TBA

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Topological Blocking Algorithm

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Two-Body Anomaly

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Three-Body Anomaly

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PHY232, Lecture 21:

Electromagnetic Waves

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An Update on IMSRG Developments

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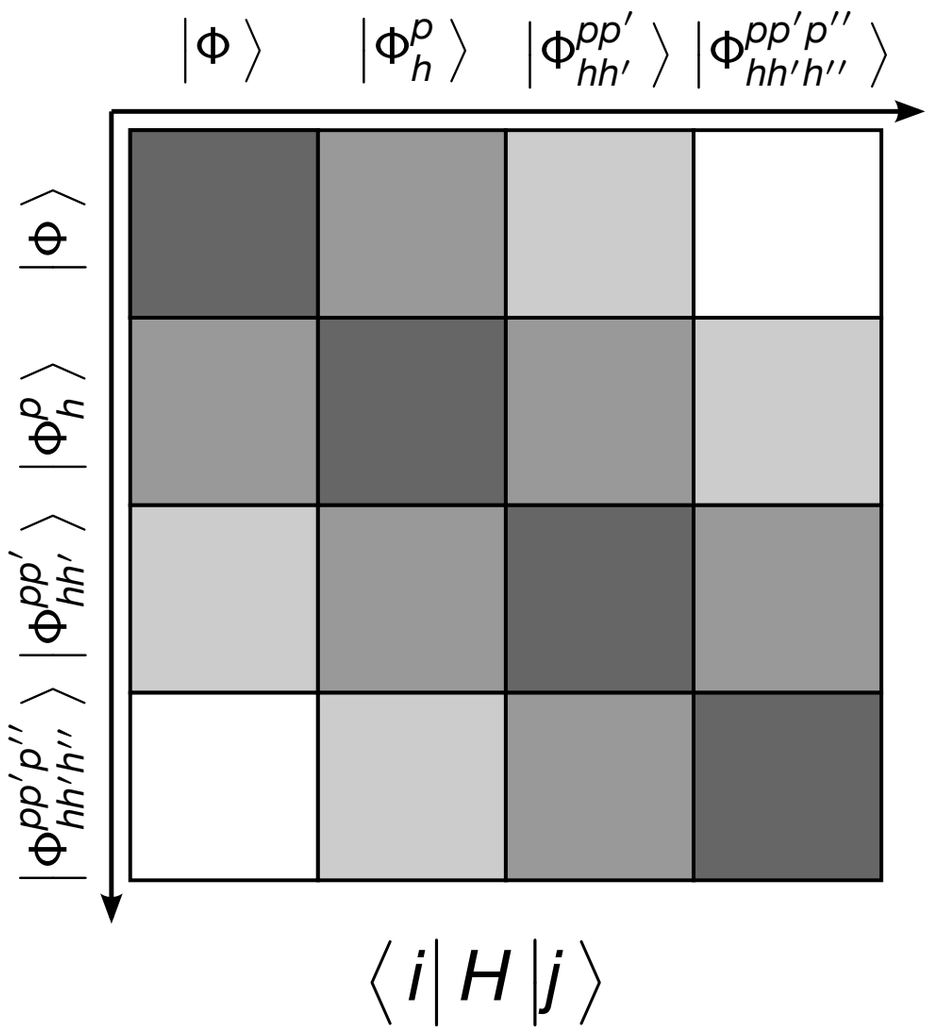
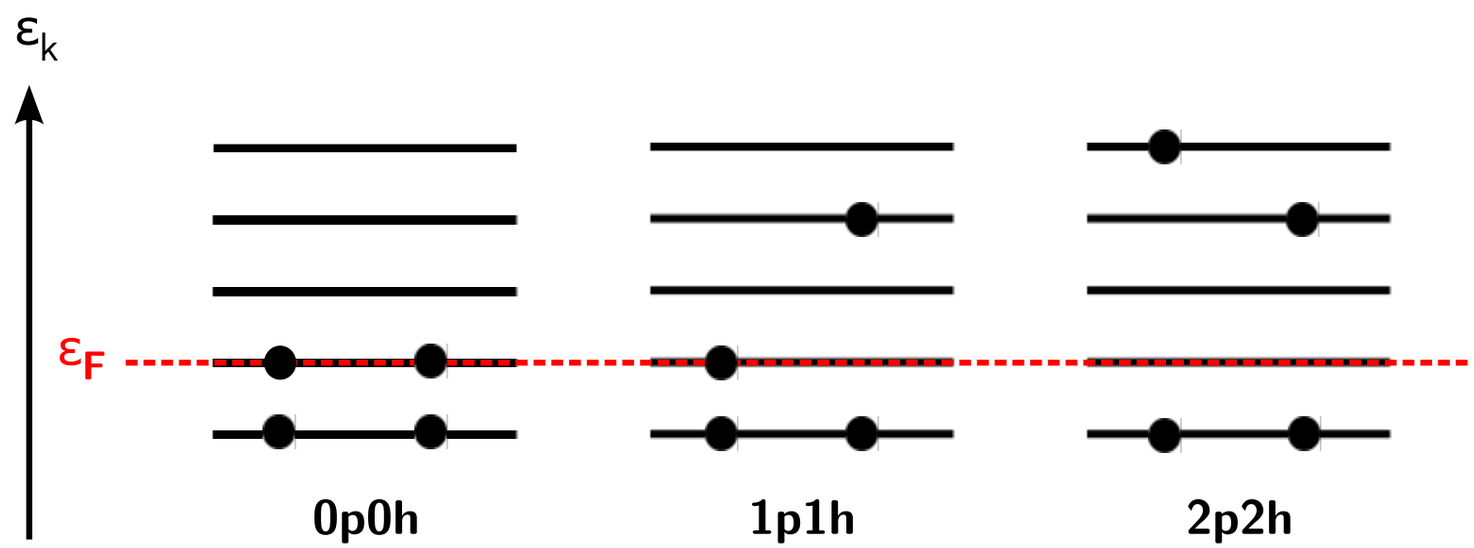
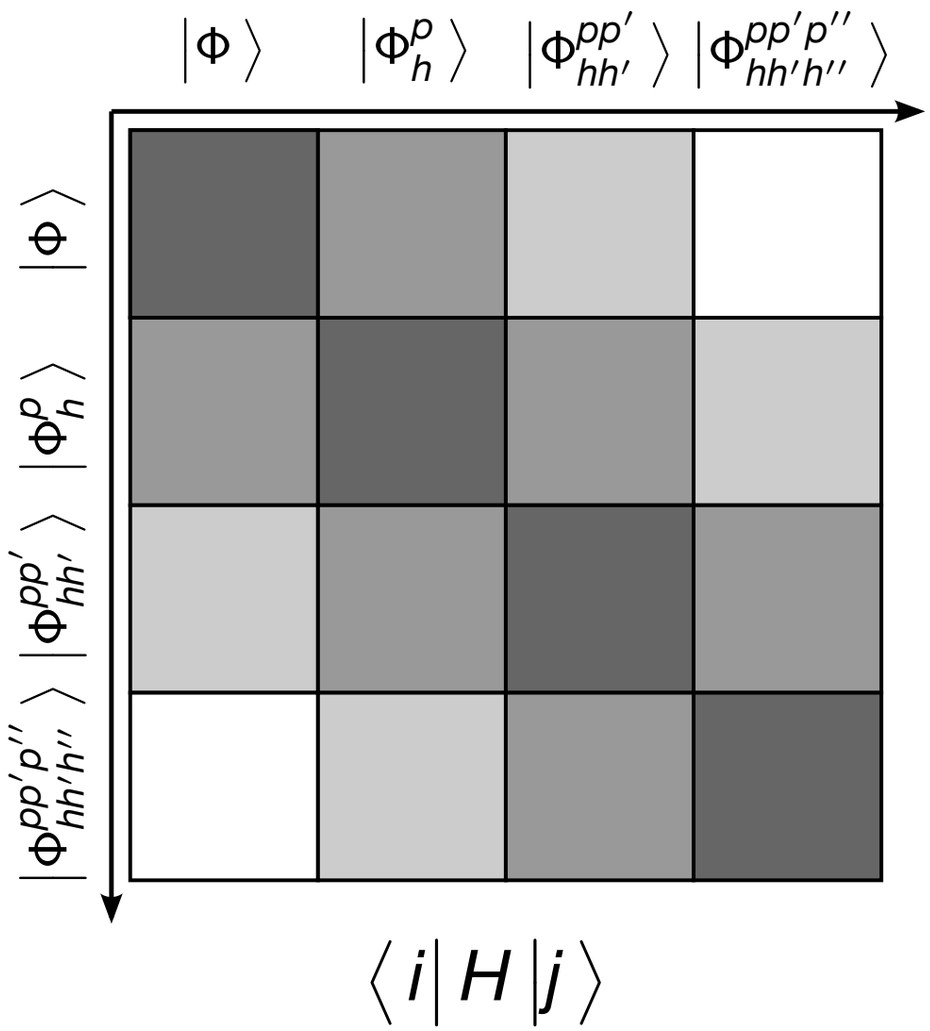
Representing the Hamiltonian

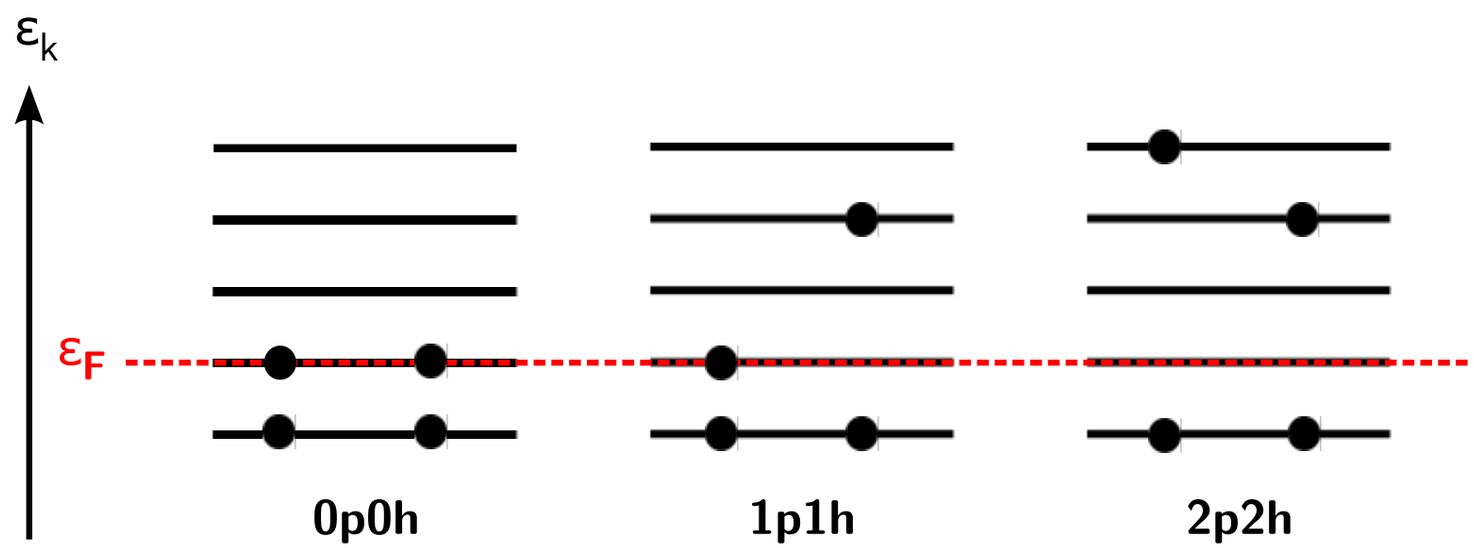




- reference state: **single Slater determinant**

Representing the Hamiltonian

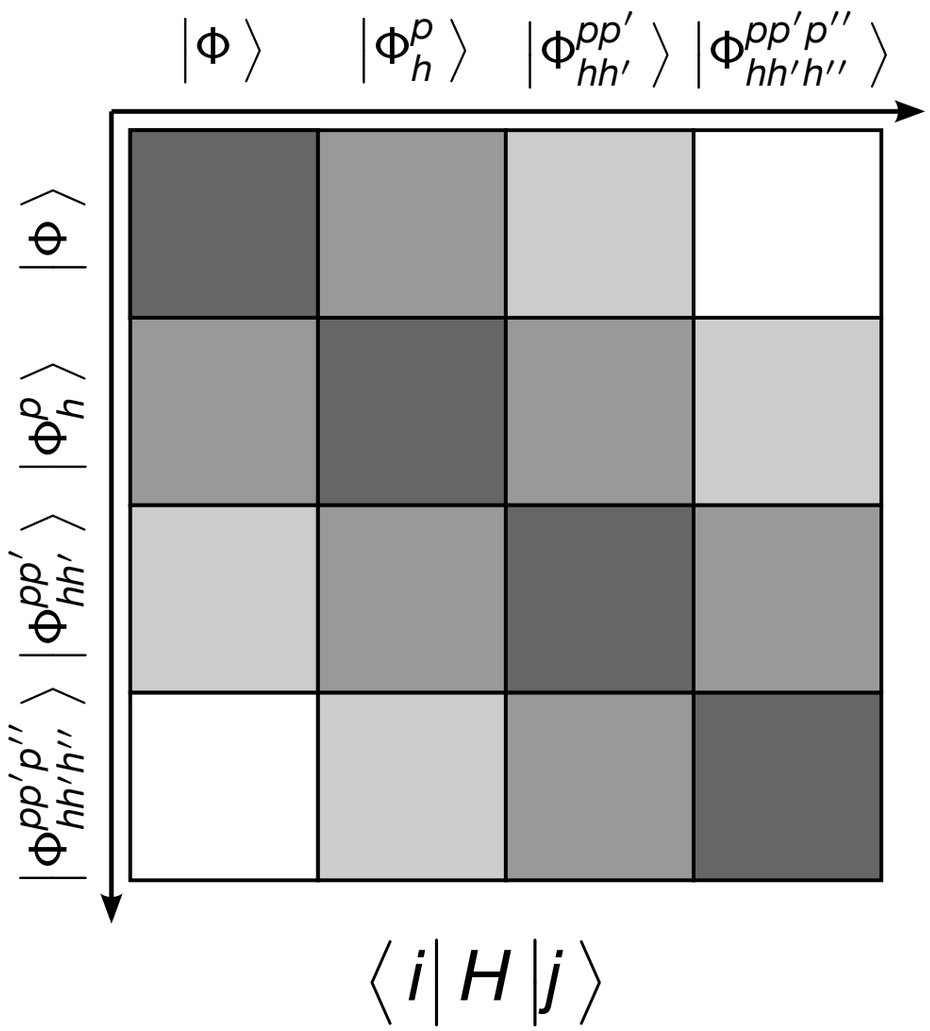




excitations relative to reference state: **normal-ordering**

- reference state: **single Slater determinant**

Single-Reference Case



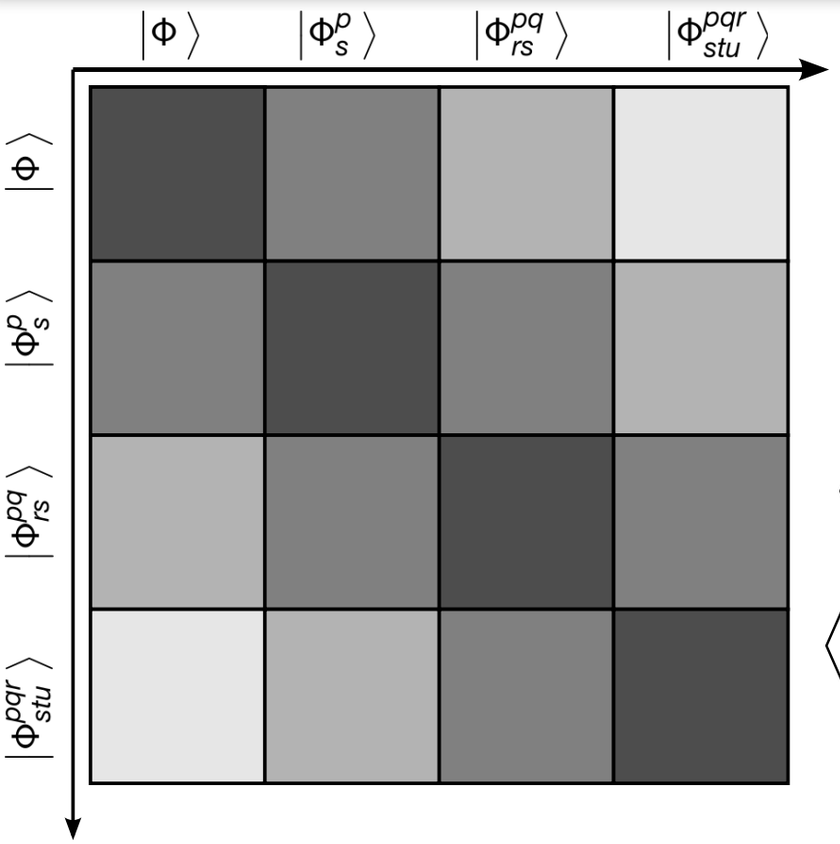
$$A^{i_1\ldots i_N}_{j_1\ldots j_N} \equiv a^\dagger_{i_1}\ldots a^\dagger_{i_N} a_{j_N}\ldots a_{j_1}$$

$$\langle {}^{p}_{h}|H|\Psi\rangle = \sum_{kl} f^k_l \langle\Psi| : A^h_p :: A^k_l : |\Psi\rangle = -n_h\bar{n}_p f^p_h$$

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

- reference state: **Slater determinant**
- normal-ordered operators **depend on occupation numbers (one-body density)**

Multi-Reference Case



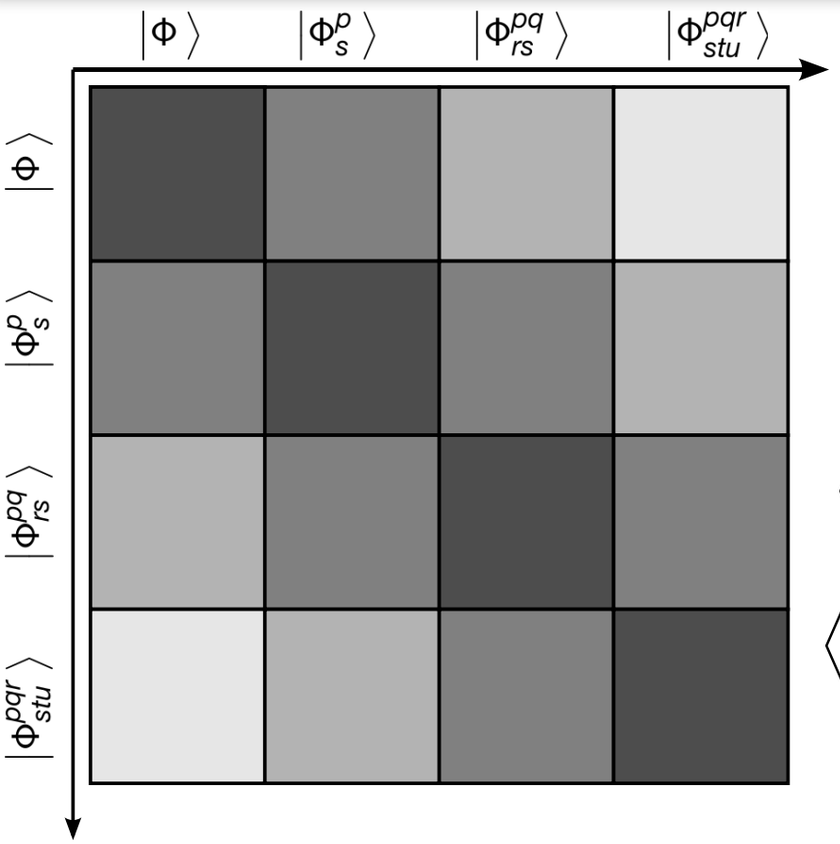
$$\left\langle {}^{p}_{s} \right| H \left| \Phi \right\rangle \sim \bar{n}_p n_s f^p_s, \sum_{kl} f^k_l \lambda^{sk}_{pl}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{skl}_{pmn}, \ldots$$

$$\left\langle {}^{pq}_{st} \right| H \left| \Phi \right\rangle \sim \bar{n}_p \bar{n}_q n_s n_t \Gamma^{pq}_{st}, \sum_{kl} \Gamma^{pk}_{sl} \lambda^{tk}_{ql}, \sum_{kl} f^k_l \lambda^{stk}_{pql}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{stkl}_{pqmn}, \ldots$$

$$\left\langle {}^{pqr}_{stu} \right| H \left| \Phi \right\rangle \sim \ldots$$

- reference state: **arbitrary**

Multi-Reference Case



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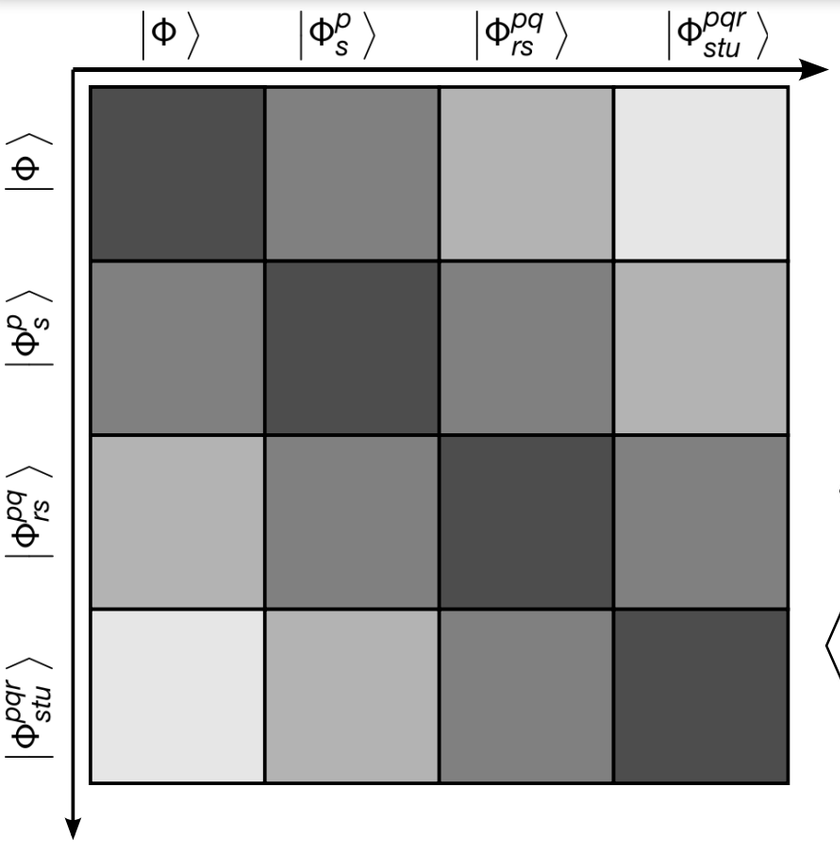
$$\left\langle {}^{pqr}_{stu} \right| H \left| \Phi \right\rangle \sim \ldots$$

- reference state: **arbitrary**
- normal-ordered operators depend on up to **irreducible n-body density matrices** of the reference state

Multi-Reference Case



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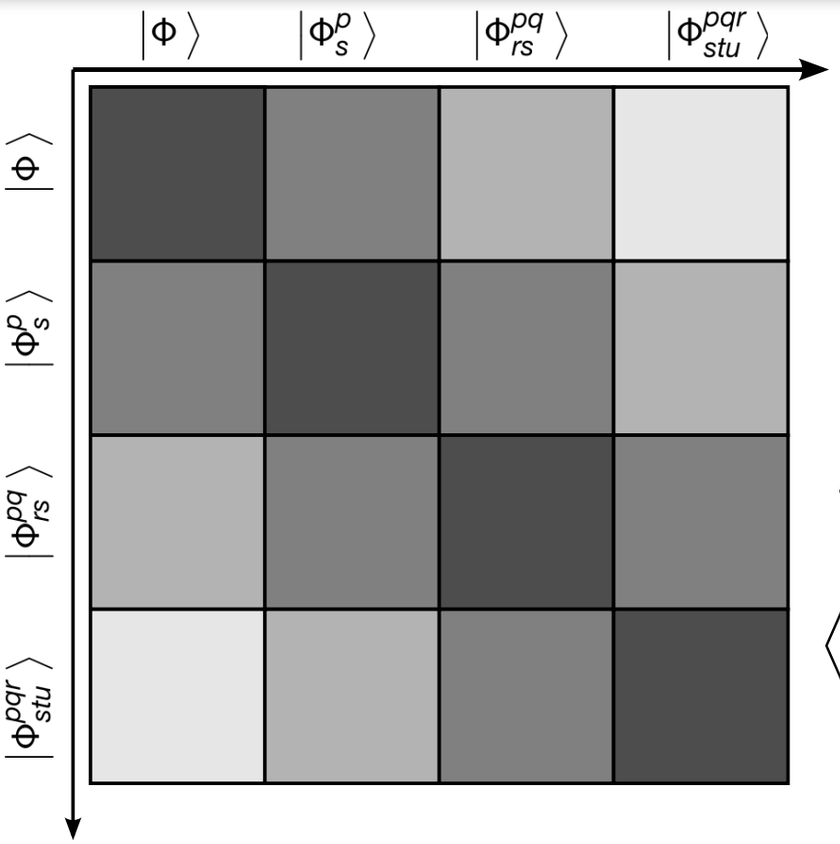
$$\rho^{kl}_{mn} = \lambda^{kl}_{mn} + \lambda^k_m \lambda^l_n - \lambda^k_n \lambda^l_m$$

$$\rho^{ijk}_{lmn} = \lambda^{ijk}_{lmn} + \lambda^i_l \lambda^{jk}_{mn} + \lambda^i_l \lambda^j_m \lambda^k_n + \text{permutations}$$

$$\ldots$$

Multi-Reference Case



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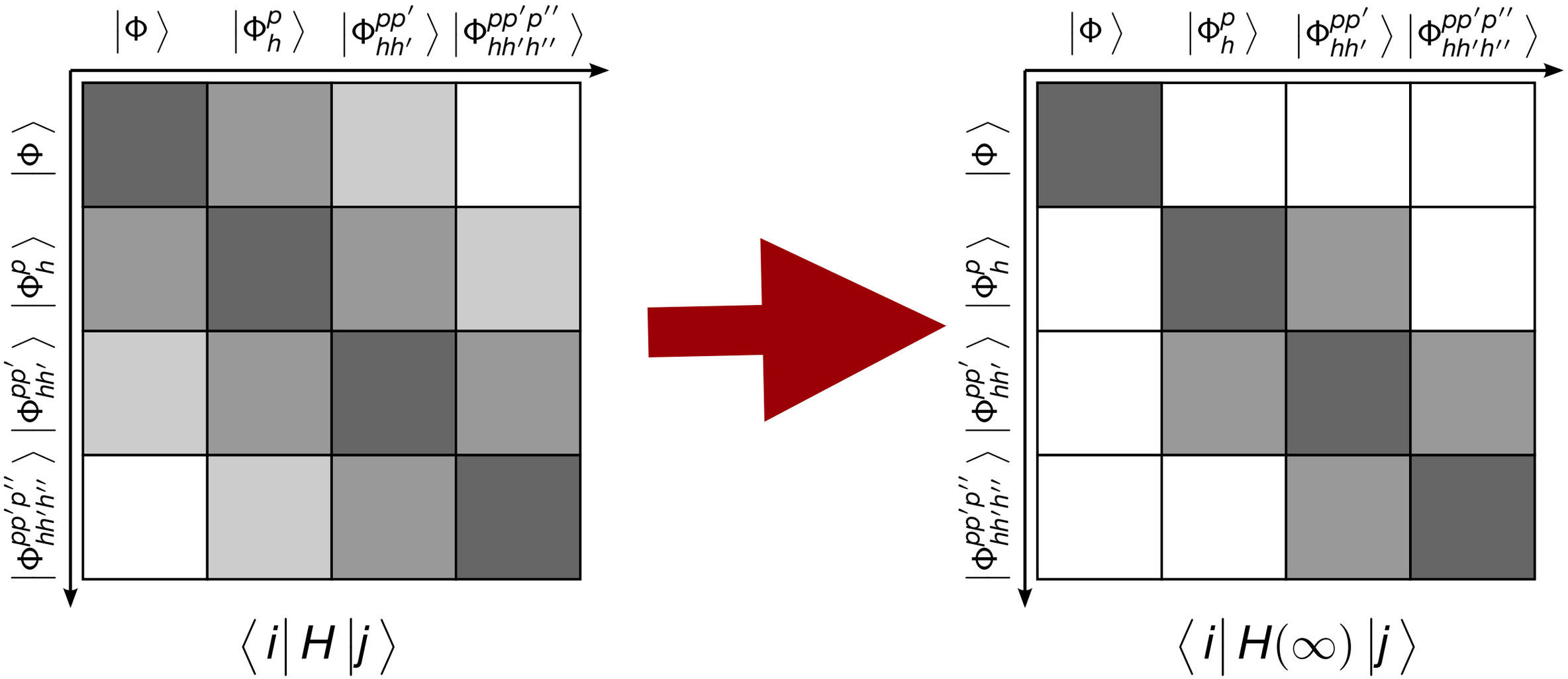
...

