Tackling large basis sizes in nuclear structure computations

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with Pepijn Demol, Thomas Duguet, Mikael Frosini, Alexander Tichai, and Urban Vernik

MITP program “Many-body theory”, August 25, 2026

Basic principle

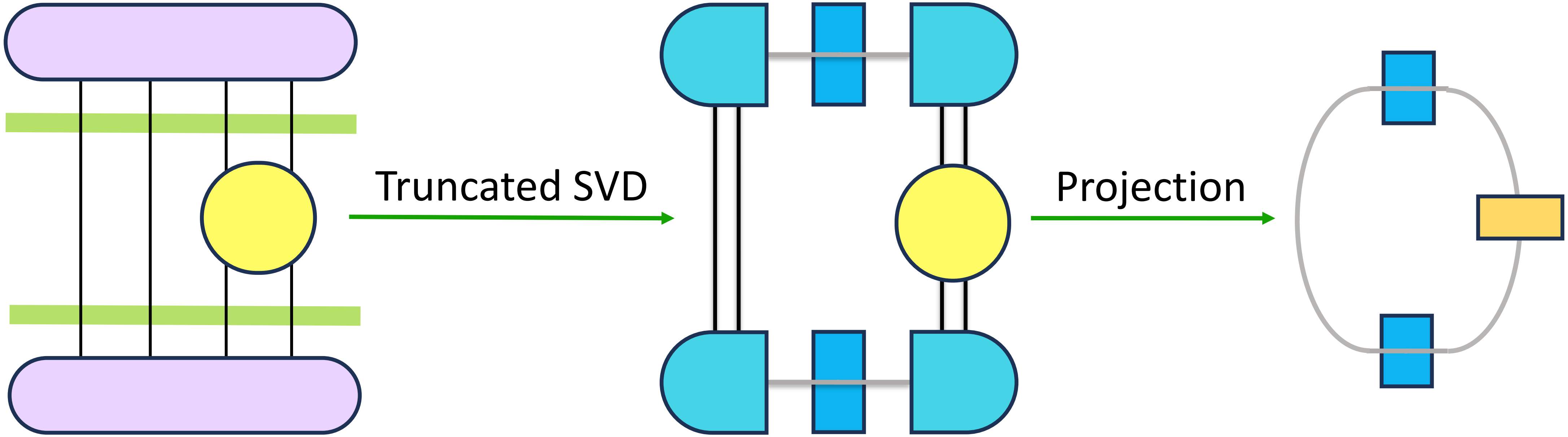
There is no point in working hard to reduce a small uncertainty when a large uncertainty is also present

Tensor decomposed many-body methods

Parrish et al., JChemPhys **150** (2019) Lesiuk, JCTC **16** (2020) Lesiuk, JCTC **18** (2022)

- Reformulate many-body methods by factorizing tensors
  - Possible decomposition strategy for (B)MBPT(3):

For BMBPT(2) see
Frosini et al., EPJA **60** (2024)
Frosini et al., EPJ Conf **302** (2024)

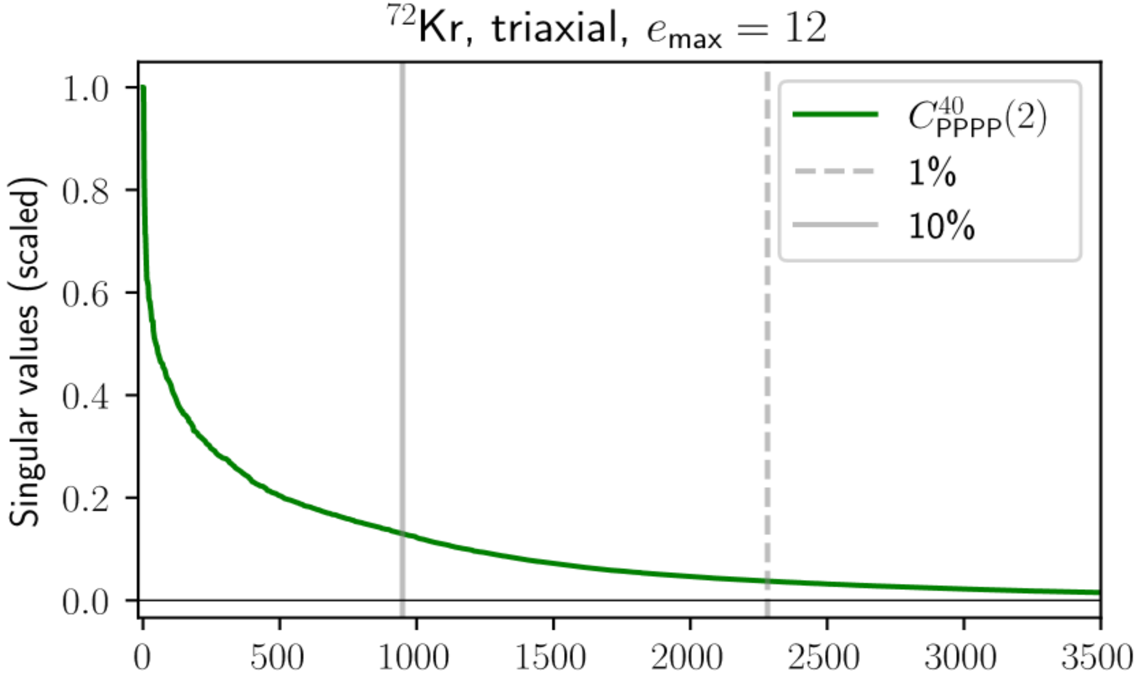


- Calculations become cheaper at the price of adding a controlled approximation

Tensor decomposed many-body methods

- Approximation introduces error → uncertainty
  - Keeping more singular values reduces error and increases computational cost

- Applying basic principle:
  keep enough singular values to not dominate uncertainty but not more



- Guideline for benchmarking different tensor decomposition approaches

Our example

- Compute ground-state energy of ^{78}Ni using 1.8/2.0 (EM) using MBPT(3)

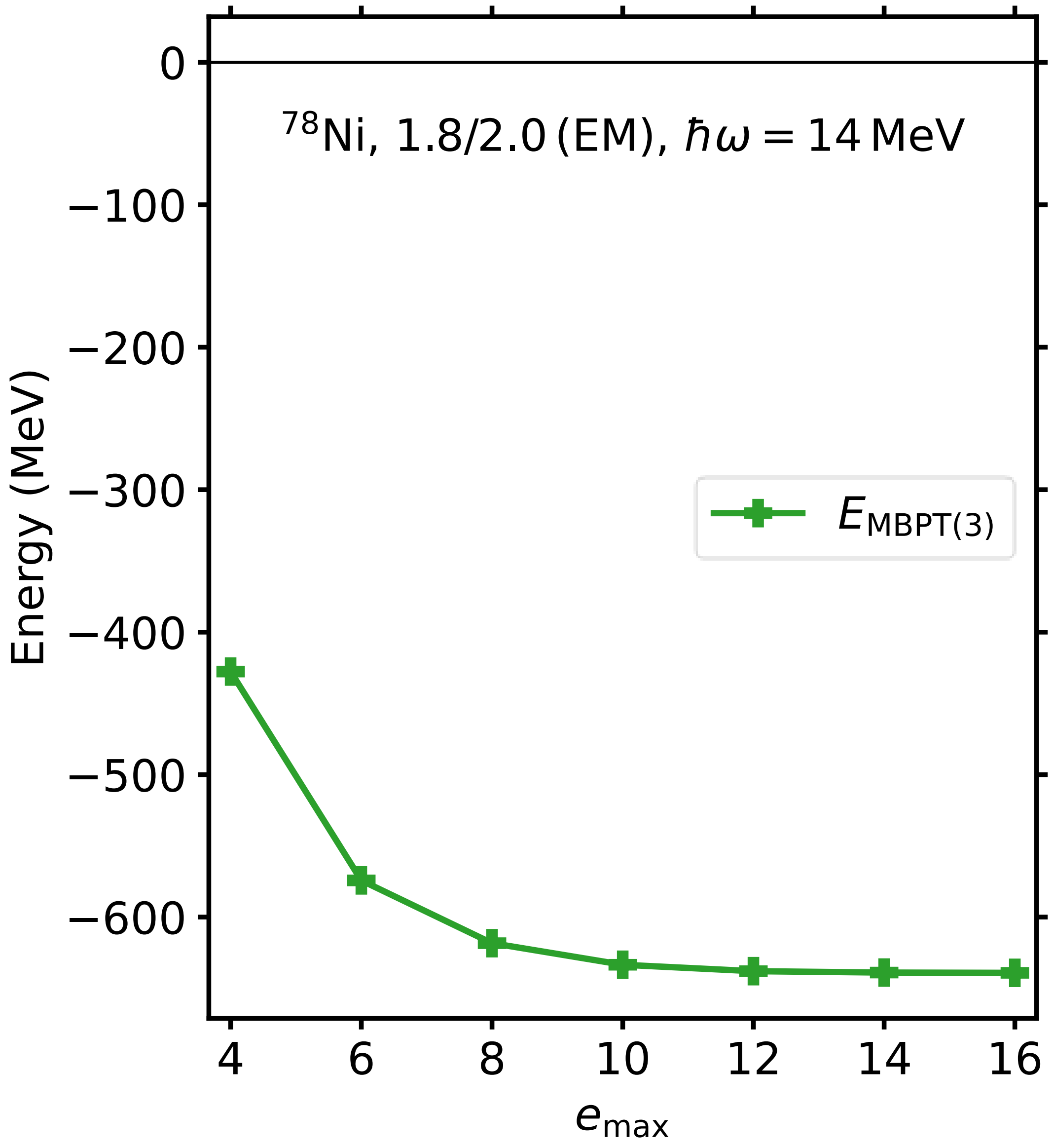
  Hebeler et al., PRC **83** (2011)

- Focus here on two types of uncertainties
  - Truncation of the correlation expansion (“many-body truncation uncertainty”)
  - Truncation of the one-body basis (“basis-size uncertainty”)

