Diagrammatic resummations for the in-medium similarity renormalization group

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ESNT Workshop "Automated tools for many-body theory"
June 8, 2023

Outline

- Introduction to the IMSRG

  Tsukiyama et al., PRL **106** (2011)
  Hergert et al., Phys. Rep. **621** (2016)
  MH et al., PRC **103** (2021)

- Connecting IMSRG and MBPT

  Hjorth-Jensen et al., Phys. Rep. **261** (1995)
  Bartlett, Shavitt, *Many-Body Methods in Chemistry and Physics* (2009)
  Hergert et al., Phys. Rep. **621** (2016)

- Approaches to improving IMSRG truncations

  Morris, PhD Thesis, MSU (2016)
  Arthuis et al., CPC **240** (2019)

Introduction to the IMSRG

Tsukiyama et al., PRL **106** (2011)
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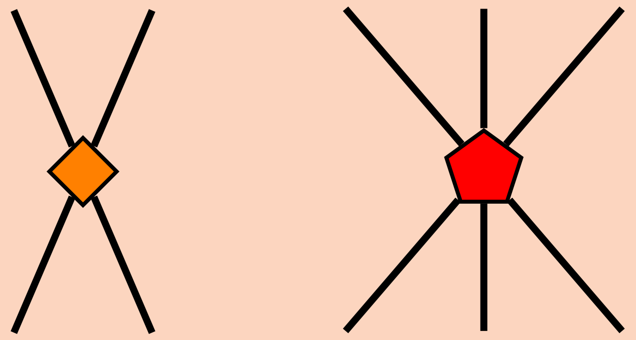
The basics



$$H = T_{\text{int}} + V_{\text{NN}} + V_{\text{3N}}$$

$$H|\Psi\rangle = E|\Psi\rangle$$

Many-body solver

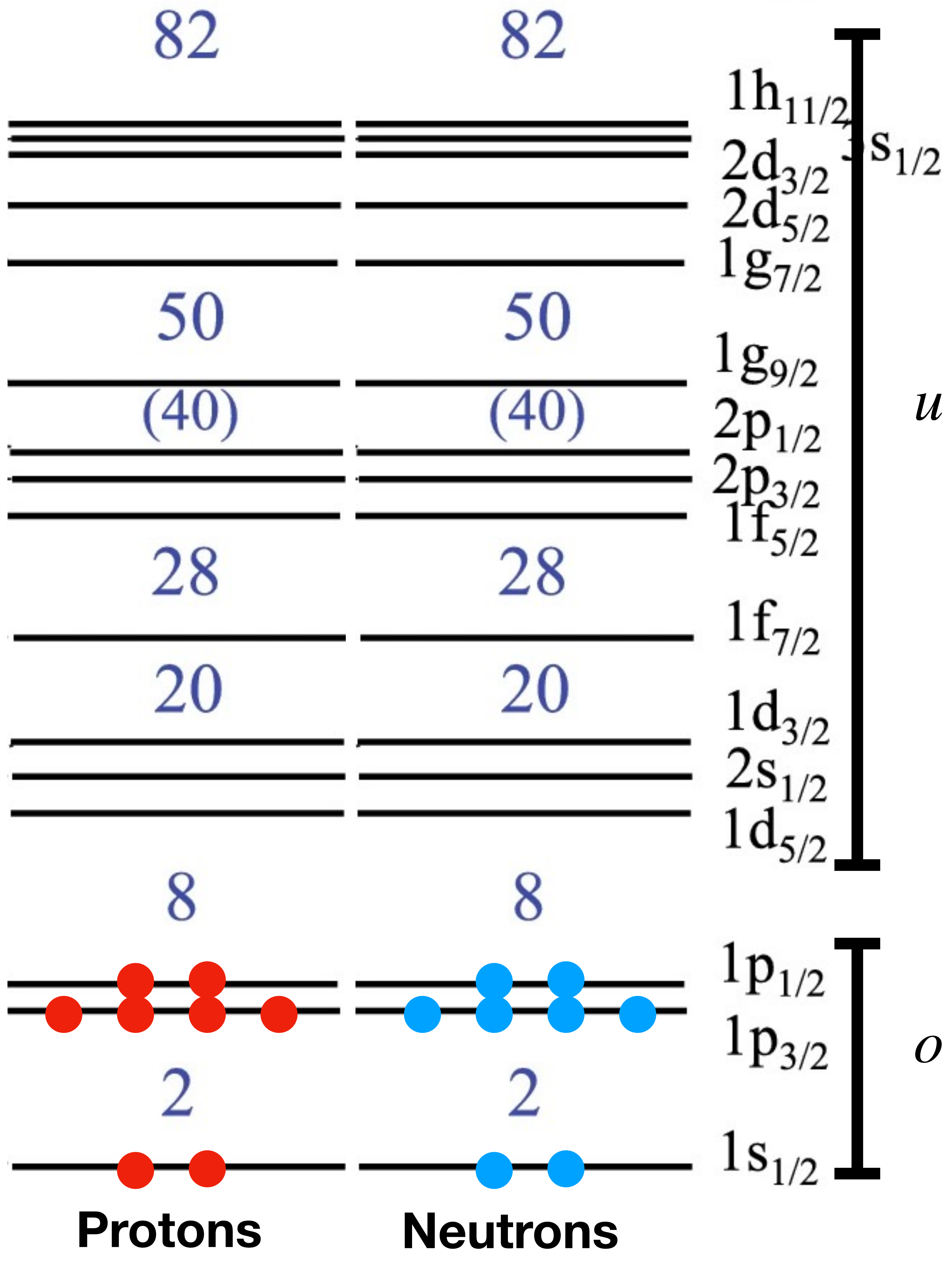
IMSRG

$$E$$

$$|\Psi\rangle = U|\Phi\rangle = e^{\Omega}|\Phi\rangle$$

$\langle R_p^2 \rangle, \ldots$ $\quad \overline{H} \rightarrow$ spectra

Solving the many-body problem



Hagino et al., Found. Chem. **22** (2020)

$$|\Phi\rangle \sim \prod_{i=1}^{o} |\phi_i\rangle$$ mean-field reference state

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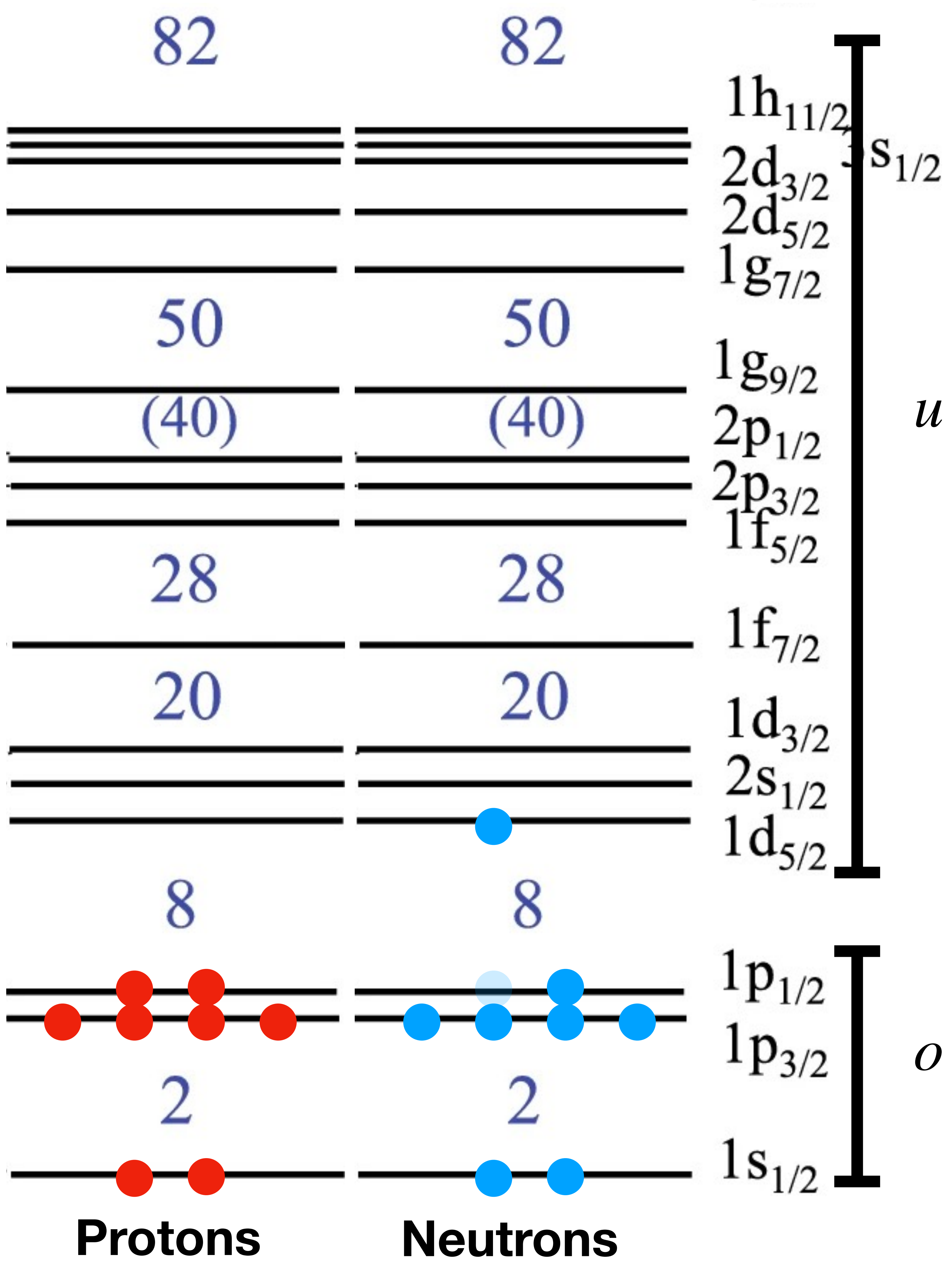

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$|\Phi_i^a\rangle$ 1p1h excitation ($\binom{o}{1}\binom{u}{1}$ states)

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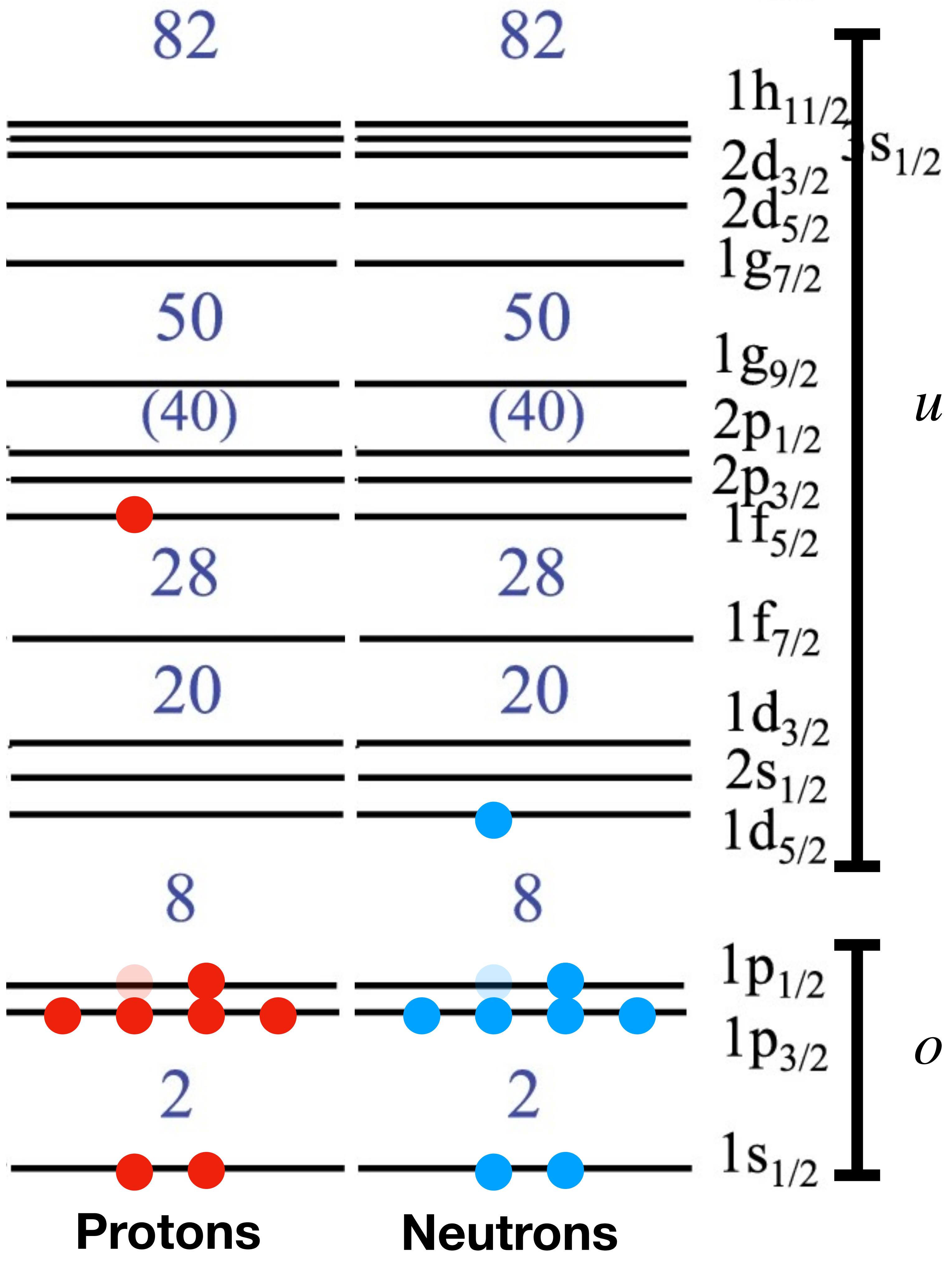

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$|\Phi_{ij}^{ab}\rangle$ 2p2h excitation ($\binom{o}{2}\binom{u}{2}$ states)

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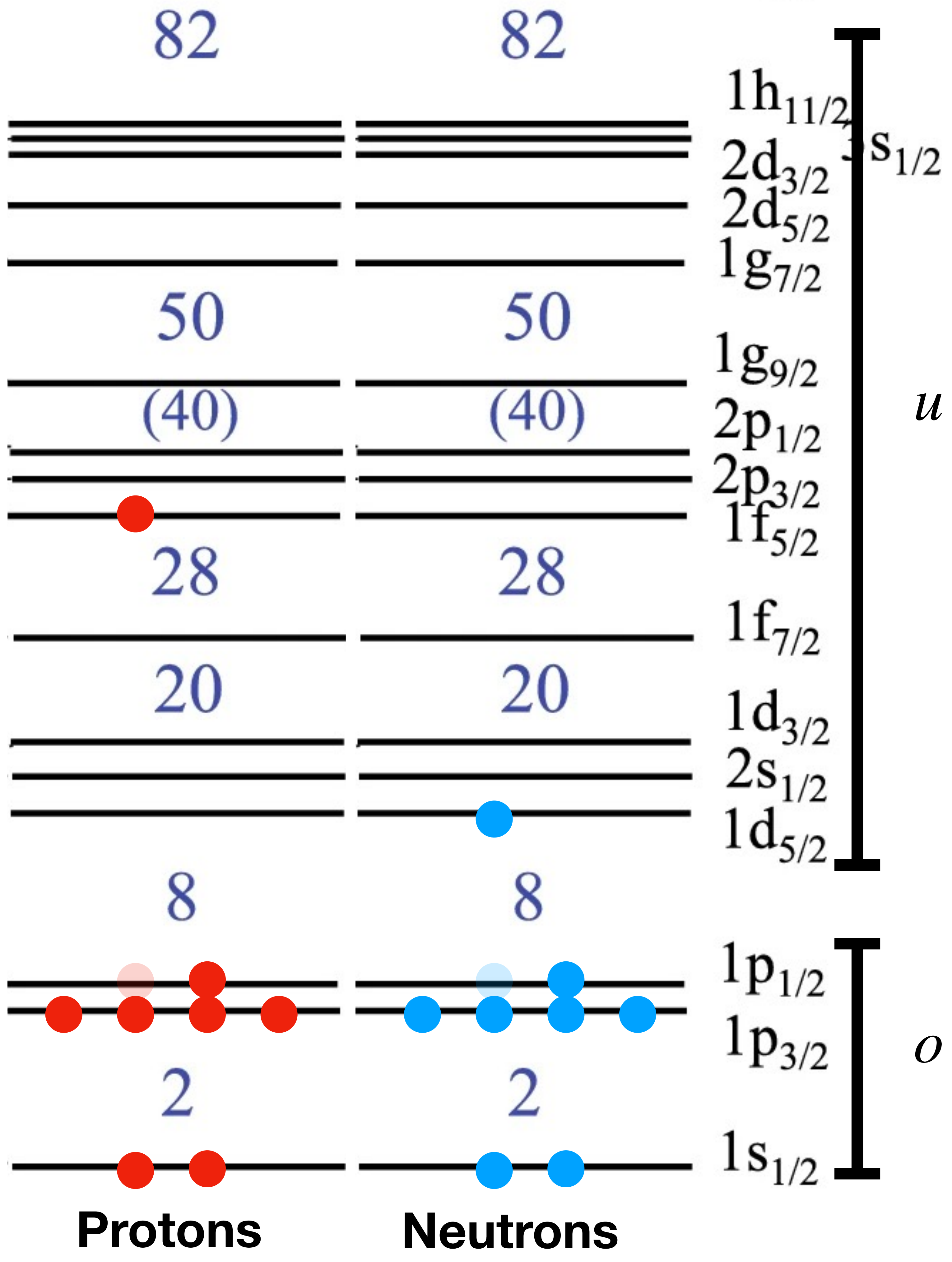

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Scales factorially in o and u.

Obvious scalability problem.

The IMSRG

in-medium similarity renormalization group

- IMSRG generates unitary transformation of Hamiltonian

$$\frac{dH}{ds} = [\eta, H]$$

- Normal order with respect to $|\Phi\rangle$ approximately handles **3N forces** and **induced many-body forces**

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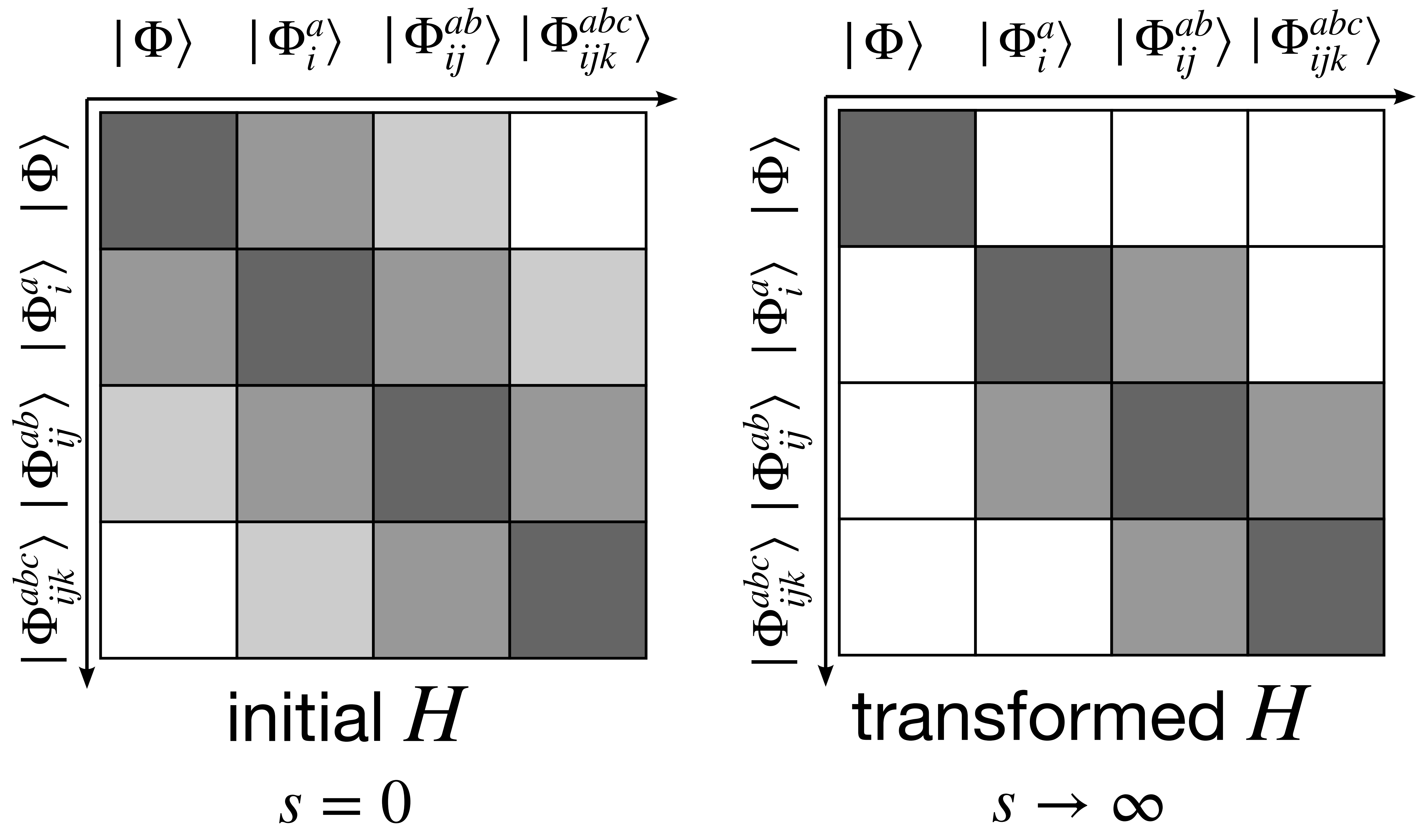

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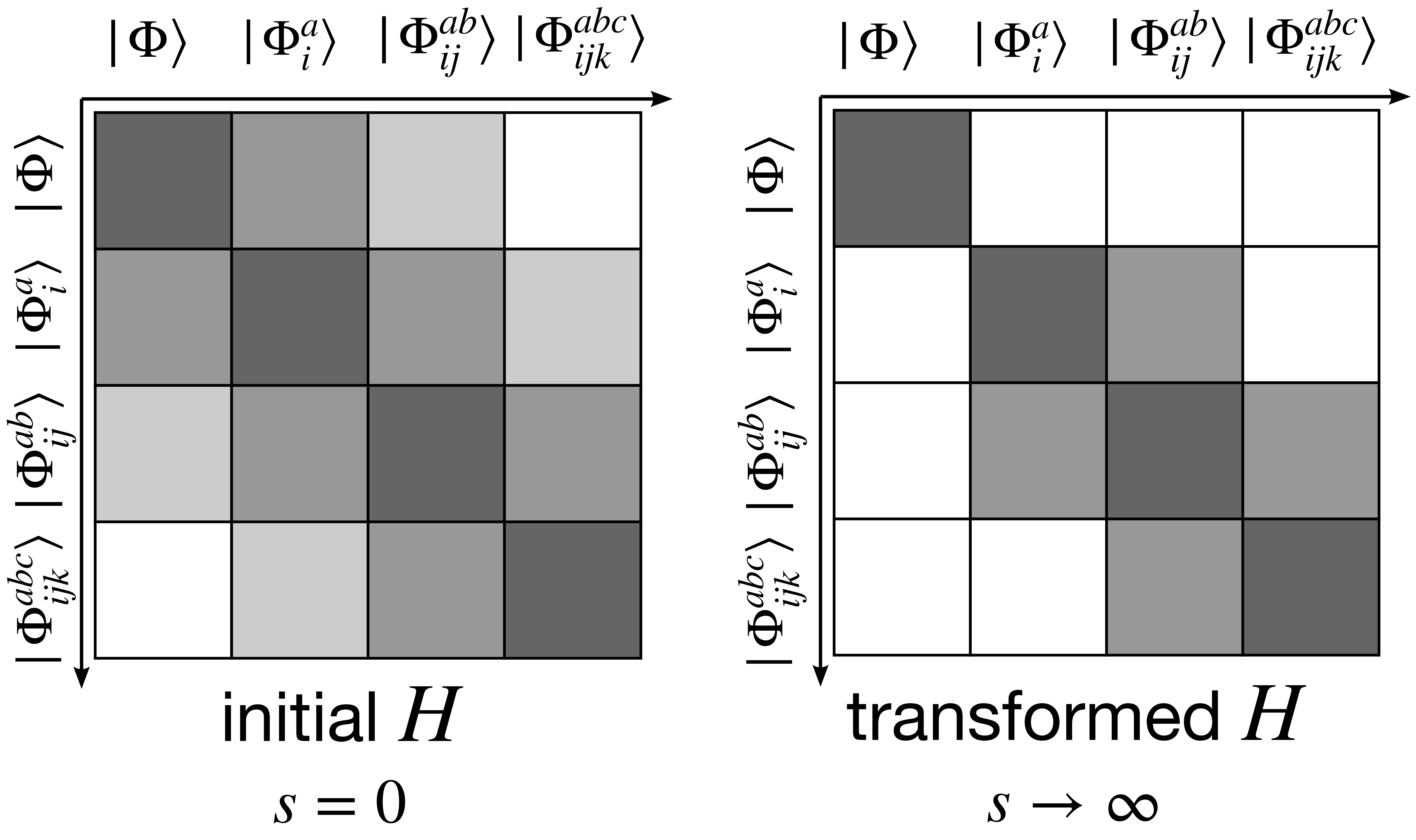


Hergert et al., Phys. Rep. **621** (2016)

Truncation necessary!

- Standard = IMSRG(2)
- More refined = **IMSRG(3)** **MH** et al., PRC **103** (2021)

Normal ordering

Hagen et al., PRC **76** (2007)
Roth et al., PRL **109** (2012)
Miyagi et al., PRC **105** (2022)
Hebeler, ..., **MH** et al., PRC **107** (2023)

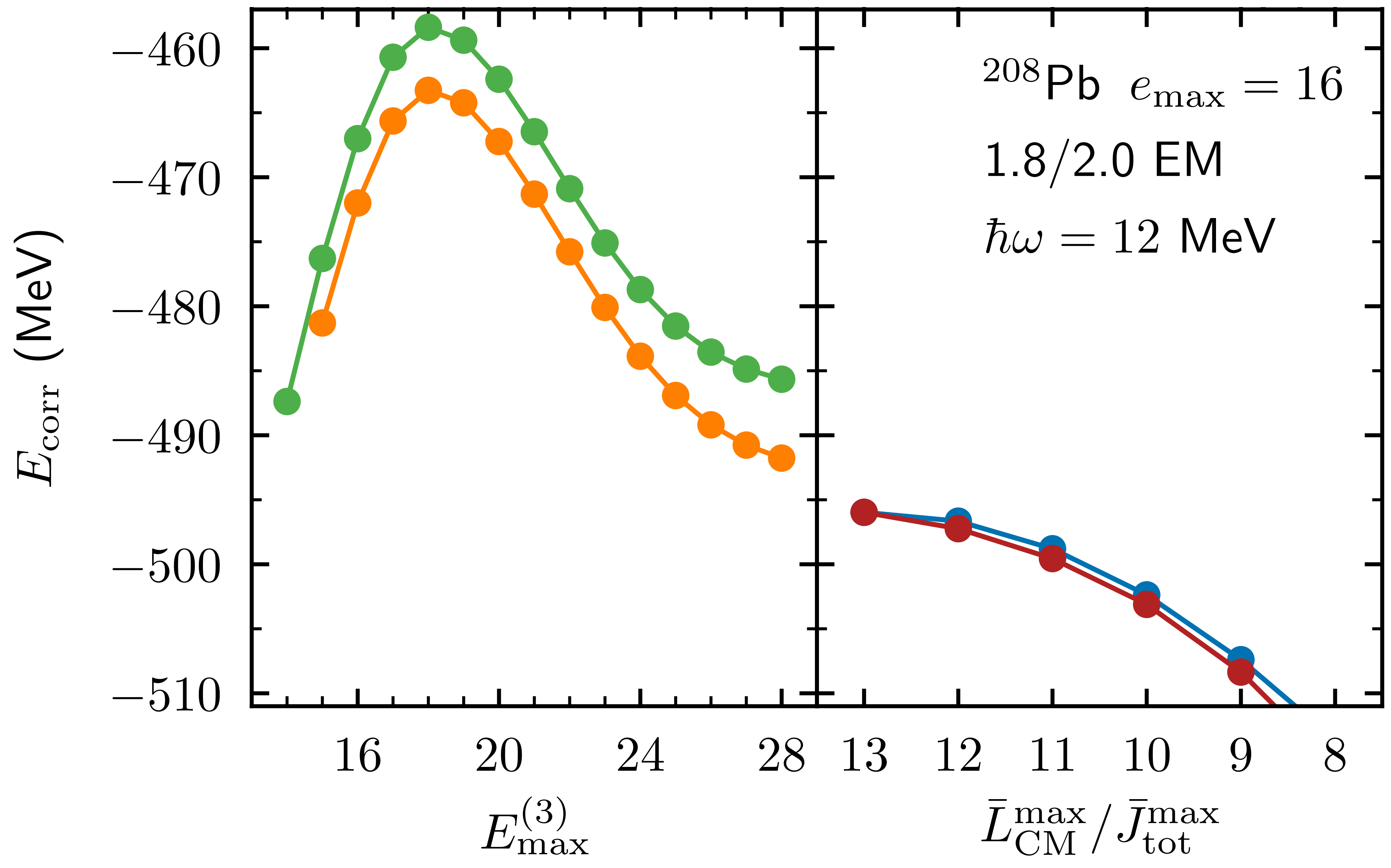
- Normal ordering w.r.t. $|\Phi\rangle$ gives us effective interactions

$$\Gamma_{pqrs} = V_{\mathrm{NN},pqrs} + \sum_i n_i V_{\mathrm{3N},pqirsi}$$

Discard

$$W_{pqrstu} = V_{\mathrm{3N},pqrstu}$$

- Single-particle representation of V_{3N} is expensive (100s of GB or TB)



Hebeler, ..., **MH** et al., PRC **107** (2023)

IMSRG truncation

Generator η gives decoupling

$$\langle \Phi_i^a | H(\infty) | \Phi \rangle \stackrel{!}{=} 0$$
$$\langle \Phi_{ij}^{ab} | H(\infty) | \Phi \rangle \stackrel{!}{=} 0$$

...

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

Truncate operators in many-body rank

$$H(0) = E_0 + f + \Gamma$$
$$\eta(0) = \eta^{(1B)} + \eta^{(2B)}$$

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IMSRG(3)

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MH et al., PRC **103** (2021)

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IMSRG(3)

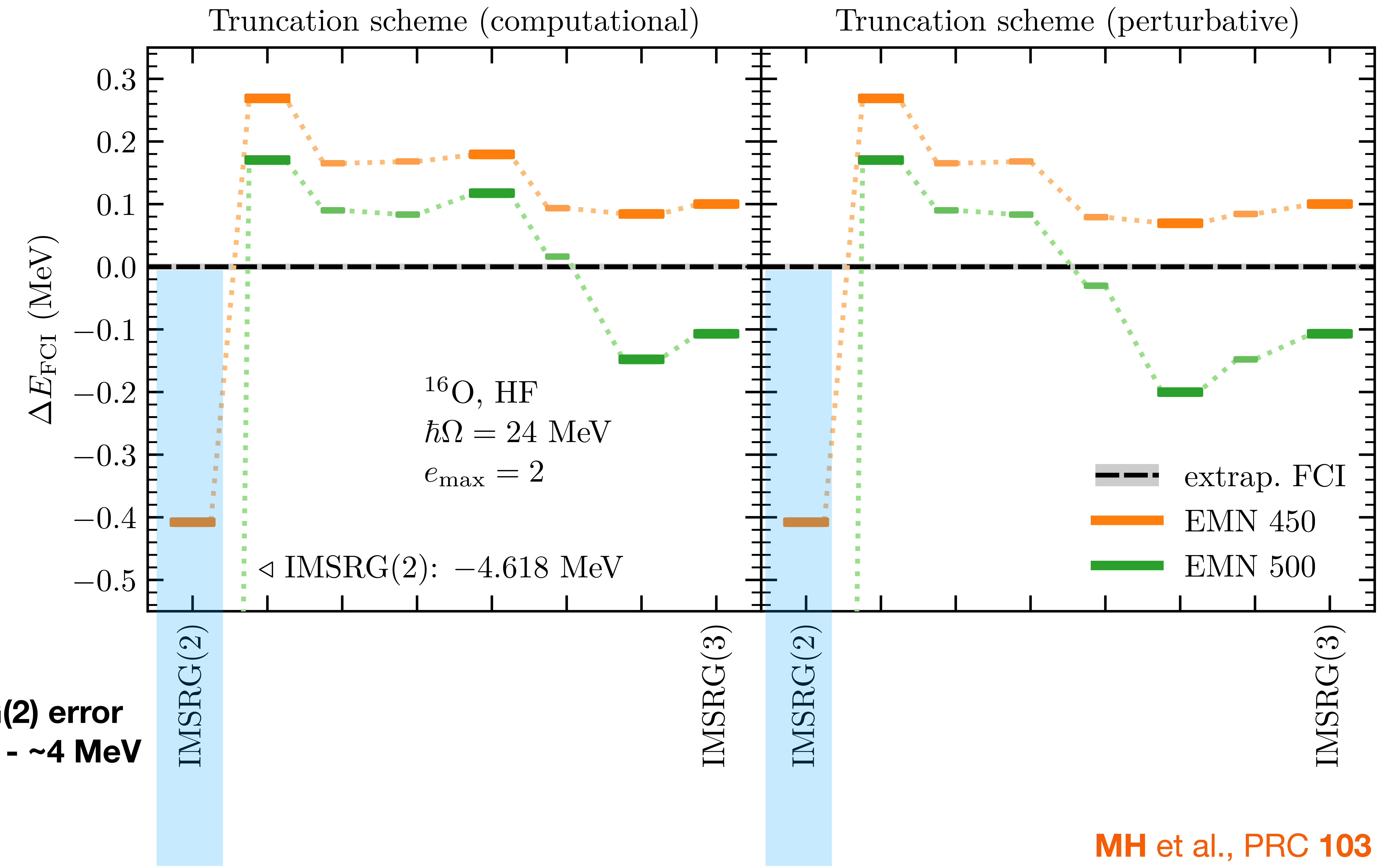
$$H(0) = E_0 + f + \Gamma$$
$$\eta(0) = \eta^{(1B)} + \eta^{(2B)}$$

MH et al., PRC **103** (2021)

IMSRG(3) = more precision, but higher cost [$\mathcal{O}(N^9)$, $\mathcal{O}(N^7)$ with approx]:

- Automated derivation with Drudge — Zhao, Scuseria, https://github.com/tschijnmo/drudge (2021)
- Angular momentum coupling with AMC — Tichai et al., EPJA **56** (2020)
- **No automatic code generation yet**

Where does IMSRG(3) matter?