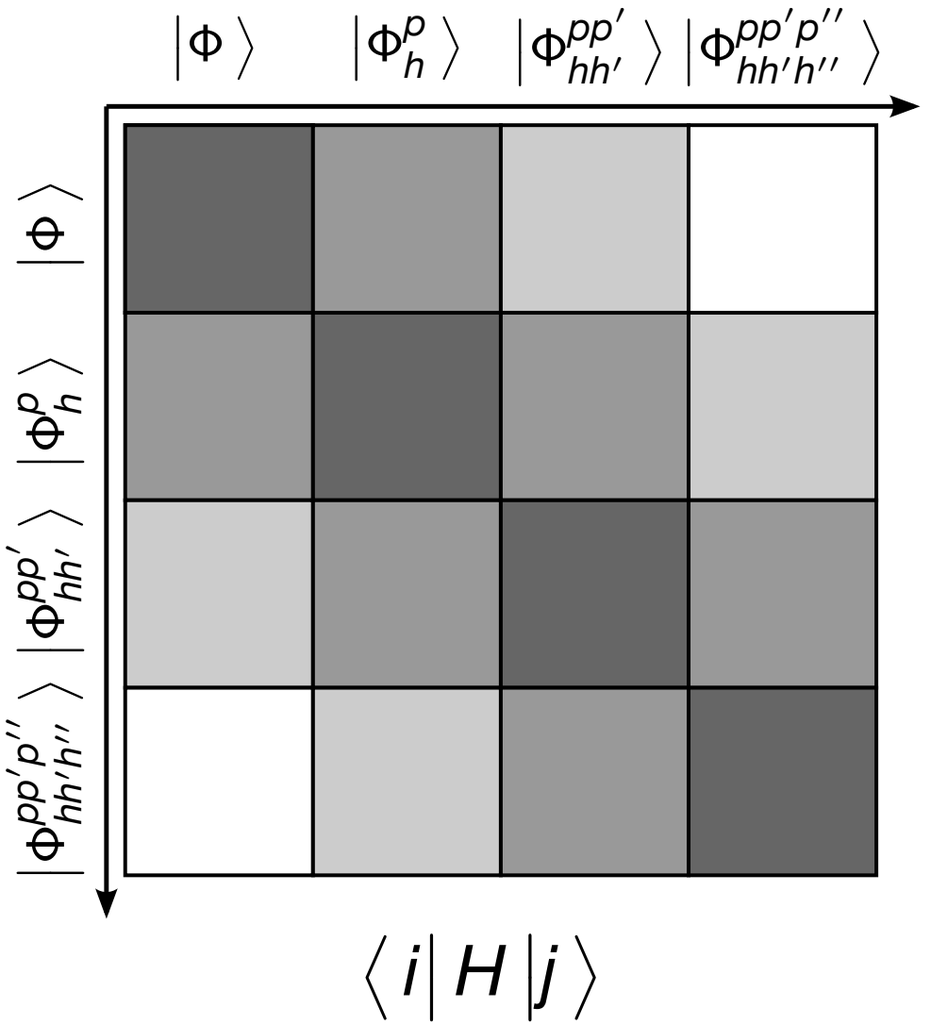
irreducible density matrices encode correlations

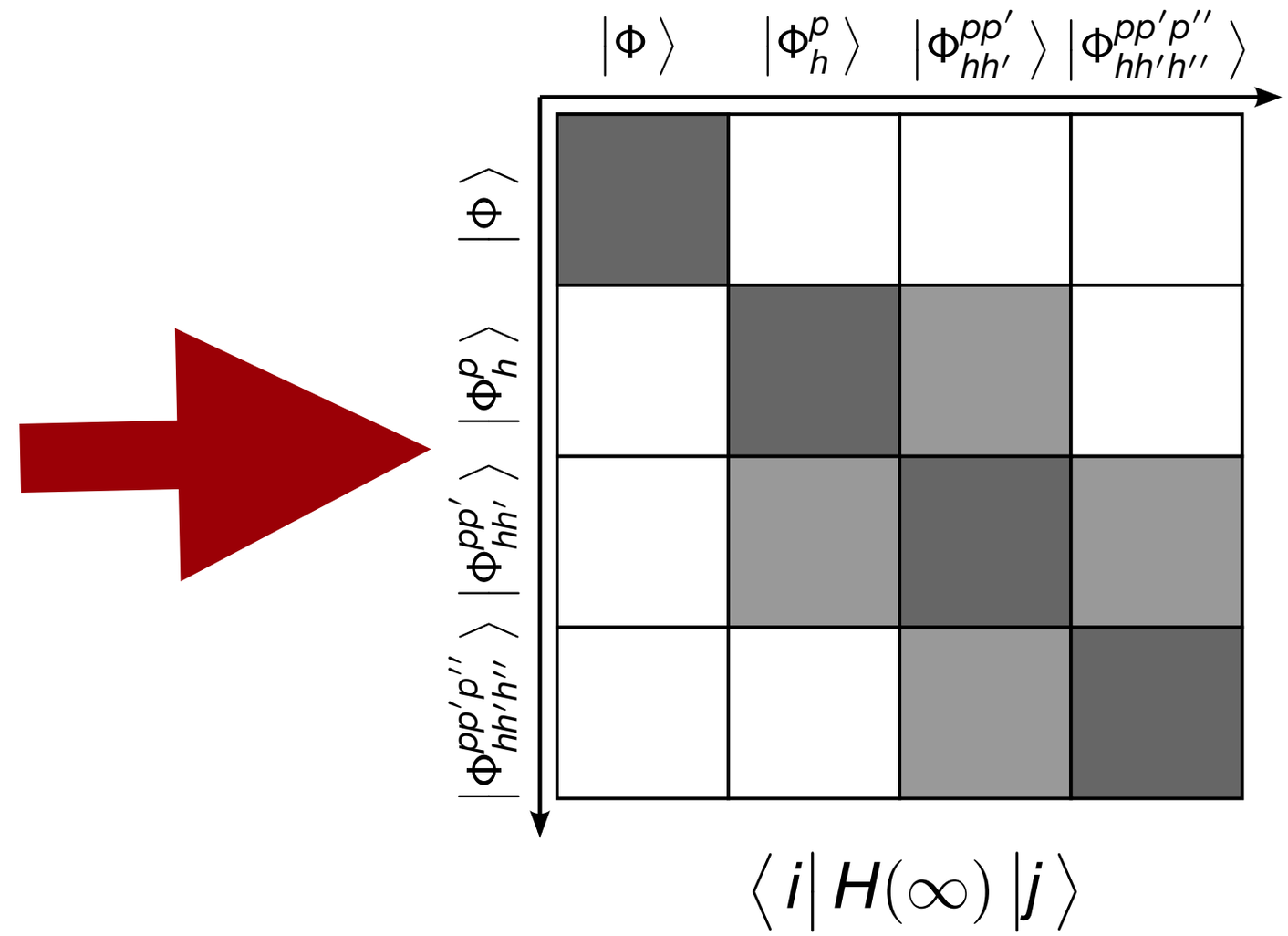
Decoupling in A-Body Space



aim: decouple reference state $|\Phi\rangle$
from excitations

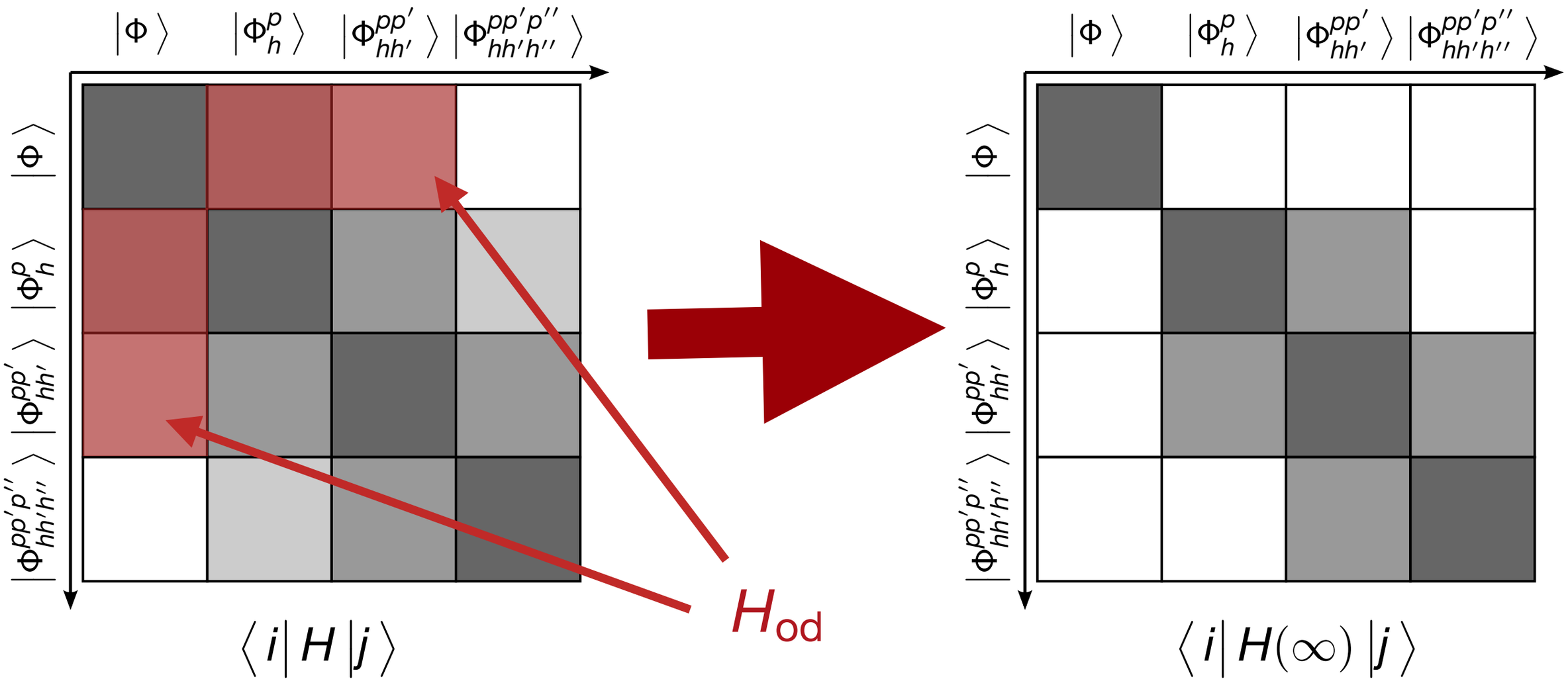
Flow Equation





$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \text{e.g.,} \quad \eta(s) \equiv \left[H_d(s), H_{od}(s)\right]$$

Flow Equation



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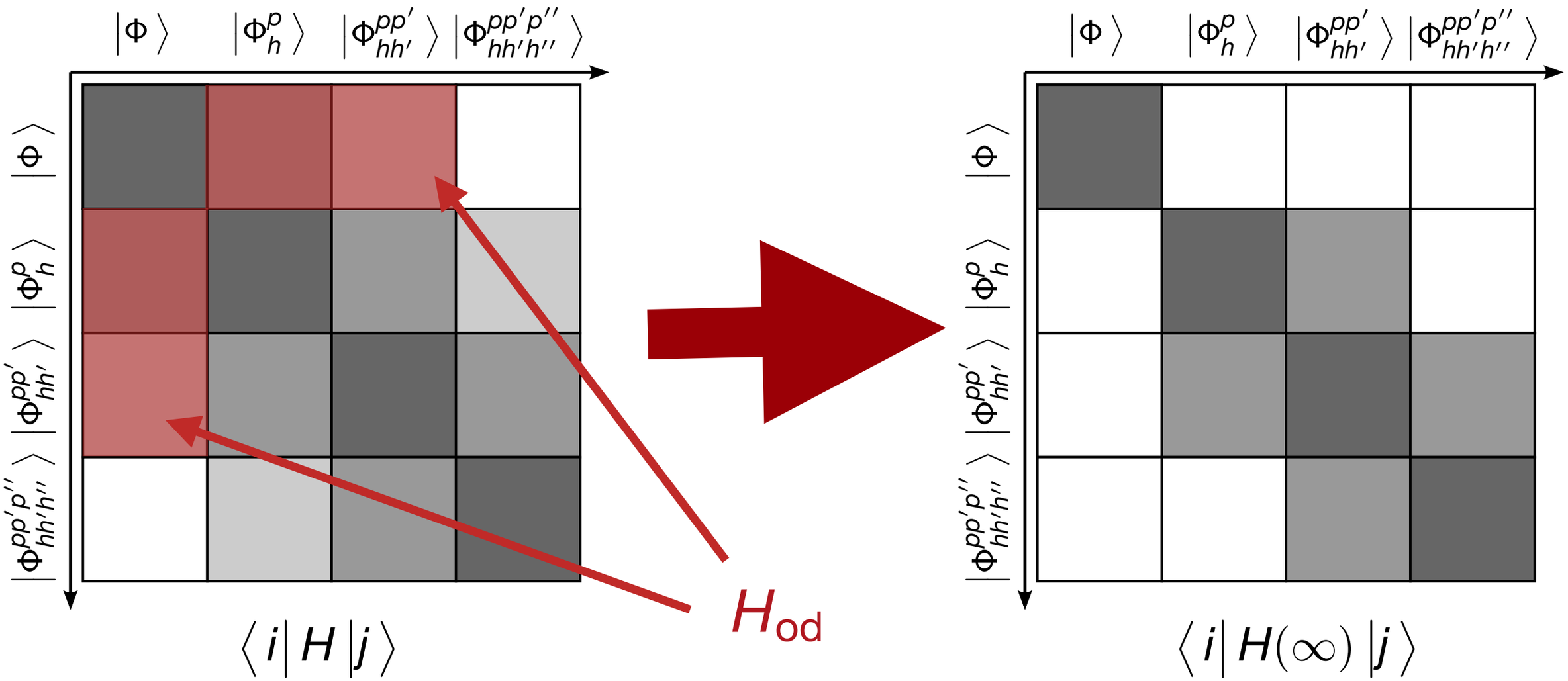
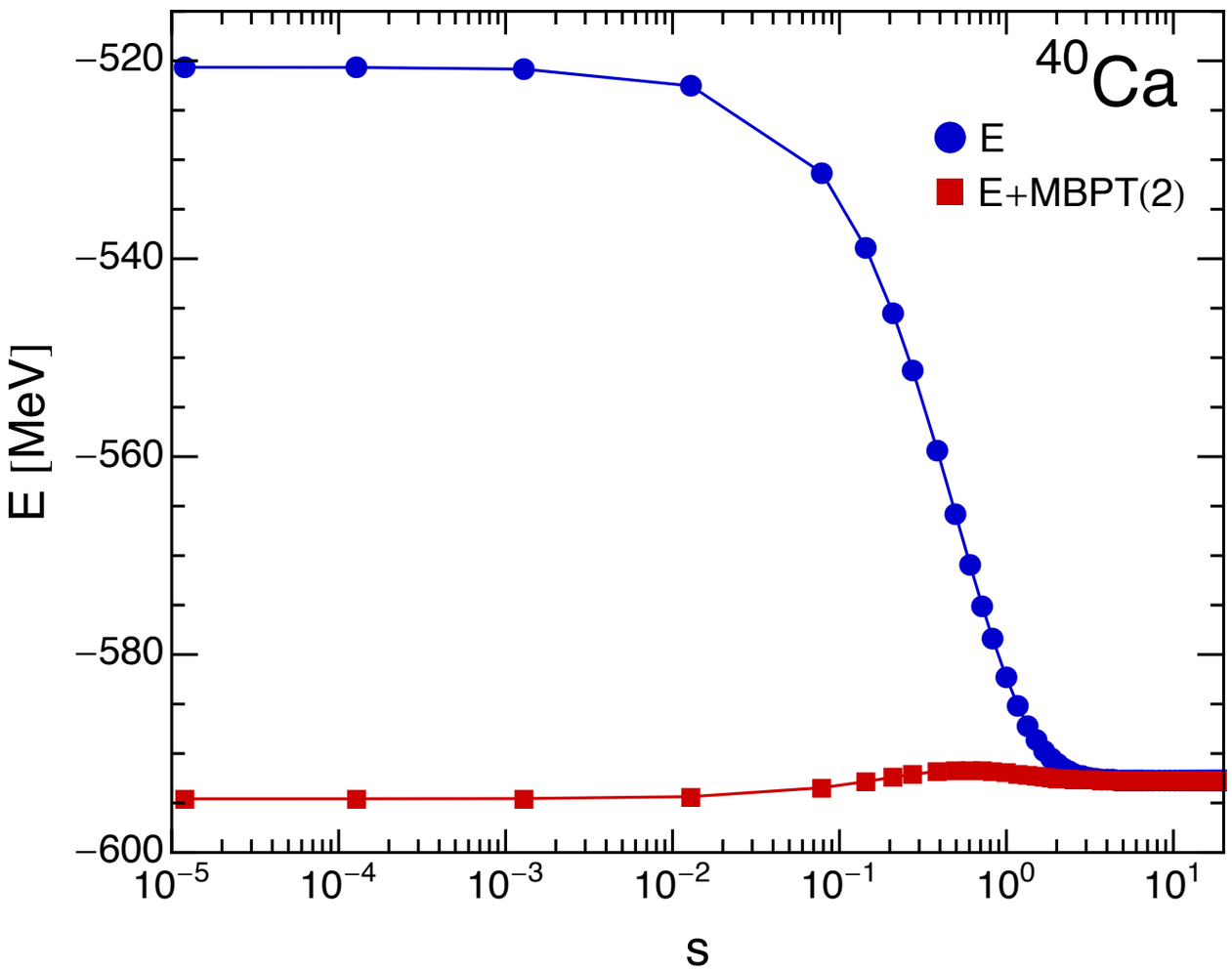
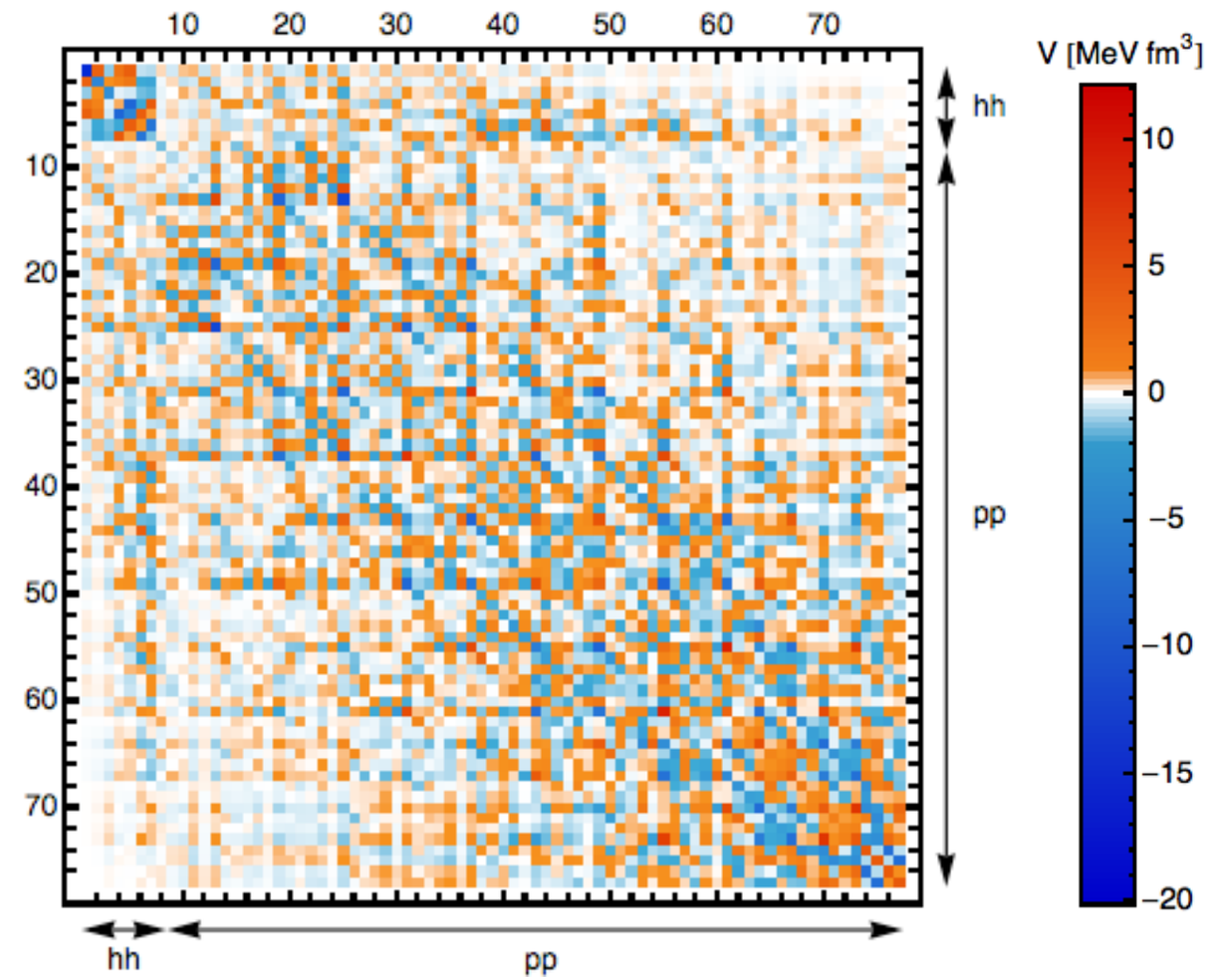