Our example

- Spherical harmonic oscillator basis is characterized by the HO frequency $\hbar\omega$
- In practice, truncate based on the principal quantum number

$$e = 2n + l \leq e_{\max}$$



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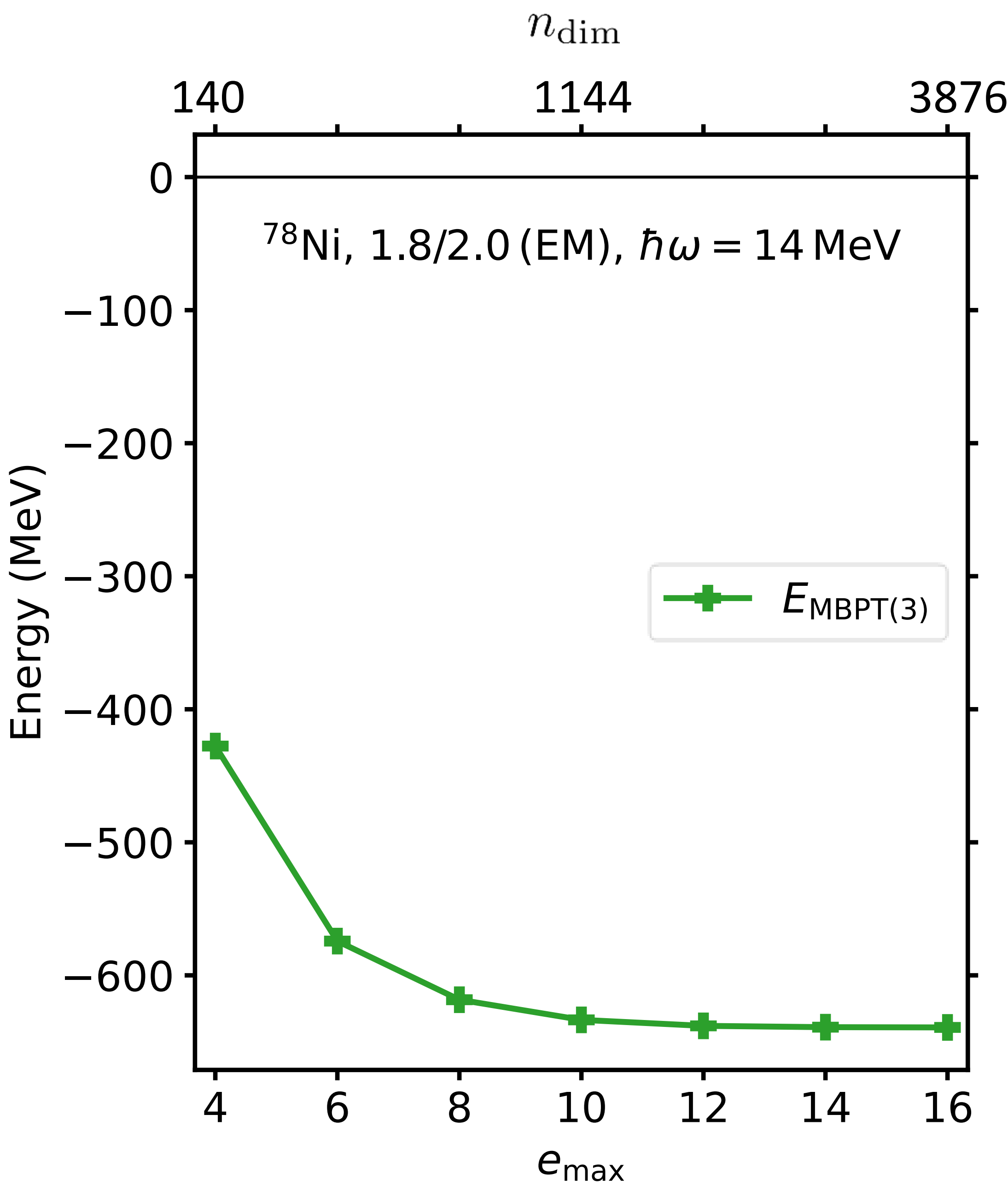
$$e = 2n + l \leq e_{\text{max}}$$

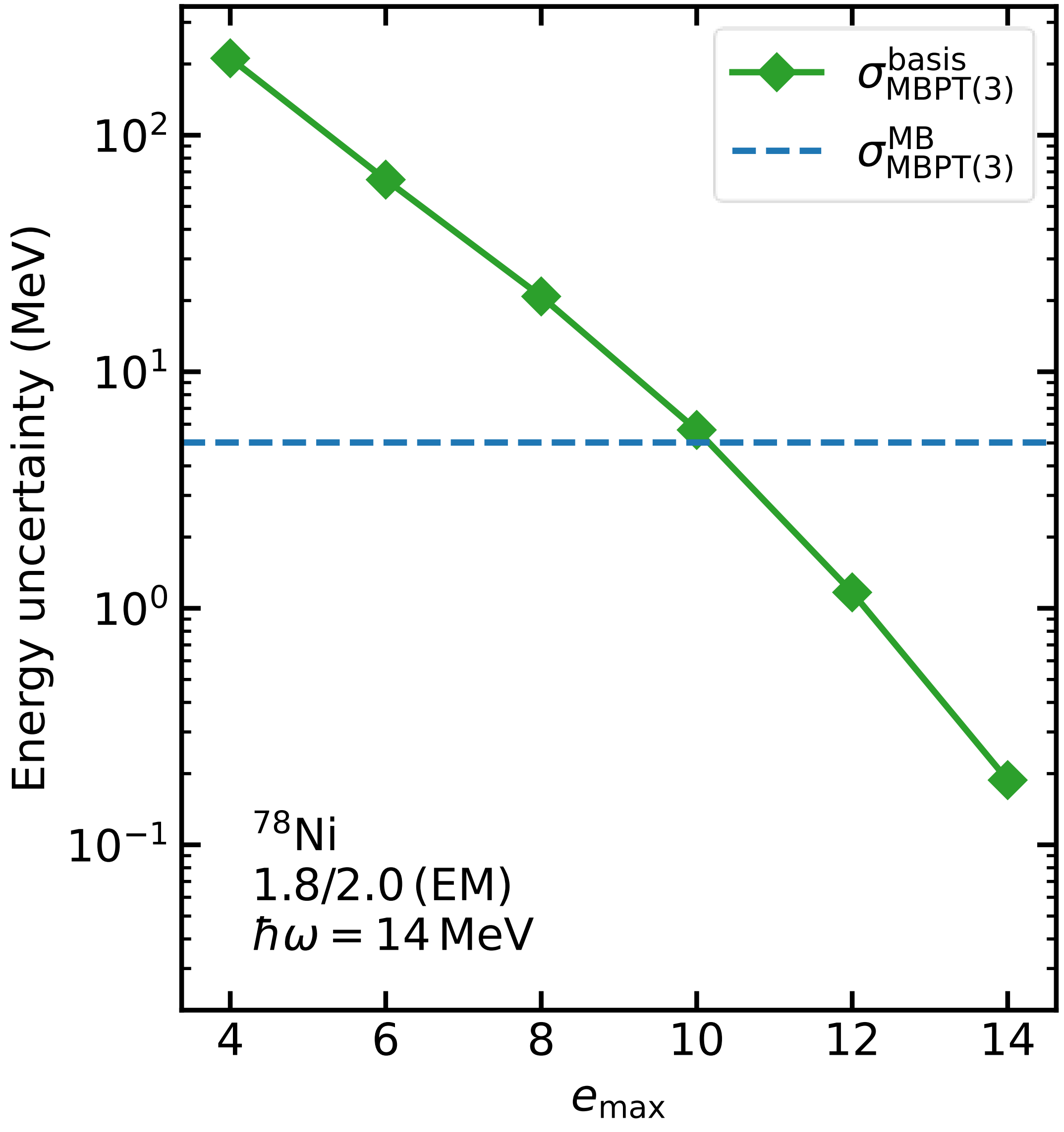
$$n_{\text{dim}} = \mathcal{O}(e_{\text{max}}^3)$$

- Cost of MBPT(3) $= \mathcal{O}(A^2 n_{\text{dim}}^4)$
- Which basis sizes should we use for our calculation?



Balancing uncertainties

- Uncertainty intrinsic to MBPT(3): many-body truncation uncertainty σ^{MB}
- Basis-size uncertainty σ^{basis} reduces with increasing e_{max}



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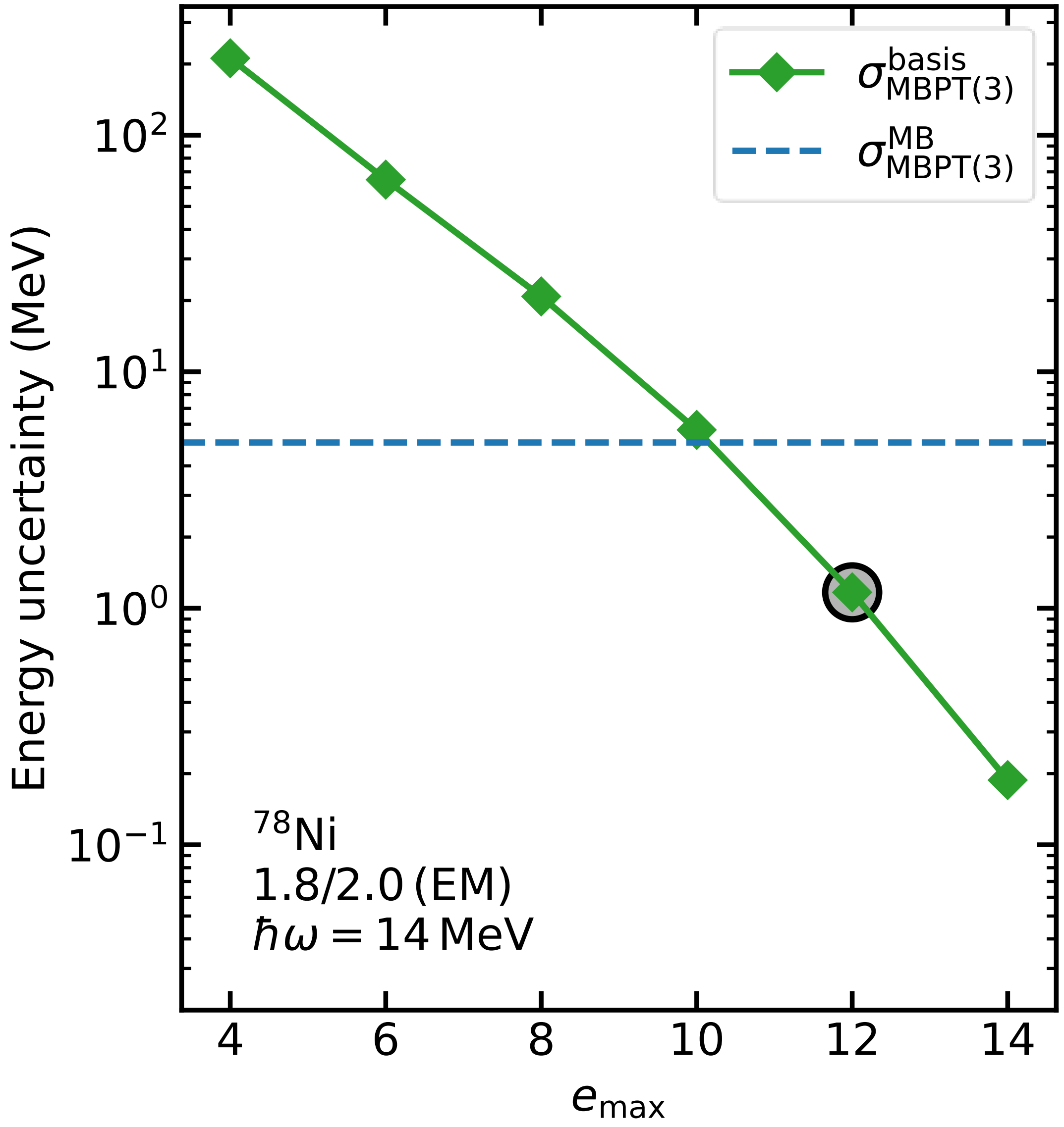