IMSRG(2) error
400 keV - ~4 MeV

MH et al., PRC **103** (2021)

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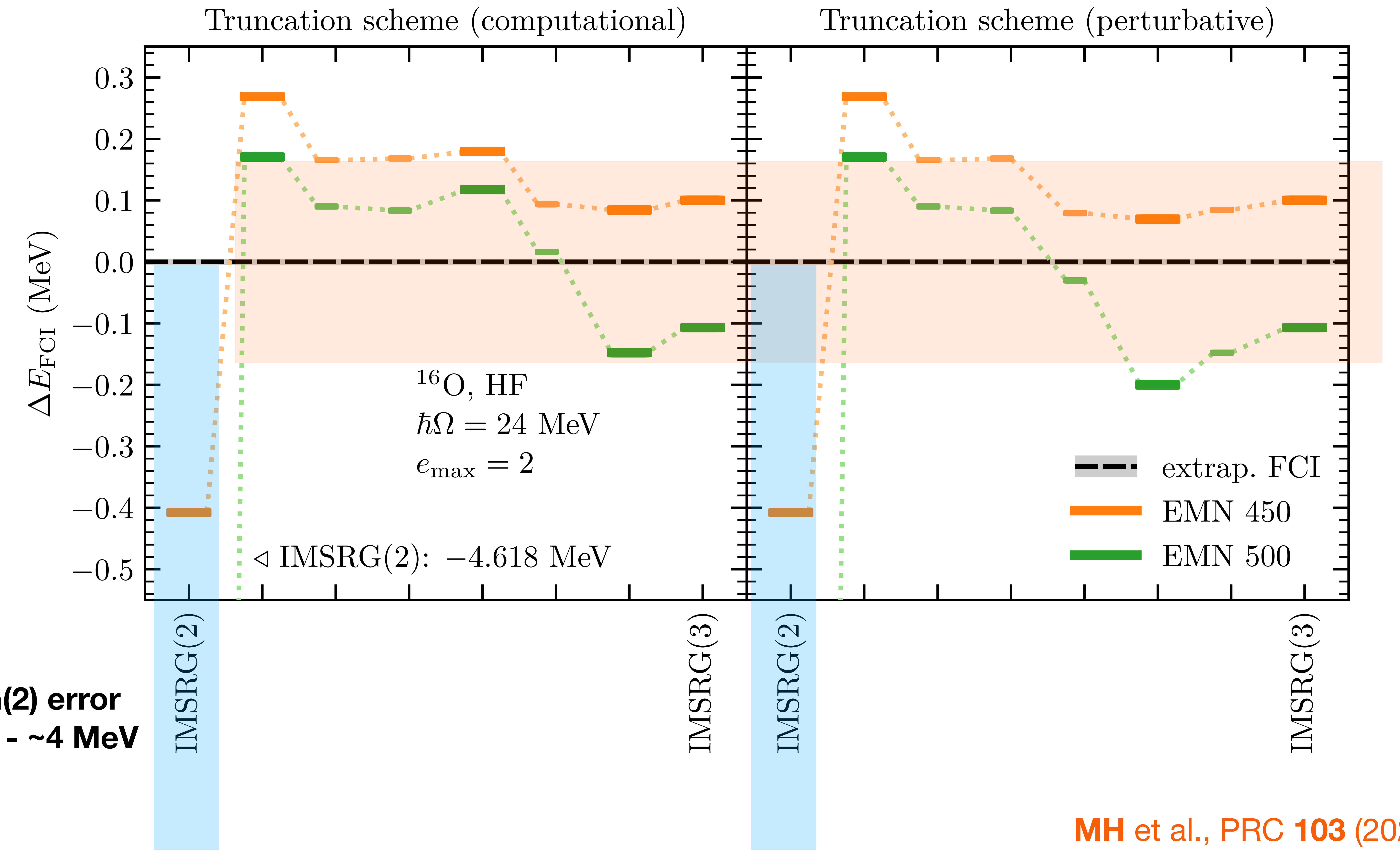
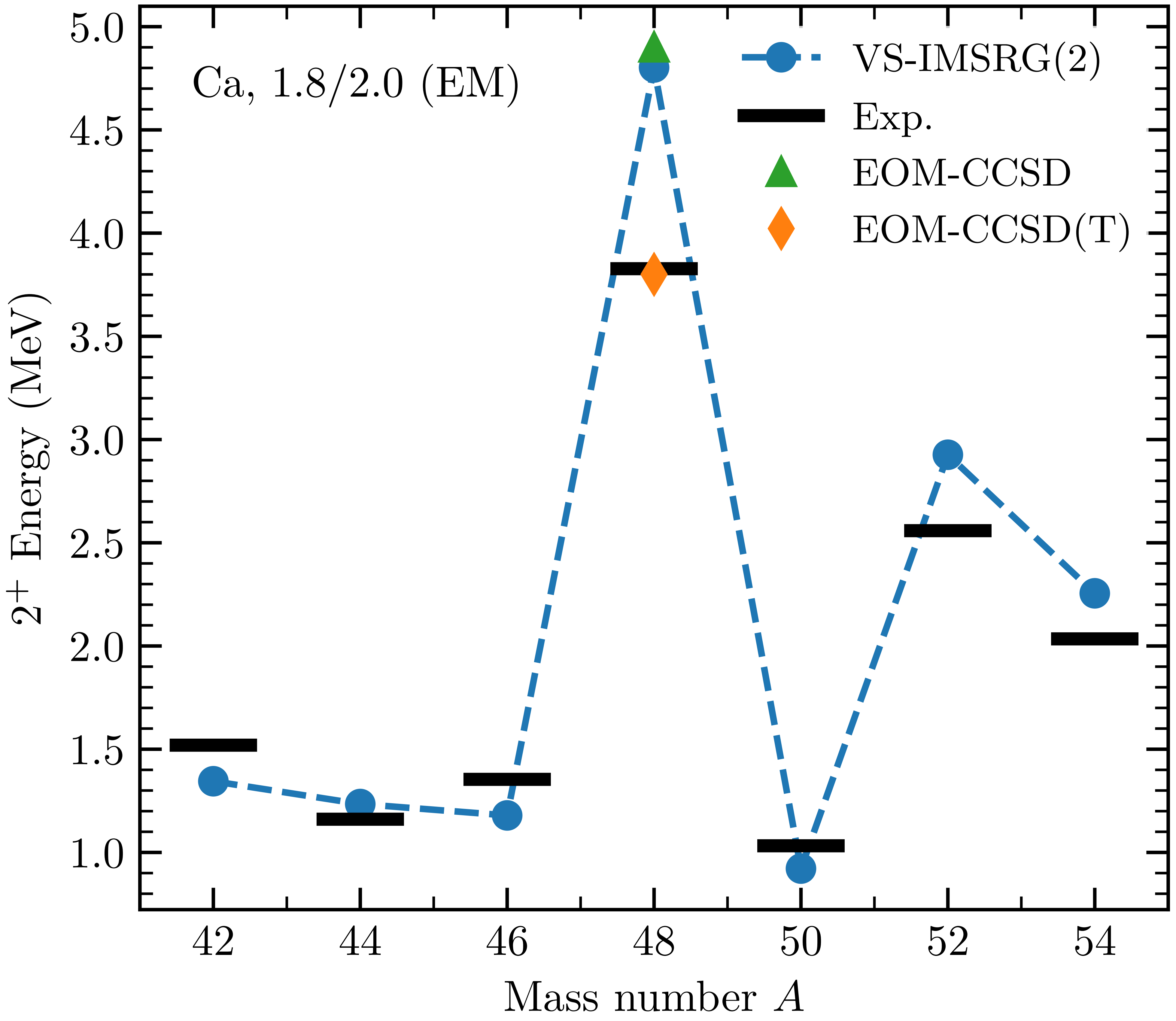


IMSRG(3) error ~150 keV

IMSRG(2) error 400 keV - ~4 MeV

MH et al., PRC **103** (2021)

Where does IMSRG(3) matter?



Hagen et al., PRL **117** (2016)

Simonis et al., PRC **96** (2017)

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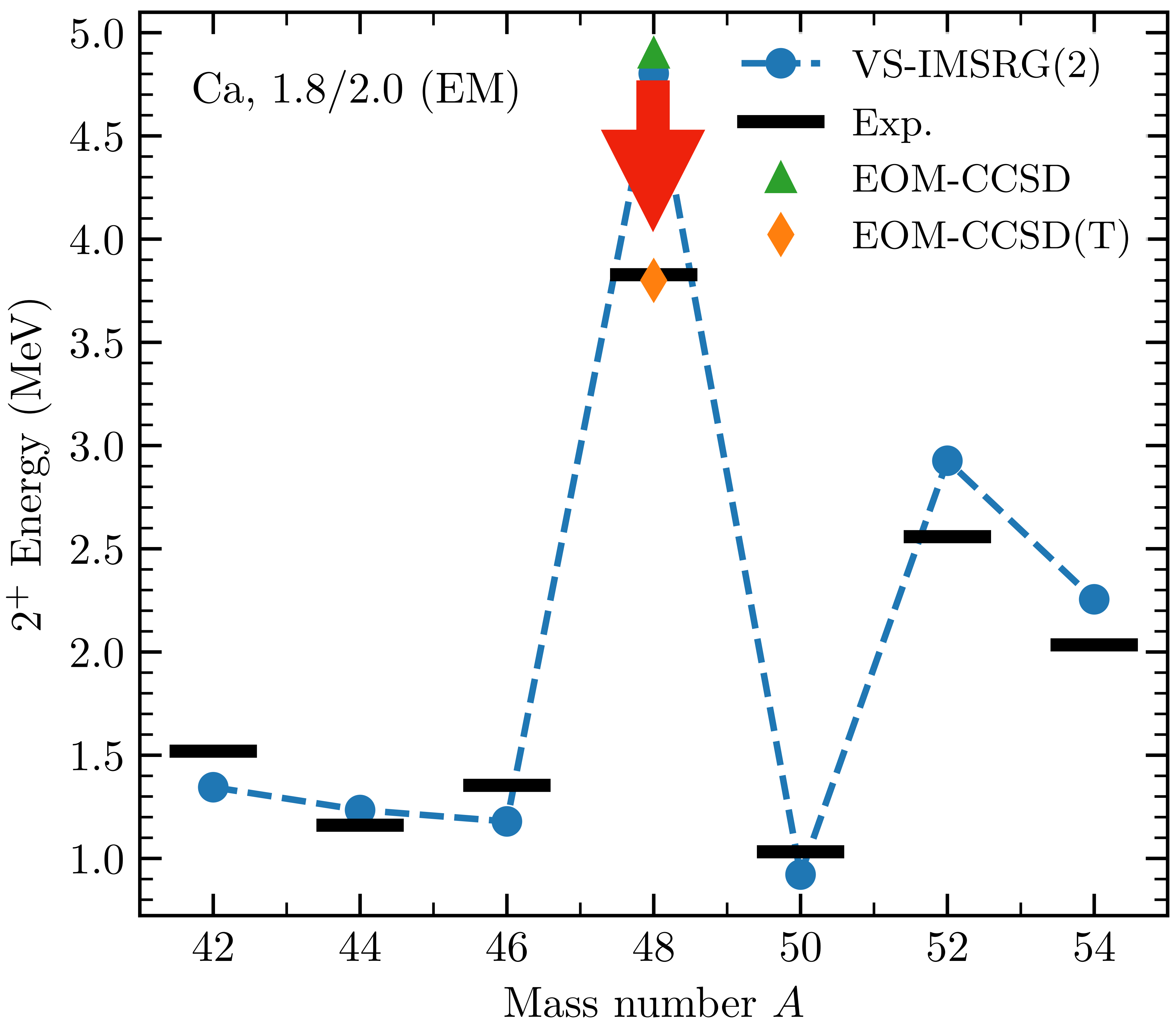

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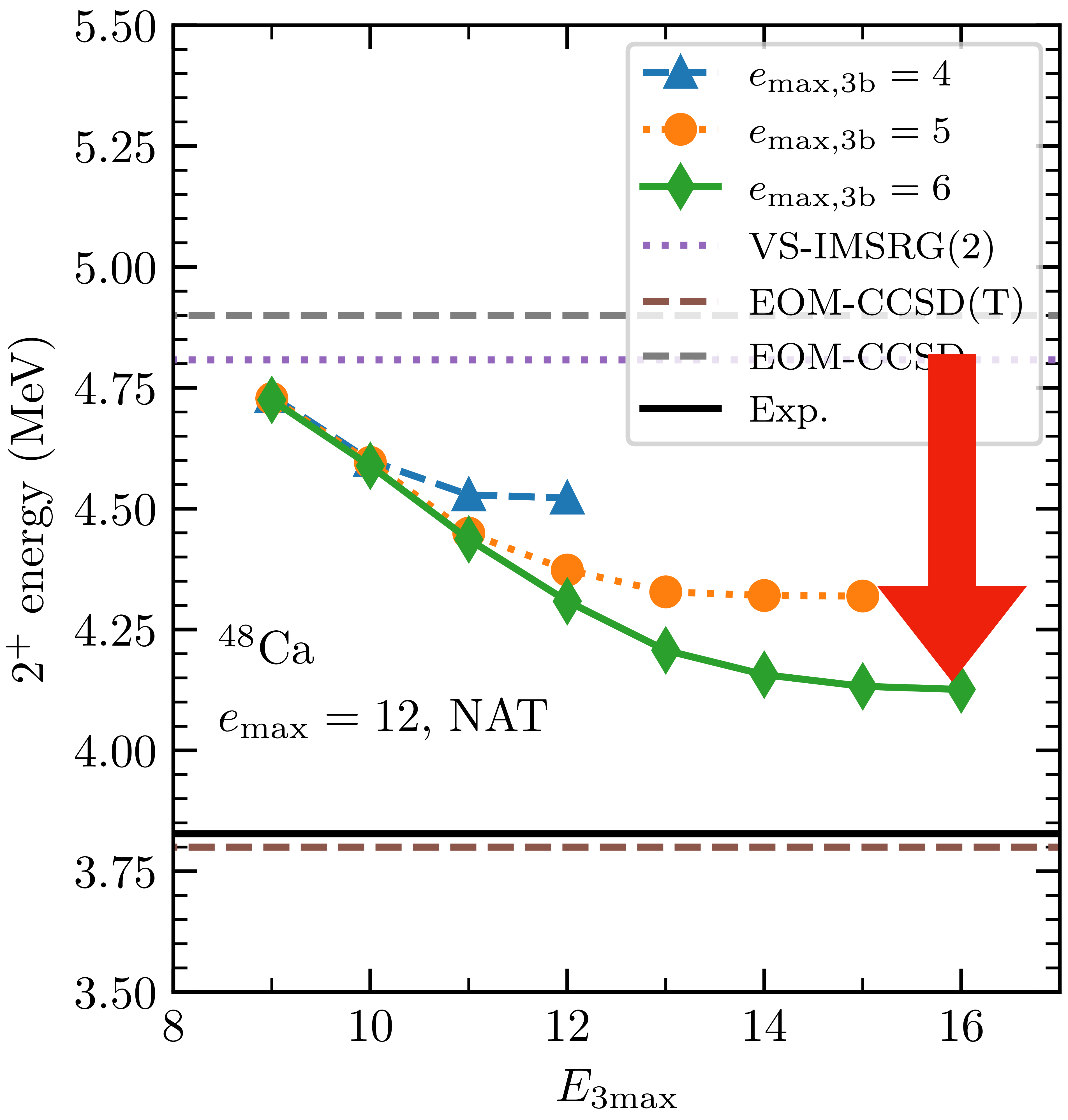


Comparing IMSRG to CC

IMSRG

- ODE solution
- Similarity transformation
- No factorization (binary contractions)
- $|\Psi\rangle = \exp(\Omega)|\Phi\rangle$, with (for example) $\Omega^{(2)} = \frac{1}{4}\sum_{pqrs} \Omega^{(2)}_{pqrs} a^\dagger_p a^\dagger_q a_s a_r$
- **Hermitian**, unitary, BCH does not truncate, but (typically) converges
- IMSRG(3) can include residual 3B interactions

CC

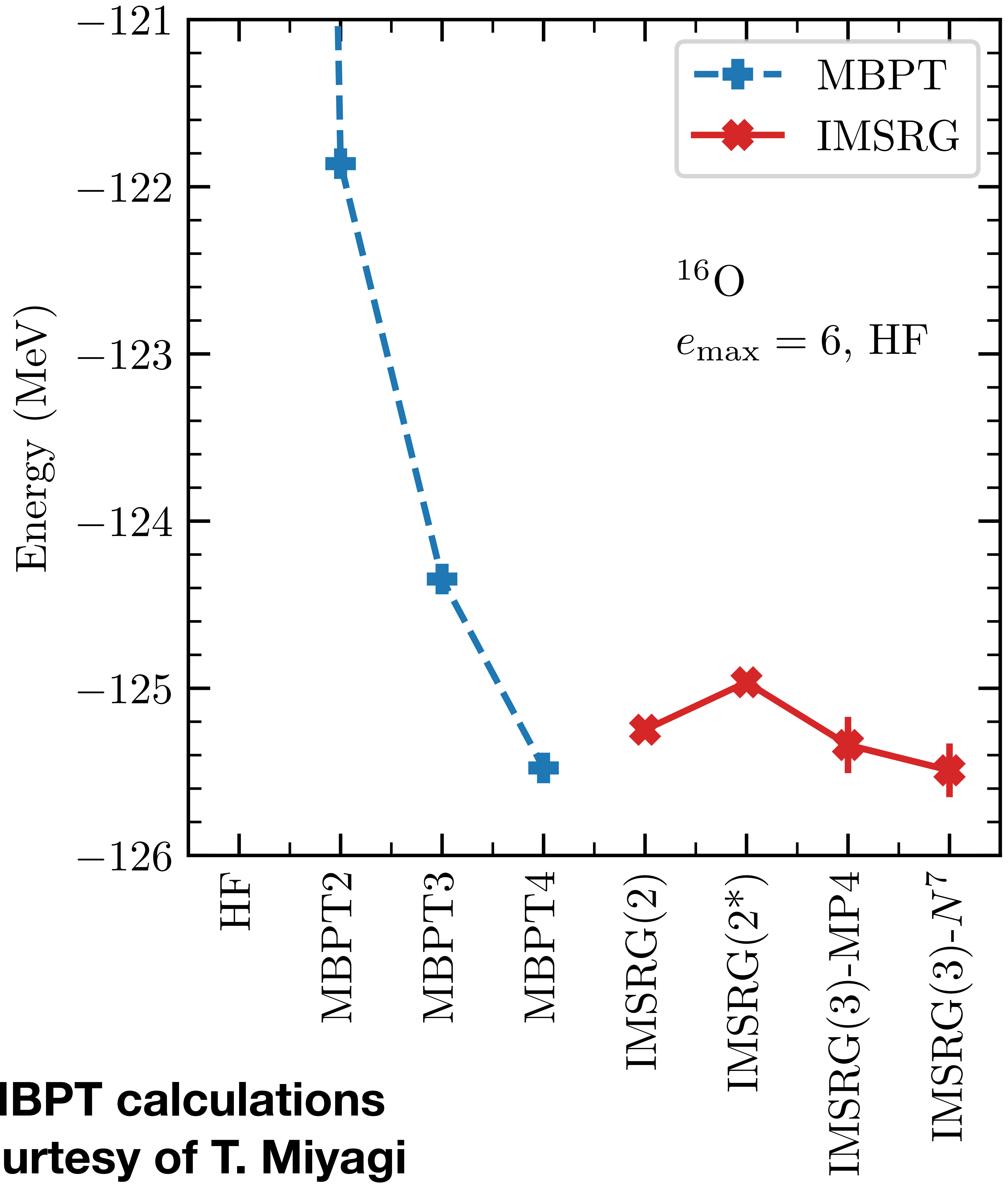
- Iterative solution
- Similarity transformation
- Factorization important
- $|\Psi\rangle = \exp(T)|\Phi\rangle$, with (for example) $T^{(2)} = \frac{1}{4}\sum_{abij} T^{(2)}_{abij} a^\dagger_a a^\dagger_b a_j a_i$
- Non-Hermitian, unitary, BCH truncates after finite commutators
- CCSDT (NO2B) $\neq$ CC with 3B interactions

**90% correct

Connecting IMSRG and MBPT

Hjorth-Jensen et al., Phys. Rep. **261** (1995)
Bartlett, Shavitt, *Many-Body Methods in Chemistry and Physics* (2009)
Hergert et al., Phys. Rep. **621** (2016)

IMSRG truncations in detail



MBPT calculations courtesy of T. Miyagi

IMSRG(2)

- Complete up to **MPBT3**
- Some higher-order effects + **nonperturbative** ladders and rings

IMSRG(3)-MP4

- Complete up **MBPT4**

IMSRG(3)-N^7

- Perturbatively less important terms also included

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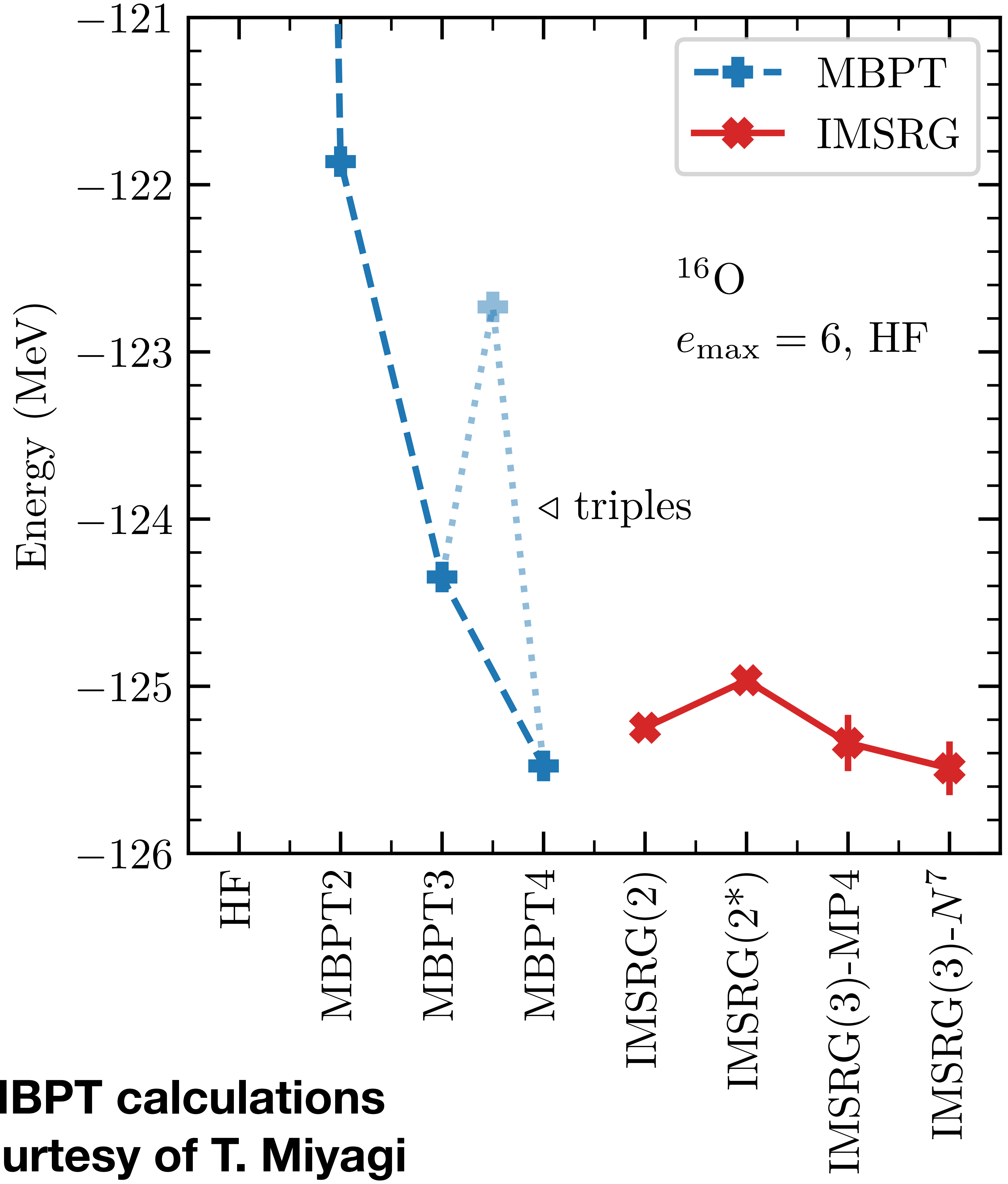

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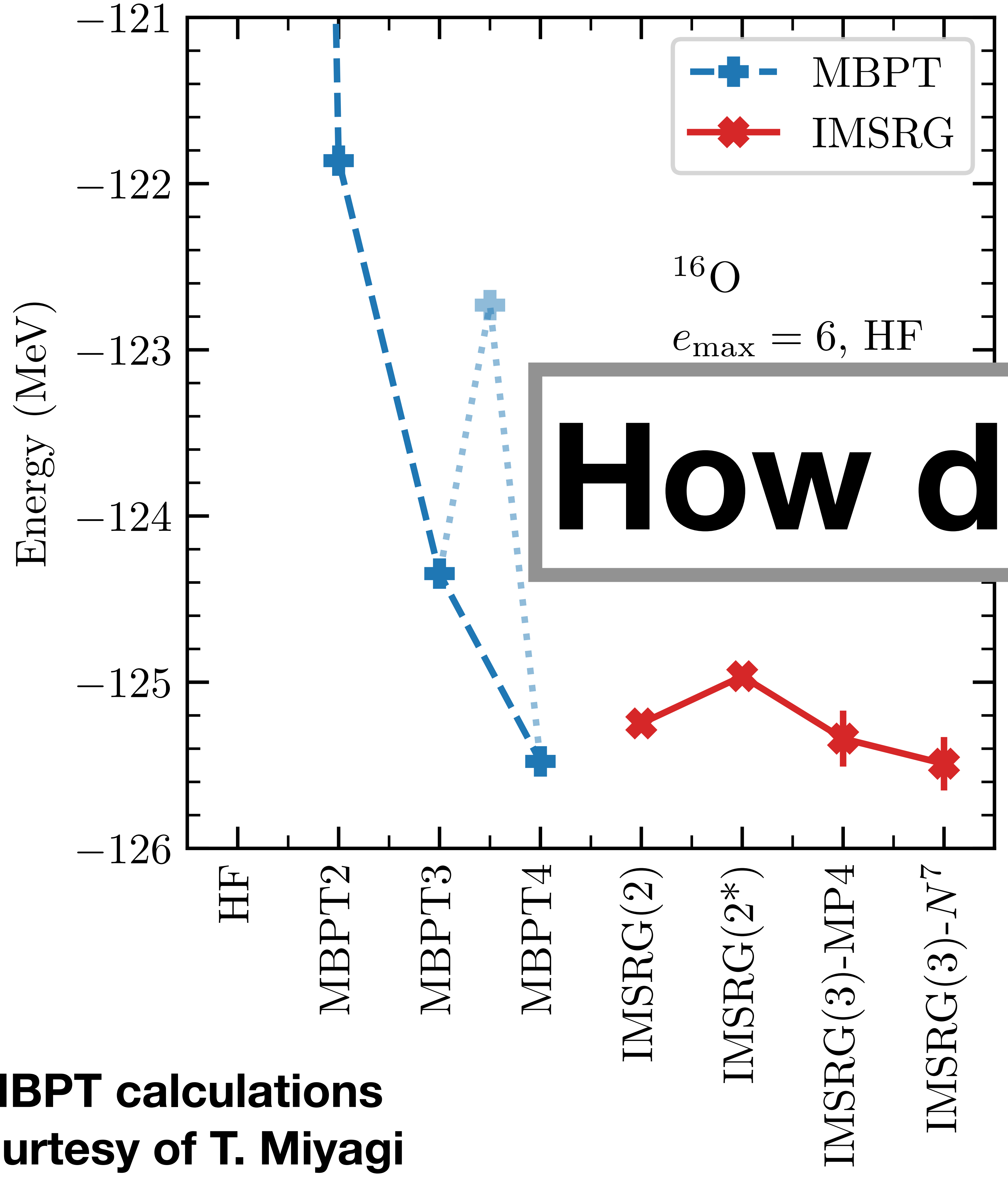


MBPT calculations courtesy of T. Miyagi

IMSRG(2)

- Complete up to **MPBT3**
- Some higher-order effects + ...nd rings

How do we know this?

