# Medium-Mass Nuclei from the In-Medium SRG

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THE OHIO STATE UNIVERSITY

# Outline

- Similarity Renormalization Group
- In-Medium SRG for Closed-Shell Nuclei
- Open-Shell Nuclei from the Multi-Reference IM-SRG
- Outlook

# Similarity Renormalization Group

**Review:**

S. Bogner, R. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65** (2010), 94

E. Anderson, S. Bogner, R. Furnstahl, and R. Perry, Phys. Rev. **C82** (2011), 054001

E. Jurgenson, P. Navratil, and R. Furnstahl, Phys. Rev. **C83** (2011), 034301

R. Roth, S. Reinhardt, and H. H., Phys. Rev. **C77** (2008), 064003

H. H. and R. Roth, Phys. Rev. **C75** (2007), 051001

# Similarity Renormalization Group

## Basic Concept

continuous unitary transformation of the Hamiltonian to band-diagonal form w.r.t. a given "uncorrelated" many-body basis

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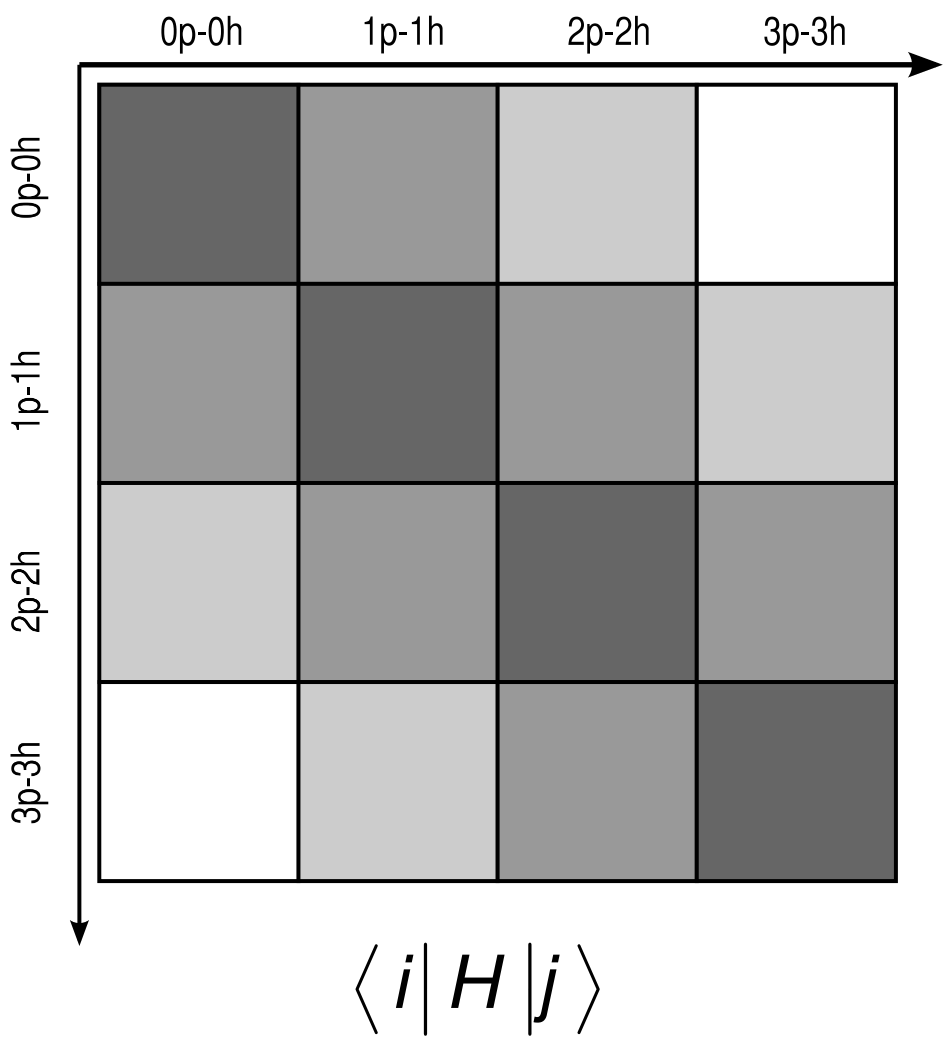
- choose $\eta(s)$ to achieve desired behavior, e.g. decoupling of momentum or energy scales

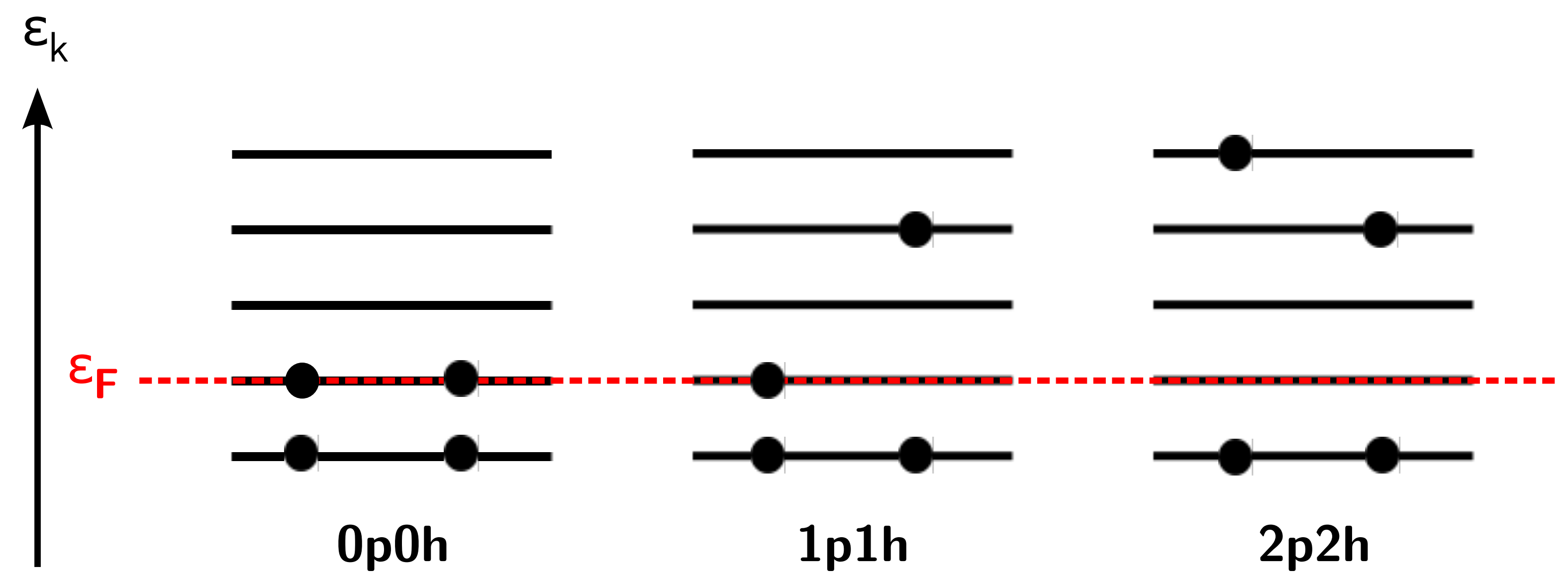
- consistently evolve observables of interest

# In-Medium SRG for Closed-Shell Nuclei

H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013)
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011)

# Decoupling in A-Body Space



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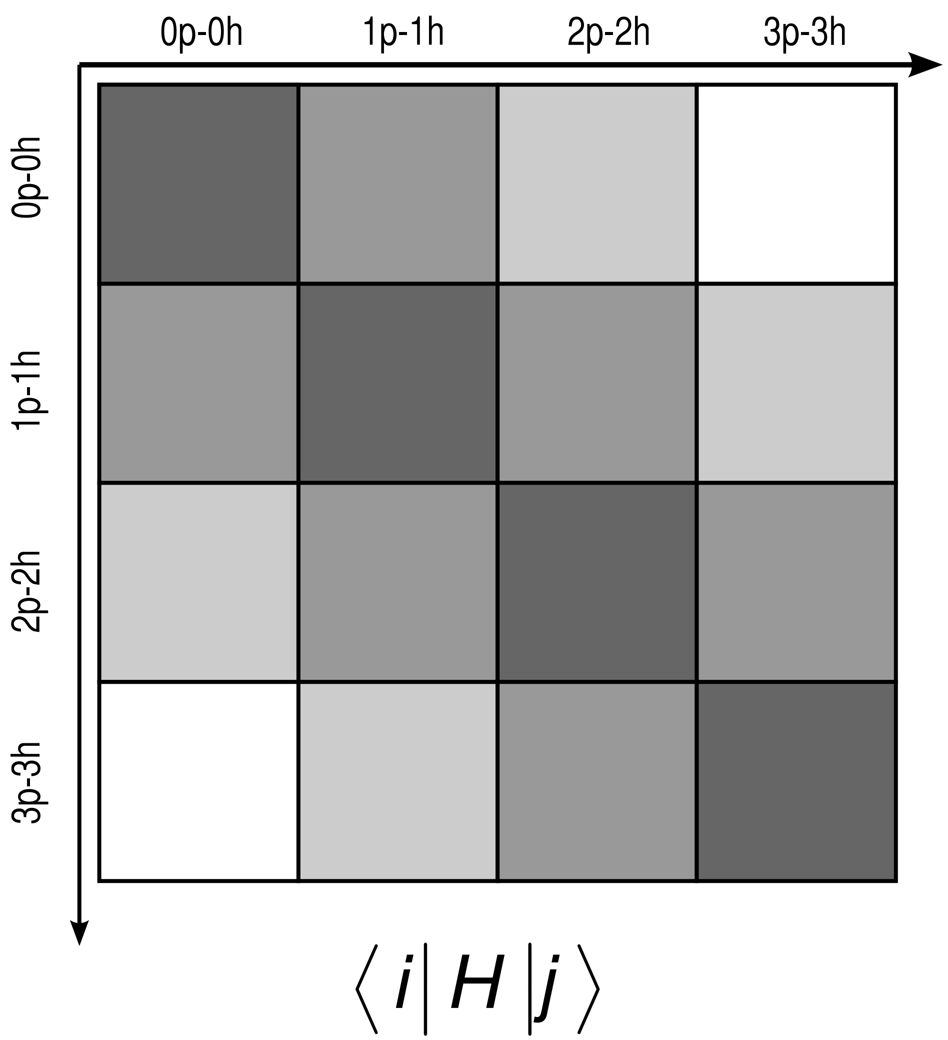


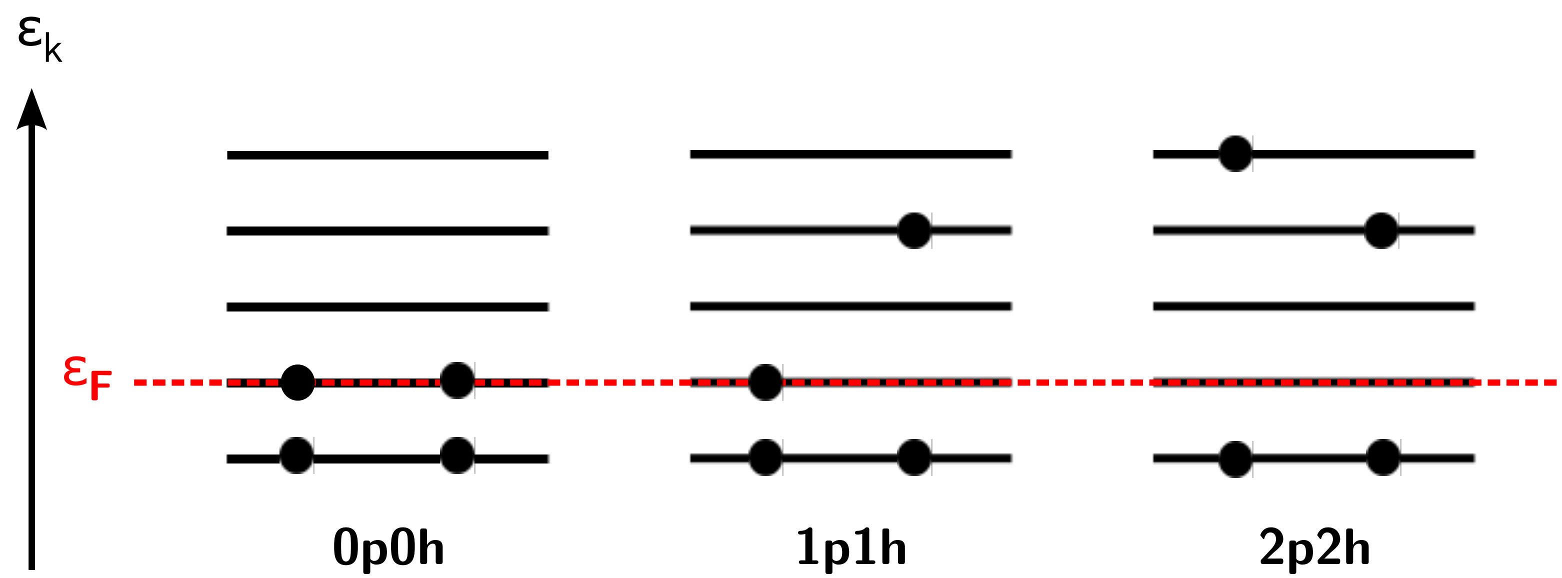


excitations relative to reference state:
→ normal-ordering

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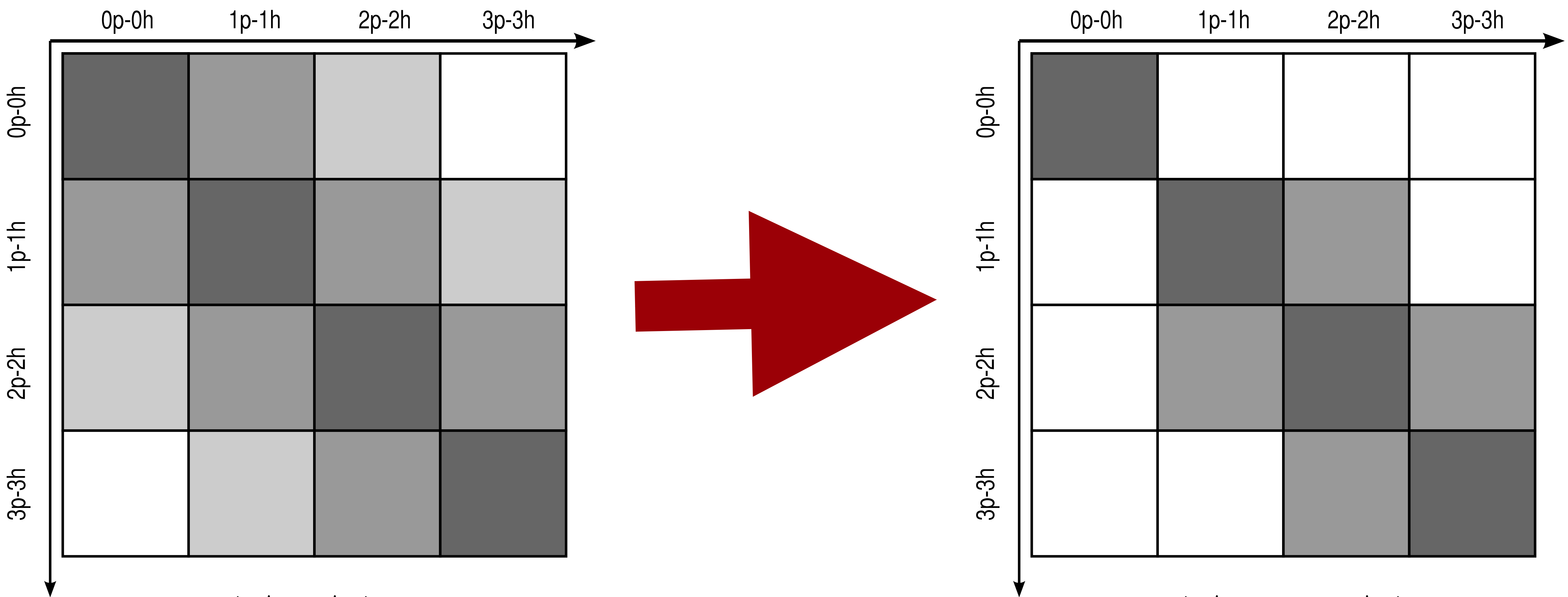


$\langle i | H | j \rangle$ $\qquad$ $\langle i | H(\infty) | j \rangle$

aim: decouple reference state $|\Phi\rangle$ (0p-0h) from excitations

# Normal Ordering

- second quantization: $A^{k_1 \ldots k_N}_{l_1 \ldots l_N} = a^{\dagger}_{k_1} \ldots a^{\dagger}_{k_N} a_{l_N} \ldots a_{l_1}$

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- Wick's theorem gives simplified expansions (fewer terms!) for products of normal-ordered operators

# Normal-Ordered Hamiltonian

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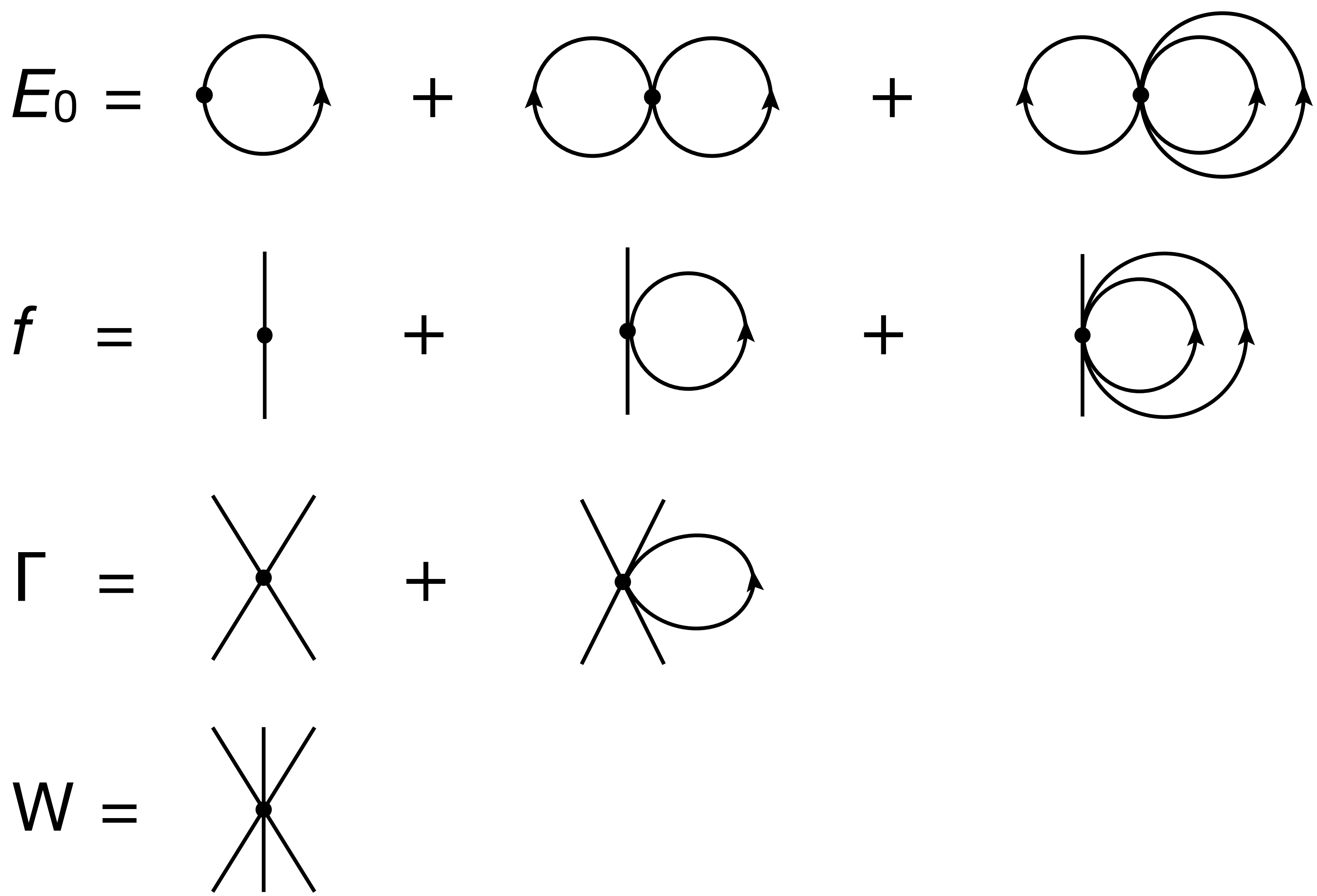
$$H = E_0 + \sum_{kl} f^k_l :A^k_l: + \frac{1}{4}\sum_{klmn} \Gamma^{kl}_{mn} :A^{kl}_{mn}: + \frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn} :A^{ijk}_{lmn}:$$



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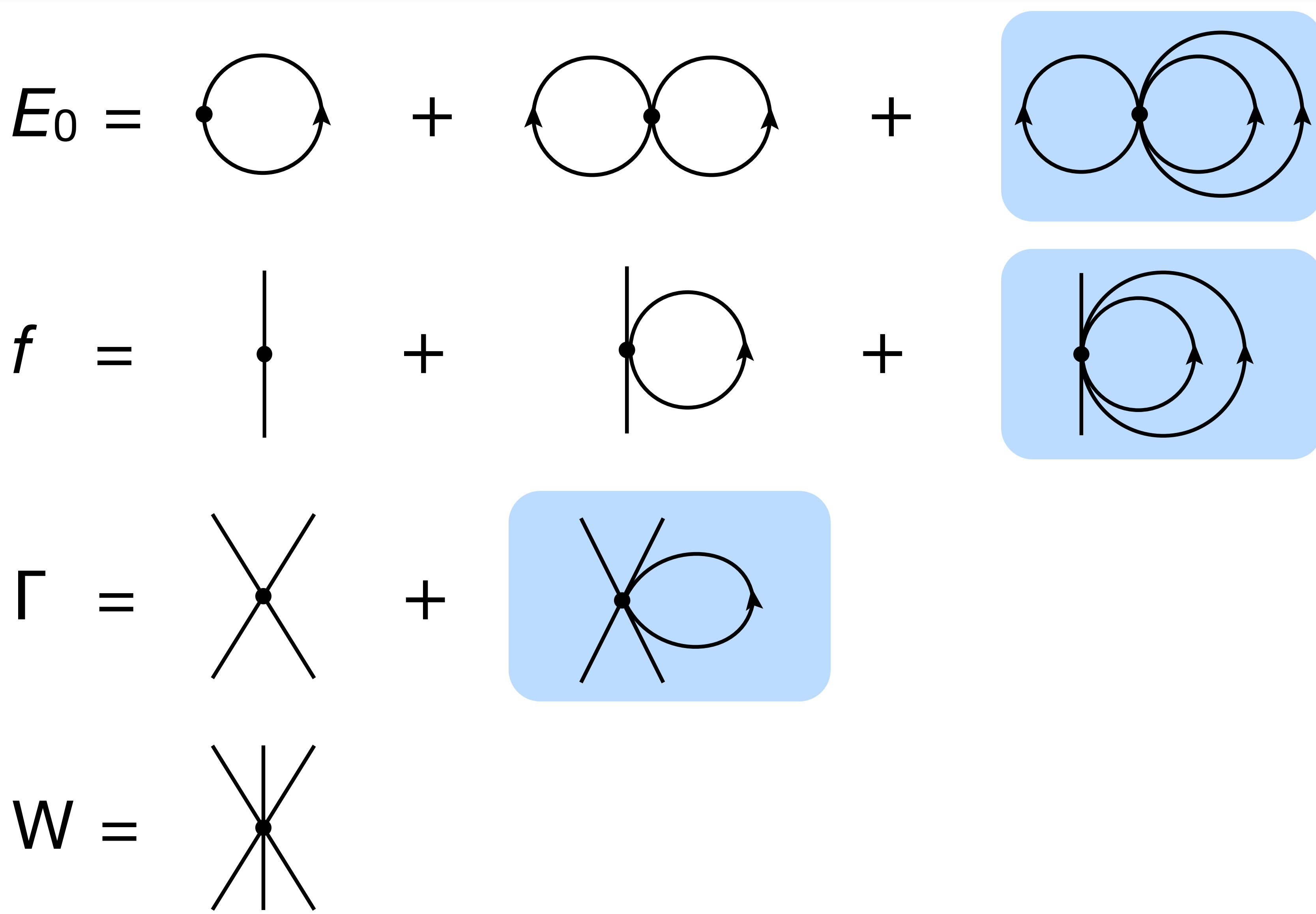

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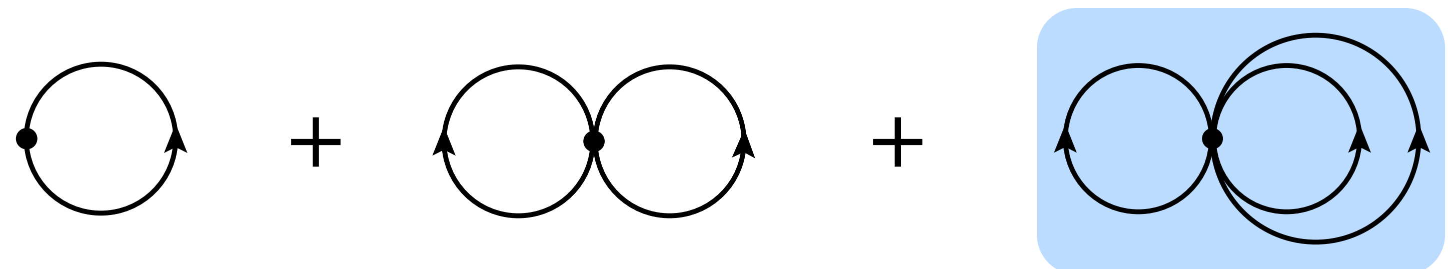
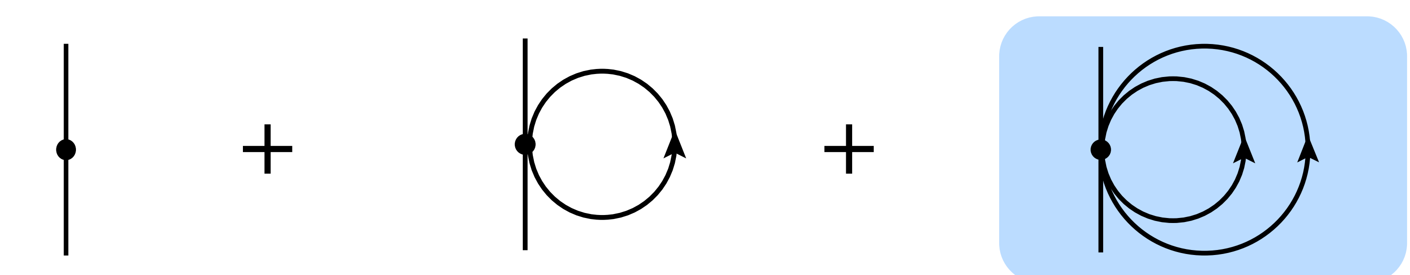
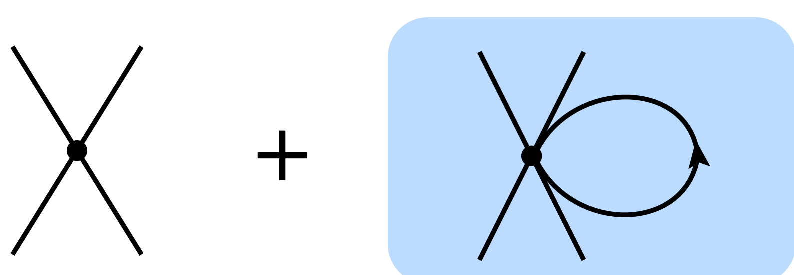
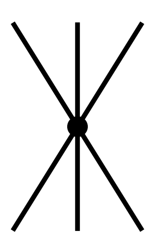
$E_0 =$ 

$f =$ 

$\Gamma =$ 

$W =$ 

two-body formalism with in-medium contributions from three-body interactions

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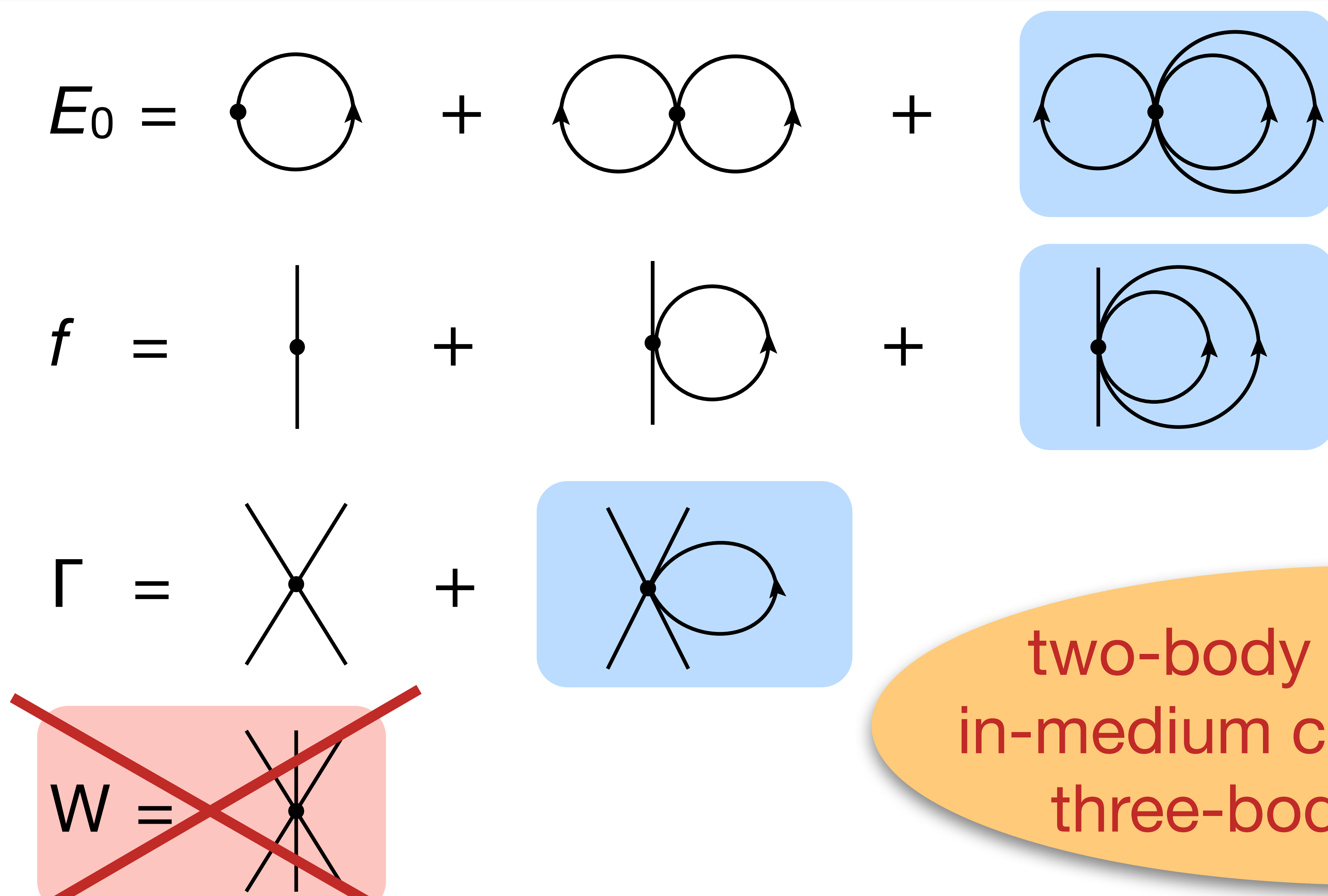


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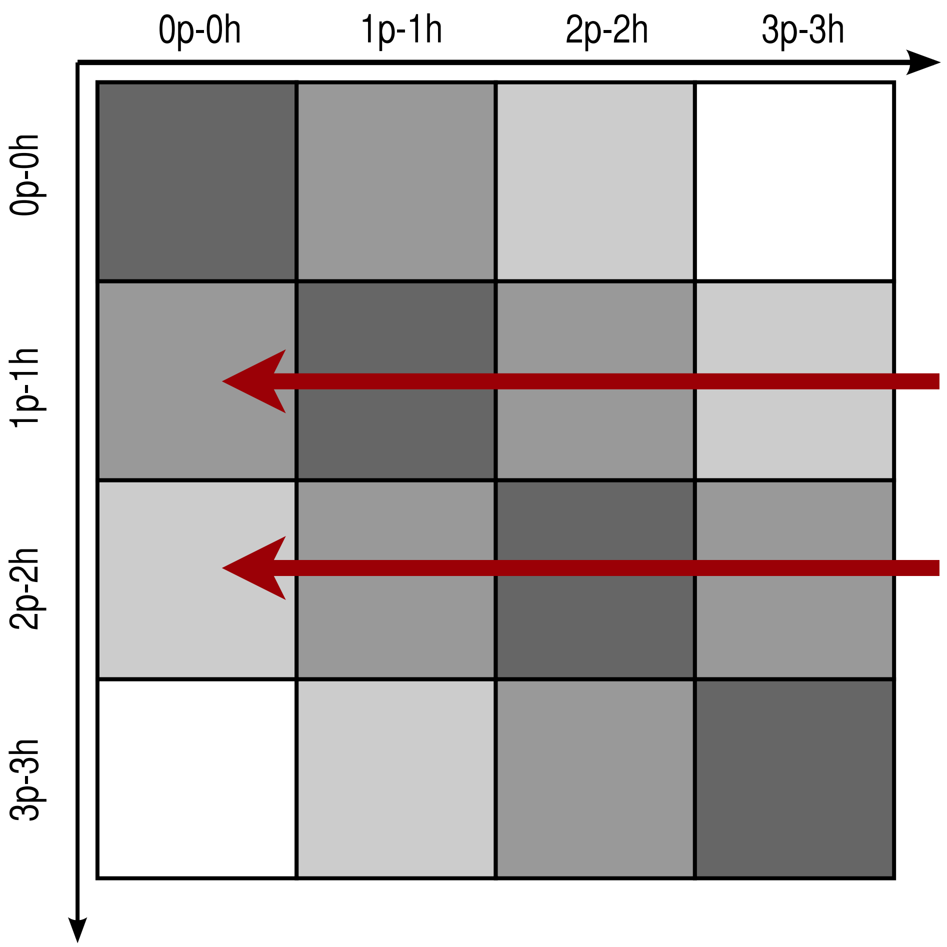
# Choice of Generator




$$\left\langle {}^{p}_{h} \right| H \left| \Psi \right\rangle = \sum_{kl} f^{k}_{l} \left\langle \Psi \right| :A^{h}_{p} :: A^{k}_{l} : \left| \Psi \right\rangle = -n_h \bar{n}_p f^{p}_{h}$$

$$\left\langle {}^{pp'}_{hh'} \right| H \left| \Psi \right\rangle = \sum_{klmn} \Gamma^{kl}_{mn} \left\langle \Psi \right| :A^{hh'}_{pp'} :: A^{kl}_{mn} : \left| \Psi \right\rangle \sim \Gamma^{pp'}_{hh'}$$

