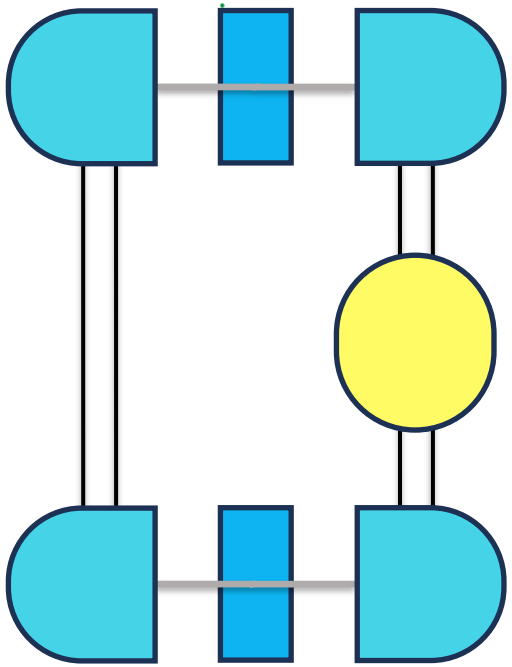
$$C^{40}_{k_1k_2k_3k_4}(2) \approx \sum_{\mu=1}^{r} F^{\mu}_{k_1k_2}\, s_\mu\, G^{\mu}_{k_3k_4}$$



SVD-BMBPT(3)

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

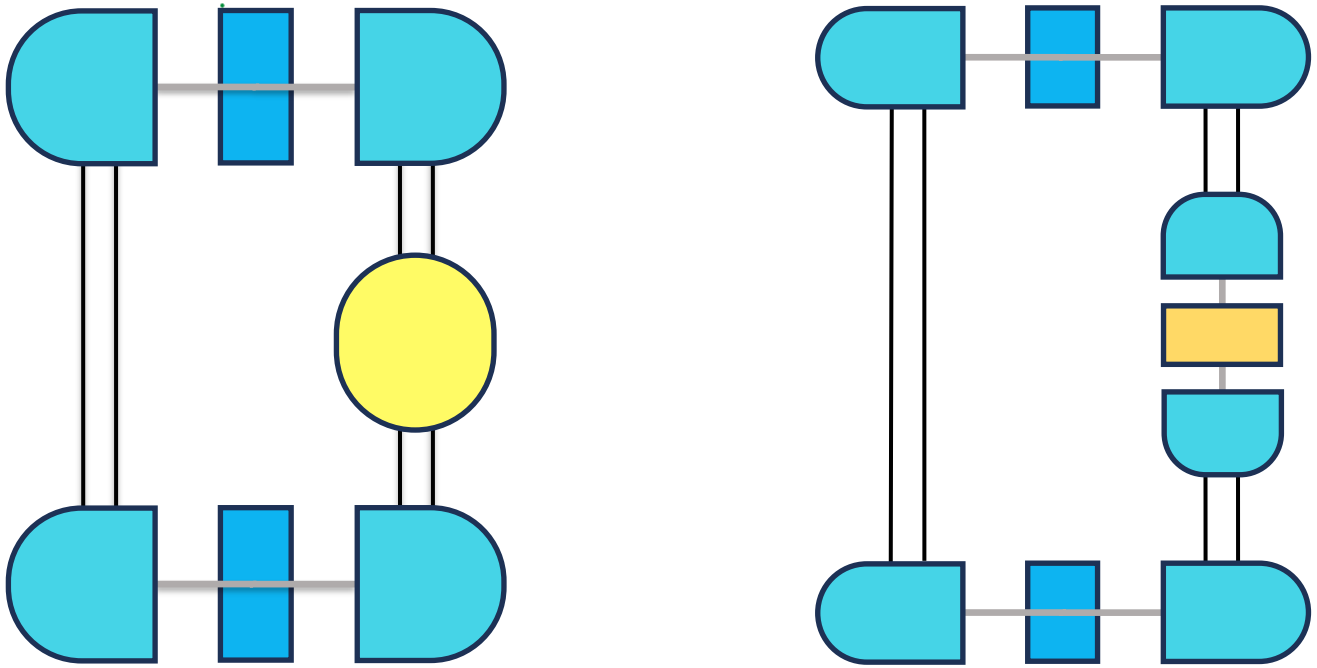
$$s'_{\mu\nu} = \sum_{k_1 \ldots k_4} F^{\mu *}_{k_1 k_2} H^{22}_{k_1 k_2 k_3 k_4} F^{\nu}_{k_3 k_4}$$