IMSRG(3)-MP4

- Complete up **MBPT4**

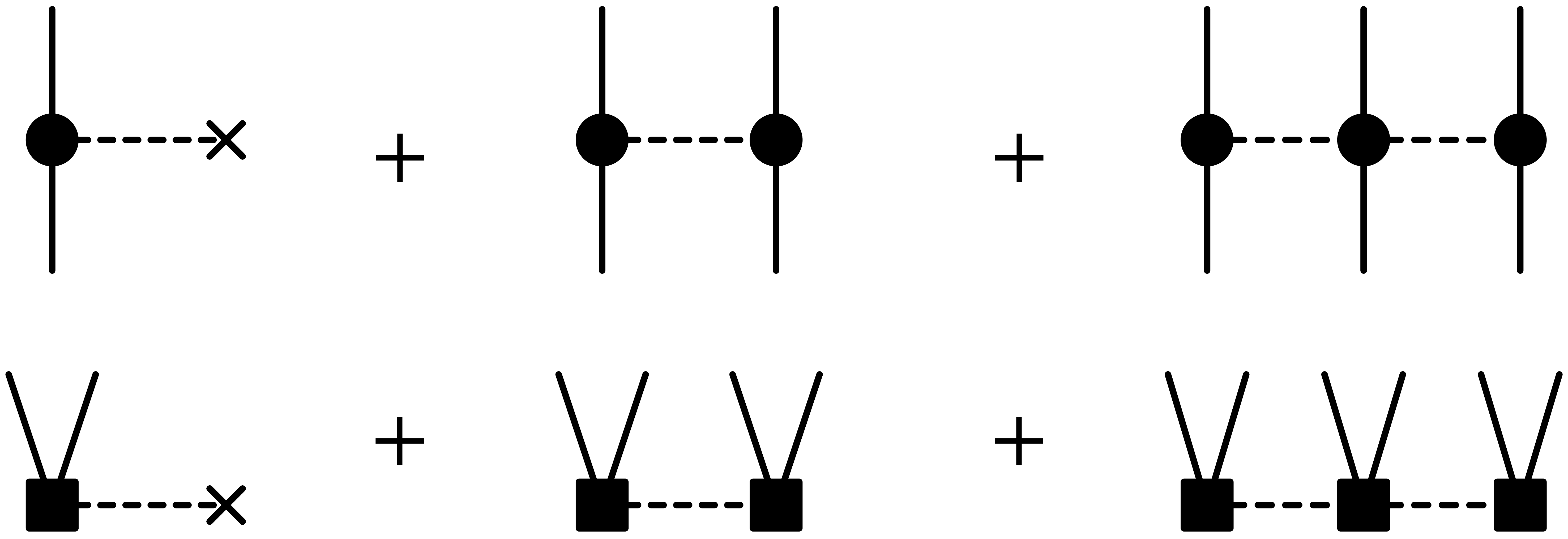
IMSRG(3)-N^7

- Perturbatively less important terms also included

IMSRG ingredients (to start)

$H(s=0) =$

$\eta(s=0) =$



f_{ia}/ε_i^a $\Gamma_{ijab}/\varepsilon_{ij}^{ab}$ $W_{ijkabc}/\varepsilon_{ijk}^{abc}$

Solving $\dfrac{dH}{ds} = [\eta(s), H(s)]$ generates new diagrams out of η and H vertices

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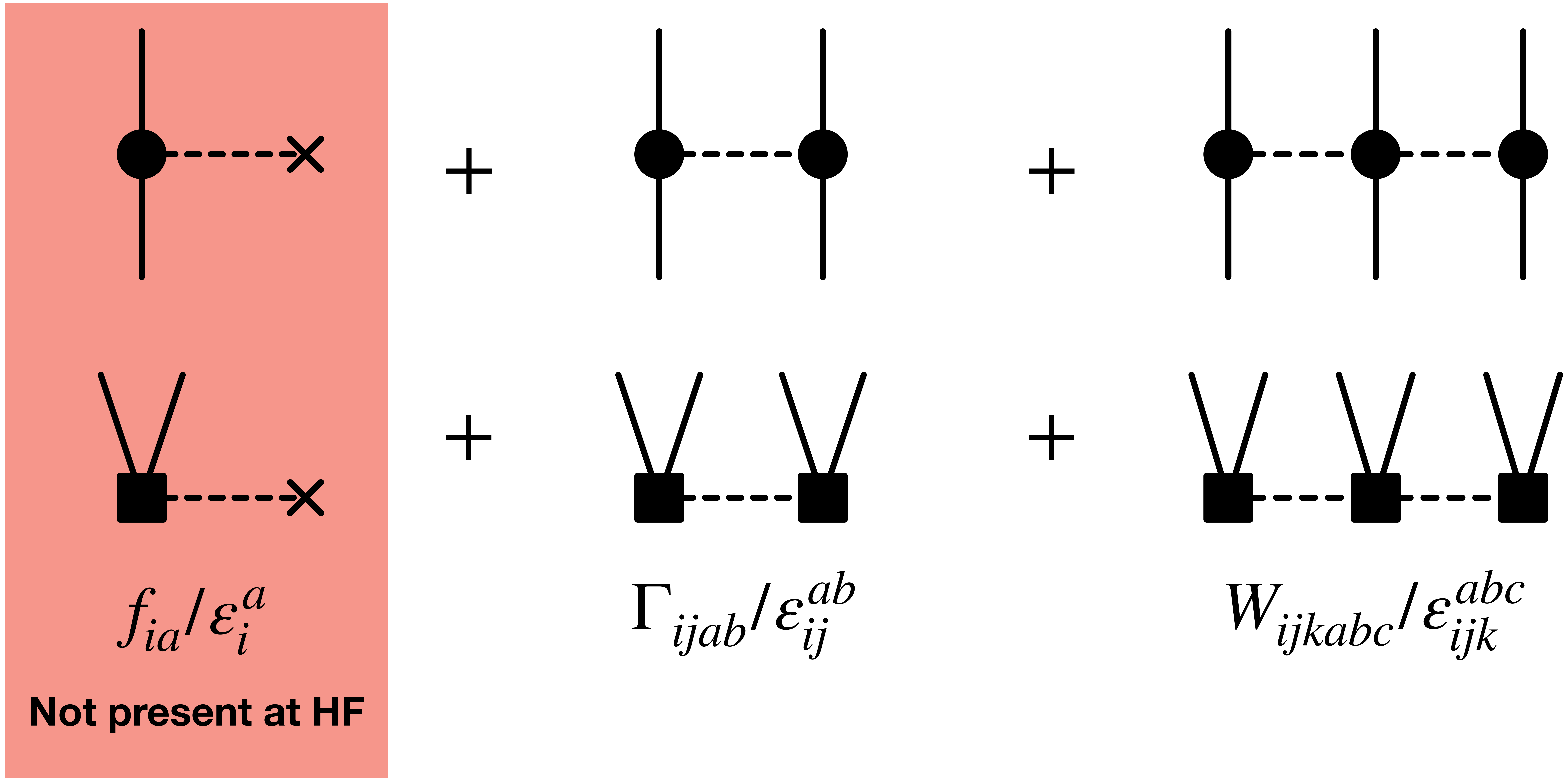

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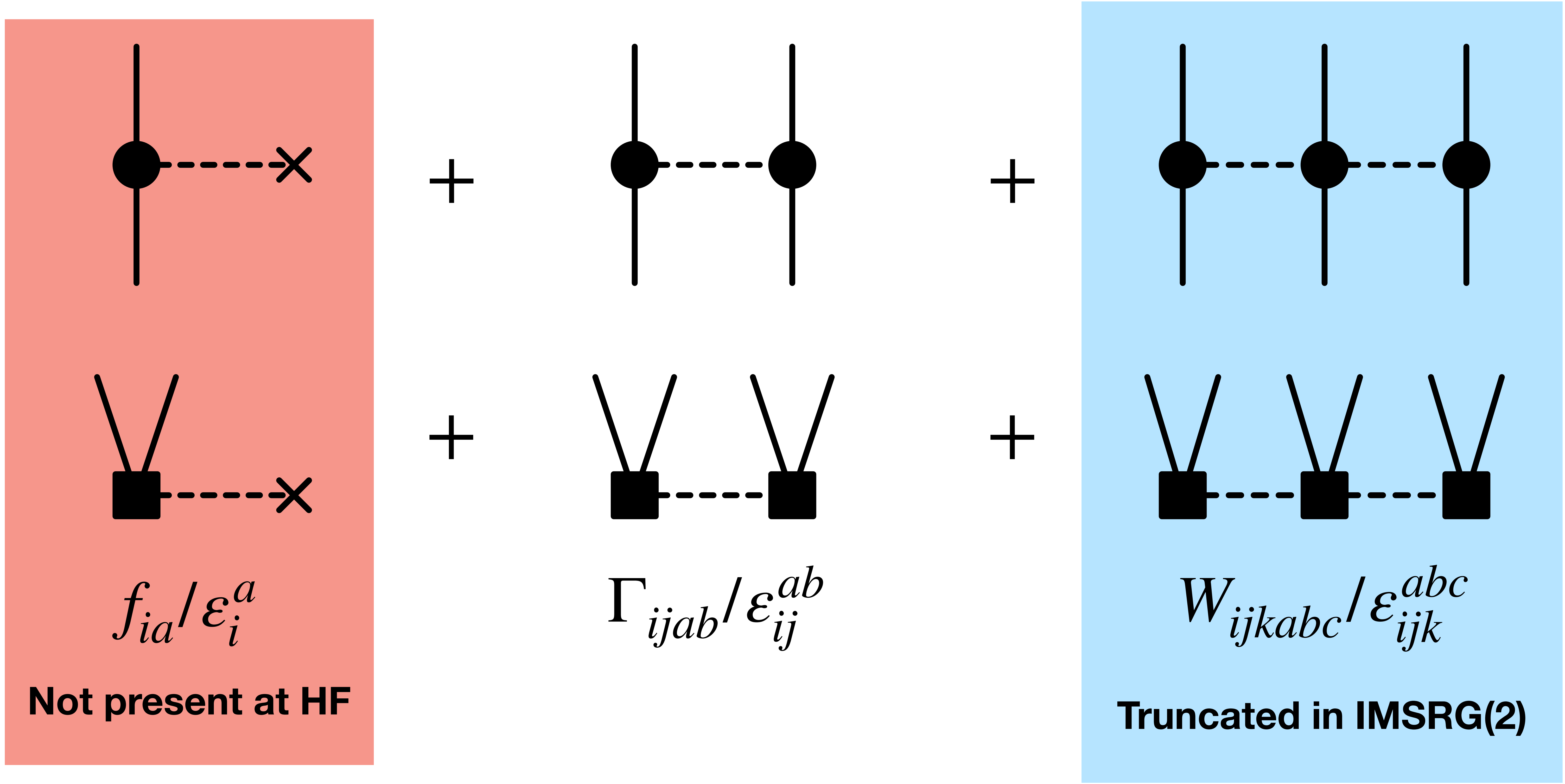
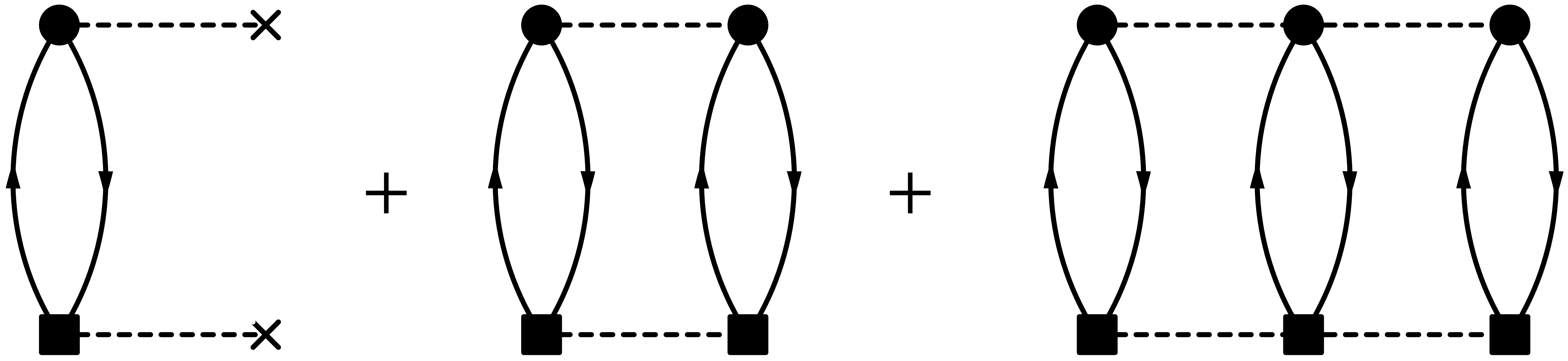


Solving $\dfrac{dH}{ds} = [\eta(s), H(s)]$ generates new diagrams out of η and H vertices

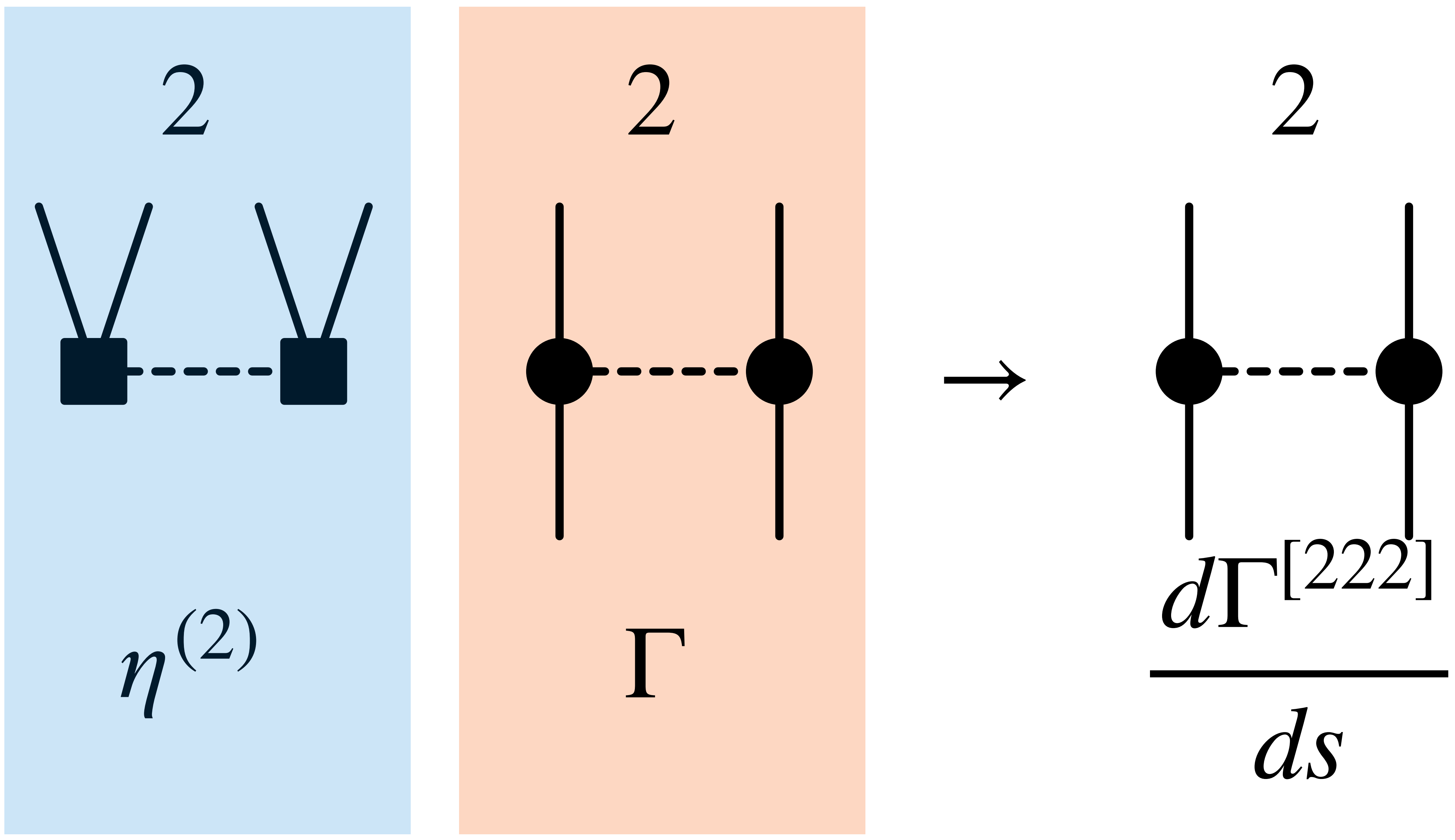
Energy contributions

$$\frac{dH^{(0B)}}{ds} = \frac{dE}{ds} = $$



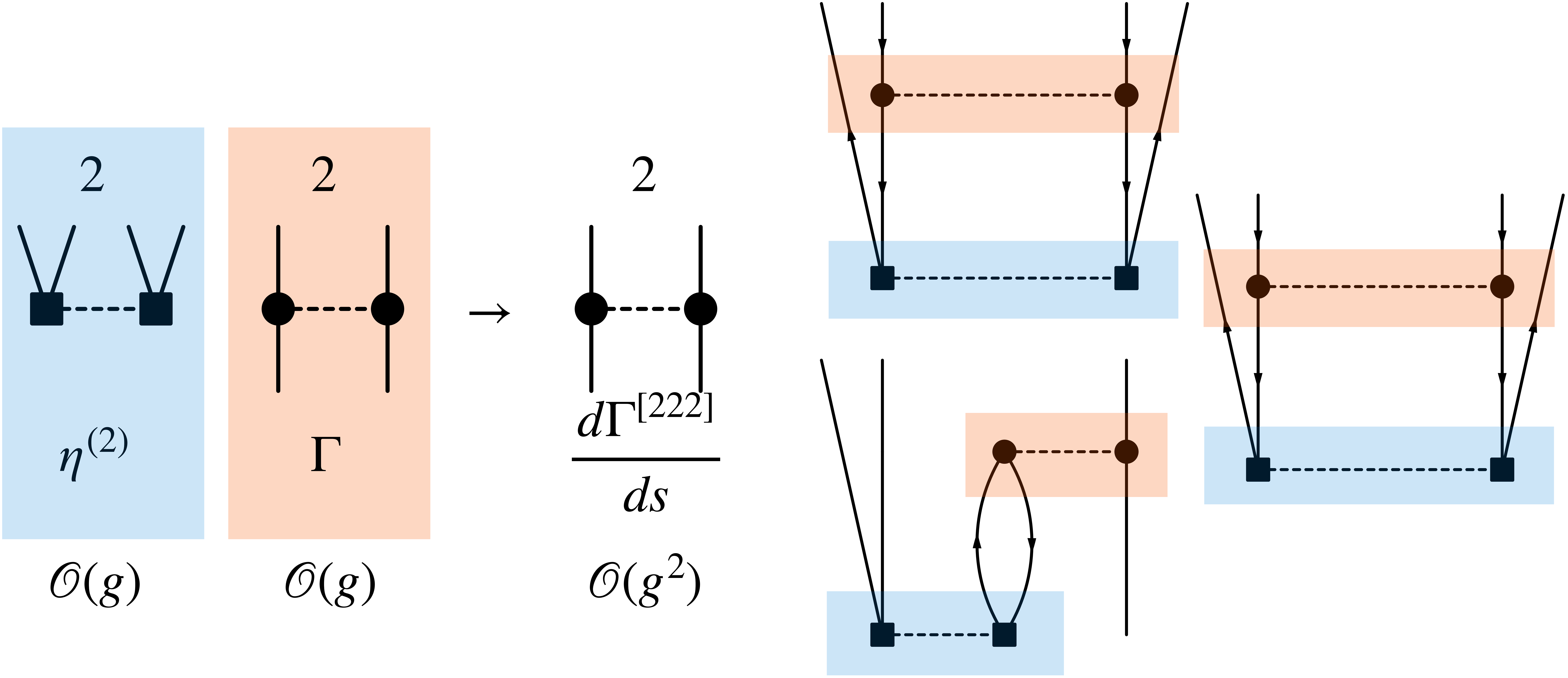
- Zero-body part produces MBPT2-like energy contributions
- Insertion of $H(s = 0)$ and $\eta(s = 0)$ gives MBPT2

Effective 2B interactions



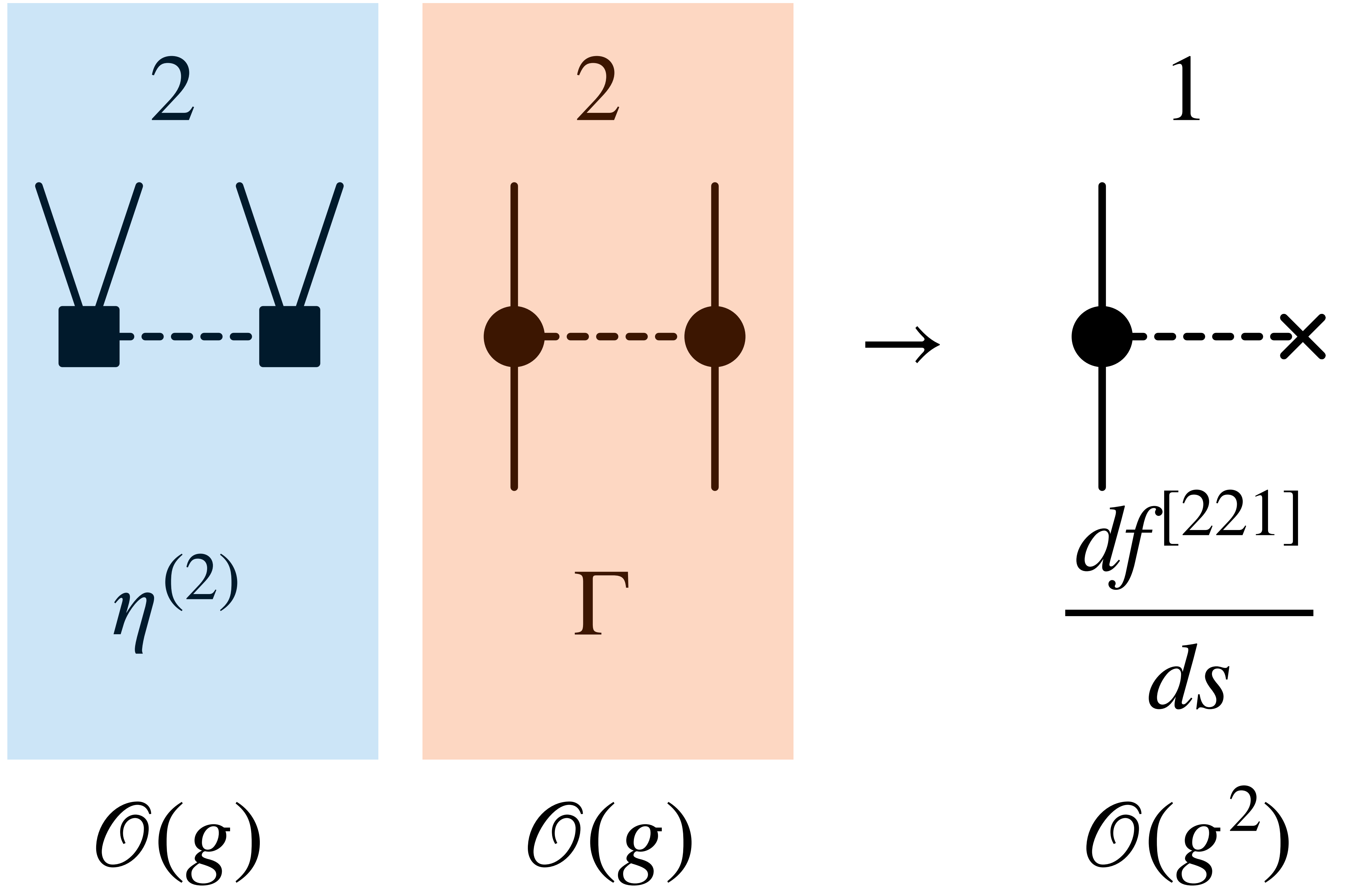
$\mathcal{O}(g)$ $\mathcal{O}(g)$ $\mathcal{O}(g^2)$

Effective 2B interactions



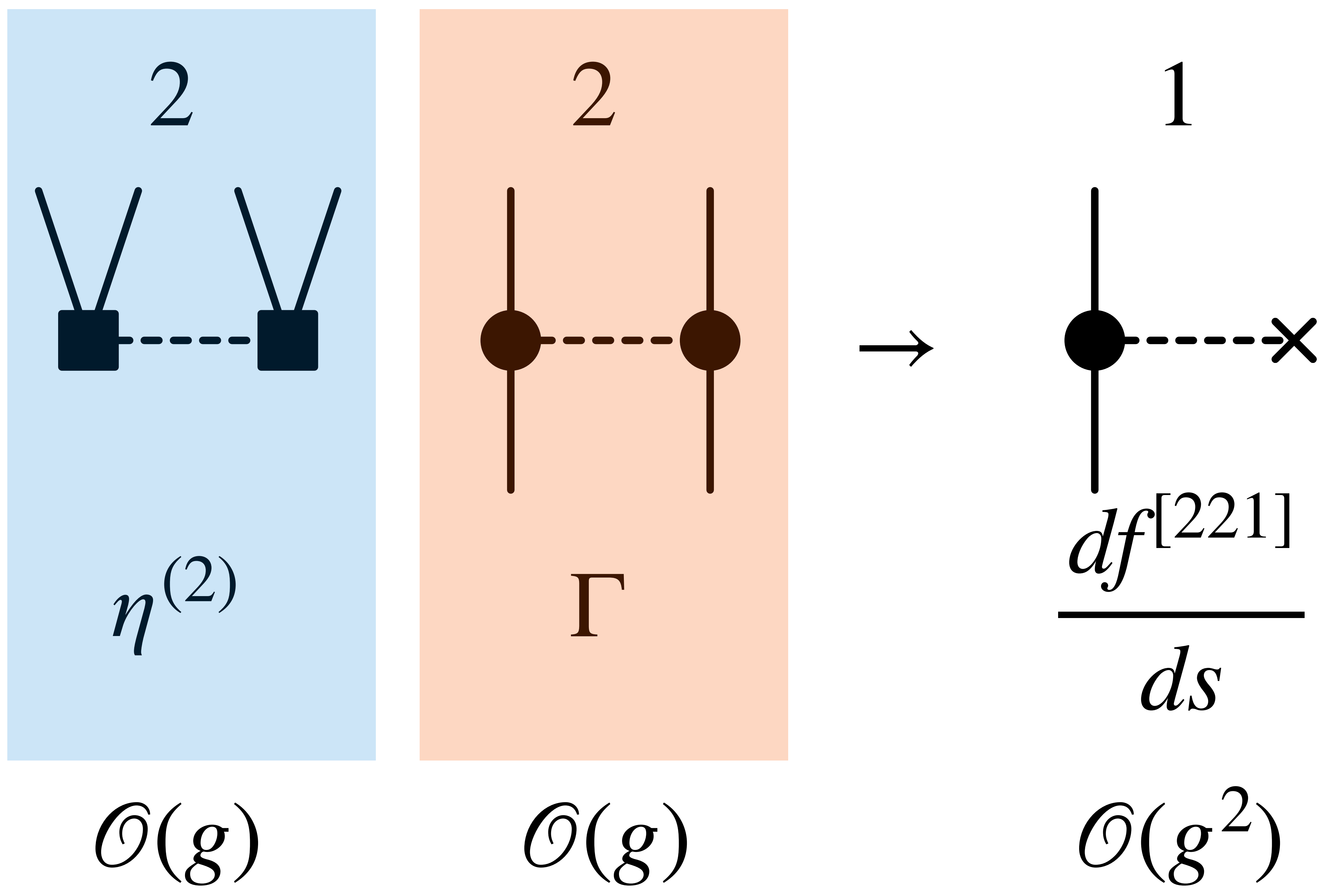
Effective 2B interactions generated to get MBPT3 right.

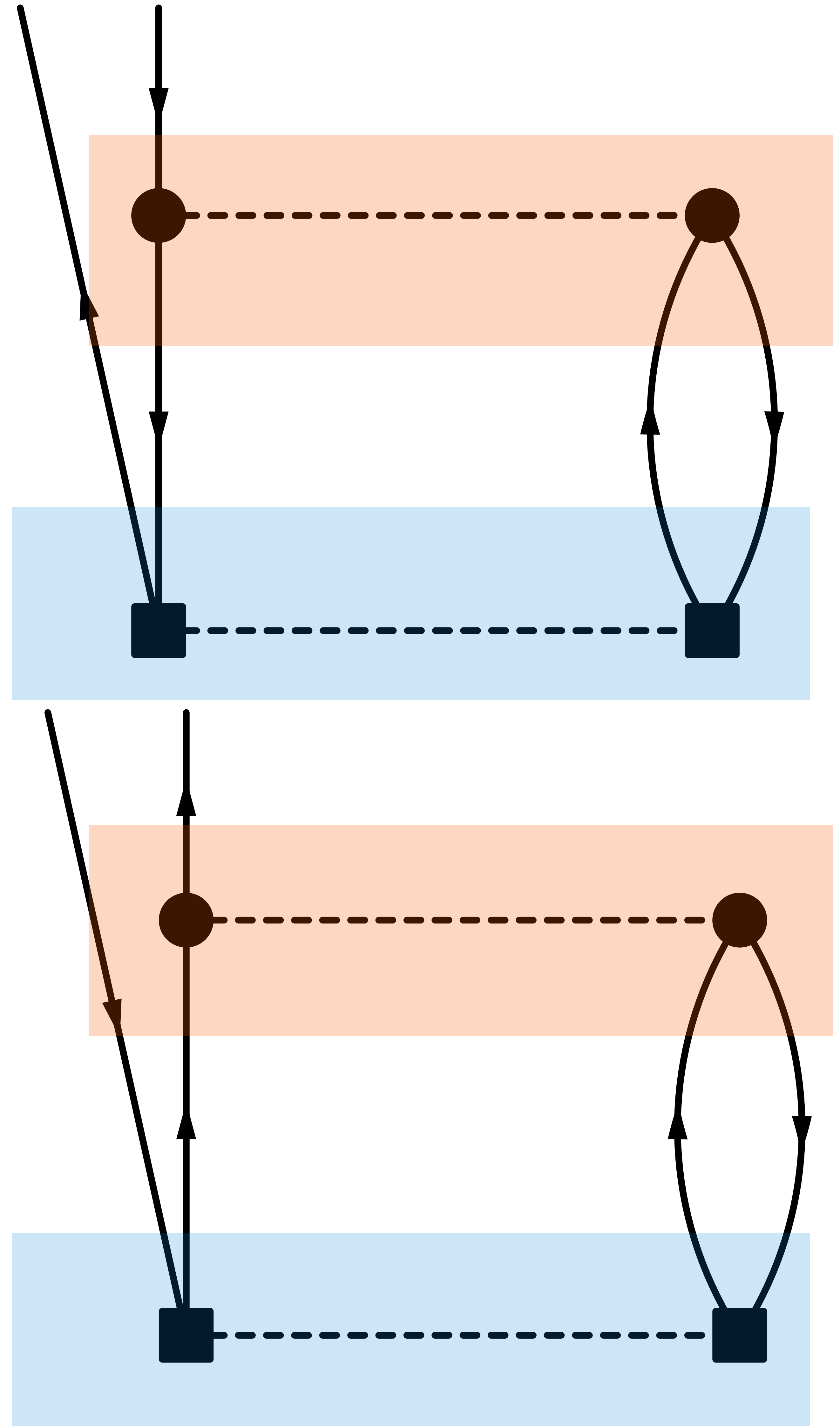
Effective 1B interactions



IMSRG "induces" effective 1B interactions

Effective 1B interactions





IMSRG "induces" effective 1B interactions

Technical details

1. Consider diagrams generated by $[\eta(s=0), H(s=0)]$ within truncation
   - IMSRG(2): **No induced effective 3B interactions**
2. Repeat up to desired perturbative order ($\mathcal{O}(g^3)$, $\mathcal{O}(g^4)$)
3. Look at what diagrams are generated and compare with MBPT

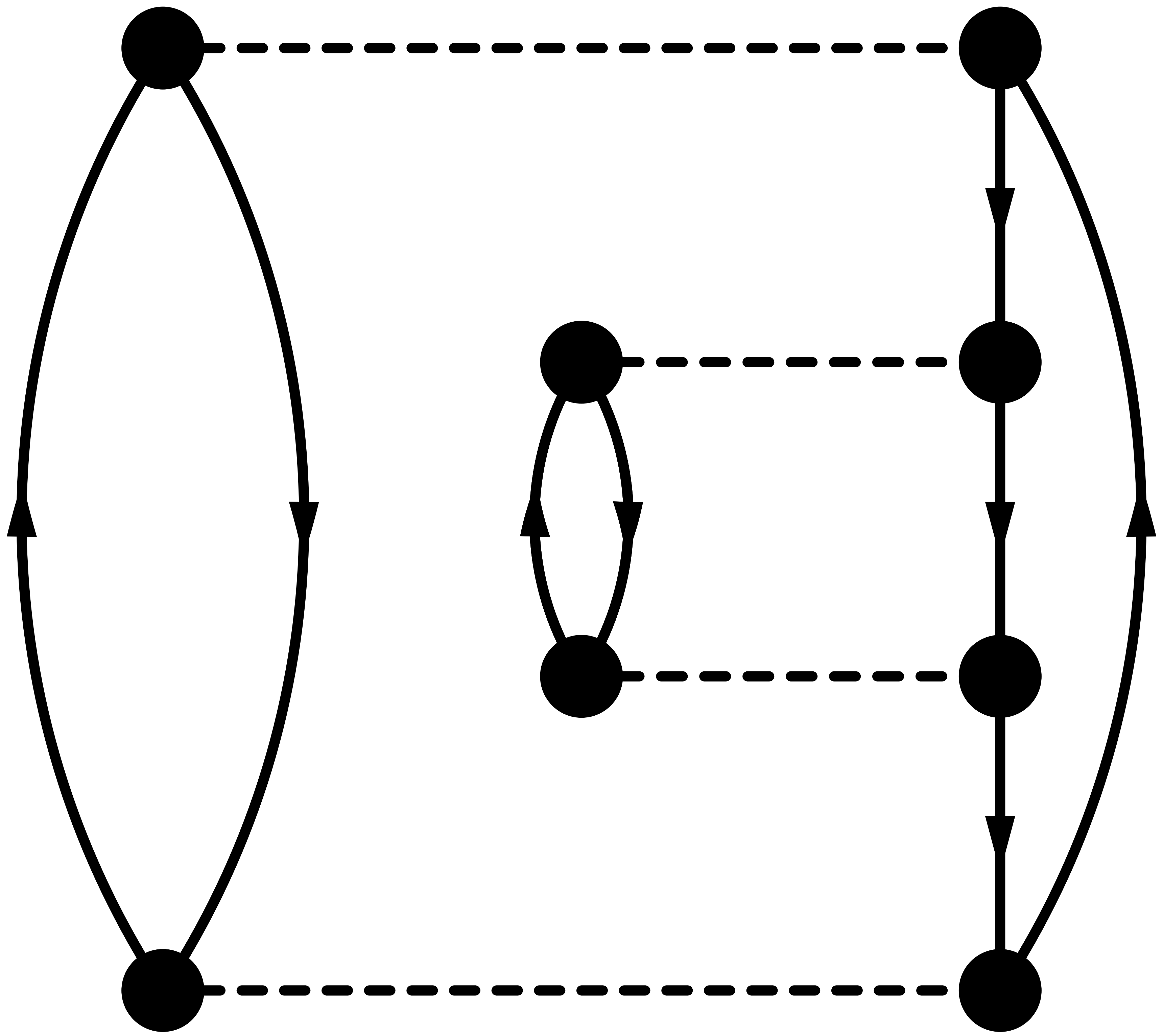
Technical complications (**missing 10%):

- Integrating in s
- Dealing with complementary diagrams (at and beyond MBPT4)

Improving the IMSRG(2)

Morris, PhD Thesis, MSU (2016)
Arthuis et al., CPC **240** (2019)

Triples (MBPT4) missing in IMSRG(2)



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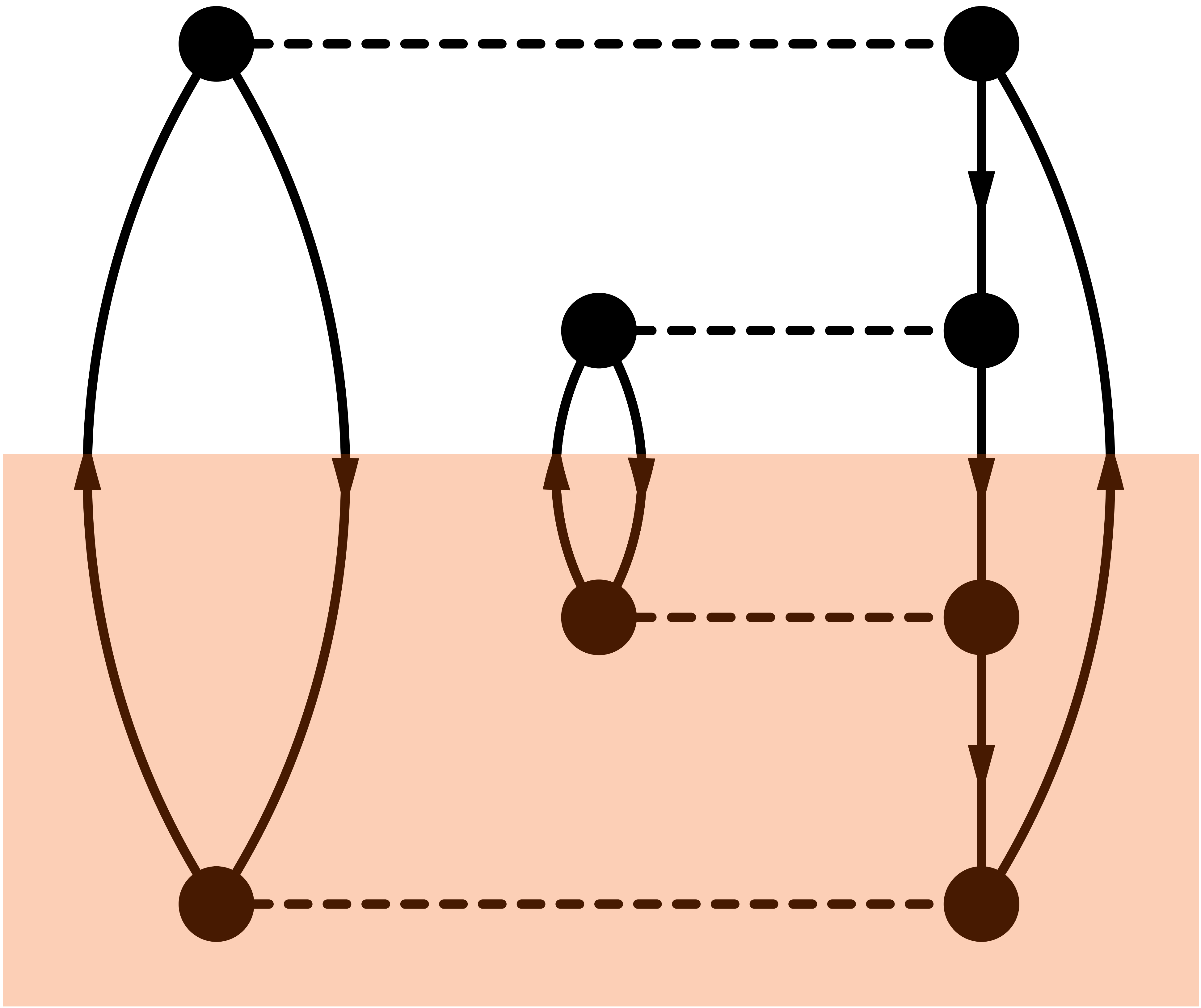