## Off-Diagonal Hamiltonian & Generator

$$H^{od} \equiv f^{od} + \Gamma^{od}\,, \quad f^{od} \equiv \sum_{ph} f^{p}_{h} :A^{p}_{h}: + \text{H.c.}\,, \quad \Gamma^{od} \equiv \sum_{pp'hh'} \Gamma^{pp'}_{hh'} :A^{pp'}_{hh'}: + \text{H.c.}$$

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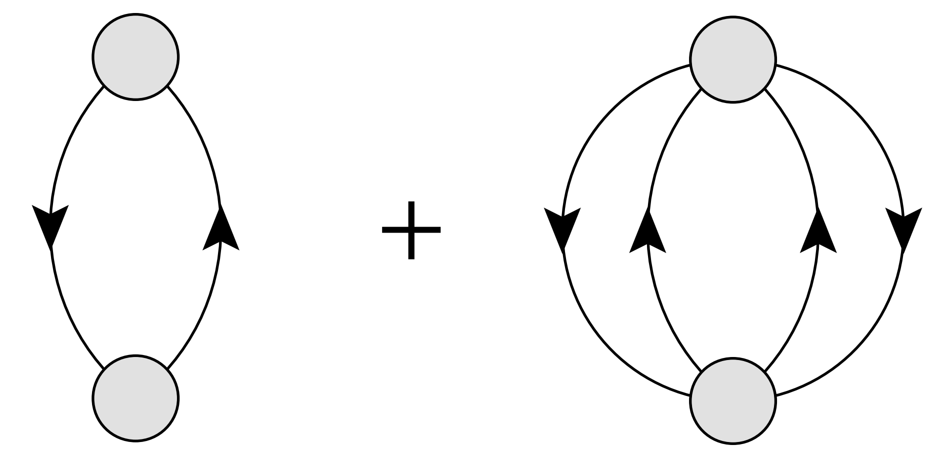
- off-diagonal matrix elements are suppressed like $e^{-\Delta^2 s}$ (Wegner), $e^{-s}$ (White), and $e^{-|\Delta| s}$ (imaginary time)
- g.s. energies ($s \to \infty$) differ by $\ll 1\%$

# In-Medium SRG Flow Equations

## 0-body Flow

$$\frac{dE}{ds} =$$



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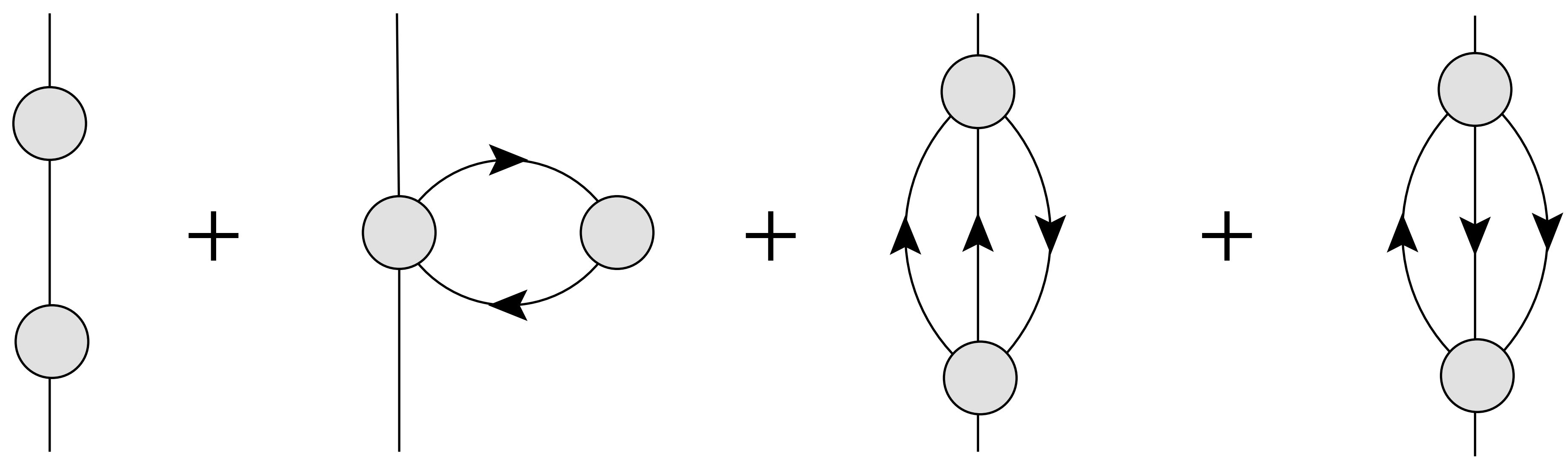

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~ 2nd order MBPT for *H(s)*

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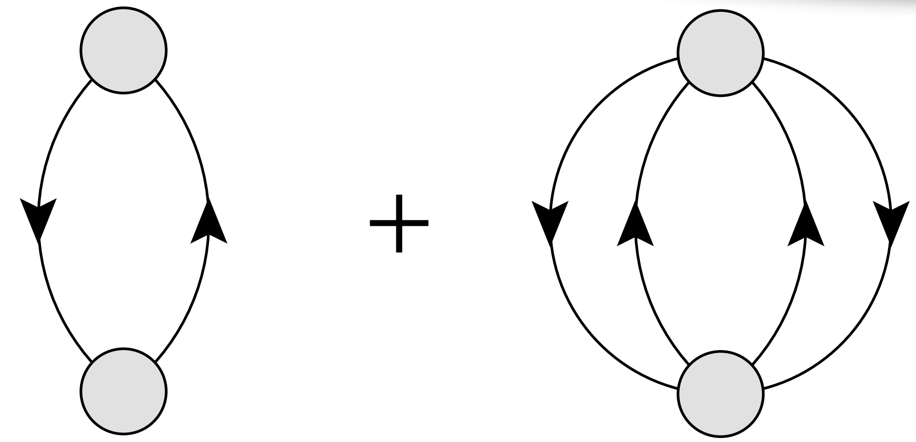

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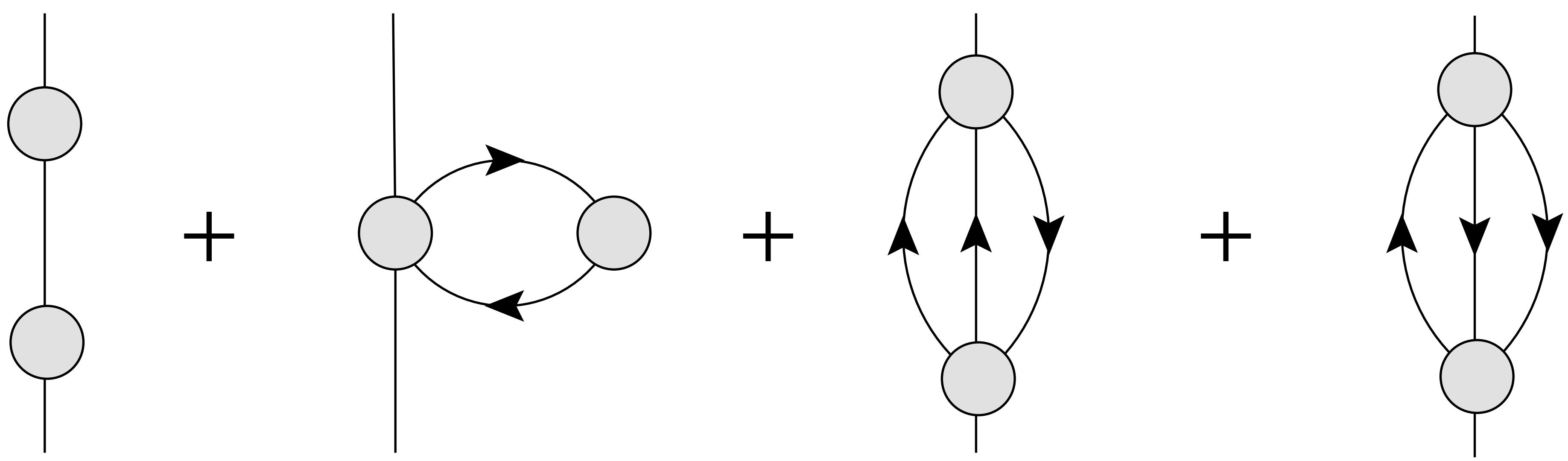

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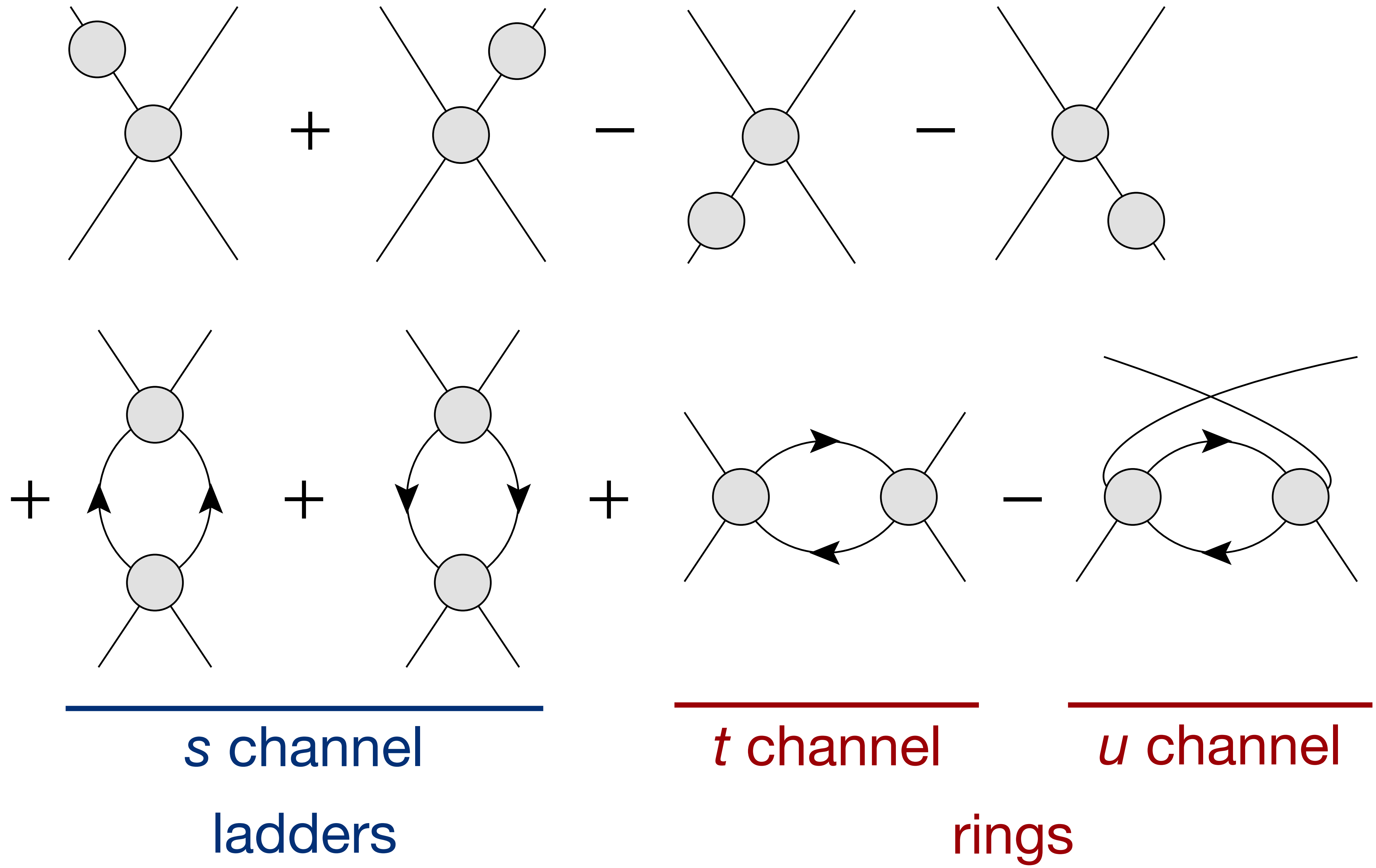

# In-Medium SRG Flow Equations

## 2-body Flow

O(N$^6$) scaling
(before particle/hole distinction)

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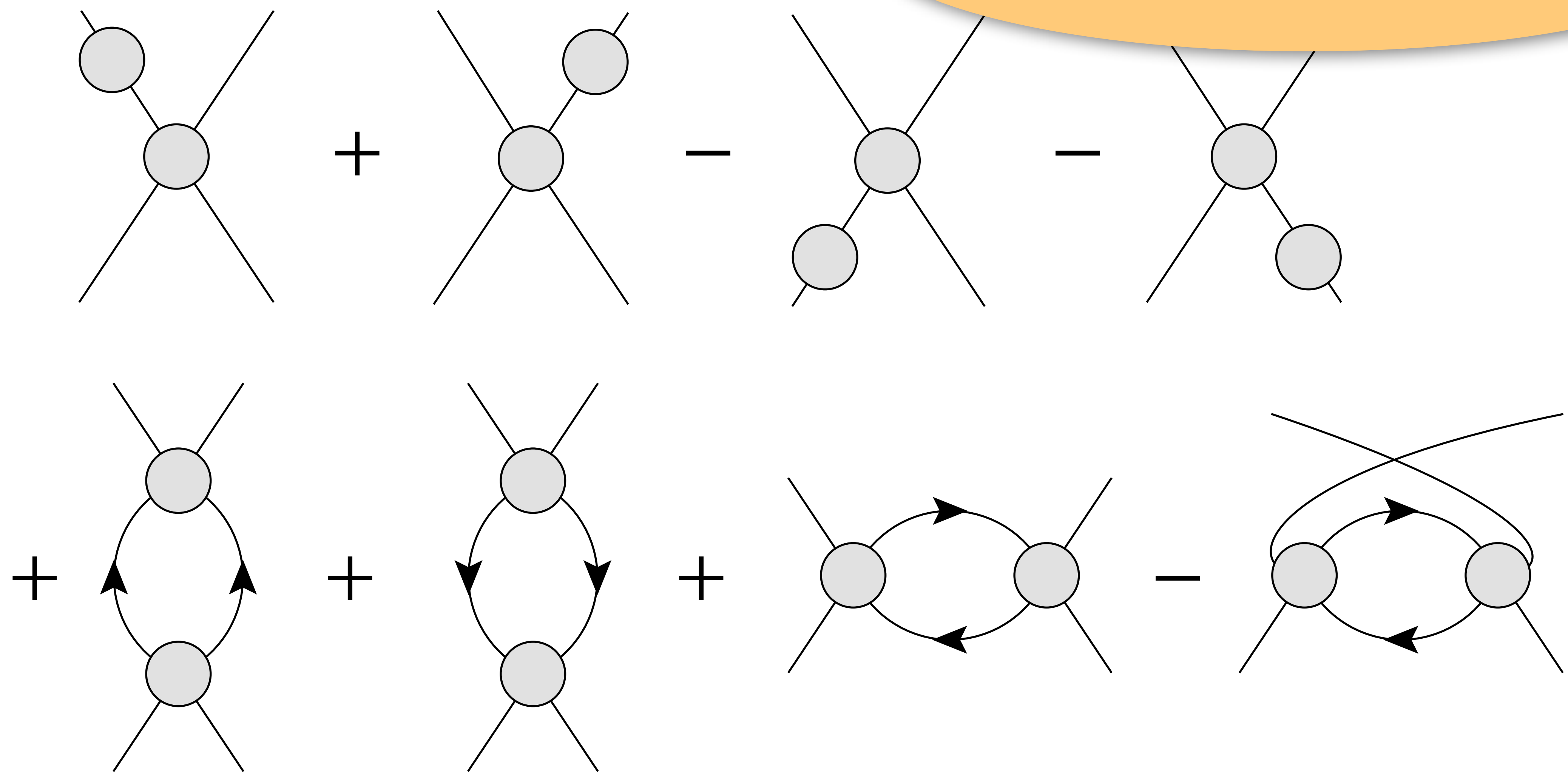


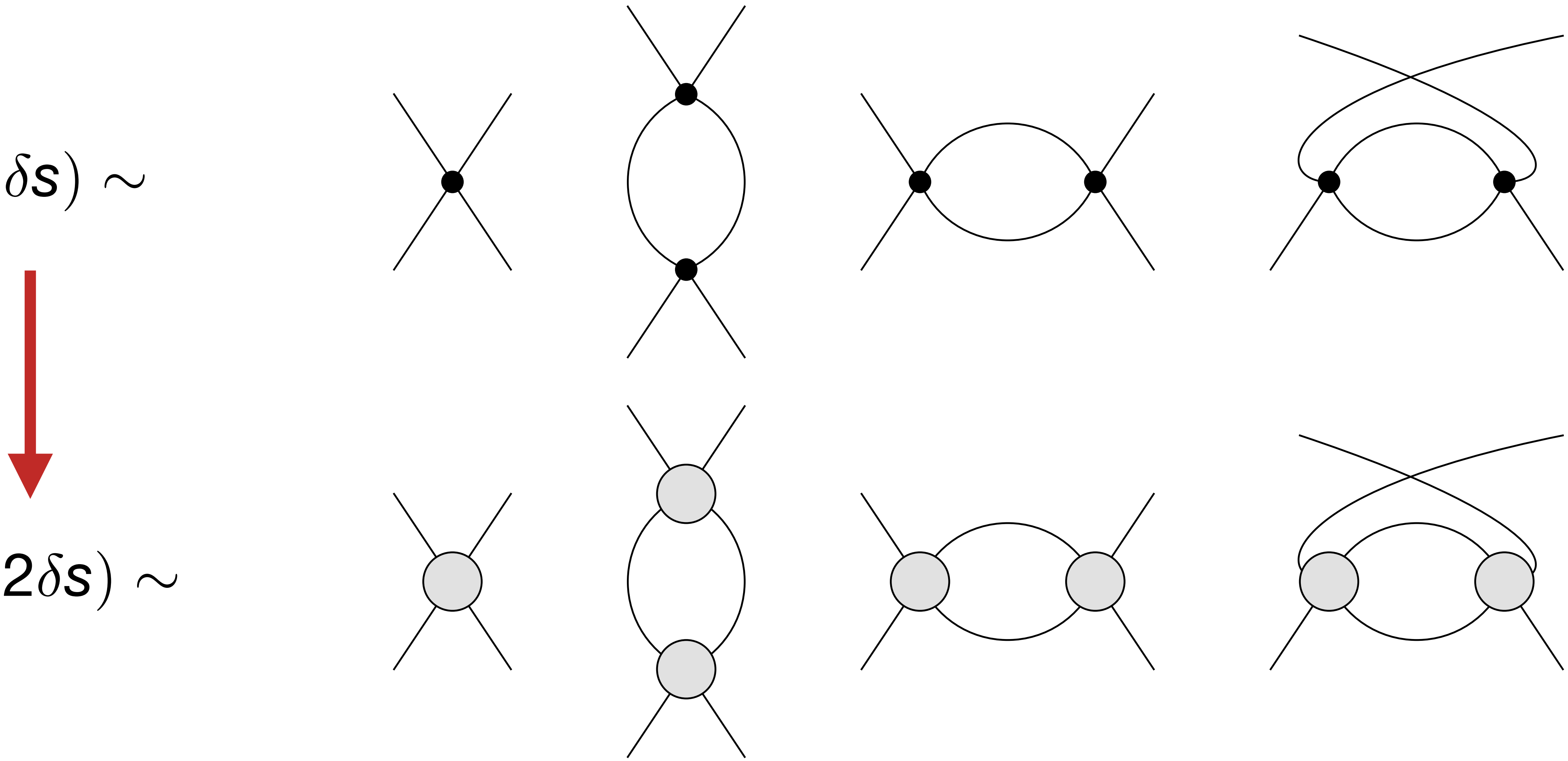
*s* channel — ladders

*t* channel, *u* channel — rings

# In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

$\Gamma(2\delta s) \sim$



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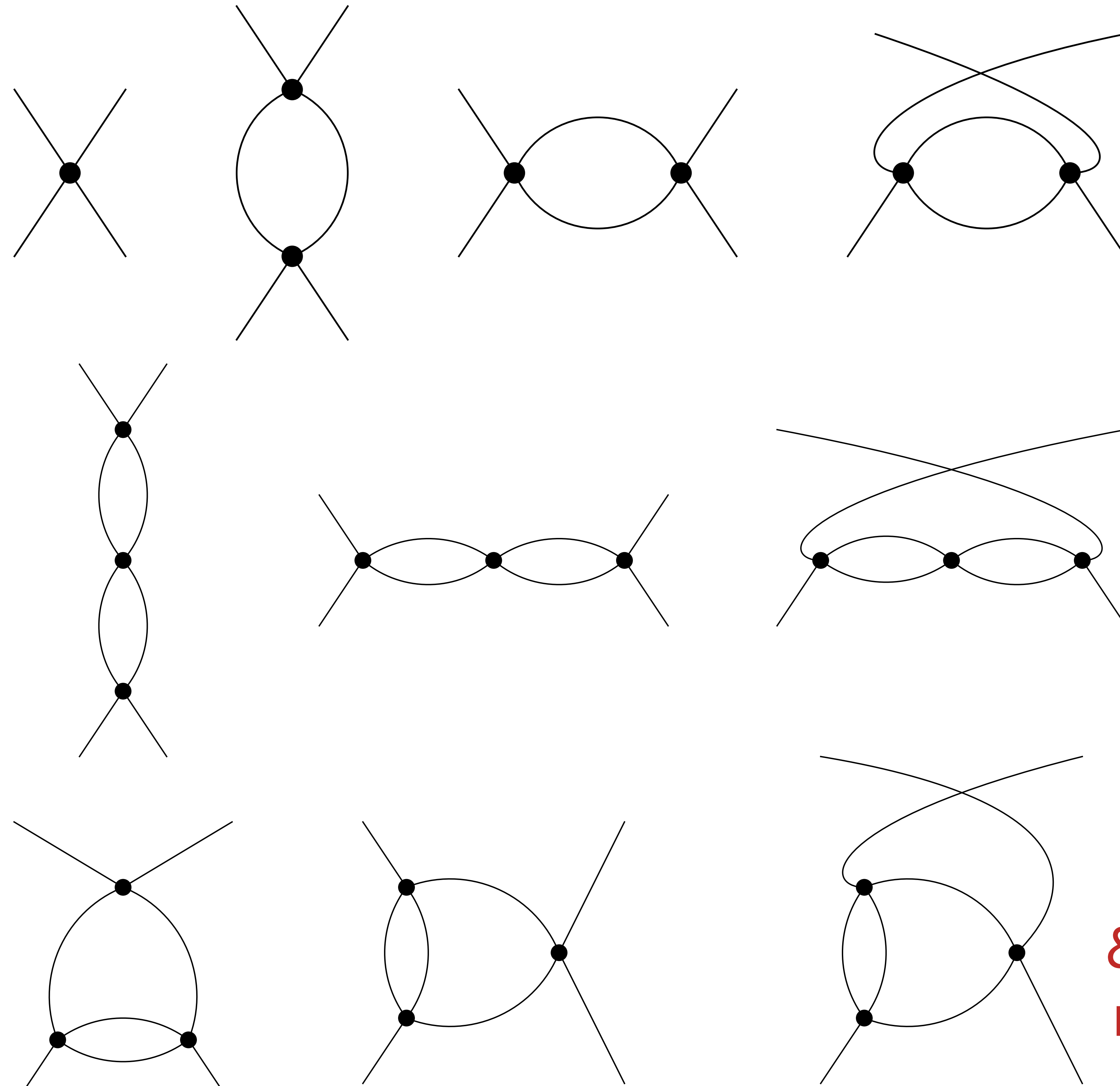

& many more...

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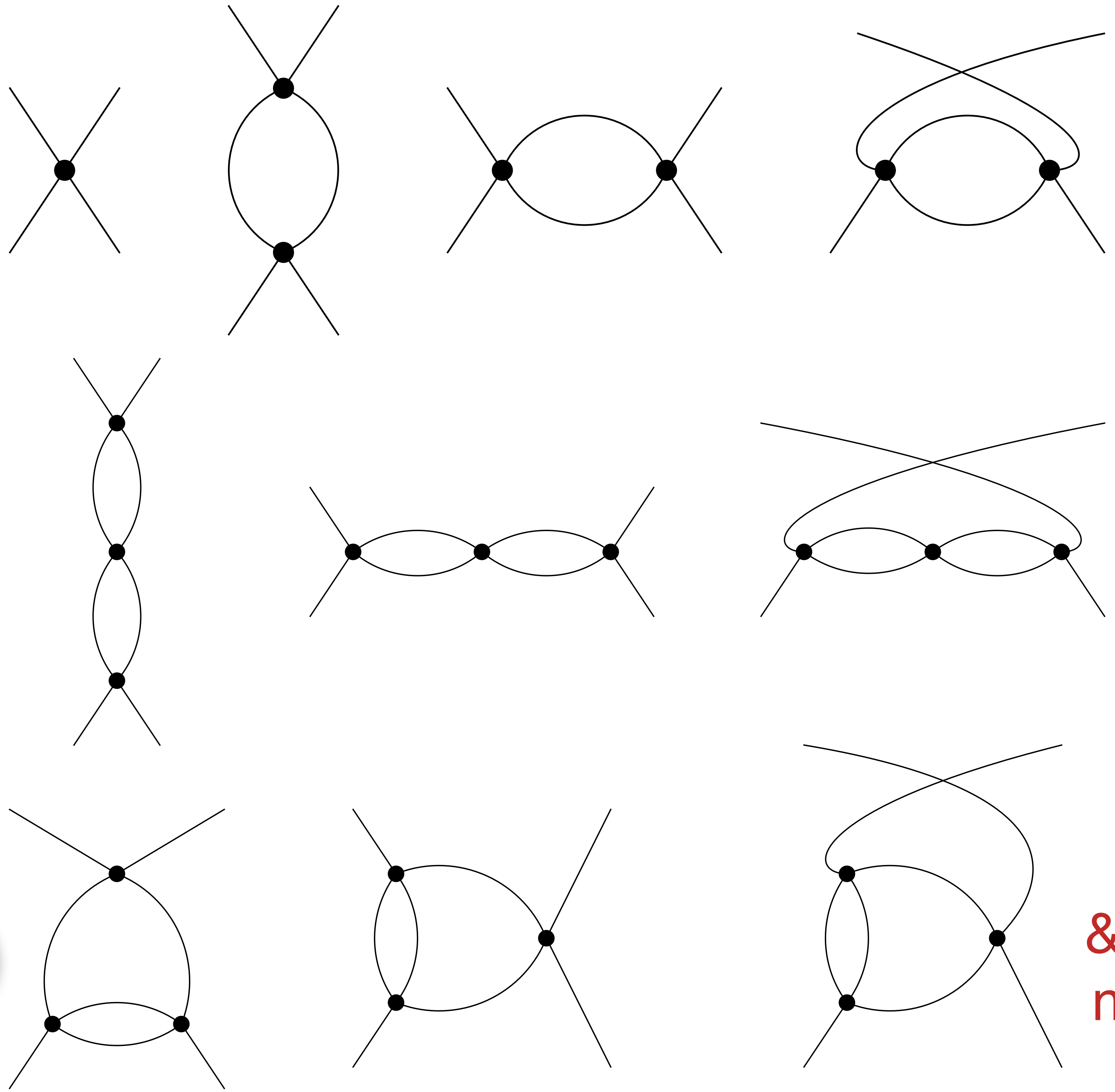

non-perturbative resummation

& many more...

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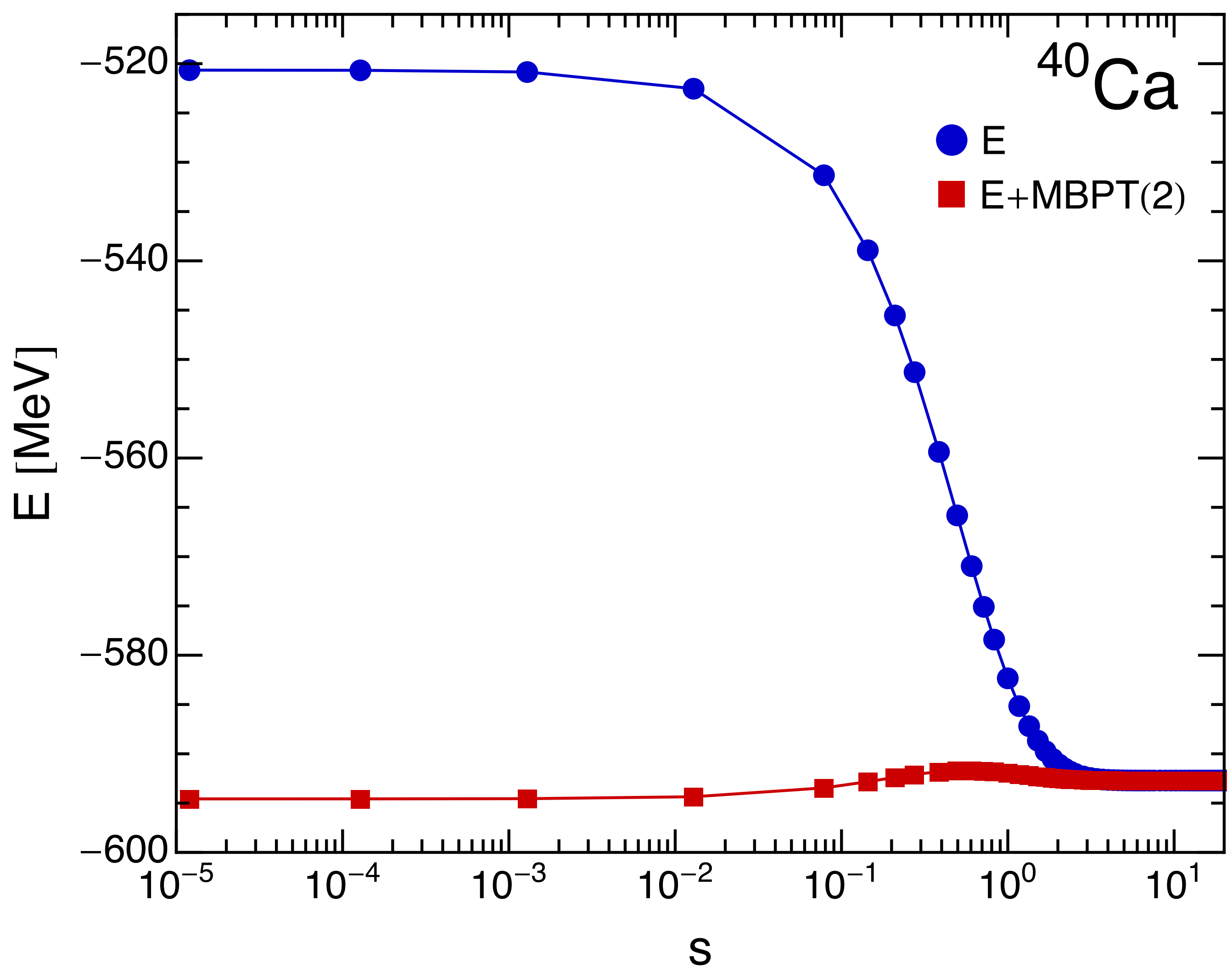