SVD-BMBPT(3)

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

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

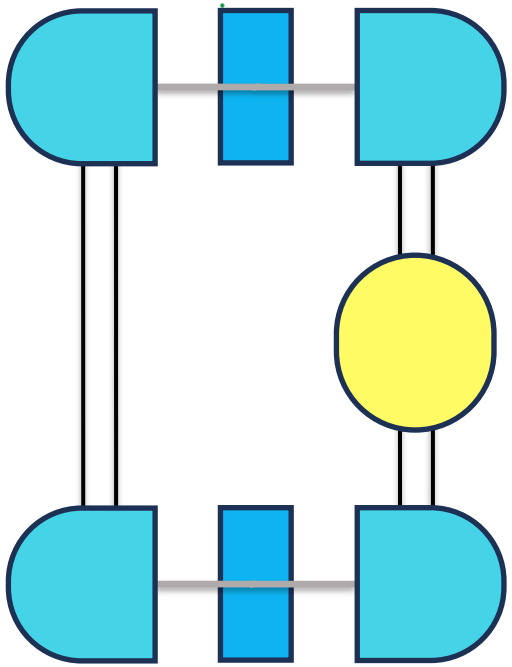


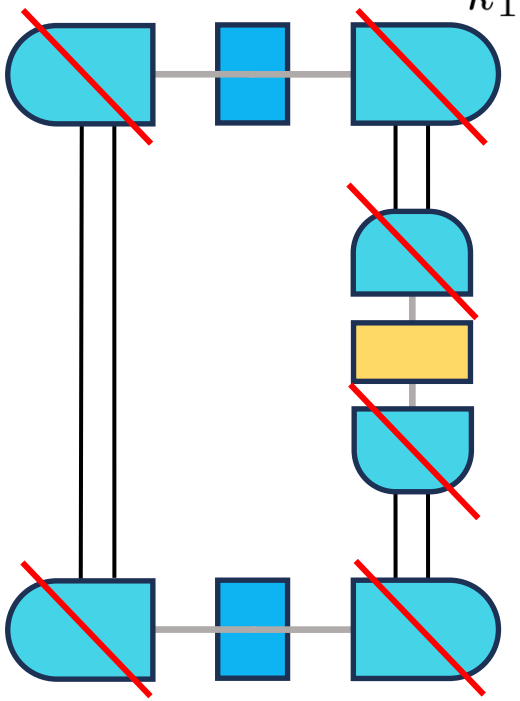
SVD-BMBPT(3)