$$\frac{d}{ds}H(s) = [\eta(s), H(s)]$$

Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

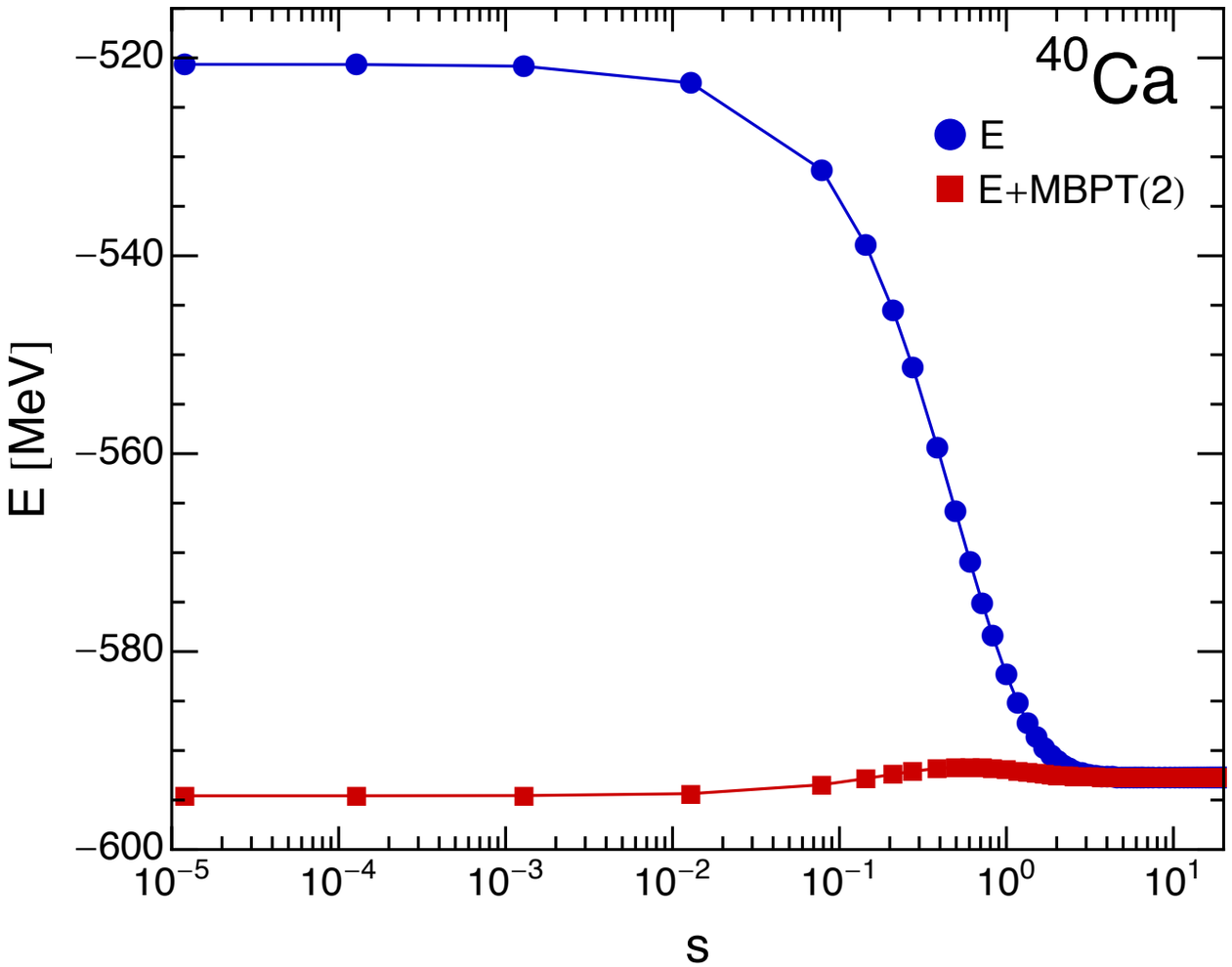
Decoupling

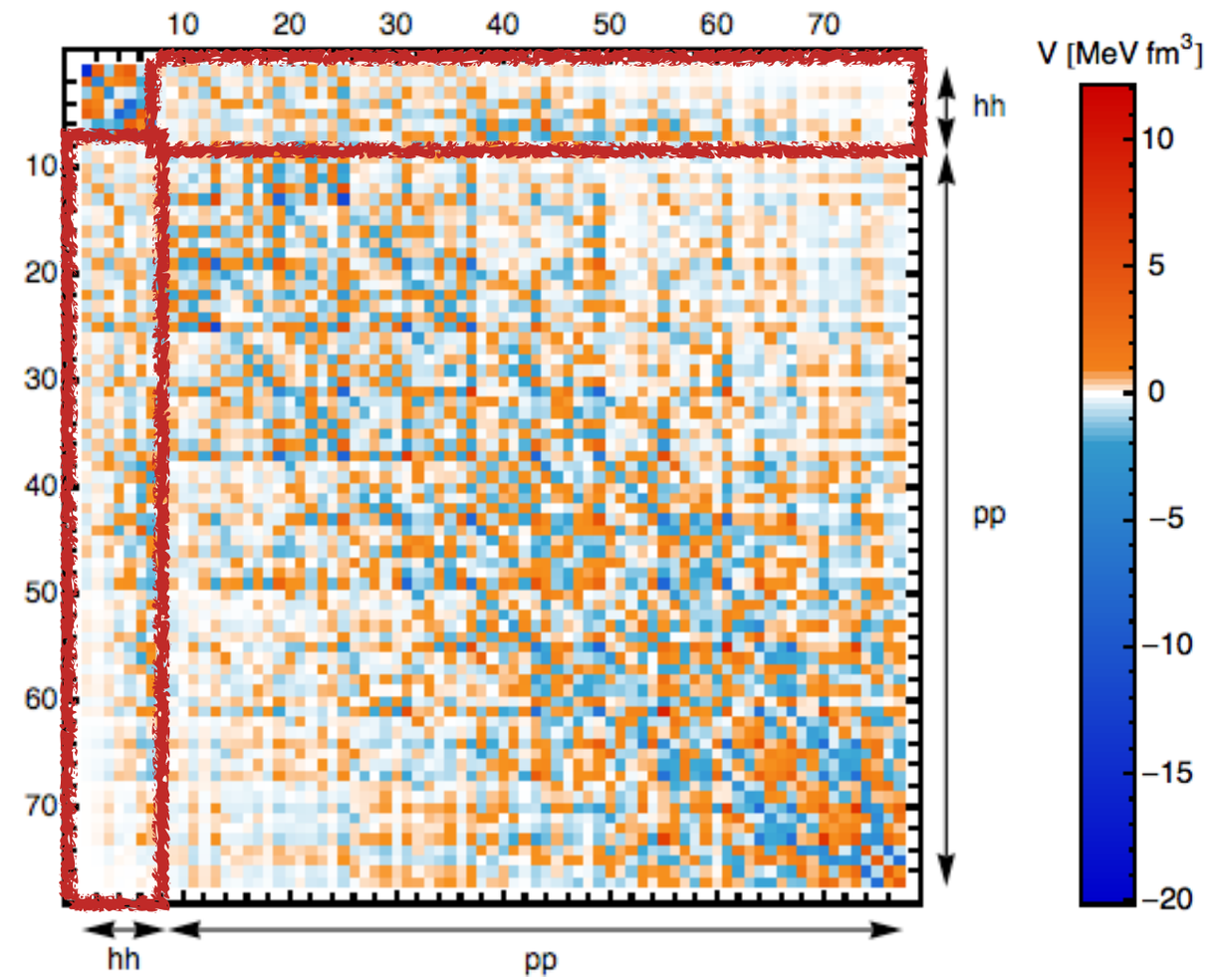




N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

Decoupling





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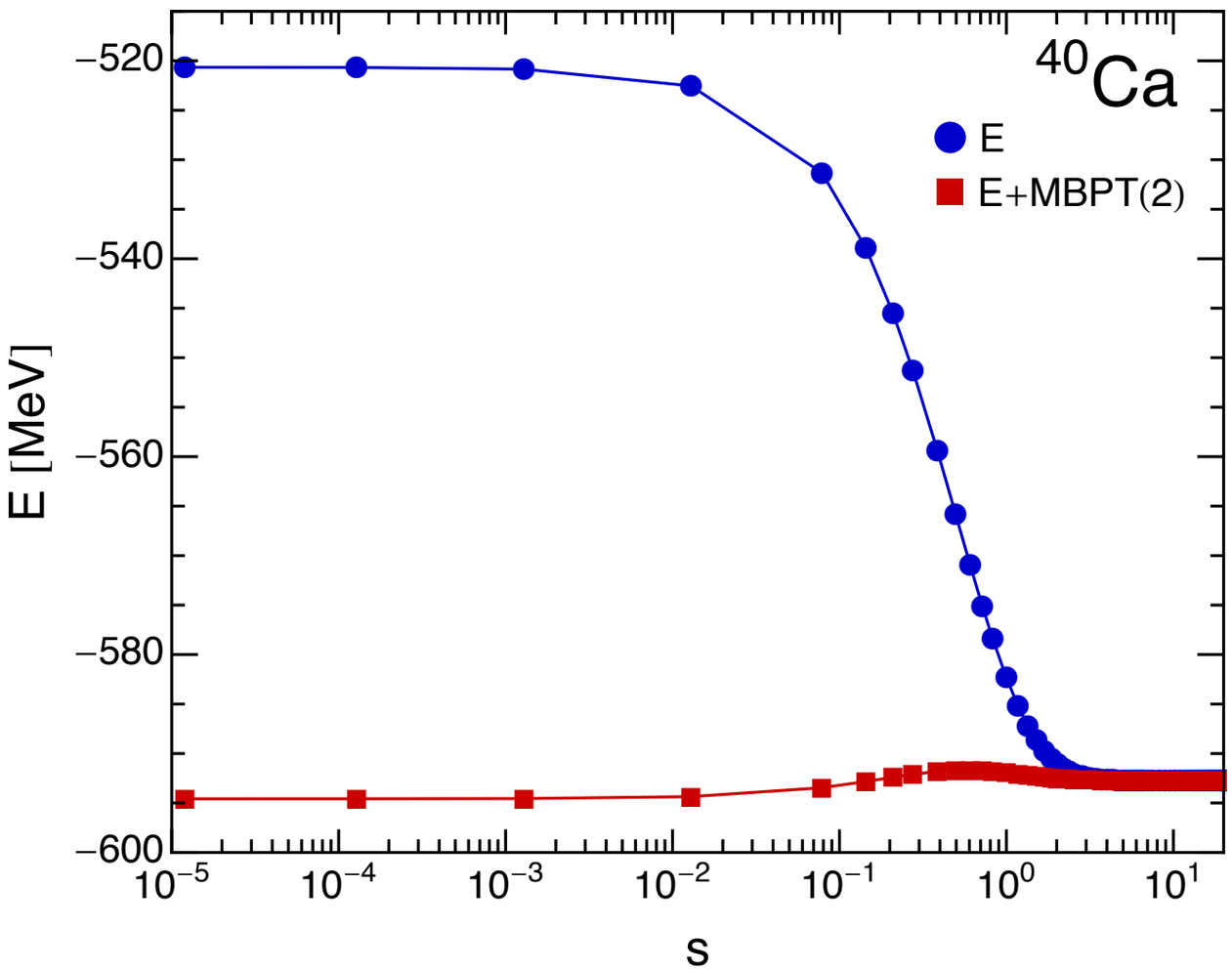

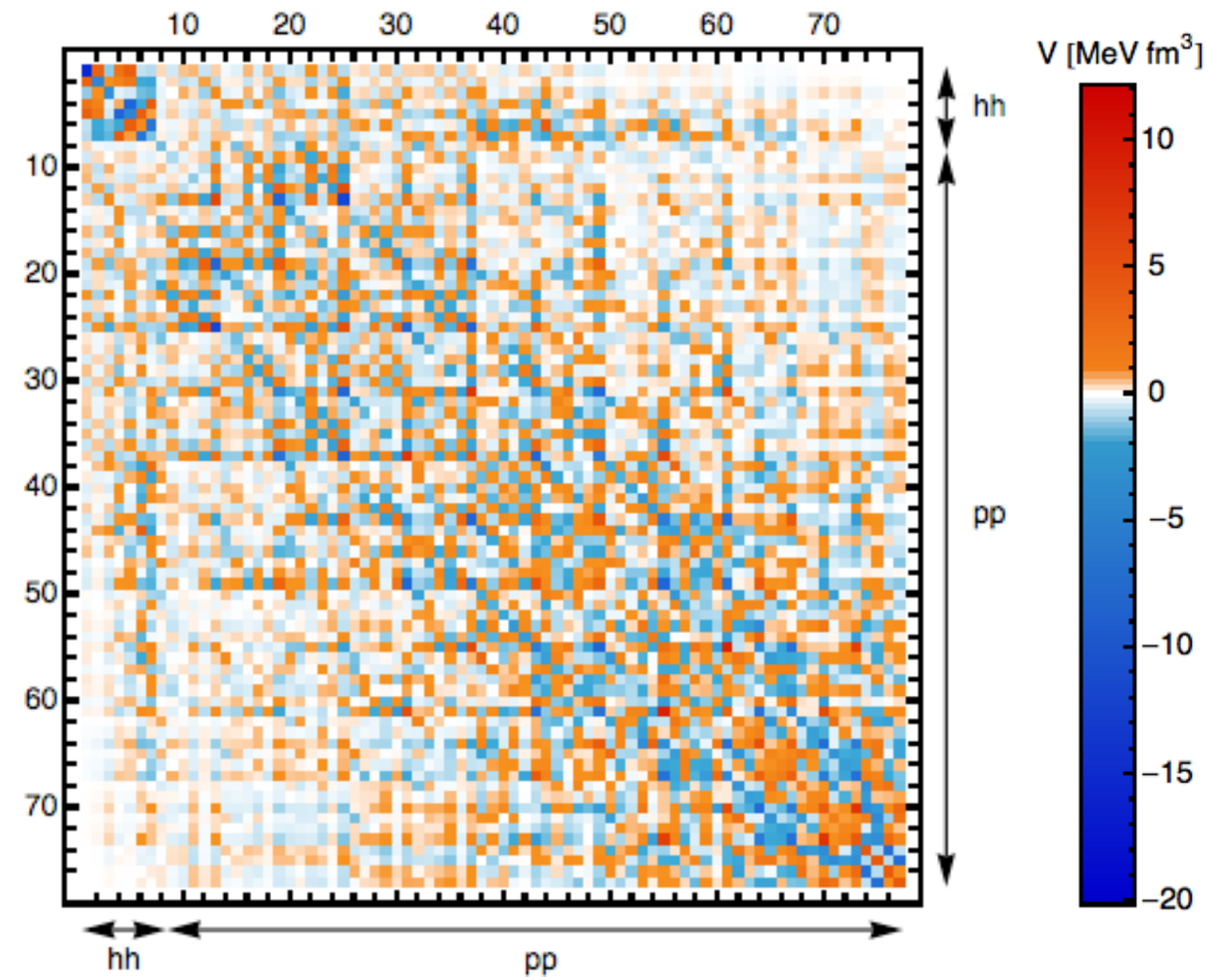

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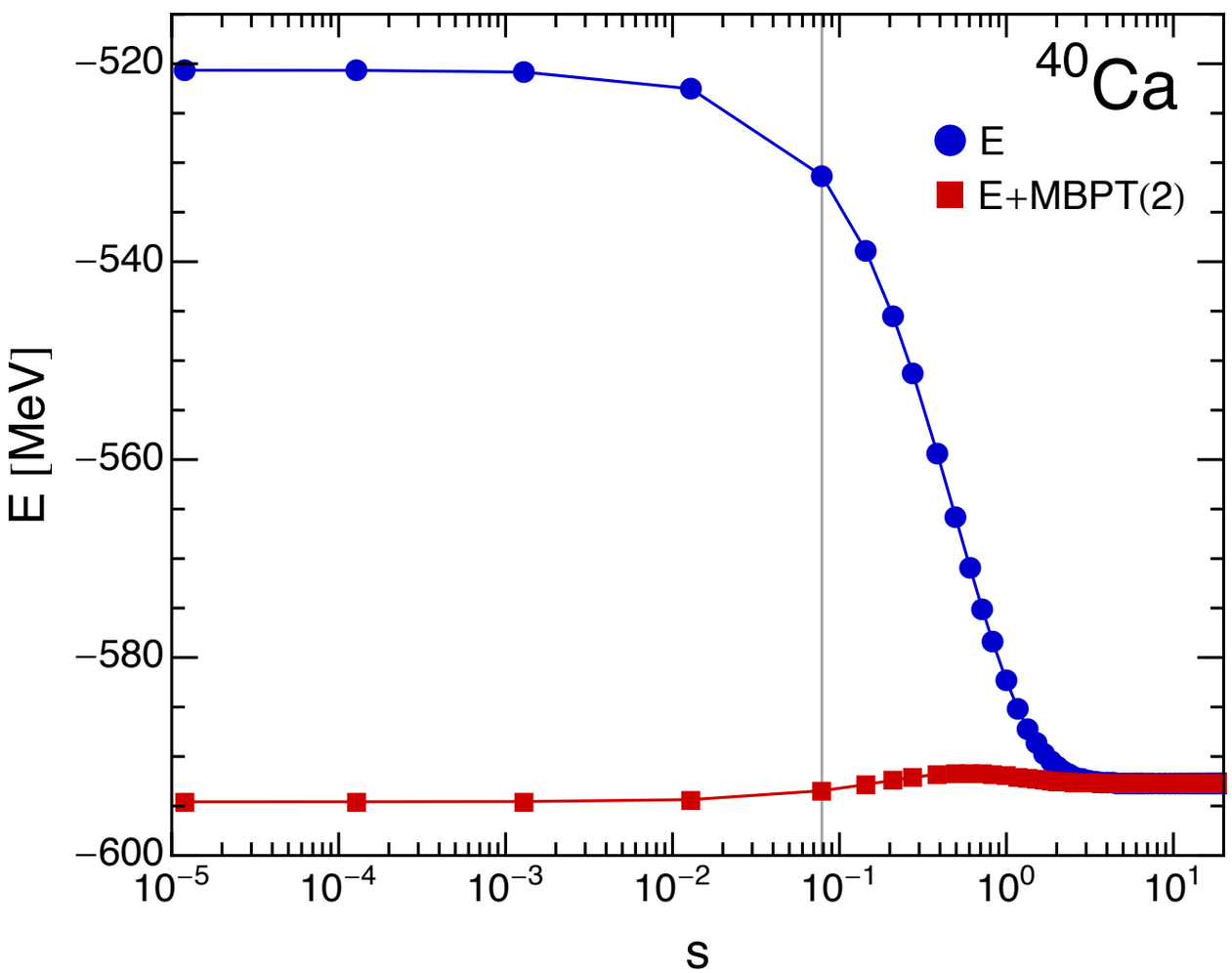

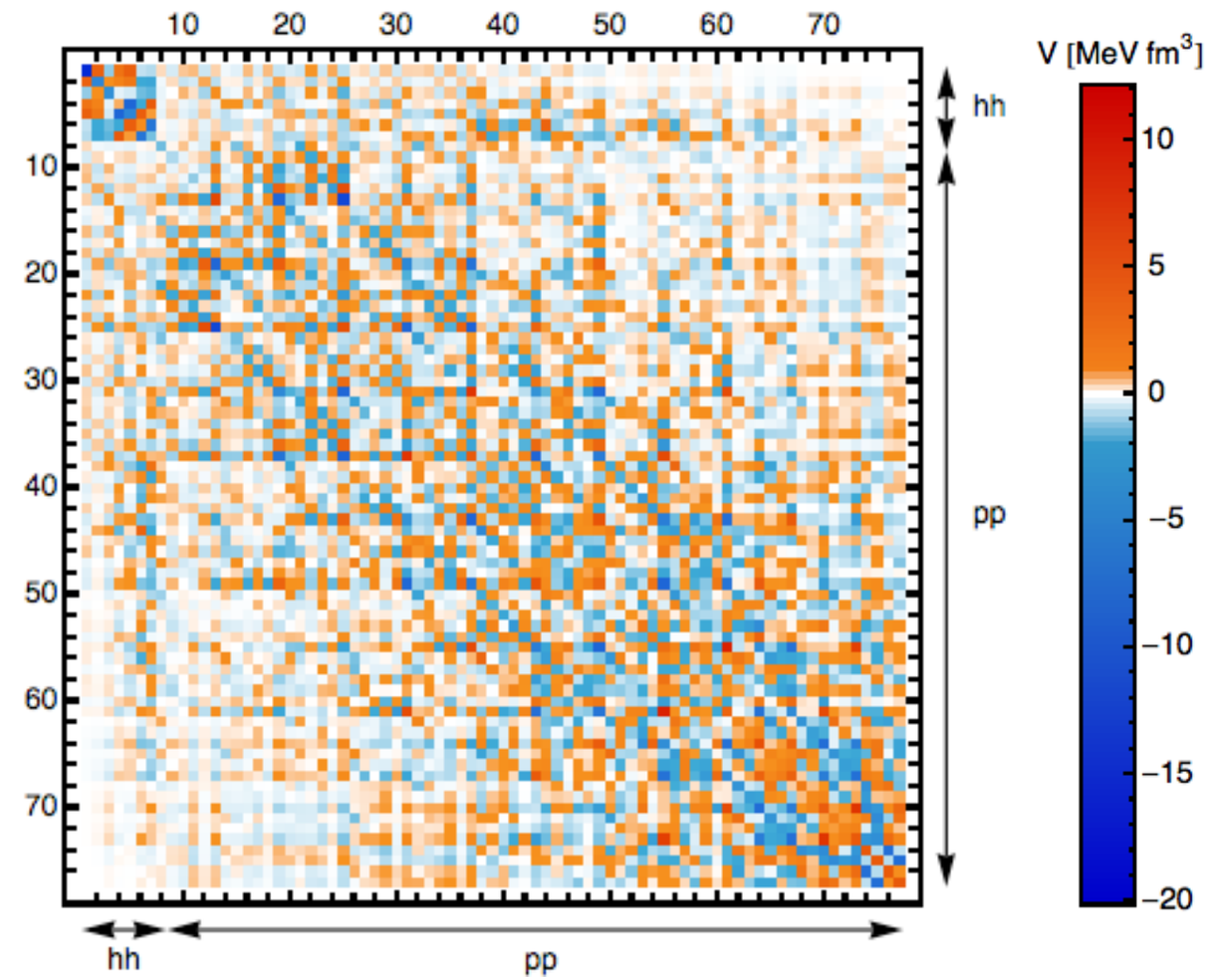

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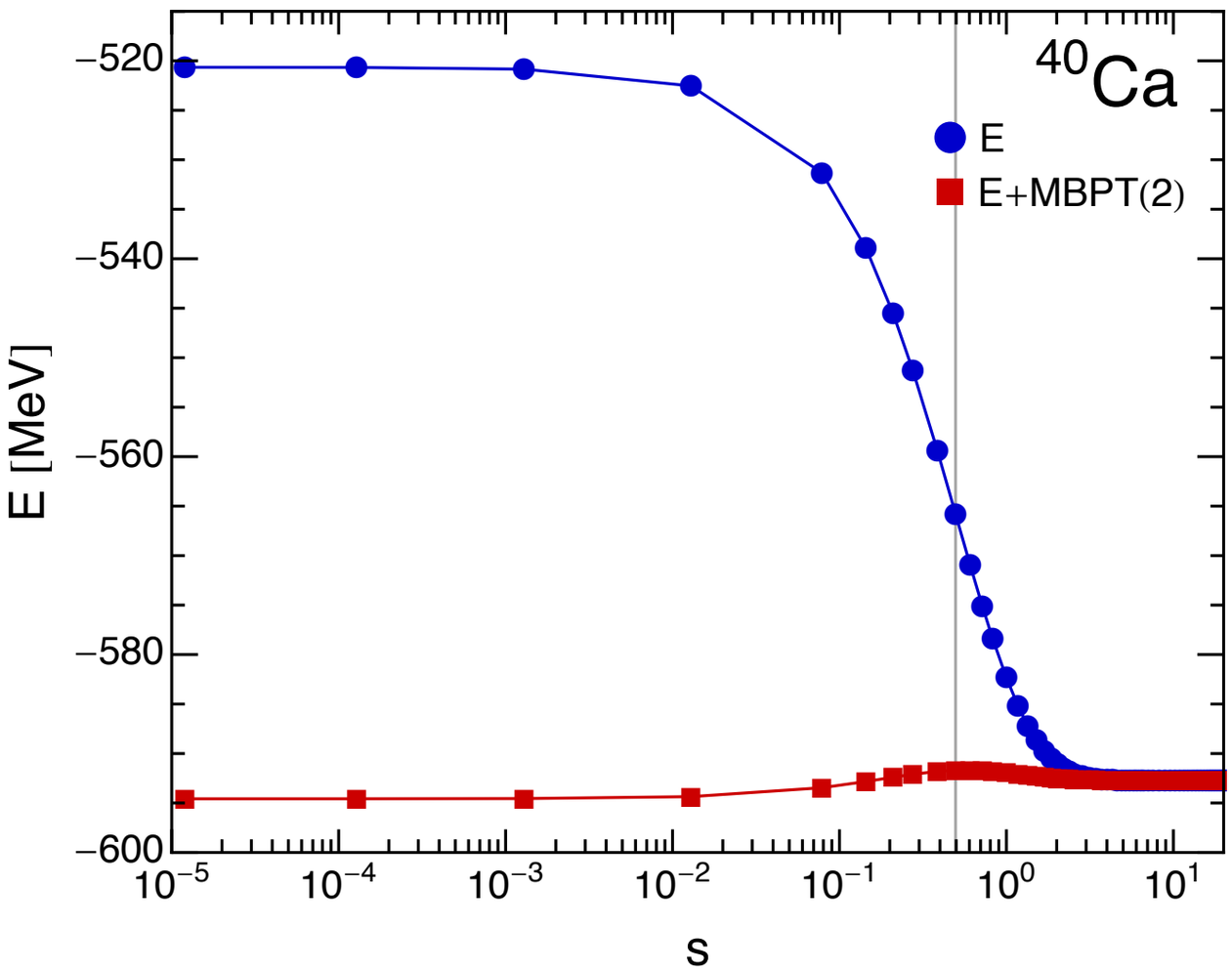