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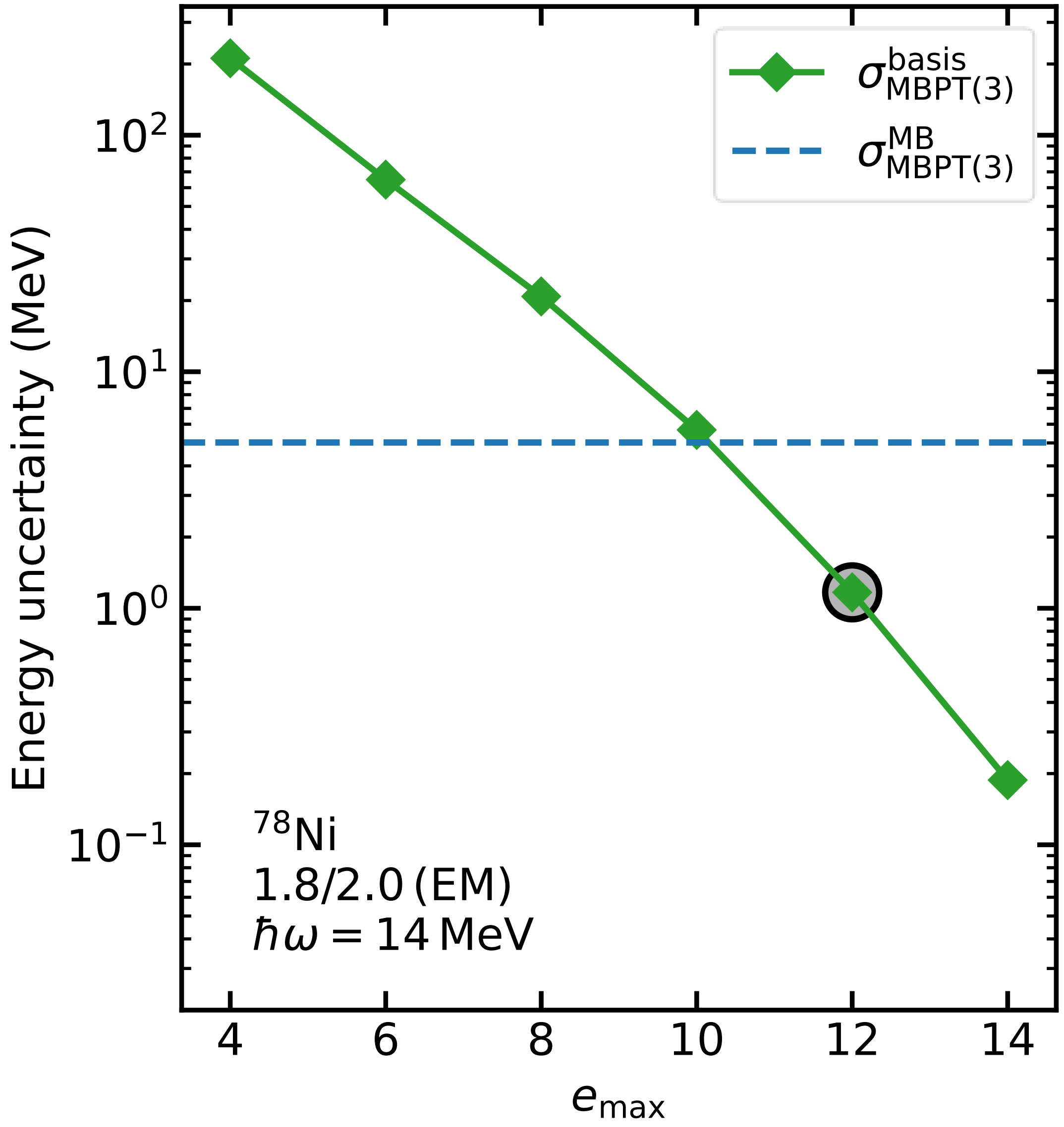
- Location of balancing point depends on how uncertainties are modeled



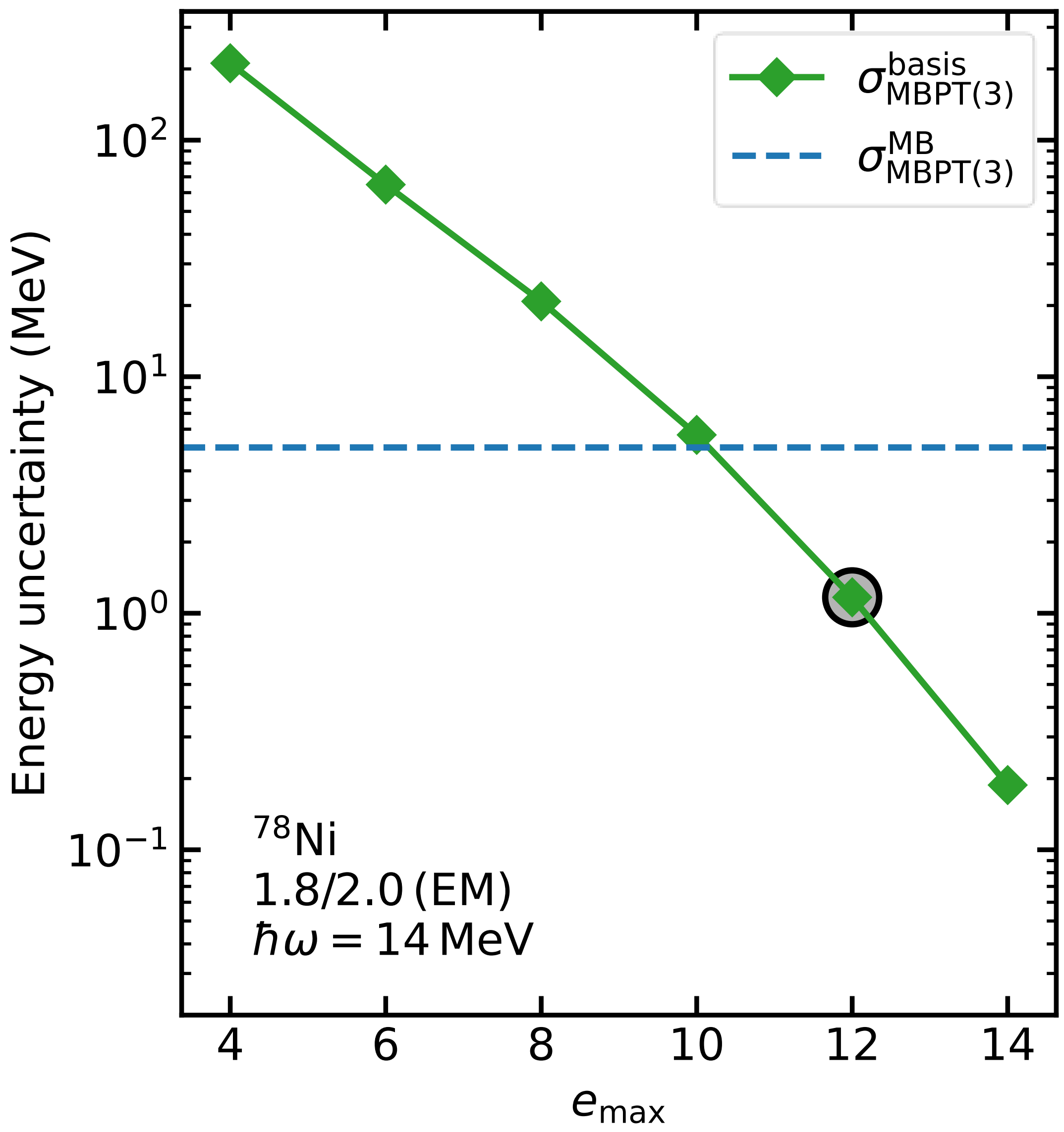
Uncertainty models

- $E_{\mathrm{MBPT(3)}} = E_{\mathrm{HF}} + E^{(2)} + E^{(3)}$
- $\sigma^{\mathrm{MB}}_{\mathrm{MBPT(3)}} \approx |E^{(4)}|$

$$\approx R^{(3)} |E^{(3)}(e_{\max} = 16)|$$

- $R^{(3)} \approx 0.44$ for 1.8/2.0(EM)