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

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

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



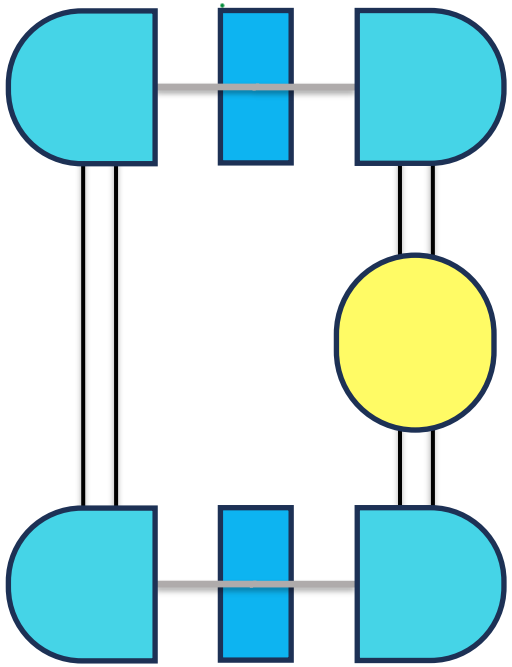


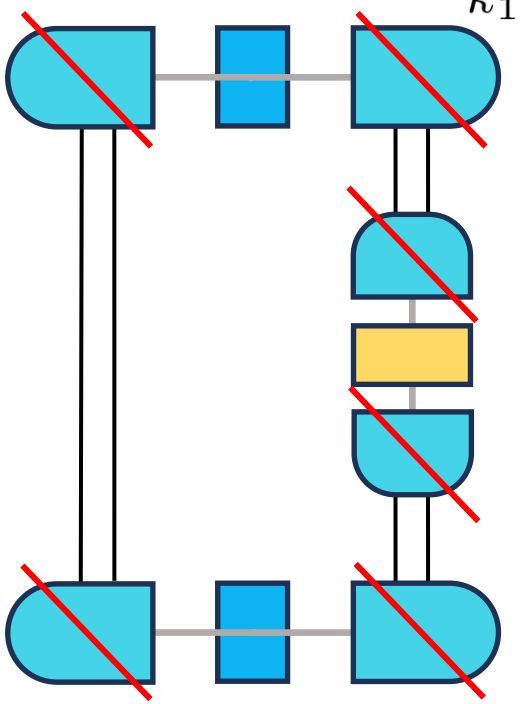
SVD-BMBPT(3)

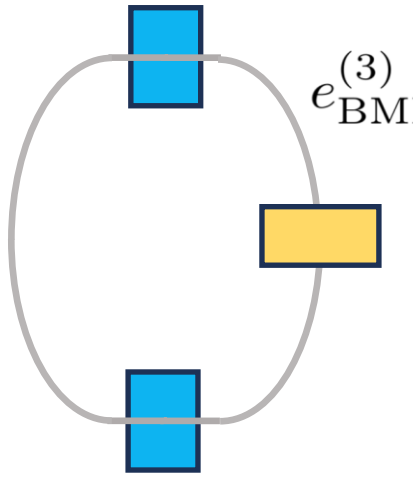
- Project H^{22} to both sides on subspace spanned $C^{40}(2)$ by singular vectors

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

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







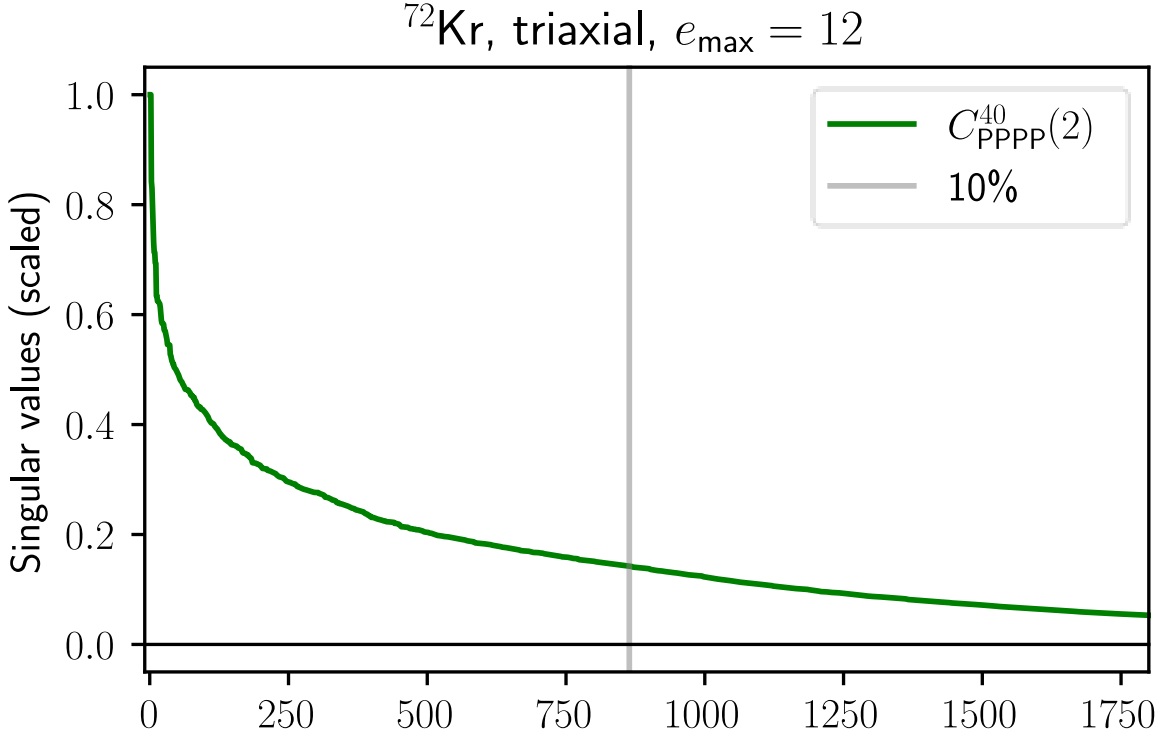
$$e^{(3)}_{\mathrm{BMBPT}} = \frac{1}{8} \sum_{\mu} s^2_{\mu} s'_{\mu\mu}$$