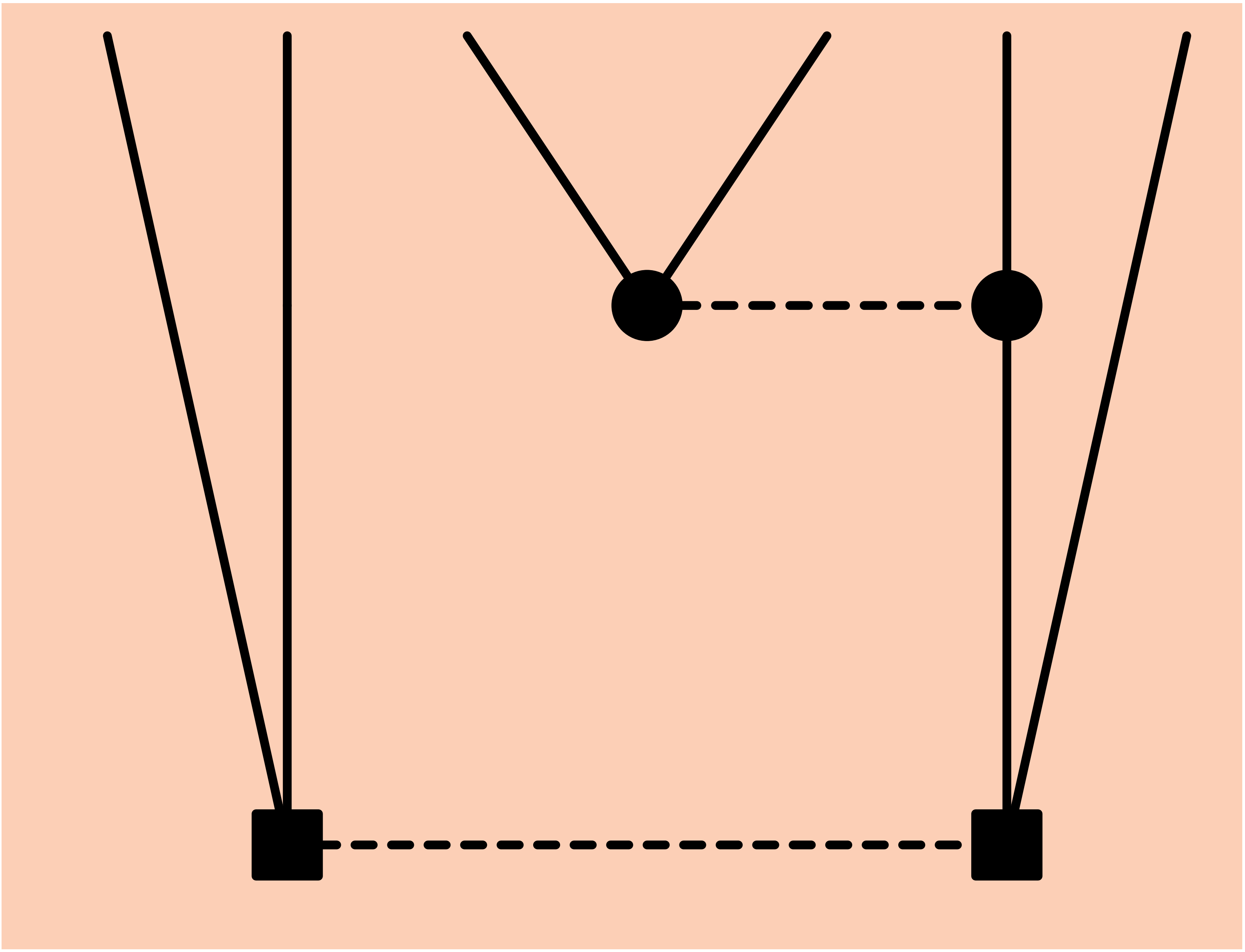

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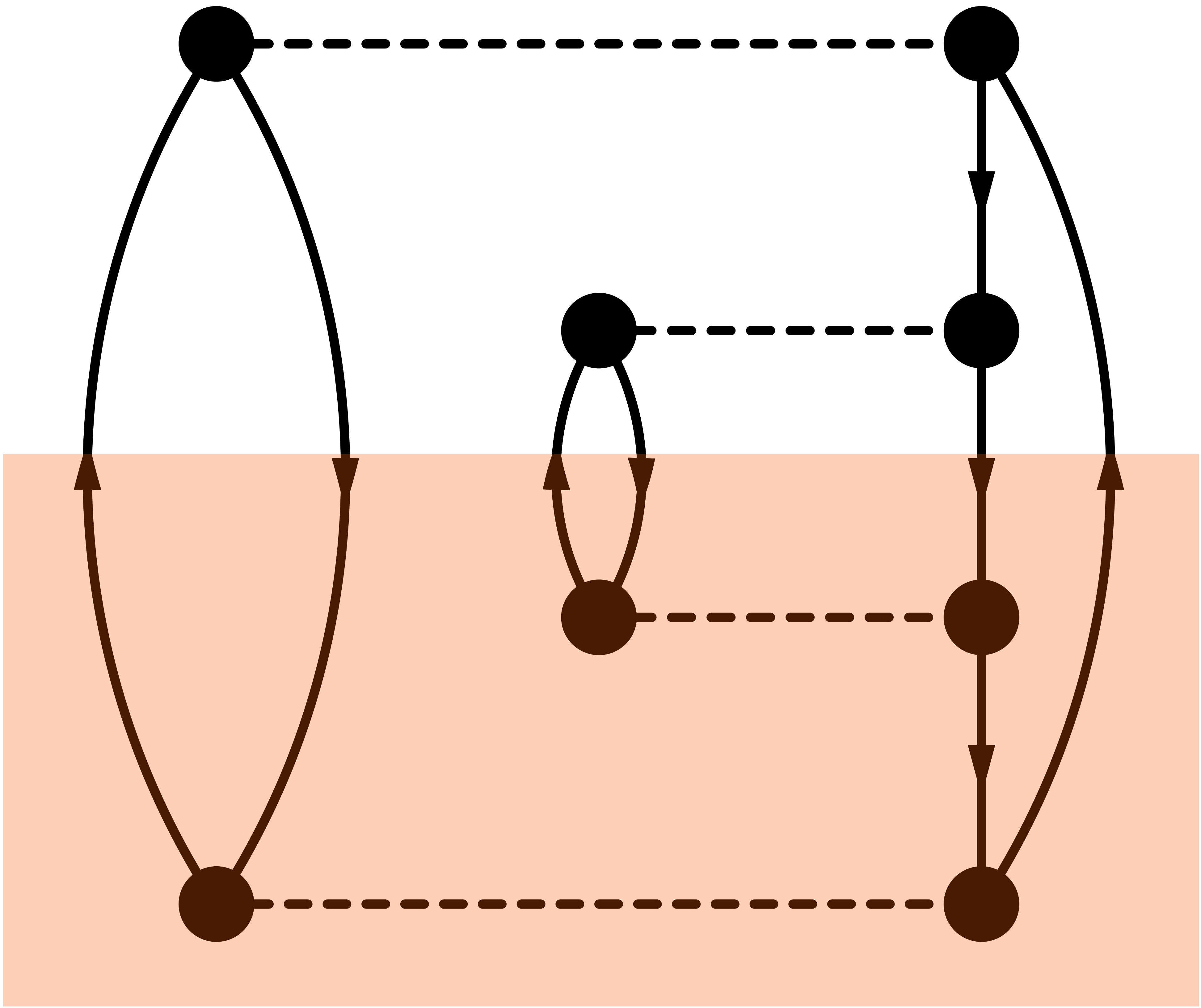

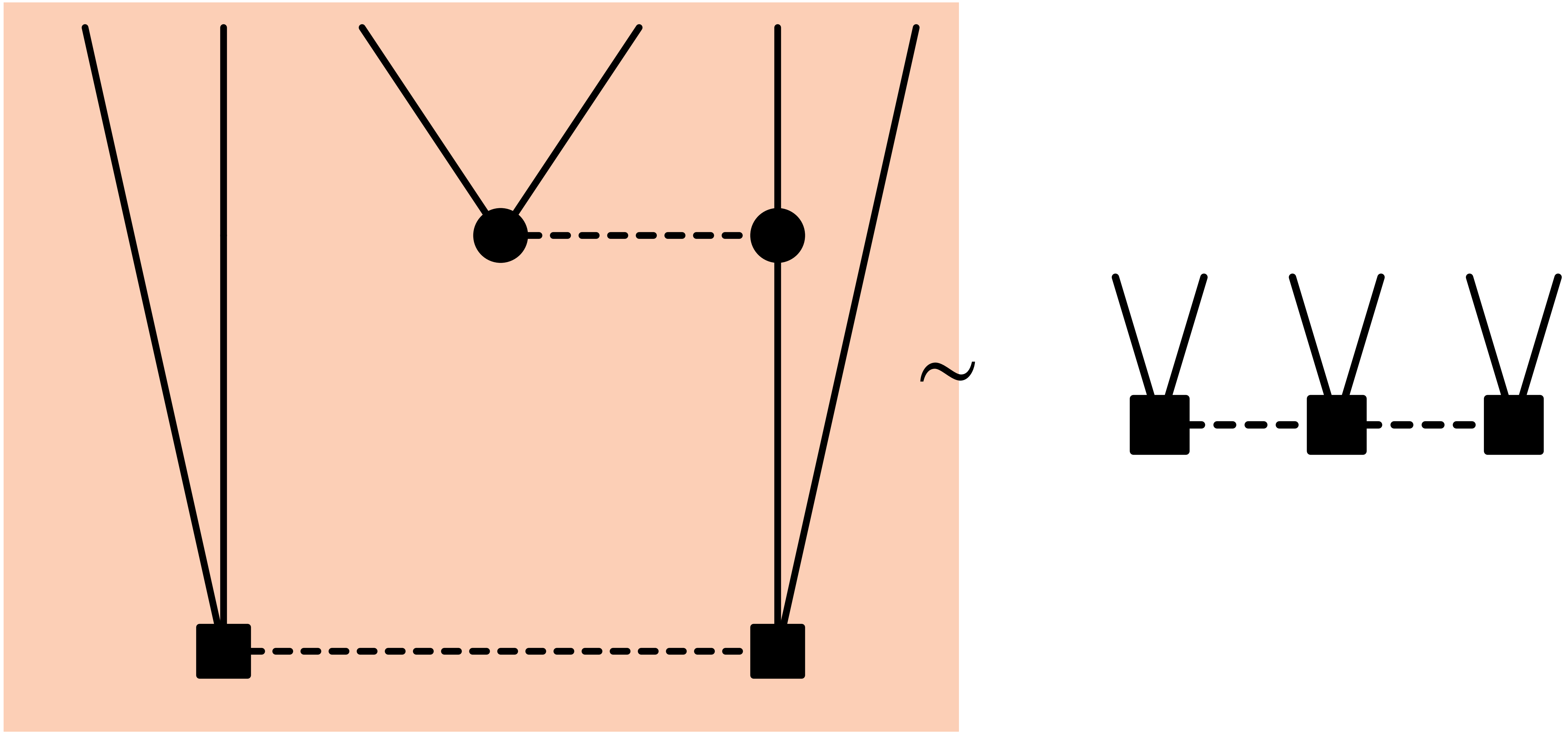

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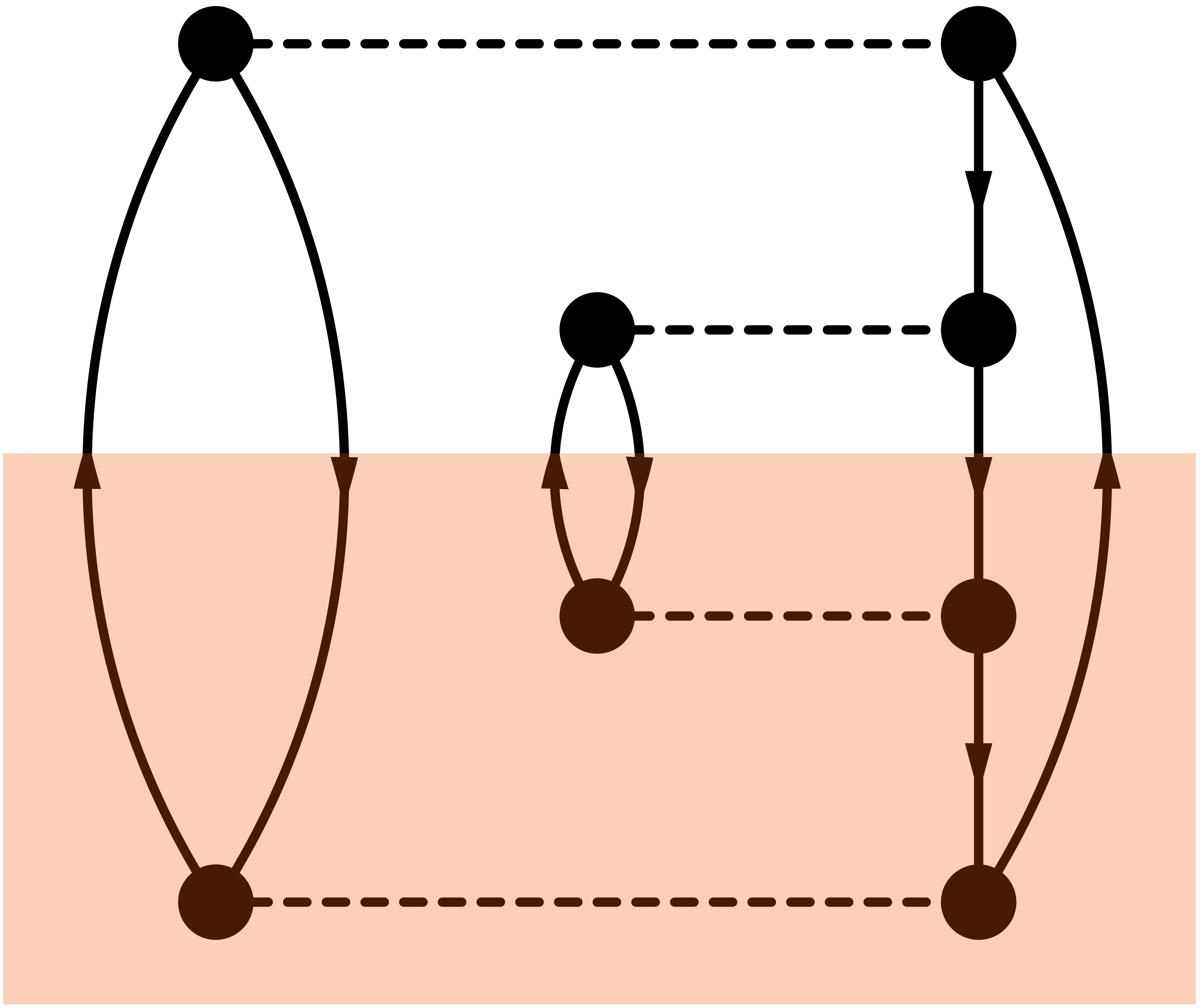

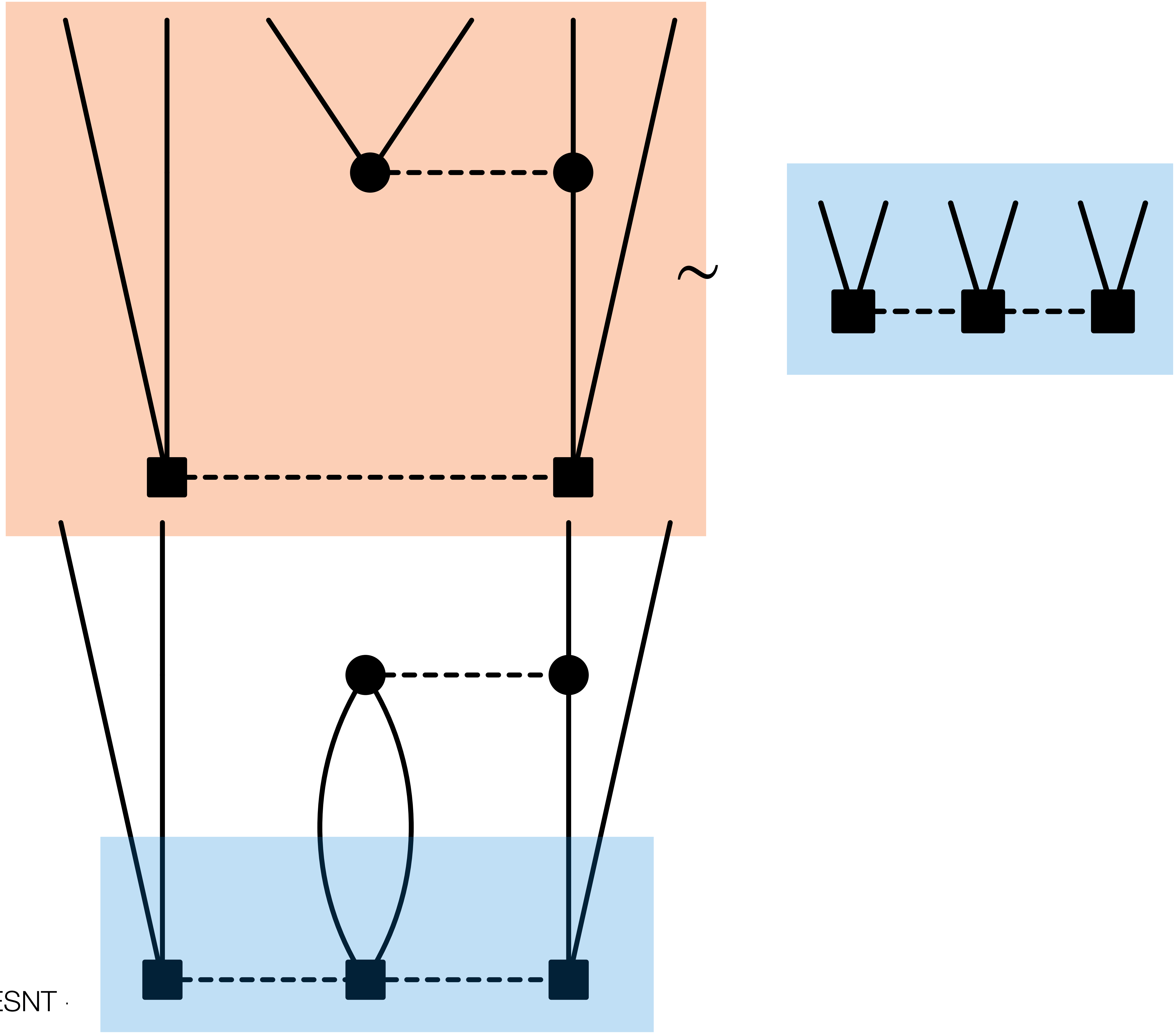

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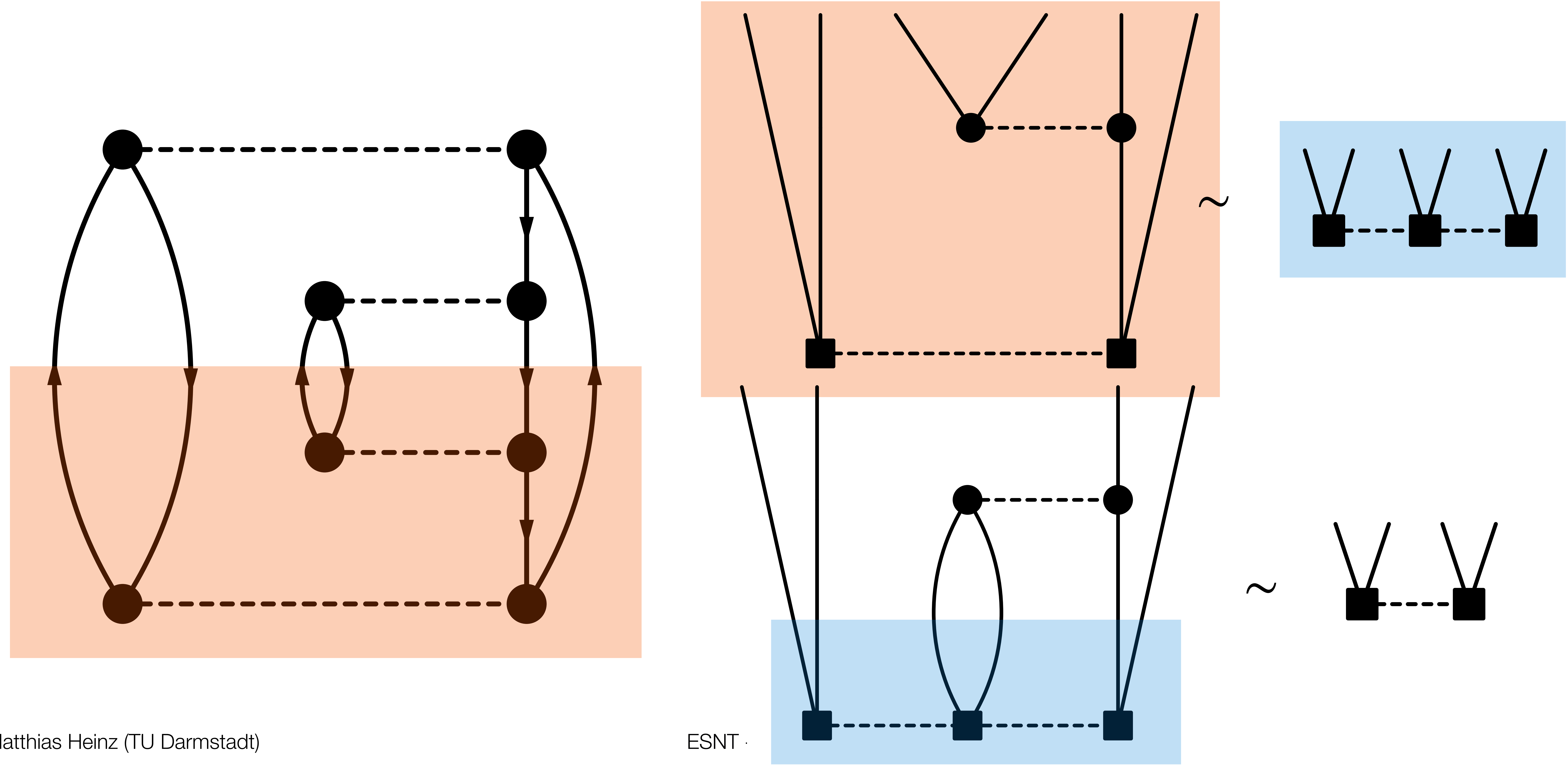
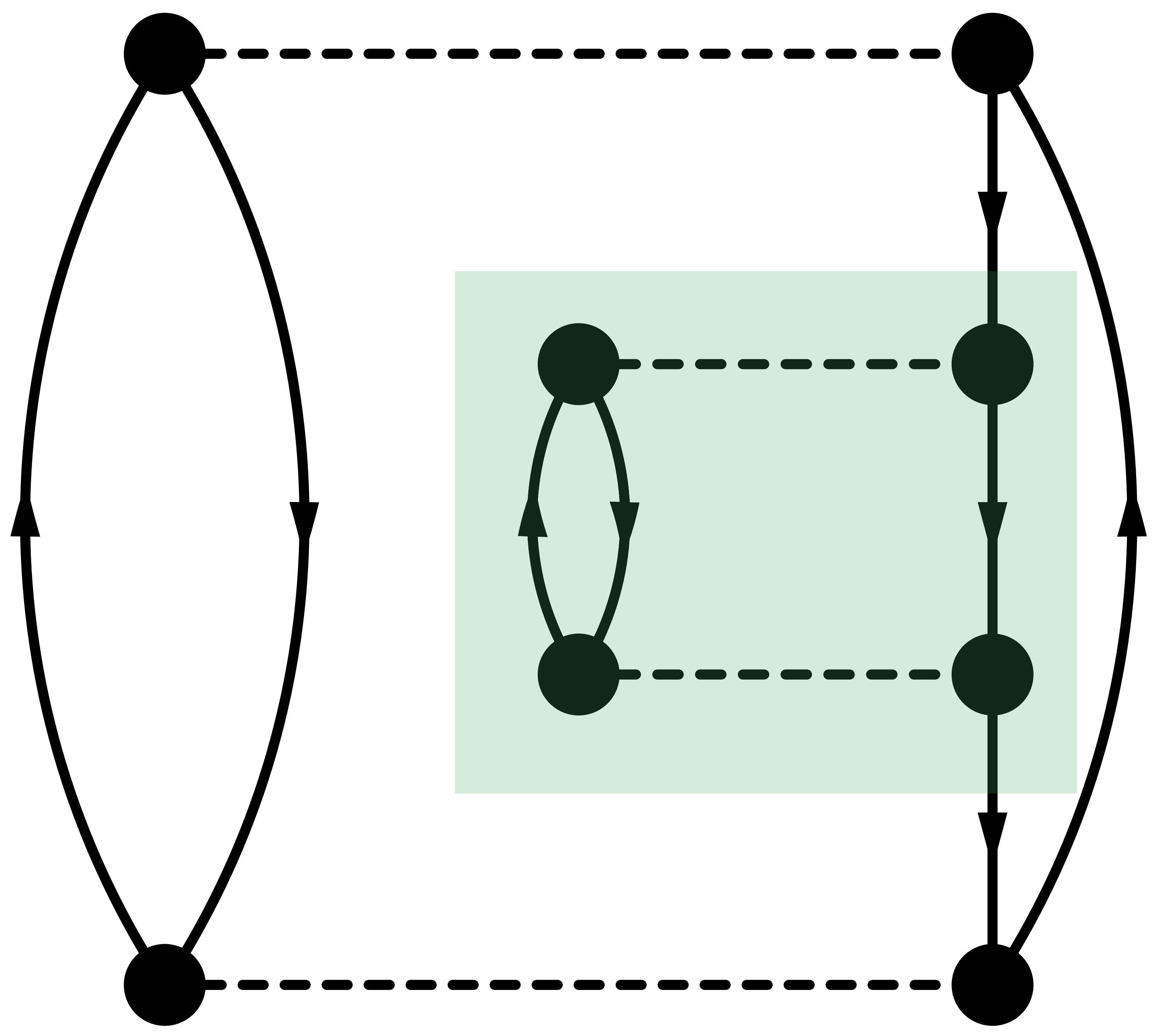
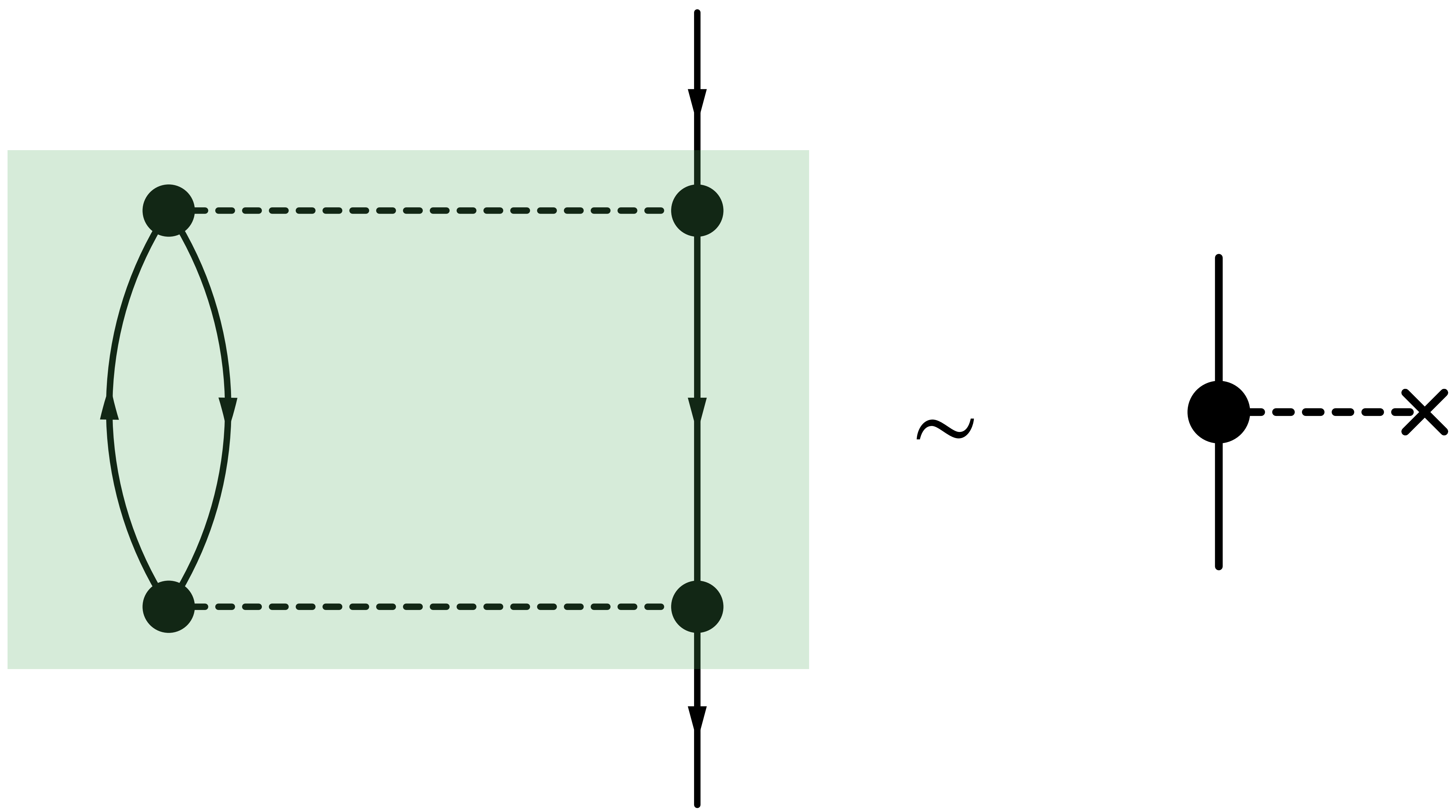


Alternative approach: effective interactions





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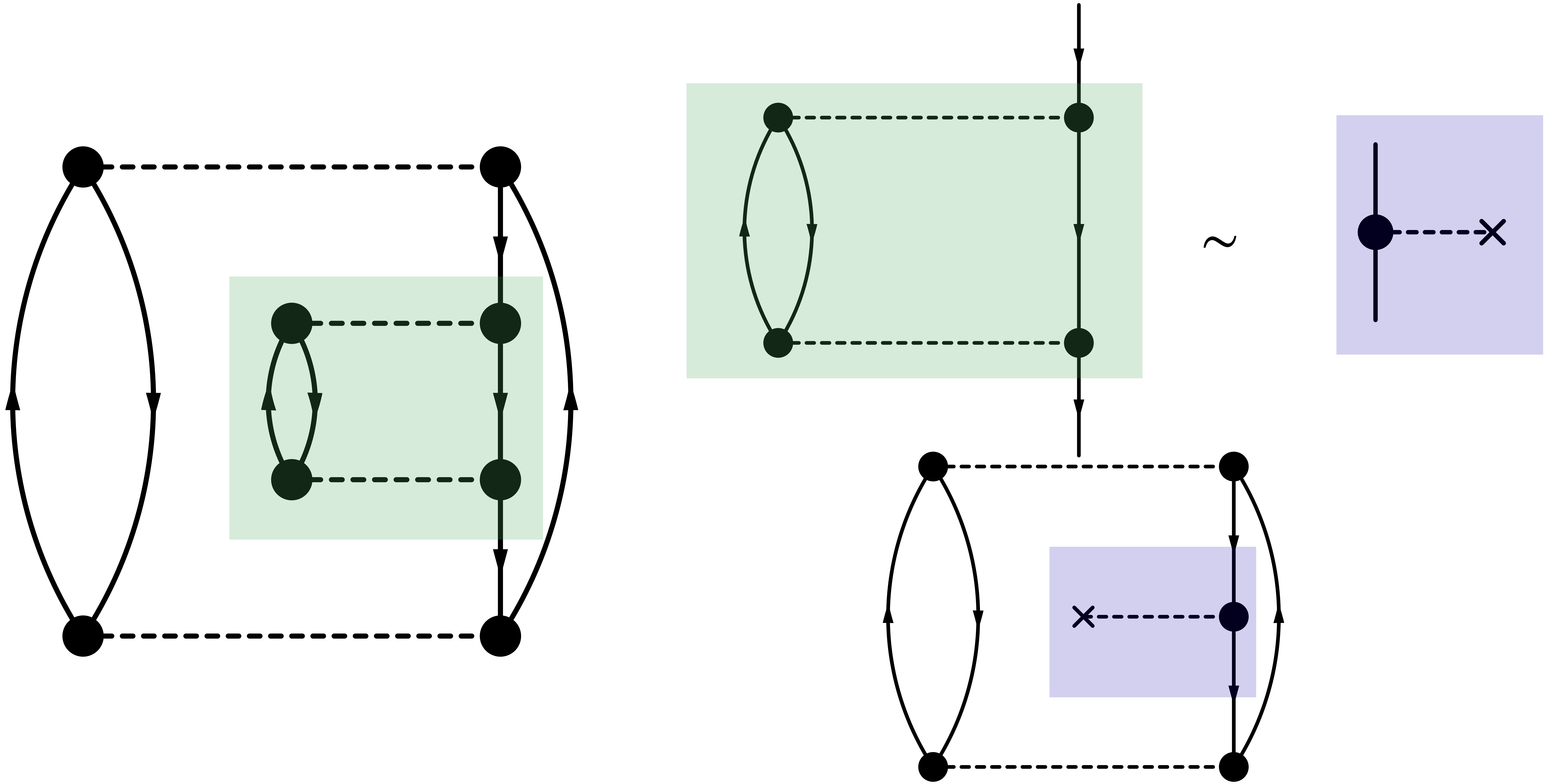