Z. Li et al., arXiv:2607.00119



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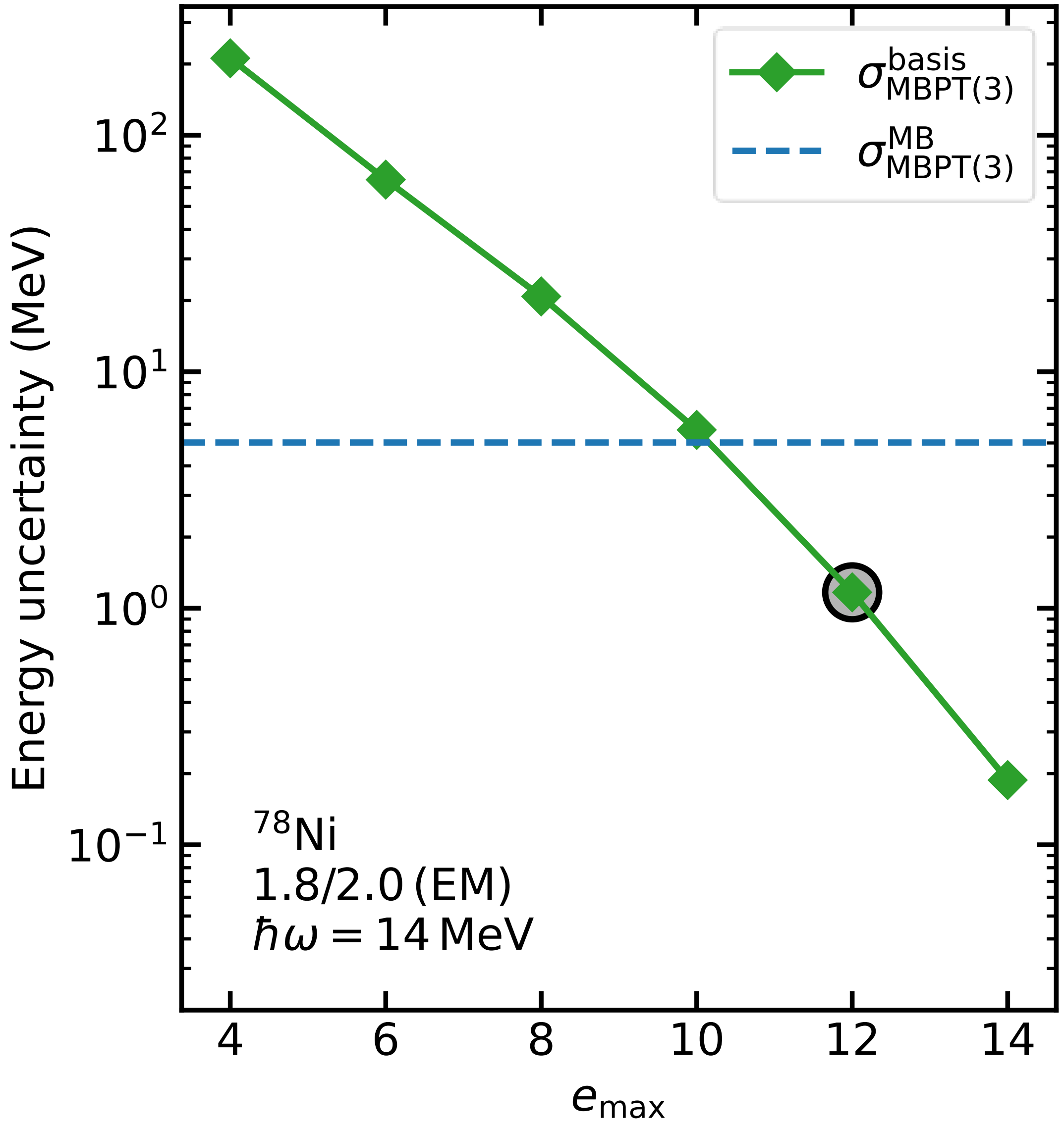
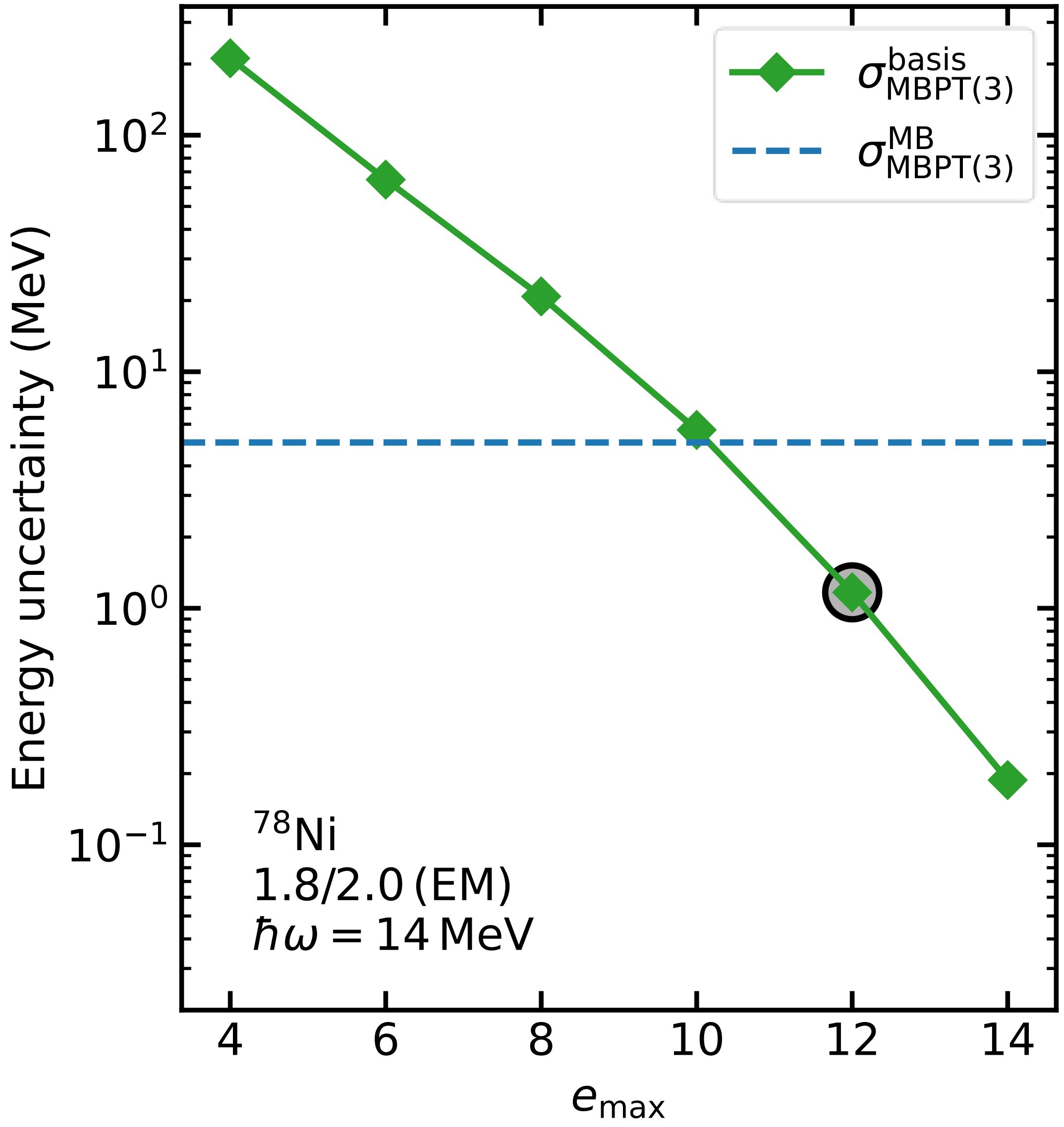
- $\sigma^{\mathrm{basis}}_{\mathrm{MBPT(3)}}(e_{\mathrm{max}})$
  $= |E_{\mathrm{MBPT(3)}}(e_{\mathrm{max}}) - E_{\mathrm{MBPT(3)}}(16)|$



Balancing uncertainties

- How can one find the balancing point without accessing large e_{max} for evaluating the uncertainties?
  - E.g., for another correlation expansion method or interaction



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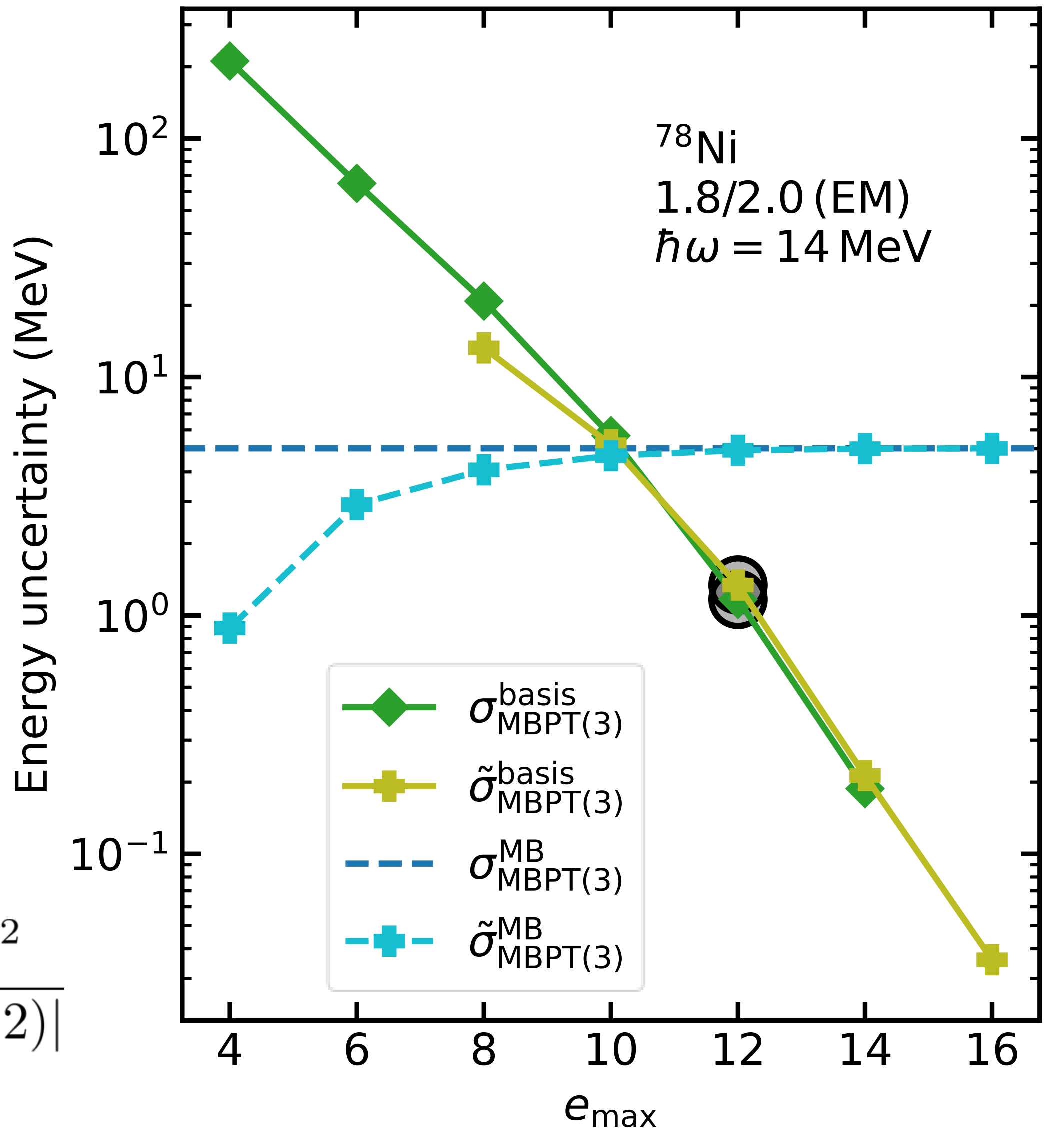
- Uncertainty models using information only from computed e_{max} work well

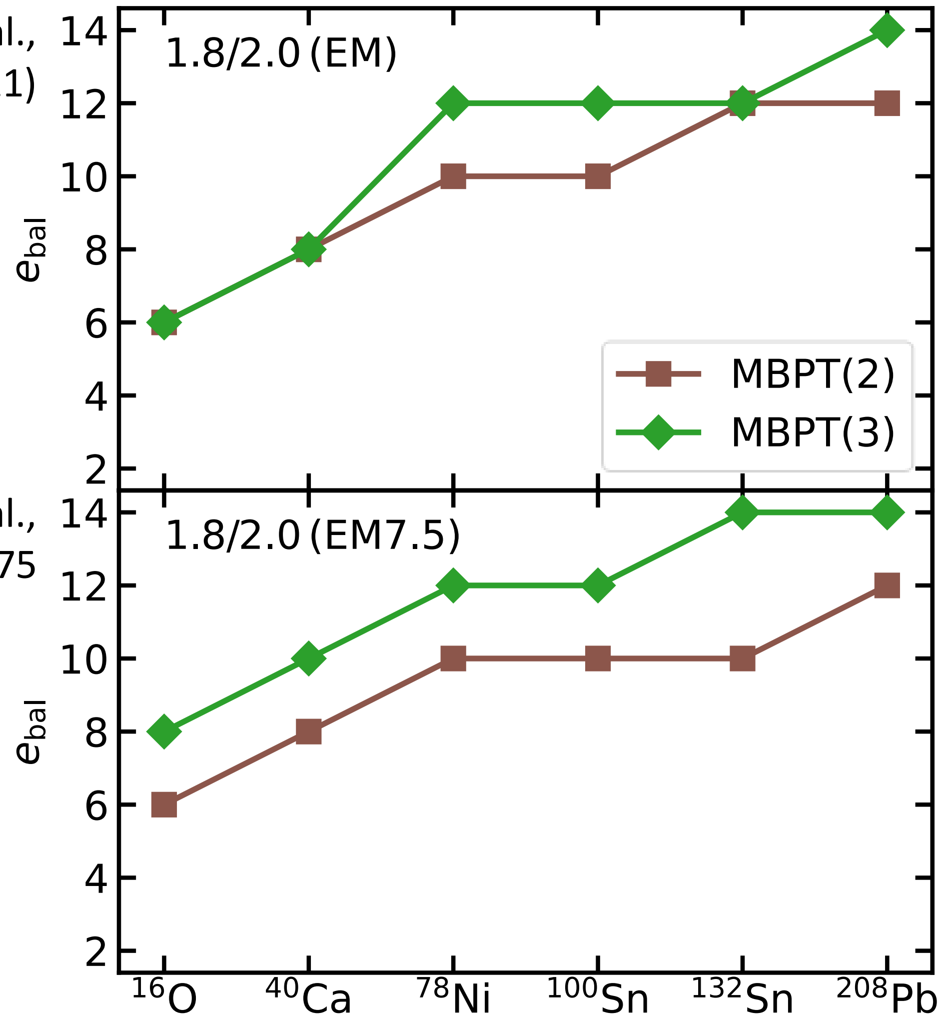
$$\tilde{\sigma}^{\mathrm{basis}}_{\mathrm{MBPT}(P)}(e_{\mathrm{max}}) = \left|\frac{E_{\mathrm{MBPT}(P)}(e_{\mathrm{max}}-2) - E_{\mathrm{MBPT}(P)}(e_{\mathrm{max}})|^2}{|E_{\mathrm{MBPT}(P)}(e_{\mathrm{max}}-4) - E_{\mathrm{MBPT}(P)}(e_{\mathrm{max}}-2)|}\right.$$