SVD-BMBPT(3)

- Memory usage: $\mathcal{O}(rN^2) \leq \mathcal{O}(N^4)$
- CPU time: $\mathcal{O}(rN^4) \leq \mathcal{O}(N^6)$

SVD-BMBPT(3)

- Memory usage: $\mathcal{O}(rN^2) \ll \mathcal{O}(N^4)$
- CPU time: $\mathcal{O}(rN^4) \ll \mathcal{O}(N^6)$
- Need only r ~ 1000 singular values to reach desired accuracy



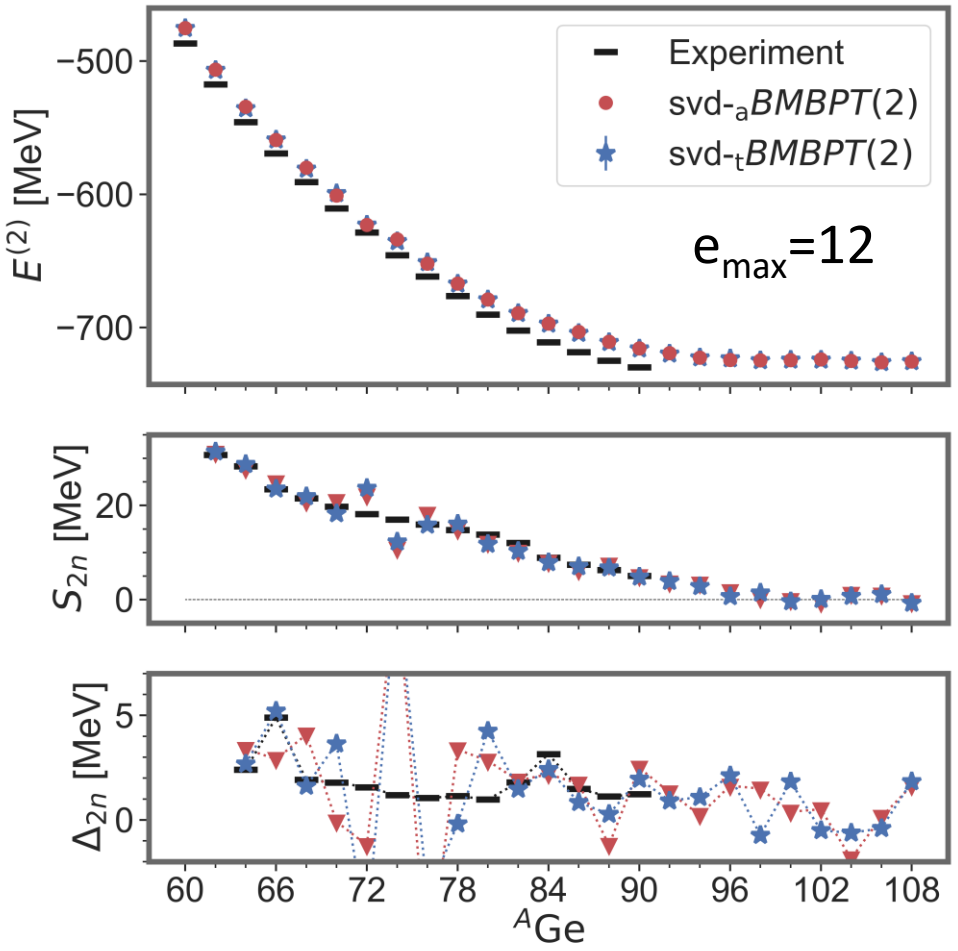
Full rank: $8 \cdot 10^5$

Summary

- SVD selects efficient subspace to compute BMBPT corrections

- Dimensionality reduction through tensor factorization makes previously unfeasible ab initio calculations possible

Frosini, …, **Zurek**, EPJ Conf **302** (2024)



Outlook

- Particle number constraint at BMBPT(3) level
- Ideas can be applied to other many-body methods

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

Parrish et al., JChemPhys **150** (2019)
Lesiuk, JCTC **18** (2022)

	BMBPT(2)	BMBPT(3)	BMBPT(4)
Traditional	$O(N^5)$	$O(N^6)$	$O(N^8)$
Tensor factorized	$O(r\ N^4)$	$O(r\ N^4)$	?