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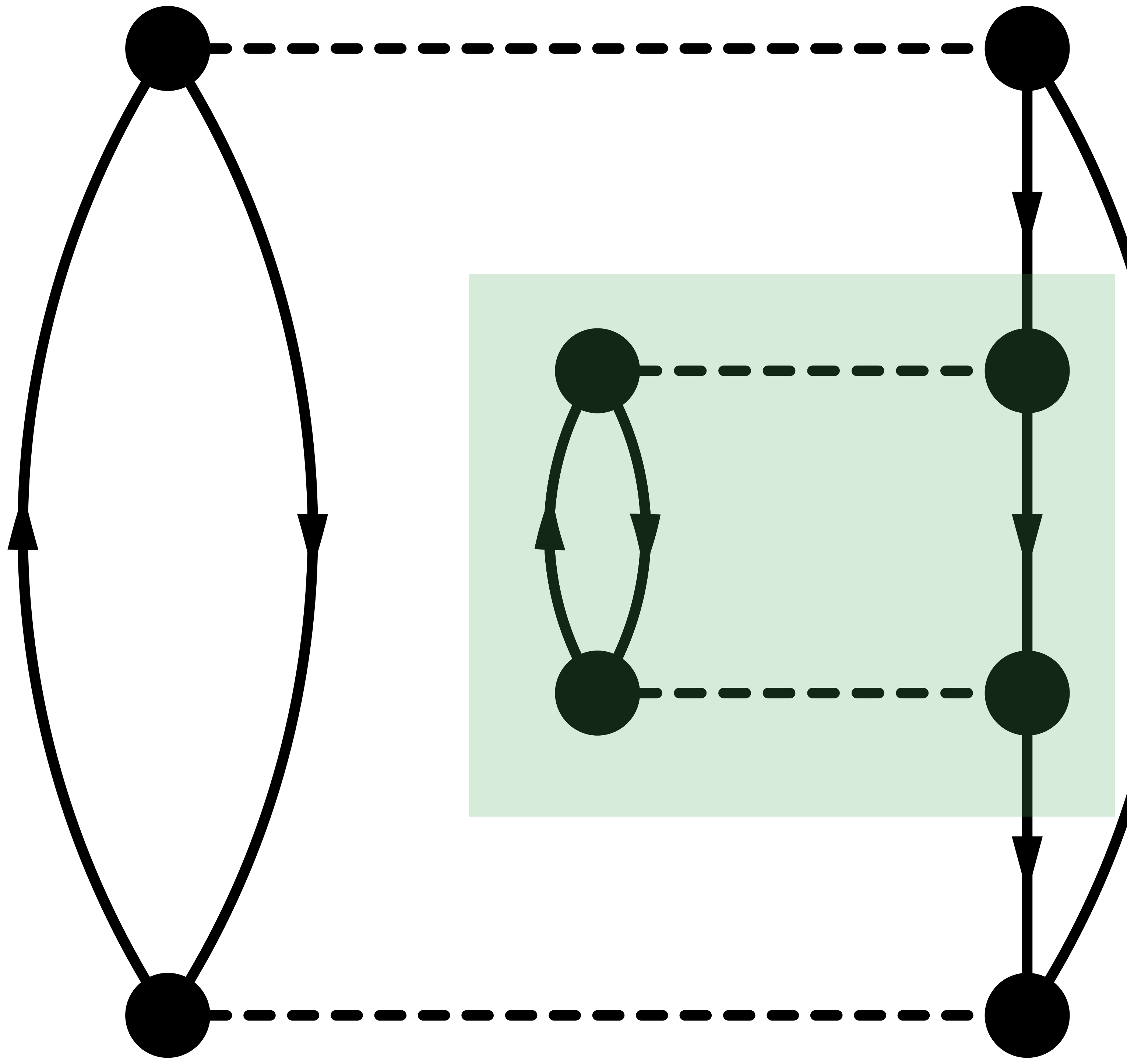
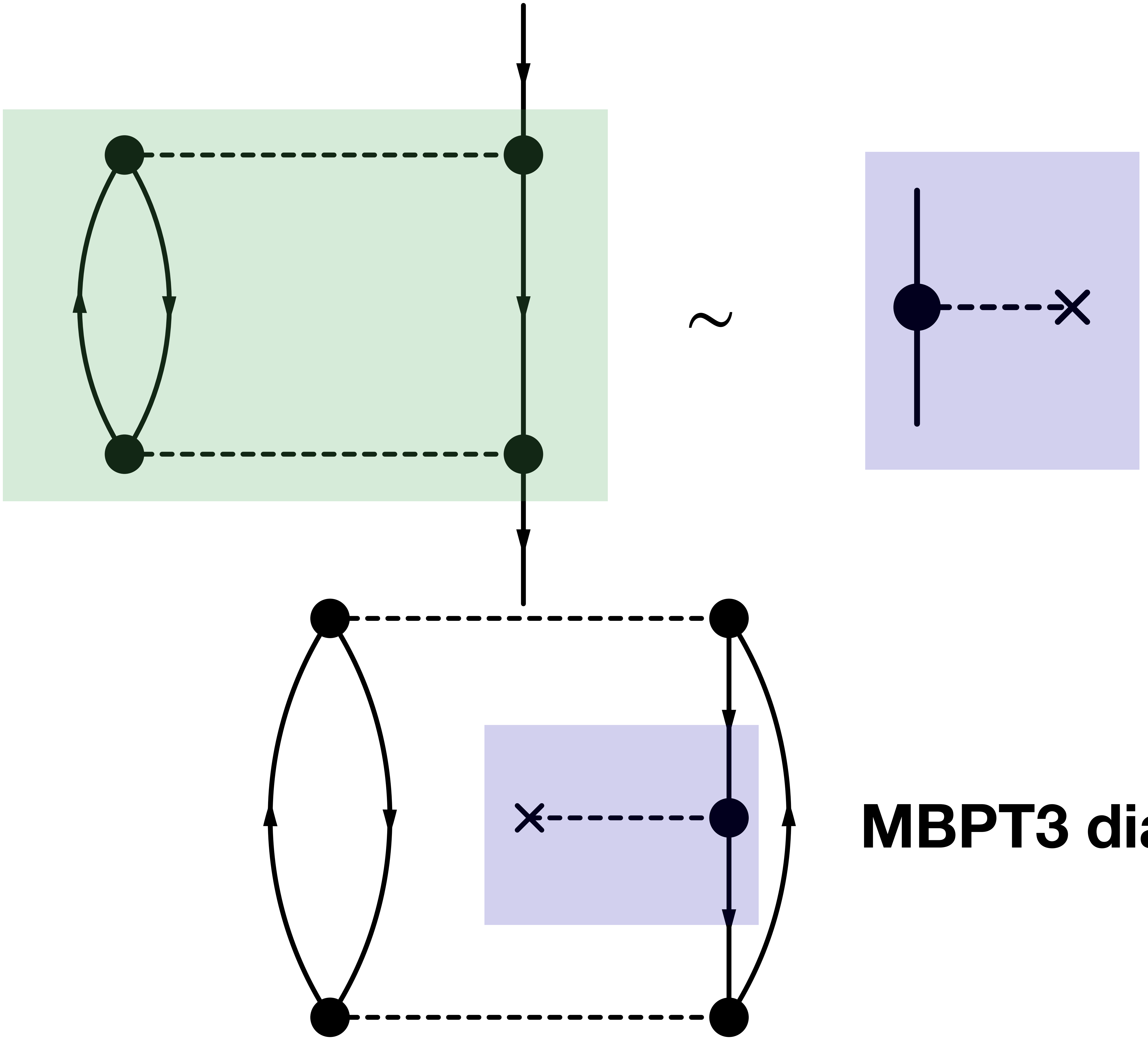
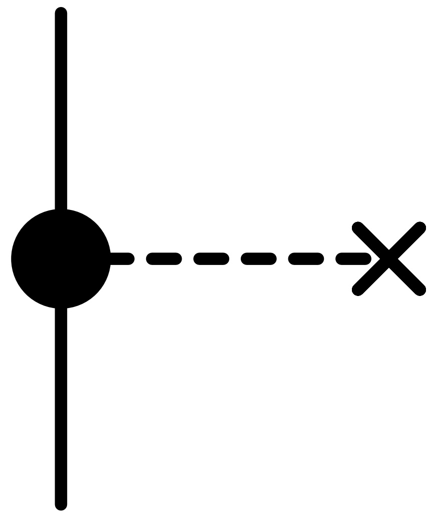




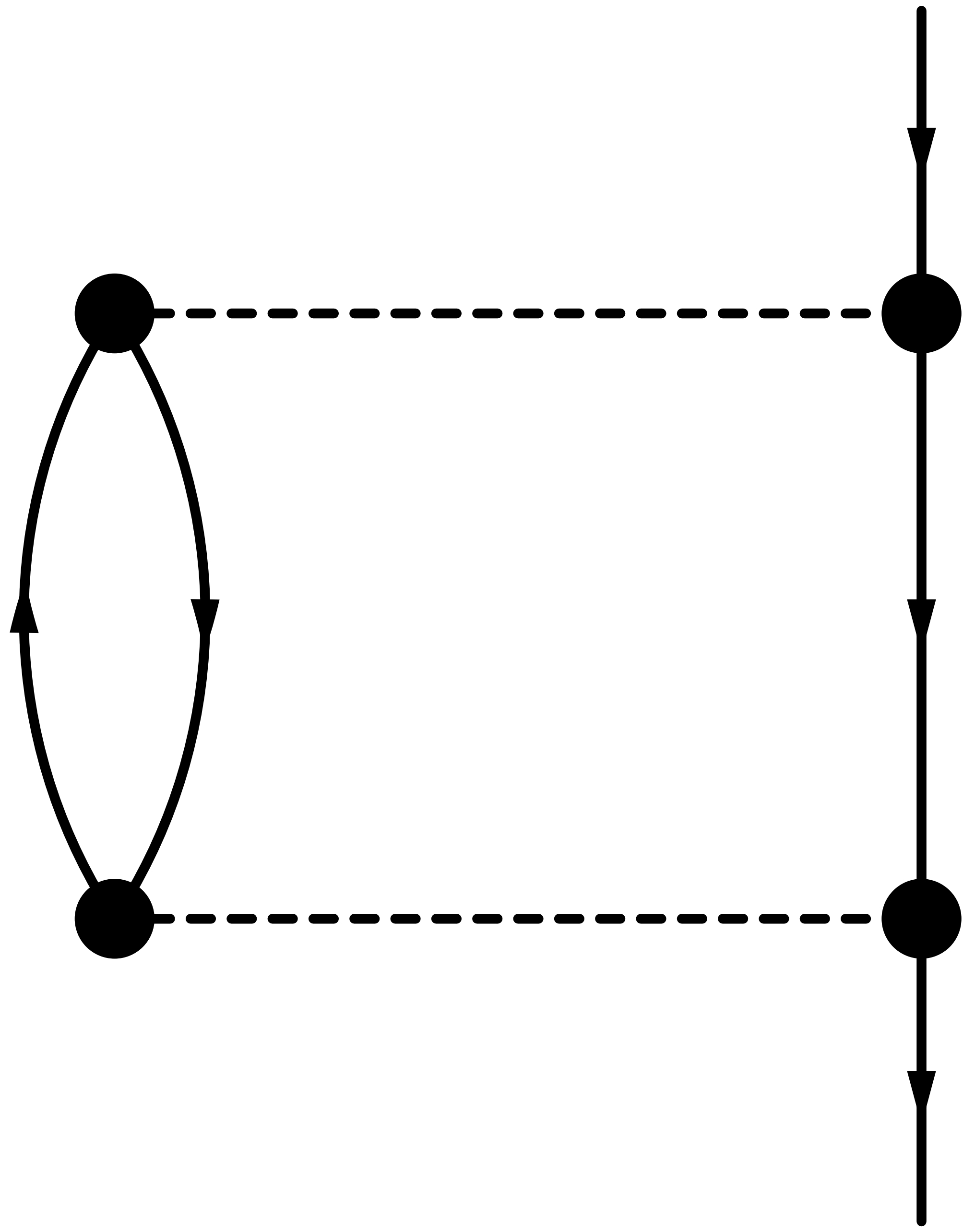
MBPT3 diagram

Alternative approach: effective interactions

Hjorth-Jensen et al., Phys. Rep. **261** (1995)



$=$



$$= -\frac{1}{2}\sum_{ija}\frac{\Gamma_{jlai}\Gamma_{aijk}}{\varepsilon_k + \varepsilon_{ij}^{a}}$$

What could possibly go wrong?

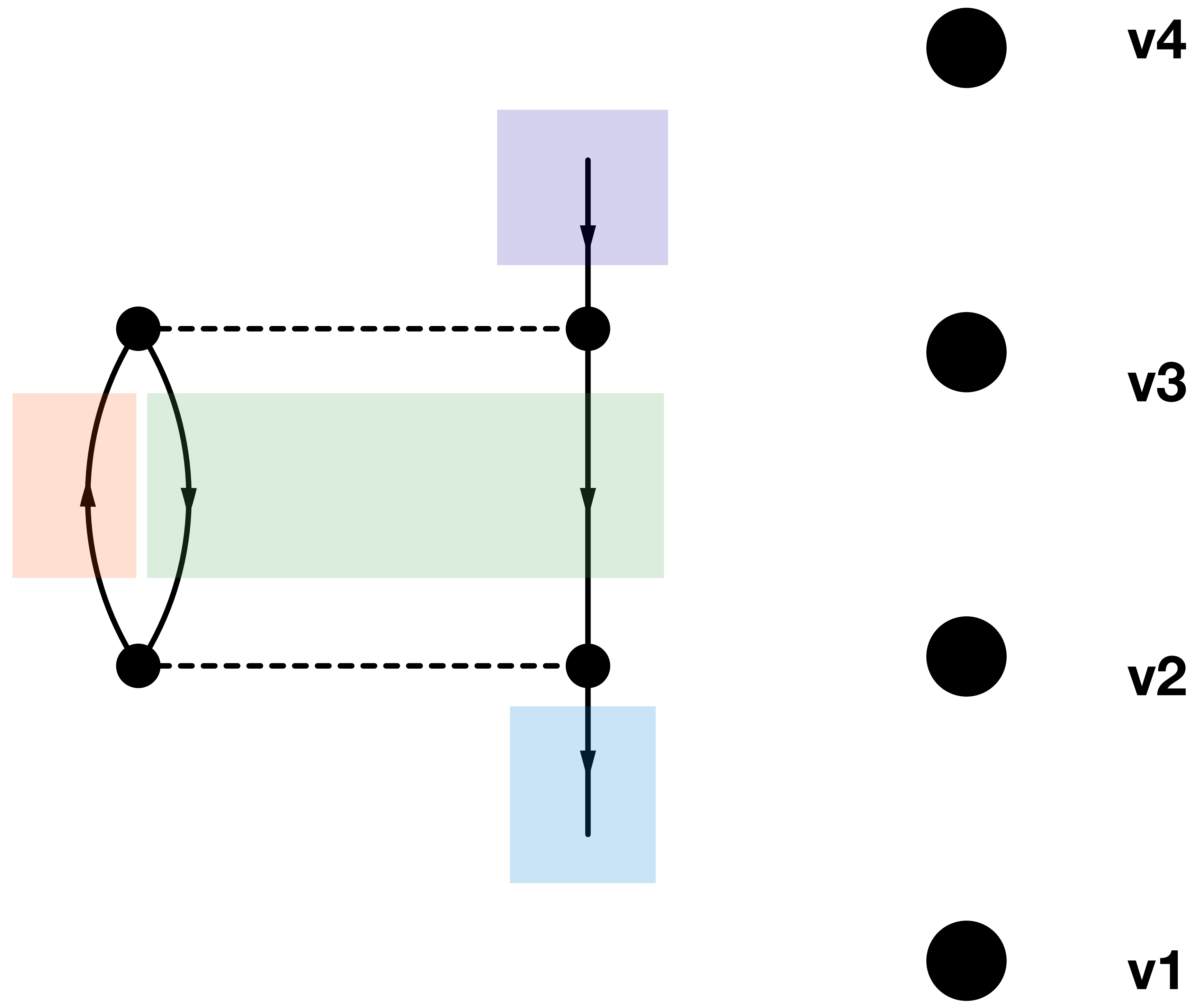
- Wrong energy denominators (unavoidable, but maybe good enough)
- **Wrong prefactor (overcounting)?**
- Fine-tuned solution, not extensible to higher IMSRG truncations

High-order diagrams with ADG

Arthuis et al., CPC **240** (2019)

- Diagrams via adjacency matrices
- Search for submatrix corresponding to effective 1B interaction

	v1	v2	v3	v4
v1	0	0	0	X
v2	1	0	1	0
v3	0	2	0	0
v4	X	0	1	0



High-order diagrams with ADG

Arthuis et al., CPC **240** (2019)

Order	4	5	6
Num diags (one hit)	1	8	206
Num diags (two hits)			2

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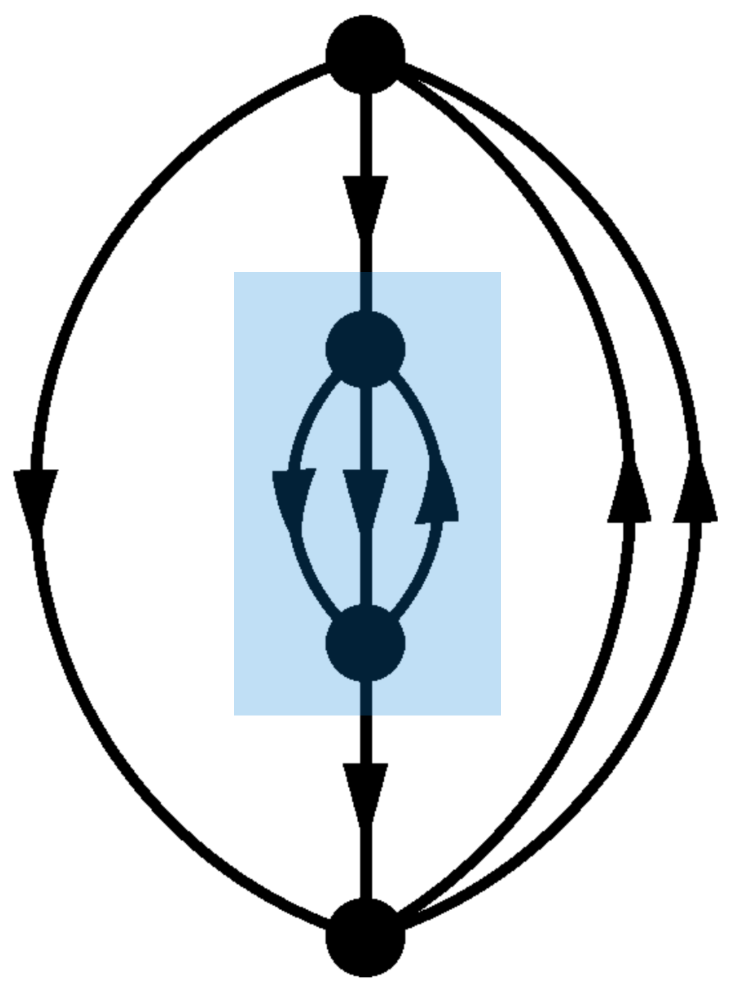

$$\frac{1}{(2!)^2} \sum \frac{v_{abnq} v_{ncop} v_{opcr} v_{qrab}}{\epsilon_{ab}^{nq} \, \epsilon_{cab}^{opq} \, \epsilon_{ab}^{qr}}$$

High-order diagrams with ADG

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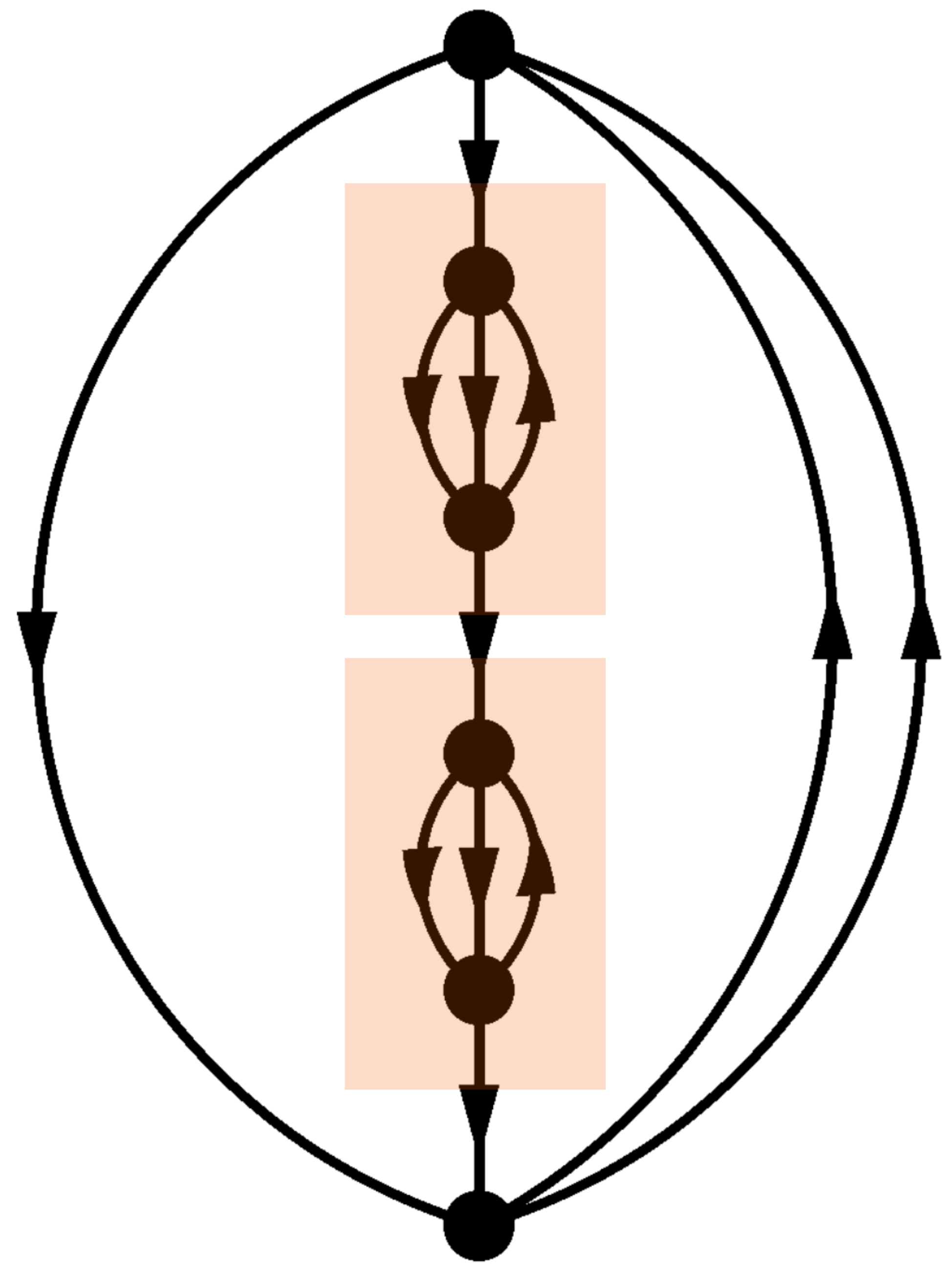
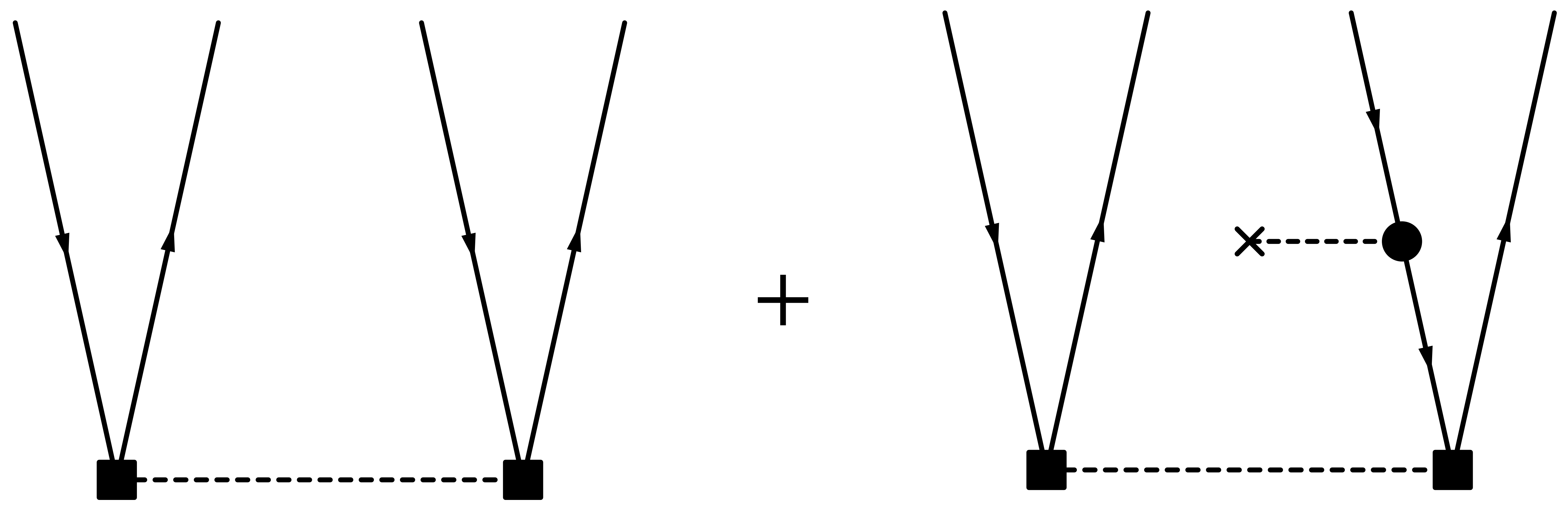


$$-\frac{1}{(2!)^3}\sum \frac{v_{abnt}v_{ncop}v_{opcq}v_{qdrs}v_{rsdu}v_{tuab}}{\epsilon^{nt}_{ab}\,\epsilon^{opt}_{cab}\,\epsilon^{qt}_{ab}\,\epsilon^{rst}_{dab}\,\epsilon^{tu}_{ab}}$$

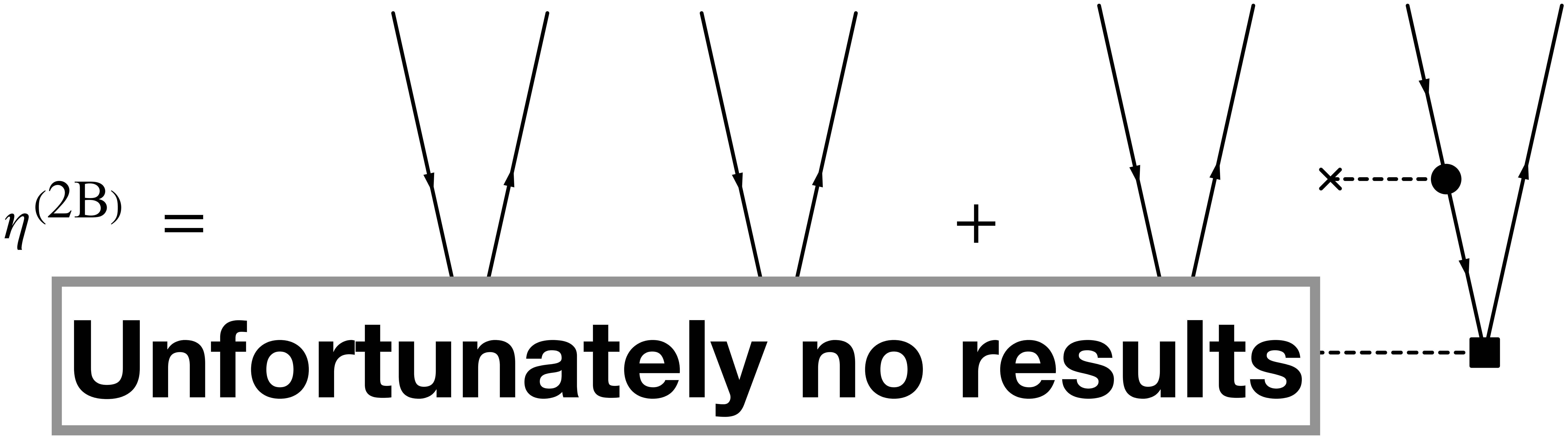
"Correcting" the IMSRG(2)

$\eta^{(2B)} =$



- Improved generator has same decoupling condition $\langle \Phi_{ij}^{ab} | H(\infty) | \Phi \rangle \stackrel{!}{=} 0$
- Gets important triples at MBPT4 approximately right
- But also higher order contributions due to nonperturbative power in IMSRG

"Correcting" the IMSRG(2)



Unfortunately no results

- Improved generator has same decoupling condition $\langle \Phi_{ij}^{ab} | H(\infty) | \Phi \rangle \overset{!}{=} 0$
- Gets important triples at MBPT4 approximately right
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Main takeaways

- IMSRG is a powerful many-body method for nuclear physics

- Perturbative improvements in IMSRG are complicated due to **ODE form**
- But they can give **insight into many-body error**

- Analysis connecting IMSRG and MBPT is complex
    - **Possibly automate perturbative analysis to get effective interactions?**
- Automated tools (ADG) can **support efforts** to validate improvements
- **TODO: Automated code generation using generic contraction engine**

Acknowledgments

Thanks to:

- **Jan Hoppe**, **Pierre Arthuis**, **Takayuki Miyagi**, **Alex Tichai**, Ragnar Stroberg, Kai Hebeler, Achim Schwenk
- TU Darmstadt "STRONGINT" group
- ORNL Nuclear Theory and **Titus Morris**
- **... and all of you for your attention**

Backup

Details for matrix elements

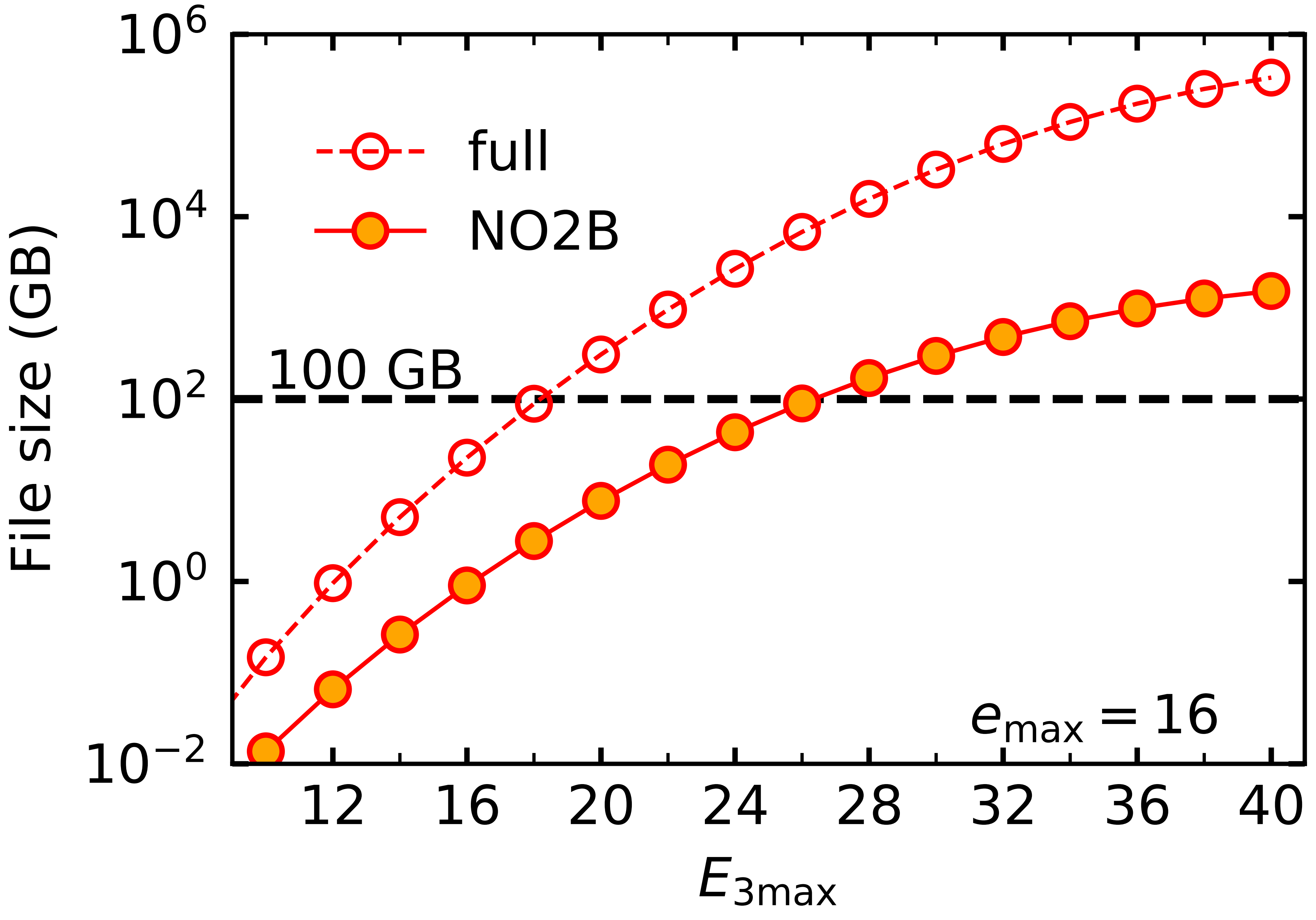
Coupled

- 2B basis: $|(pq)JM_J\rangle$, ignore trivial M_J dependence, block sparse in $(\Pi = \Pi_p + \Pi_q, T_z = t_{z,p} + t_{z,q}, J)$
- 3B basis: $|[(pq)J_{pq}r]JM_J\rangle$, ignore trivial M_J dependence, block sparse in $(\Pi = \Pi_p + \Pi_q + \Pi_r, T_z = t_{z,p} + t_{z,q} + t_{z,r}, J)$