Balancing across the nuclear chart

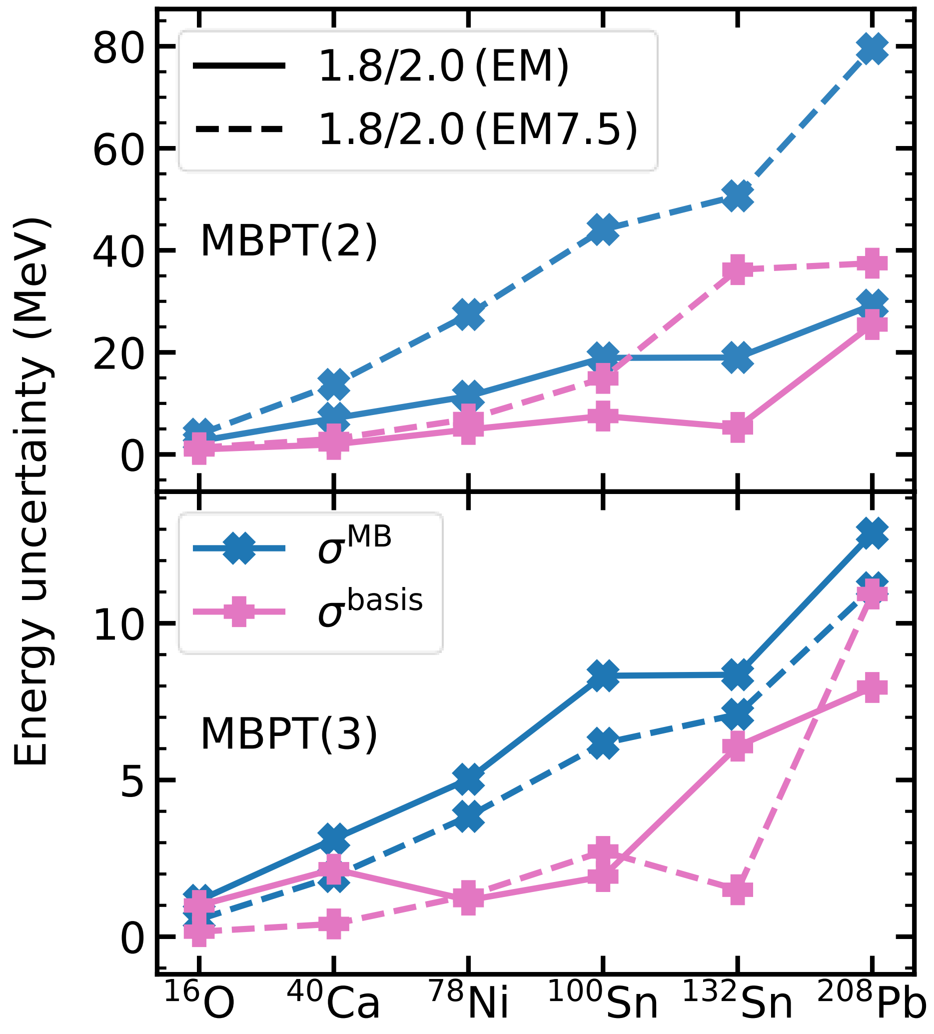
Hebeler et al., PRC **83** (2011)

Arthuis et al., 2401.06675



- Required basis size grows with order and (slightly sublinear) with mass
- Difference between balancing points for MBPT(2) and MBPT(3) smaller for 1.8/2.0(EM) because of large $R^{(3)}$
- Balancing points at MBPT(2) level almost identical for the two interactions

Balancing across the nuclear chart



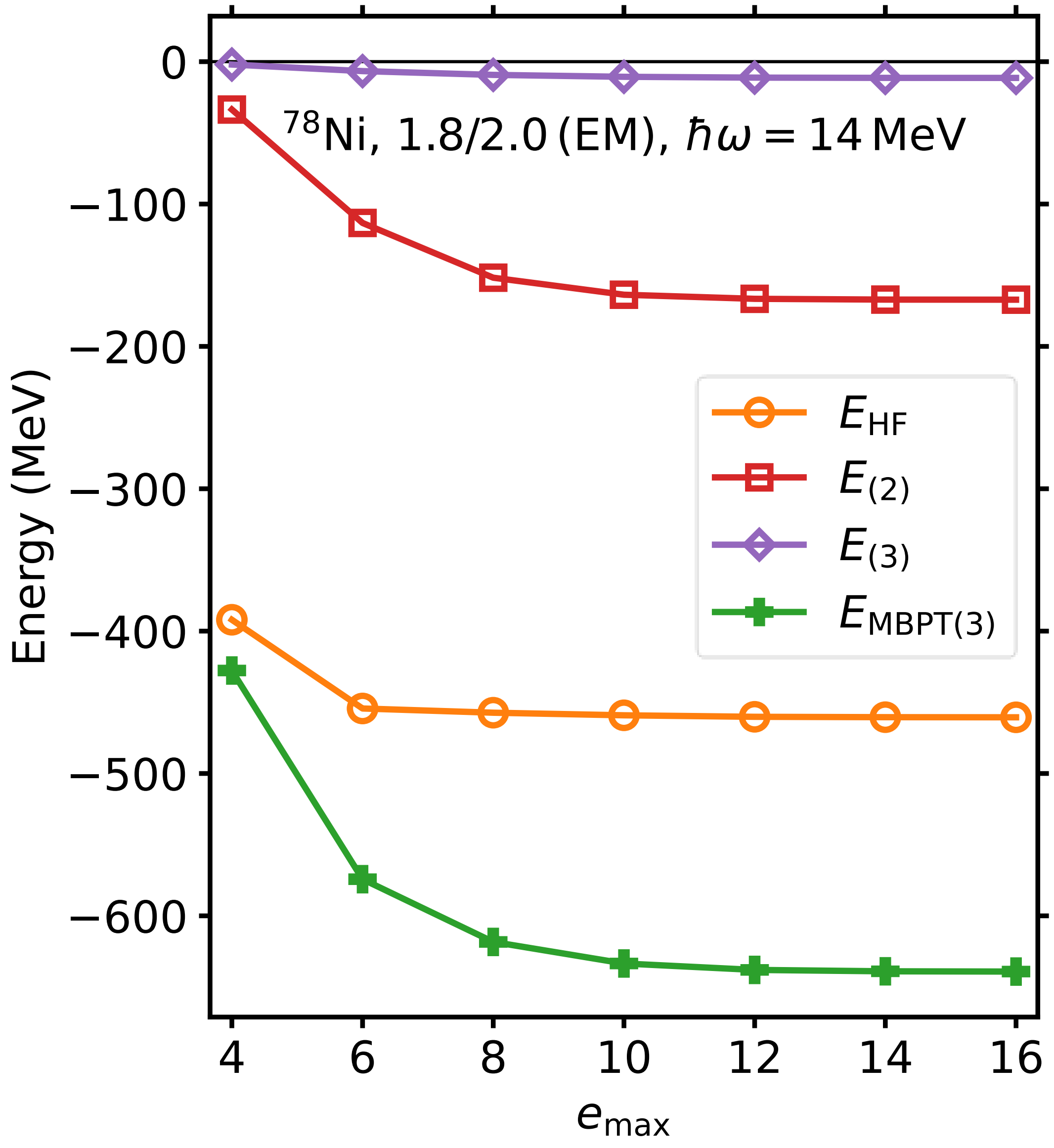
- Uncertainties at MBPT(2) level much larger for 1.8/2.0 (EM7.5) than for 1.8/2.0(EM)

- Many-body truncation uncertainties for the two interactions similar at MBPT(3) level (about 0.7% of total energy)

Contributions from different orders

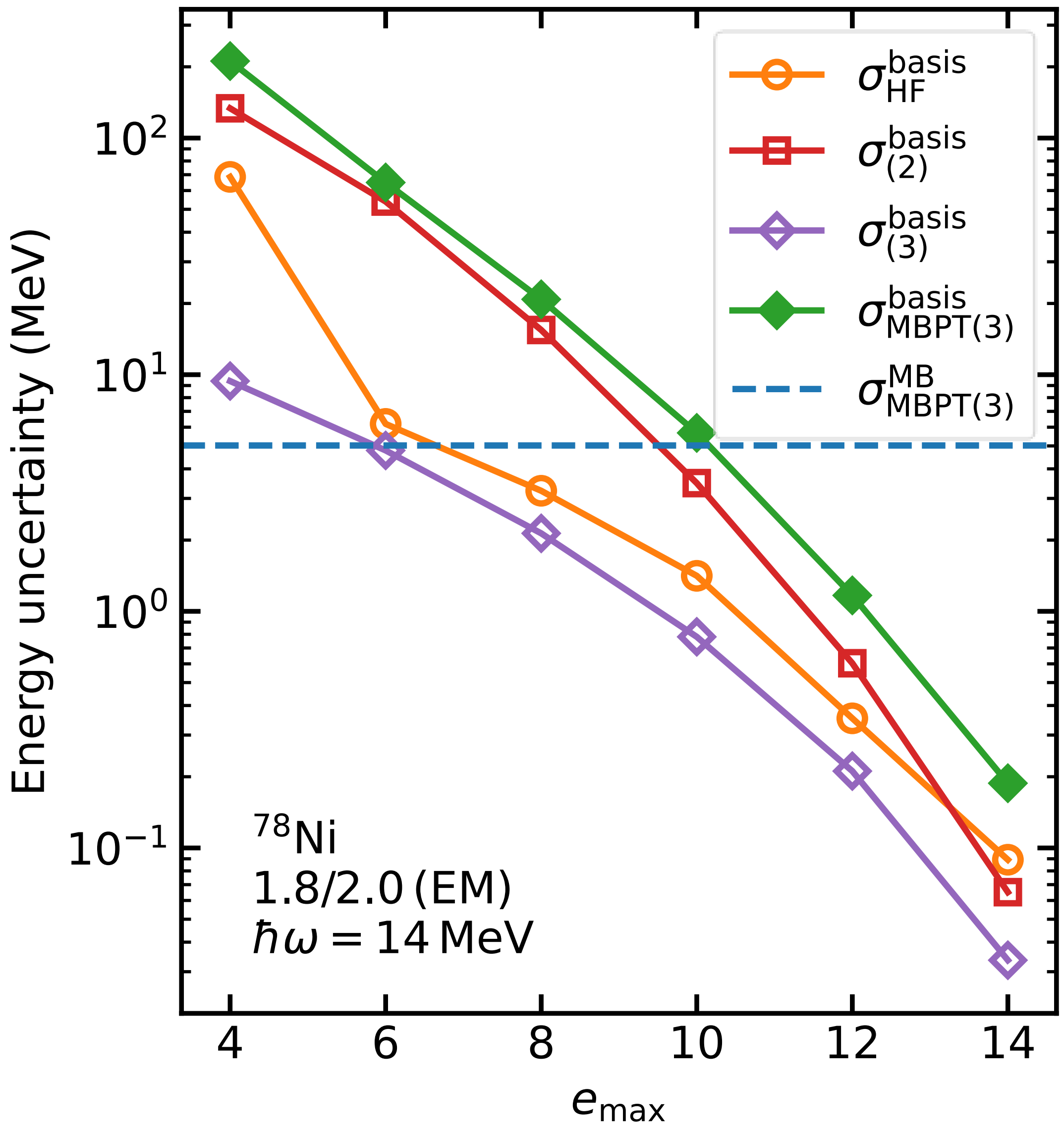
- $E_{\mathrm{MBPT}(3)} = E_{\mathrm{HF}} + E^{(2)} + E^{(3)}$