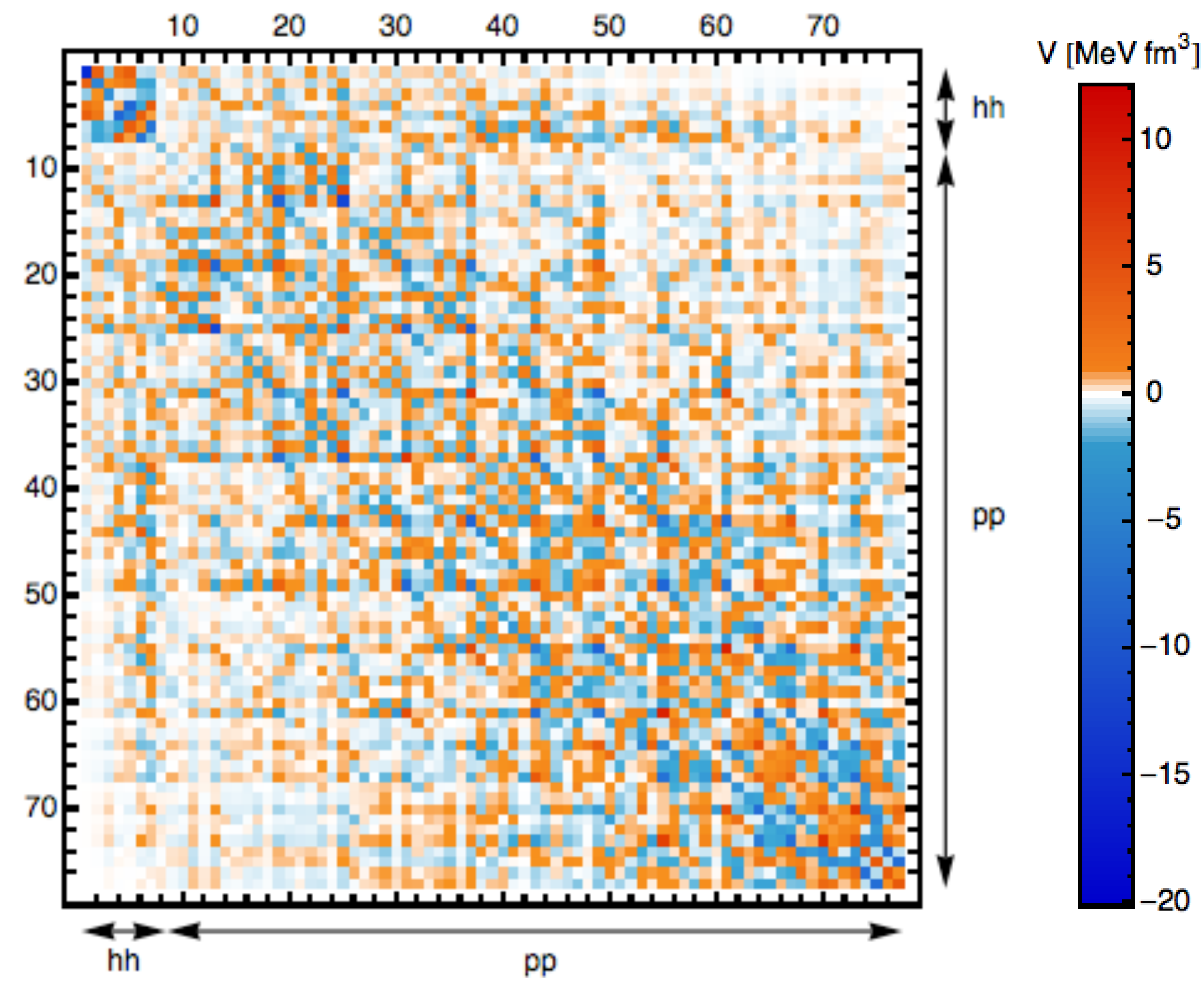


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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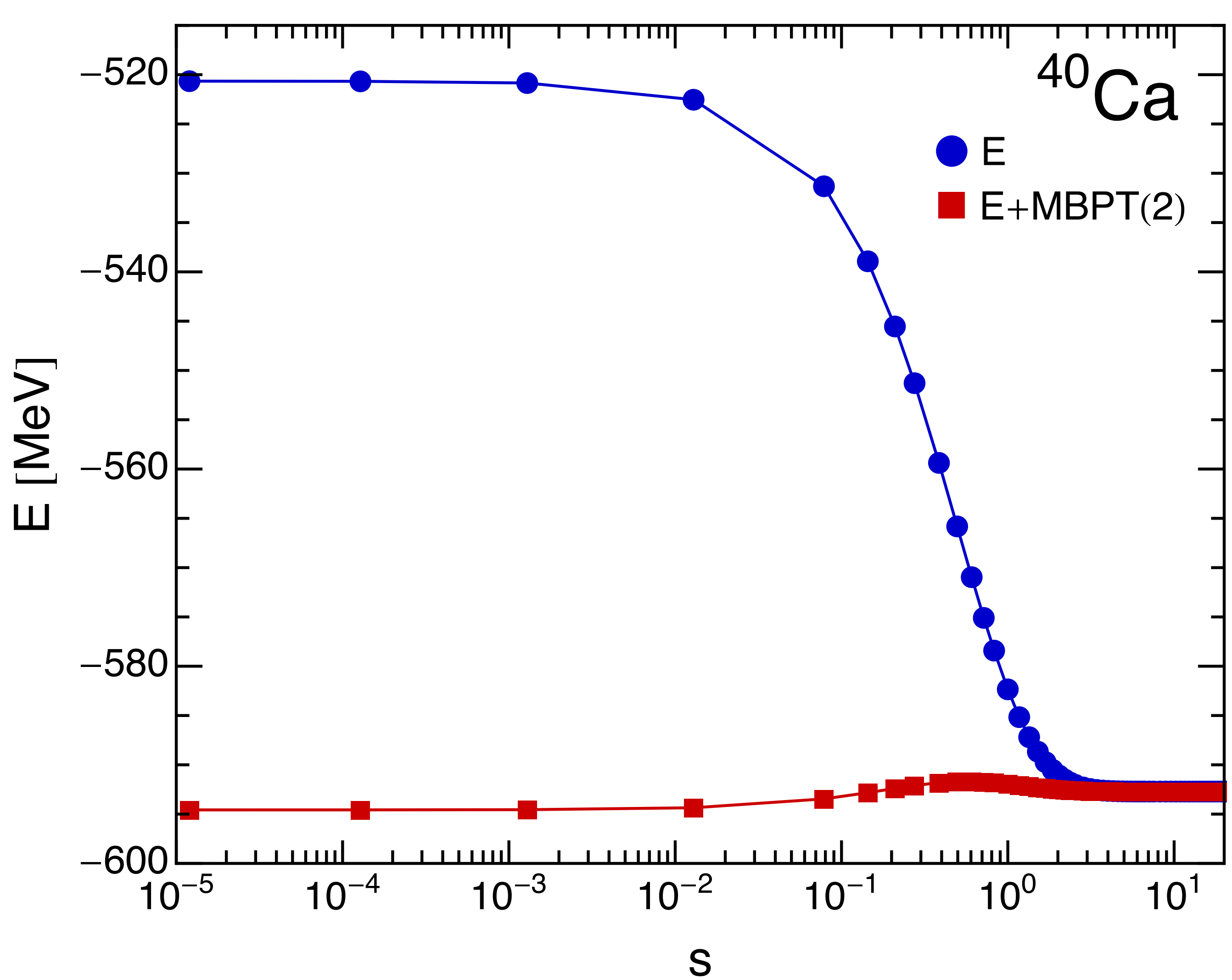


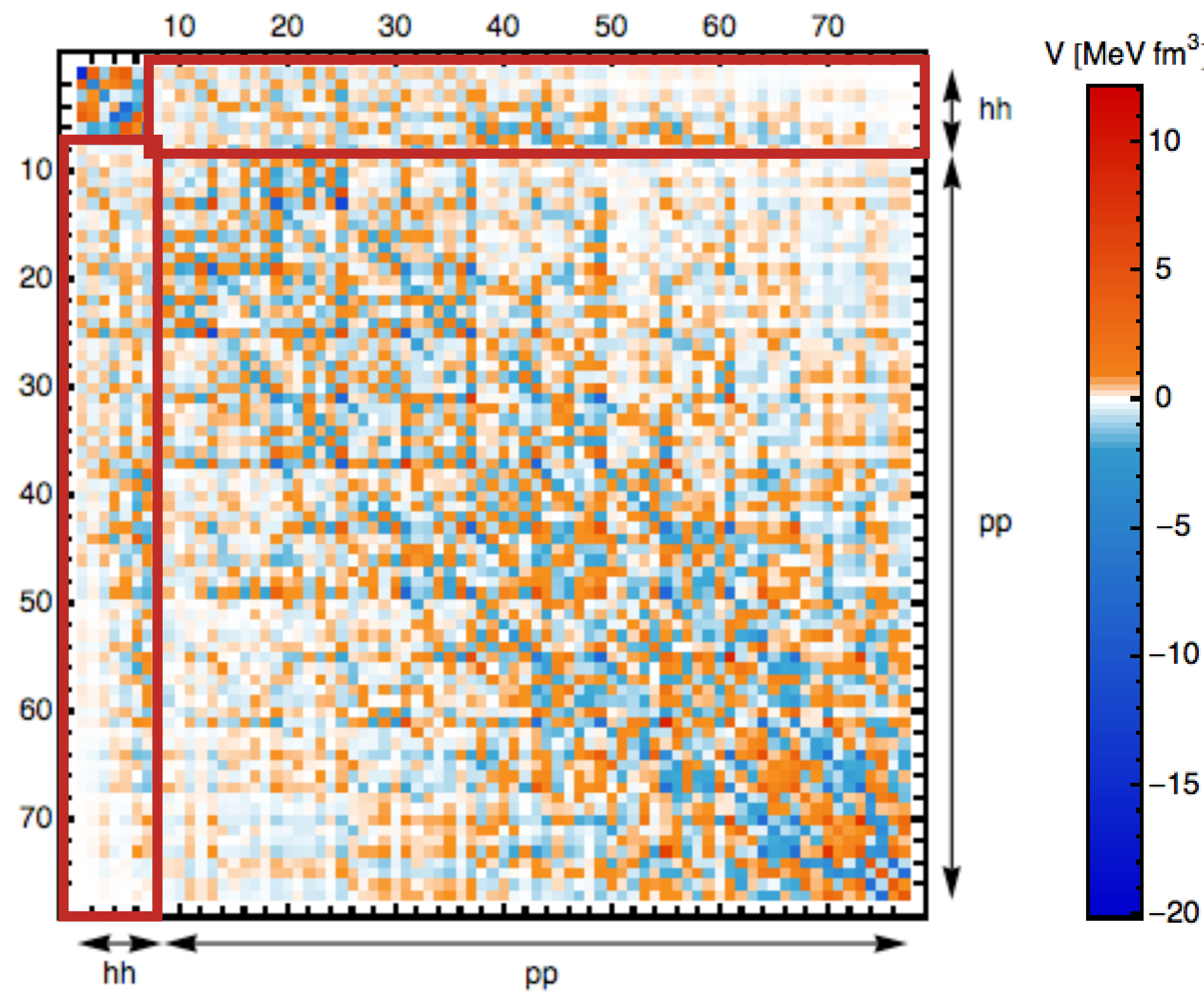


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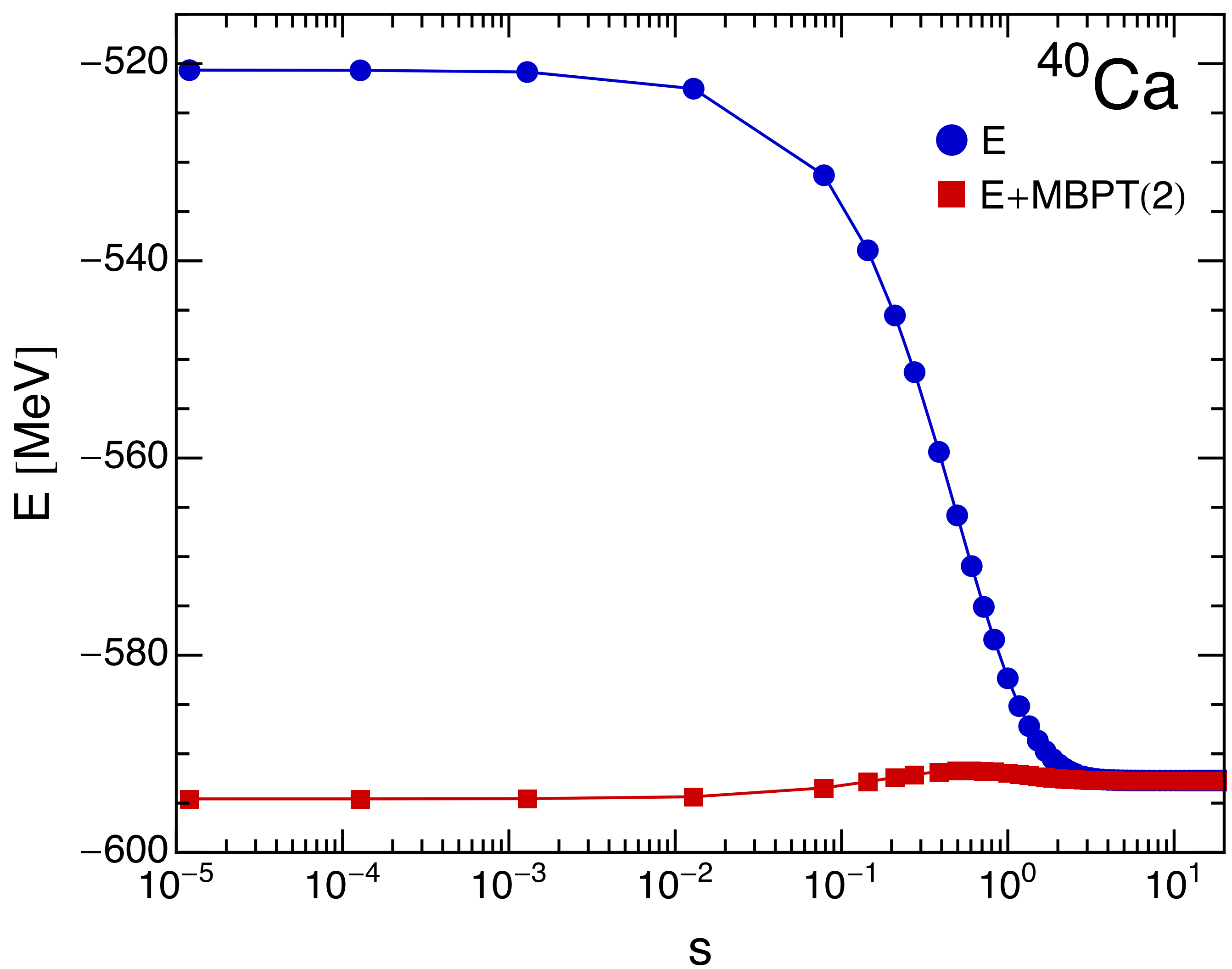


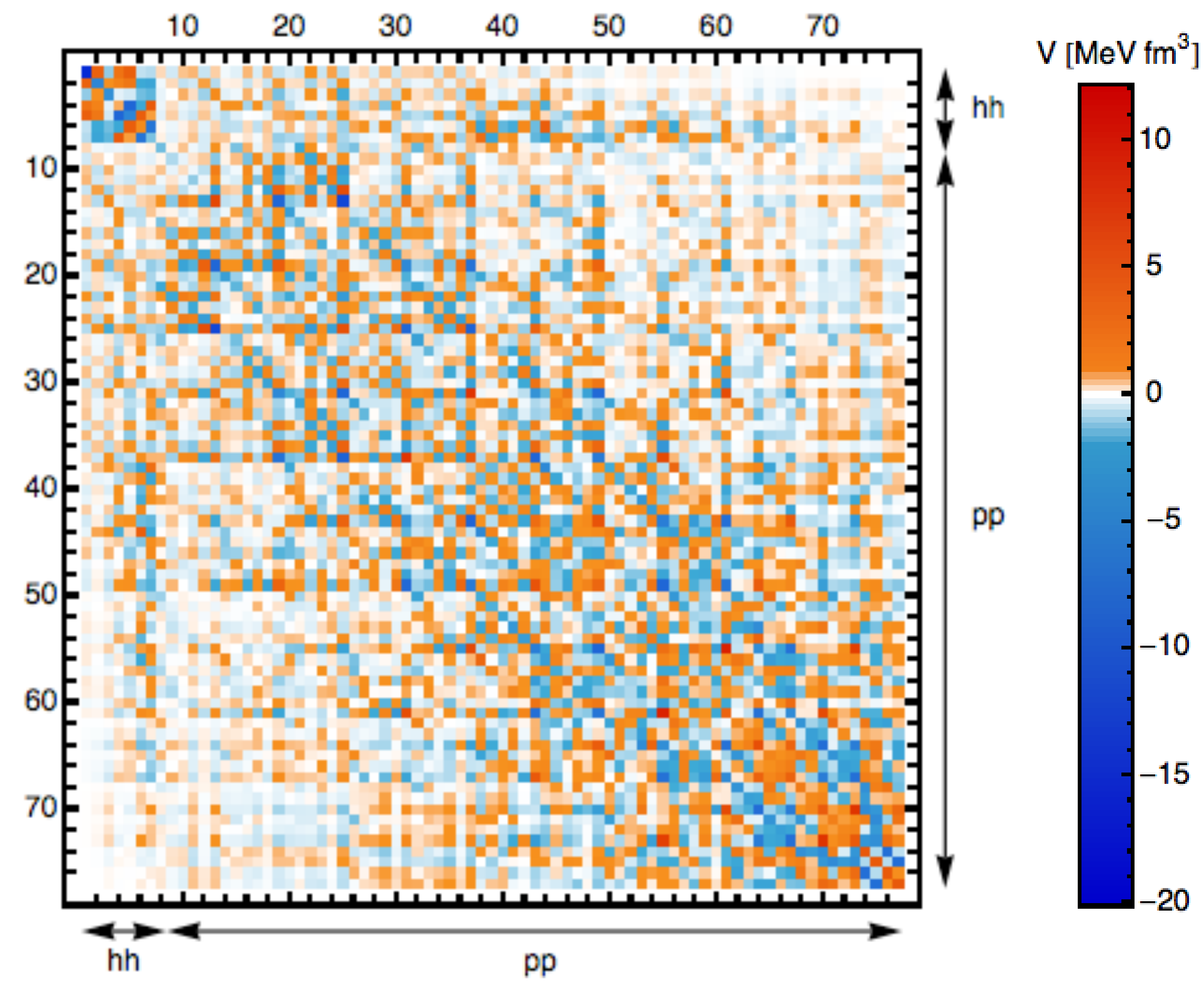


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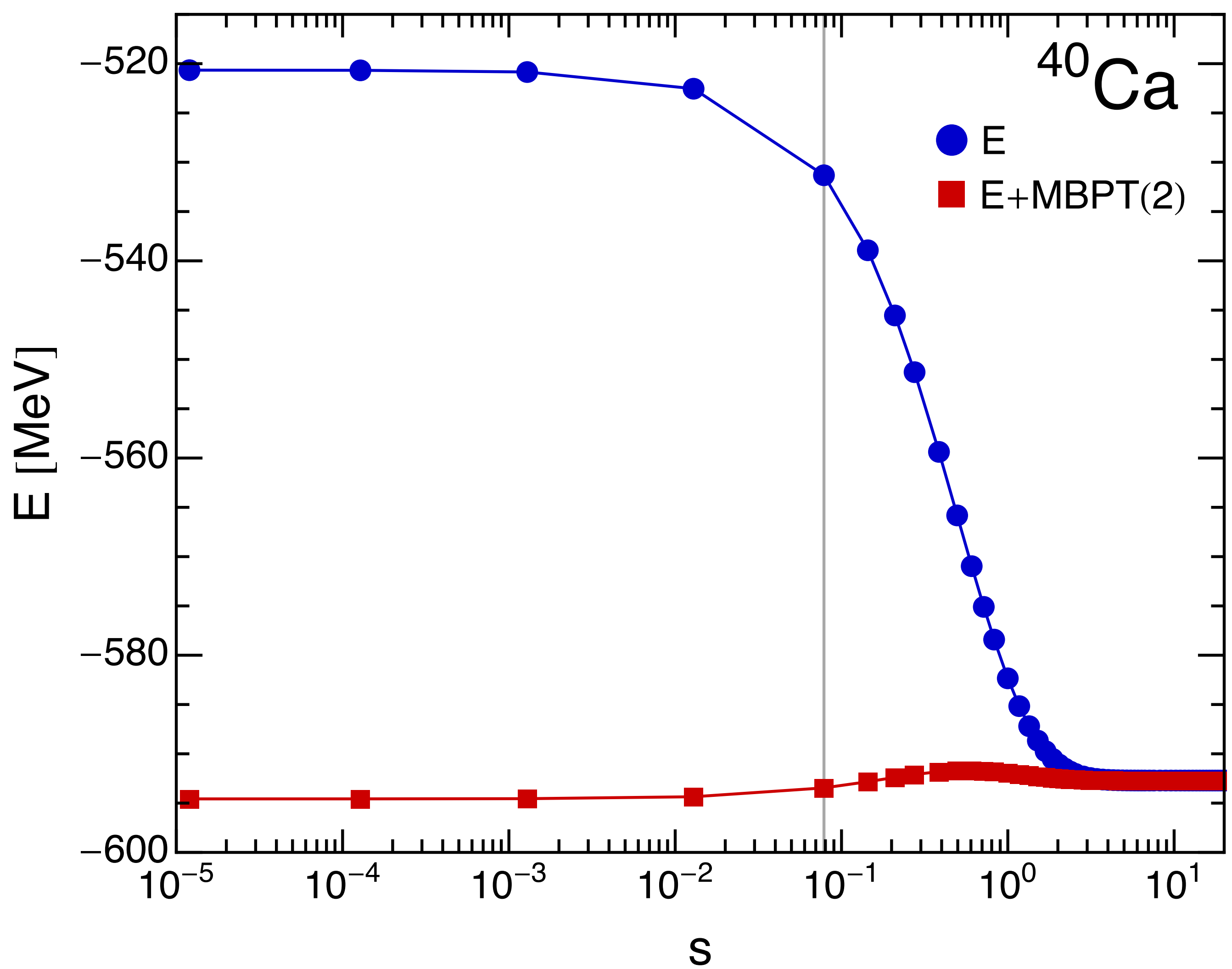


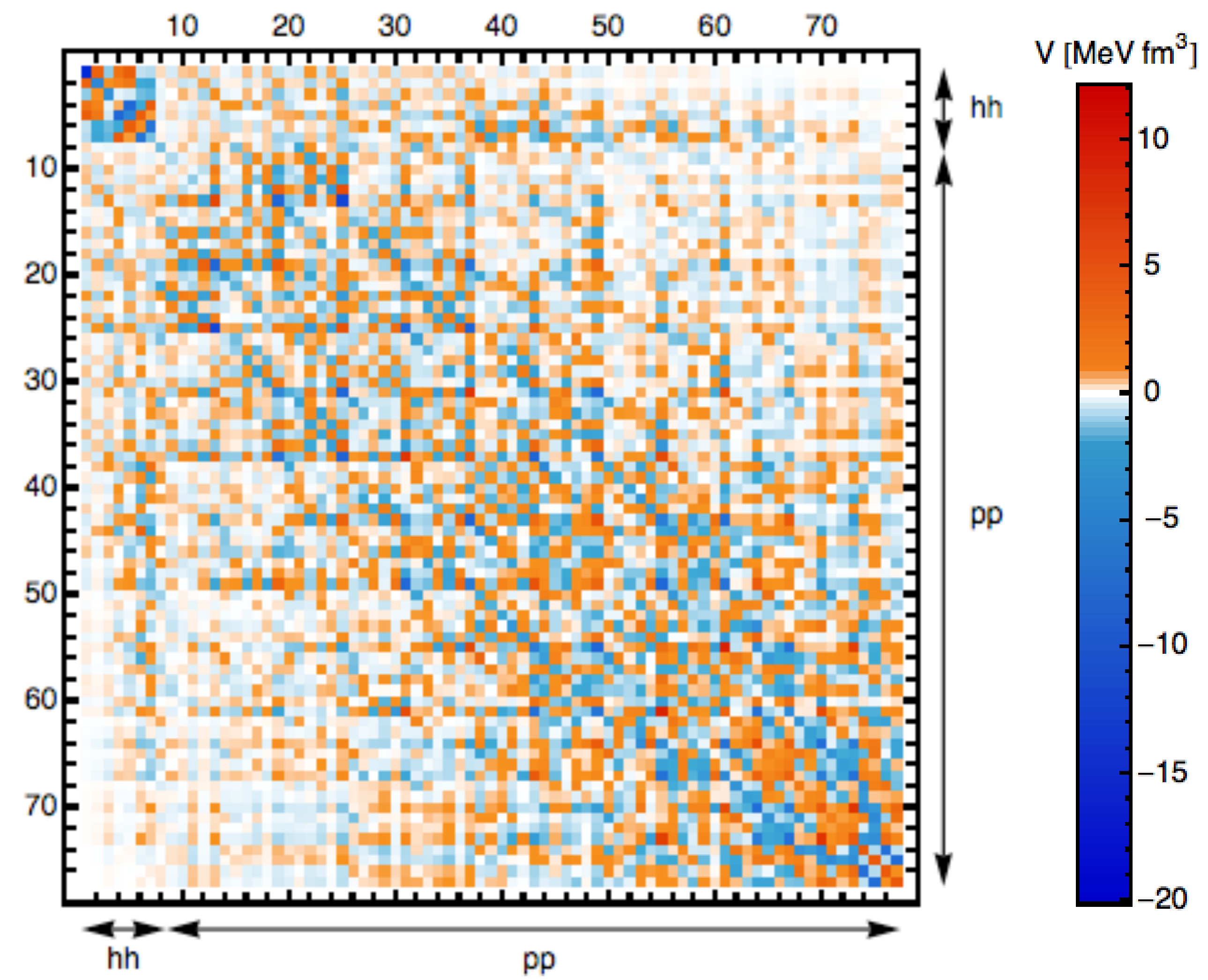


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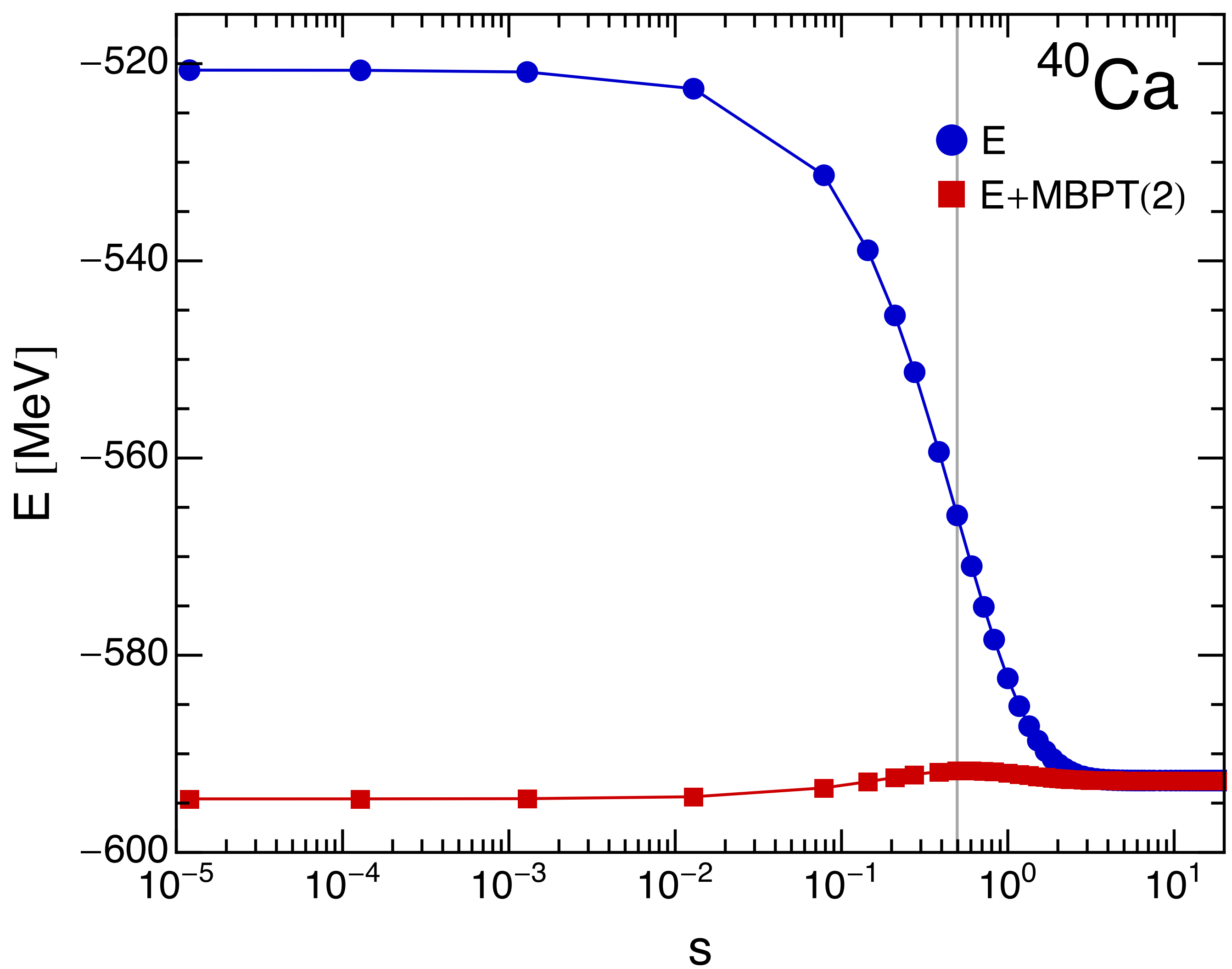


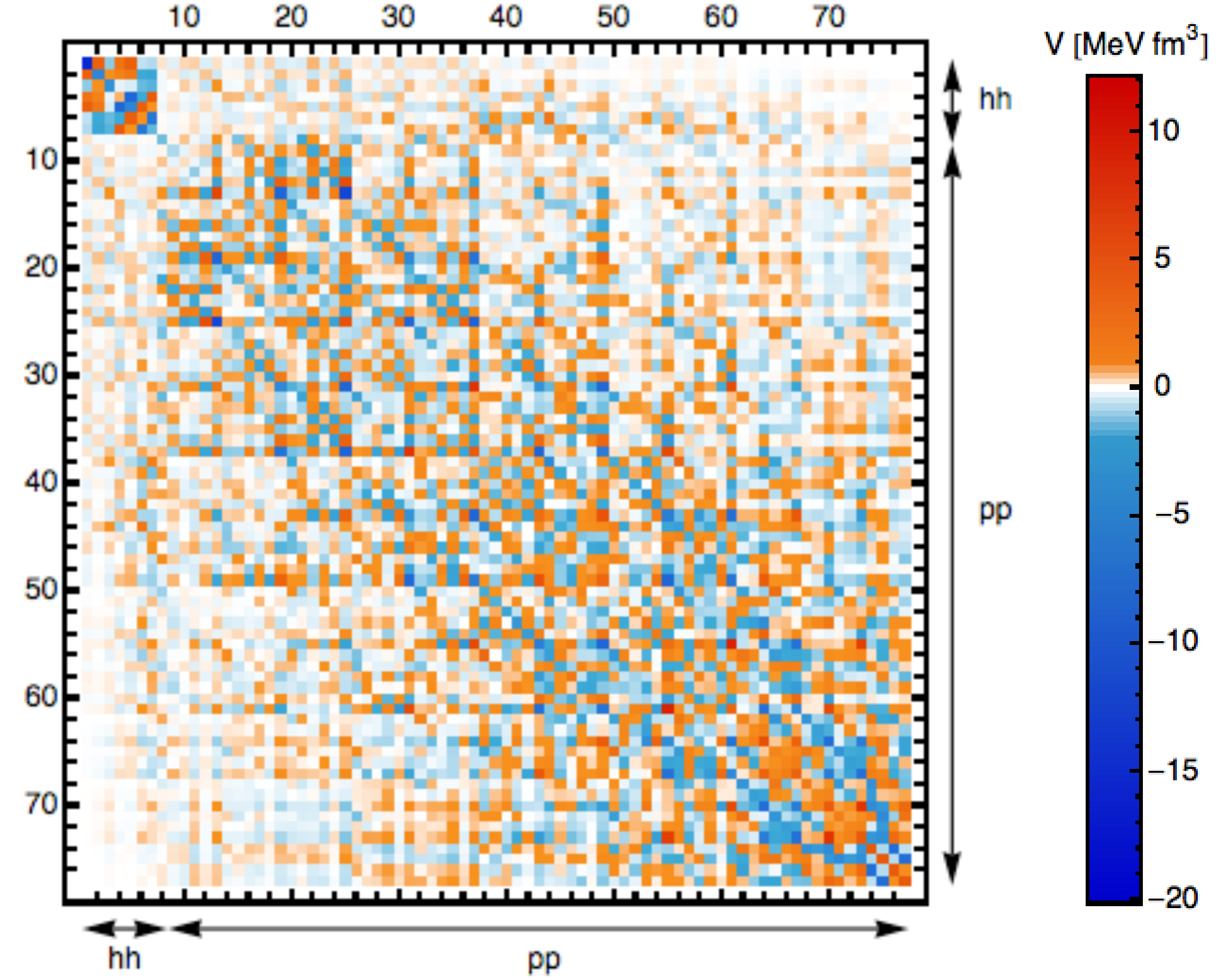


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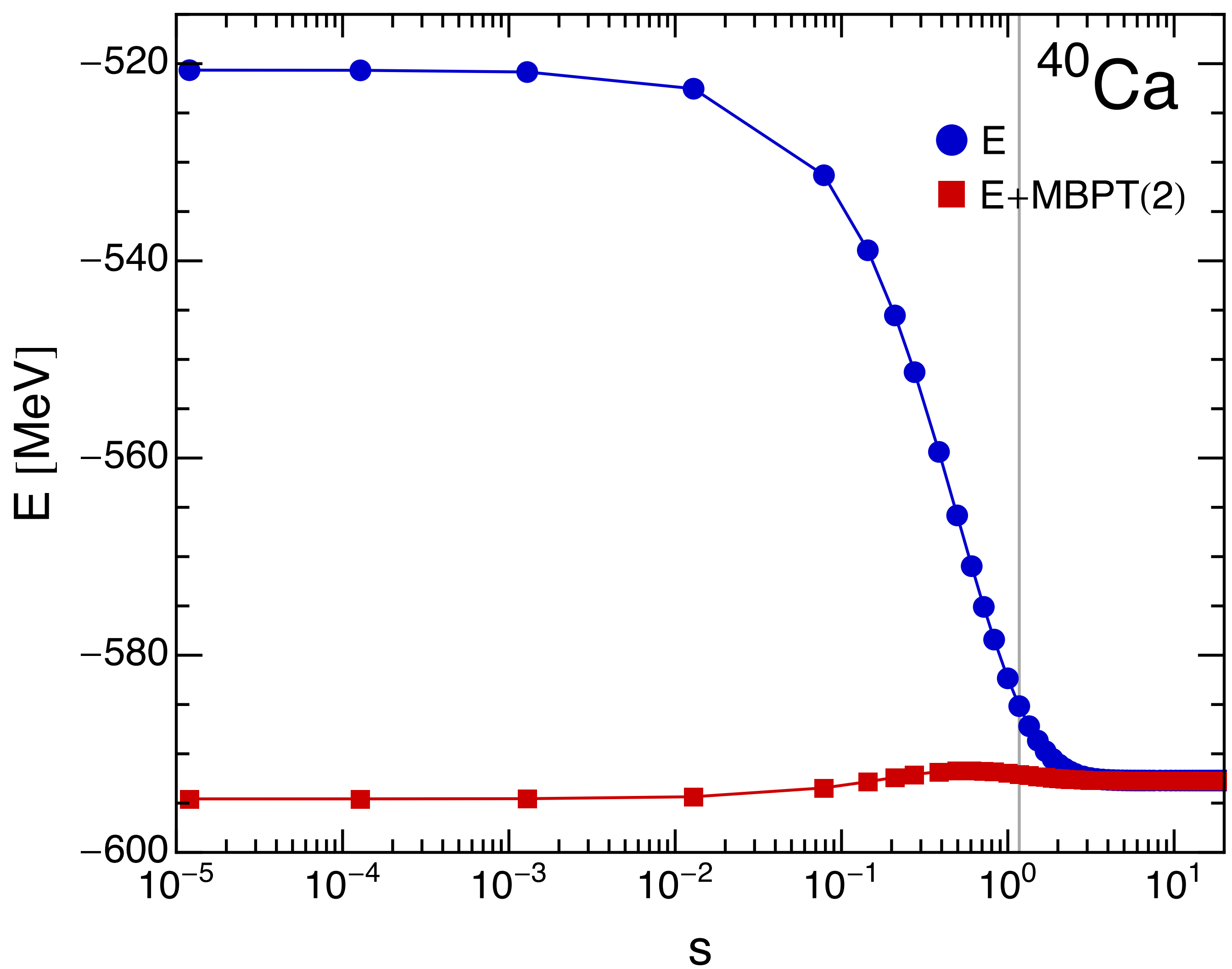