Uncoupled

- 2B basis: $|pq\rangle$, block sparse in $(\Pi, T_z, M_J = m_p + m_q)$
- 3B basis: $|pqr\rangle$, block sparse in $(\Pi, T_z, M_J = m_p + m_q + m_r)$
- **Typically partition 3B basis blocks into 2B symmetry sublocks**

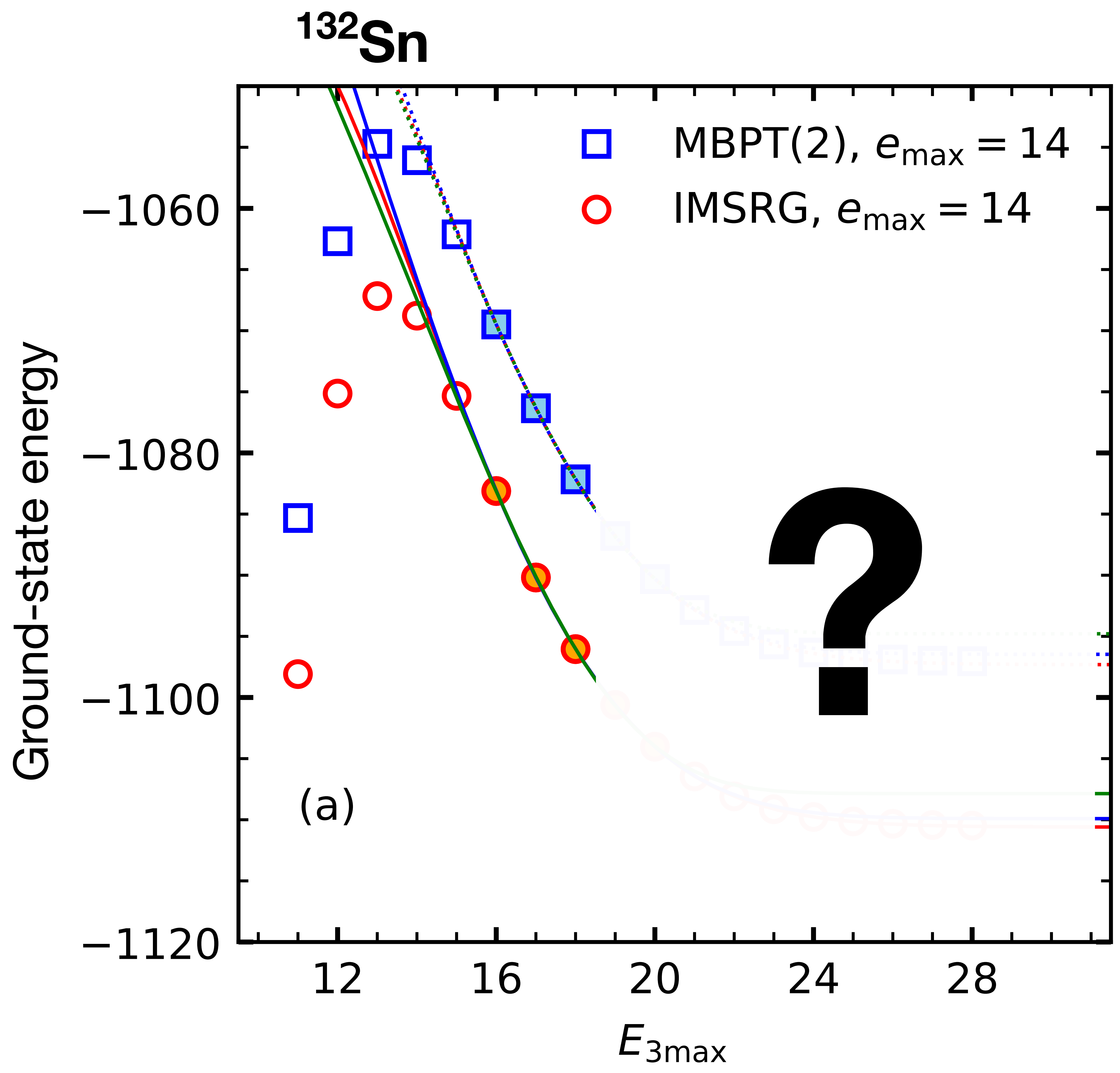
Converged calculations for heavy nuclei



Miyagi et al., PRC **105** (2022)

- Ab initio calculations of heavy nuclei constrained by three-body force convergence ($E_{3,\max}$)
- Novel storage scheme reduces storage costs by 2-3 orders of magnitude
- First converged calculations of Sn-132
- Opens up frontier of heavy nuclei

Converged calculations for heavy nuclei



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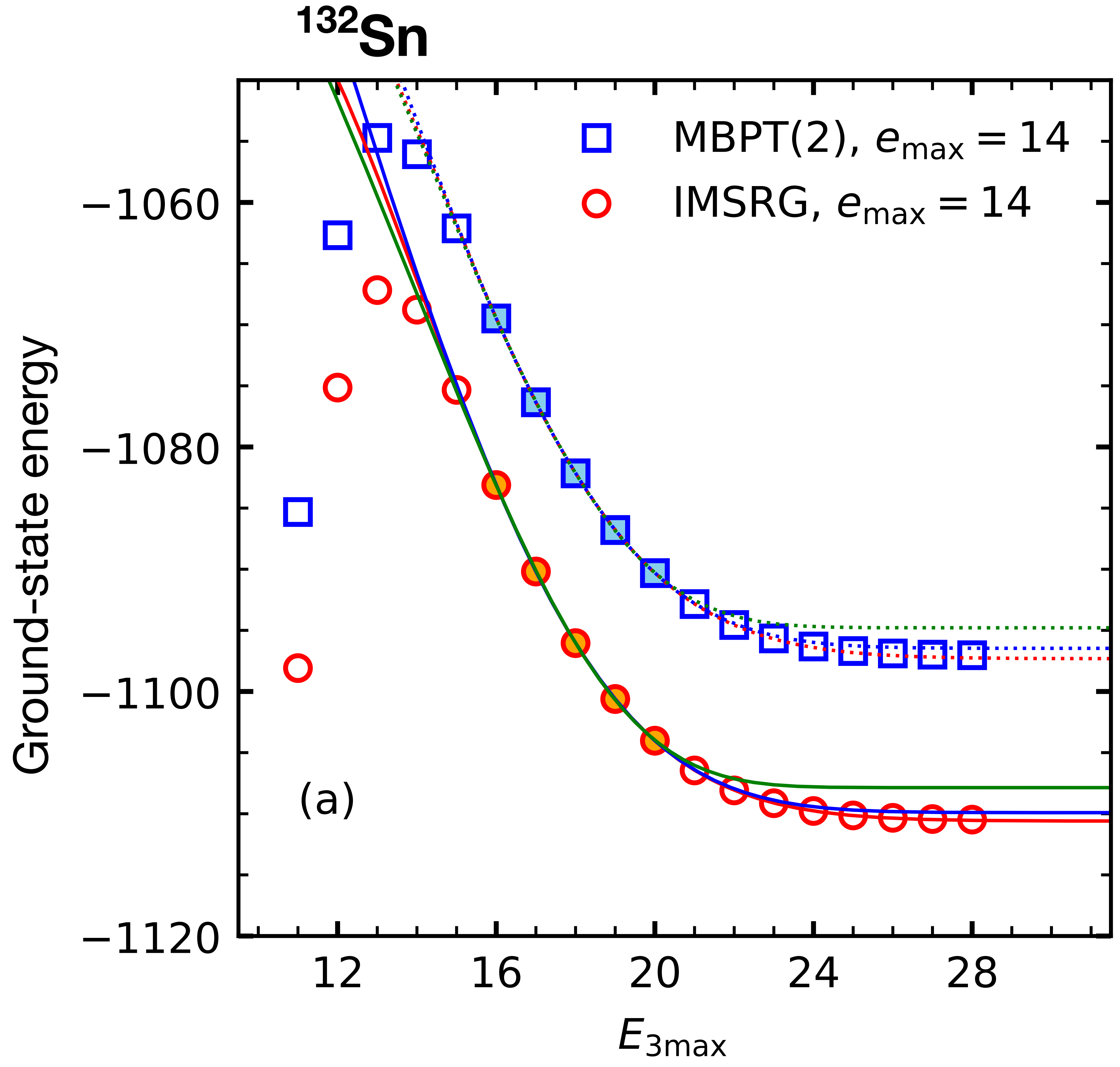

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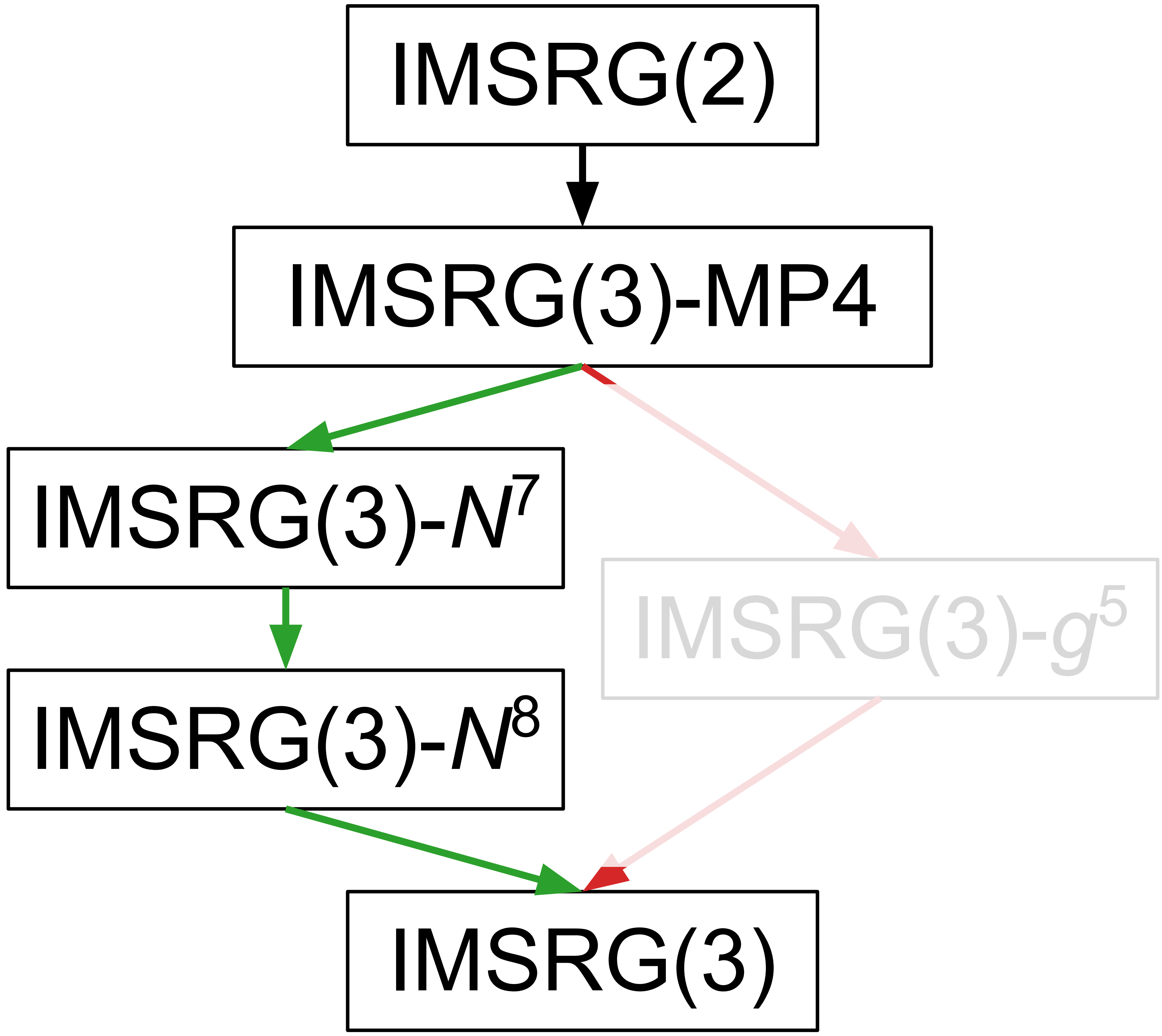
Unlocking IMSRG(3) (approximately)

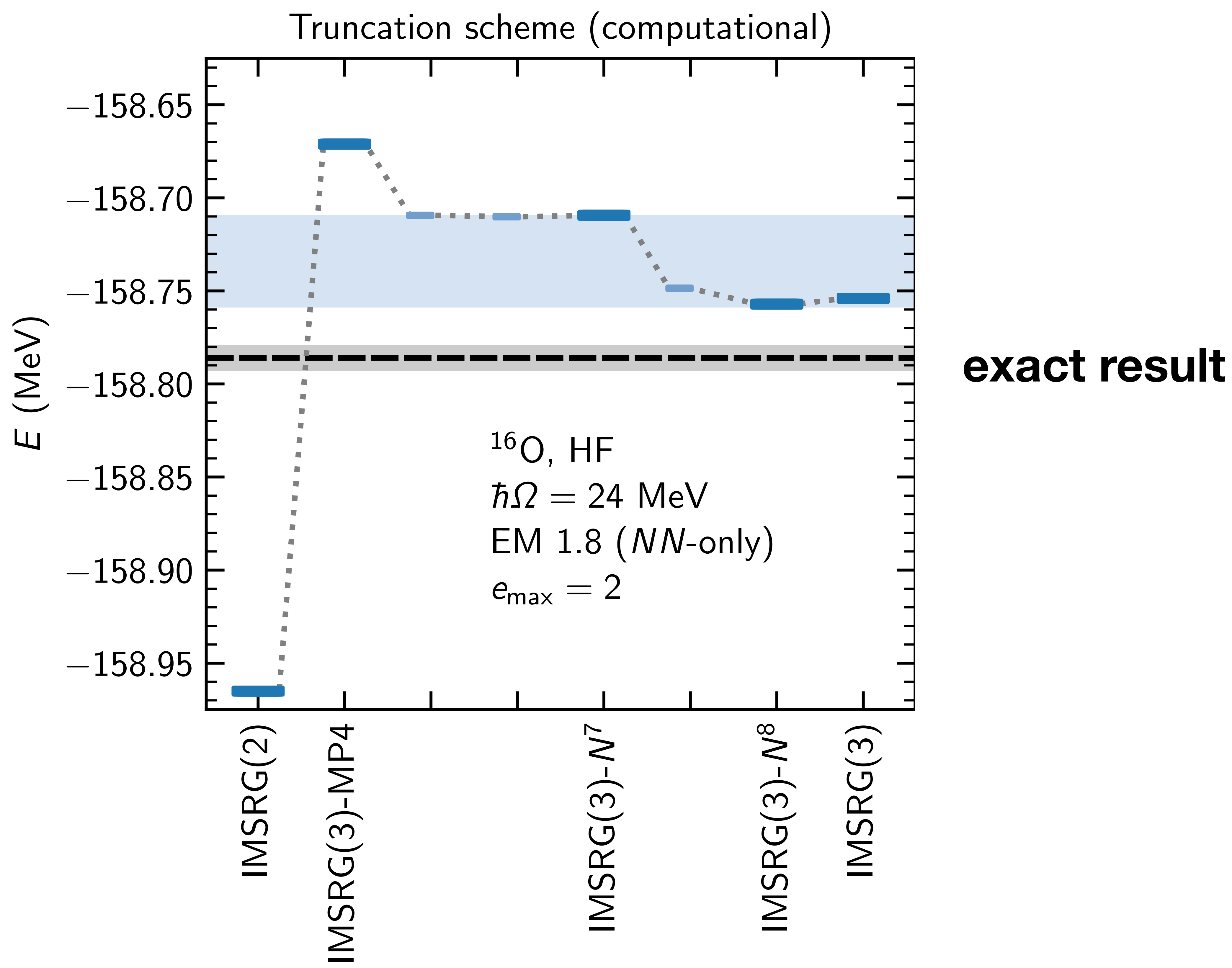
Heinz et al., PRC **103** (2021)

- IMSRG(3) is too expensive
- Systematic approximation based on computational cost
- Study in restricted setting to understand many-body convergence



Unlocking IMSRG(3) (approximately)

Heinz et al., PRC **103** (2021)



- Systematic convergence to exact result
- IMSRG(2) does very well ...
- ... but IMSRG(3) (and approximations) perform even better
- Benefits of IMSRG(3) largely present in approximations (e.g., IMSRG(3)-N^7)

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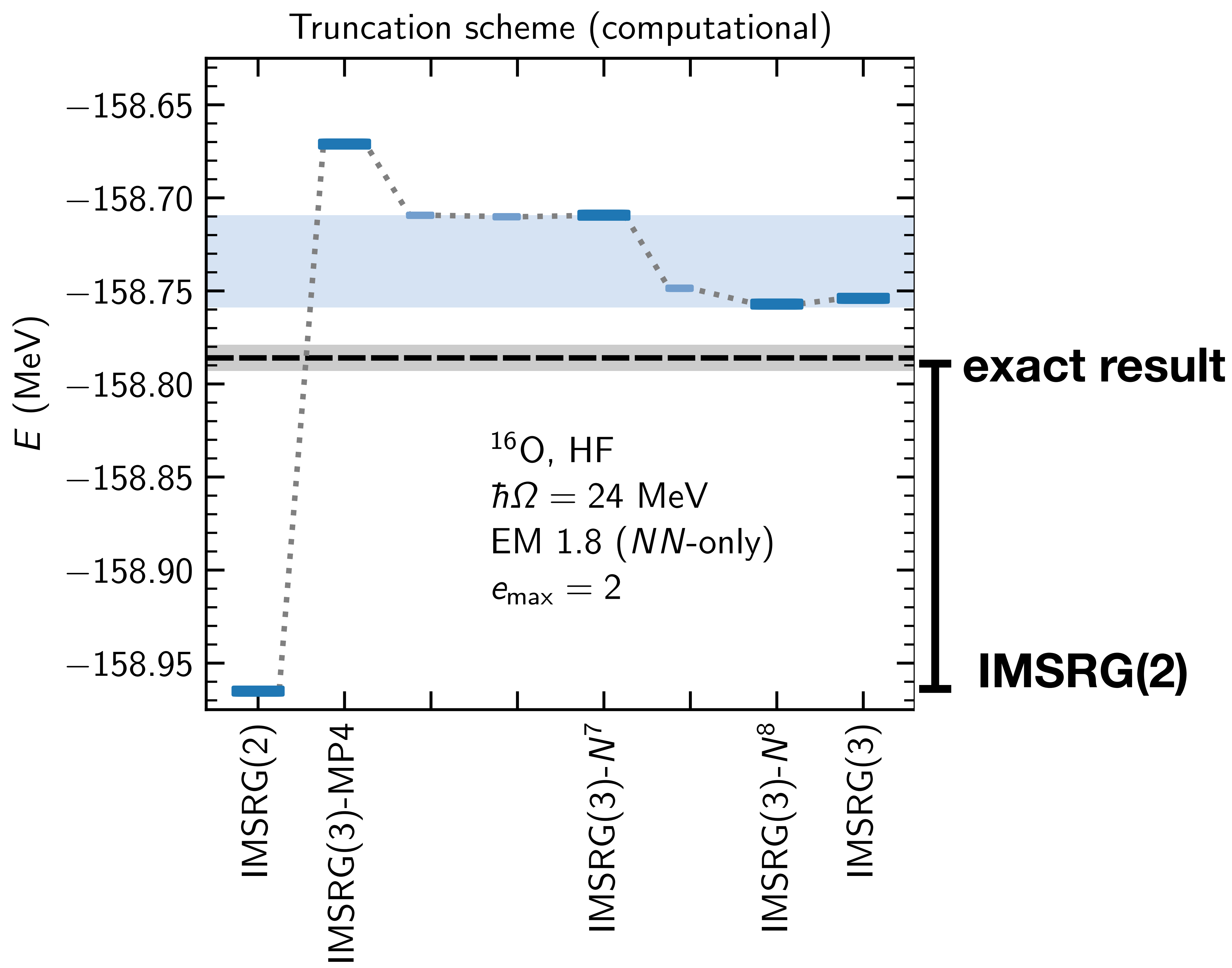
Heinz et al., PRC **103** (2021)



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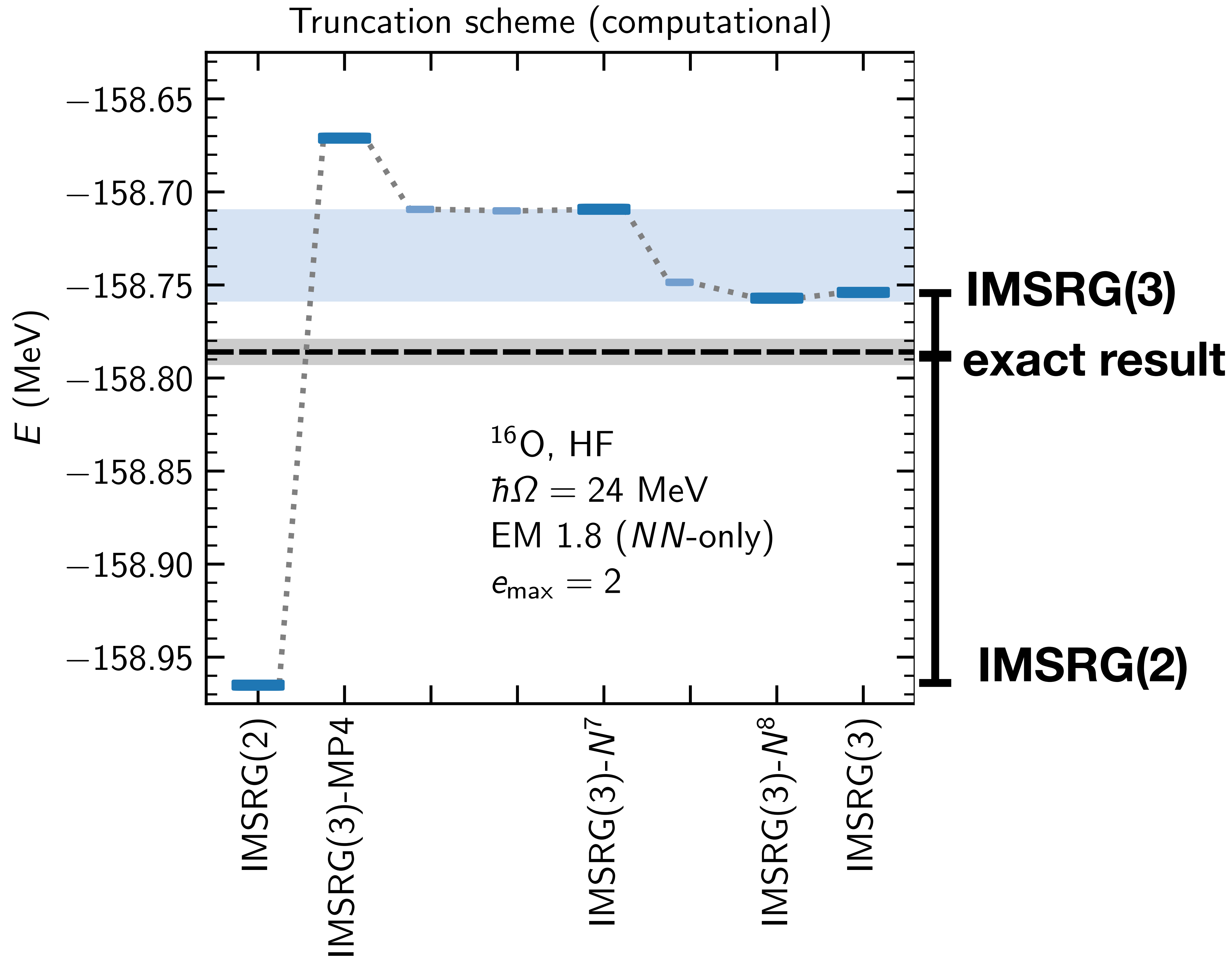

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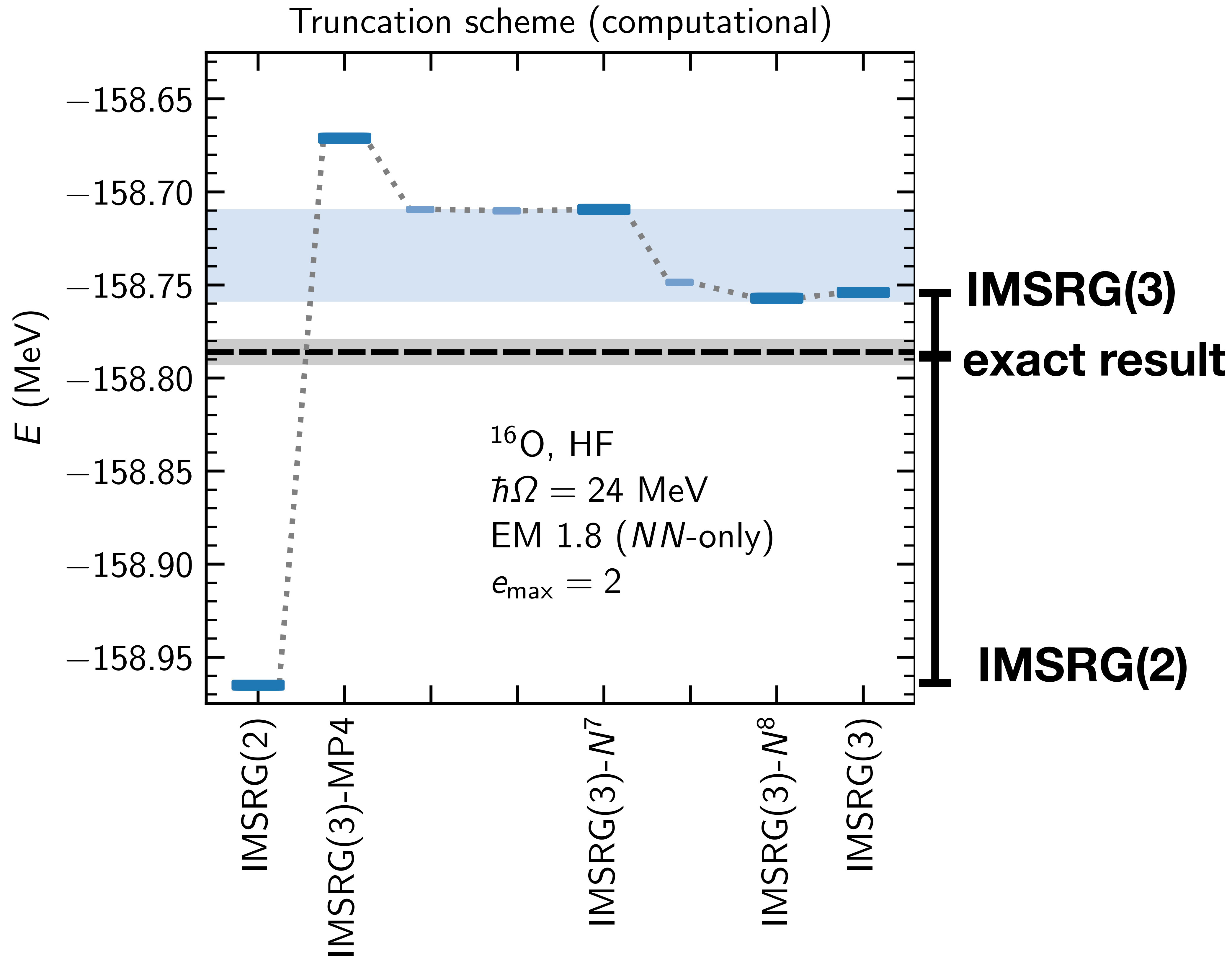

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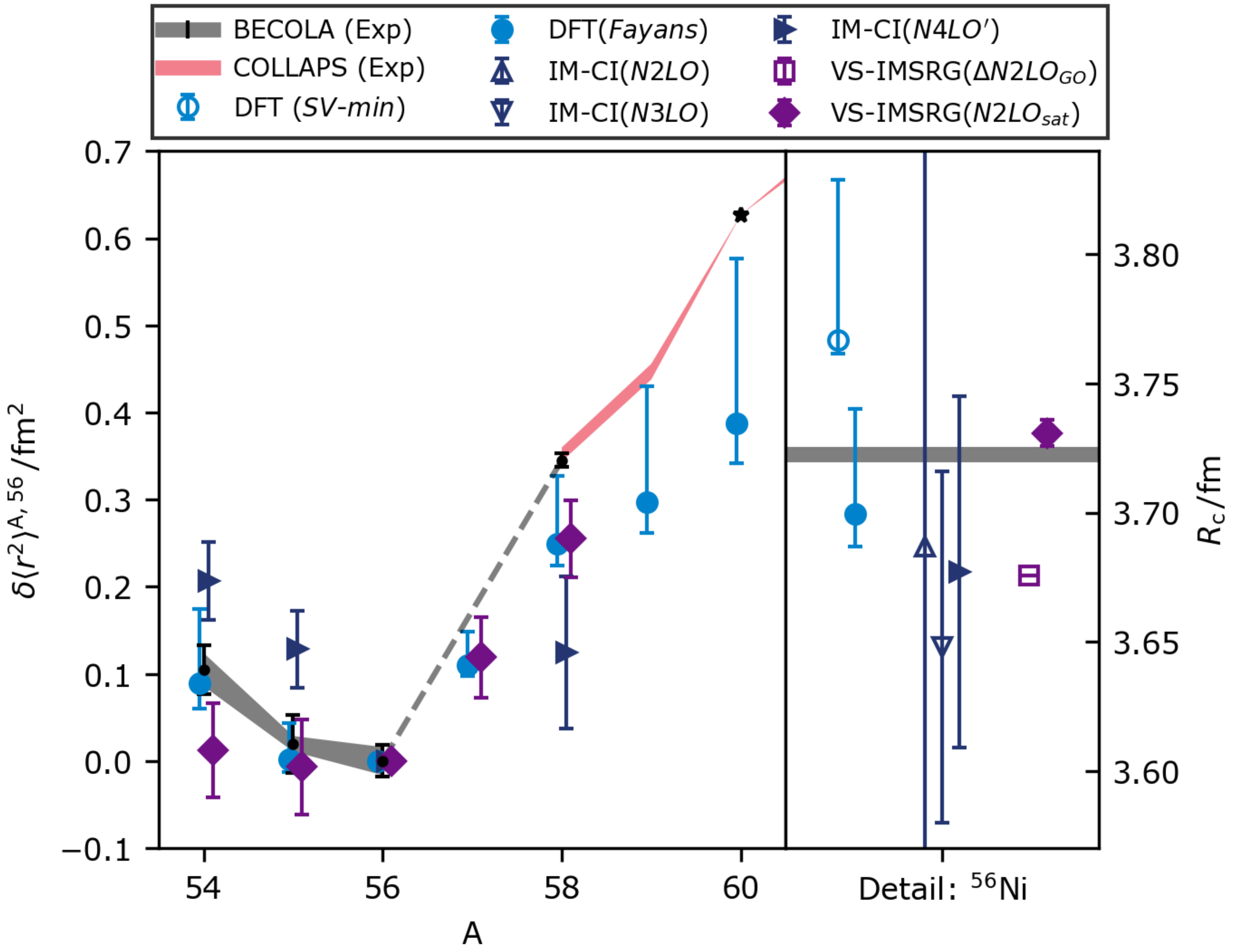
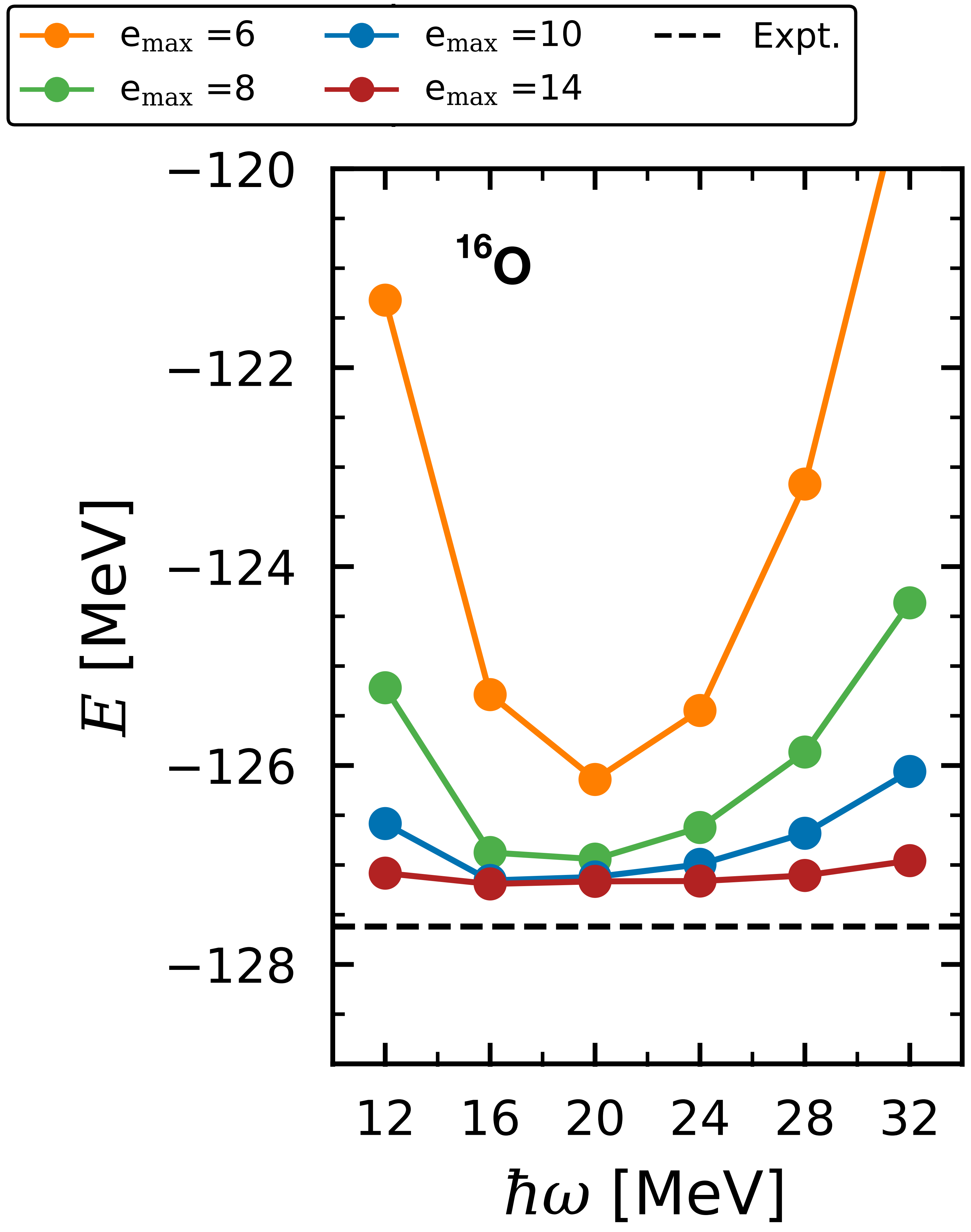
Goal: Use IMSRG(3) approximations to improve many-body calculations and quantify uncertainties