- Different contributions differ in sizes and convergence speeds



Contributions from different orders

- $\sigma_{(3)}^{\text{basis}} < \sigma_{(2)}^{\text{basis}}$
- We can choose different $e_{\max}$ for the individual contributions to achieve uncertainty balancing



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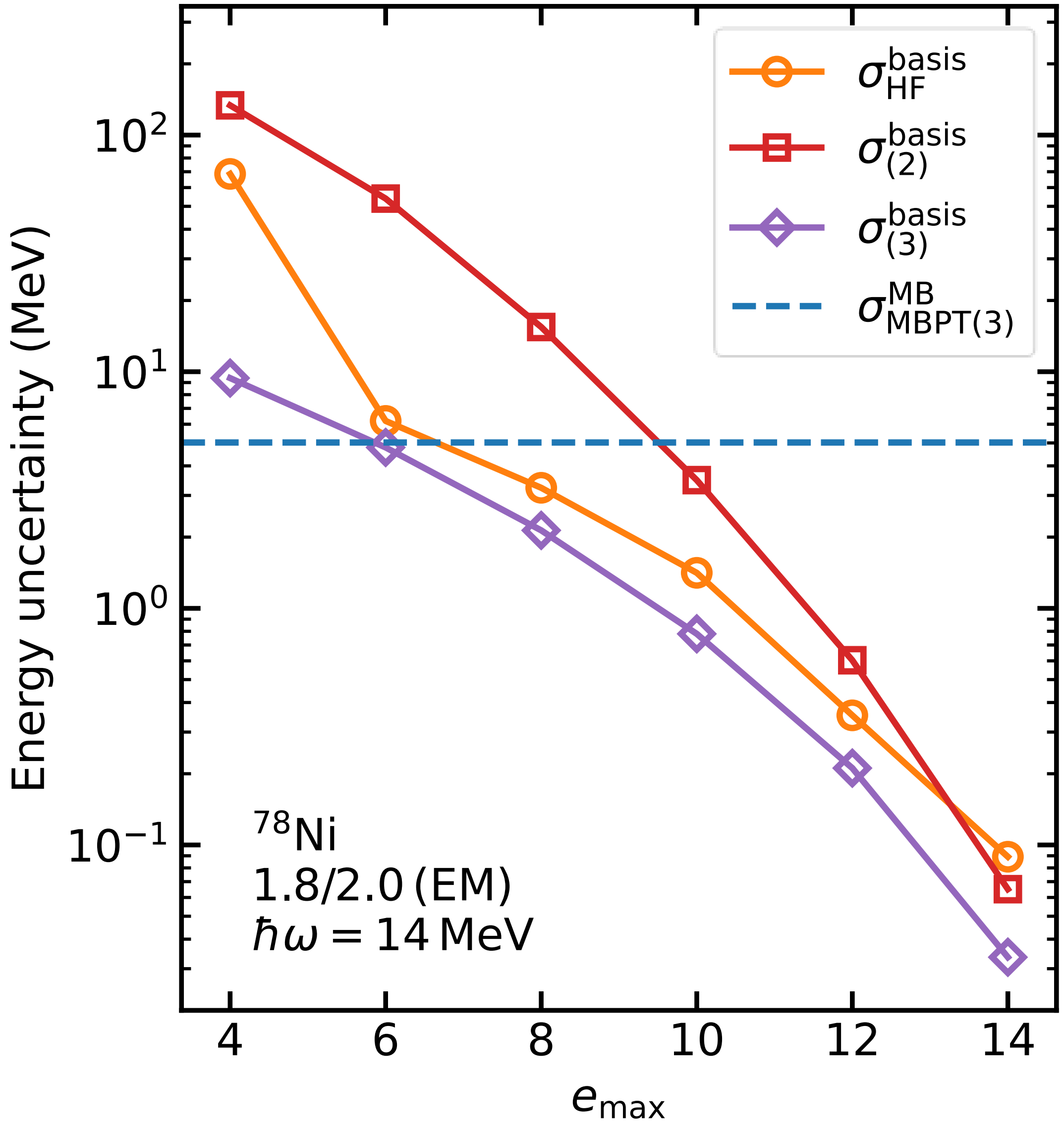

Contributions from different orders

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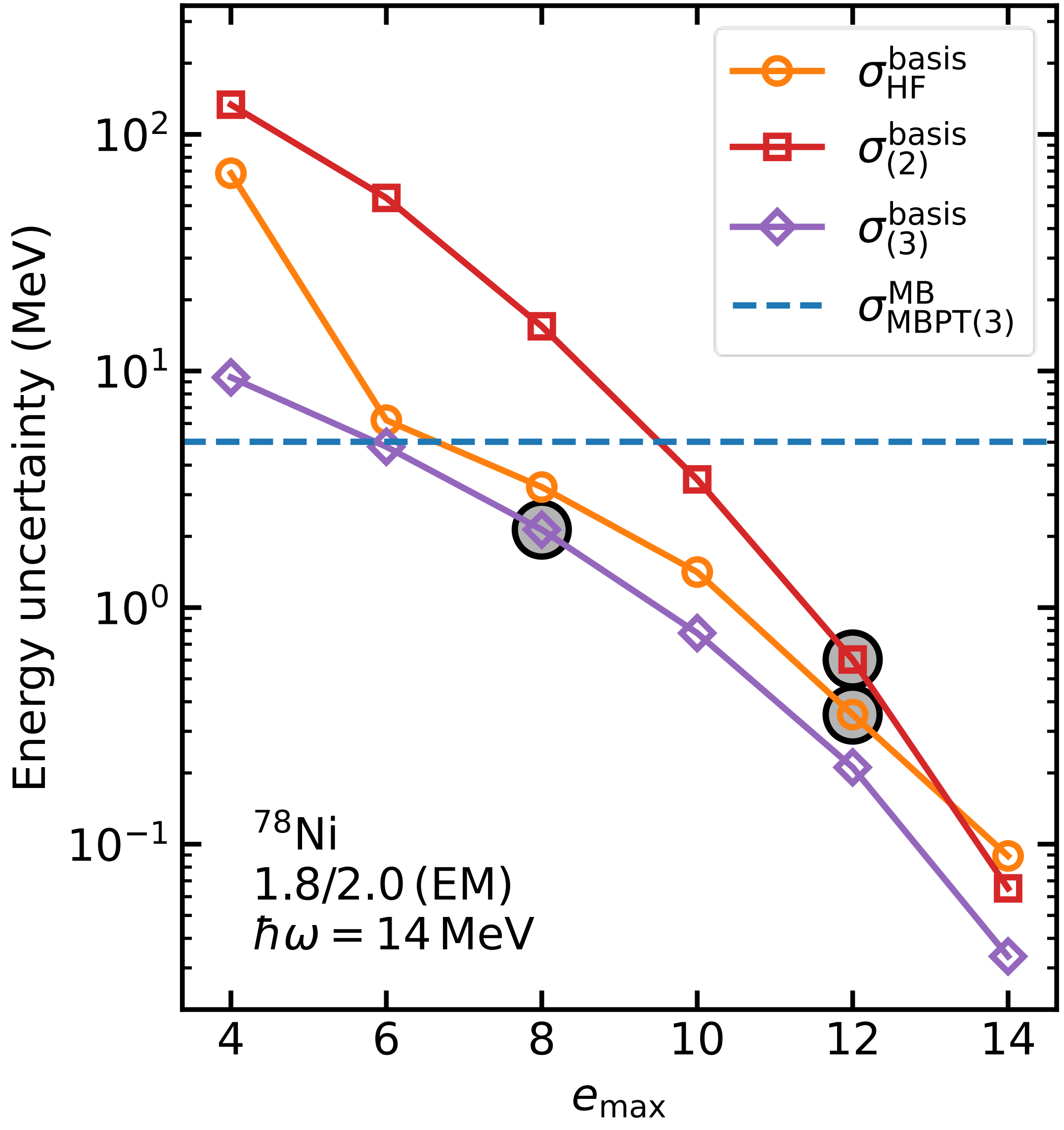
- We can choose different e_{max} for the individual contributions to achieve uncertainty balancing
- Instead of one MBPT(3) calculation with e_{max}=12, compute third- and second-order correction in separate calculations