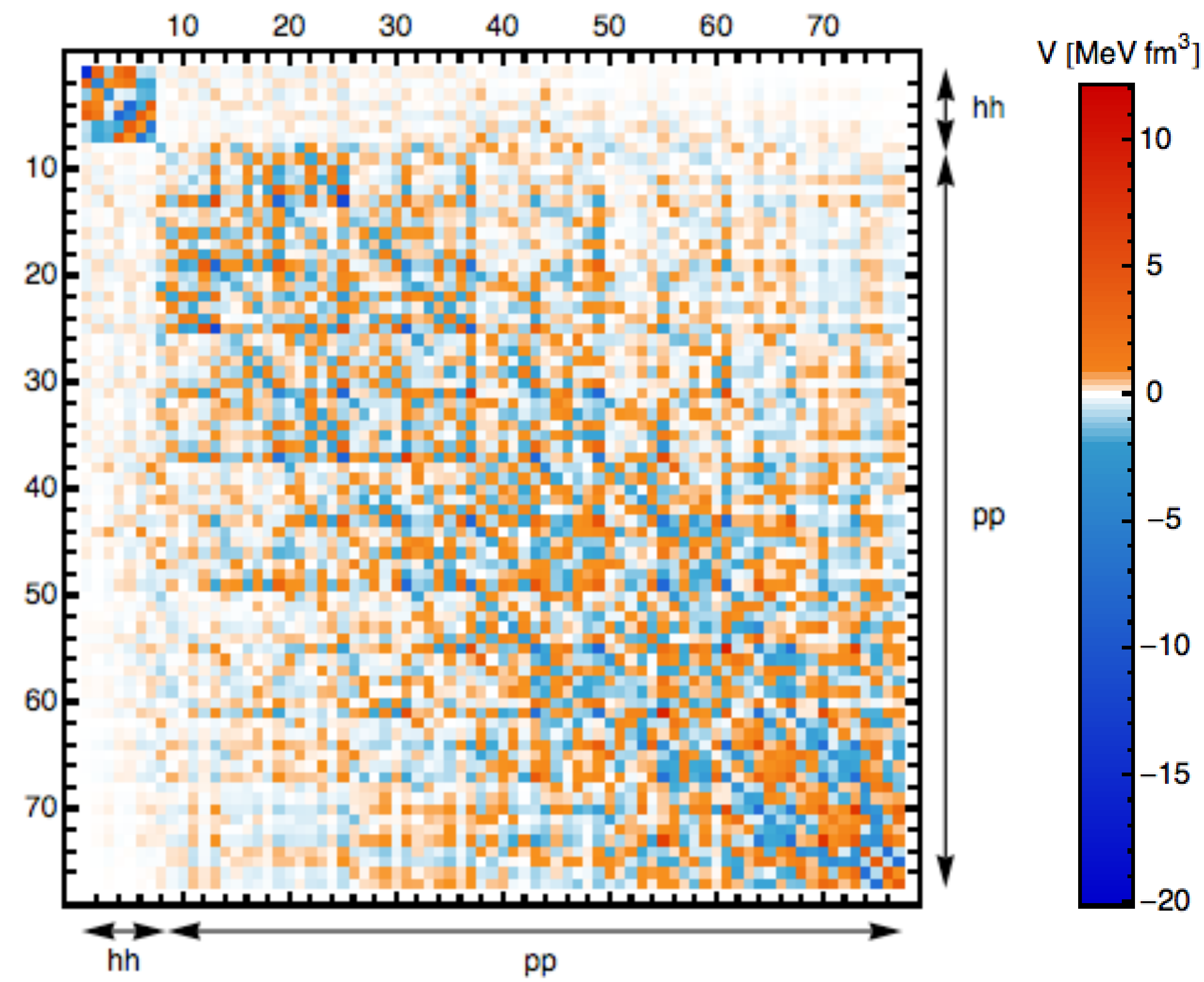


N3LO, $\lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

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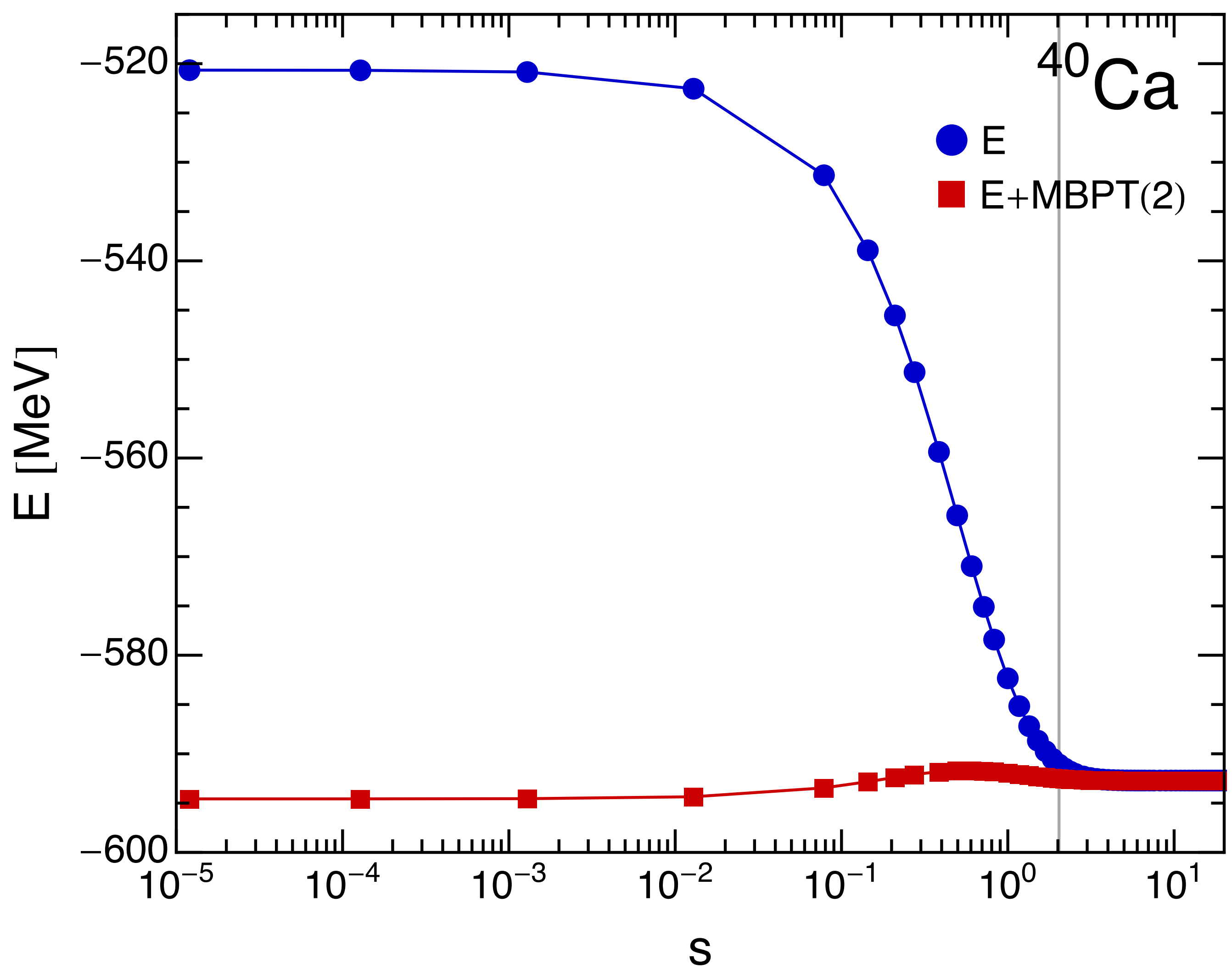


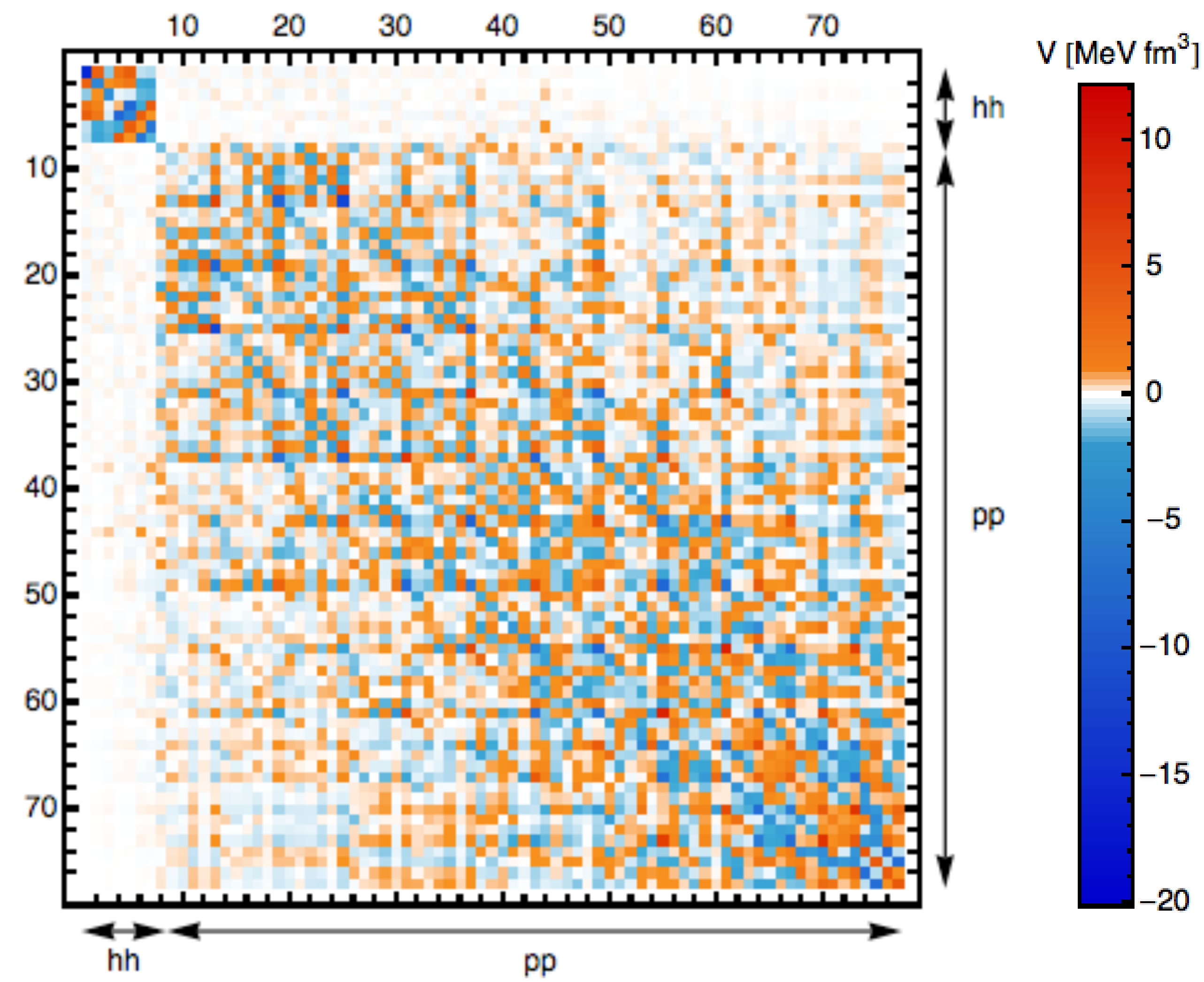


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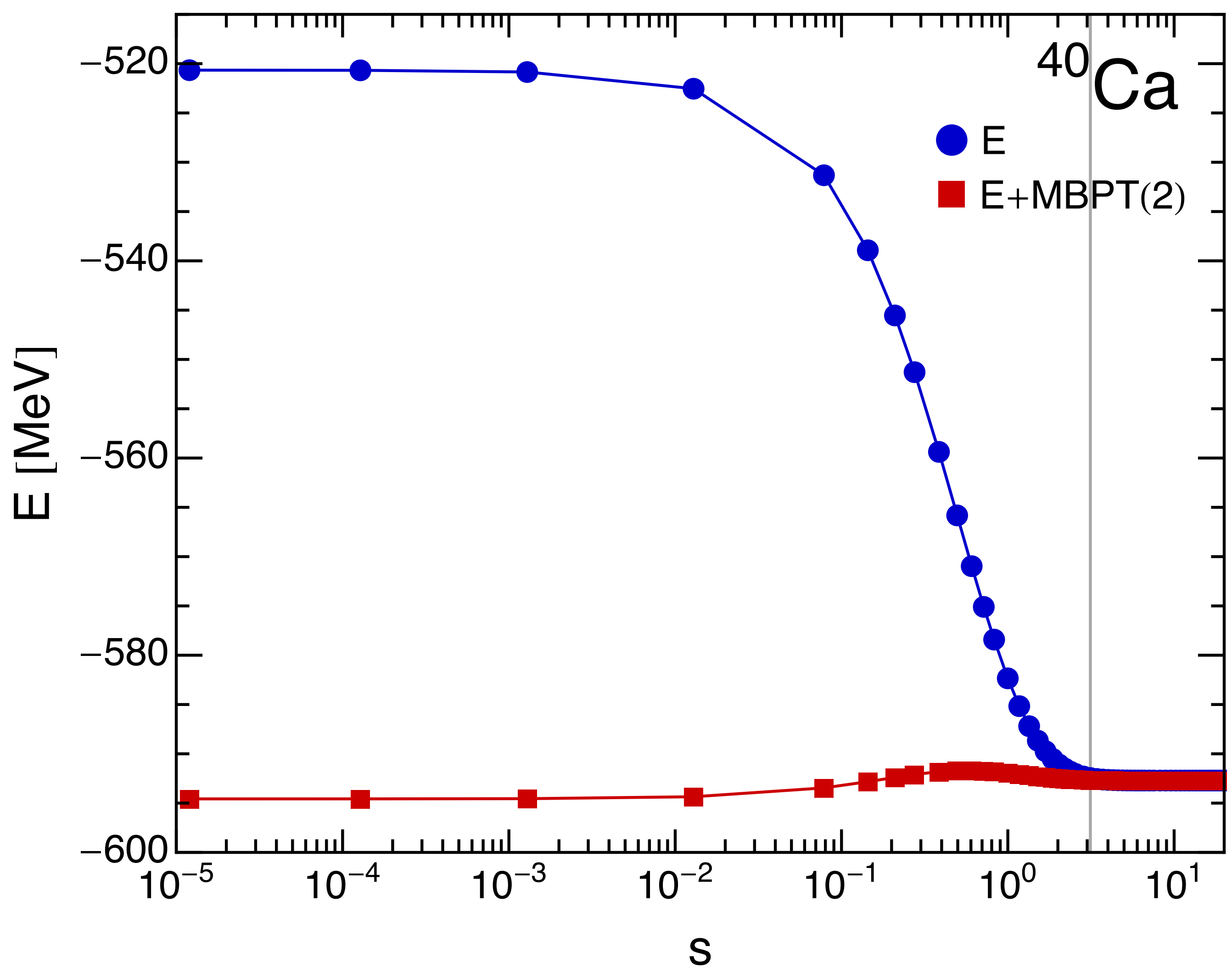


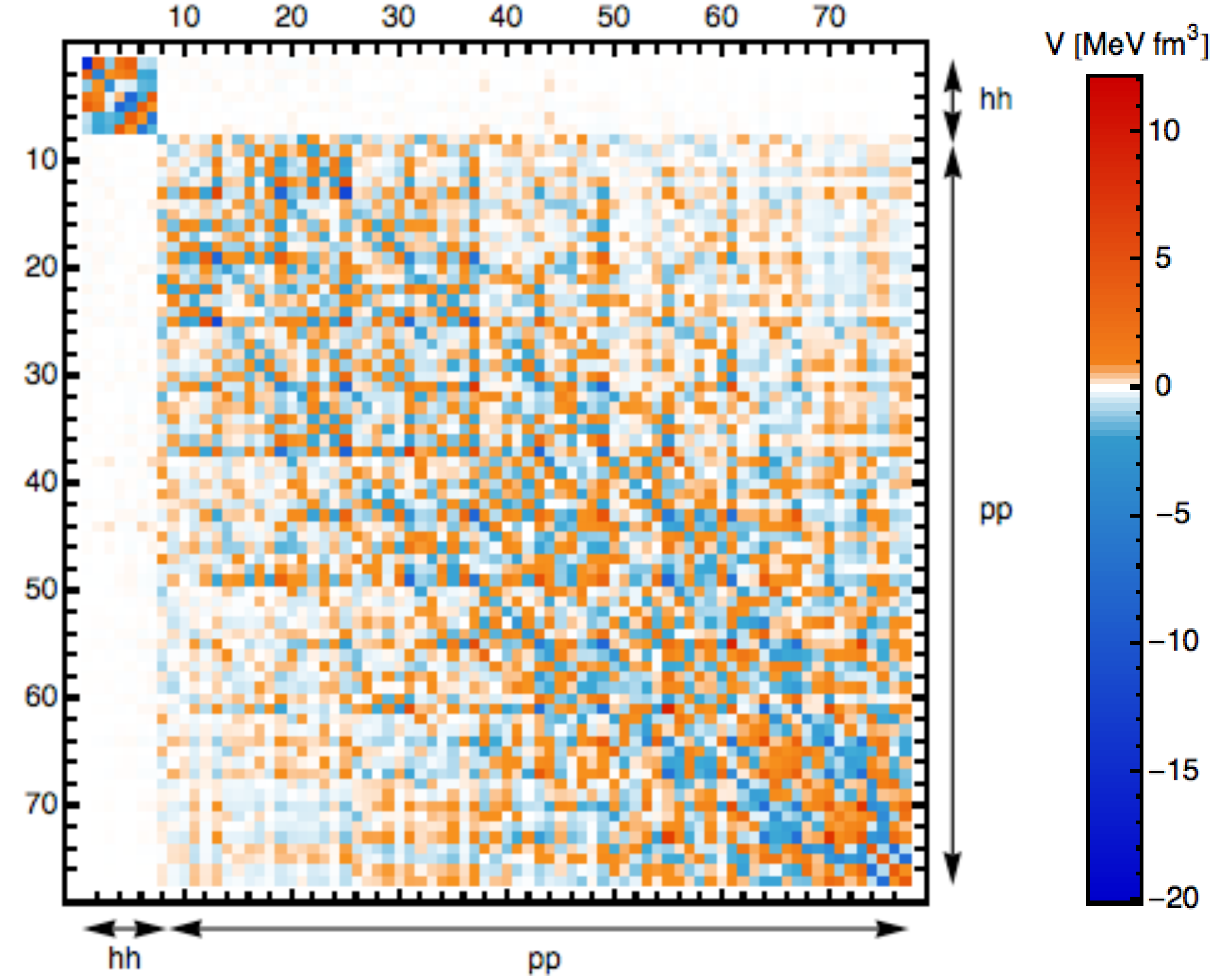


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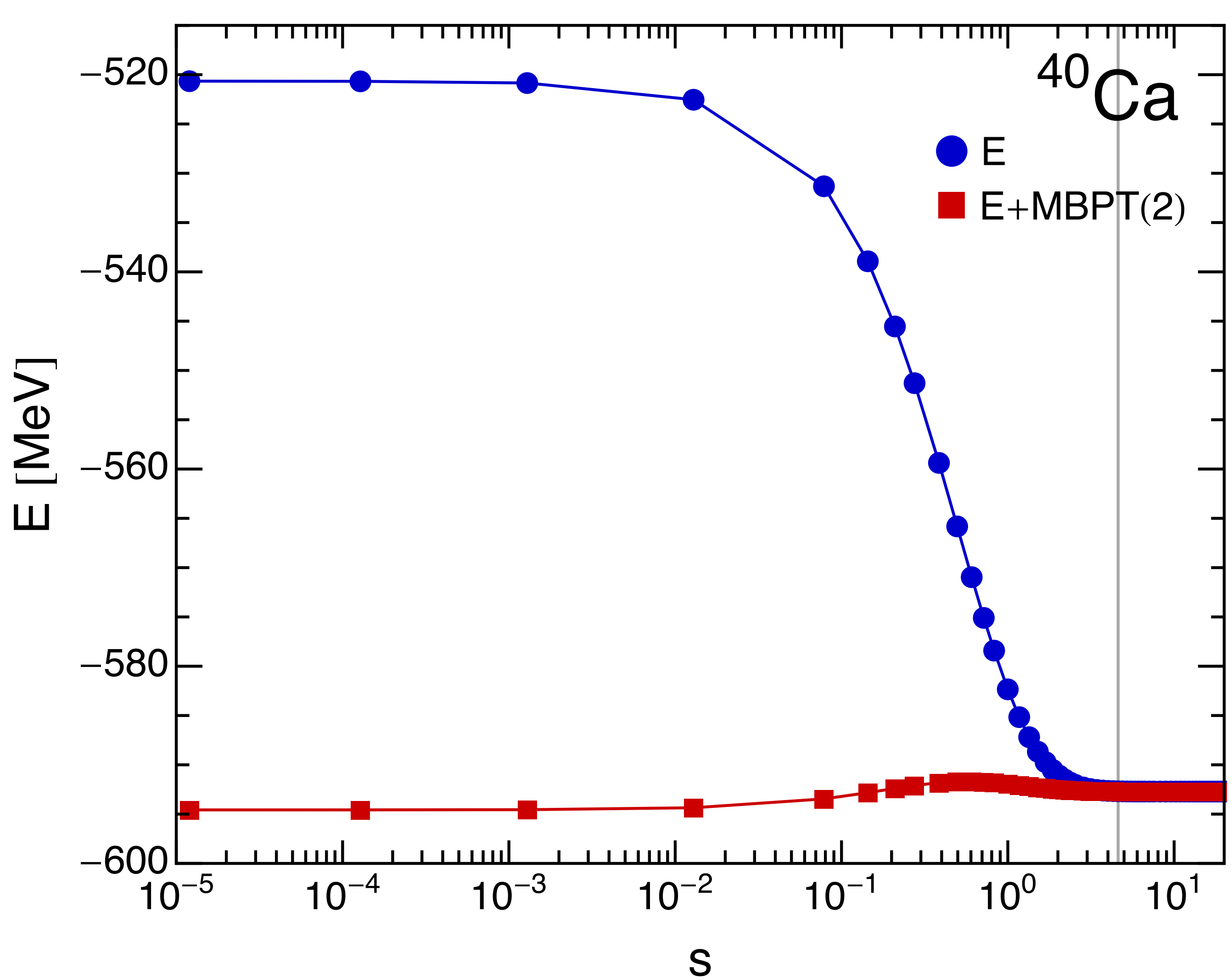


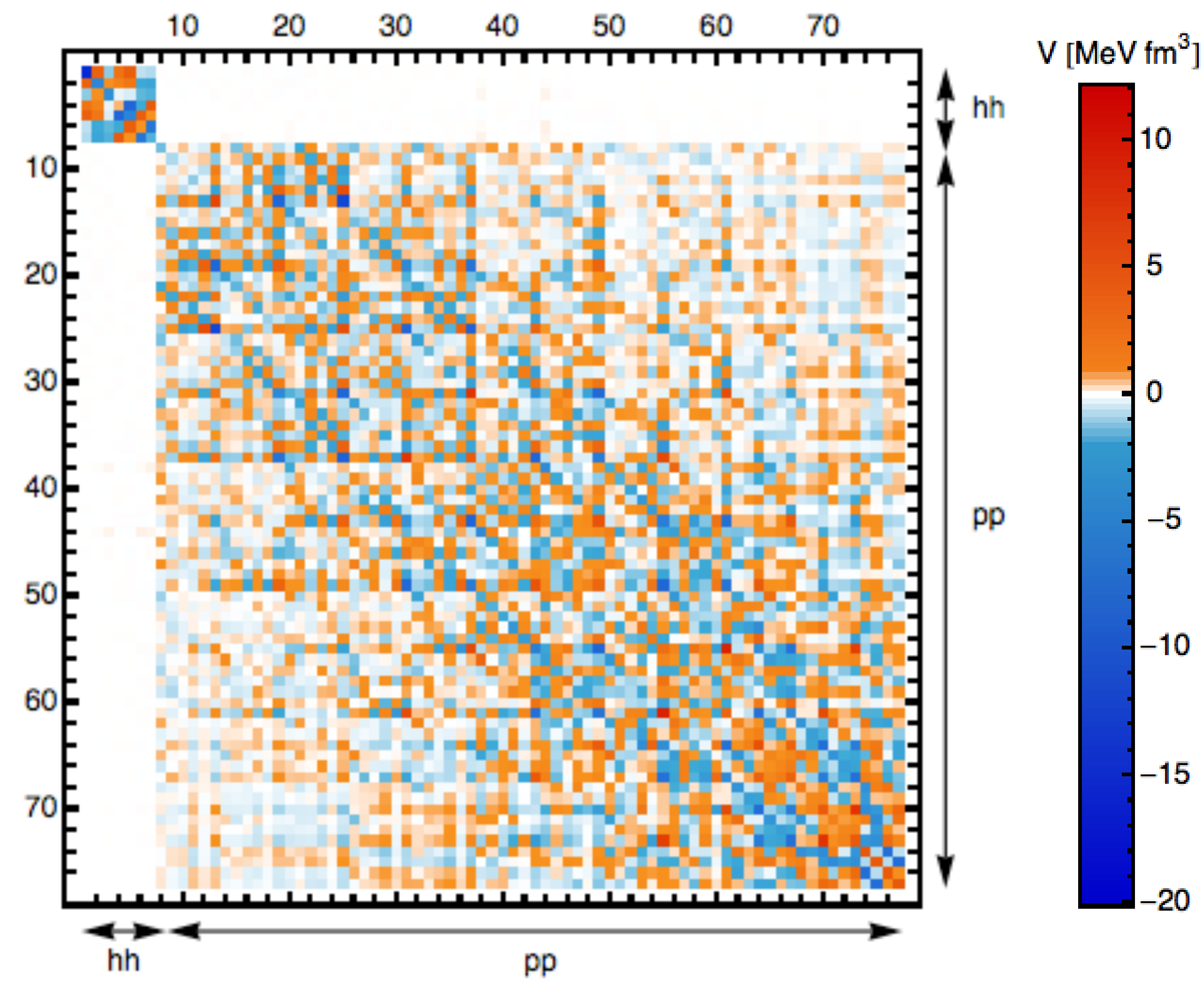


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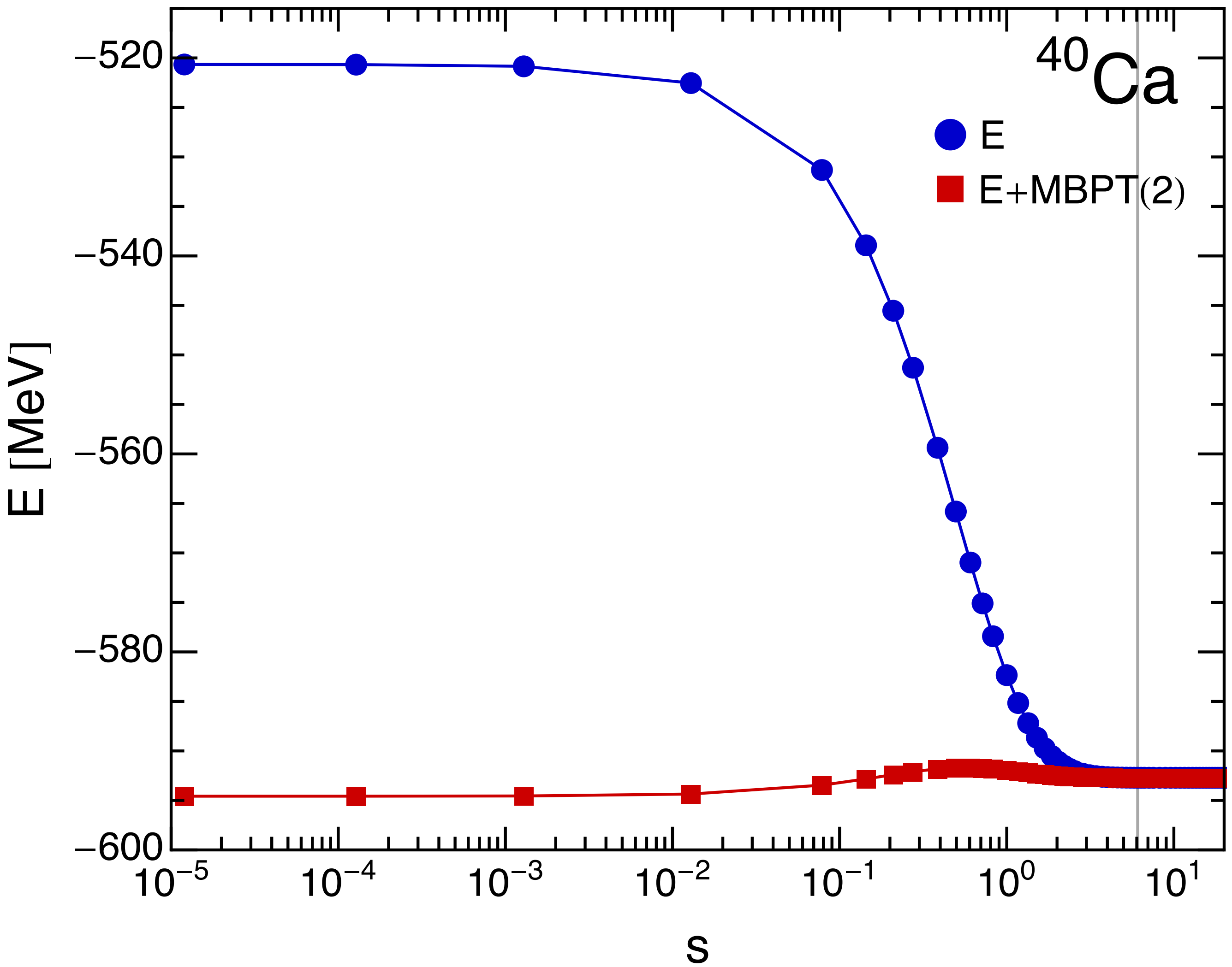


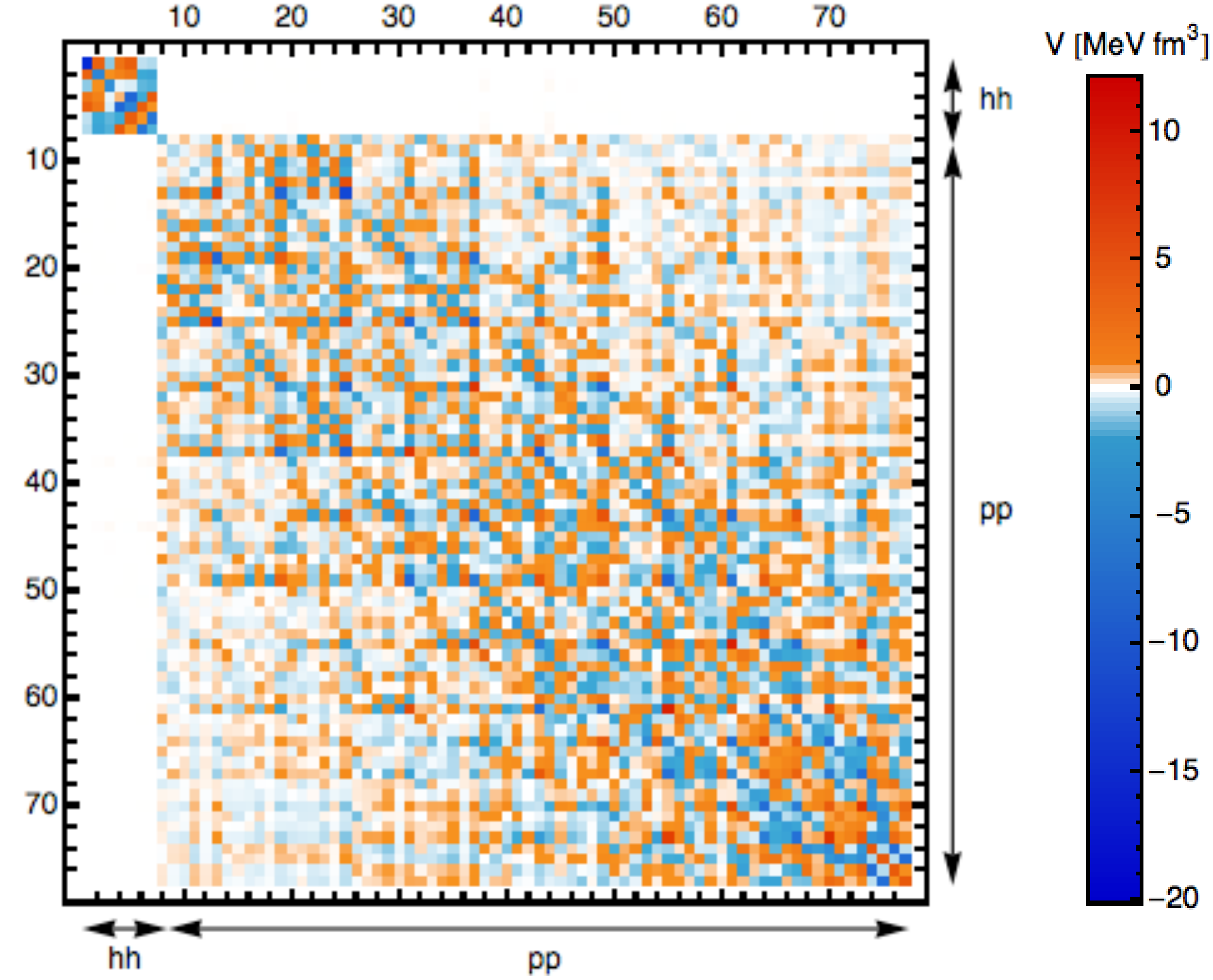


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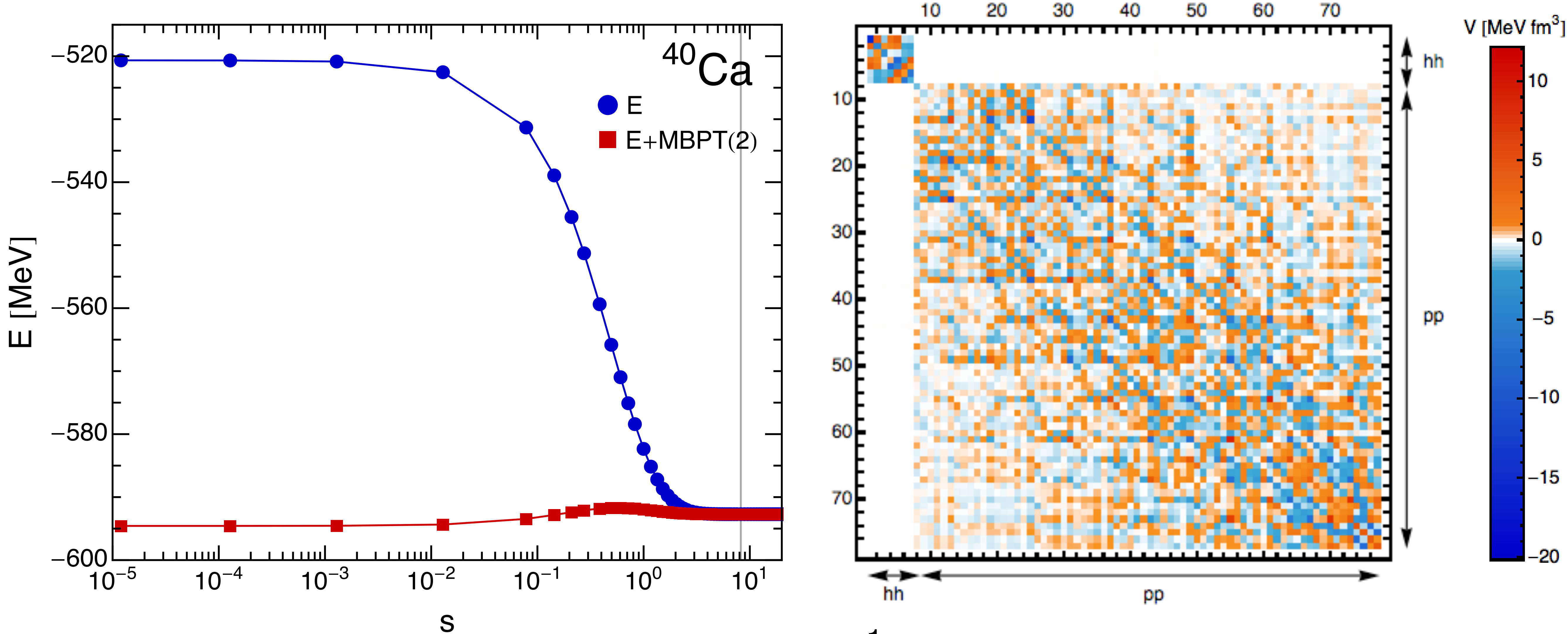