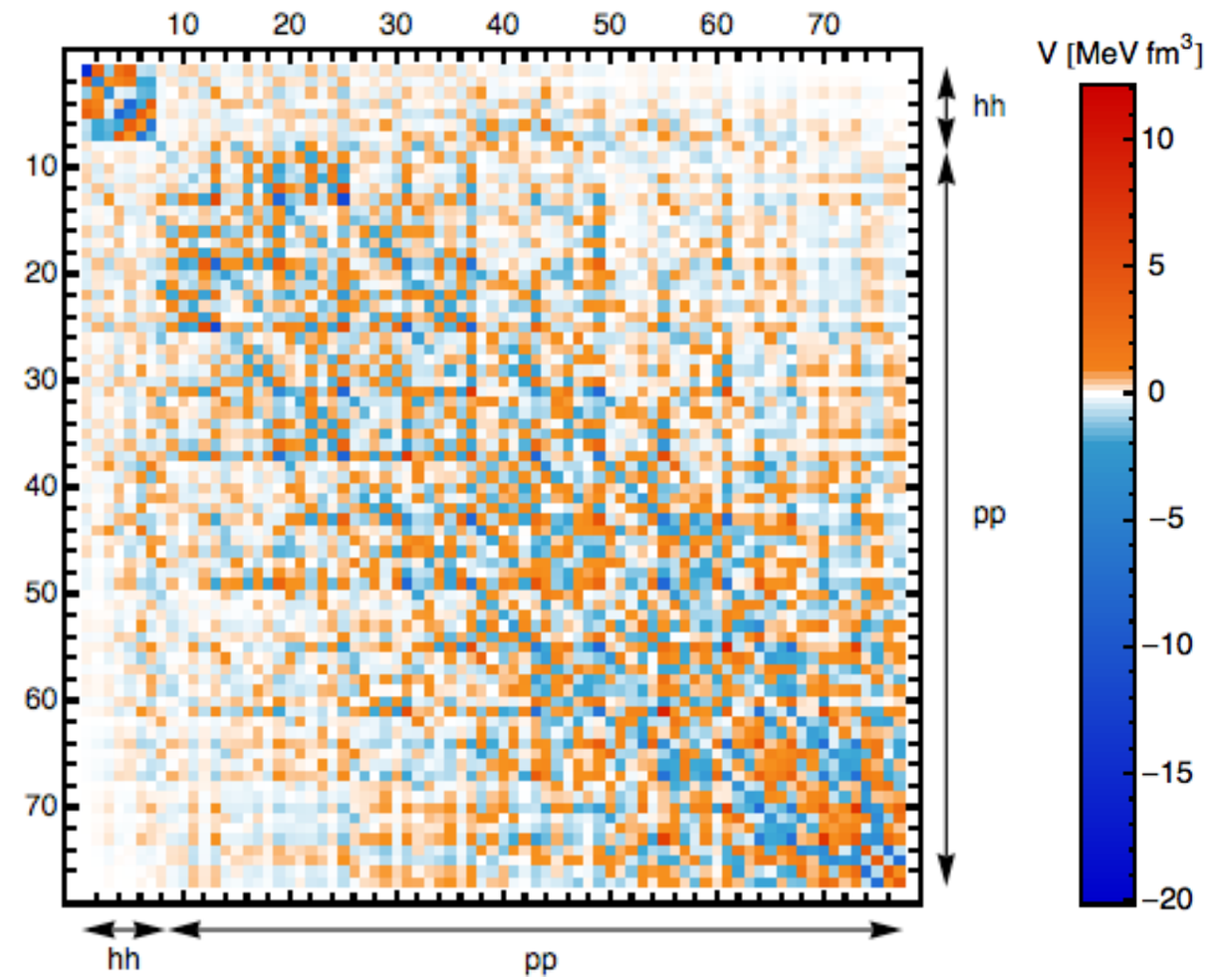

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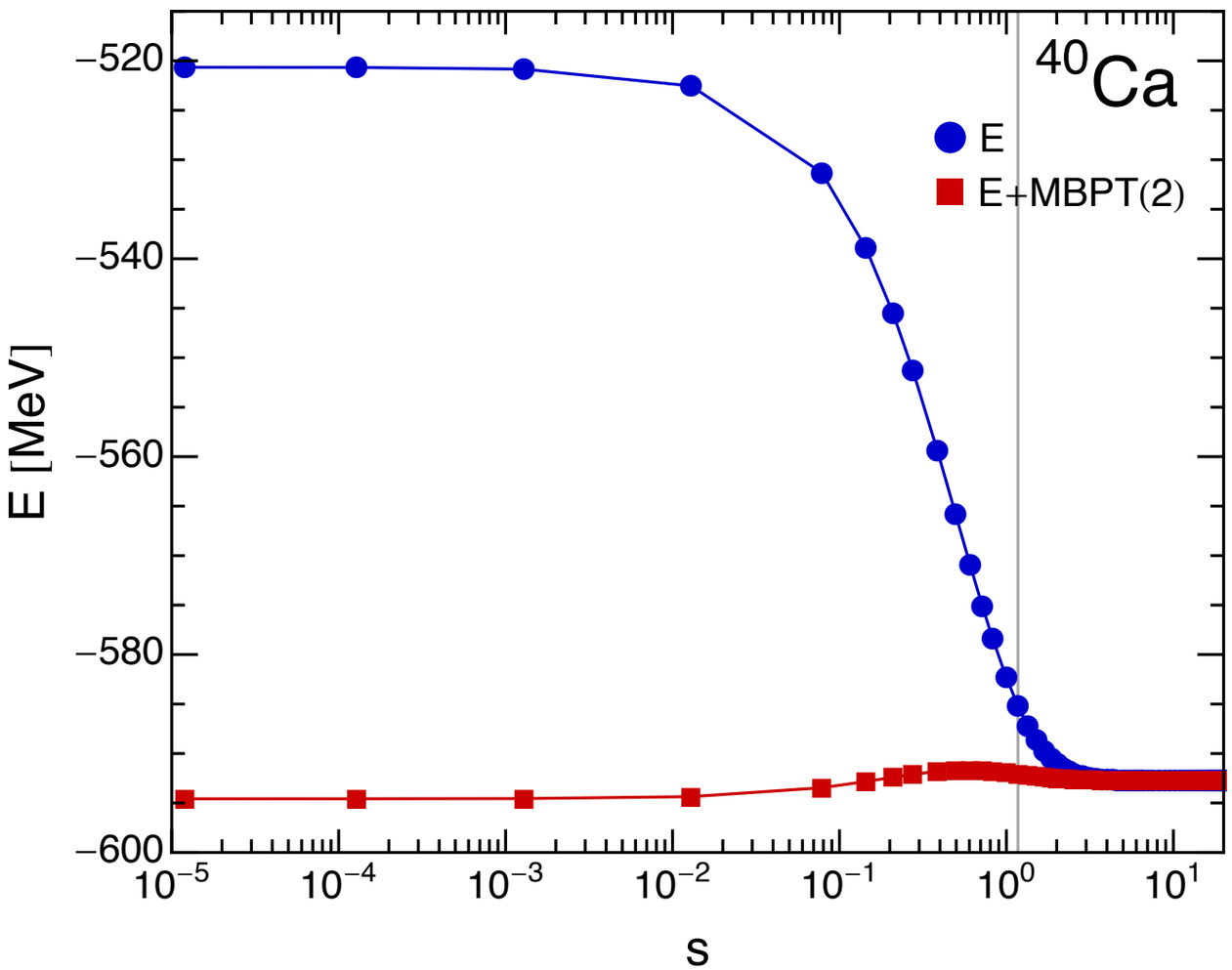

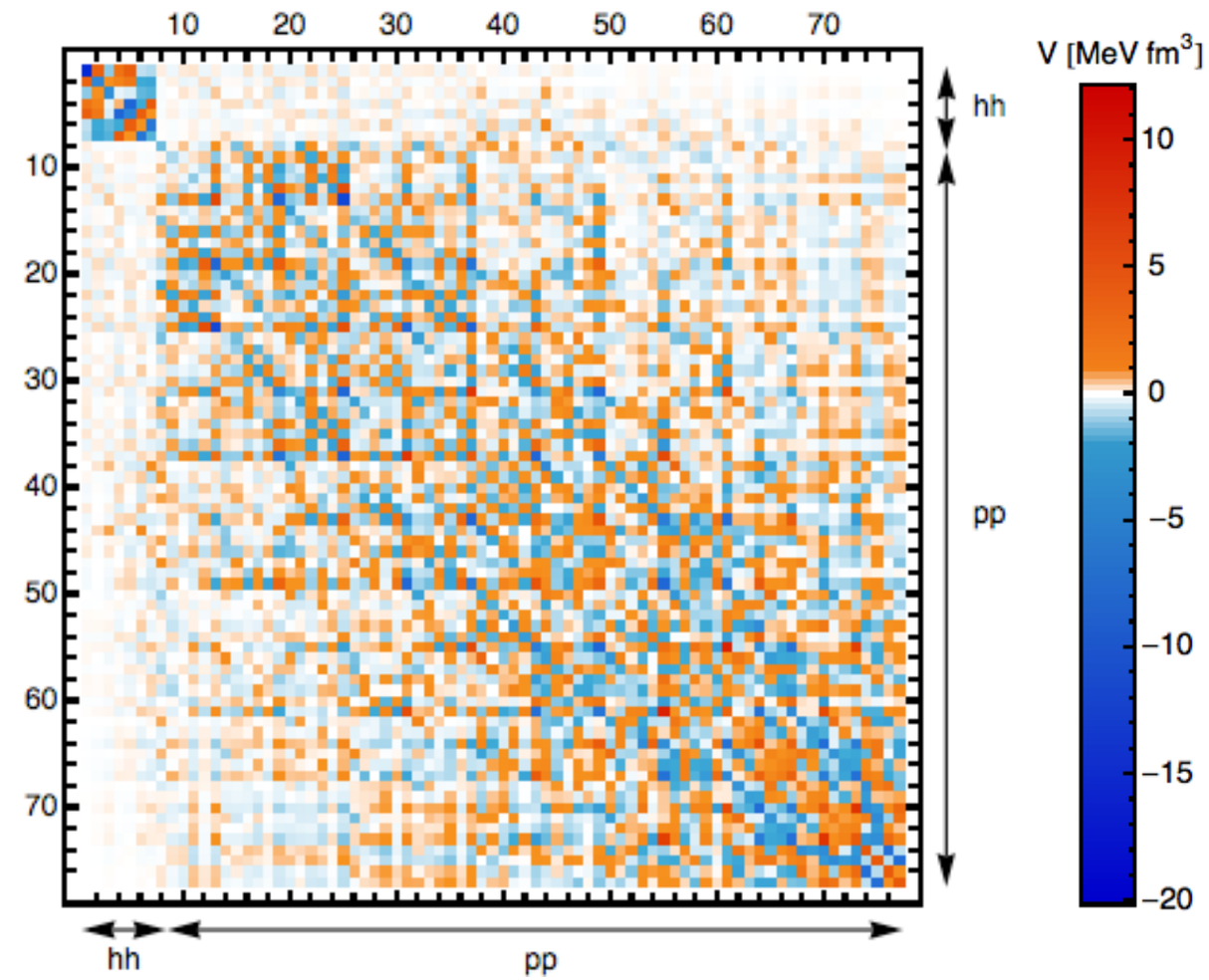

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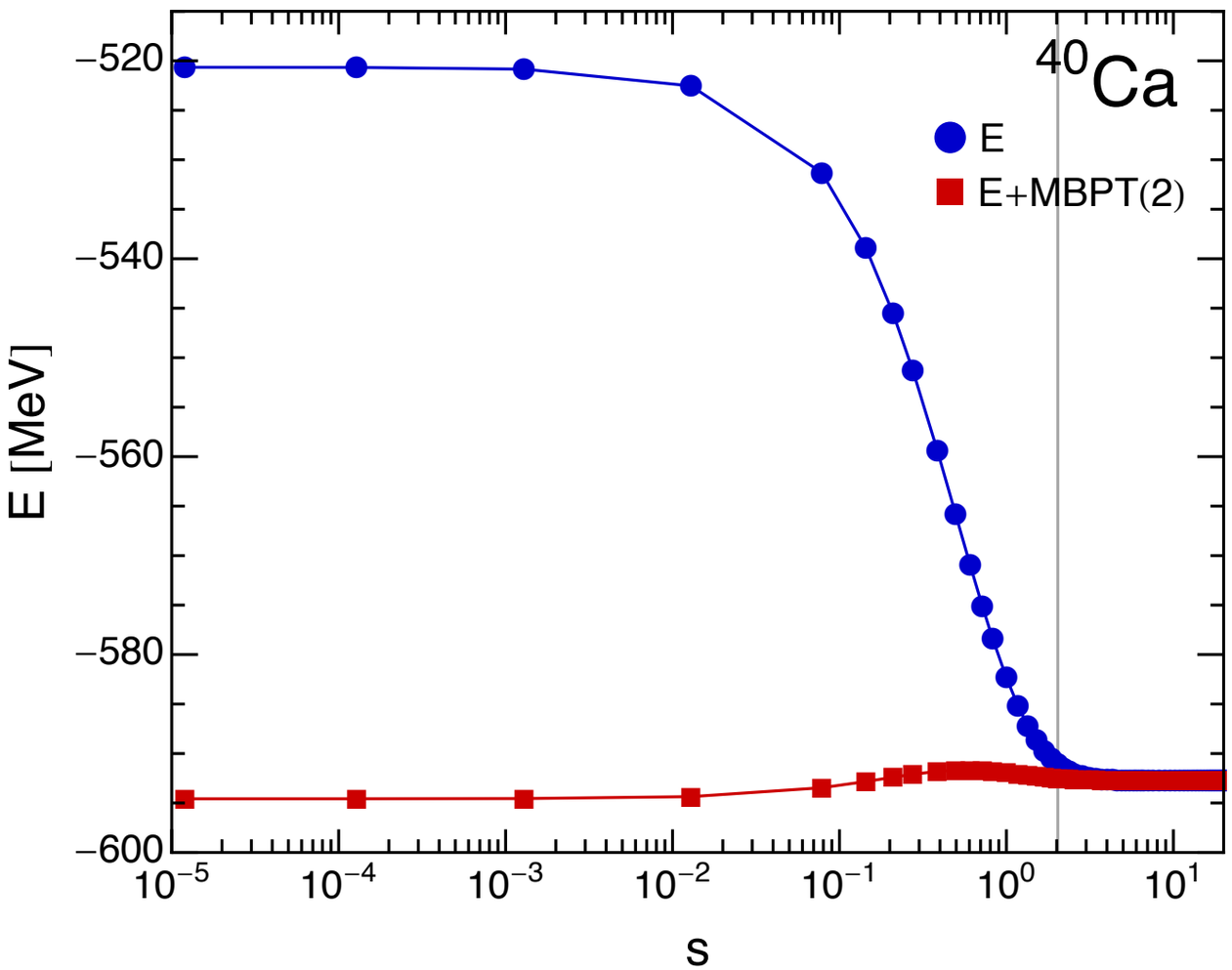

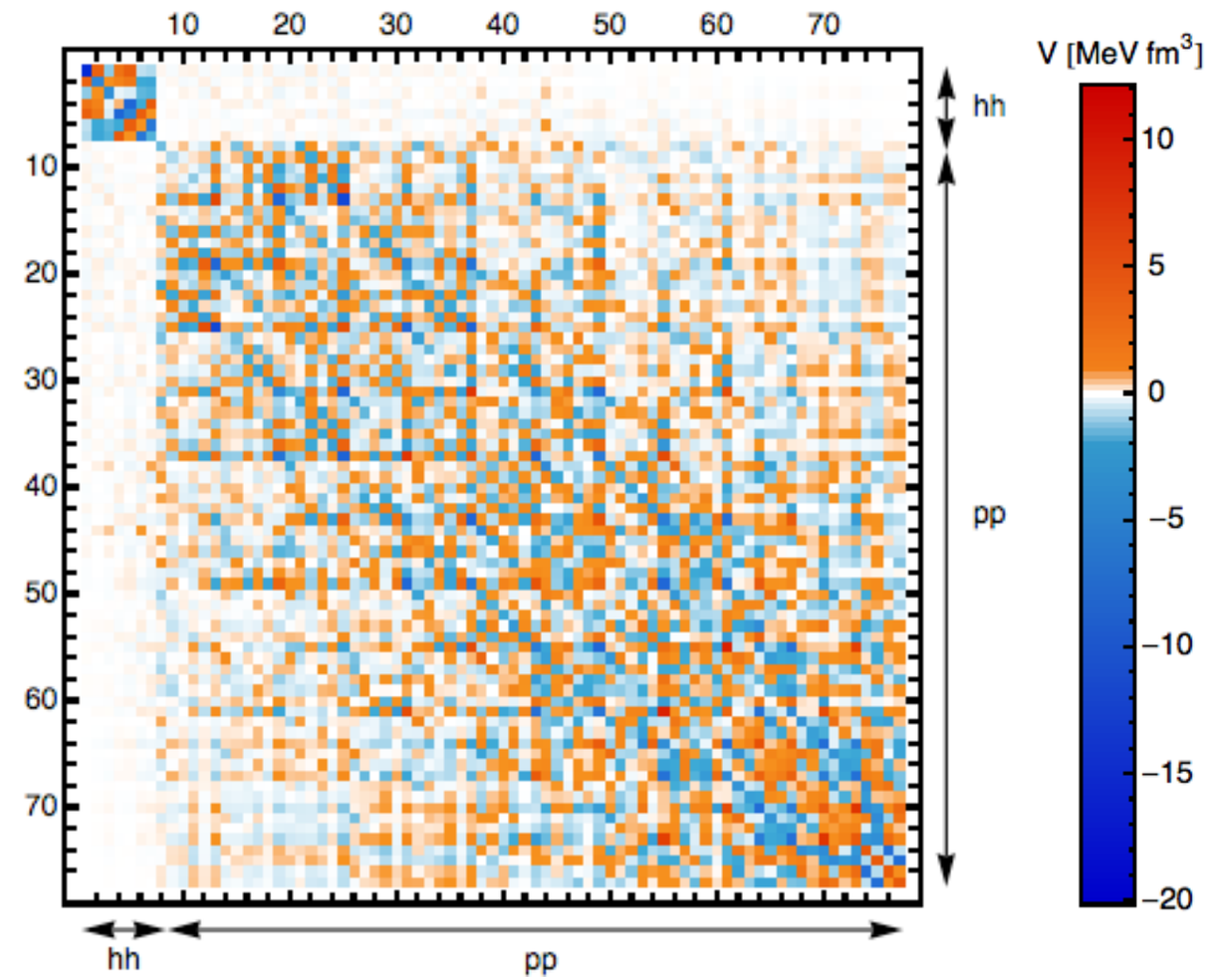

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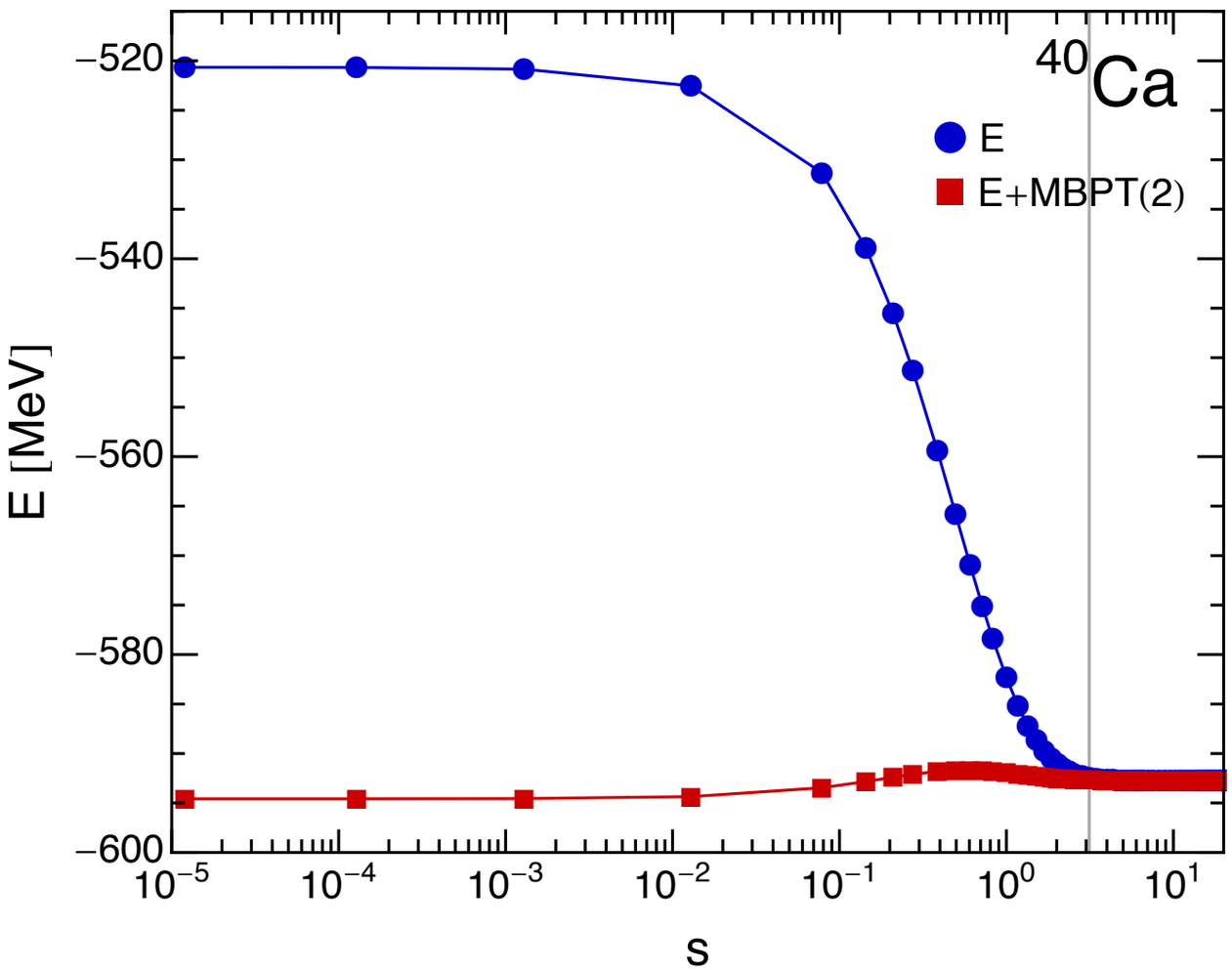

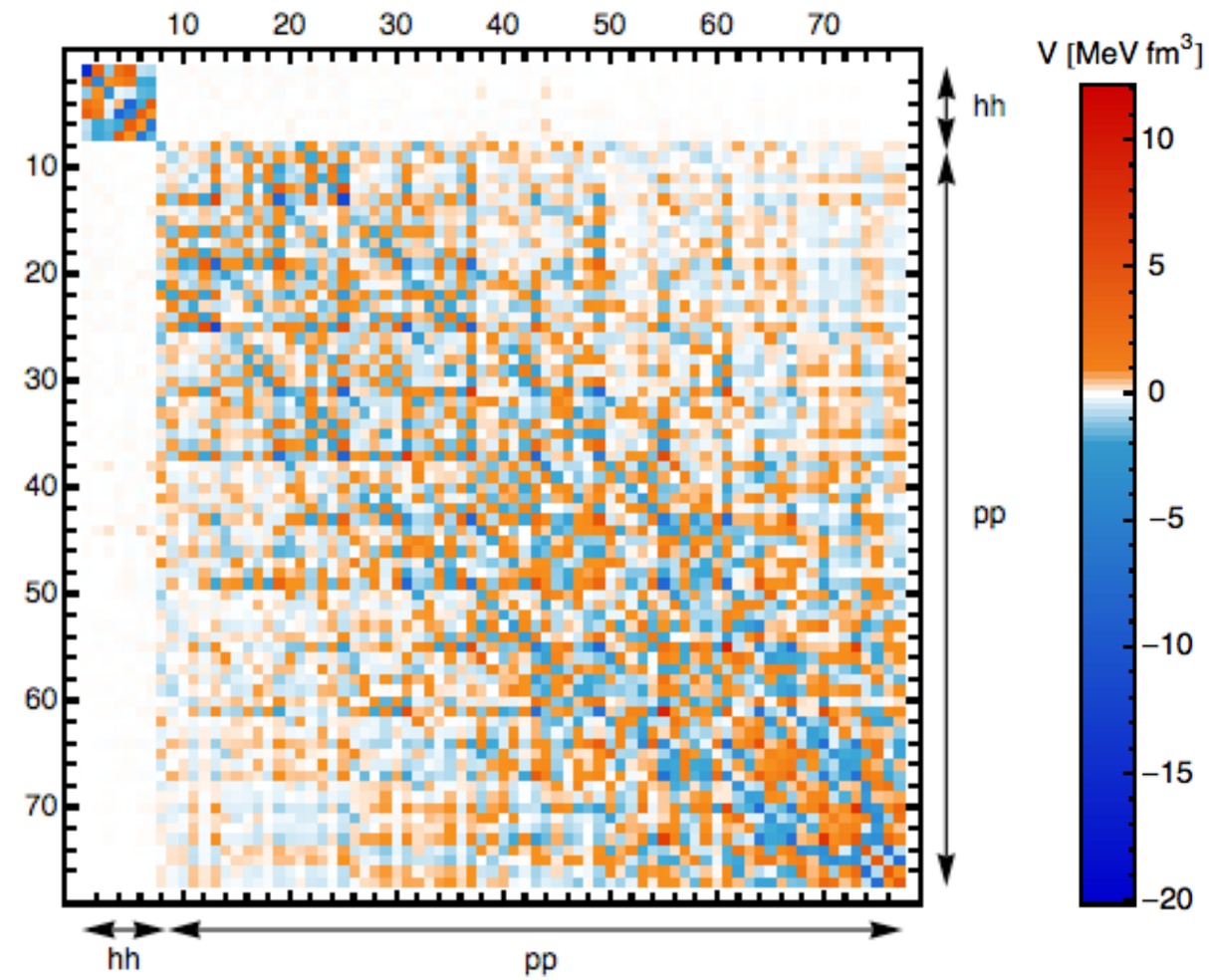

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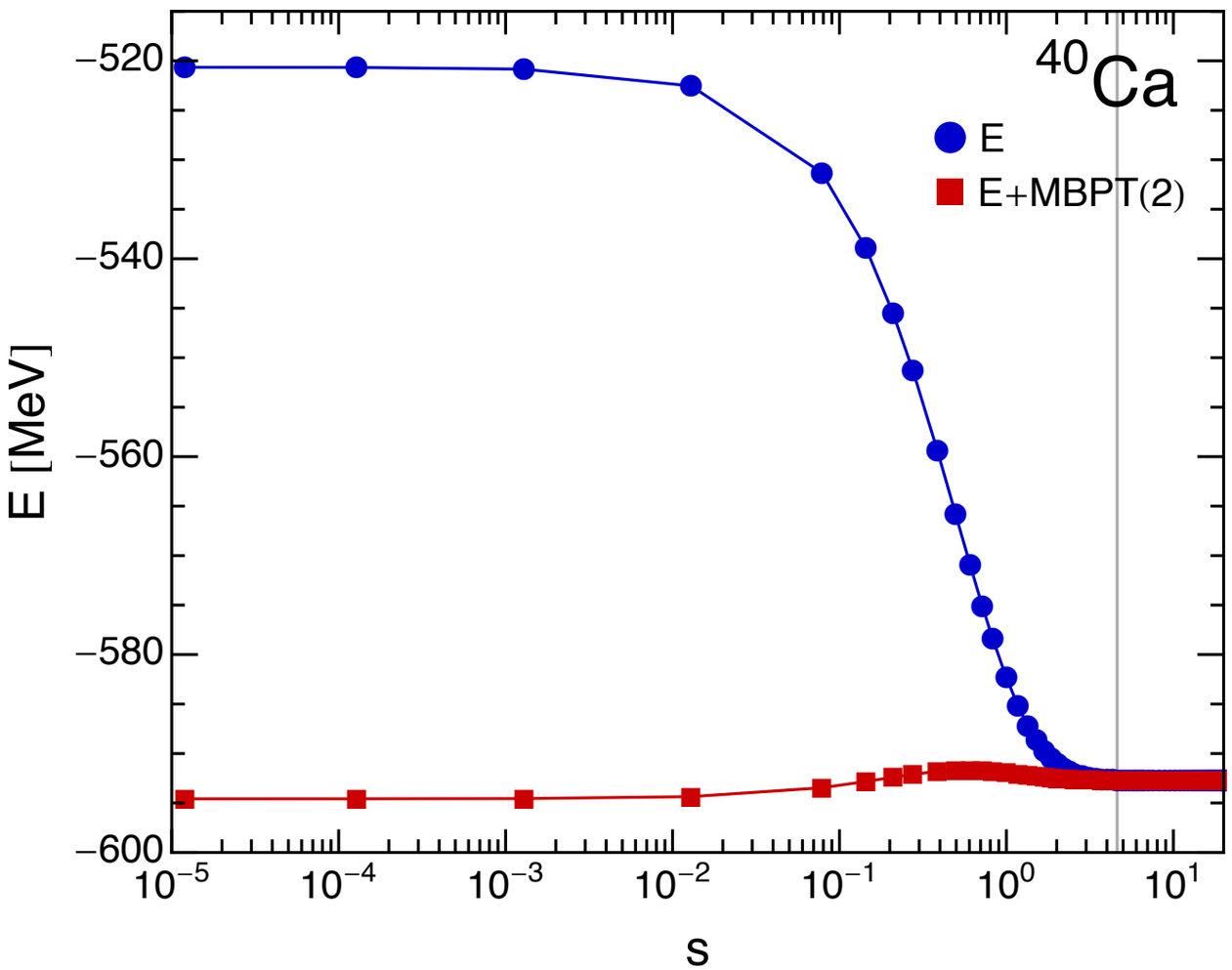