Outlook

- Particle number constraint at BMBPT(3) level
- Ideas can be applied to other many-body methods

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

Parrish et al., JChemPhys **150** (2019)
Lesiuk, JCTC **18** (2022)

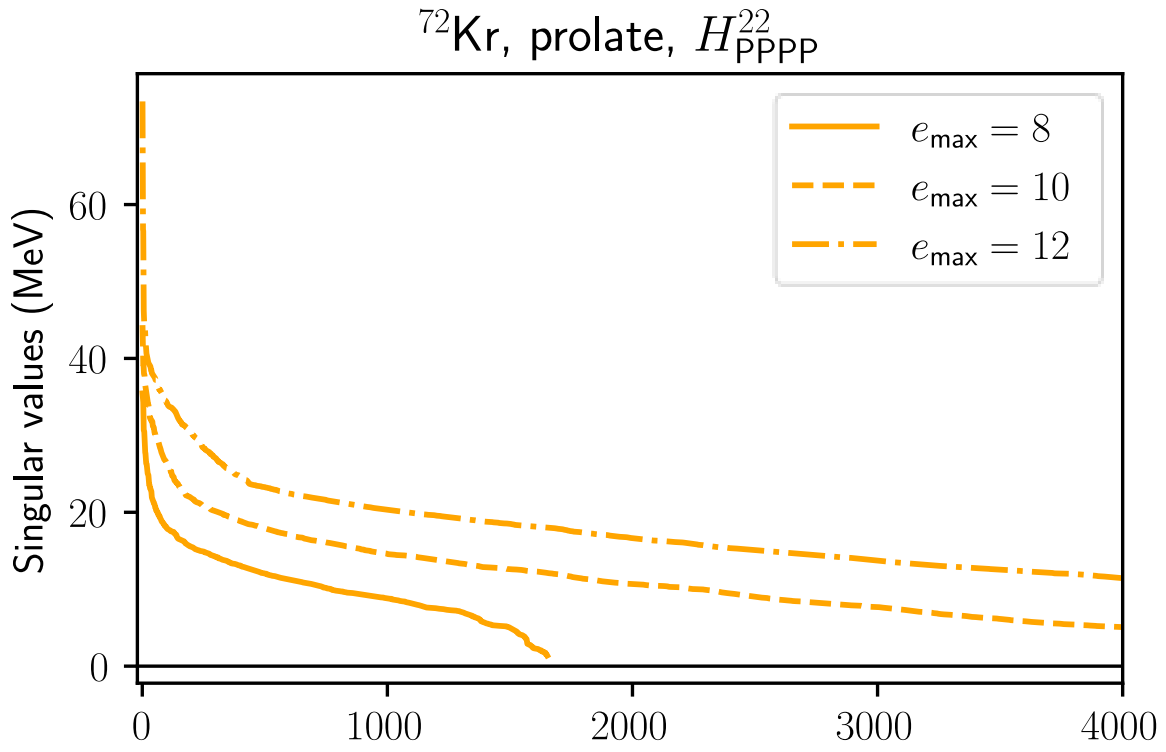
	BMBPT(2)	BMBPT(3)	BMBPT(4)
Traditional	$O(N^5)$	$O(N^6)$	$O(N^8)$
Tensor factorized	$O(r\ N^4)$	$O(r\ N^4)$	?