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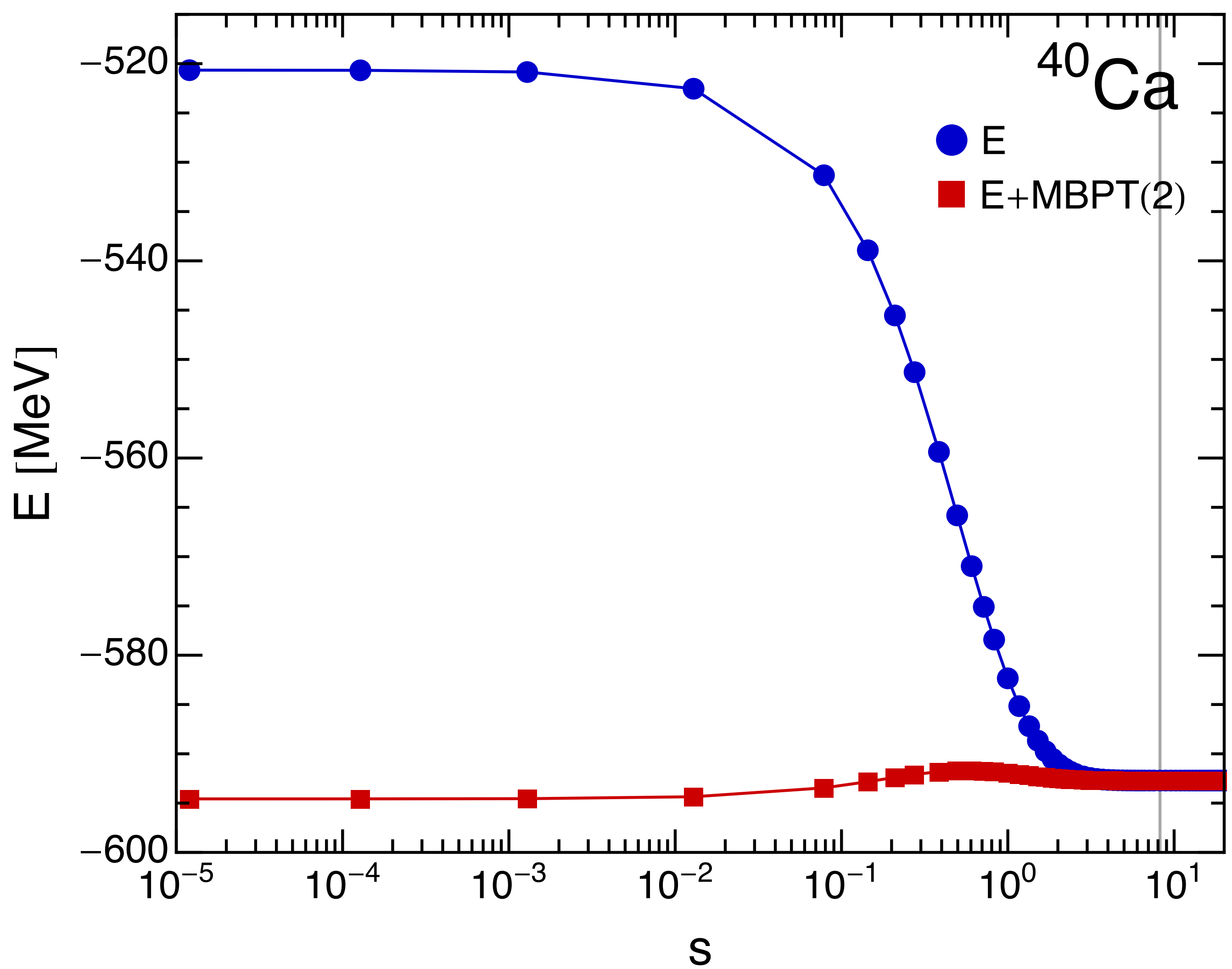


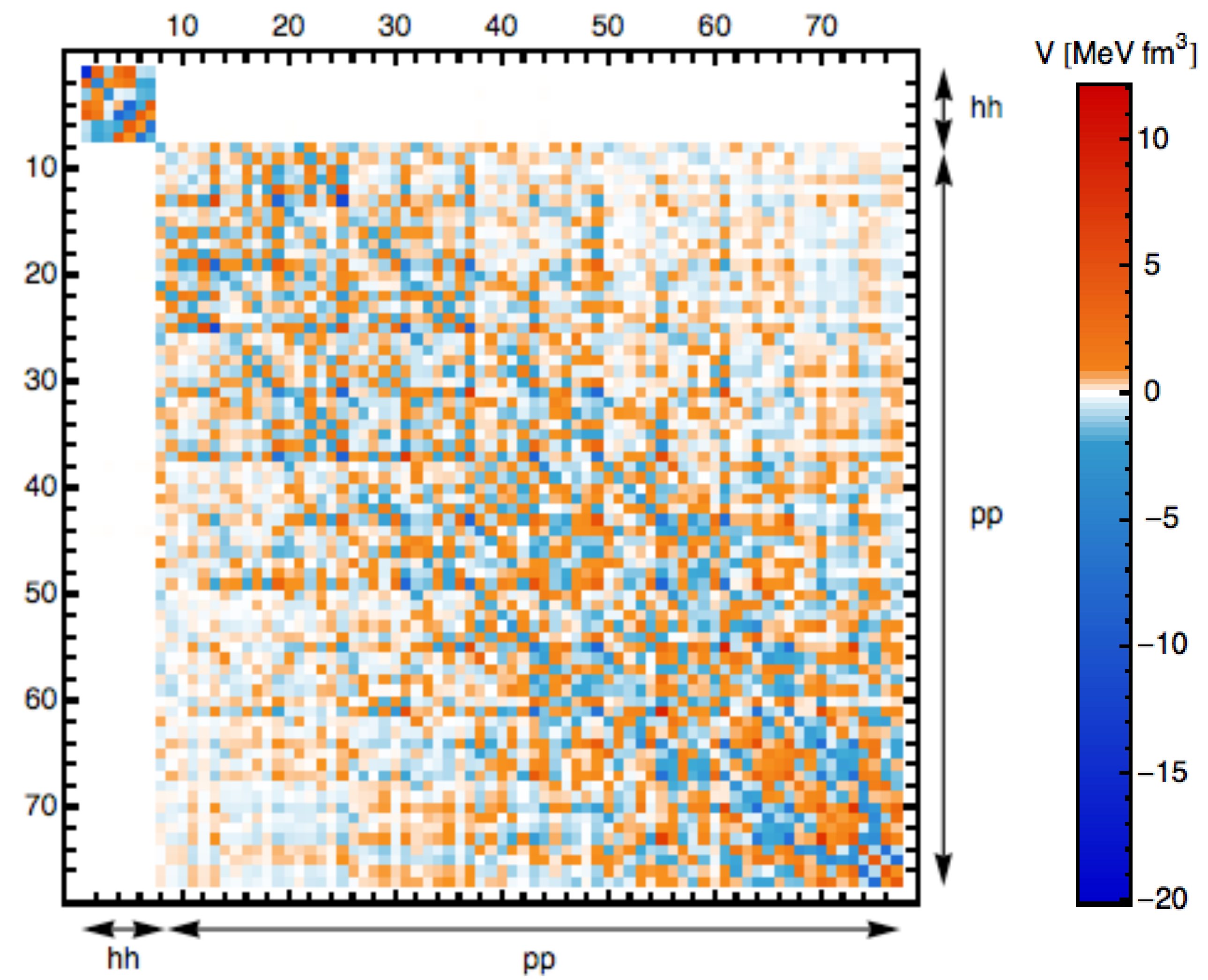


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off-diagonal couplings are rapidly driven to zero

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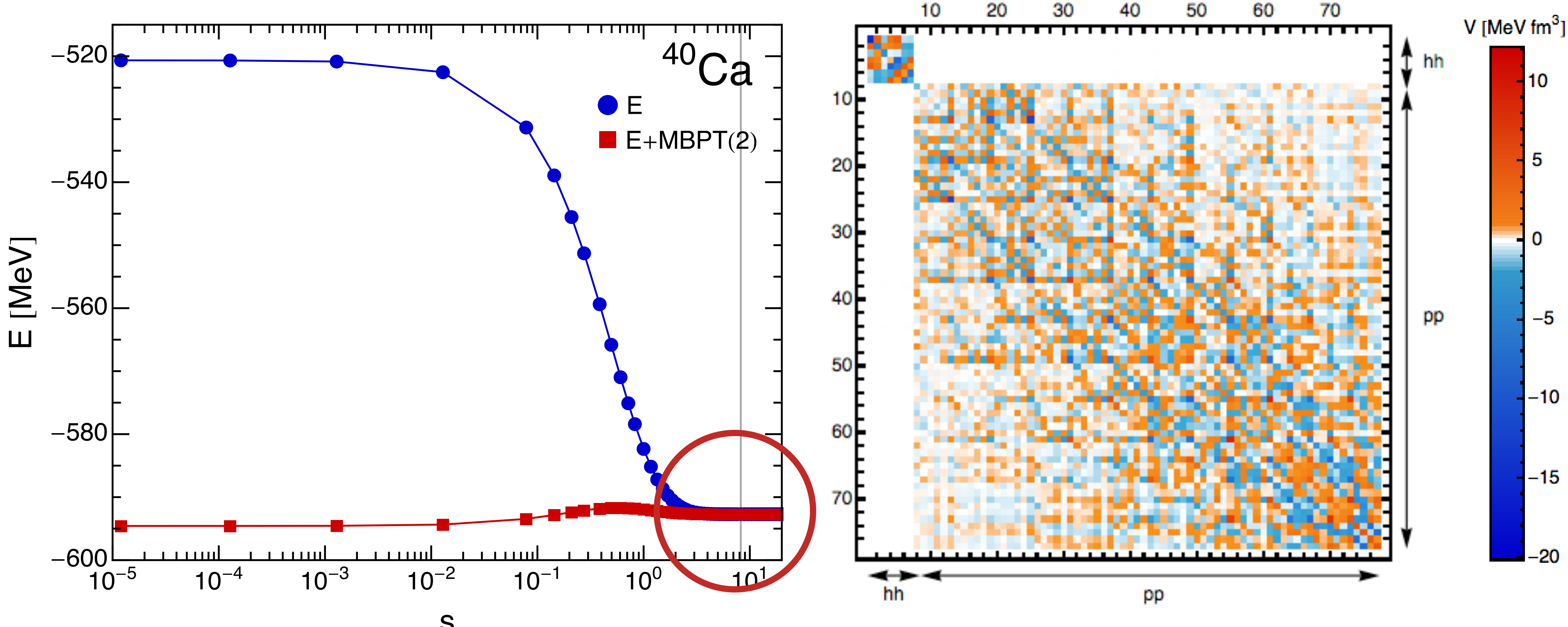



N3LO, $\lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

# Hamiltonians

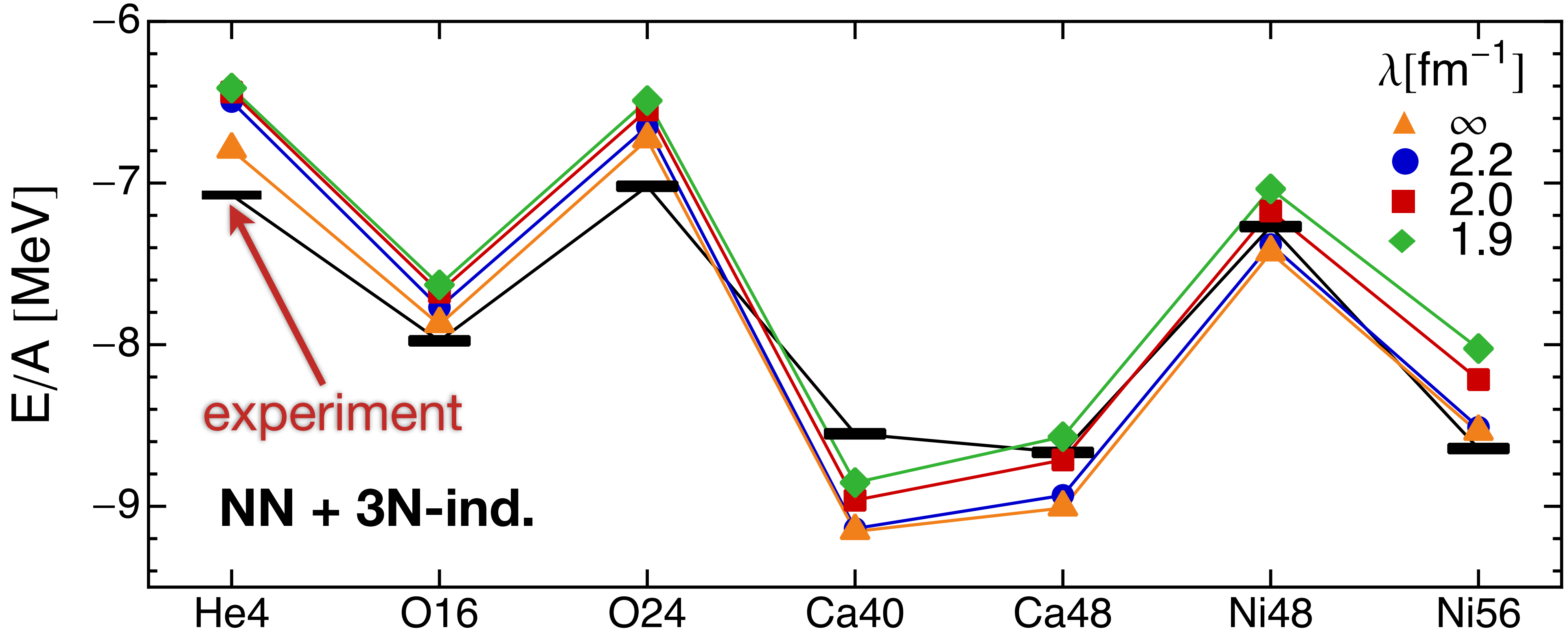
## Initial Hamiltonian

- NN: chiral interaction at $N^3LO$ (Entem & Machleidt)
- 3N: chiral interaction at $N^2LO$ ($c_D$,$c_E$ fit to $^3H$ energy & half-life)

## SRG-Evolved Hamiltonians

- **NN + 3N-induced:** start with initial NN Hamiltonian, keep two- and three-body terms
- **NN + 3N-full:** start with initial NN + 3N Hamiltonian, keep two- and three-body terms

# Results: Closed-Shell Nuclei




Phys. Rev. C **87**, 034307 (2013), arXiv: 1212.1190 [ nucl-th]

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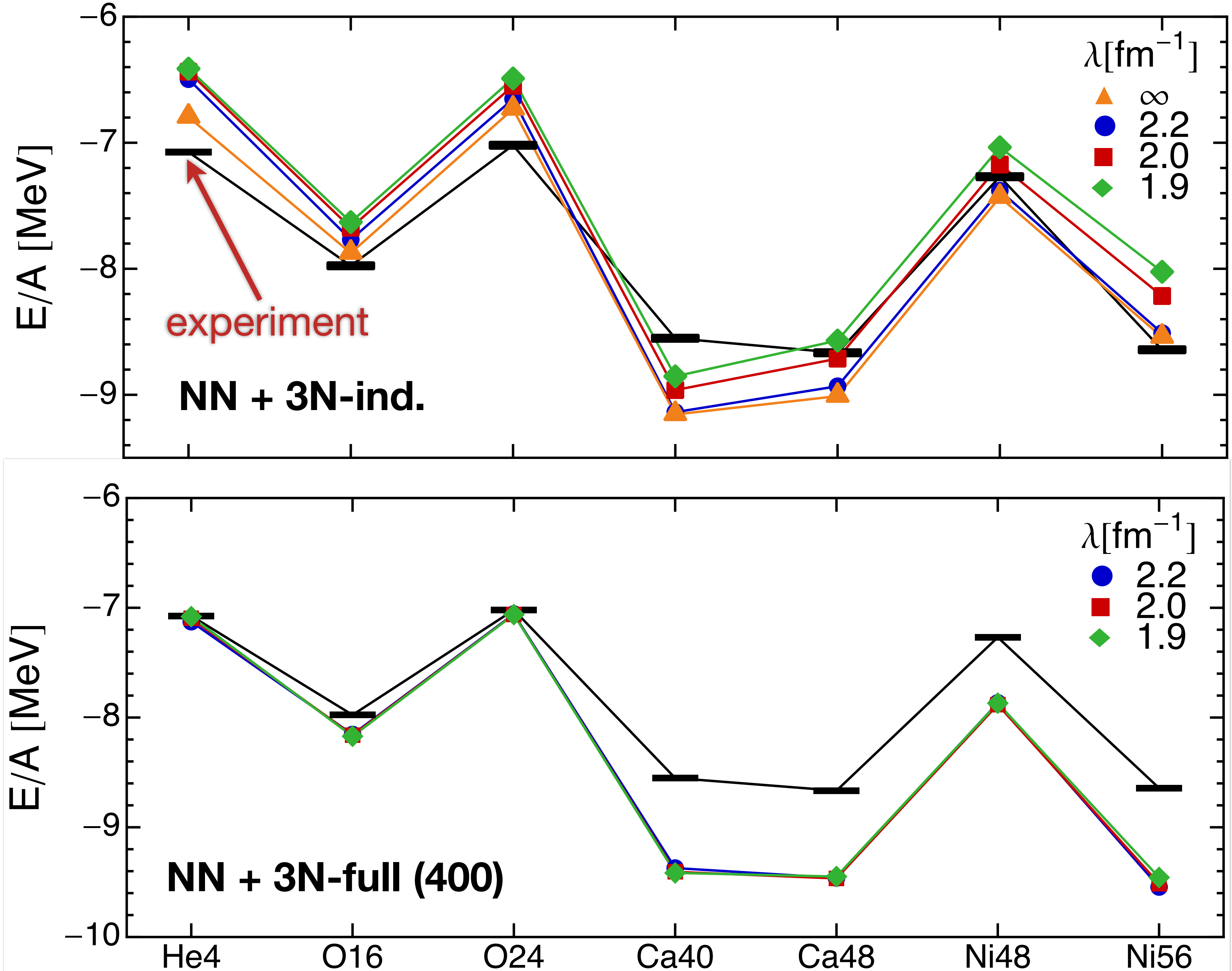


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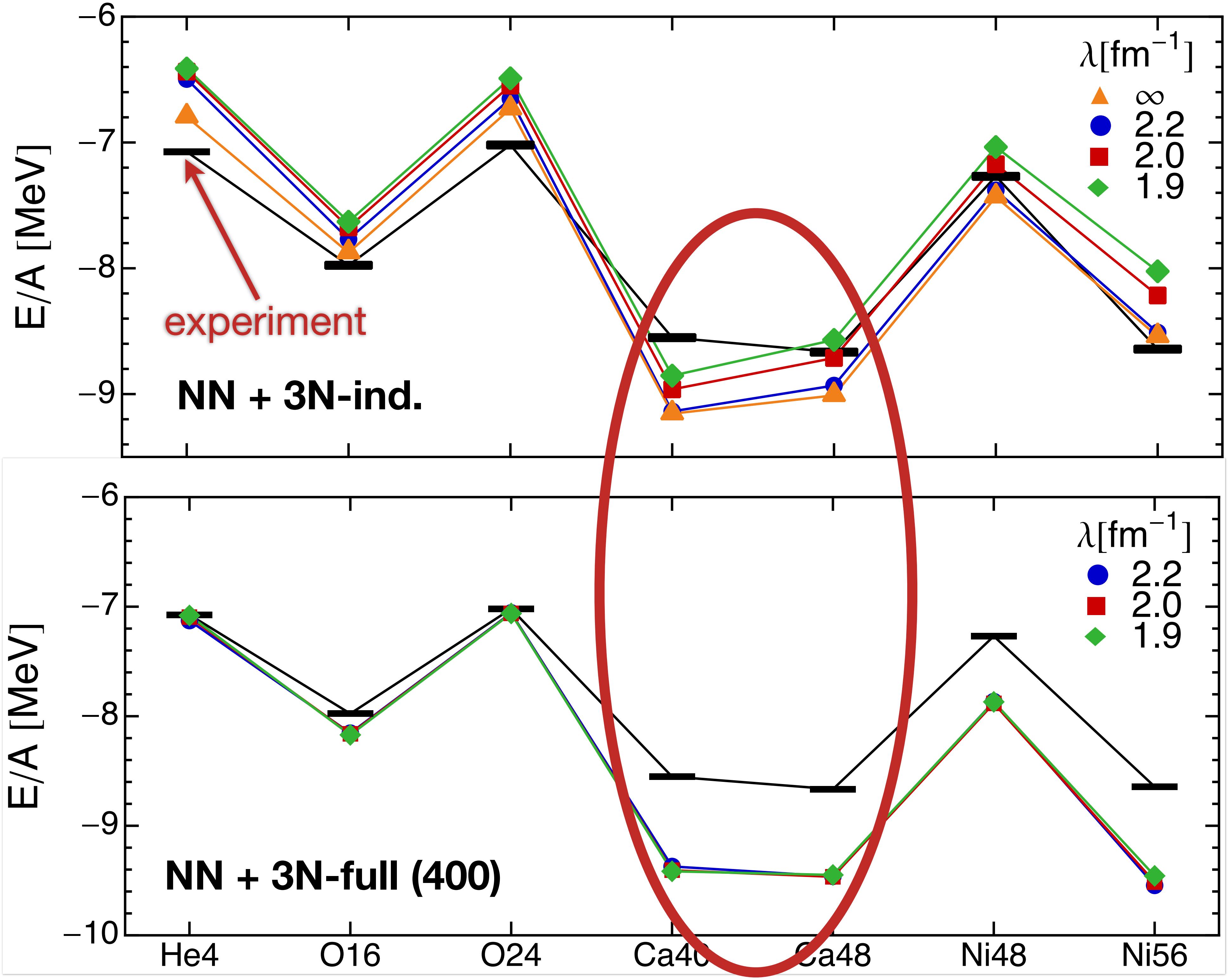


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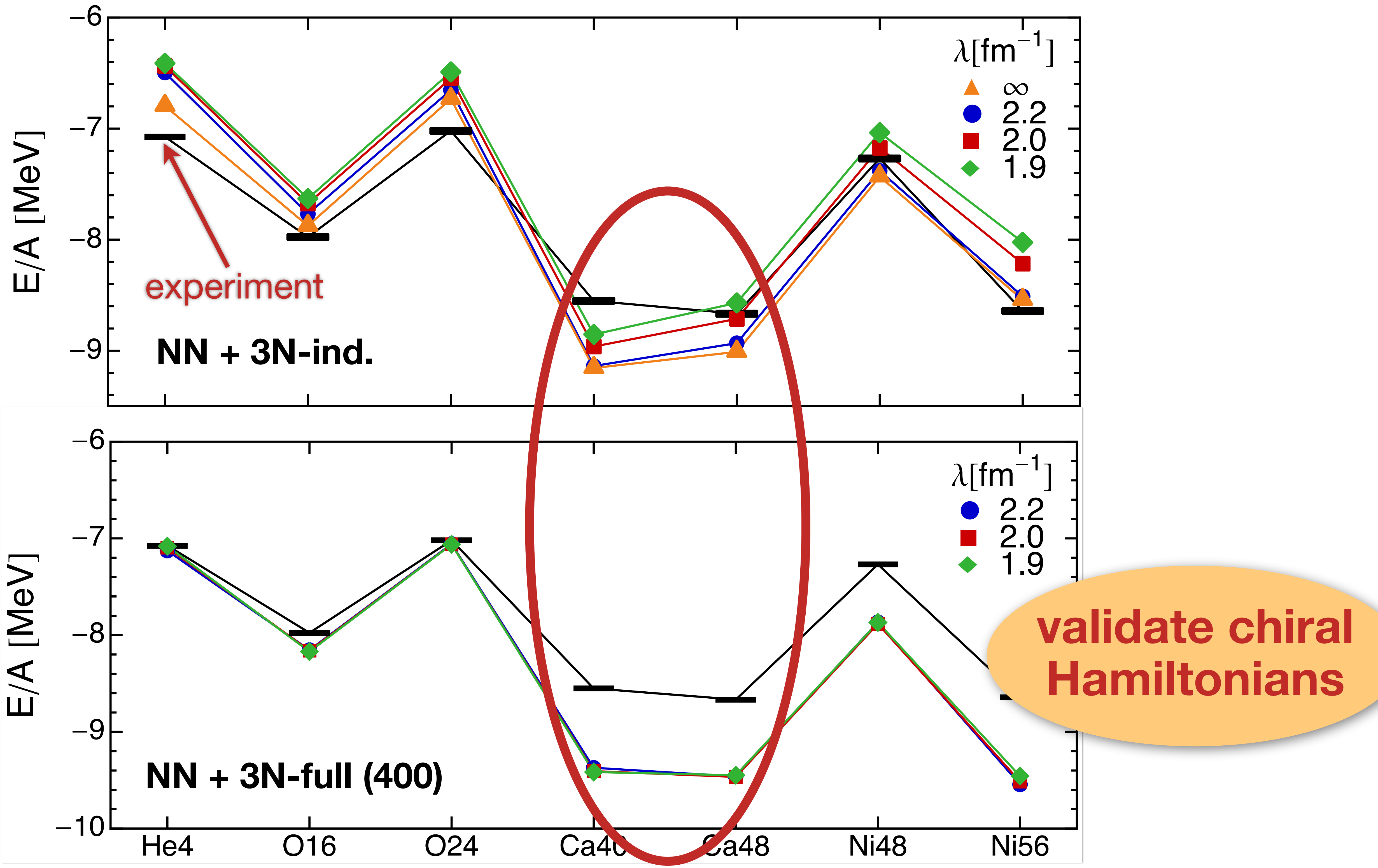


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# Open-Shell Nuclei from the Multi-Reference IM-SRG

H. H., S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

# Generalized Normal Ordering

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- define irreducible n-body density matrices of reference state:

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$$\cdots$$

**two-body flow unchanged, $O(N^6)$ scaling preserved**

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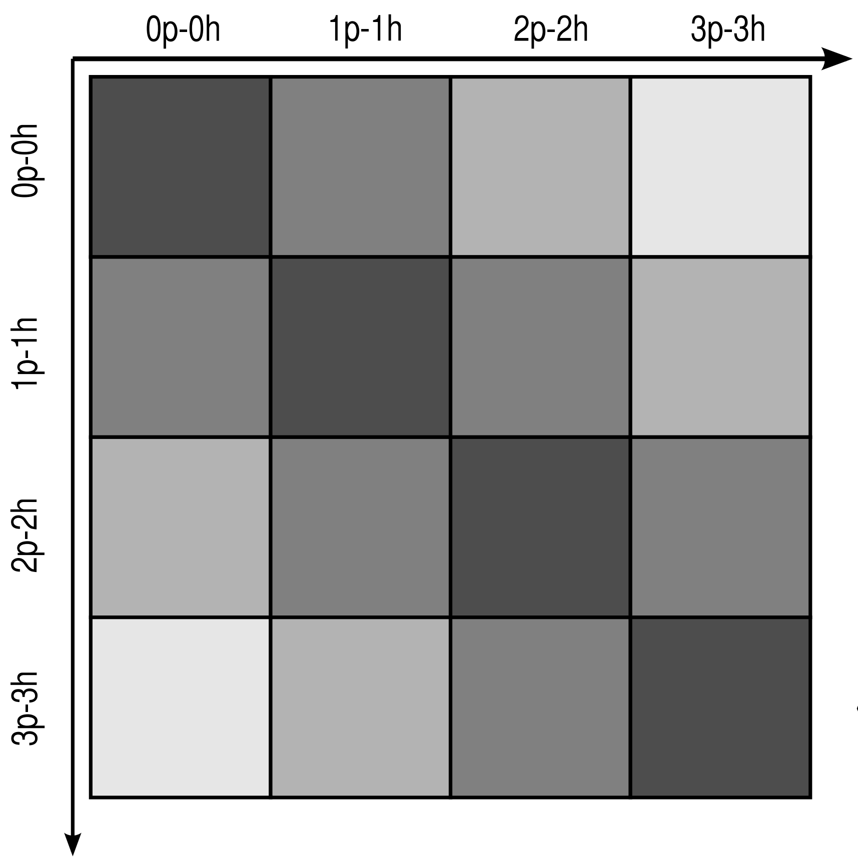


$$\langle {}^{p}_{h} | H | \Psi \rangle \sim f^{p}_{h}, \sum_{kl} f^{k}_{l} \lambda^{hk}_{pl}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{hkl}_{pmn}, \dots$$

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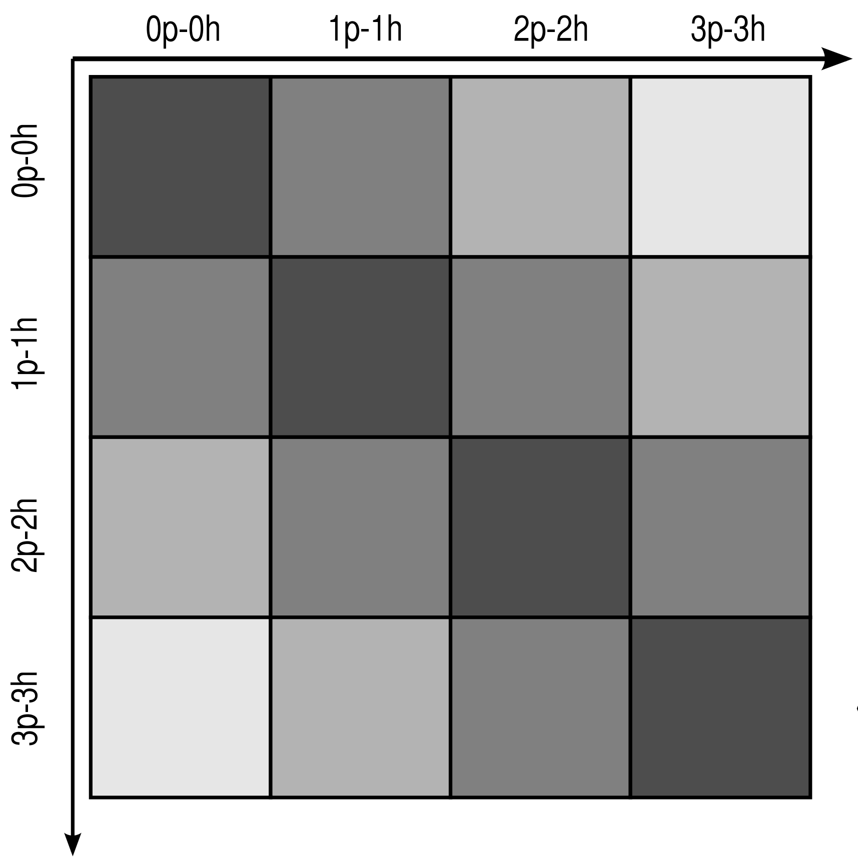