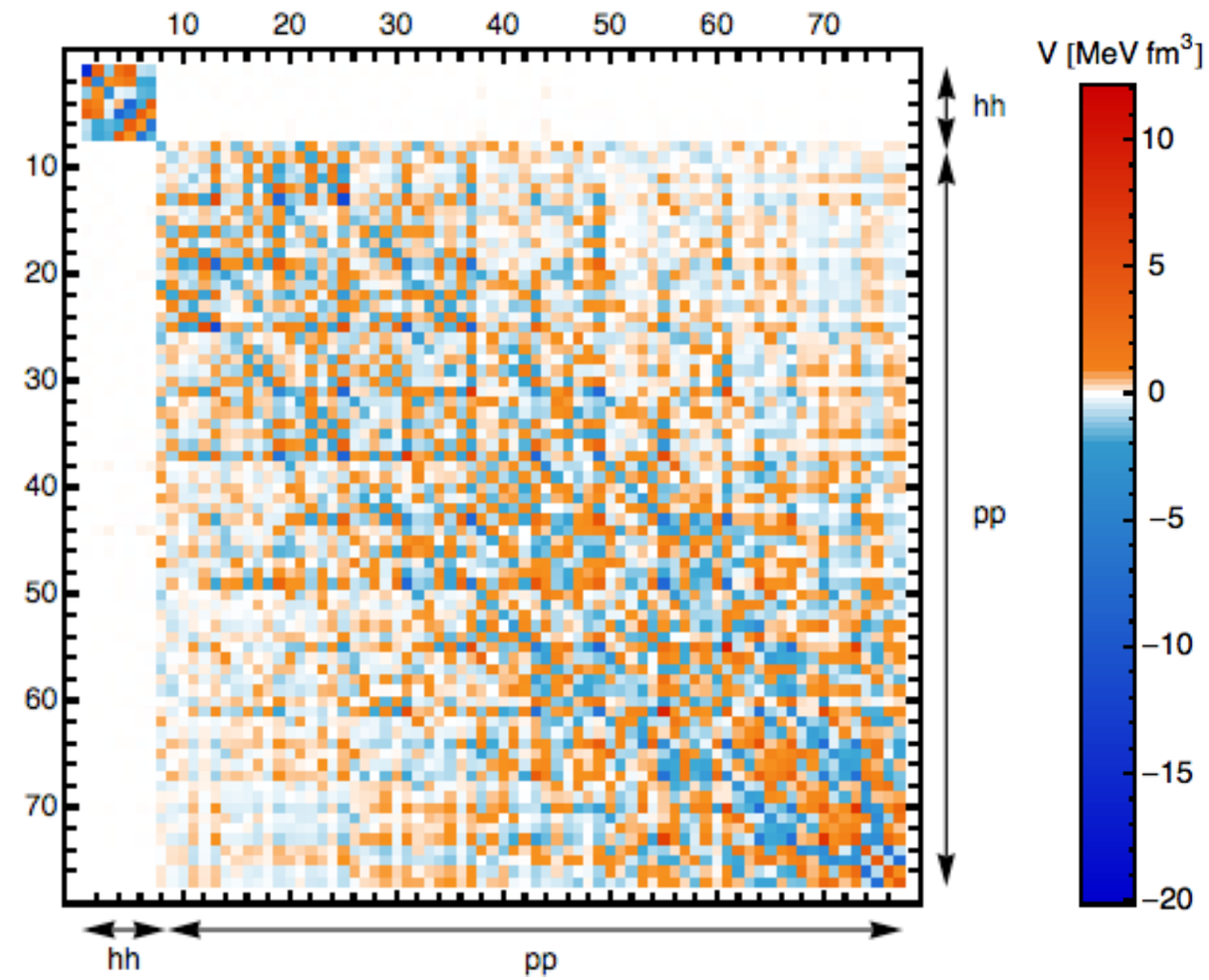

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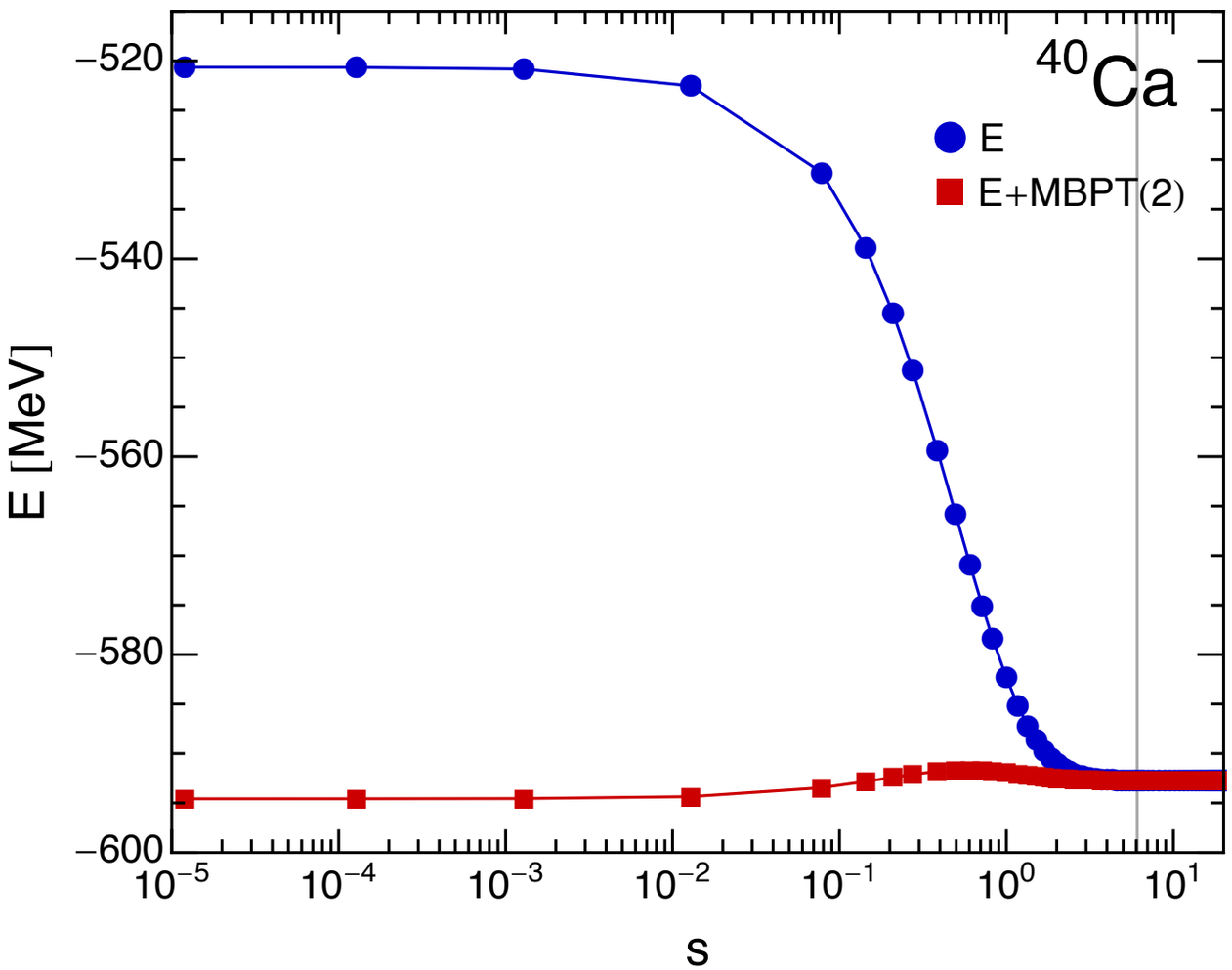

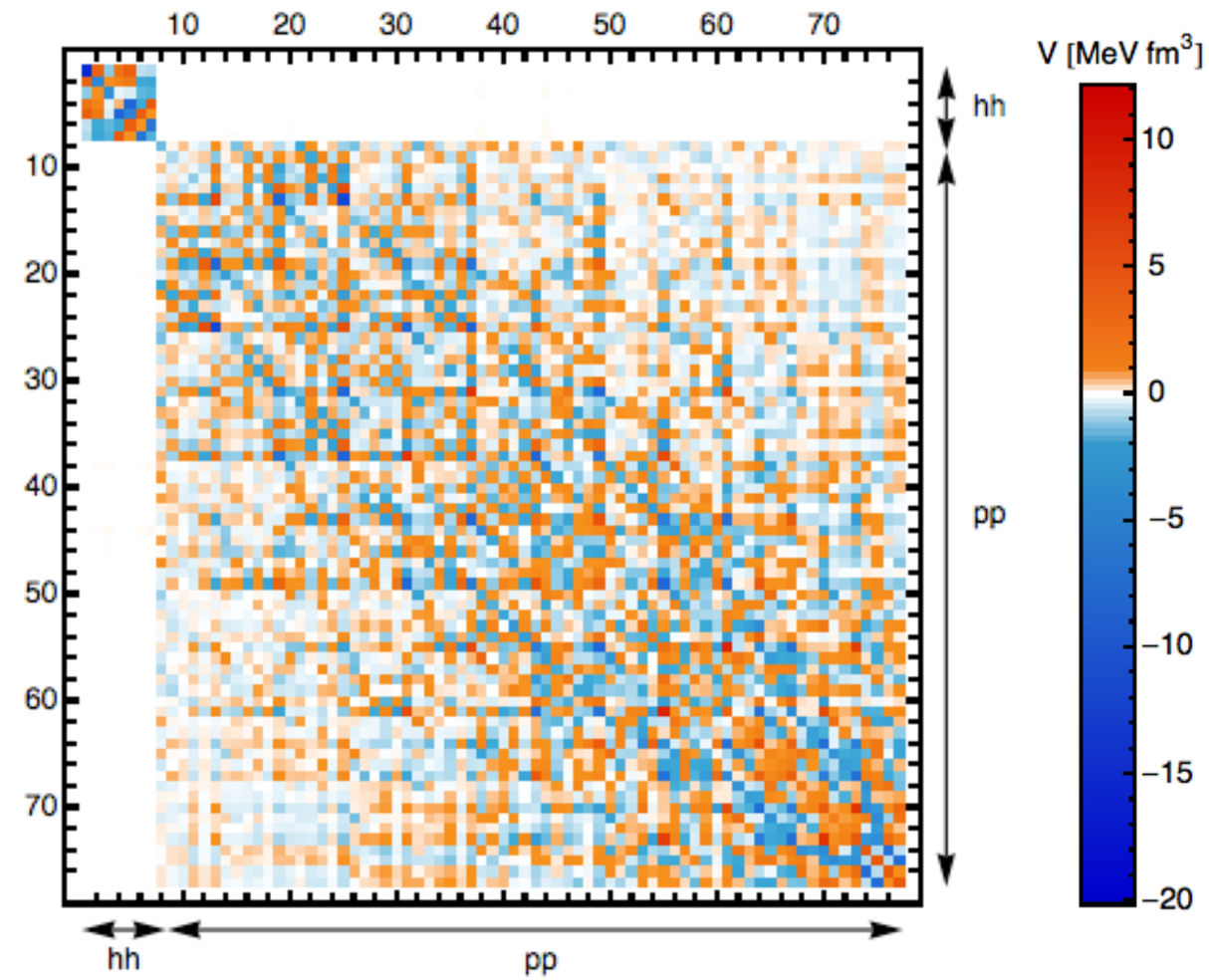

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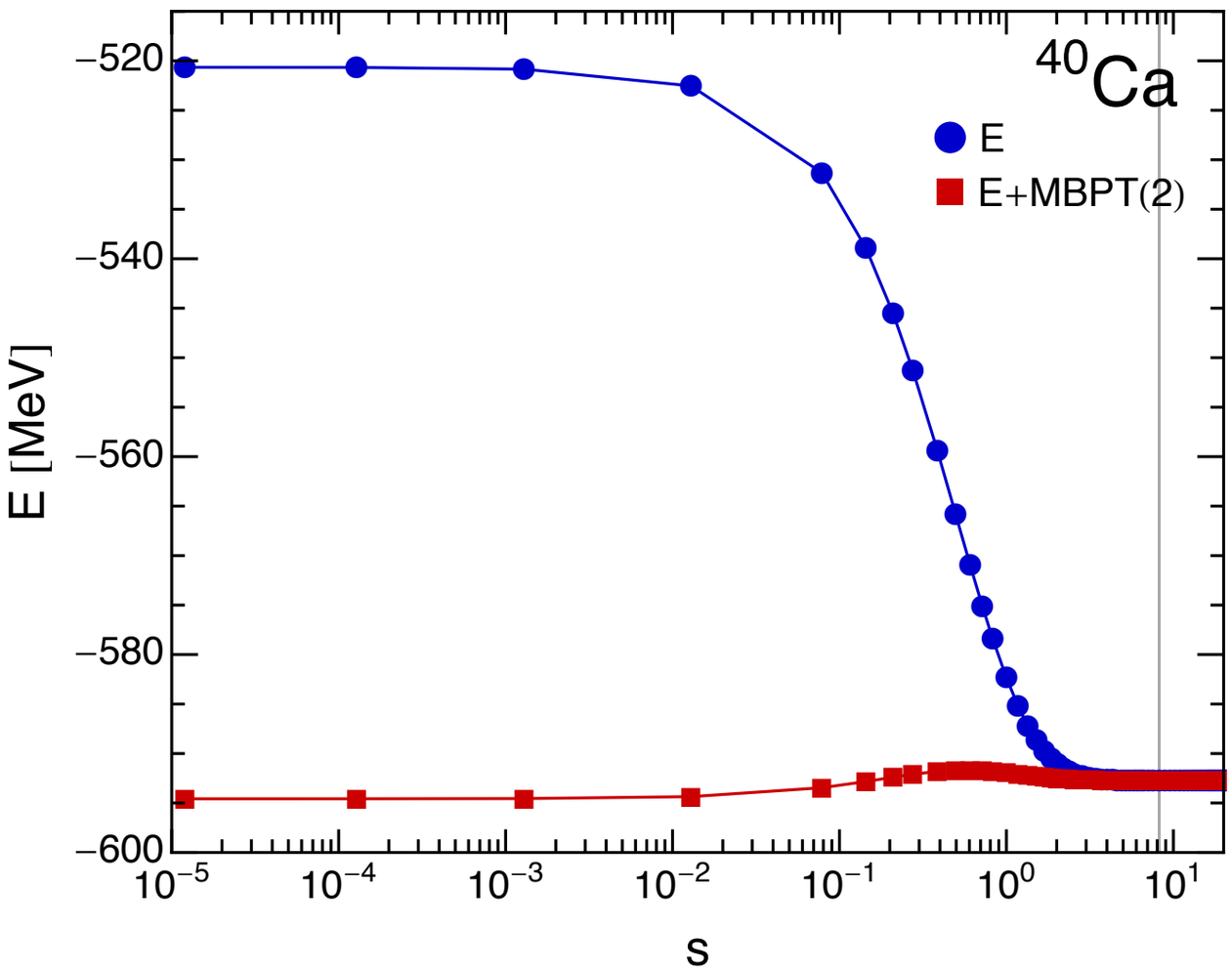

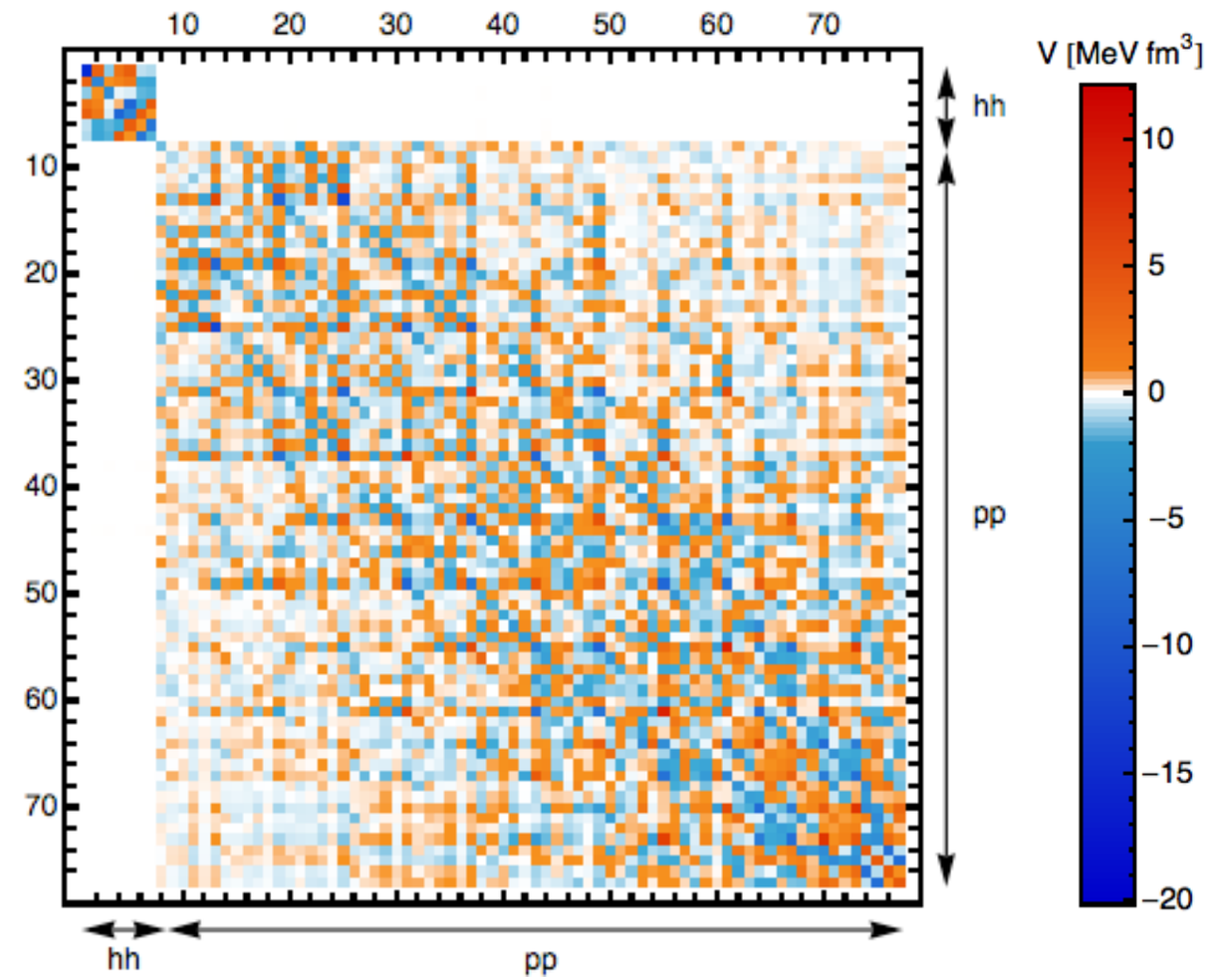

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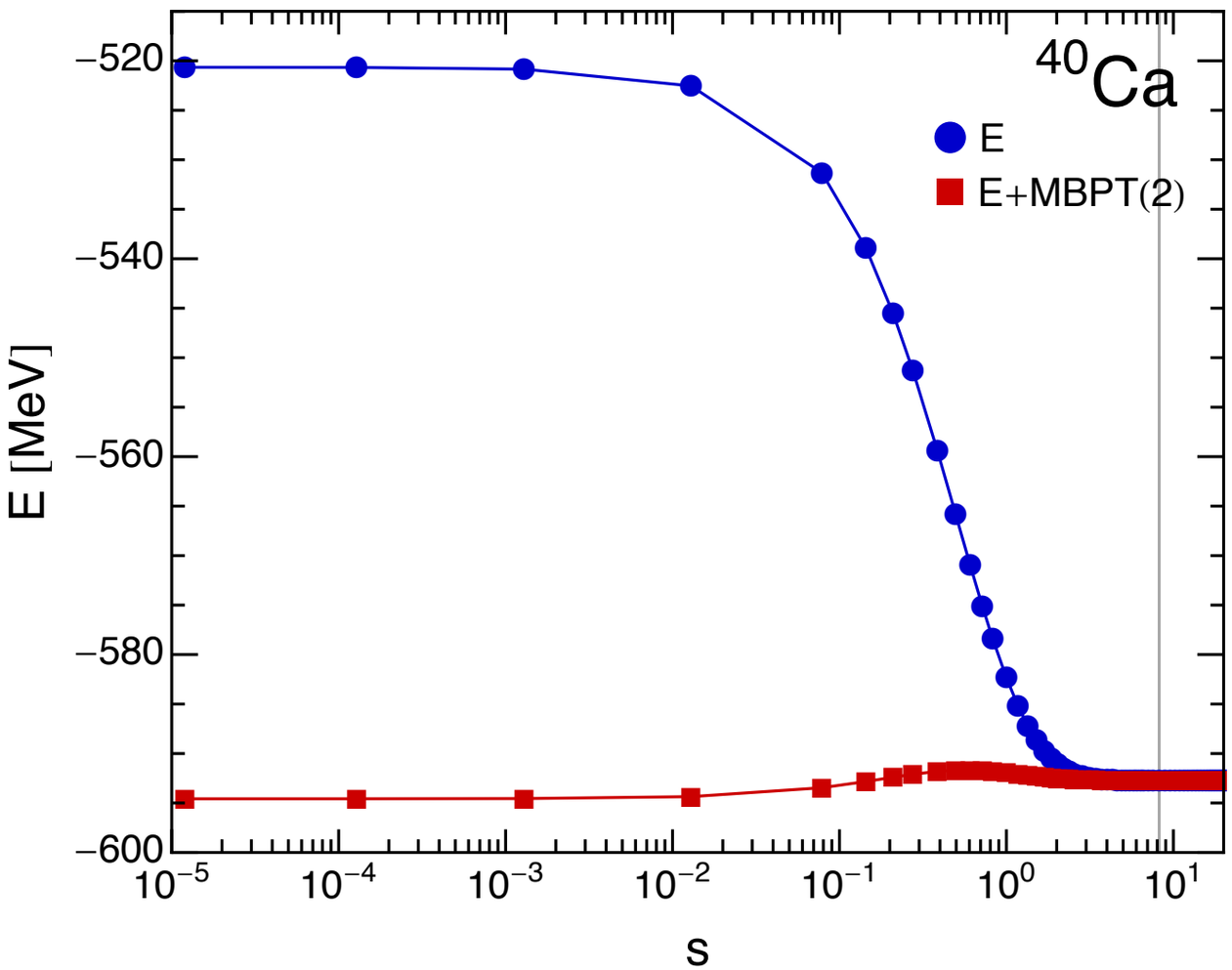
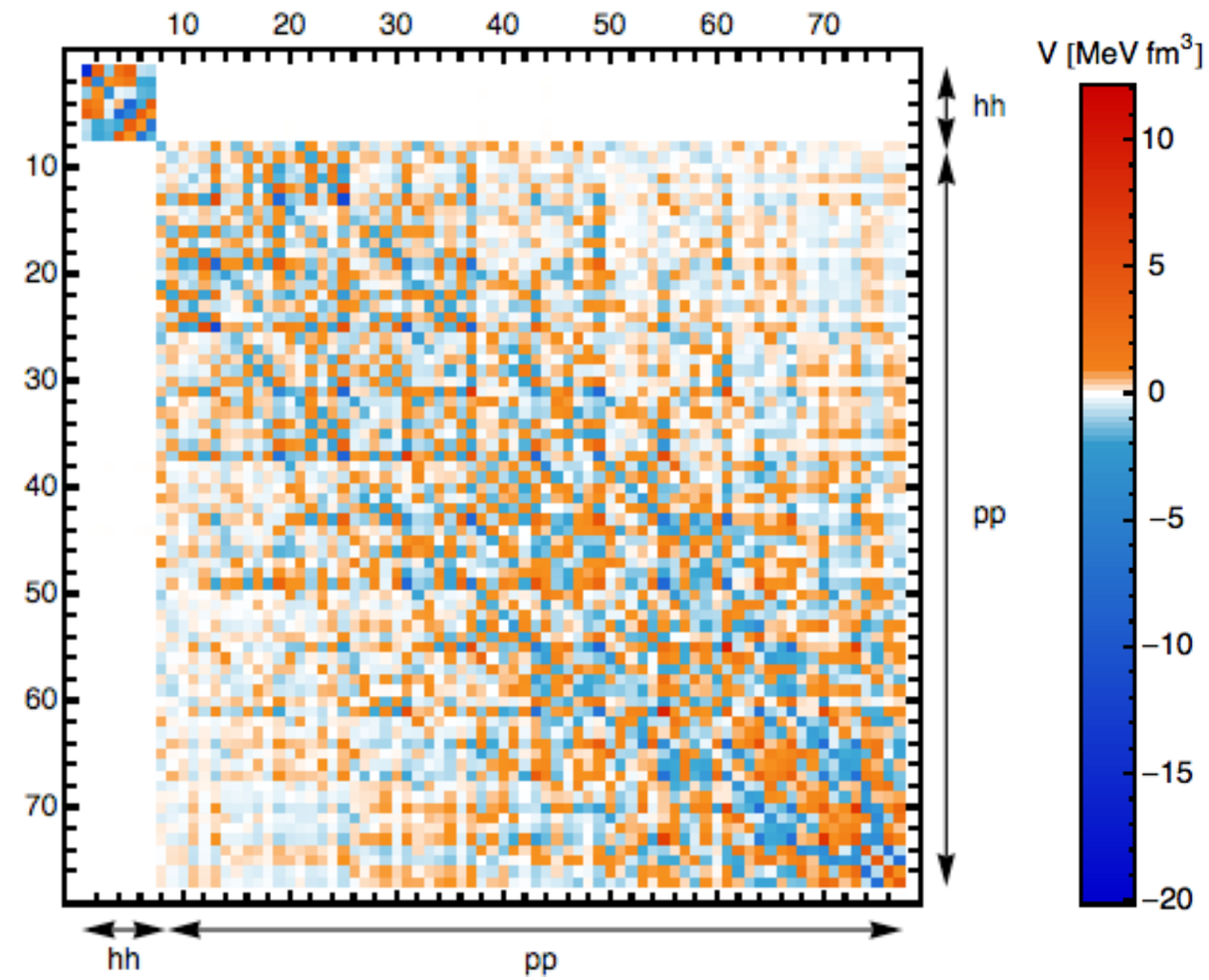
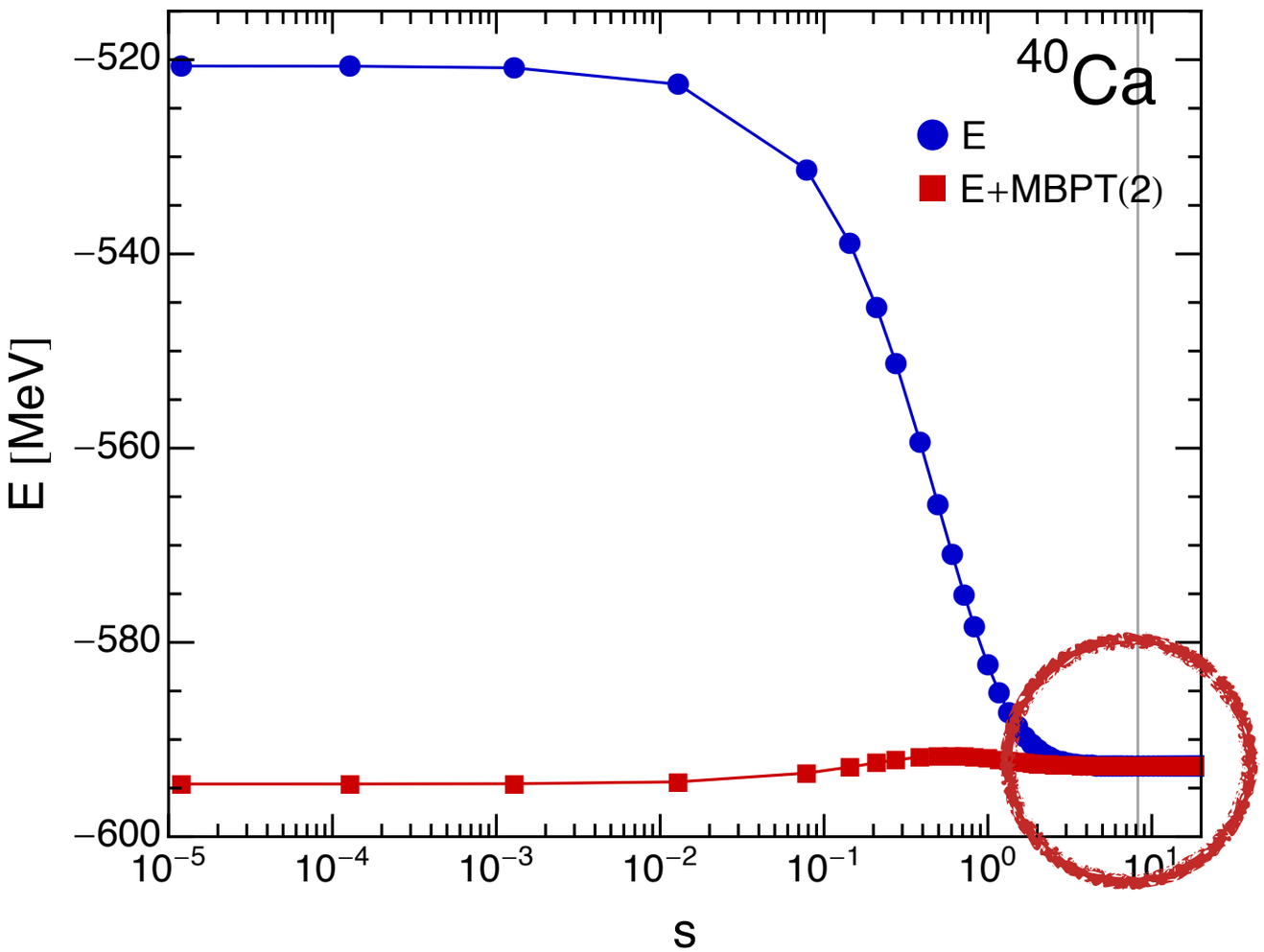