→ Expensive third-order contribution can be computed with smaller e_{max}=8



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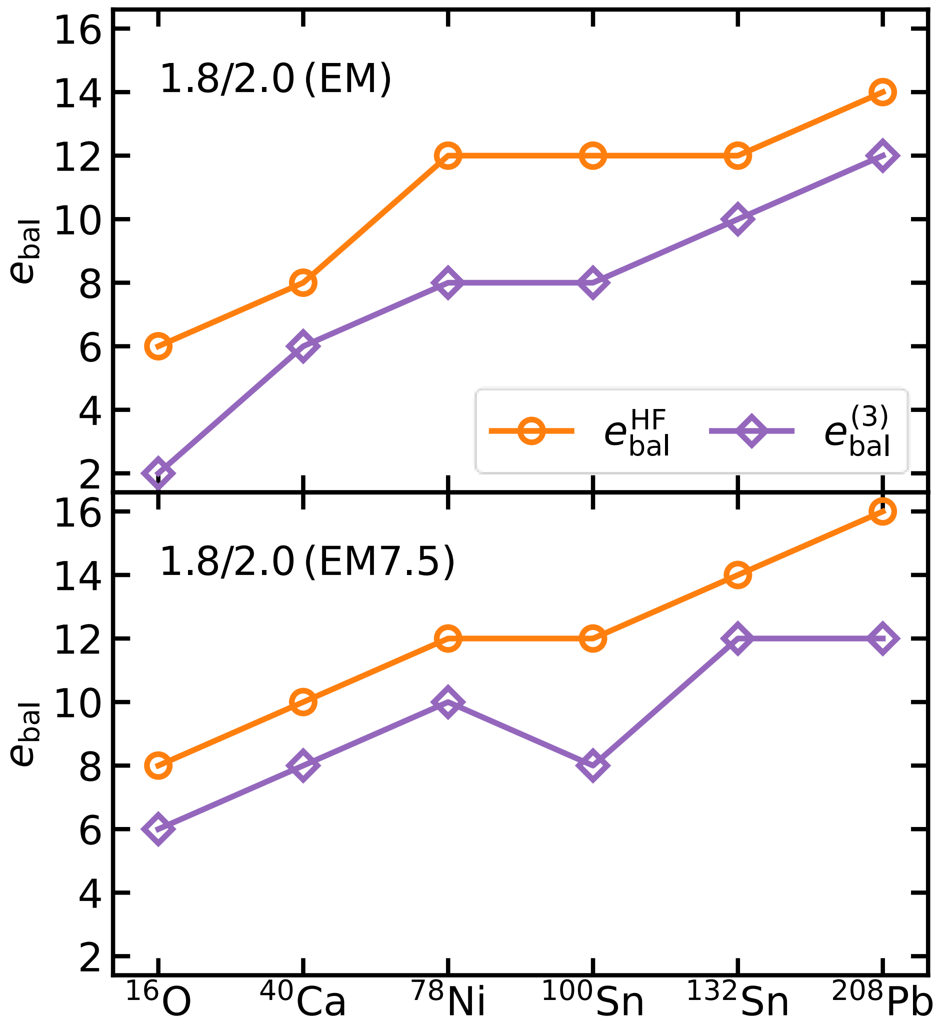

- Almost always $e_{\rm bal}^{\rm HF} = e_{\rm bal}^{(2)}$
- The e_{max} needed for third order corrections is 2 to 4 units smaller than the one for the leading terms

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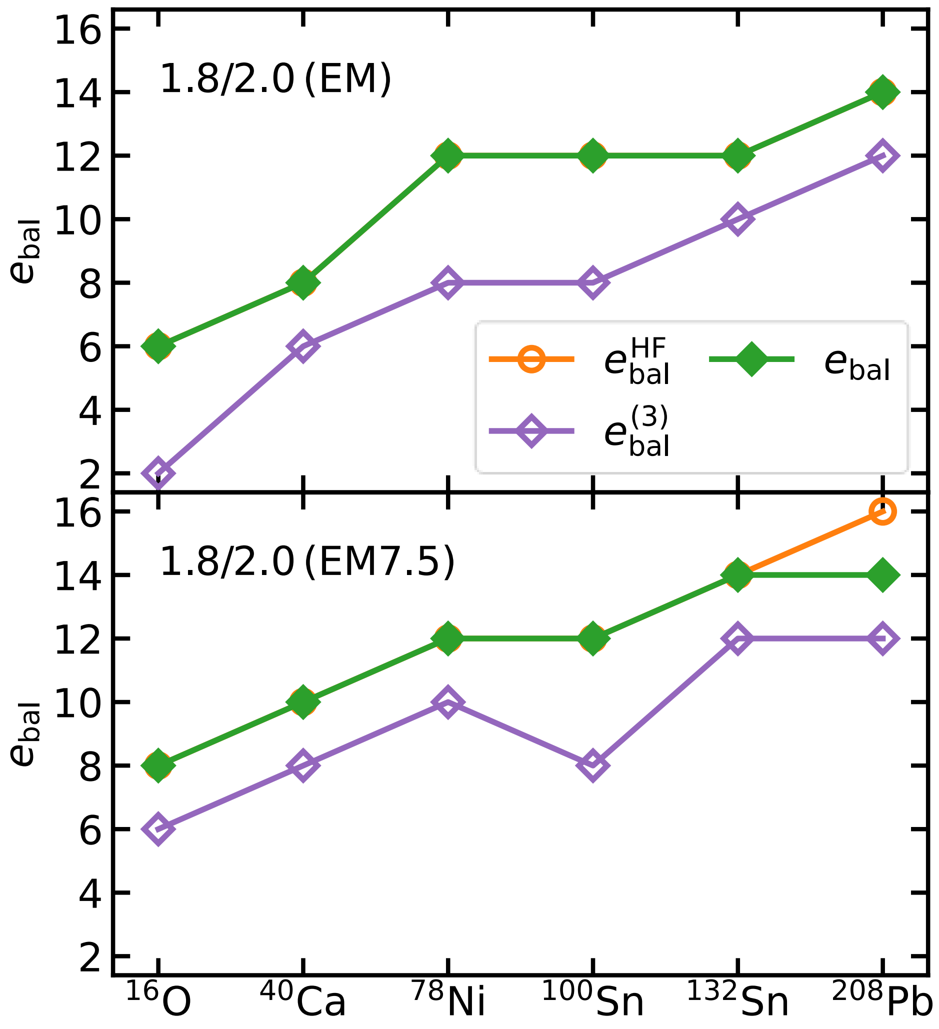

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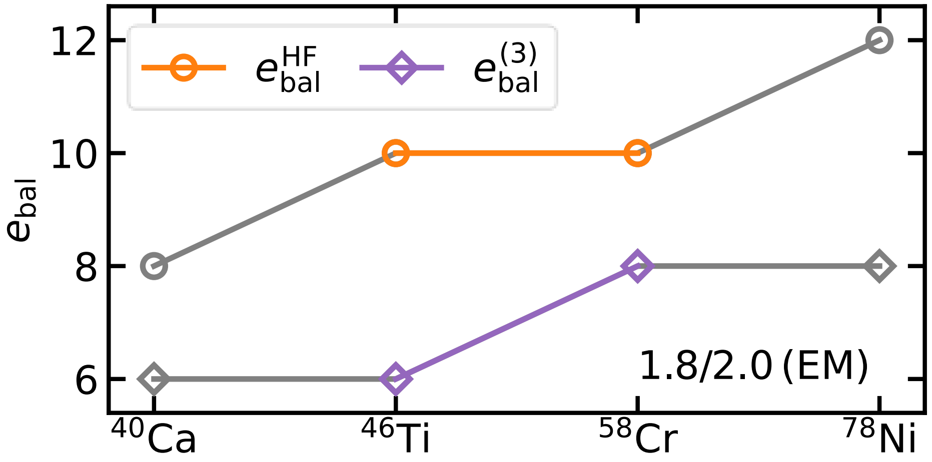
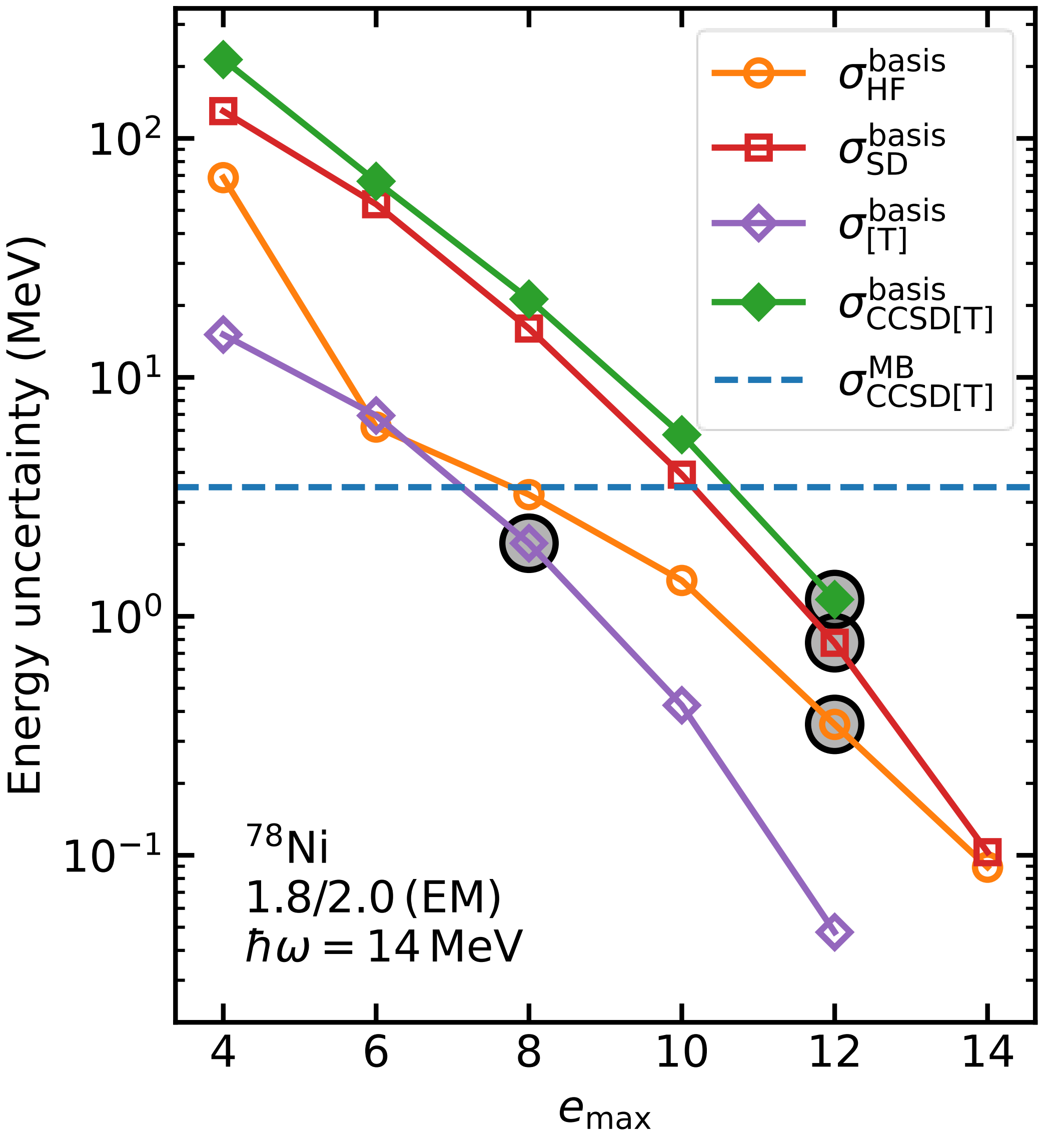


- Balancing points for open-shell nuclei align with results for closed-shell nuclei nearby
- Determined balancing points can be used as guideline for calculations of other nuclei