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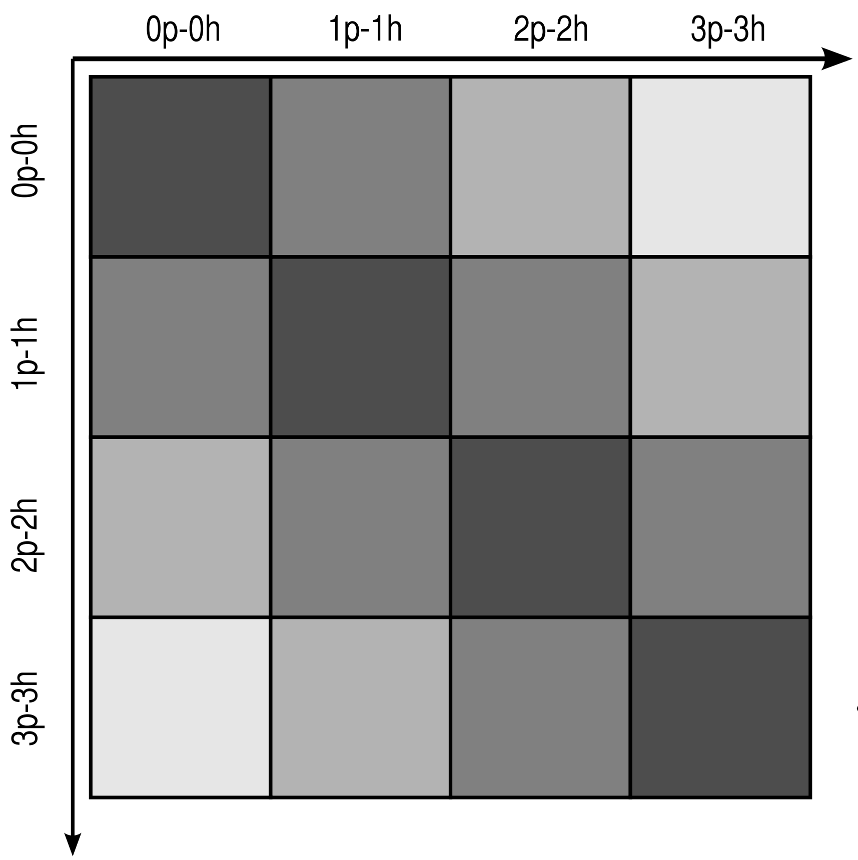


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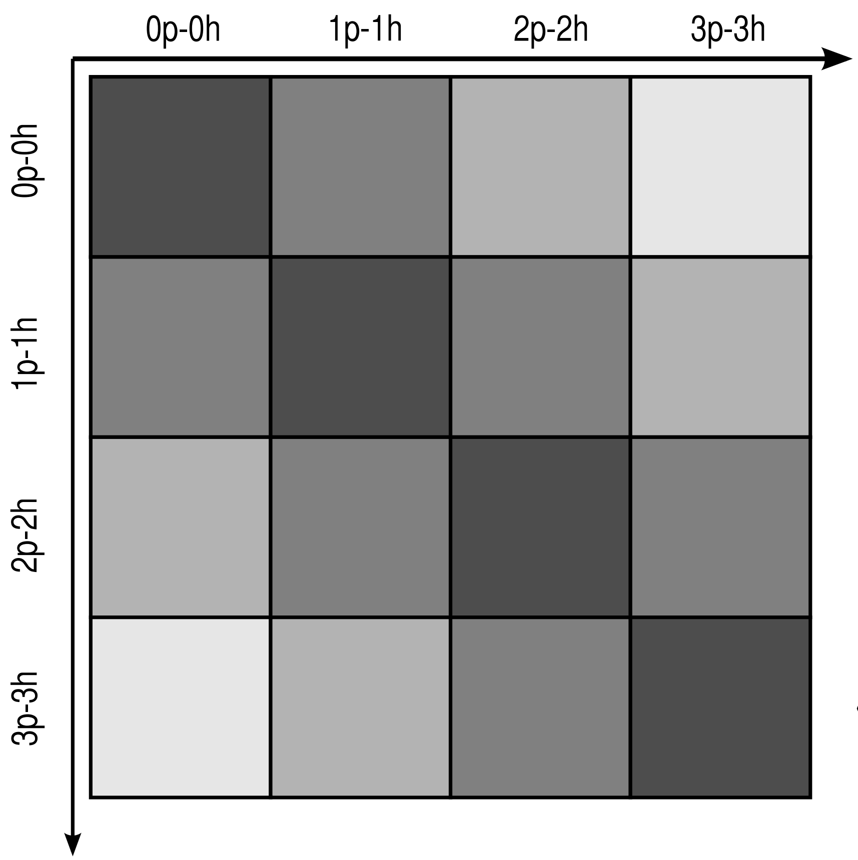


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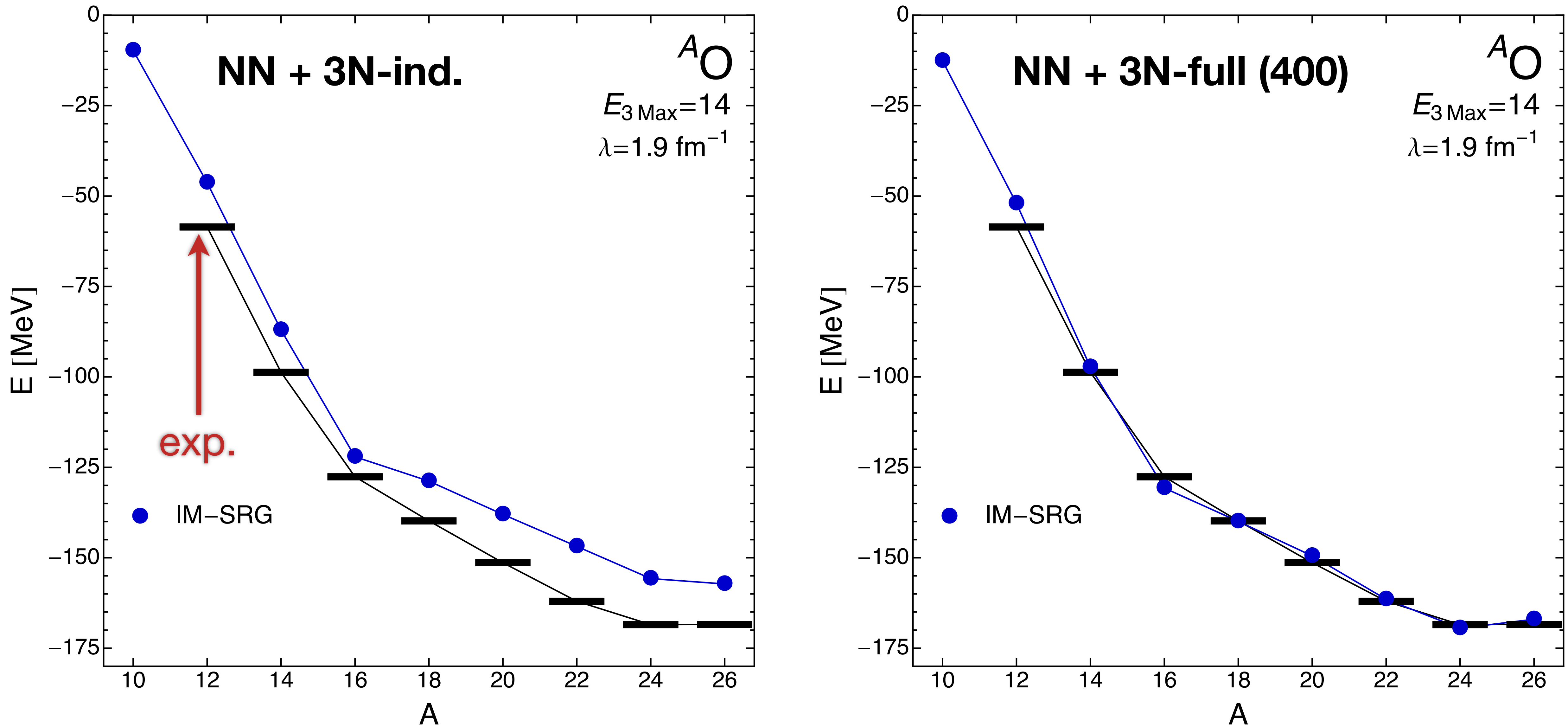
# Results: Oxygen Chain




Phys. Rev. Lett. **110**, 242501 (2013)

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- consistent results from different many-body methods

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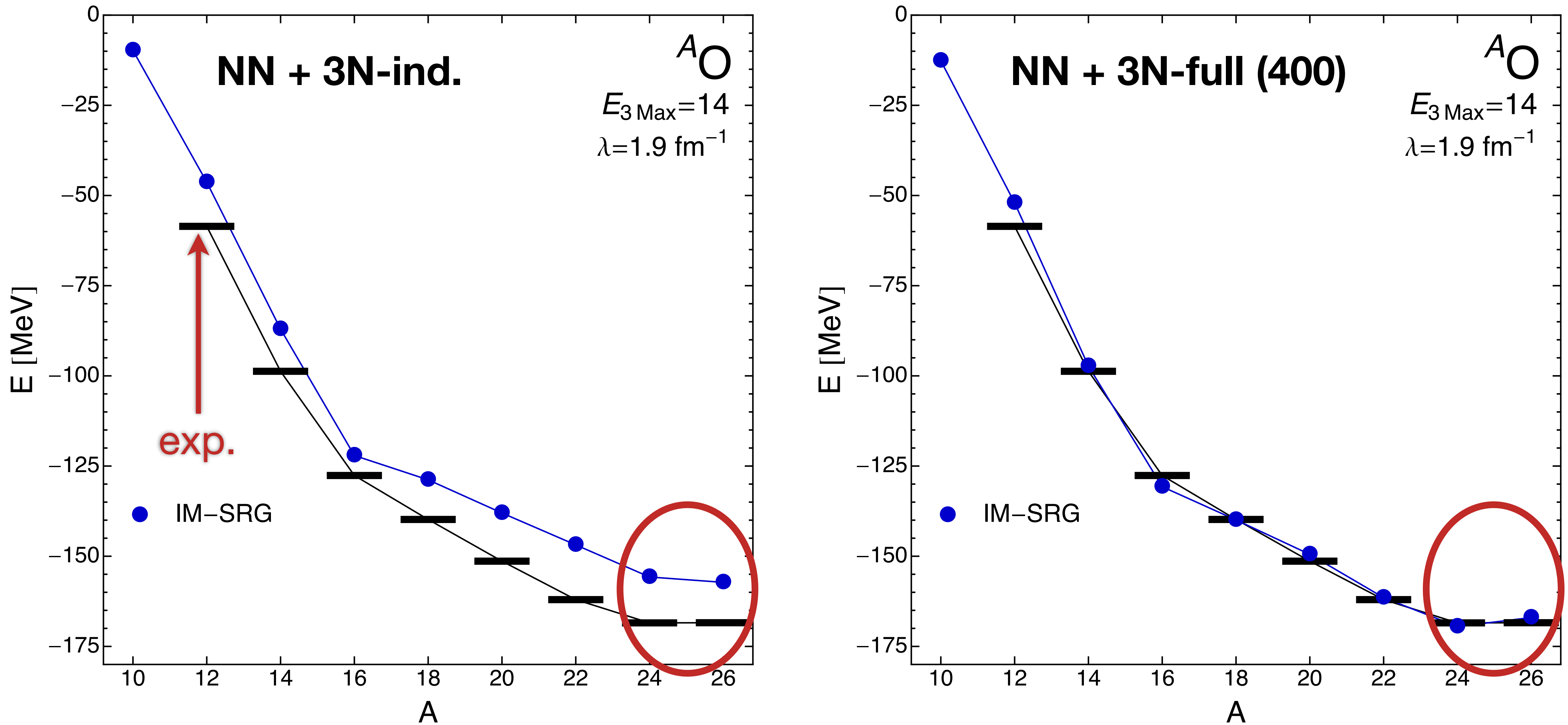


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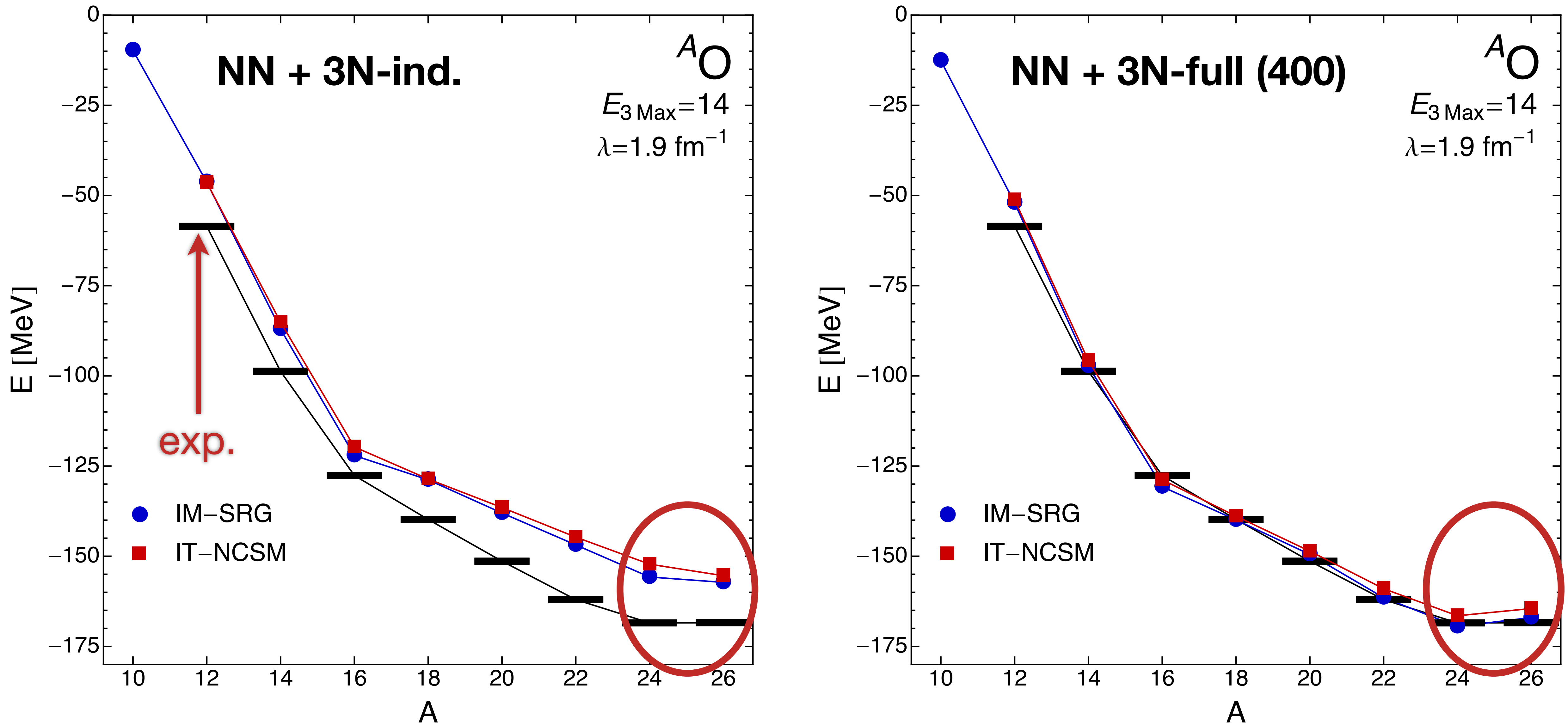


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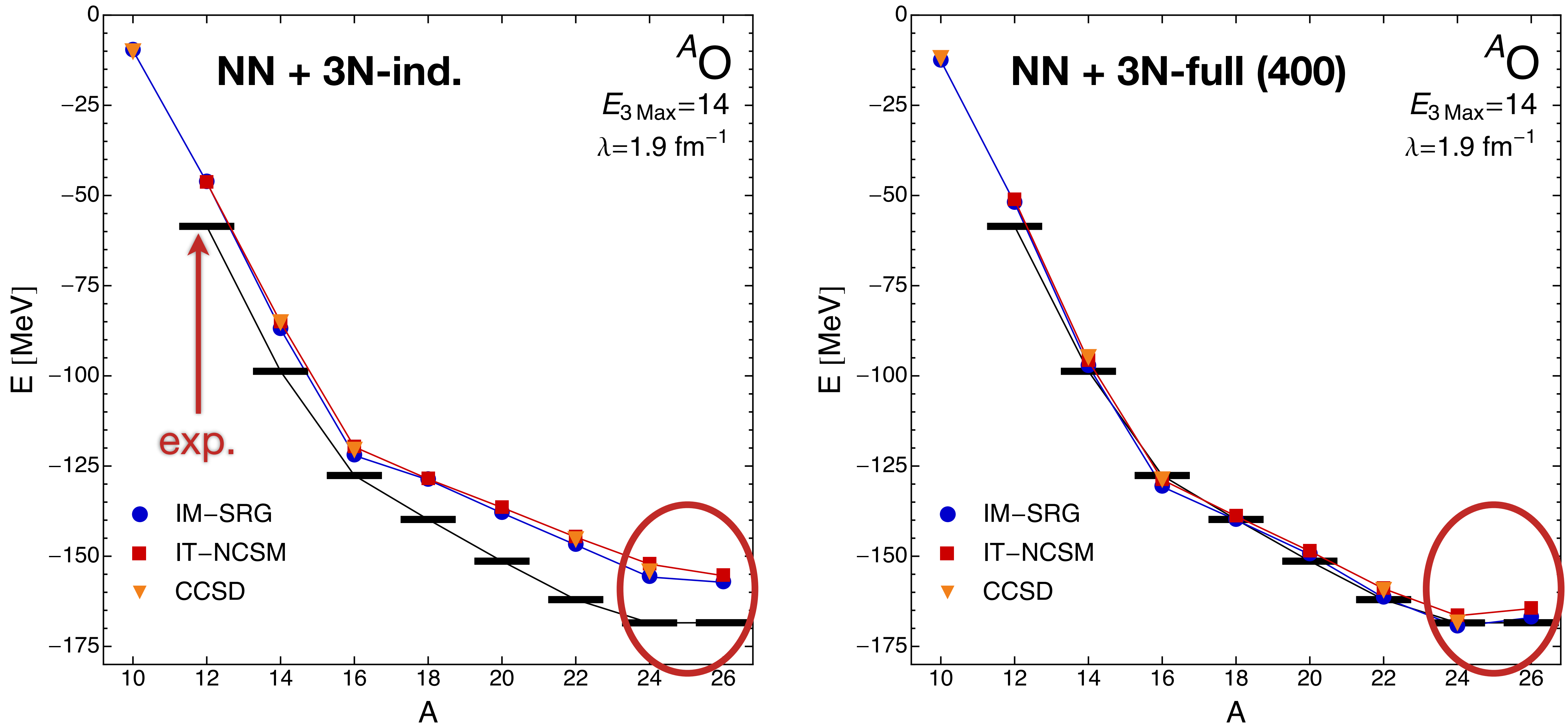


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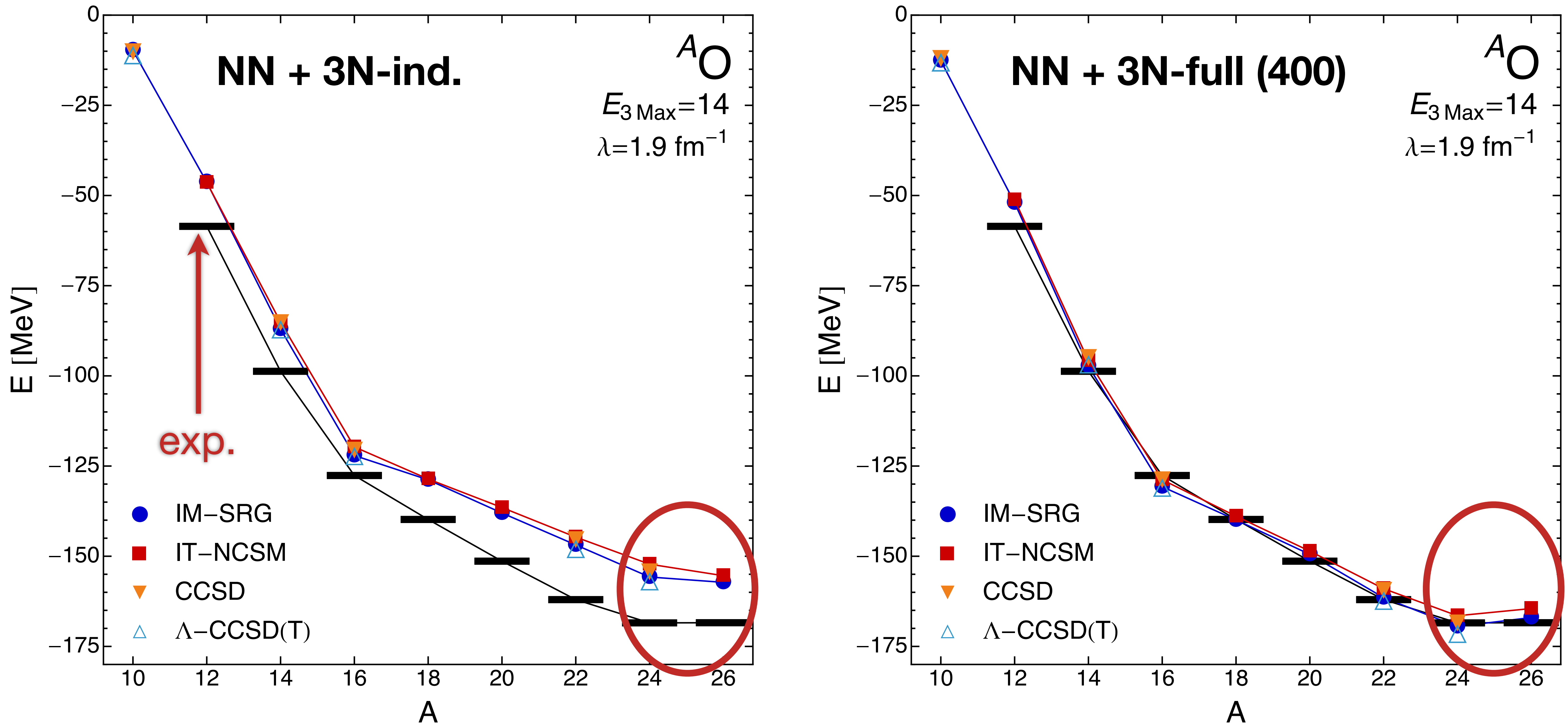


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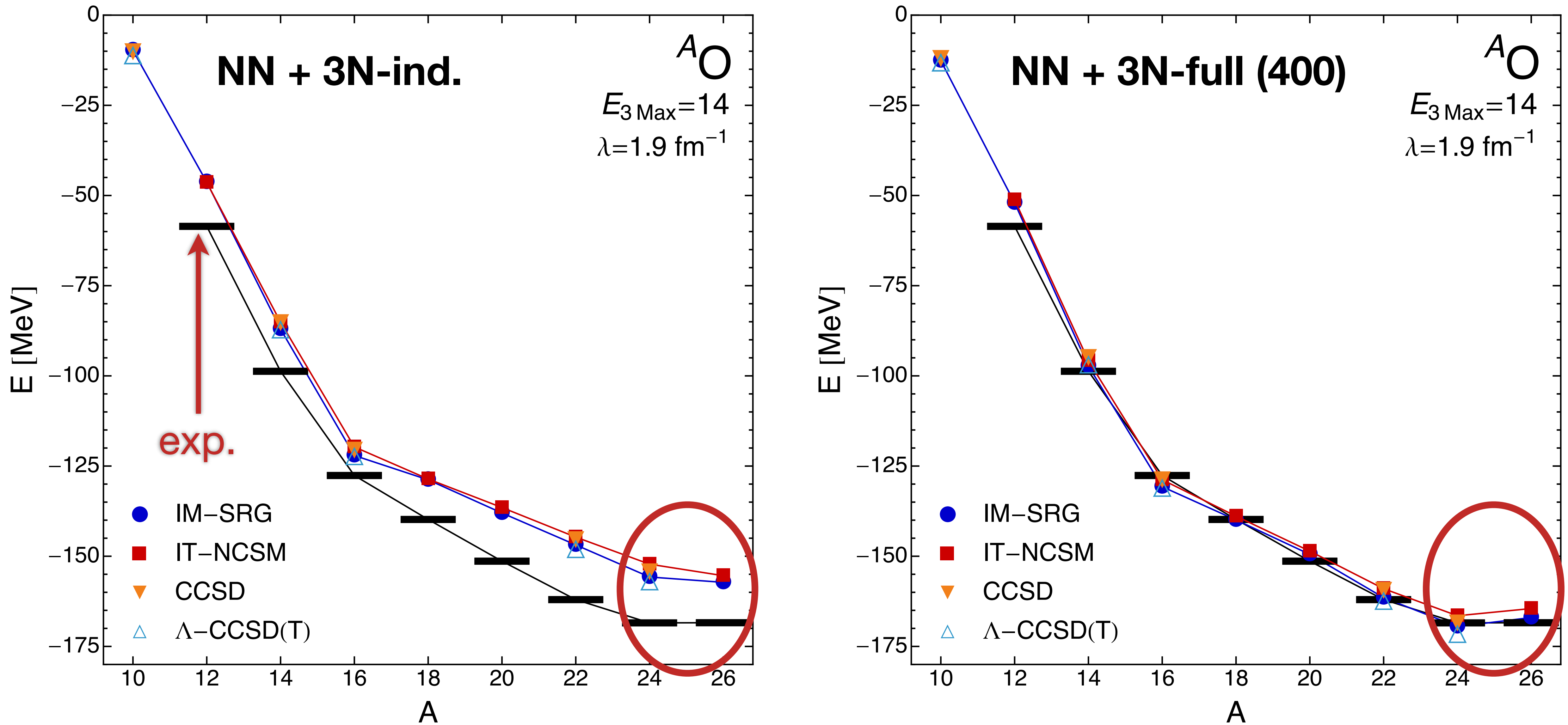


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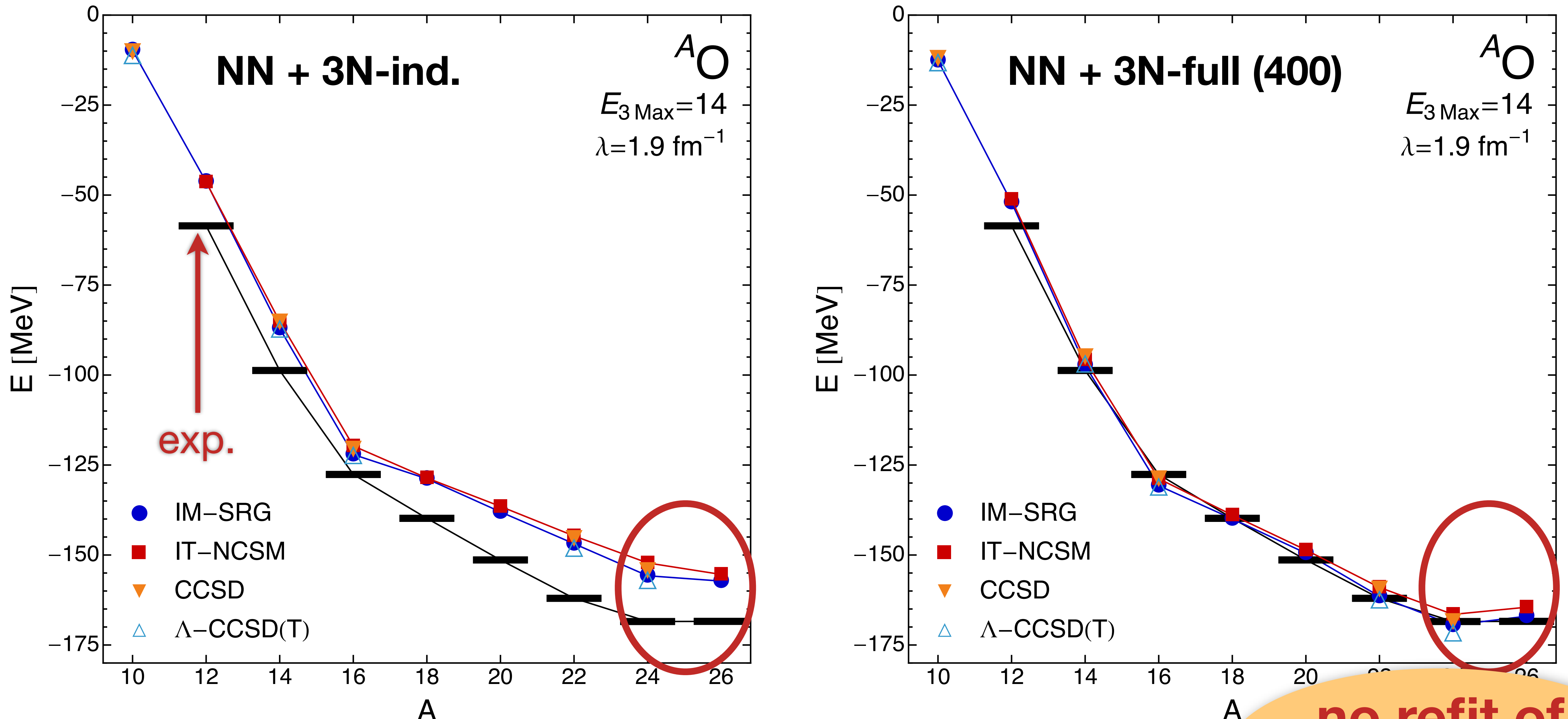


Phys. Rev. Lett. **110**, 242501 (2013)

**no refit of 3N interaction**

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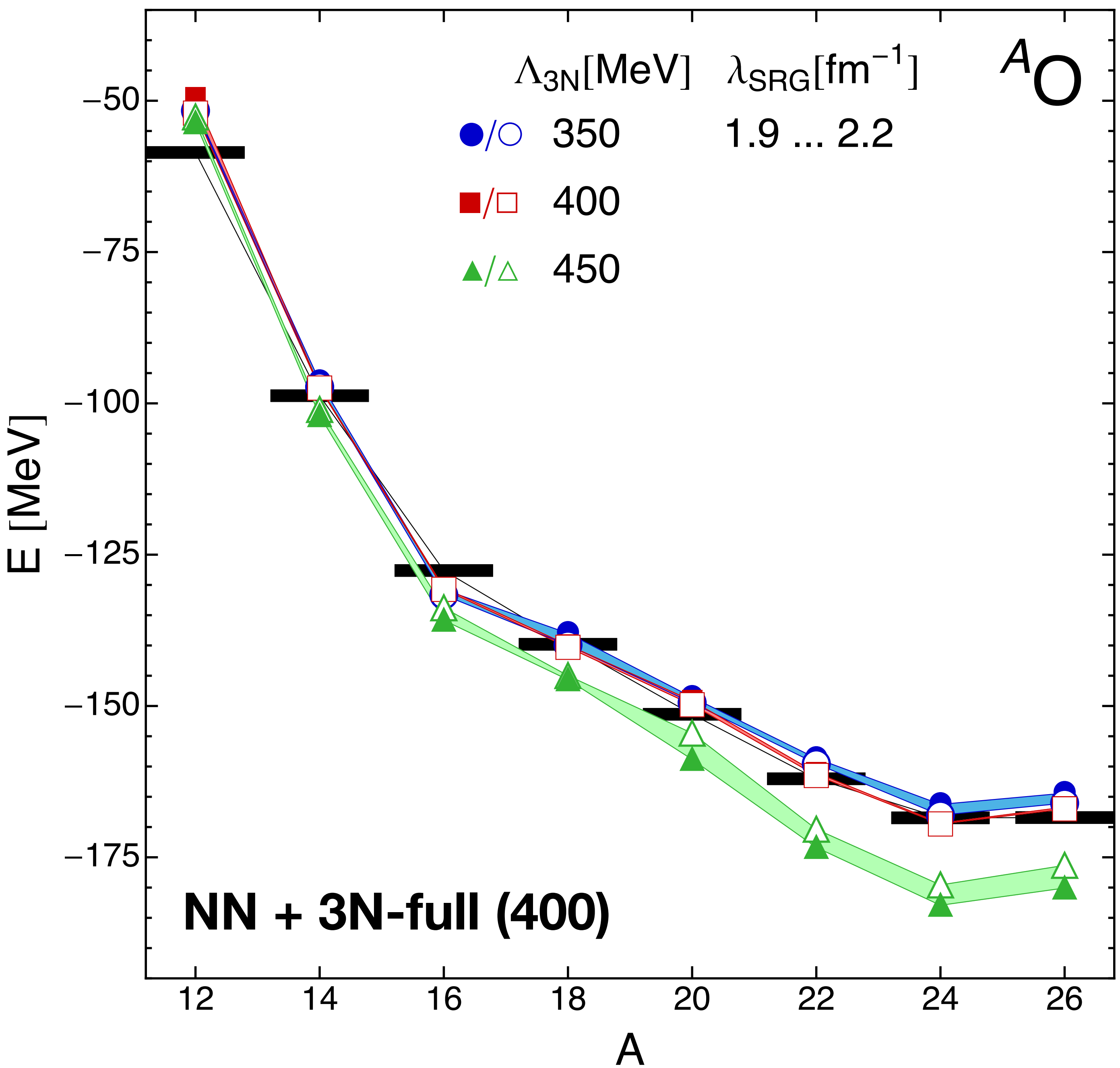
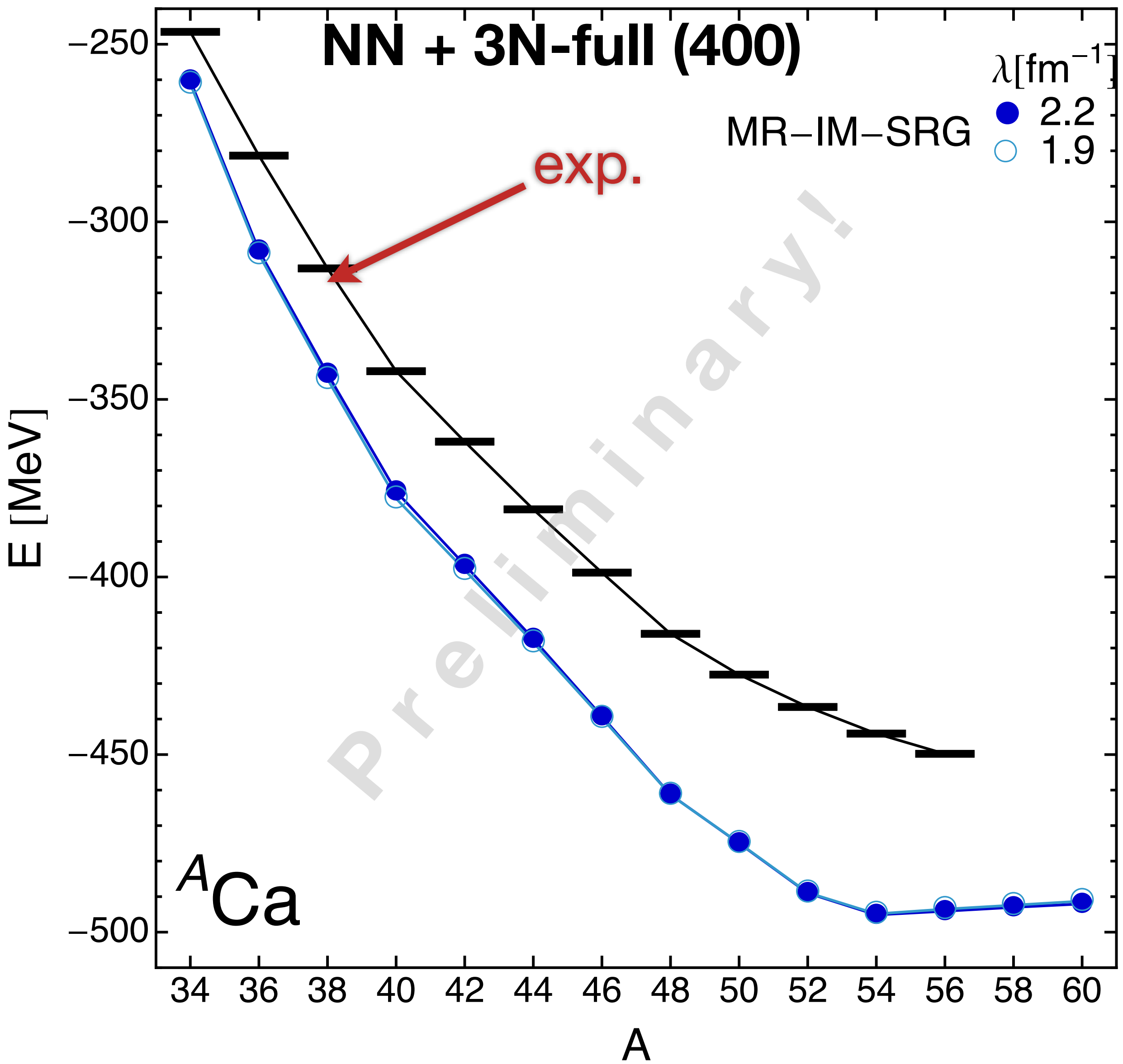
# Variation of Scales