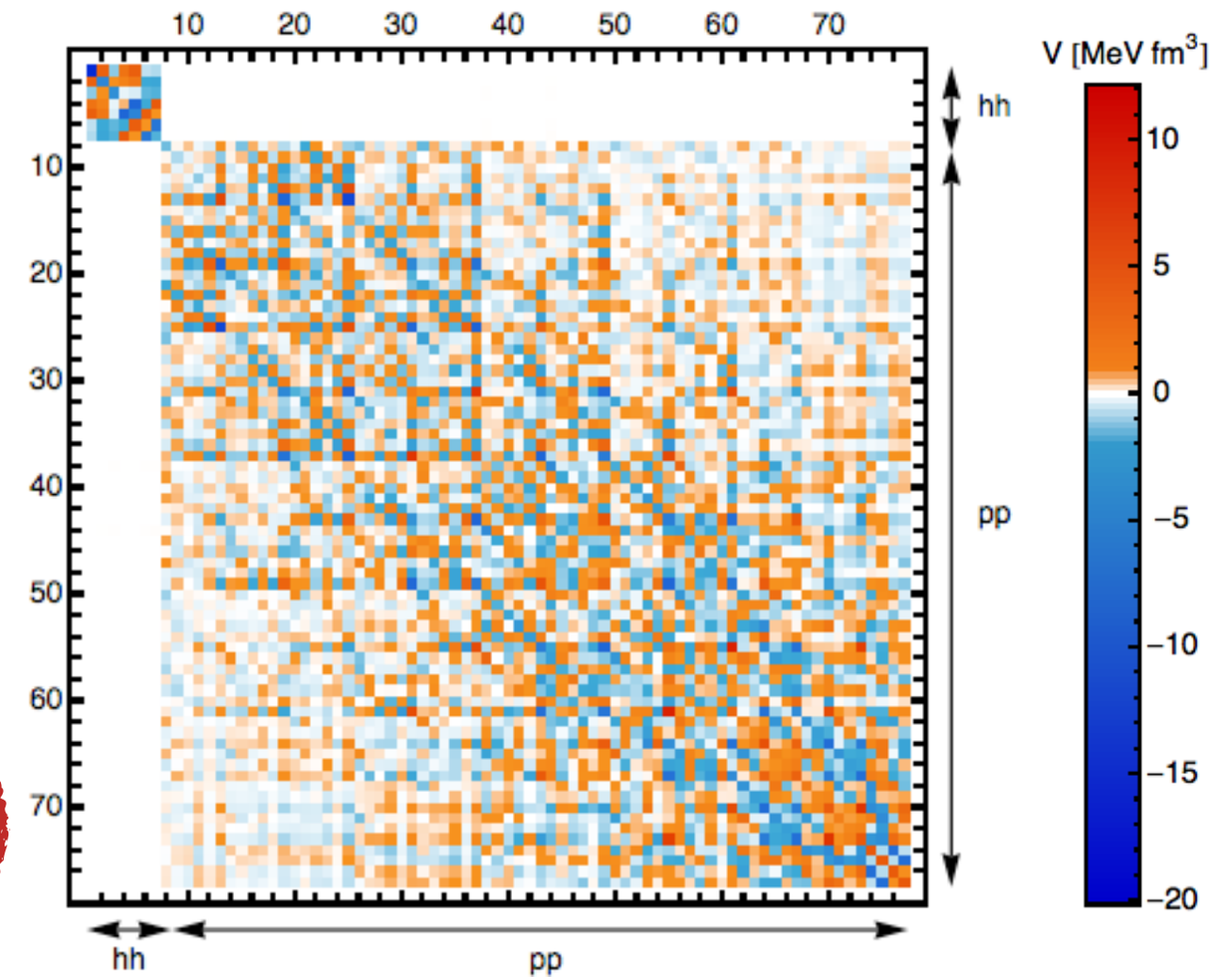


N3LO, $\lambda = 2.0$ fm^{-1}, $e_{\mathrm{Max}} = 8$

off-diagonal couplings are rapidly driven to zero

Decoupling



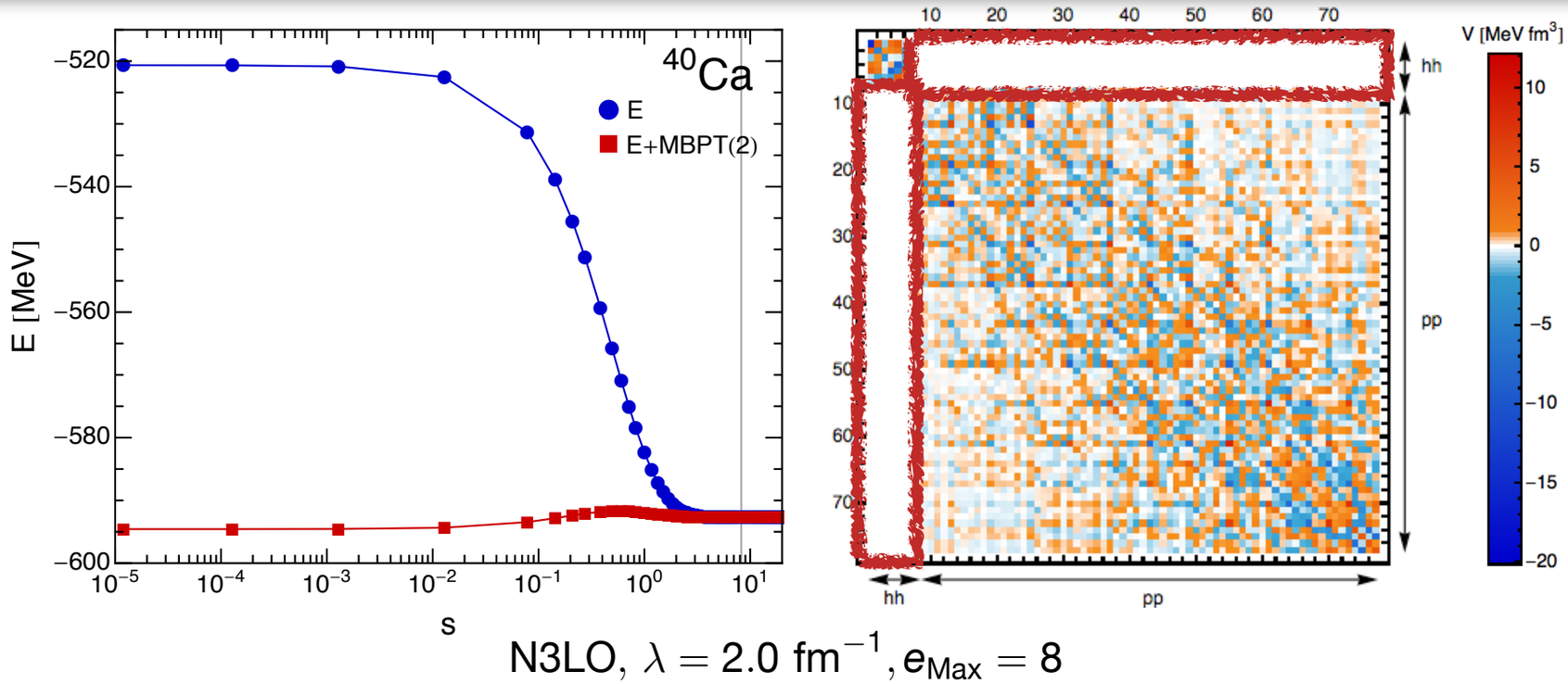


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

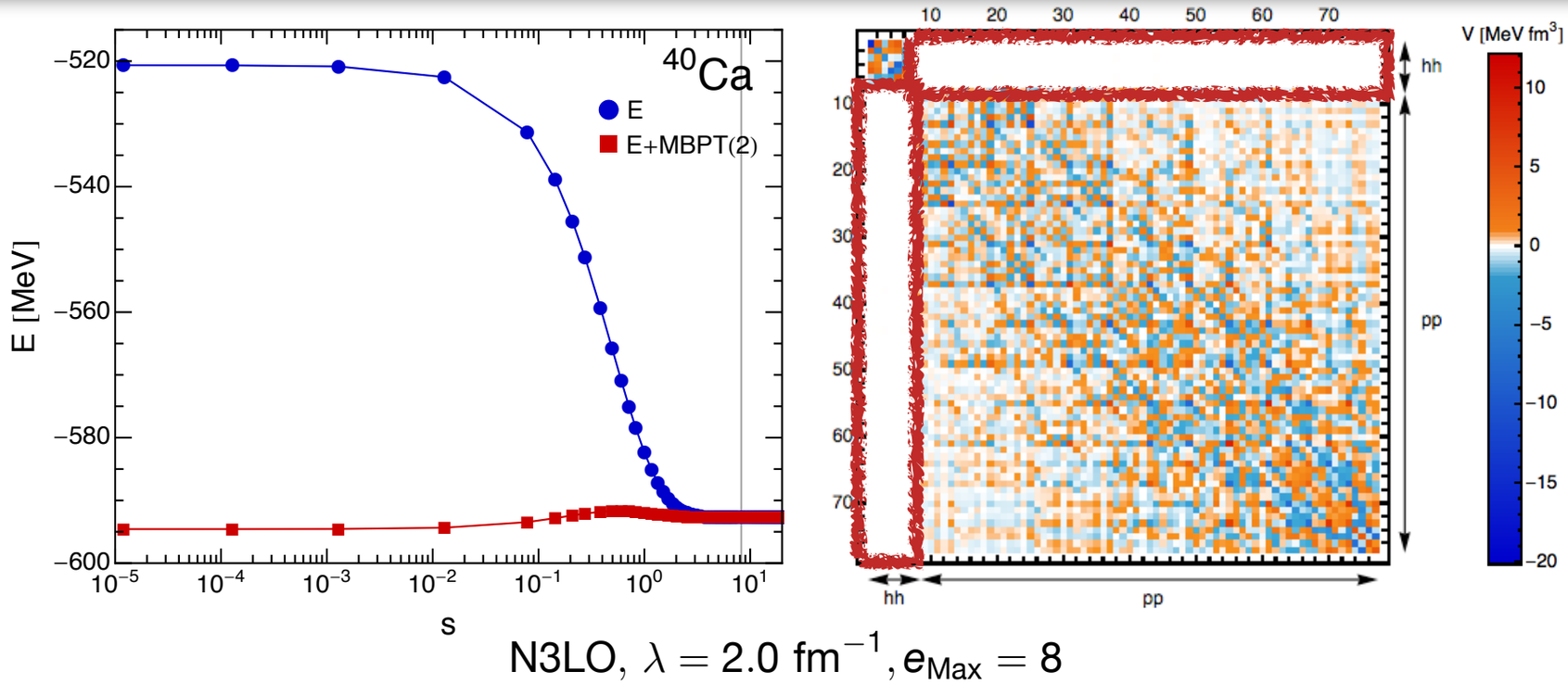
Decoupling



- absorb correlations into **RG-improved Hamiltonian**

$$U(s)HU^{\dagger}(s)U(s)\left|\Psi_n\right\rangle = E_n U(s)\left|\Psi_n\right\rangle$$

Decoupling



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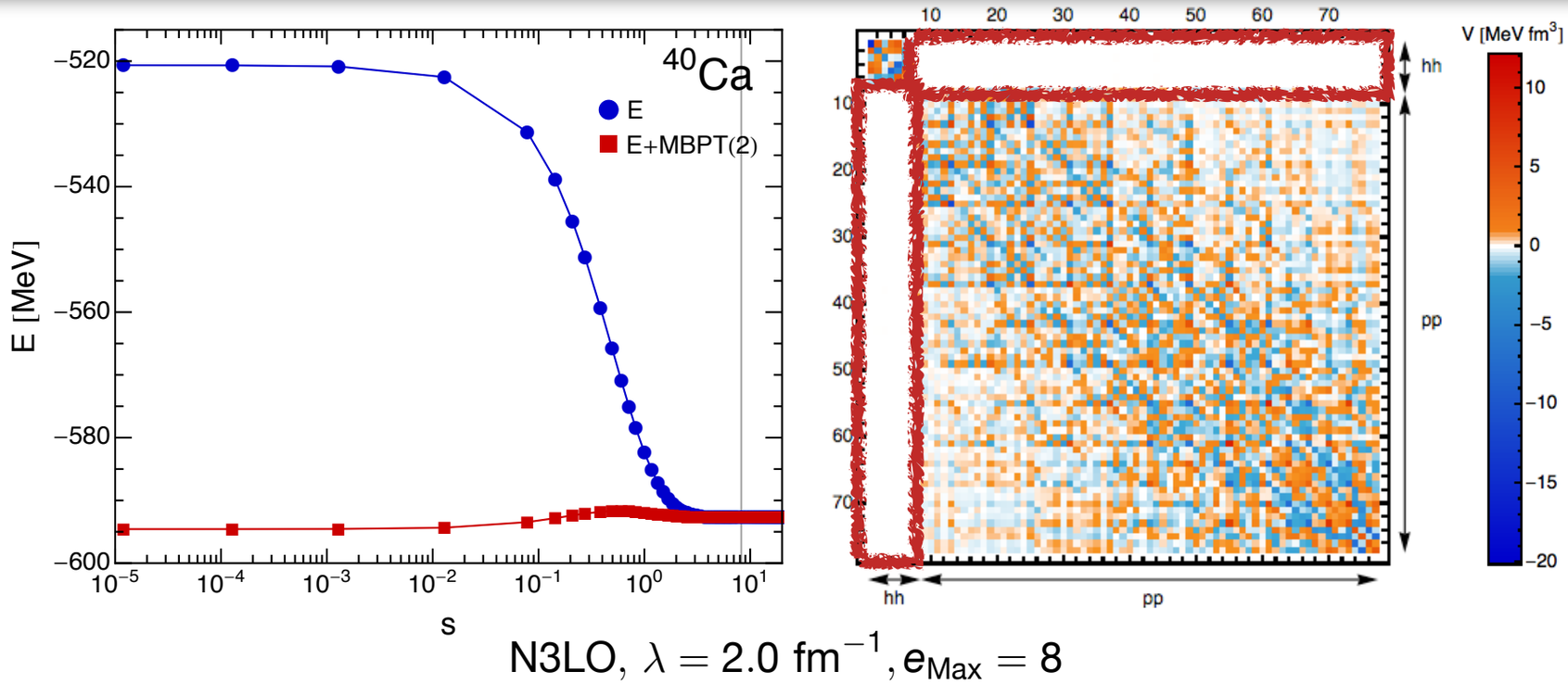
Decoupling



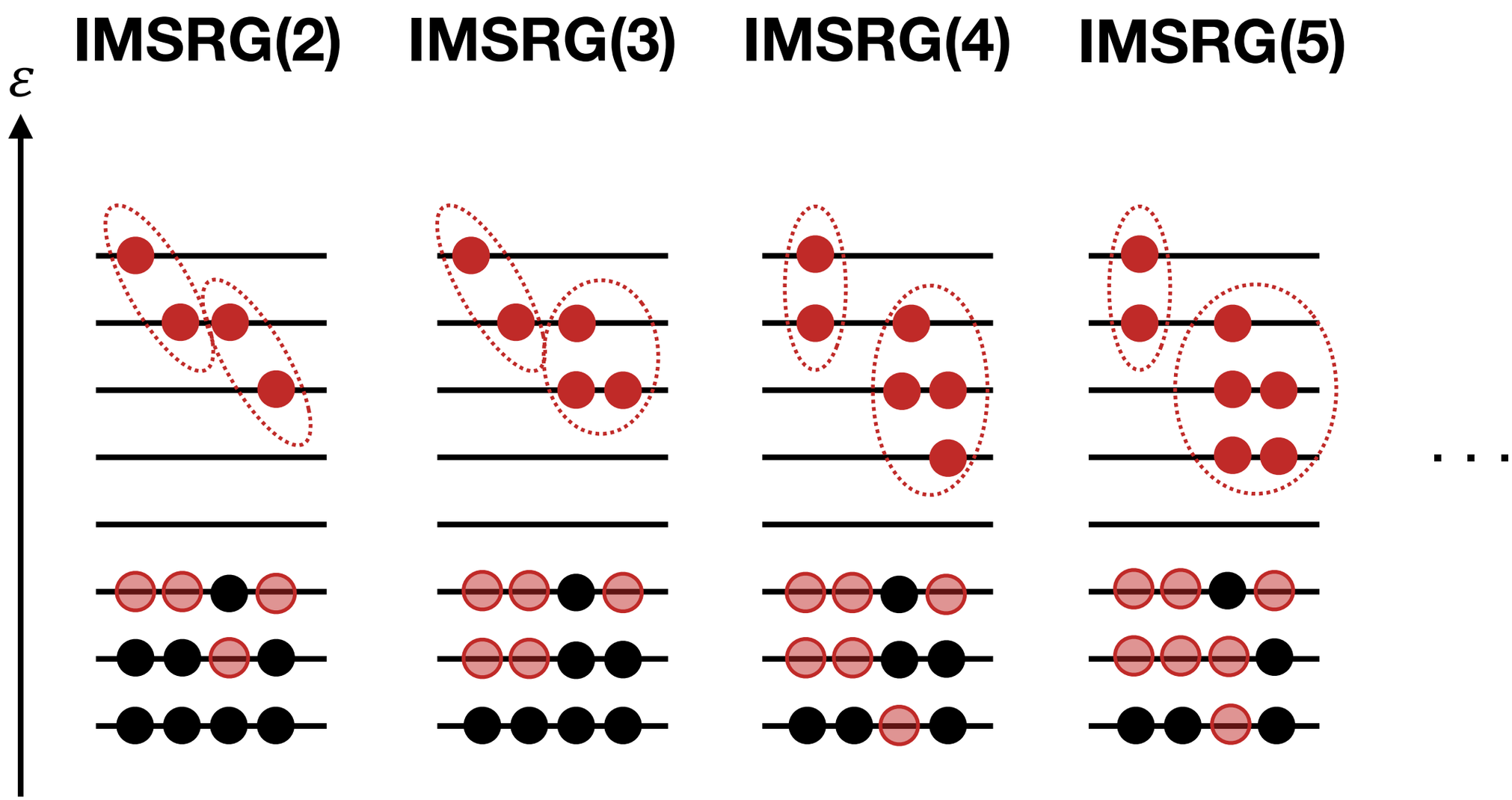
- absorb correlations into **RG-improved Hamiltonian**

$$U(s)HU^{\dagger}(s)U(s)\left|\Psi_n\right\rangle = E_n U(s)\left|\Psi_n\right\rangle$$

- reference state is ansatz for transformed, **less correlated** eigenstate:

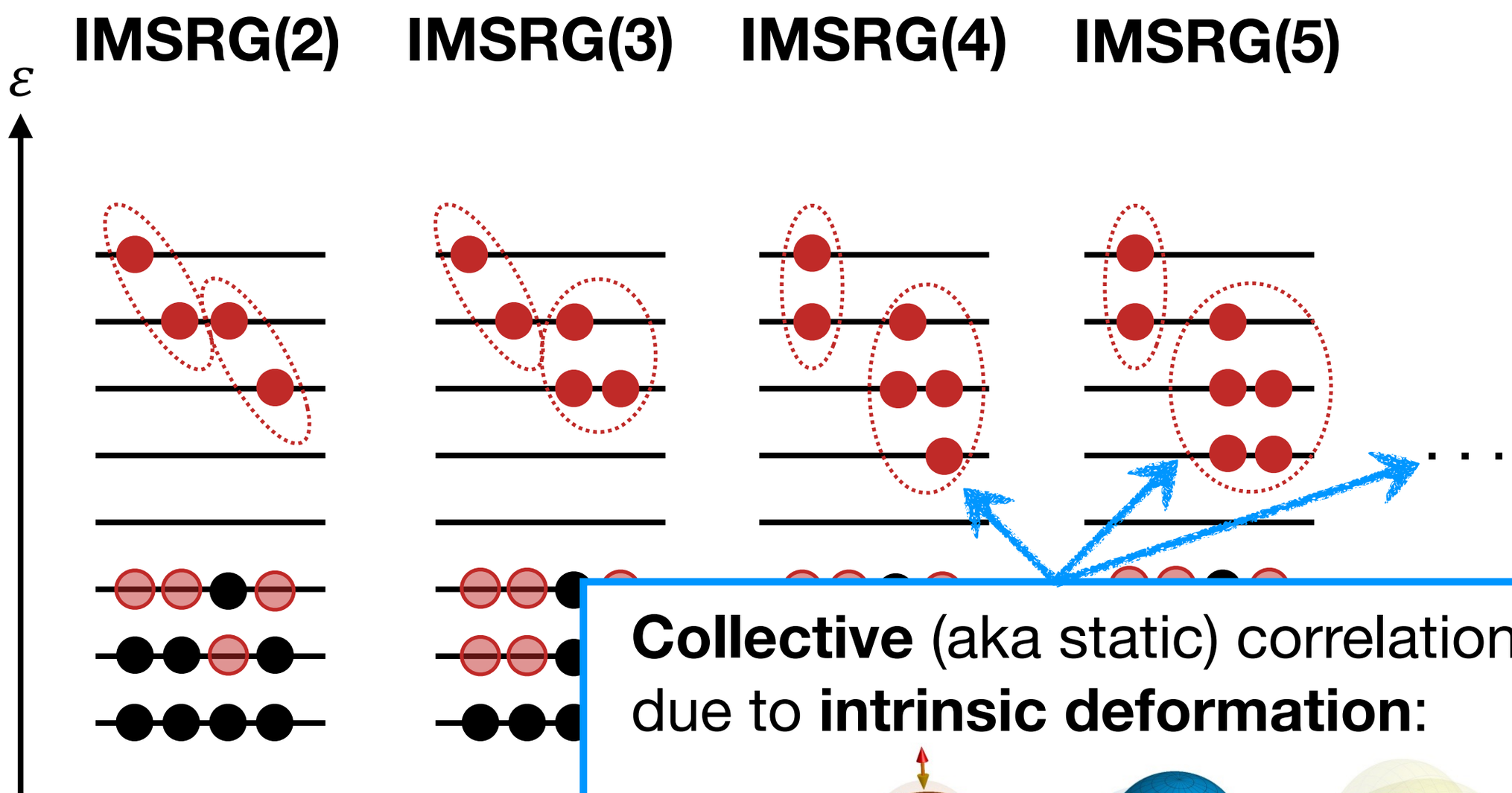
$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States



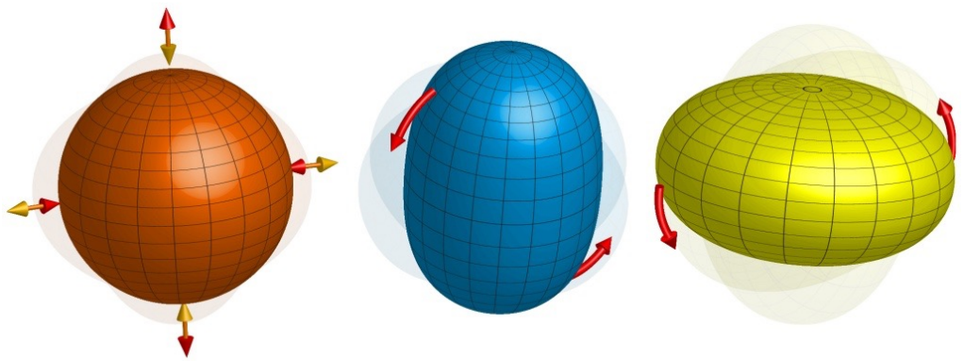
"standard" IMSRG: build correlations on top of Slater determinant (=**independent-particle state**)