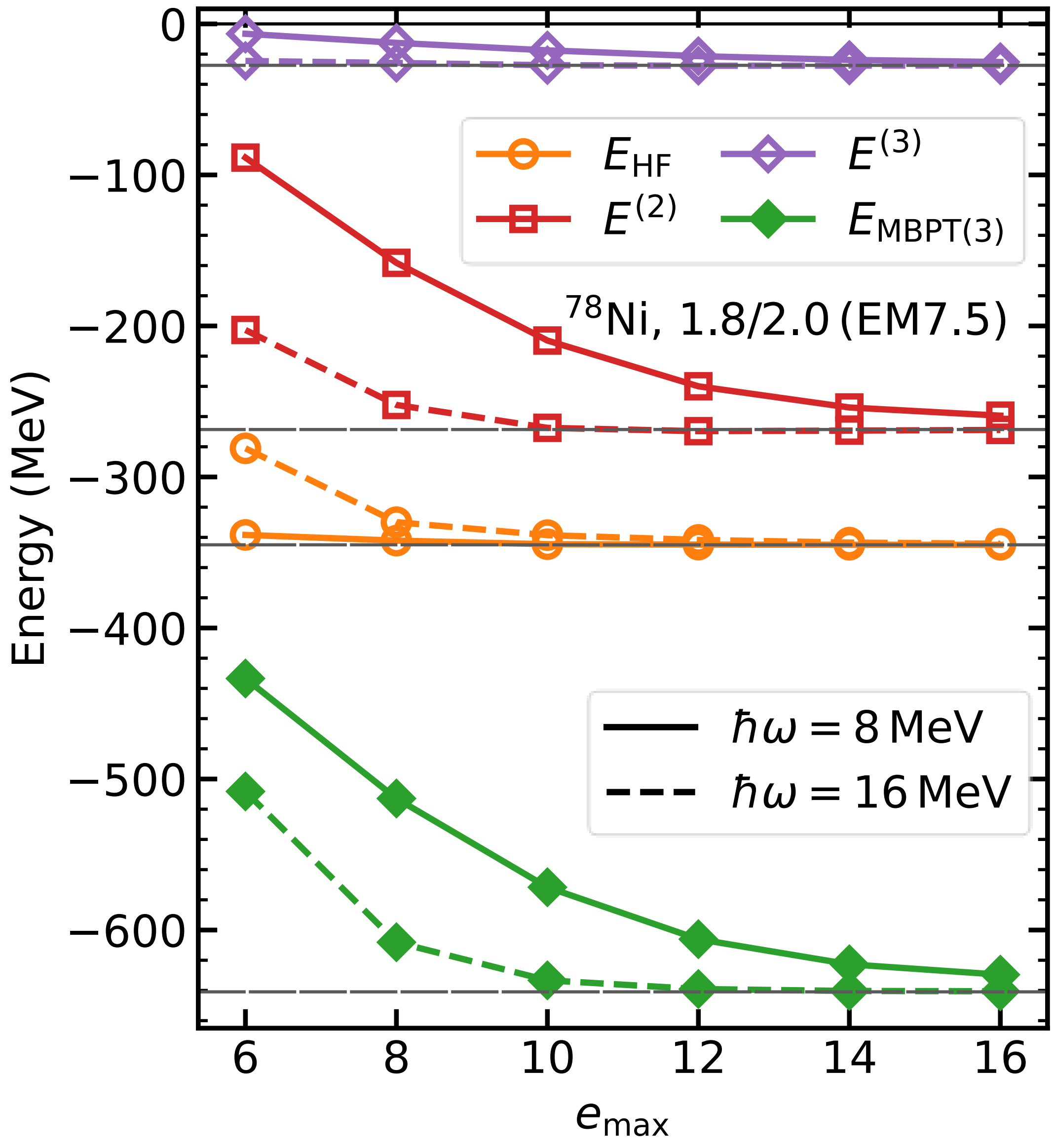
Contributions from different orders

- Coupled-cluster test case for 1.8/2.0 (EM) behaves just like MBPT



Mixing different frequencies

- Now: 1.8/2.0 (EM7.5) interaction



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  → Requires small $\hbar\omega$
- Dynamical correlations are short-range physics

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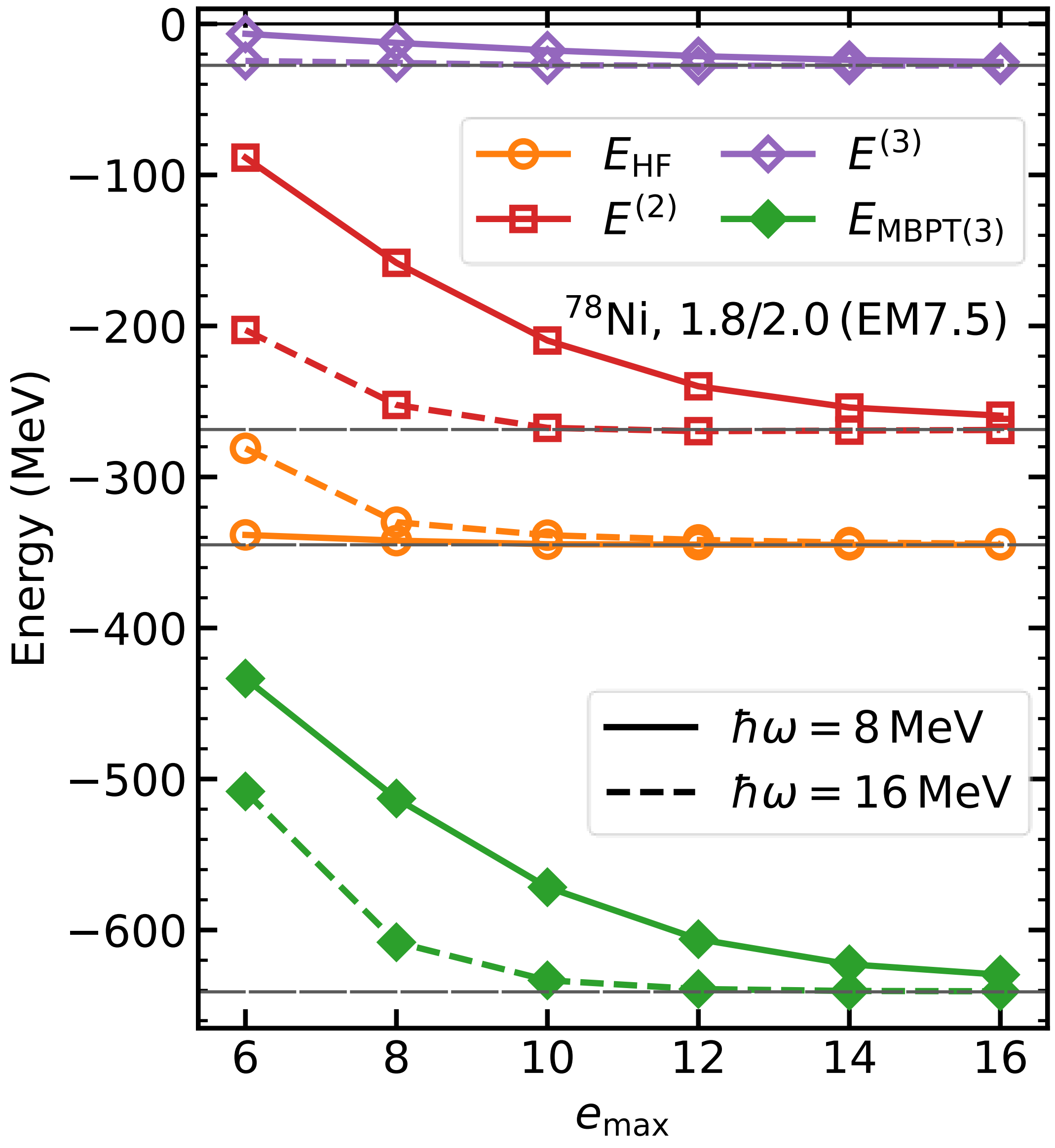

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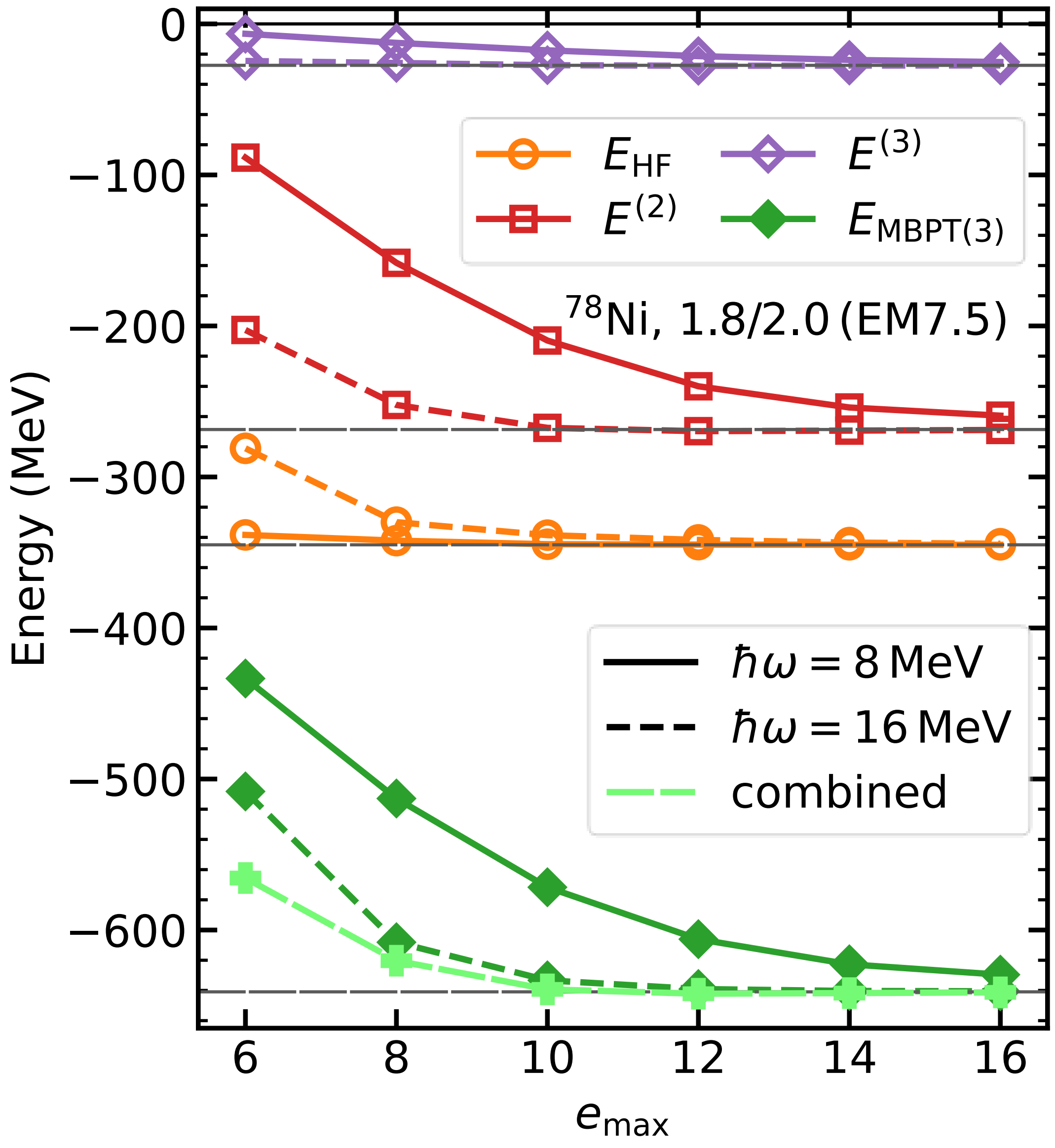
- Dynamical correlations are short-range physics

  → Requires large $\hbar\omega$
- Use different $\hbar\omega$ for the individual contributions

  → Even smaller e_{max} possible



Summary

- Avoid wasting resources by balancing uncertainties
- Compute high-order contributions with smaller bases

arXiv:2608.18975

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Thanks for your attention