Nickel charge radii



Sommer et al., PRL **129** (2022)

IMSRG ingredients



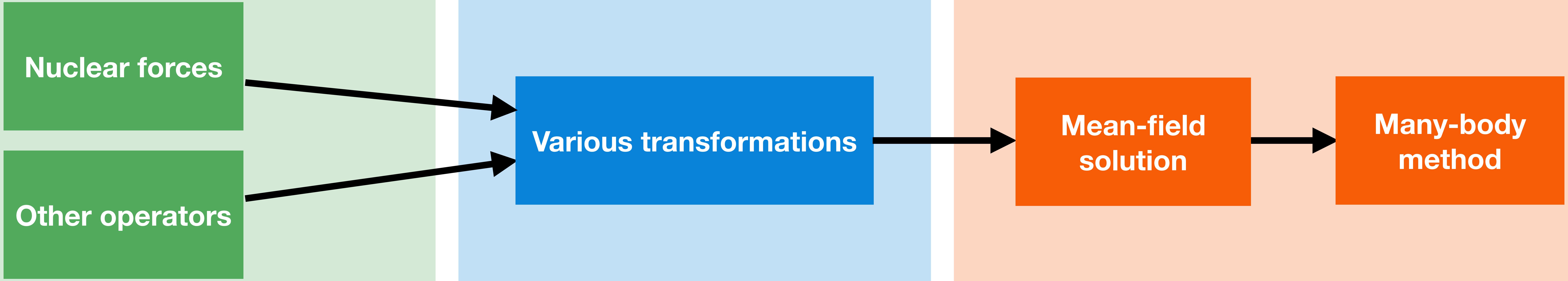
Hoppe, ..., **MH** et al., PRC **103** (2021)

1. Input Hamiltonian H
2. Solve for mean field (Hartree-Fock)
   - Input dependence: H, e_{max}, $E_{3\text{max}}$, $\hbar\omega$
   - Output: reference state $|\Phi\rangle$, basis $\{\phi_p\}$
3. Solve for many-body correlations [IMSRG(2)]
   - Input dependence: $\underbrace{H, |\Phi\rangle}$, $\{\phi_p\}$, other ops ...

     normal ordering
     Hebeler, ..., **MH** et al., PRC **107** (2023)
   - Output: $|\Phi\rangle$, E, expectation values of ops ...

Many-body calculation uncertainties

Operator determination | **Basis transformation** | **Many-body calculation**

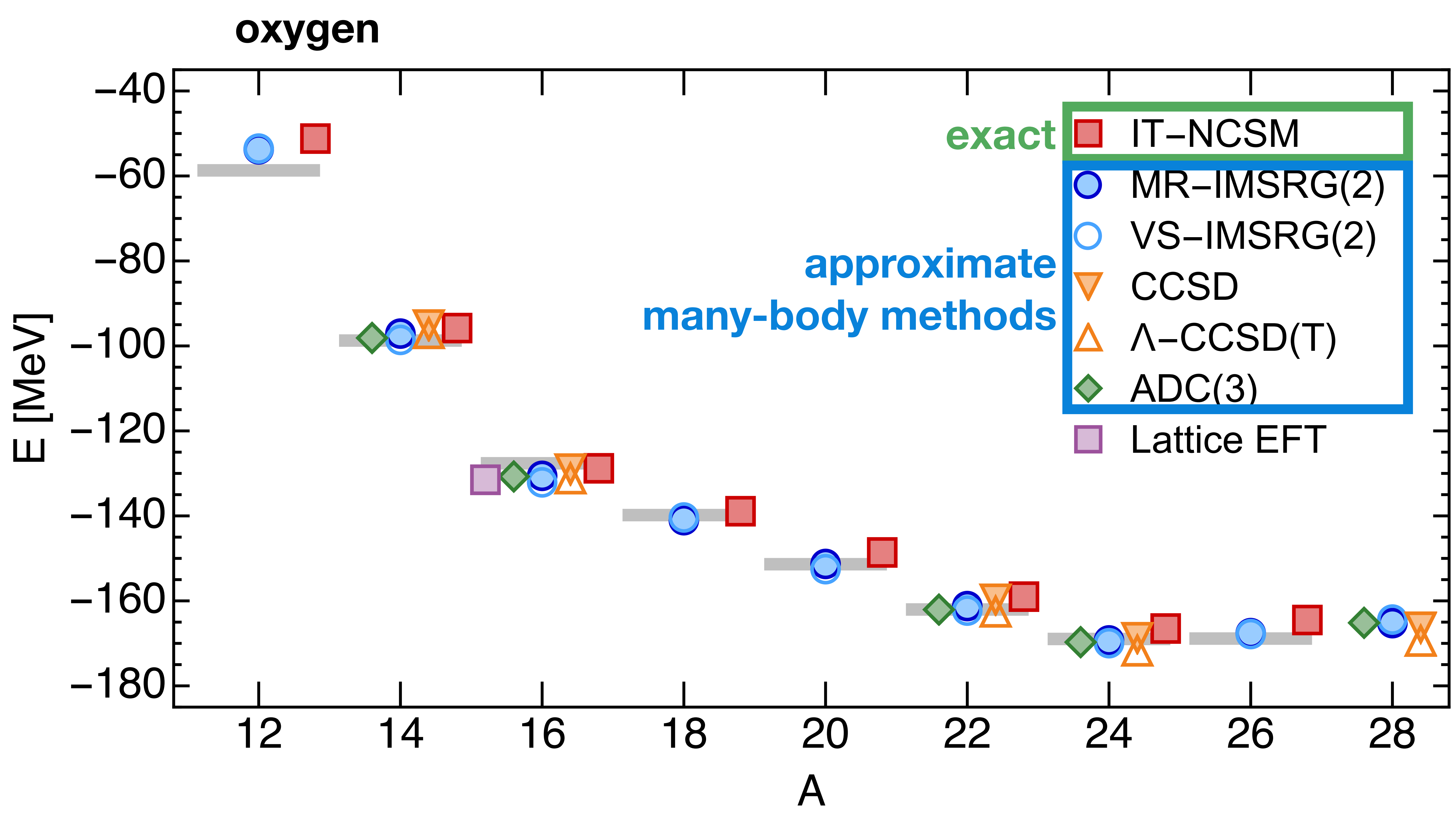


Hamiltonian uncertainty:
- **Nuclear force model**
- **Model error**
- **Fit strategy to experimental data**

Model-space uncertainty:
- **Basis truncation**
  - $e_{\text{max}}, E_{3,\text{max}}$

Many-body uncertainty:
- **Many-body method truncation**
  - **IMSRG(2), IMSRG(3)**
- **...**

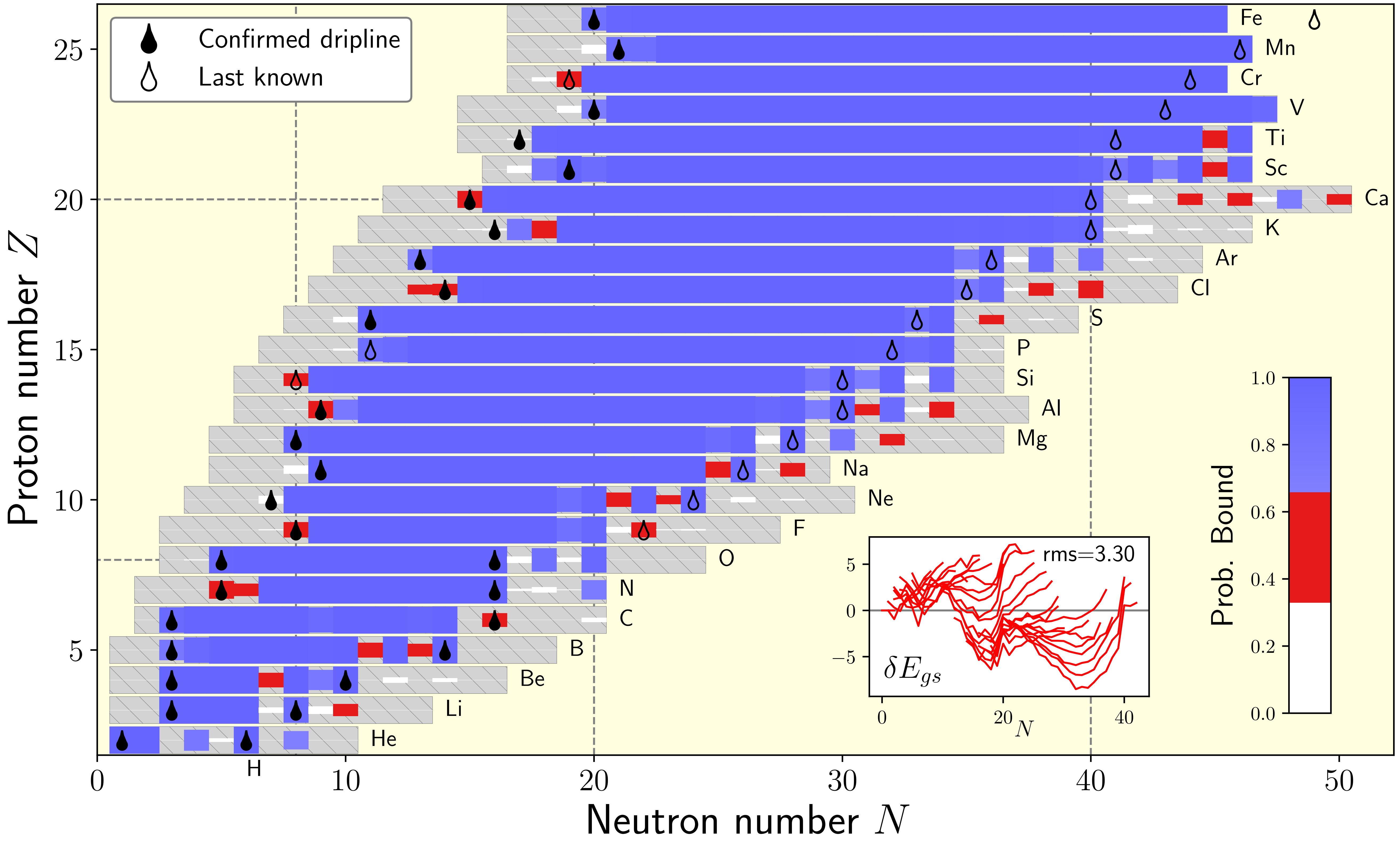
Many-body consistency in oxygen



Hergert, Front. Phys. **7** (2020)

- For given Hamiltonian, many-body methods are very consistent
- 1-2% discrepancy to **exact result** due to **many-body approximation**

Drip lines from the VS-IMSRG



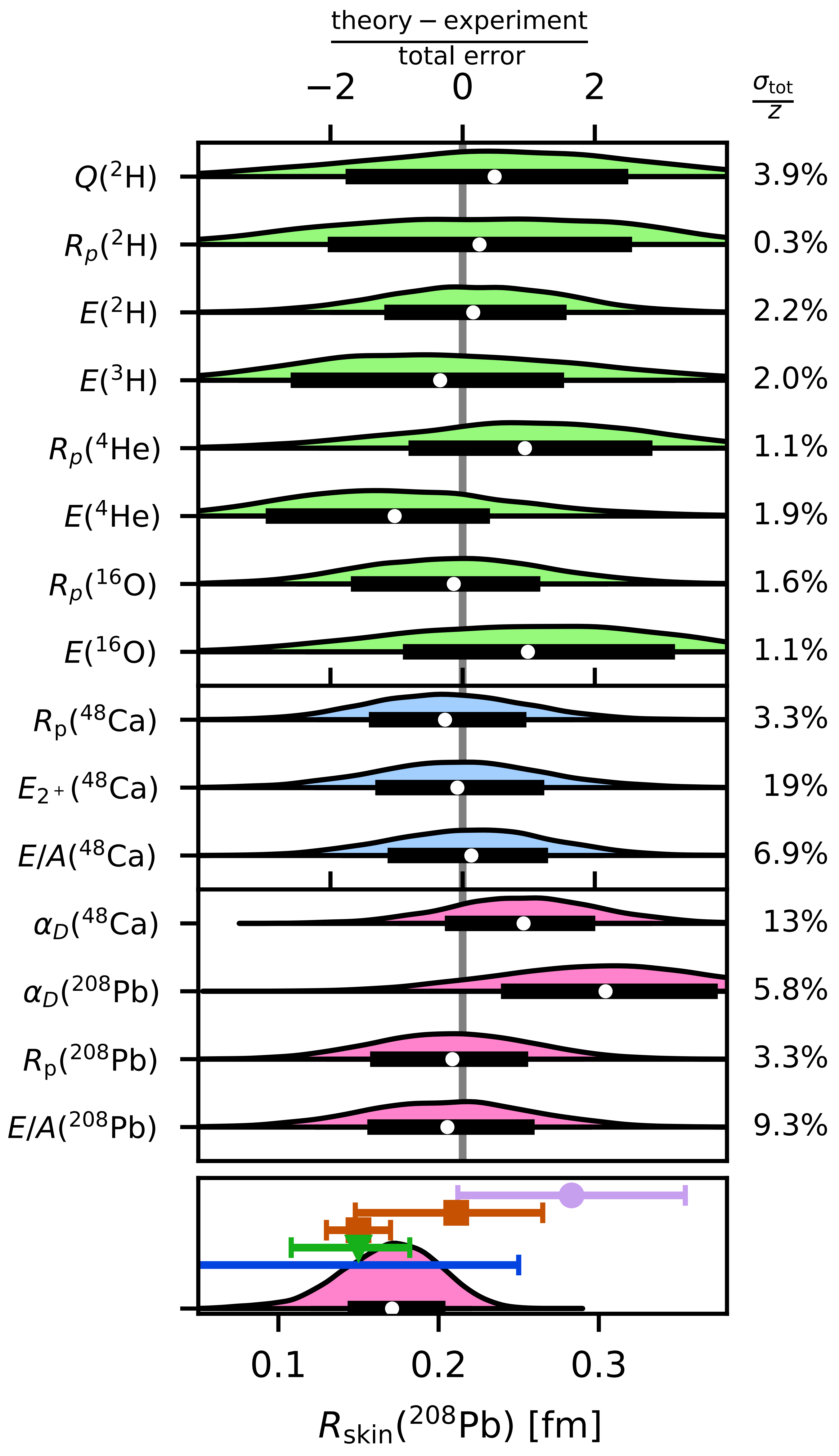
agonalization

ies based on single Hamiltonian

ors to predict limits of stability

Stroberg et al., PRL **126** (2021)

First systematic study of ^{208}Pb



Hu et al., Nature Phys. **18** (2022)

History matching:

- Start from 10^9 Hamiltonians
- Compare predictions with experiment and discard "implausible" Hamiltonians
- Final result: 34 different valid choices

Likelihood calibration:

- Assess quality of valid Hamiltonians in ^{48}Ca
- Assign importance weight based on quality

Uncertainty quantified prediction:

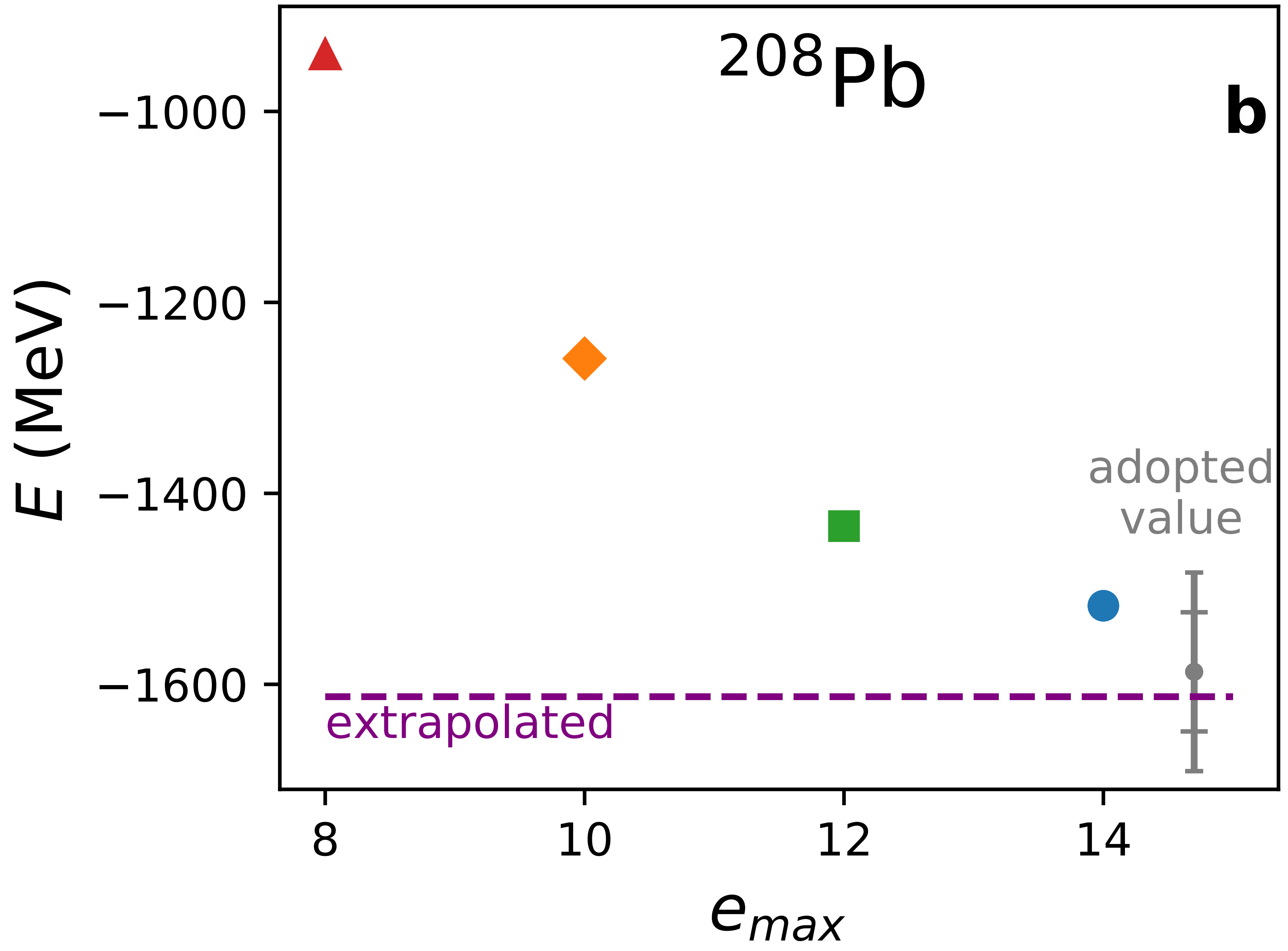
- Make many-body prediction using all valid Hamiltonians

$$R_{\text{skin}} = 0.14\text{-}0.20 \text{ fm}$$

Hamiltonian, model space, and method uncertainties accounted for at all stages!

First systematic study of ^{208}Pb

- Convergence of many-body calculation still challenging
- Hamiltonian uncertainties also very large
- Uncertainty quantification methods explicitly take errors into account
- Look at observables where correlated errors cancel?

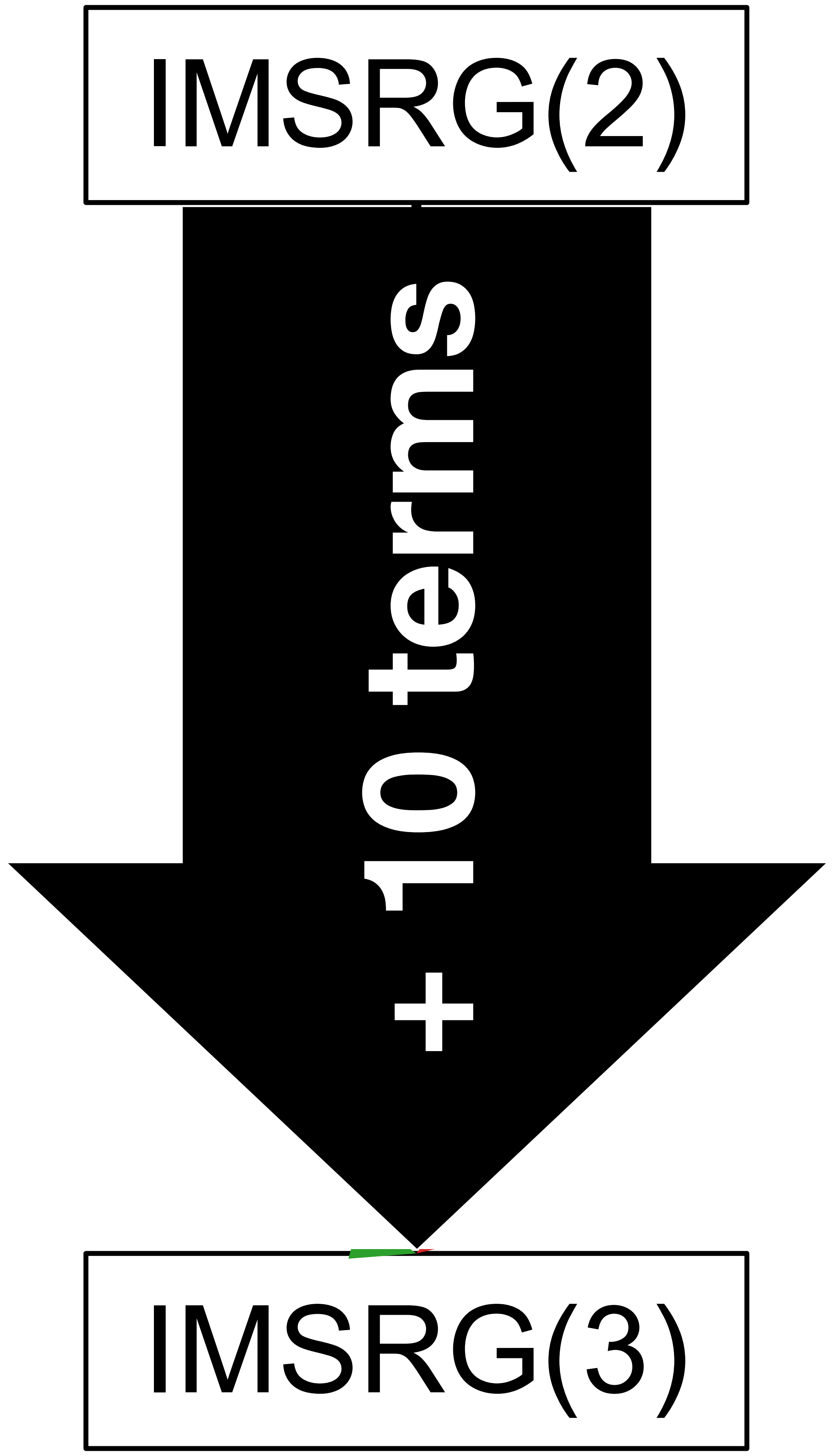


Hu et al., Nature Phys. **18** (2022)

Reaching IMSRG(3)

MH et al., PRC **103** (2021)

- IMSRG(3) is too expensive
- What can we afford?
- What is actually important?



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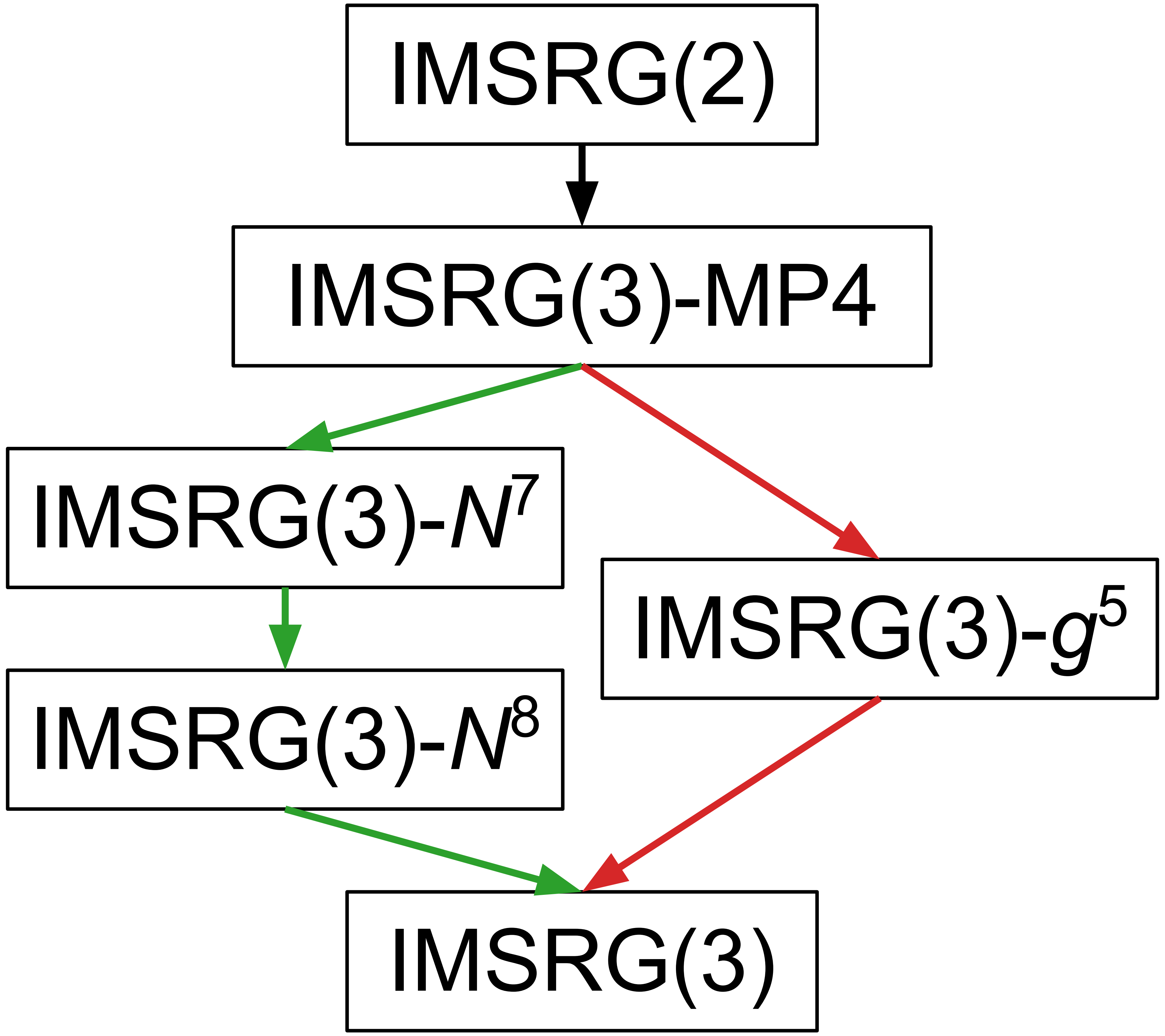
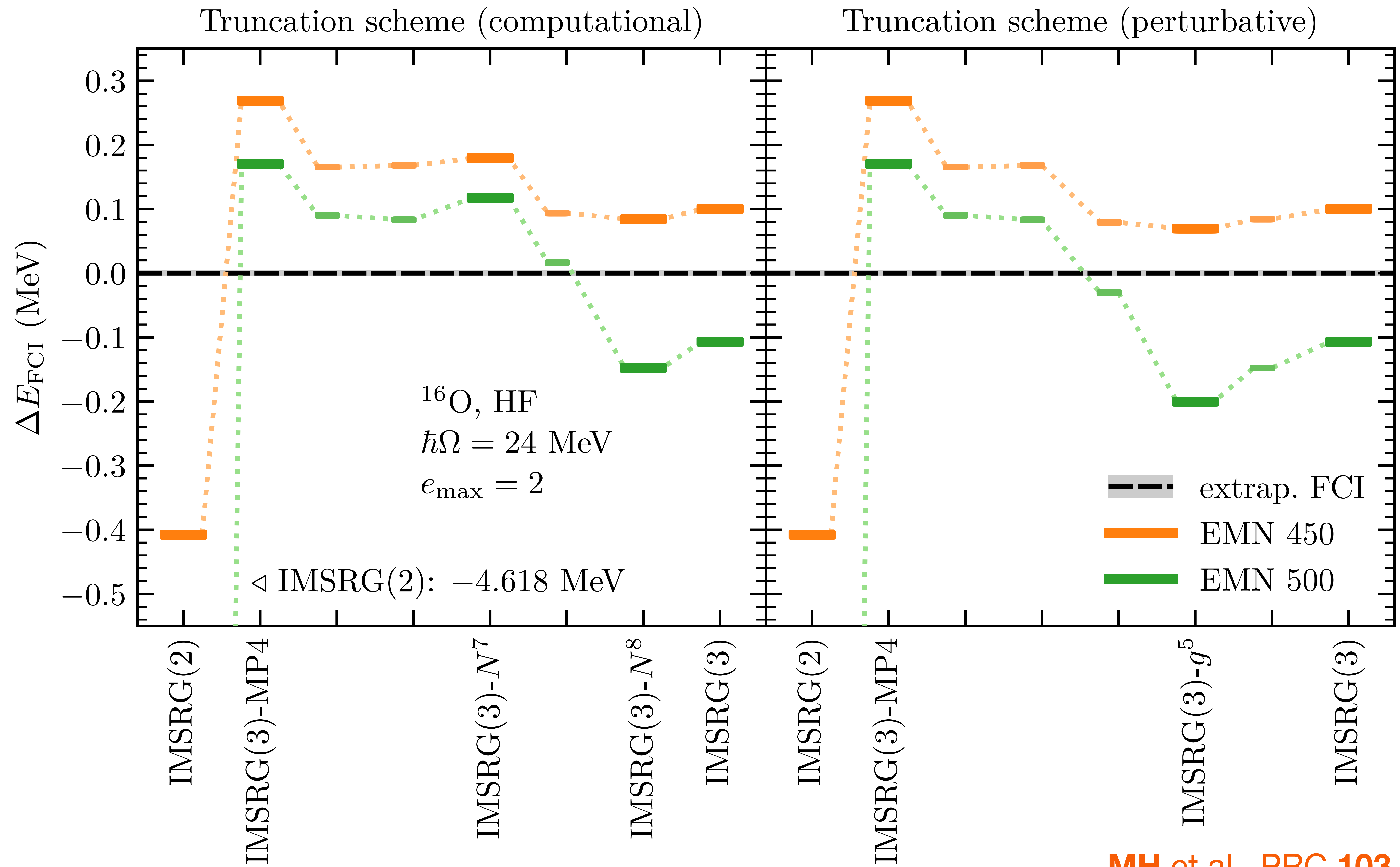
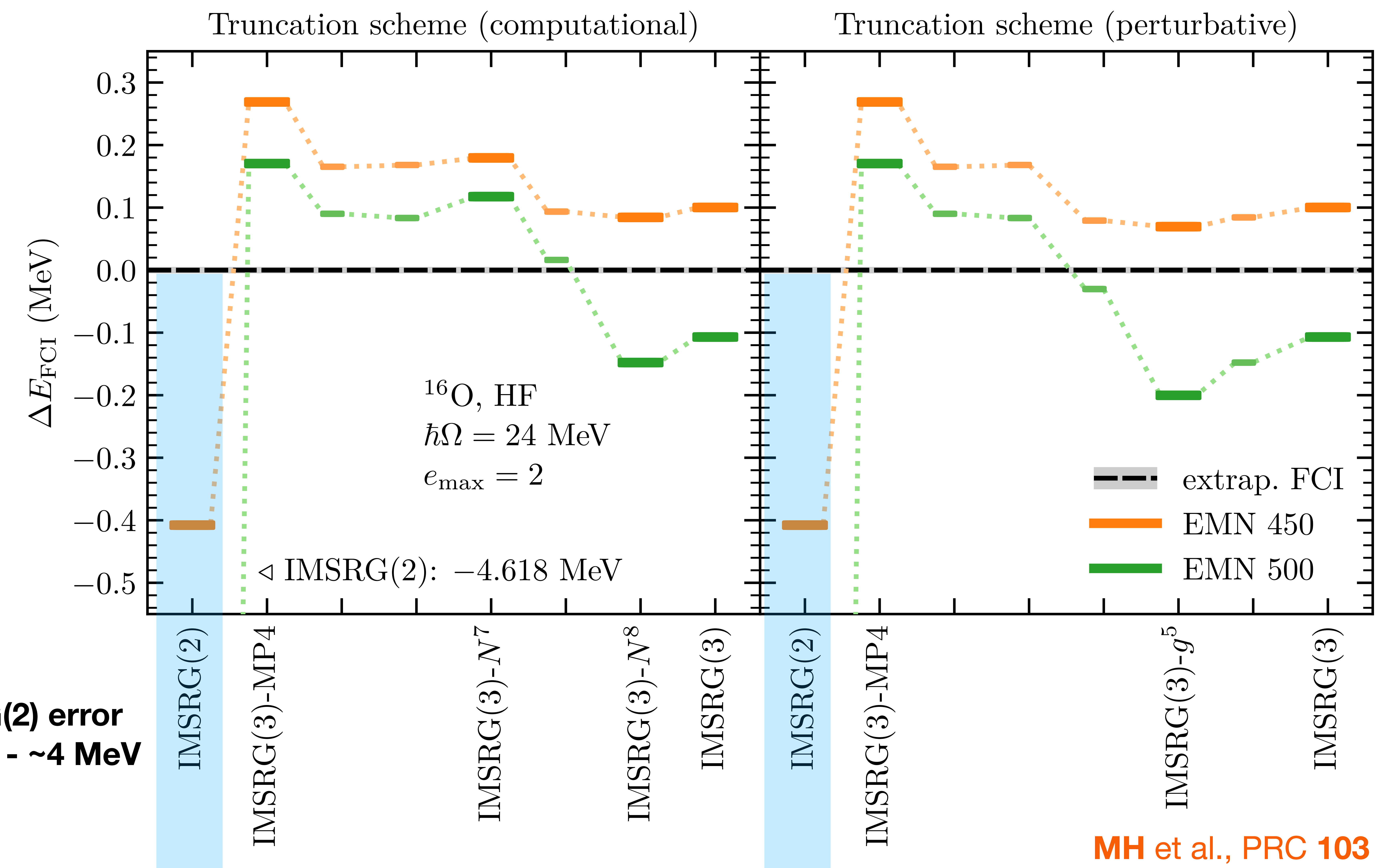