Correlated Reference States

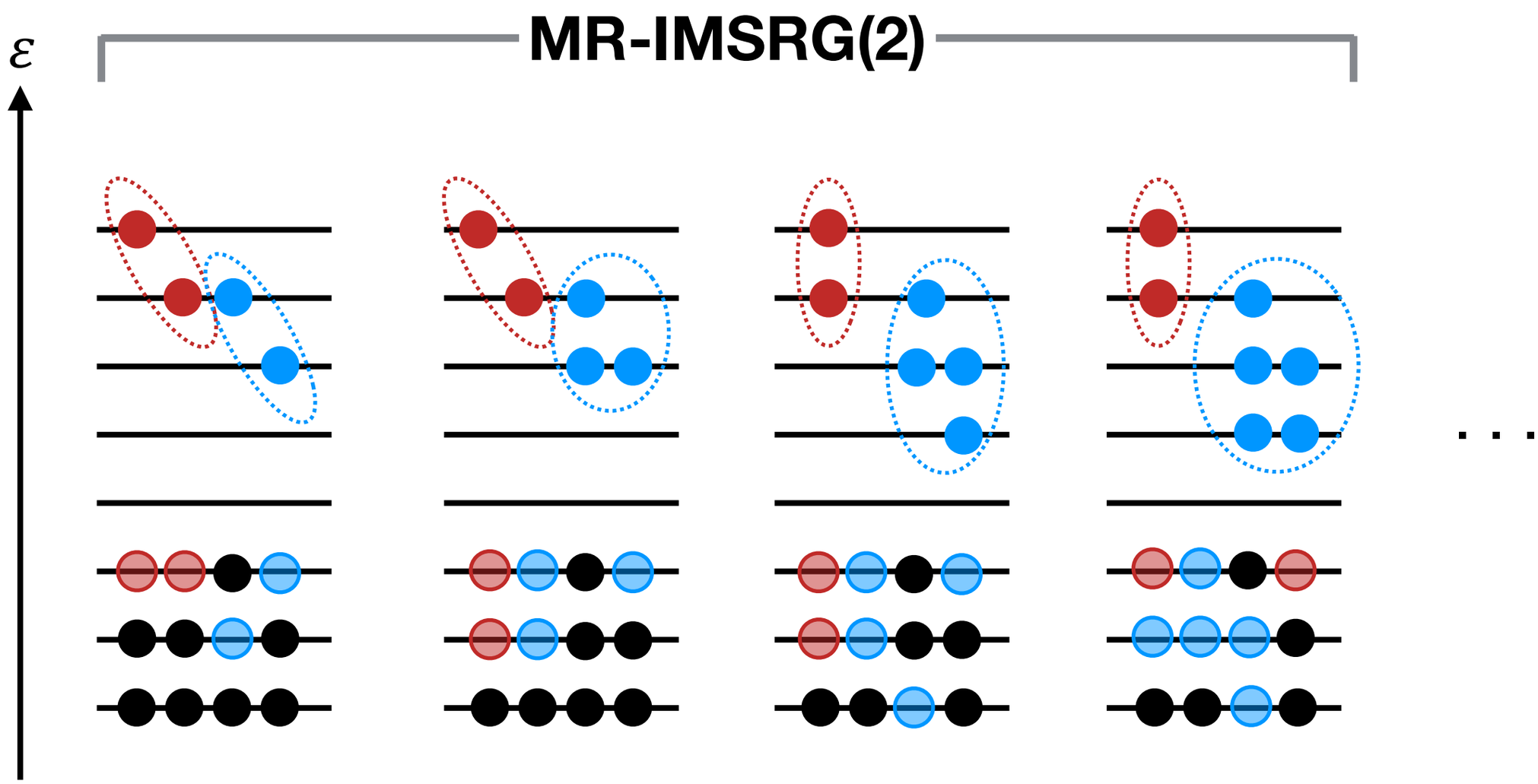


“standard” IMS
Slater determinan

Collective (aka static) correlations, e.g. due to **intrinsic deformation**:

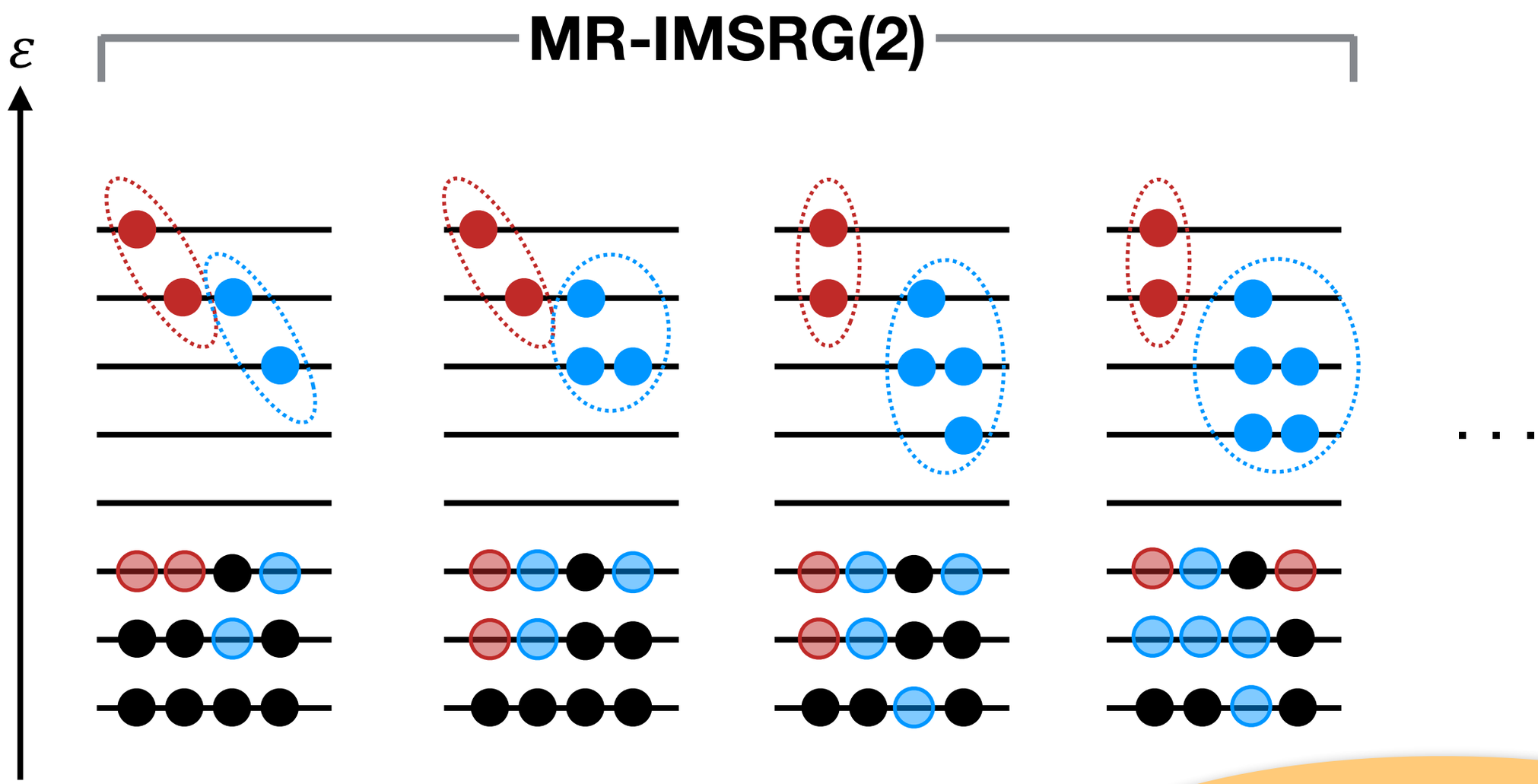


Correlated Reference States



MR-IMSRG: build correlations on top of **already correlated** state (e.g., from a method that describes static correlation well)

Correlated Reference States



MR-IMSRG: build correlations
already correlated state (e.g., fro
describes static correlation

use generalized normal ordering with 2B,... densities

MR-IMSRG References States

available

- Slater determinants (uncorrelated)
- number-projected Hartree-Fock Bogoliubov vacua
- Generator Coordinate Method (with projections)
- small-scale No-Core Shell Model

see talk by **K. Vobig**

future

- clustered states, Density Matrix Renormalization Group, tensor networks etc.

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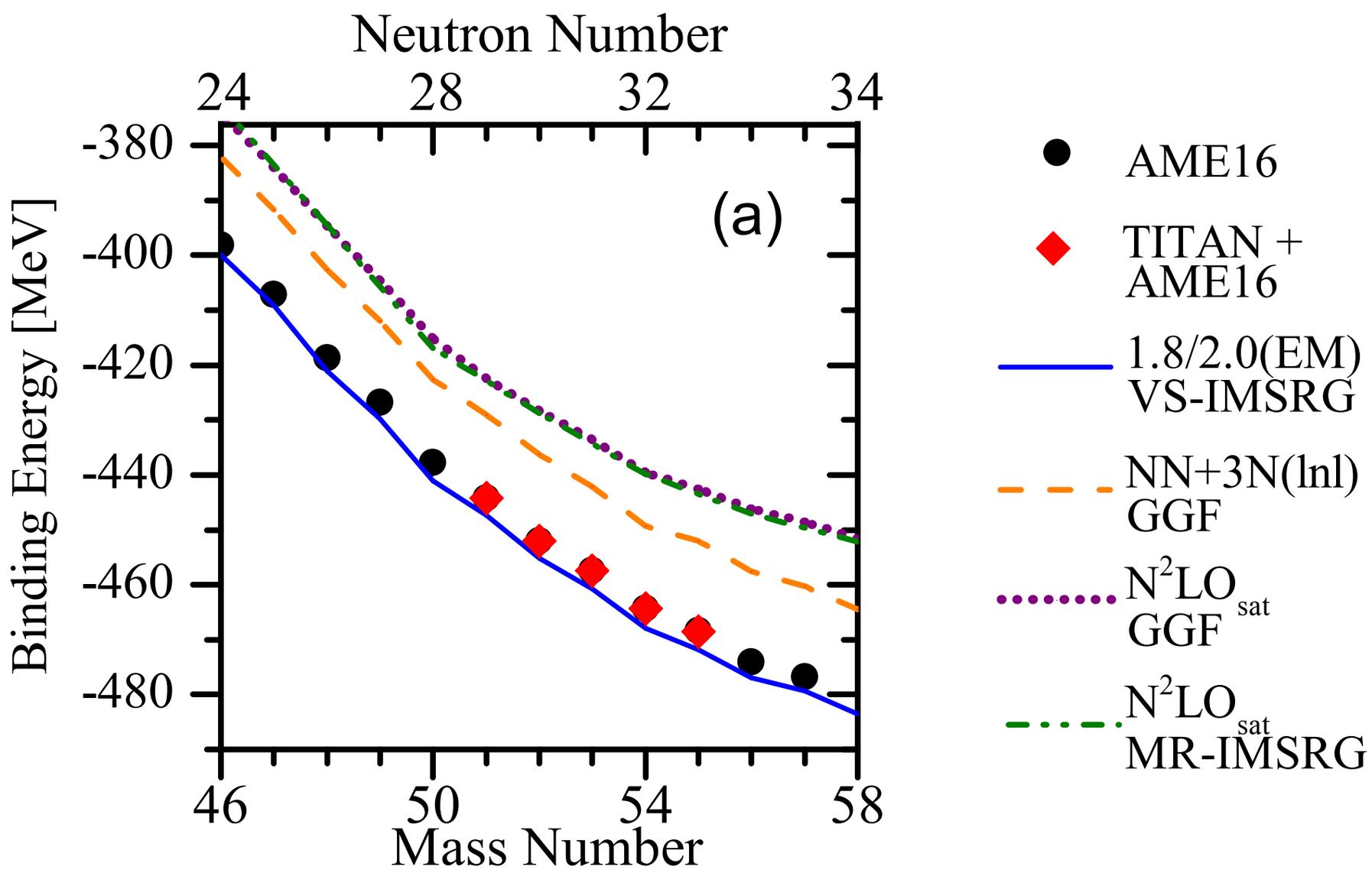
Titanium Isotopes

E. Leistenschneider et al., arXiv:1710.08537



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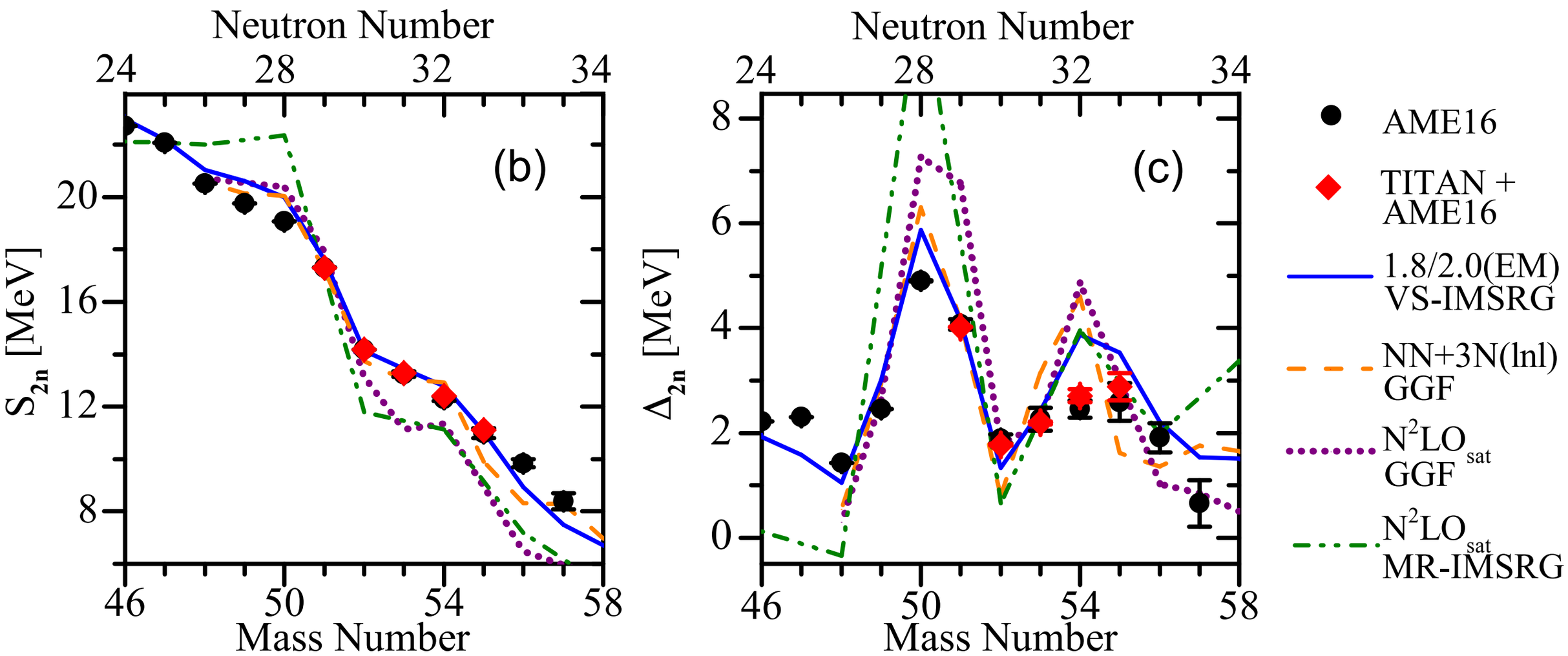

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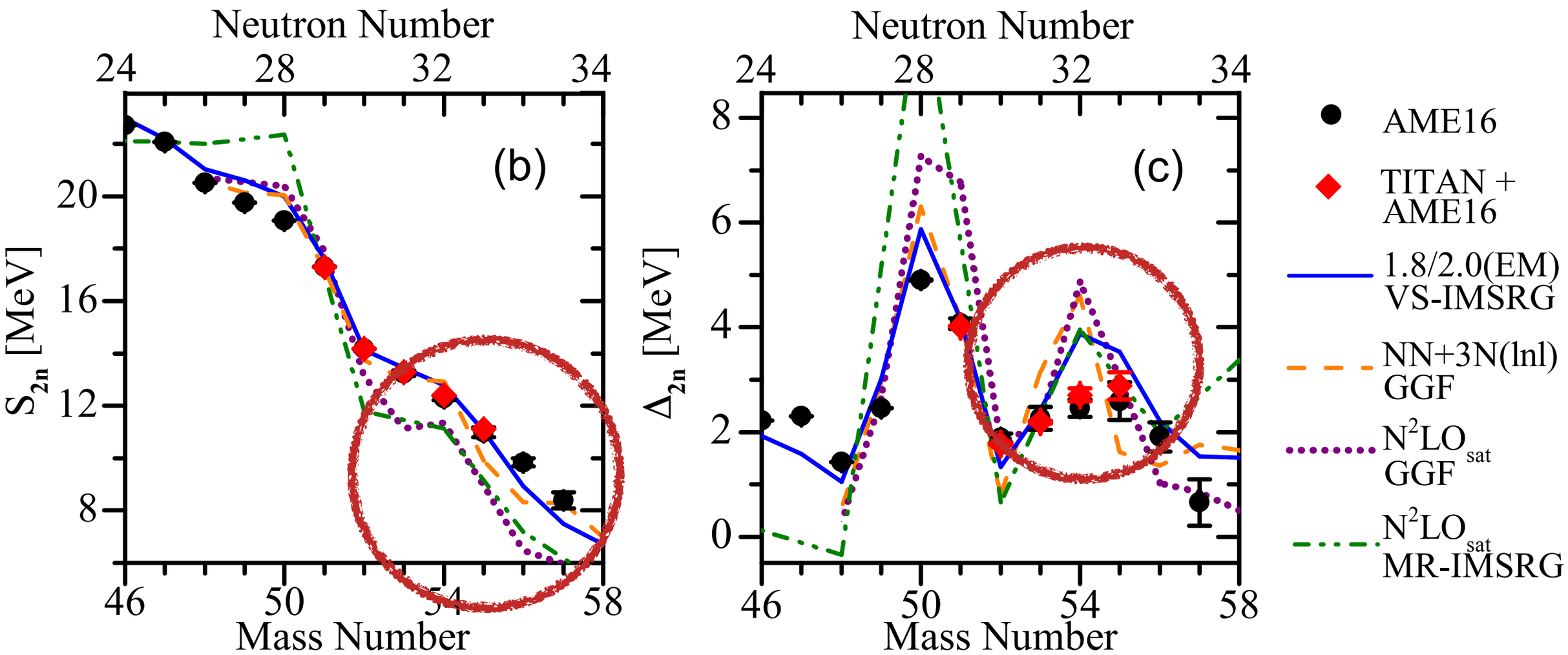

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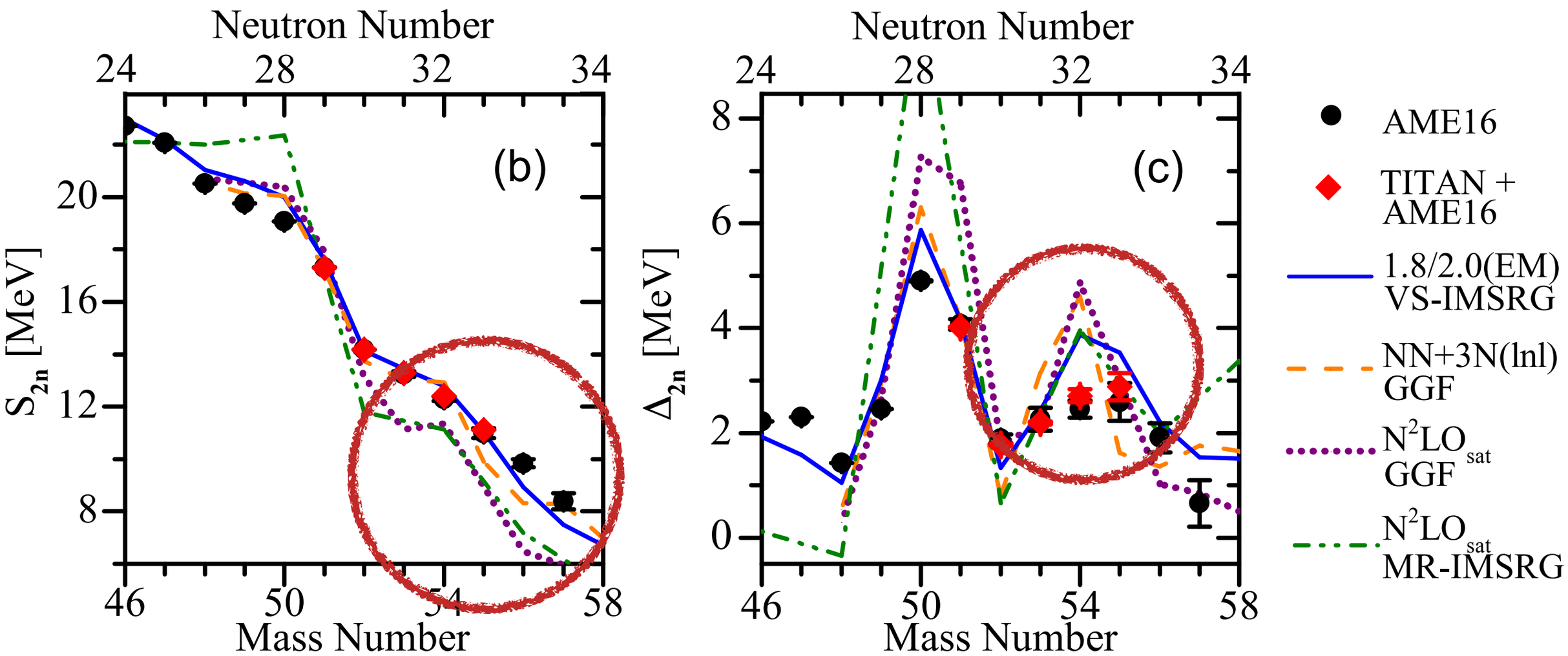
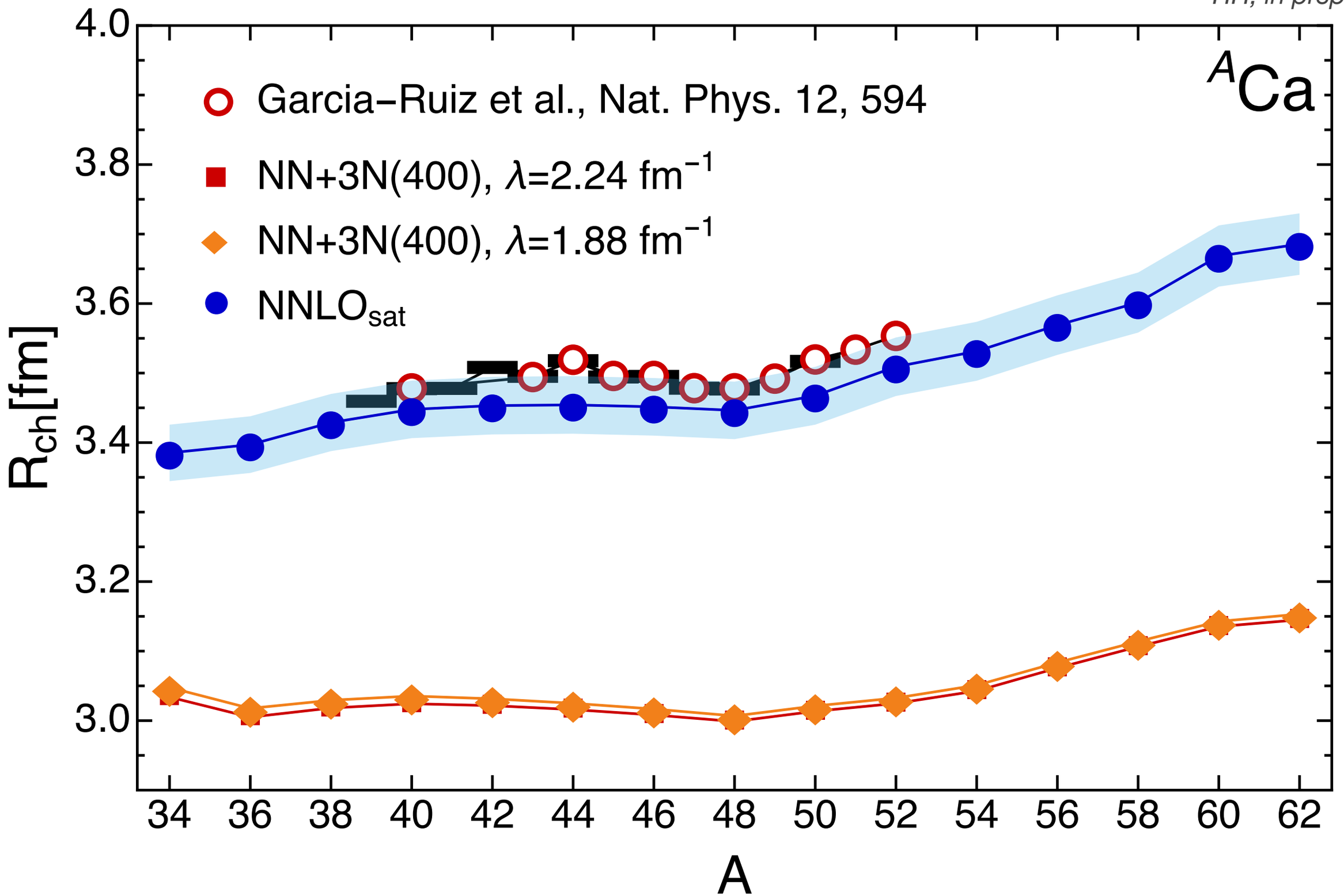


N=32 sub-shell **closure too pronounced**: combined effect of **method & interaction** !