Phys. Rev. Lett. **110**, 242501 (2013)

- variation of **initial 3N cutoff only**
- diagnostics for chiral interactions
- **dripline at A=24 is robust under variations**

# Calcium and Nickel Isotopes

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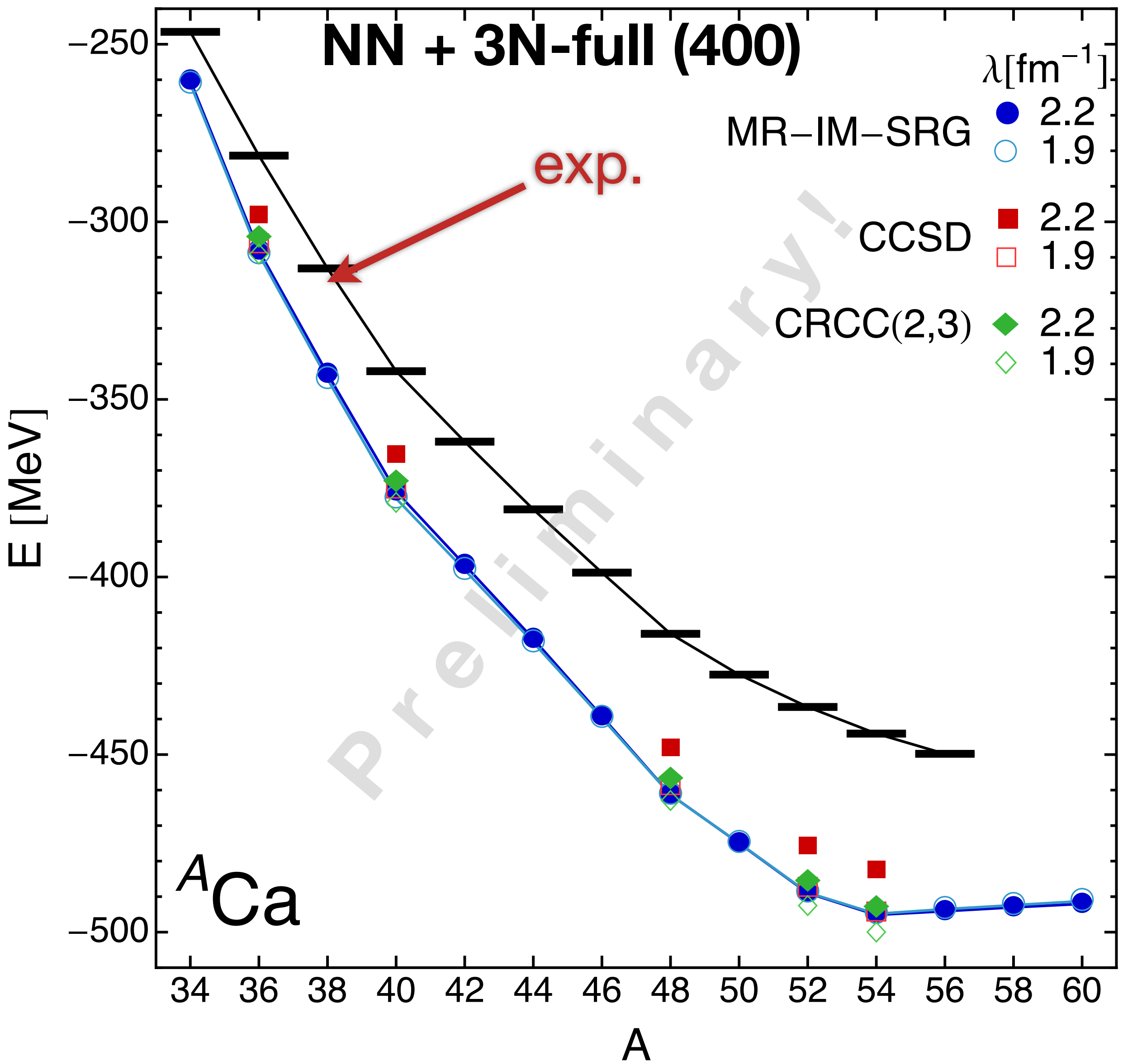


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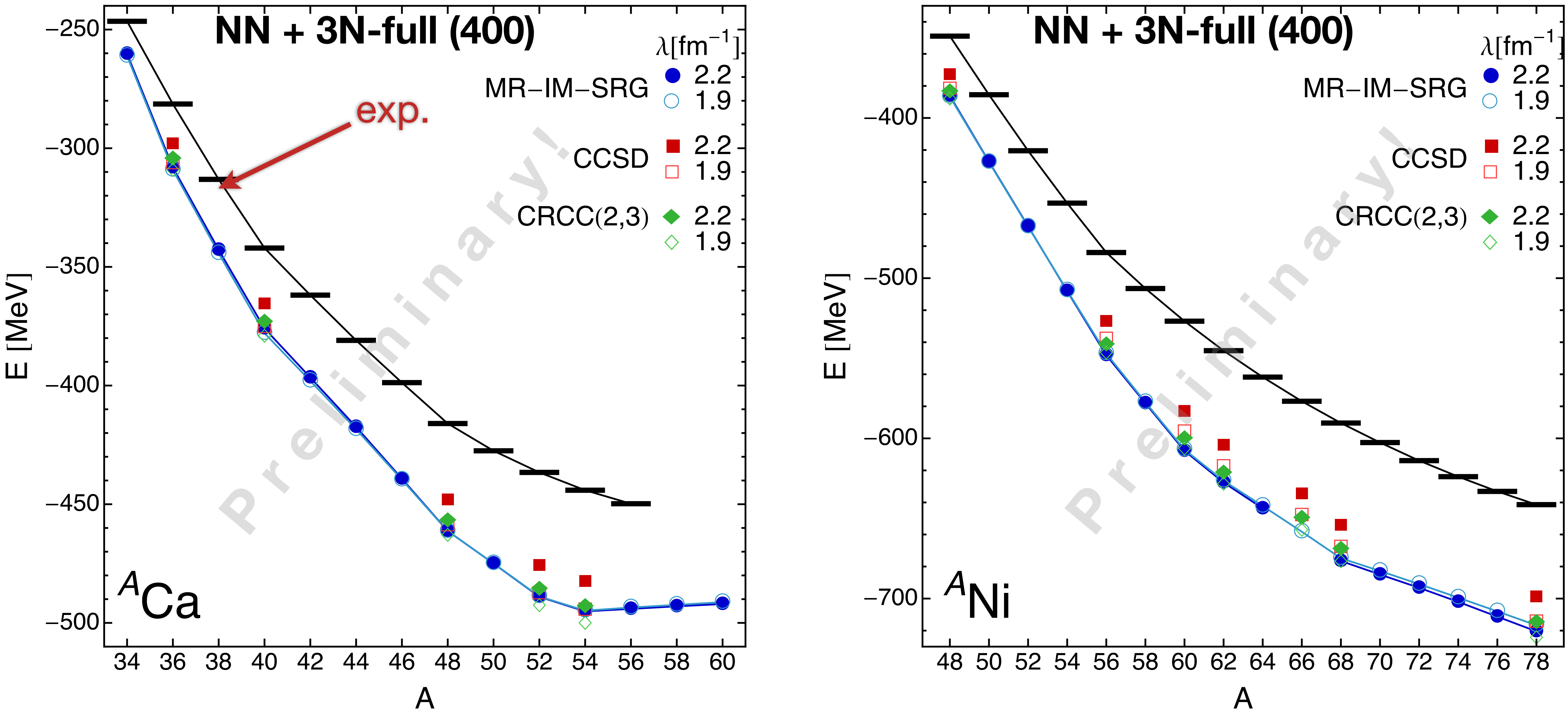


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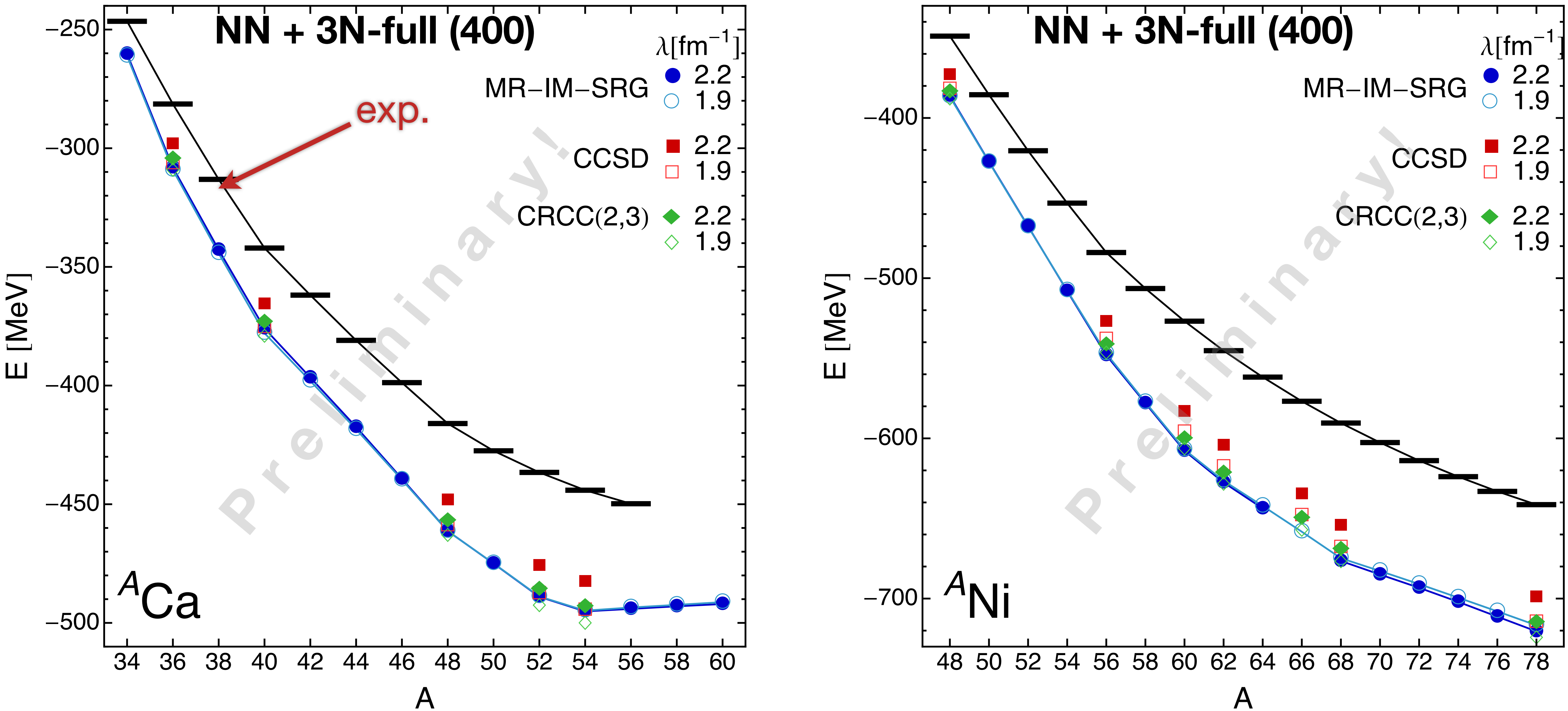


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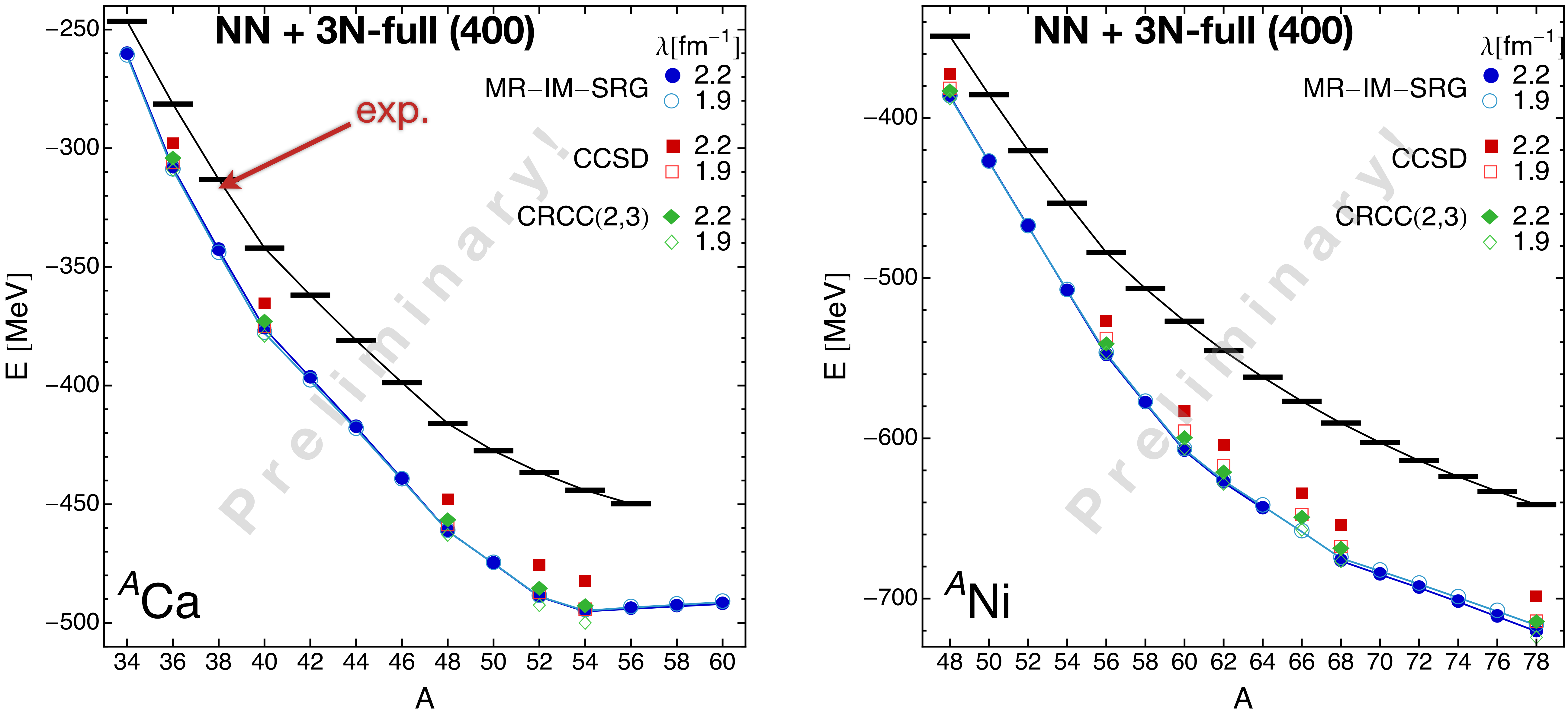


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- calculations for pf-shell nuclei in progress, **heavier nuclei in reach**

# Conclusions

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➡ excited states

# Acknowledgments

THE OHIO STATE UNIVERSITY

**S. Bogner, T. Morris**
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R. J. Furnstahl, R. J. Perry
The Ohio State University

K. A. Wendt
UT-Knoxville & Oak Ridge National Laboratory

P. Papakonstantinou
IBS / Rare Isotope Science Project, S. Korea

NSF — DEPARTMENT OF ENERGY, UNITED STATES OF AMERICA — NUCLEI Nuclear Computational Low-Energy Initiative — Ohio Supercomputer Center

# Supplements

# Normal-Ordering & Wick's Theorem

- define elementary contractions of a one-body operator w.r.t. a given reference state as

$$A^k_l \equiv a^\dagger_k a_l \,, \quad \lambda^k_l \equiv \left\langle \Psi \right| A^k_l \left| \Psi \right\rangle , \quad \xi^k_l \equiv \lambda^k_l - \delta^k_l$$

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- define normal-ordered operators recursively through all possible internal contractions:

$$A^{k_1\dots k_N}_{l_1\dots l_N} = :A^{k_1\dots k_N}_{l_1\dots l_N}: + \lambda^{k_1}_{l_1} :A^{k_2\dots k_N}_{l_2\dots l_N}: + \text{singles}$$
$$+ \left(\lambda^{k_1}_{l_1}\lambda^{k_2}_{l_2} - \lambda^{k_1}_{l_2}\lambda^{k_2}_{l_1}\right) :A^{k_3\dots k_N}_{l_3\dots l_N}: + \text{doubles} + \dots$$

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THE OHIO STATE UNIVERSITY

- define elementary contractions of a one-body operator w.r.t. a given reference state as

$$A^{k}_{l} \equiv a^{\dagger}_{k} a_{l}\,, \quad \lambda^{k}_{l} \equiv \left\langle \Psi \right| A^{k}_{l} \left| \Psi \right\rangle, \quad \xi^{k}_{l} \equiv \lambda^{k}_{l} - \delta^{k}_{l}$$

- define normal-ordered operators recursively through all possible internal contractions:

$$A^{k_1\ldots k_N}_{l_1\ldots l_N} = :A^{k_1\ldots k_N}_{l_1\ldots l_N}: + \lambda^{k_1}_{l_1} :A^{k_2\ldots k_N}_{l_2\ldots l_N}: + \text{singles}$$
$$+ \left(\lambda^{k_1}_{l_1}\lambda^{k_2}_{l_2} - \lambda^{k_1}_{l_2}\lambda^{k_2}_{l_1}\right) :A^{k_3\ldots k_N}_{l_3\ldots l_N}: + \text{doubles} + \ldots$$

- Wick's Theorem: products of normal-ordered operators can be expanded in terms of external contractions alone

$$:A^{k_1\ldots k_N}_{m_1\ldots m_N}::A^{l_1\ldots l_N}_{n_1\ldots n_N}: = (-1)^{N-1}\lambda^{k_1}_{n_1} :A^{k_2\ldots k_N l_1\ldots l_N}_{m_1\ldots m_N n_2\ldots n_N}:$$
$$+ (-1)^{N-1}\xi^{l_1}_{m_1} :A^{k_1\ldots k_N l_2\ldots l_N}_{m_2\ldots m_N n_1\ldots n_N}: + \ldots$$

# In-Medium SRG Flow Equations

## 0-body Flow

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\left(\eta^a_b f^b_a - f^a_b \eta^b_a\right) + \frac{1}{4}\sum_{abcd}\left(\eta^{ab}_{cd}\Gamma^{cd}_{ab} - \Gamma^{ab}_{cd}\eta^{cd}_{ab}\right) n_a n_b \bar{n}_c \bar{n}_d$$

## 1-body Flow

$$\frac{d}{ds}f^1_2 = \sum_a \left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b)$$
$$+ \frac{1}{2}\sum_{abcdef}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)$$

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$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\left(\eta^a_b f^b_a - f^a_b \eta^b_a\right) + \frac{1}{4}\sum_{abcd}\left(\eta^{ab}_{cd}\Gamma^{cd}_{ab} - \Gamma^{ab}_{cd}\eta^{cd}_{ab}\right) n_a n_b \bar{n}_c \bar{n}_d$$

~ 2nd order MBPT for *H(s)*

## 1-body Flow

$$\frac{d}{ds}f^1_2 = \sum_a\left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b)$$
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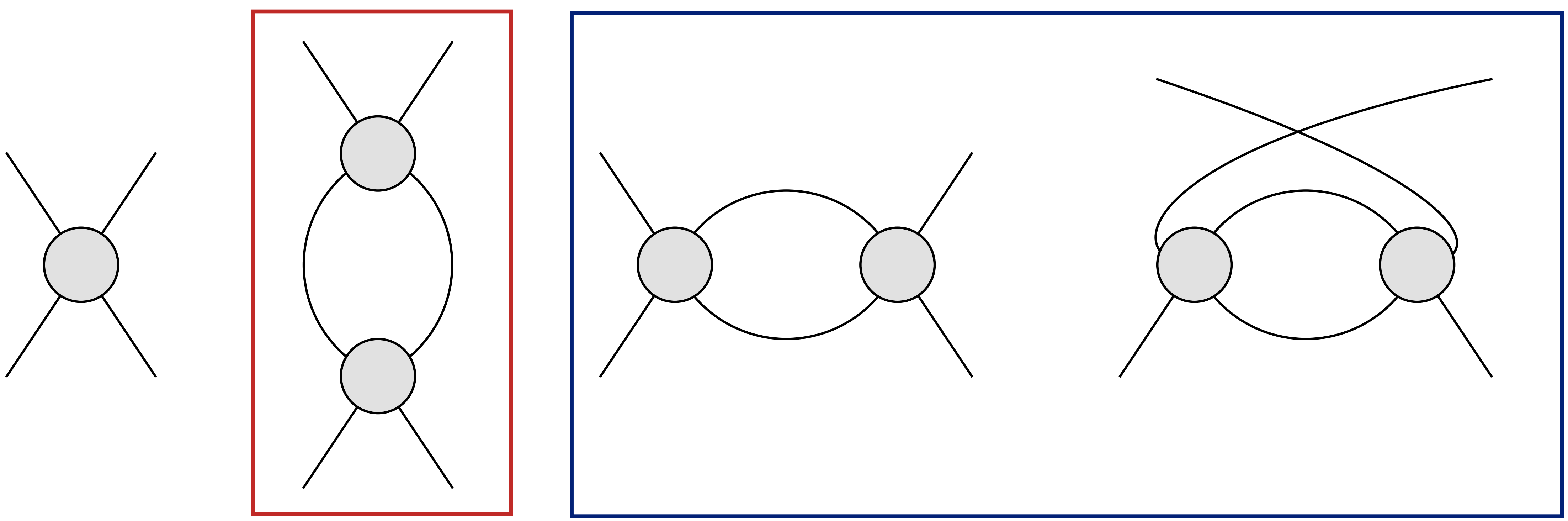
# In-Medium SRG Flow Equations

## 2-body Flow

$$\frac{d}{ds}\Gamma^{12}_{34} = \sum_a \left(\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\right)$$

$$+ \frac{1}{2}\sum_{ab}\underline{\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b)}$$

$$+ \sum_{ab}\underline{(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)}$$



# In-Medium SRG Flow Equations

## 2-body Flow

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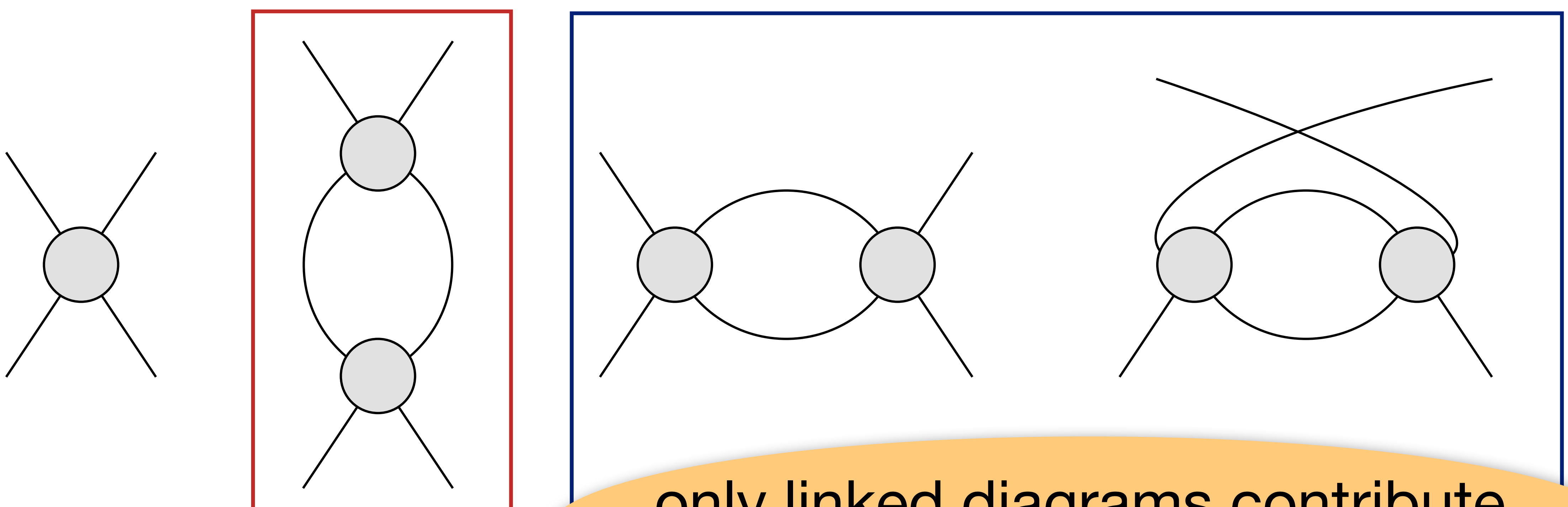

only linked diagrams contribute, IM-SRG size-extensive

# Particle-Number Projected HFB State

- HFB ground state is a superposition of states with different particle number:

$$\left|\Psi\right\rangle = \sum_{A=N,N\pm2,\dots} c_A \left|\Psi_A\right\rangle\,, \qquad \left|\Psi_N\right\rangle \equiv P_N \left|\Psi\right\rangle \equiv \frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{i\phi(\hat{N}-N)} \left|\Psi\right\rangle$$

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- calculate one- and two-body densities (project only once):

$$\lambda^k_l = \frac{\left\langle\Psi\right| A^k_l P_N \left|\Psi\right\rangle}{\left\langle\Psi\middle|\Psi\right\rangle}, \quad \lambda^{kl}_{mn} = \frac{\left\langle\Psi\right| A^{kl}_{mn} P_N \left|\Psi\right\rangle}{\left\langle\Psi\middle|\Psi\right\rangle} - \lambda^k_m \lambda^l_m + \lambda^k_n \lambda^l_m$$

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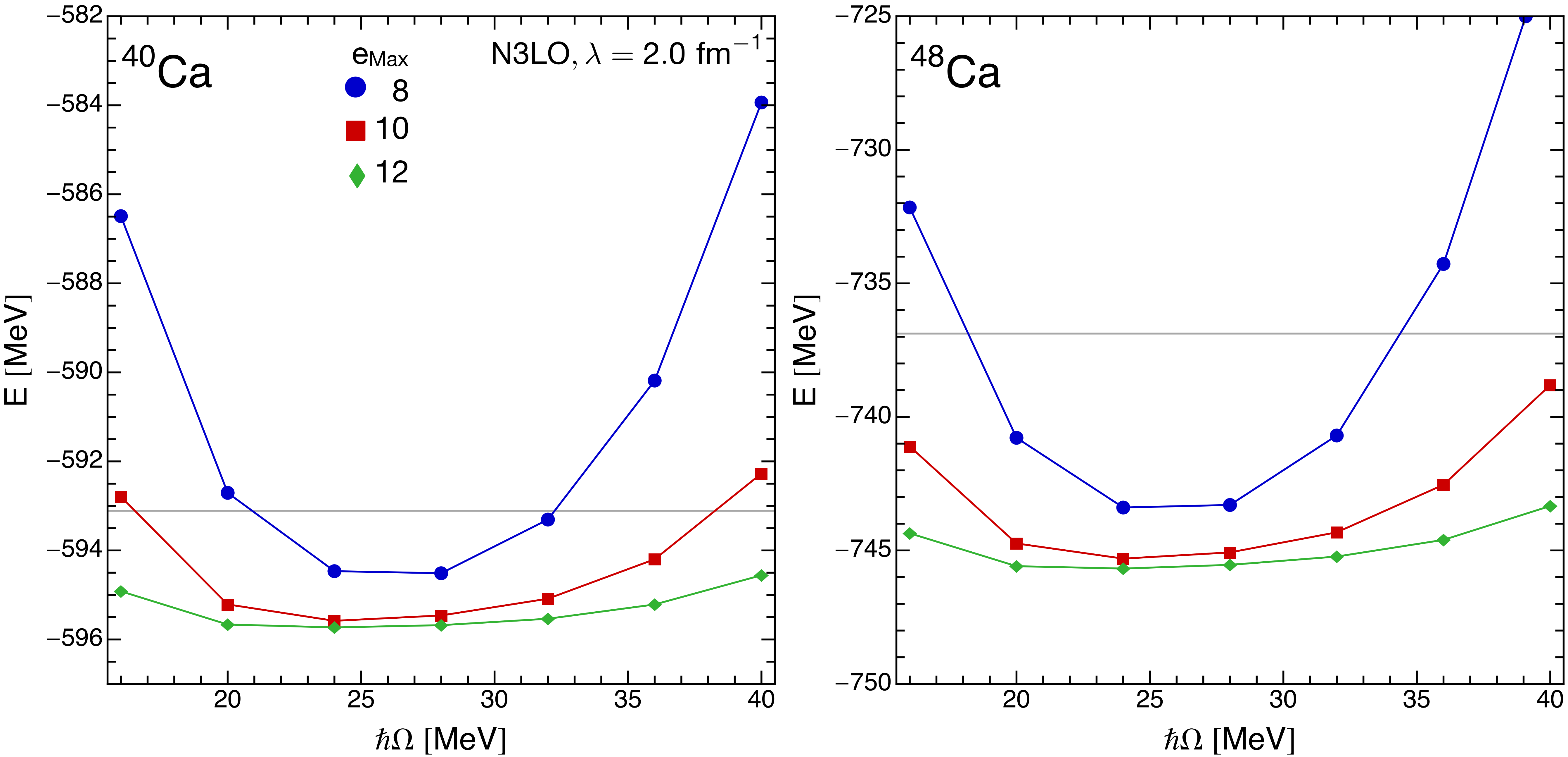
- work in natural orbitals (= HFB canonical basis):

$$\lambda^k_l = n_k\delta^k_l \left(= v_k^2\delta^k_l\right)\,, \quad 0 \le n_k \le 1$$

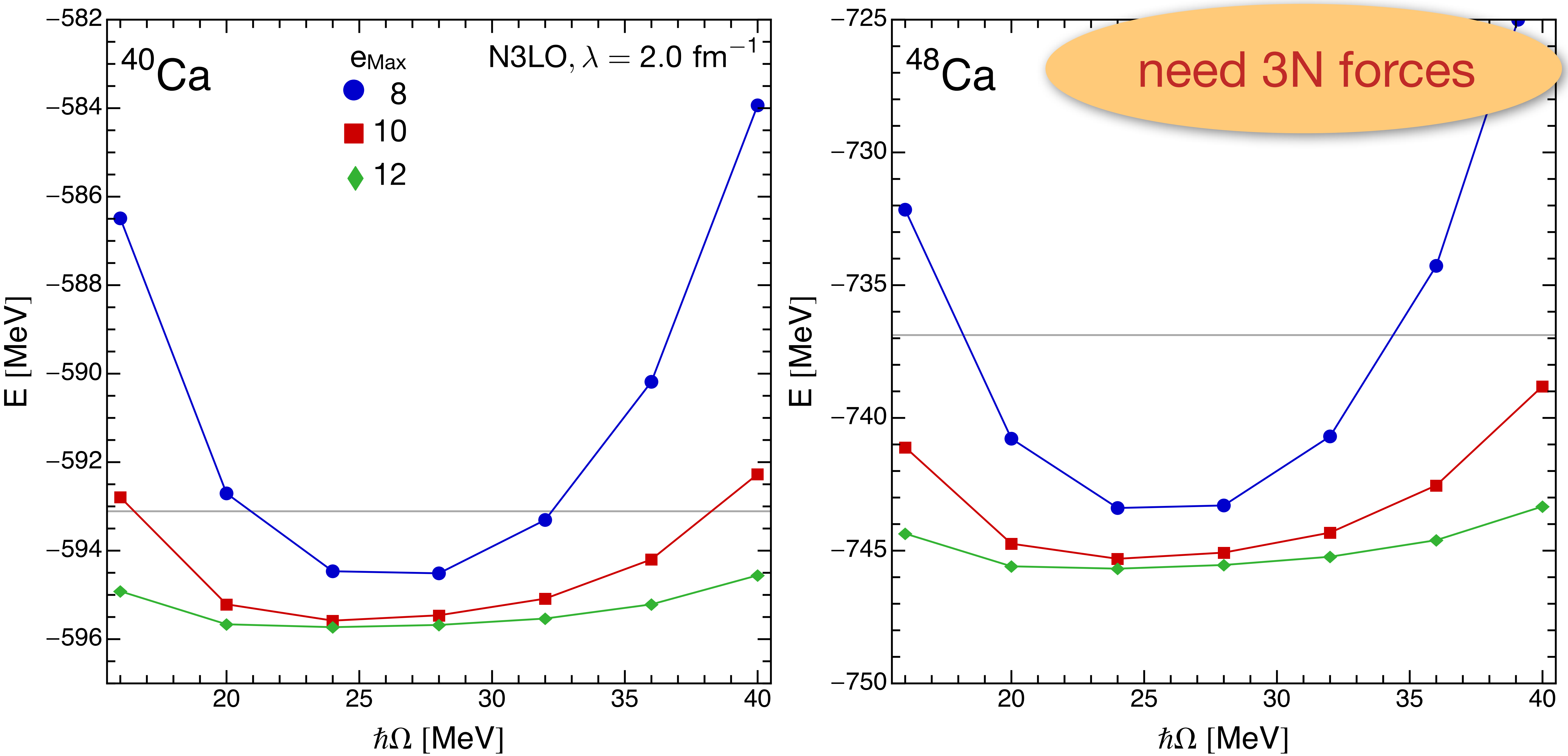
# Results




[gray lines: CCSD by S. Binder, $e_{\text{Max}} = 12, \hbar\Omega = 20$ MeV]

converged g.s. energies between CCSD and Λ-CCSD(T)