Thanks for your attention

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

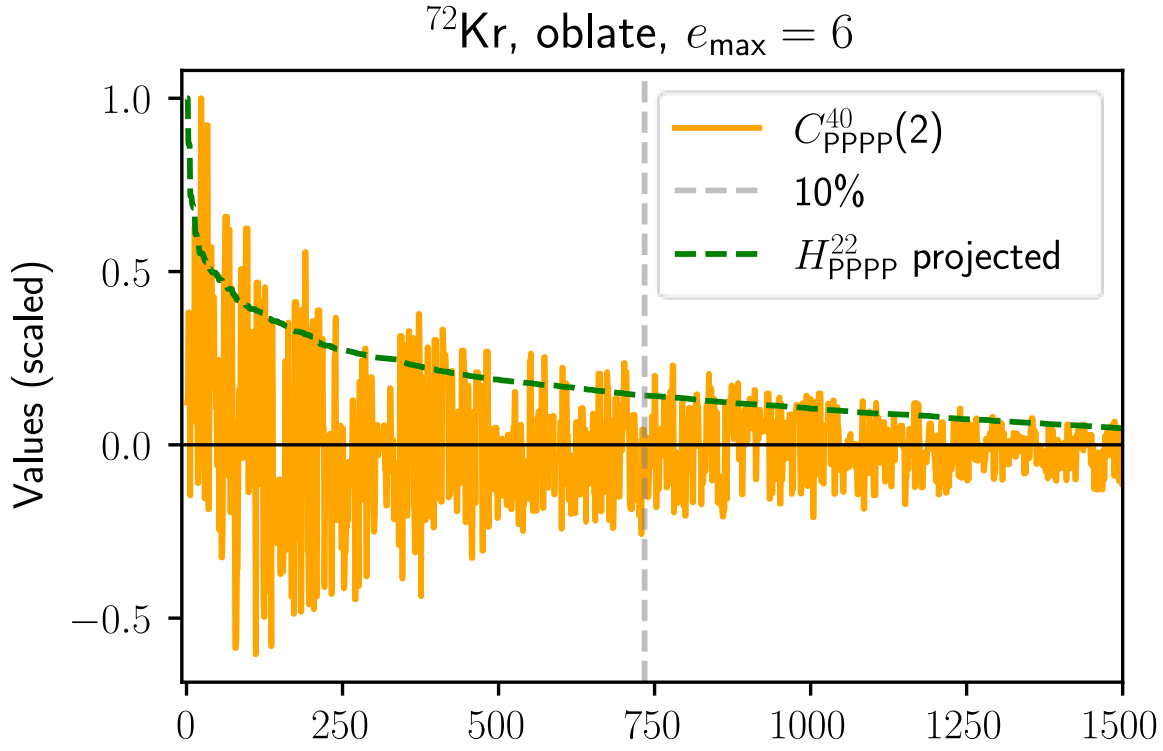
Singular spectra

- The spectrum of H^{22} does not converge with increasing e_{max}



Singular spectra

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



Required accuracy

- BMBPT as formal power series

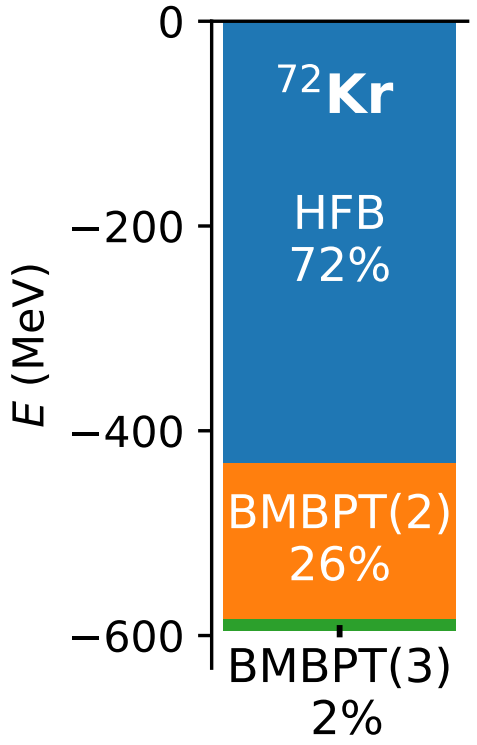
$$E^{[P]} = \langle \Phi | H \sum_{p=0}^{P-1} (R_0\, \Omega_1^{(P)})^p | \Phi \rangle_{\mathrm{c}}$$

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

- Conservative estimate of missing next-order contribution

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

→ Defines calculation accuracy goal at BMBPT(3) level



Required accuracy: needed basis size

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