The IMSRG(3) difference



MH et al., PRC **103** (2021)

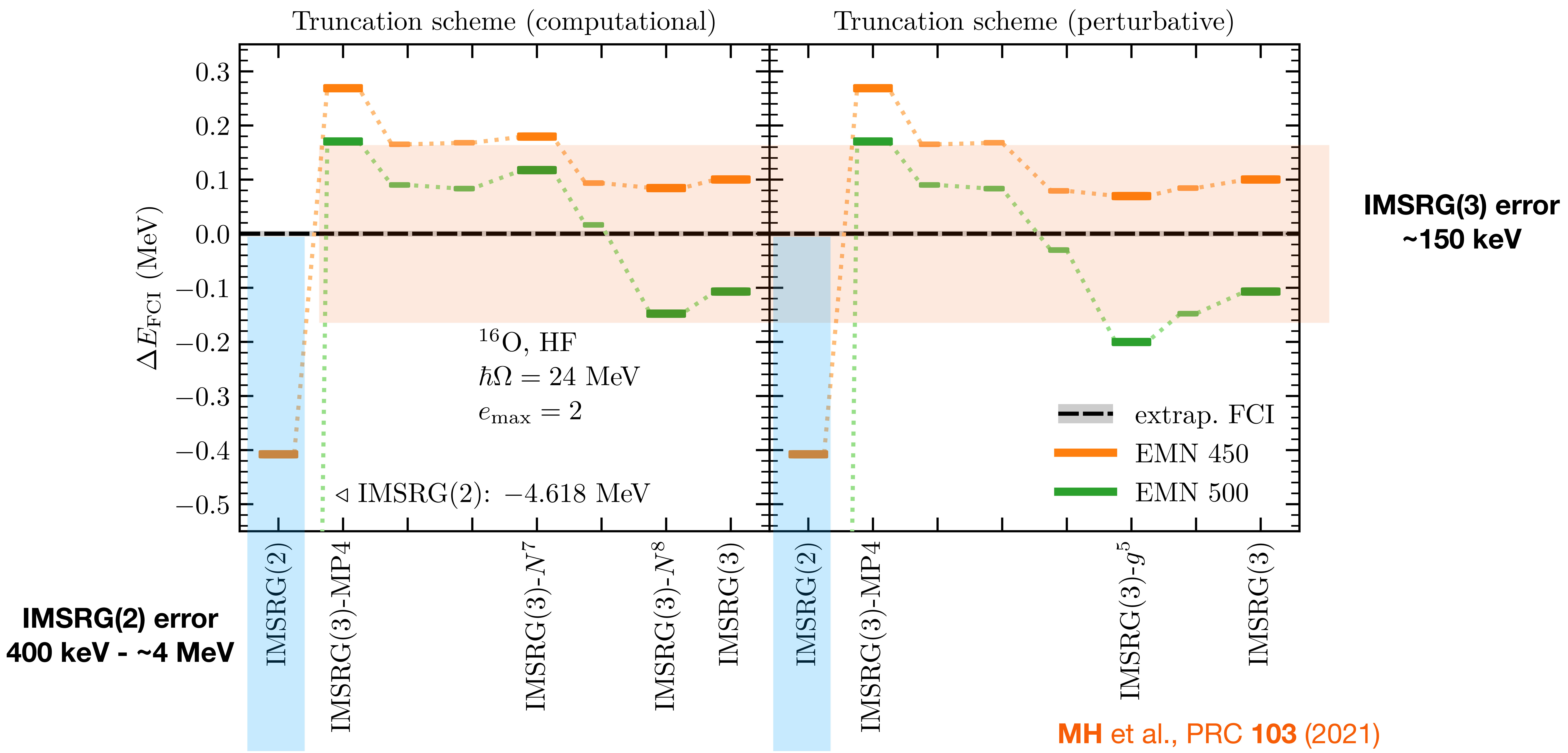
The IMSRG(3) difference



IMSRG(2) error
400 keV - ~4 MeV

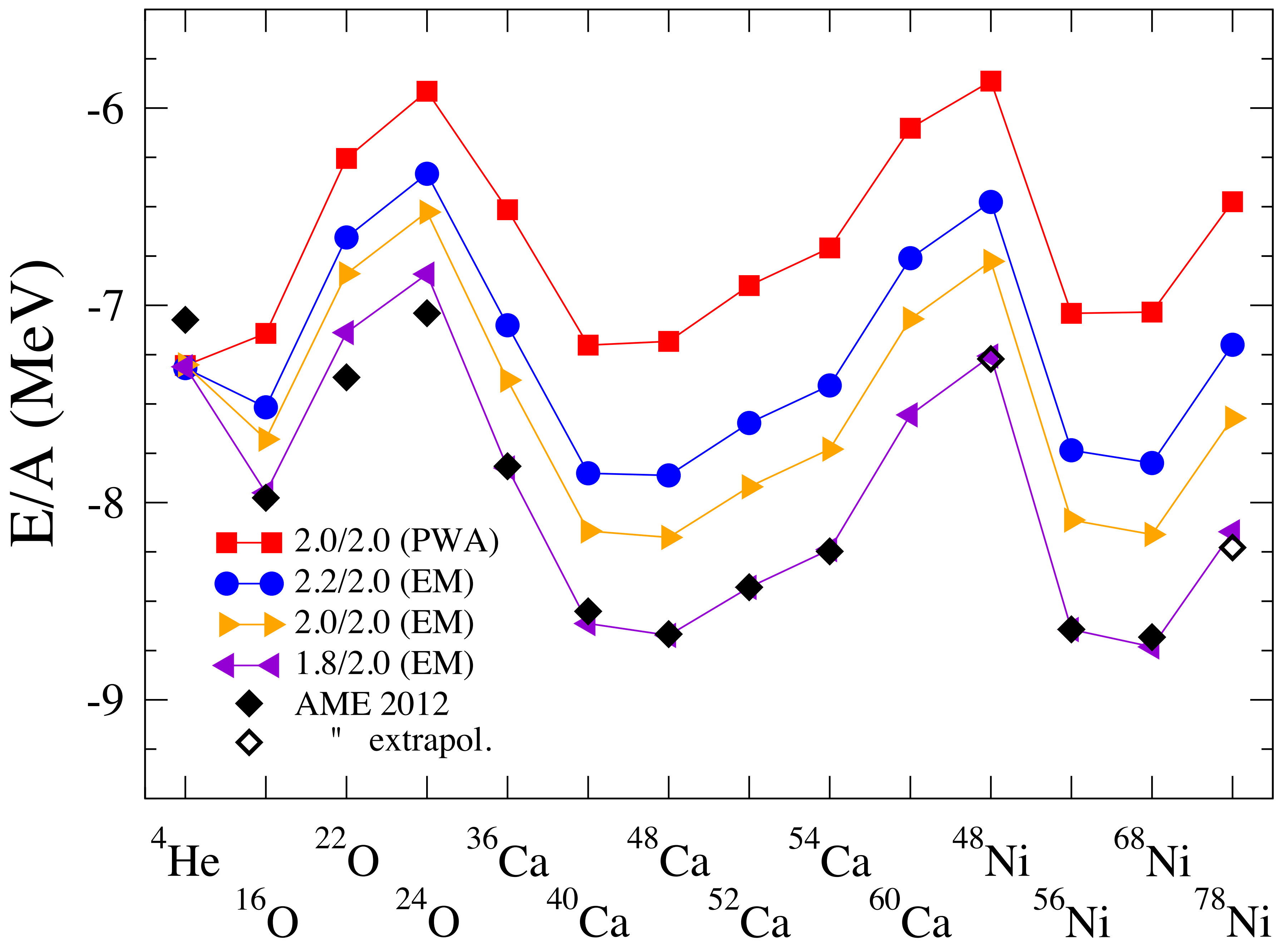
MH et al., PRC **103** (2021)

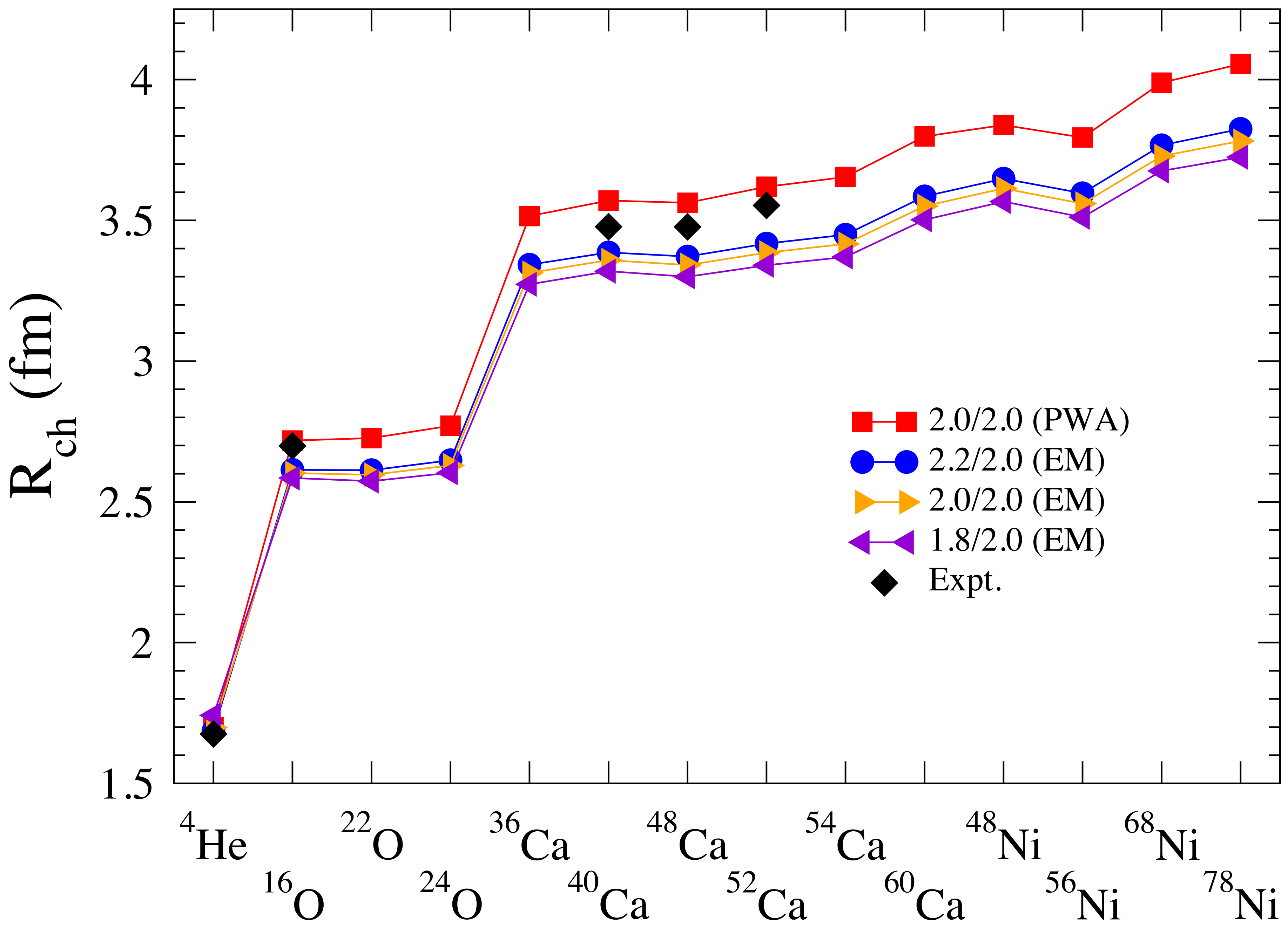
The IMSRG(3) difference



MH et al., PRC **103** (2021)

Challenge: Energies and radii

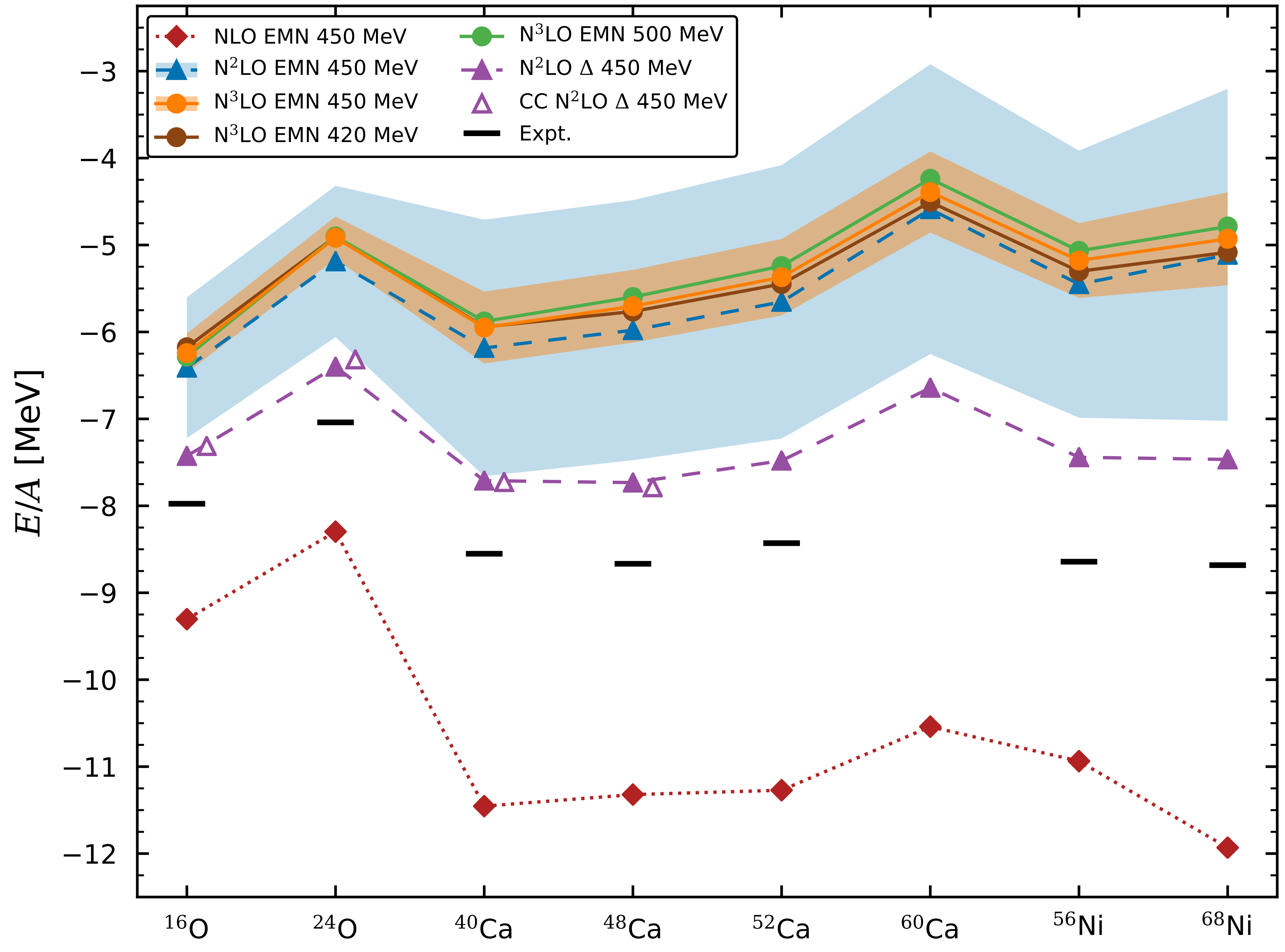


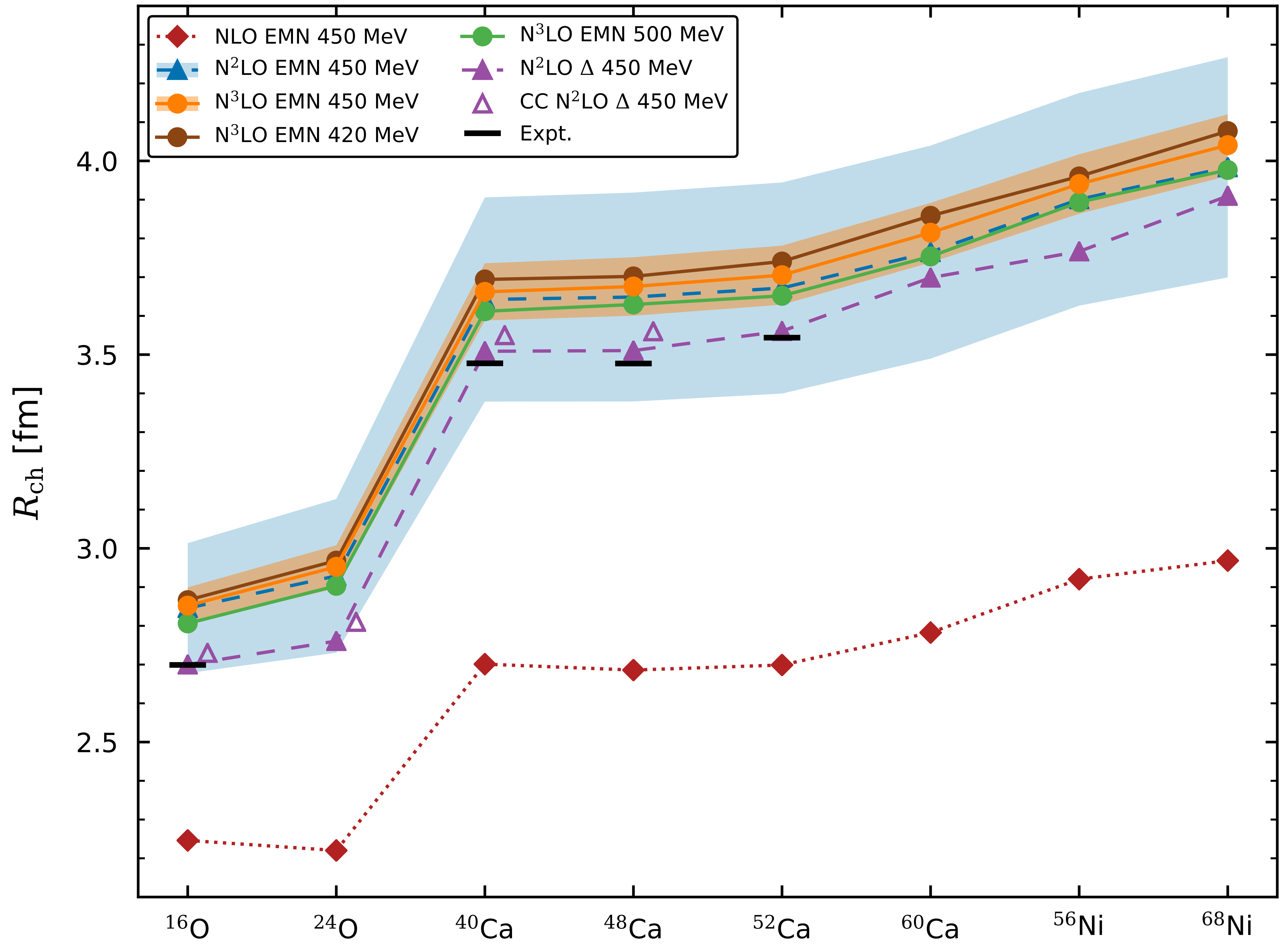


Simonis et al., PRC **96** (2017)

Accurate binding energies lead to underpredicted radii!

Challenge: Energies and radii





Hoppe et al., PRC **100** (2019)

Accurate radii lead to underpredicted binding energies!

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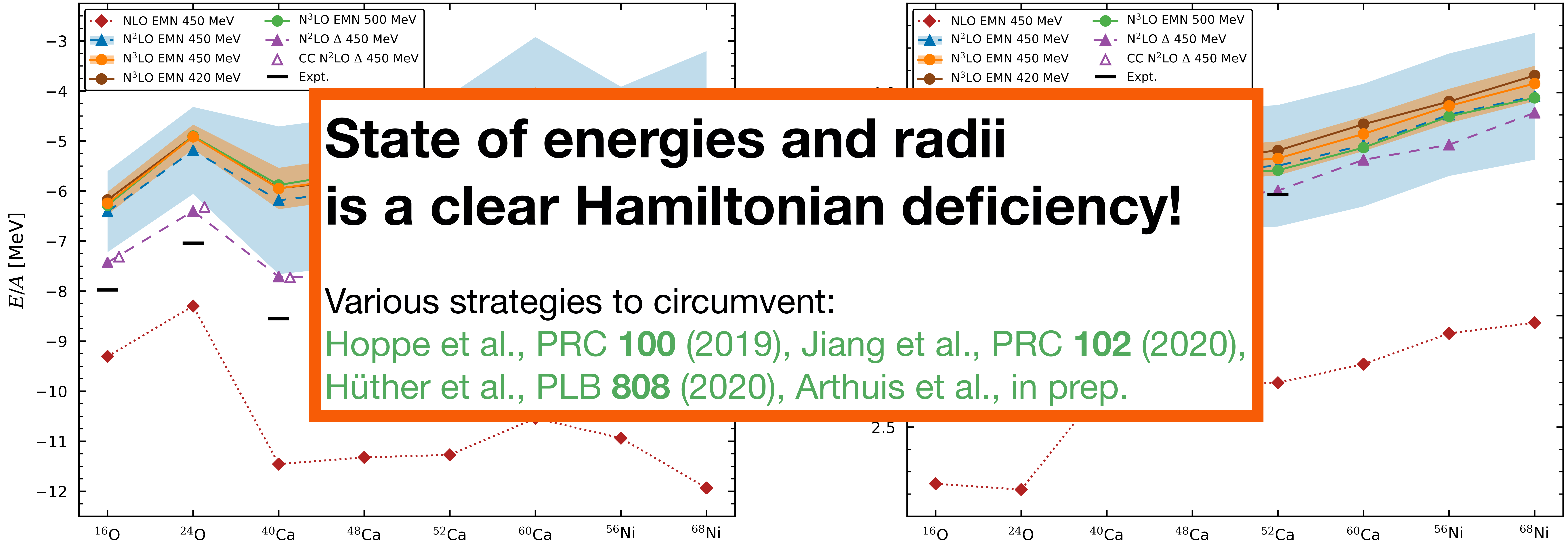


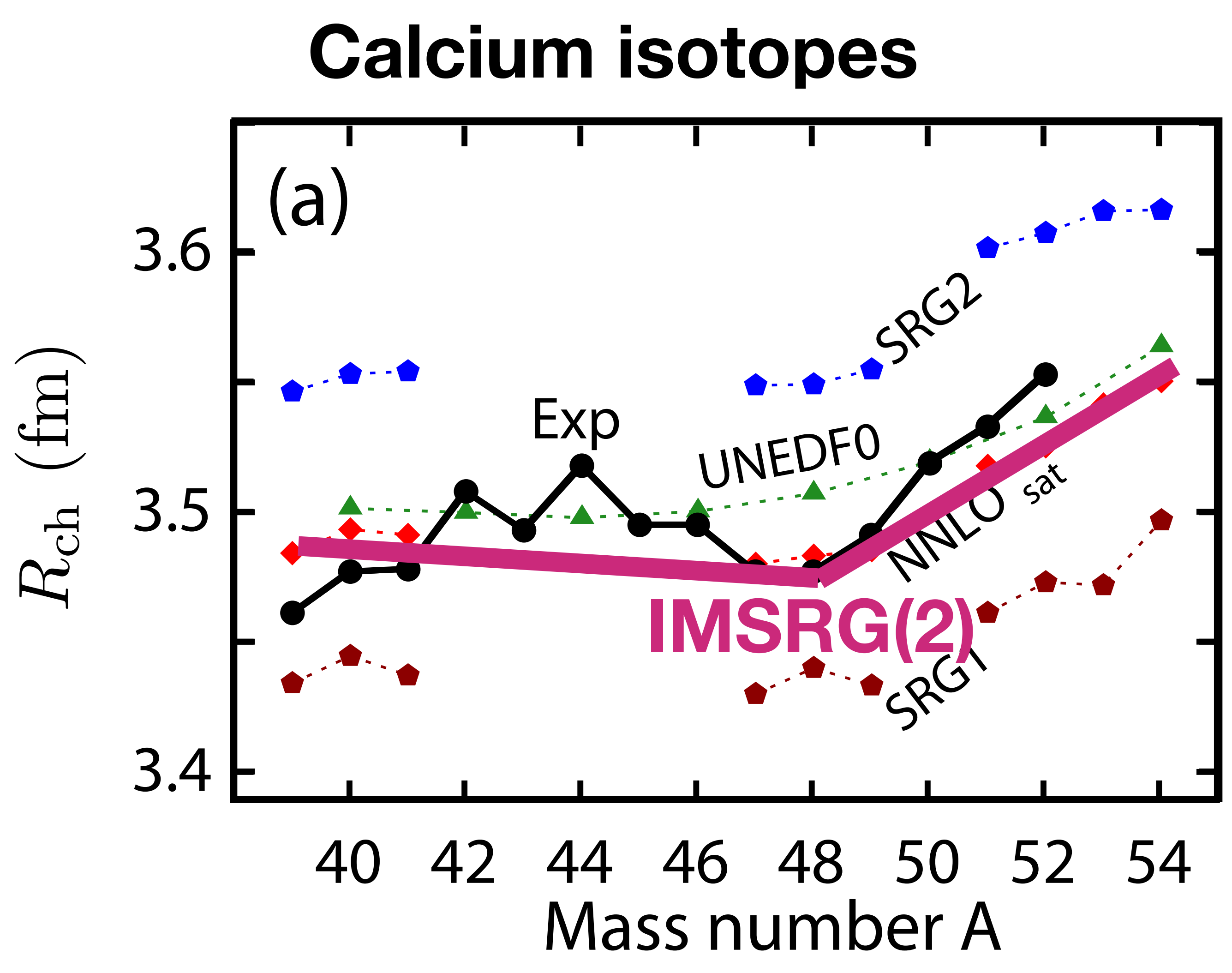
State of energies and radii is a clear Hamiltonian deficiency!

Various strategies to circumvent:
Hoppe et al., PRC **100** (2019), Jiang et al., PRC **102** (2020), Hüther et al., PLB **808** (2020), Arthuis et al., in prep.

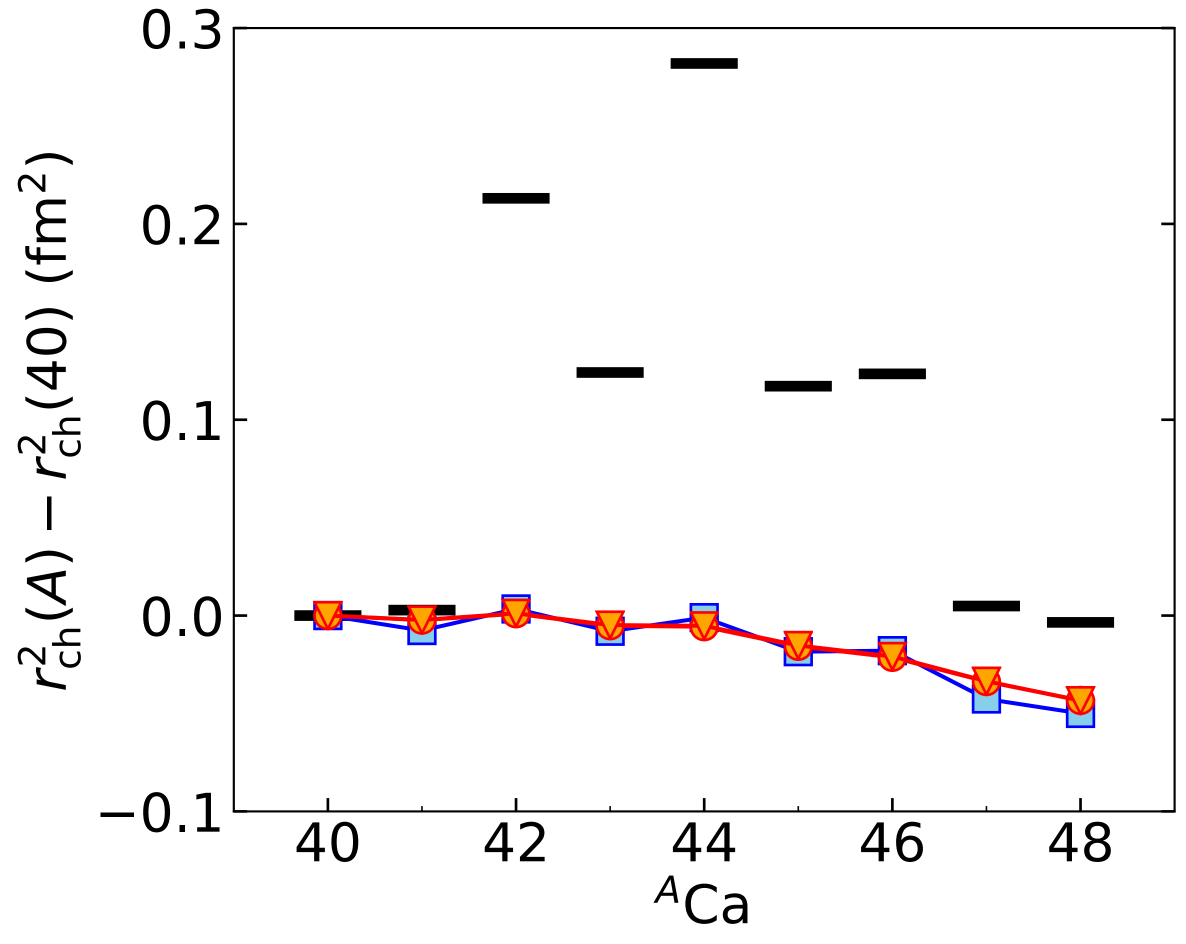
Hoppe et al., PRC **100** (2019)

Accurate radii lead to underpredicted binding energies!

Challenge: Charge radii in Ni and Ca



Garcia Ruiz et al., Nature Physics **12** (2016)



Miyagi et al., PRC **102** (2020)

- Many-body calculations have trouble reproducing
  - R_{ch} parabola between ^{40}Ca and ^{48}Ca
  - Steep increase in R_{ch} after ^{48}Ca
- Unclear whether Hamiltonian or many-body error
- Similar trend observed in nickel isotopes

  Sommer et al., PRL **129** (2022)