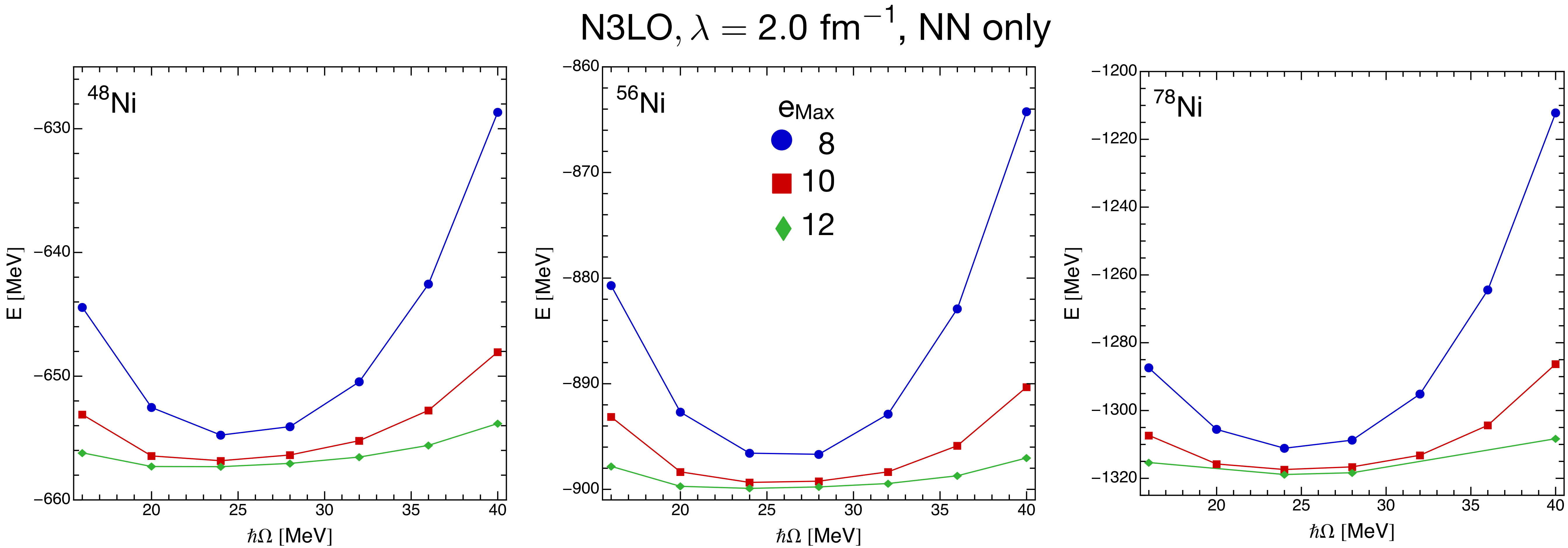
# Results




[gray lines: CCSD by S. Binder, $e_{\text{Max}} = 12, \hbar\Omega = 20$ MeV]

converged g.s. energies between CCSD and Λ-CCSD(T)

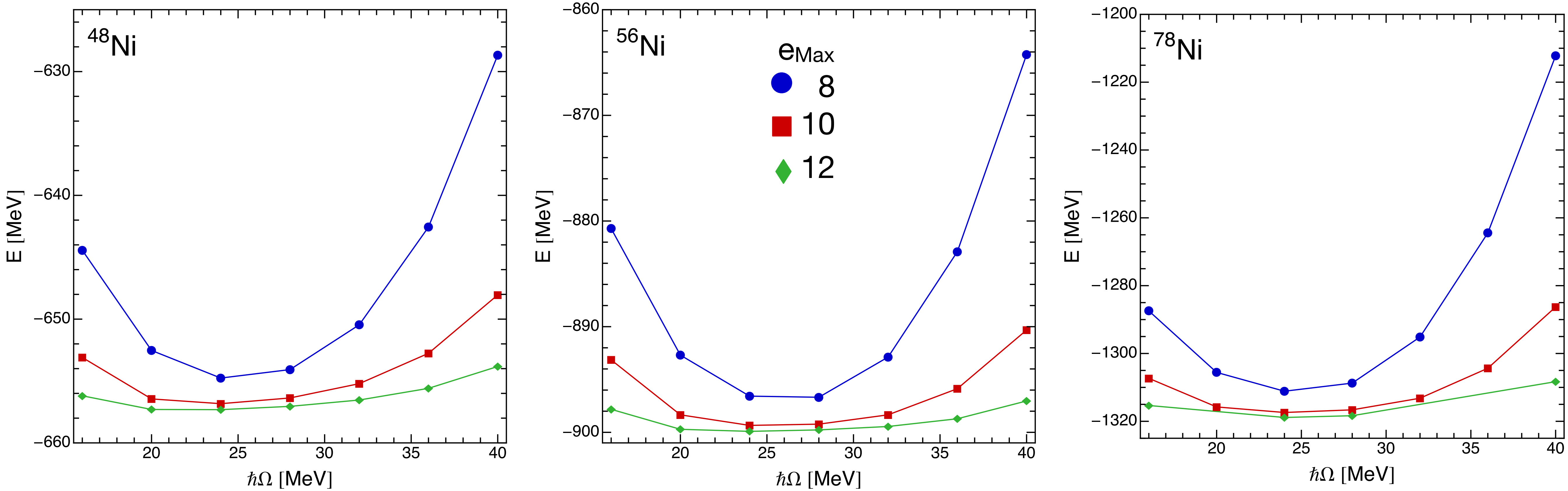
# Isotopic "Chains"




- "closed-shell" Ni and Sn isotopes can give insight into isovector interaction...

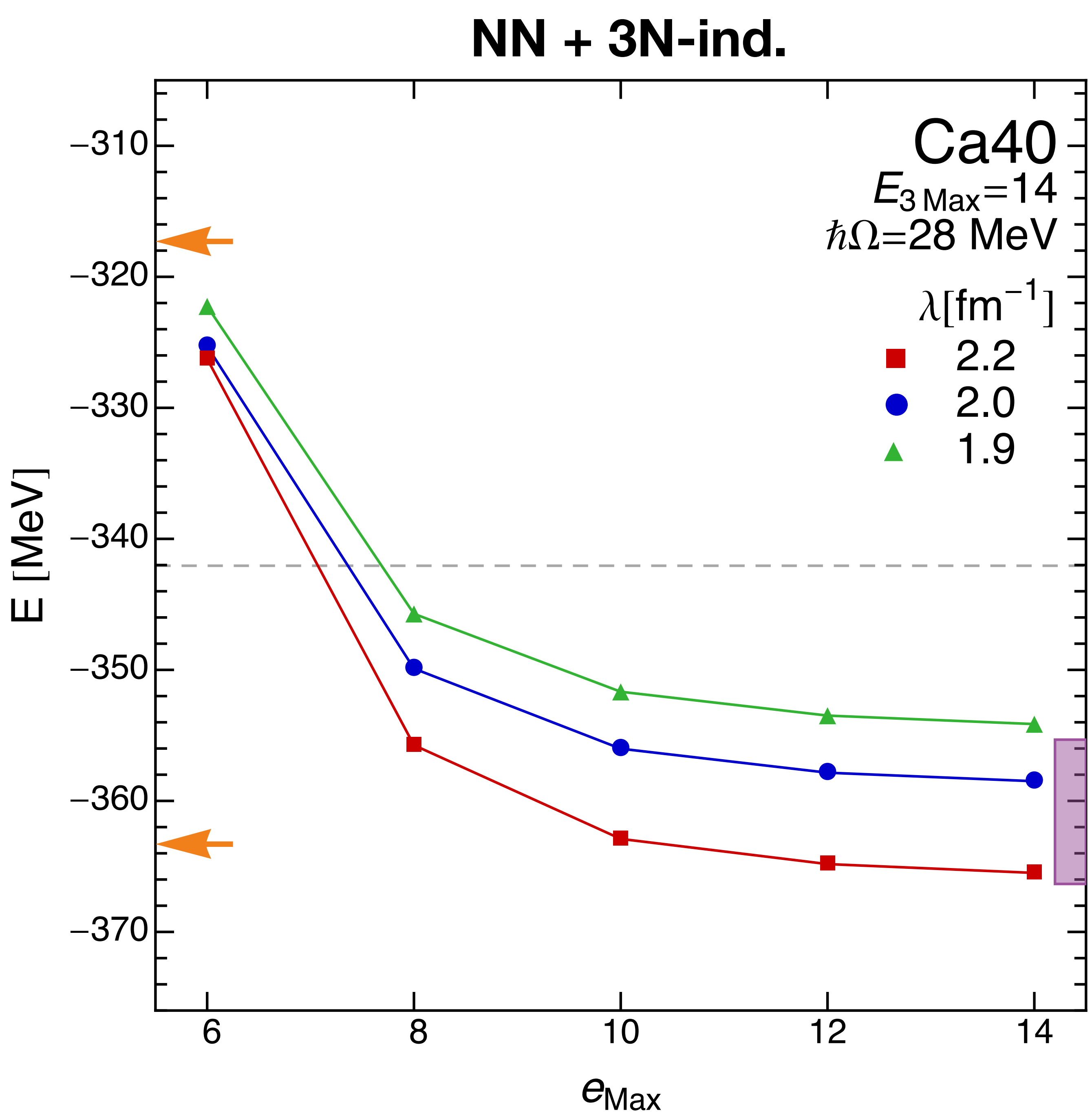
# Isotopic "Chains"

N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}$, NN only




- "closed-shell" Ni and Sn isotopes can give insight into isovector interaction...
- ... but complete isotopic chains would be preferable, i.e., devise an approach to open-shell nuclei

# Results: Closed-Shell Nuclei

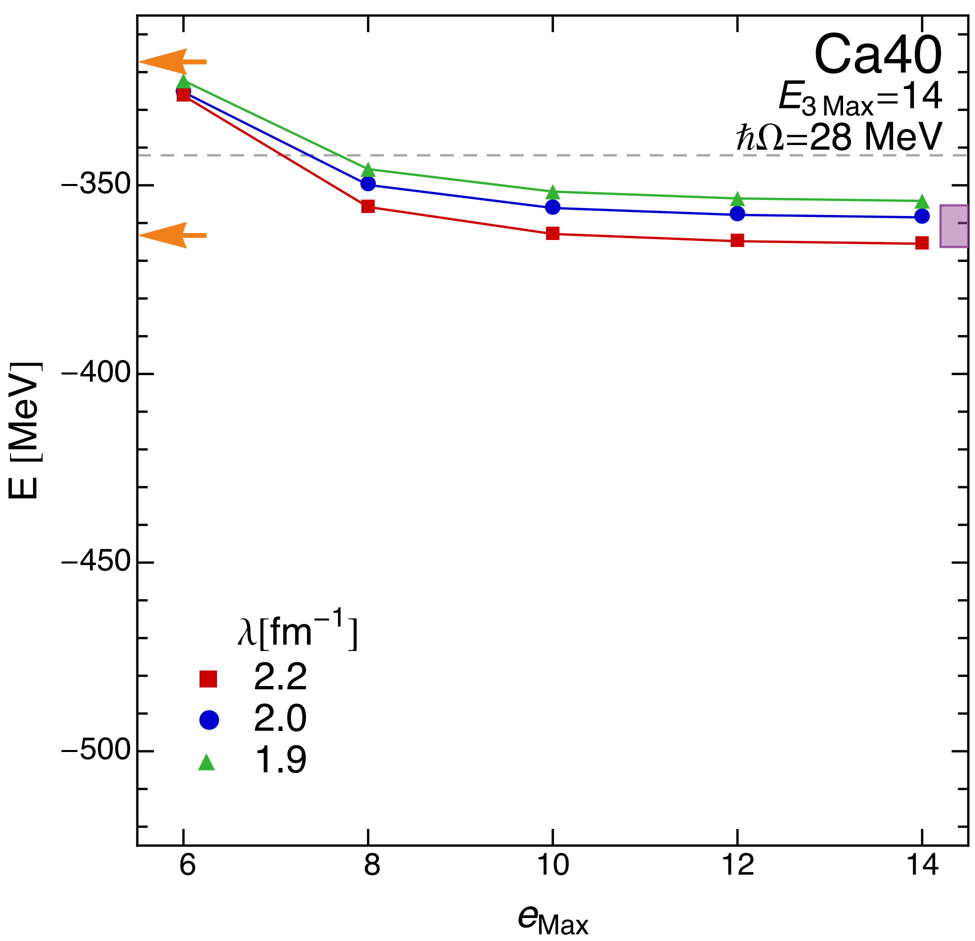



CCSD/Λ-CCSD(T), $\lambda = \infty$ , G. Hagen et al., PRL 109, 032502 (2012)

Λ-CCSD(T), $\lambda = 1.9 - 2.2\ \mathrm{fm}^{-1}$ , S.Binder et al., arXiv:1211.4748 [nucl-th] & PRL 109, 052501 (2012)

# Results: Closed-Shell Nuclei

**NN + 3N-ind.**




CCSD/Λ-CCSD(T), $\lambda = \infty$ , G. Hagen et al., PRL 109, 032502 (2012)

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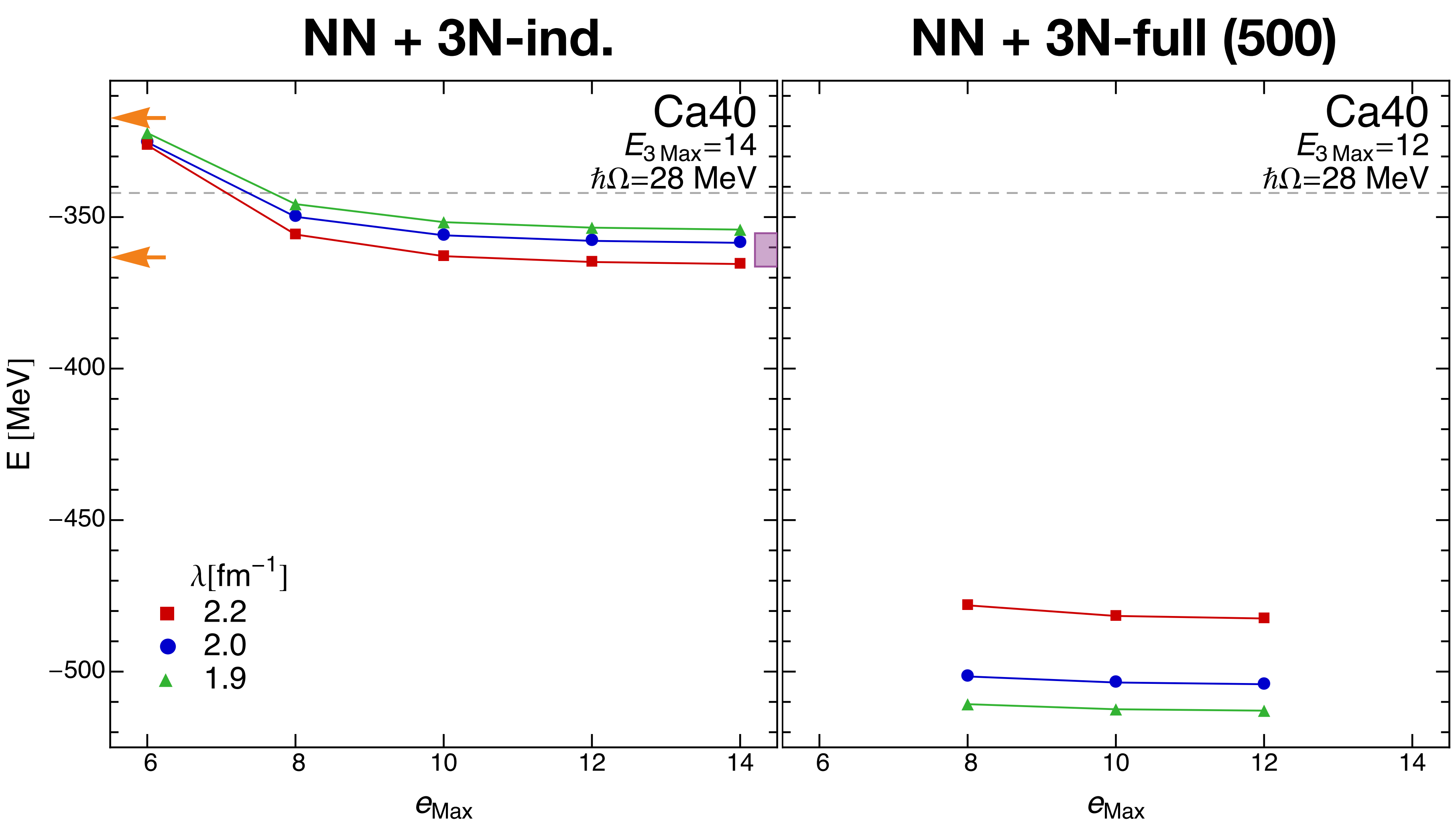


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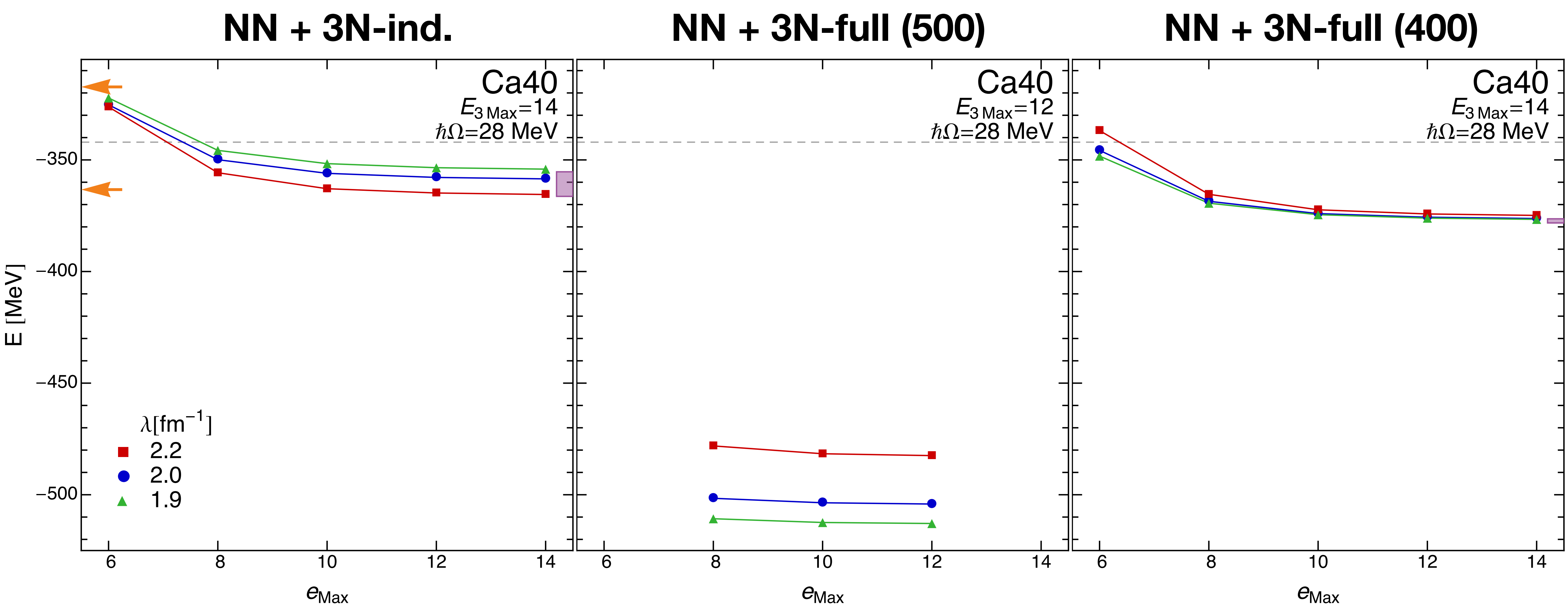


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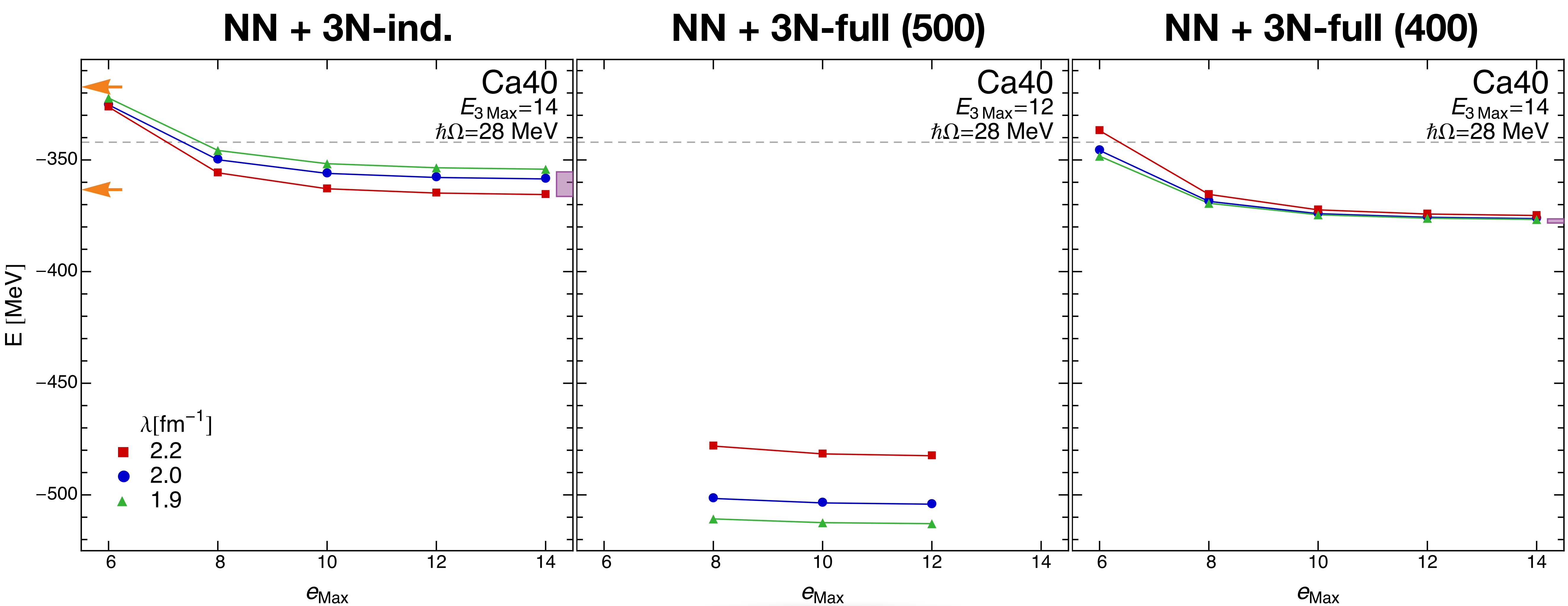
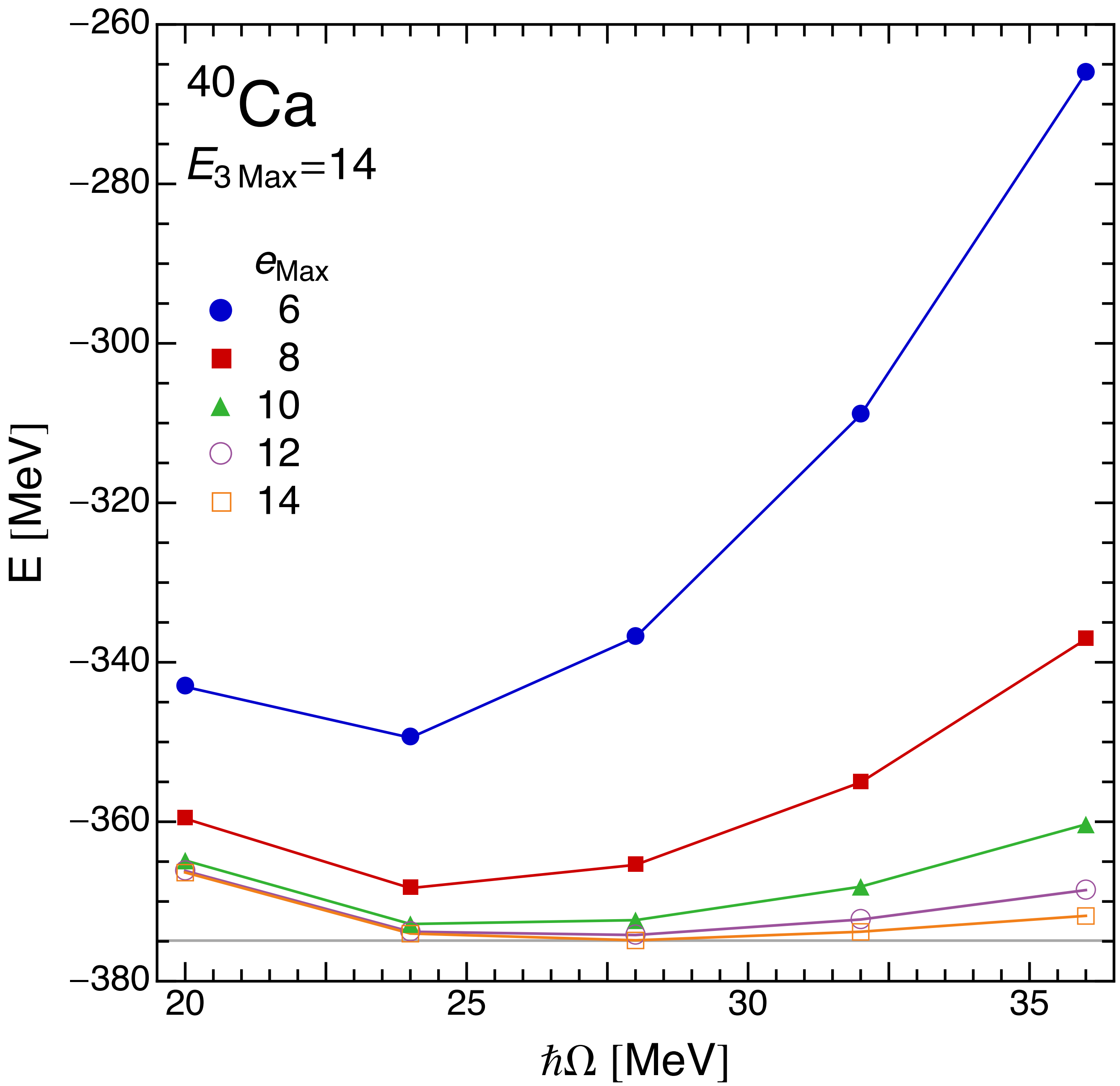


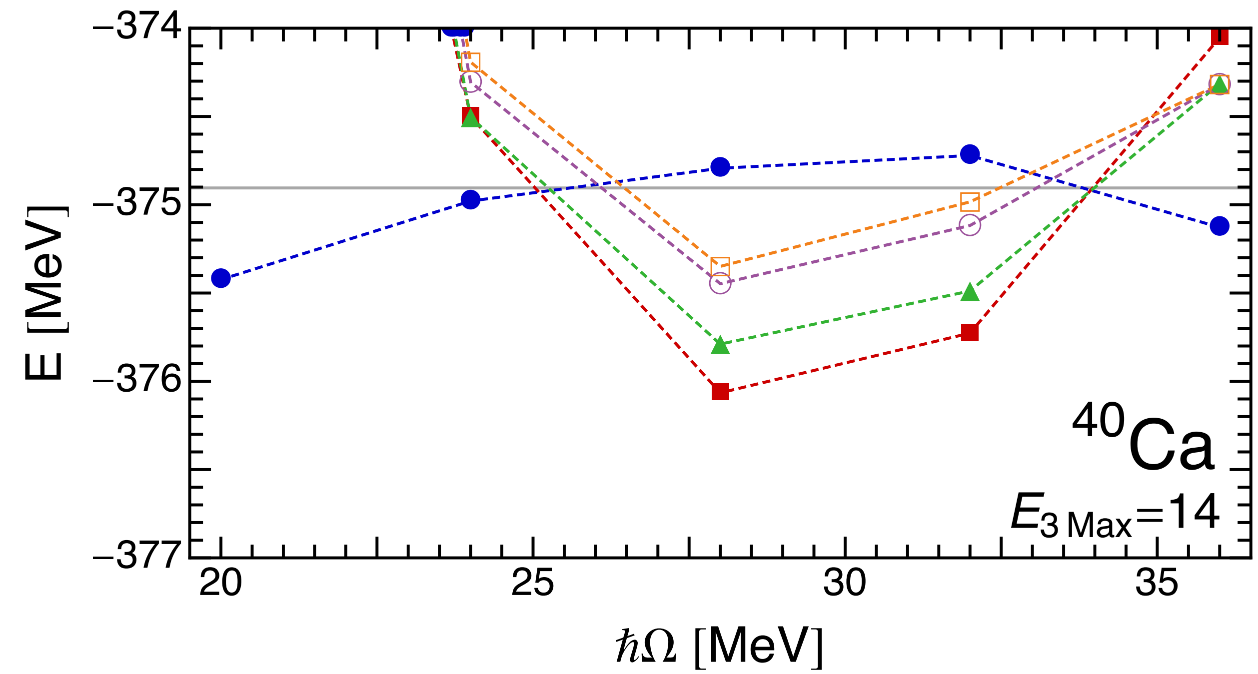

**validate chiral Hamiltonians**

CCSD/Λ-CCSD(T), $\lambda = \infty$ , G. Hagen et al., PRL 109, 032502 (2012)

Λ-CCSD(T), $\lambda = 1.9 - 2.2\ \mathrm{fm}^{-1}$ , S.Binder et al., arXiv:1211.4748 [nucl-th] & PRL 109, 052501 (2012)

# Extrapolation




max./UV momentum:

$$\Lambda_{\mathrm{UV}} = \sqrt{2m(e_{\mathrm{Max}} + 3/2)\hbar\Omega}$$

radial extent:

$$L = \sqrt{2(e_{\mathrm{Max}} + 3/2)\hbar/m\Omega}$$

simultaneous ultraviolet & infrared extrapolation:

$$E(\Lambda_{\mathrm{UV}}, L) = E_{\infty} + A_0 \exp\left(-2\Lambda_{\mathrm{UV}}^2/A_1^2\right) + A_2 \exp\left(-2k_{\infty}L\right)$$

(R. Furnstahl, G. Hagen & T. Papenbrock, PRC 86,031301 (2012))

# Multi-Reference Flow Equations

## 0-body flow:

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\left(\eta^a_b f^b_a - f^a_b \eta^b_a\right) + \frac{1}{4}\sum_{abcd}\left(\eta^{ab}_{cd}\Gamma^{cd}_{ab} - \Gamma^{ab}_{cd}\eta^{cd}_{ab}\right) n_a n_b \bar{n}_c \bar{n}_d$$

$$+ \frac{1}{4}\sum_{abcd}\left(\frac{d}{ds}\Gamma^{ab}_{cd}\right)\lambda^{ab}_{cd} + \frac{1}{4}\sum_{abcdklm}\left(\eta^{ab}_{cd}\Gamma^{kl}_{am} - \Gamma^{ab}_{cd}\eta^{kl}_{am}\right)\lambda^{bkl}_{cdm}$$

## 1-body flow:

$$\frac{d}{ds}f^1_2 = \sum_a\left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b)$$

$$+ \frac{1}{2}\sum_{abcdef}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)$$

$$+ \frac{1}{4}\sum_{abcde}\left(\eta^{1a}_{bc}\Gamma^{de}_{2a} - \Gamma^{1a}_{bc}\eta^{de}_{2a}\right)\lambda^{de}_{bc} + \sum_{abcde}\left(\eta^{1a}_{bc}\Gamma^{be}_{2d} - \Gamma^{1a}_{bc}\eta^{be}_{2d}\right)\lambda^{ae}_{cd}$$

$$- \frac{1}{2}\sum_{abcde}\left(\eta^{1a}_{2b}\Gamma^{cd}_{ae} - \Gamma^{1a}_{2b}\eta^{cd}_{ae}\right)\lambda^{cd}_{be} + \frac{1}{2}\sum_{abcde}\left(\eta^{1a}_{2b}\Gamma^{bc}_{de} - \Gamma^{1a}_{2b}\eta^{bc}_{de}\right)\lambda^{ac}_{de}$$

# Multi-Reference Flow Equations

2-body flow:

$$\frac{d}{ds}\Gamma^{12}_{34} = \sum_a \left(\eta^1_a\Gamma^{a2}_{34} + \eta^2_a\Gamma^{1a}_{34} - \eta^a_3\Gamma^{12}_{a4} - \eta^a_4\Gamma^{12}_{3a} - f^1_a\eta^{a2}_{34} - f^2_a\eta^{1a}_{34} + f^a_3\eta^{12}_{a4} + f^a_4\eta^{12}_{3a}\right)$$

$$+ \frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b)$$

$$+ \sum_{ab}(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)$$

2-body flow unchanged