Calcium Isotopes

HH, in preparation



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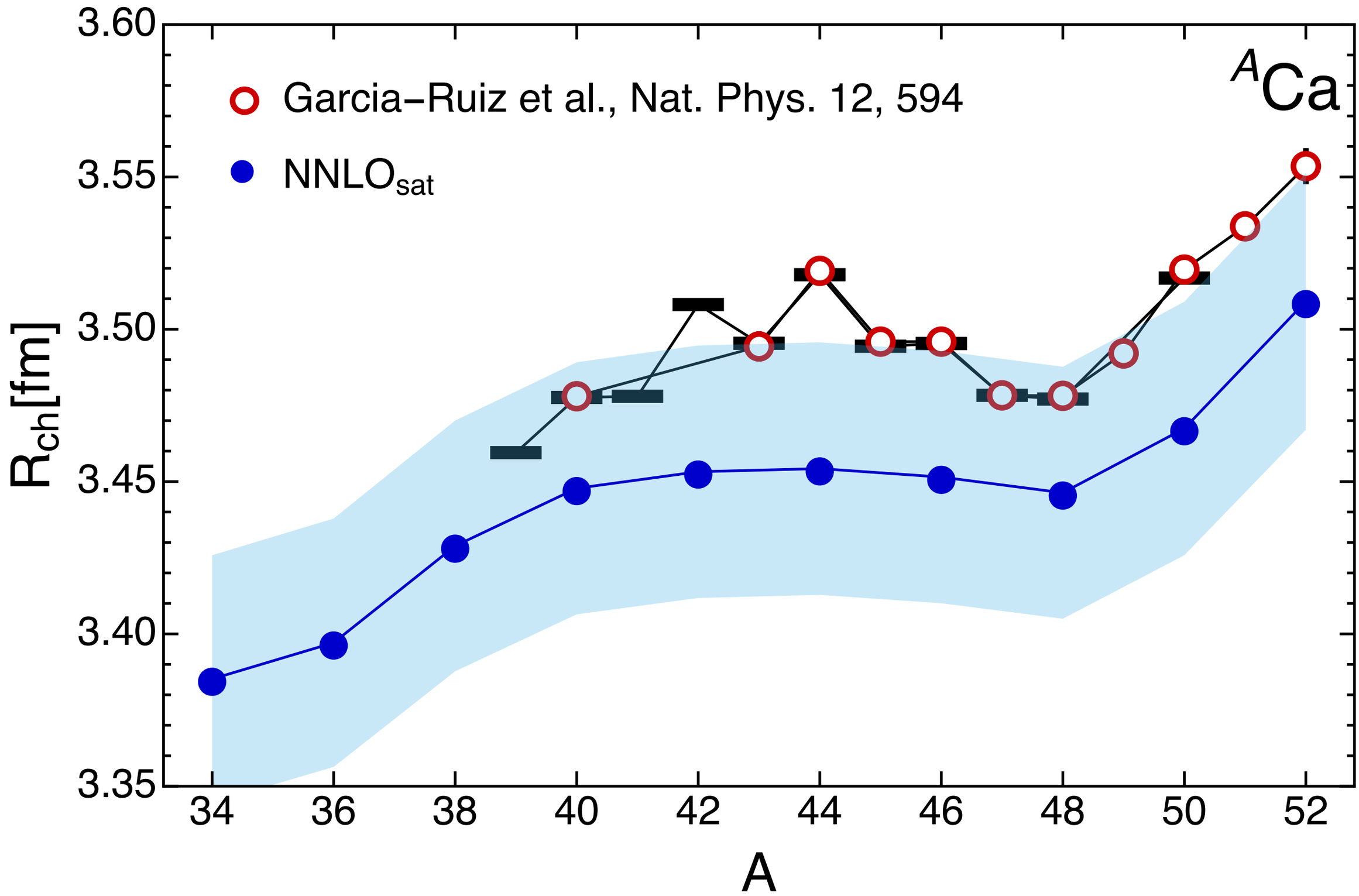

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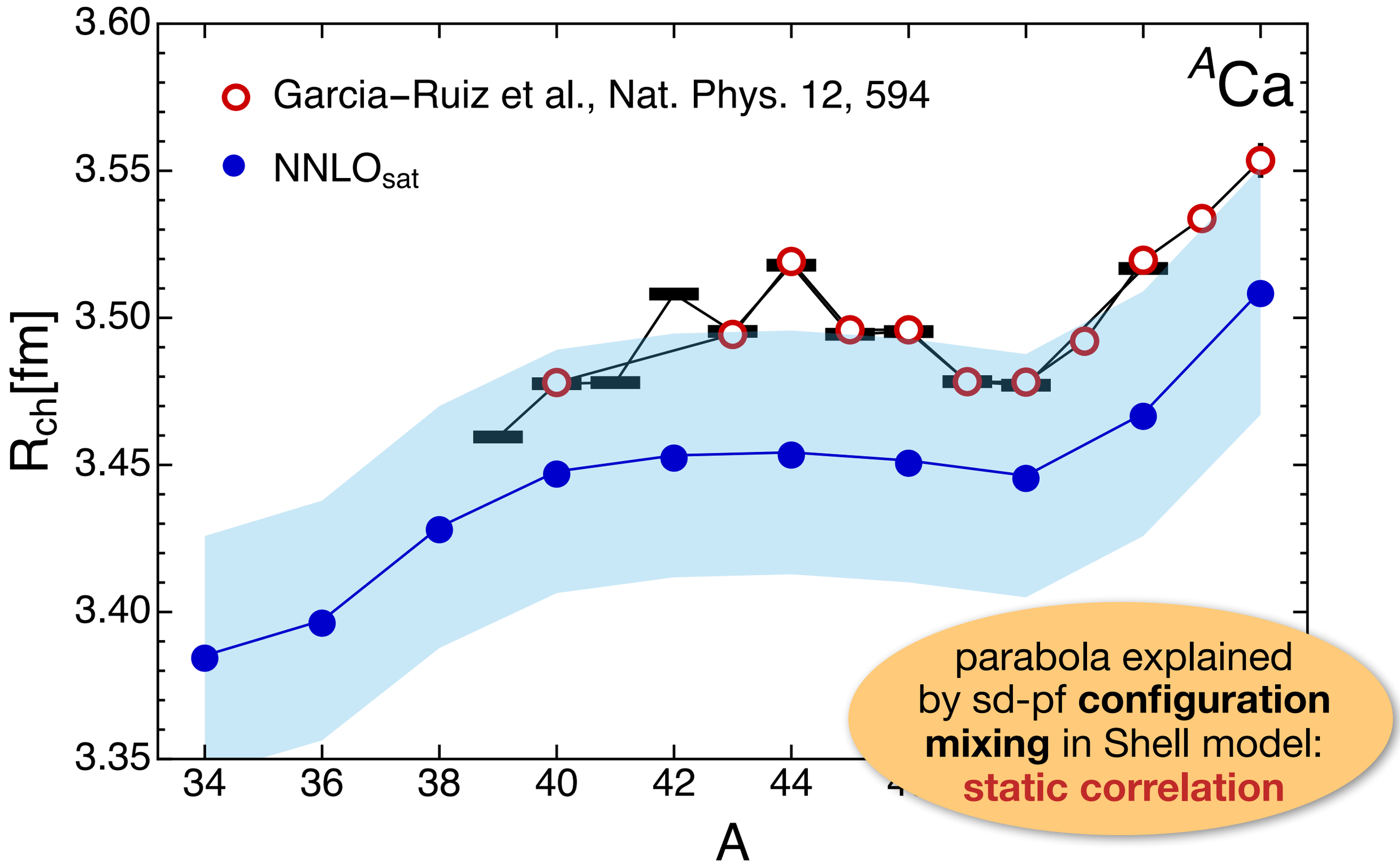

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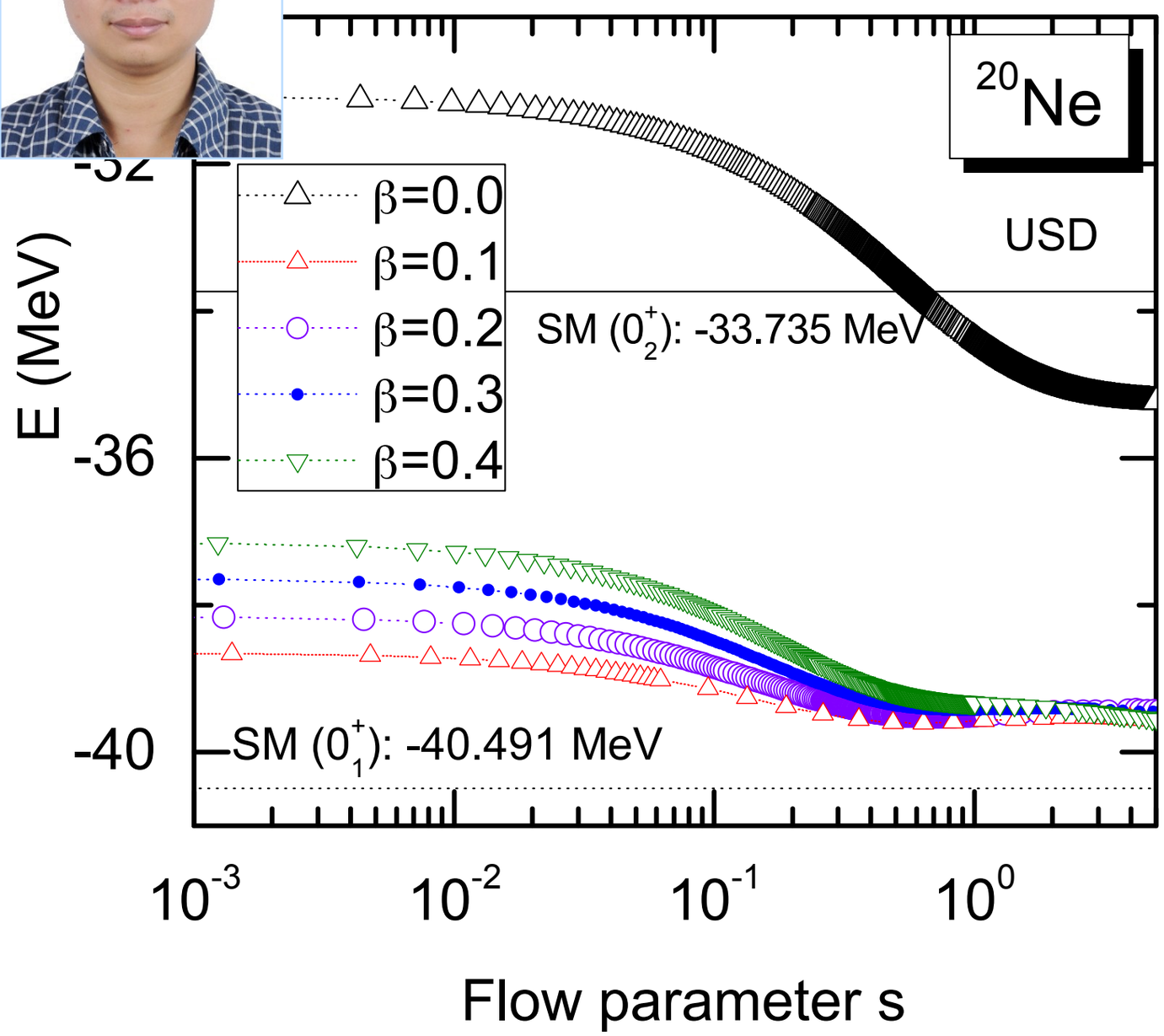
Example: ^{20}Ne

J. Yao, T. D. Morris, HH, J. Engel, in prep.



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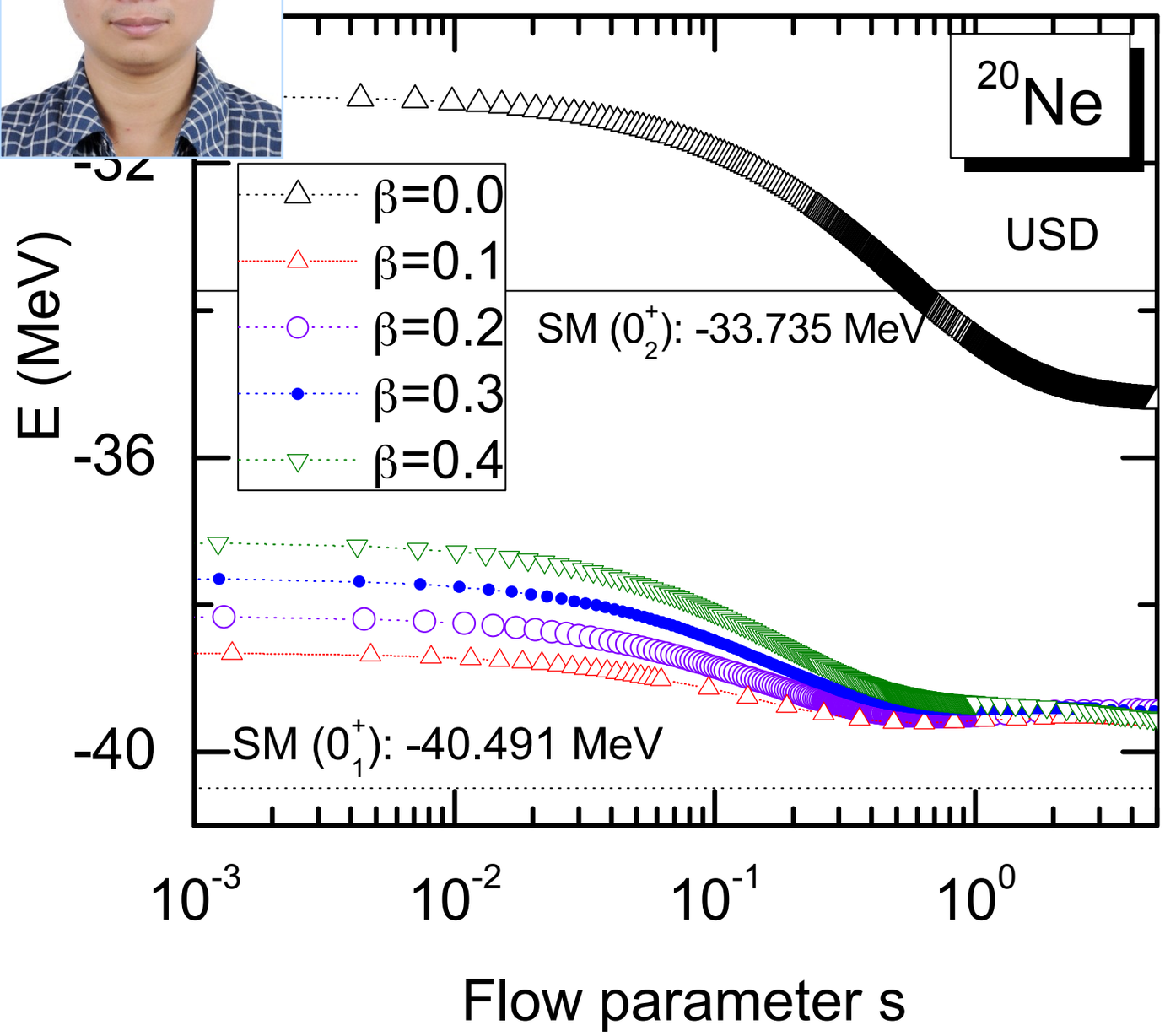

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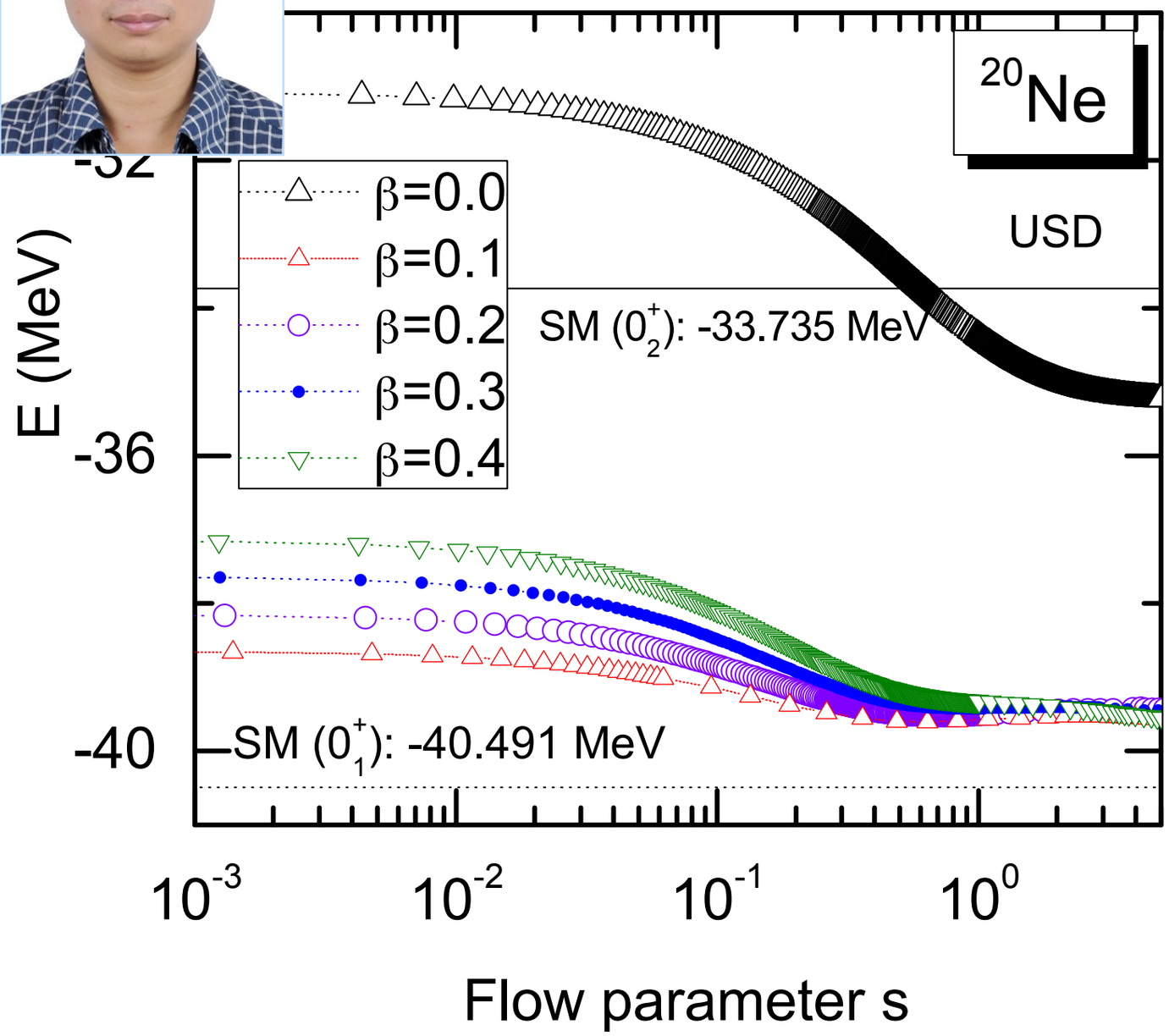
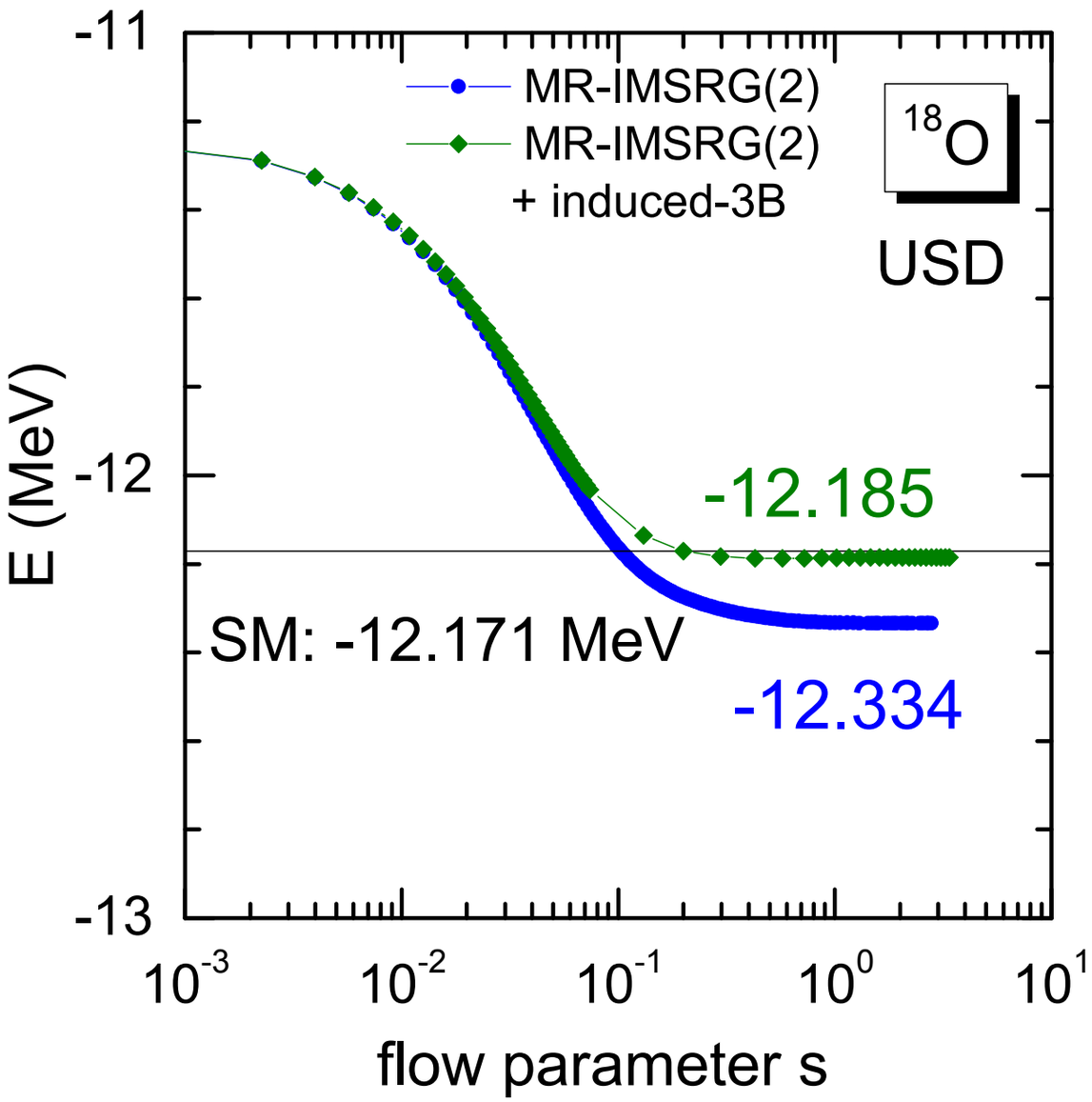
J. Yao, T. D. Morris, HH, J. Engel, in prep.



- reference: particle-number & angular-momentum projected HFB
- **range of deformed reference states flow to the ^{20}Ne ground state**
- deviation from Shell model result: **correlations beyond MR-IMSRG(2)**

Approximate MR-IMSRG(3)

J. Yao, T. D. Morris, HH, J. Engel, in prep.



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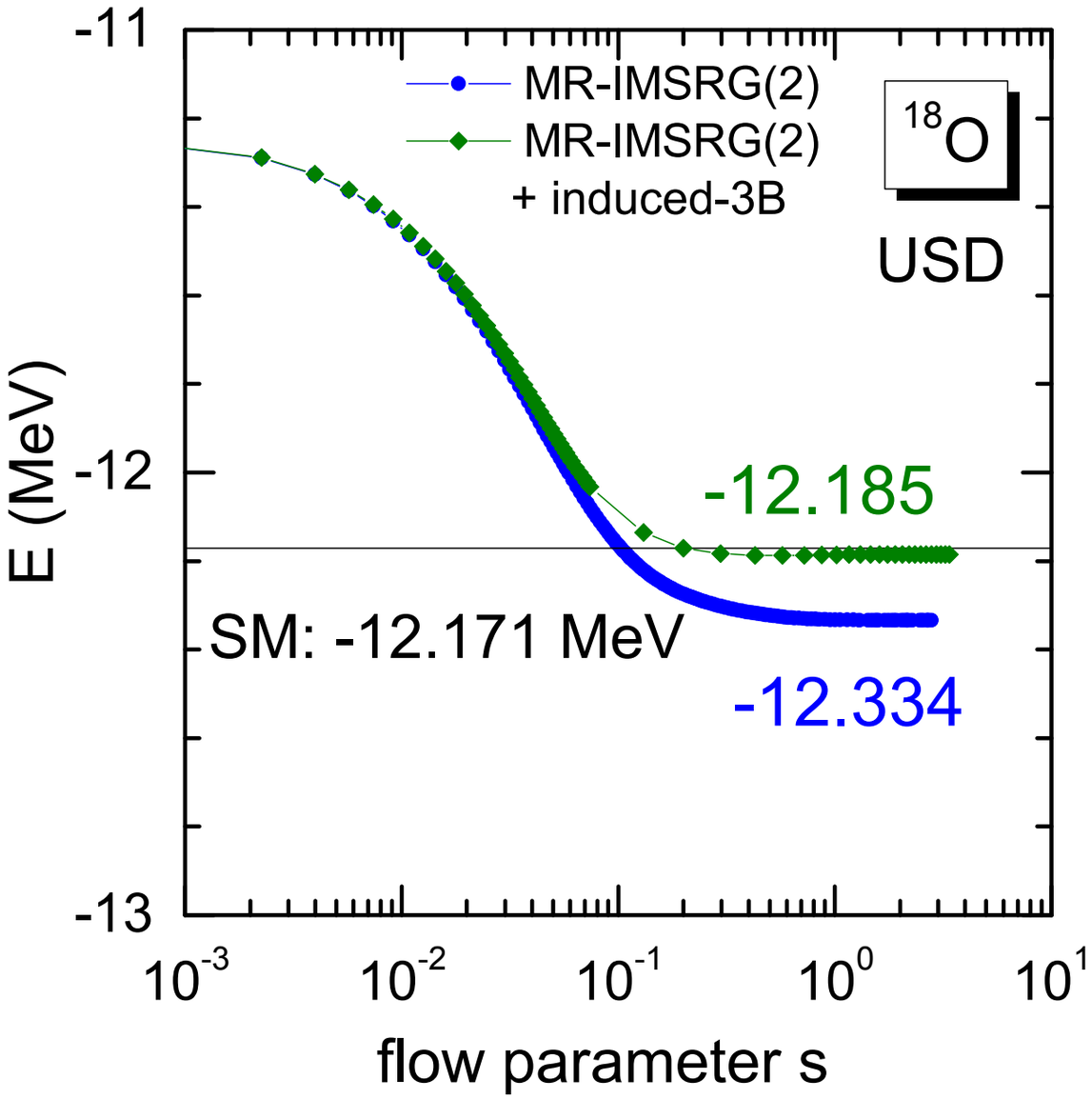

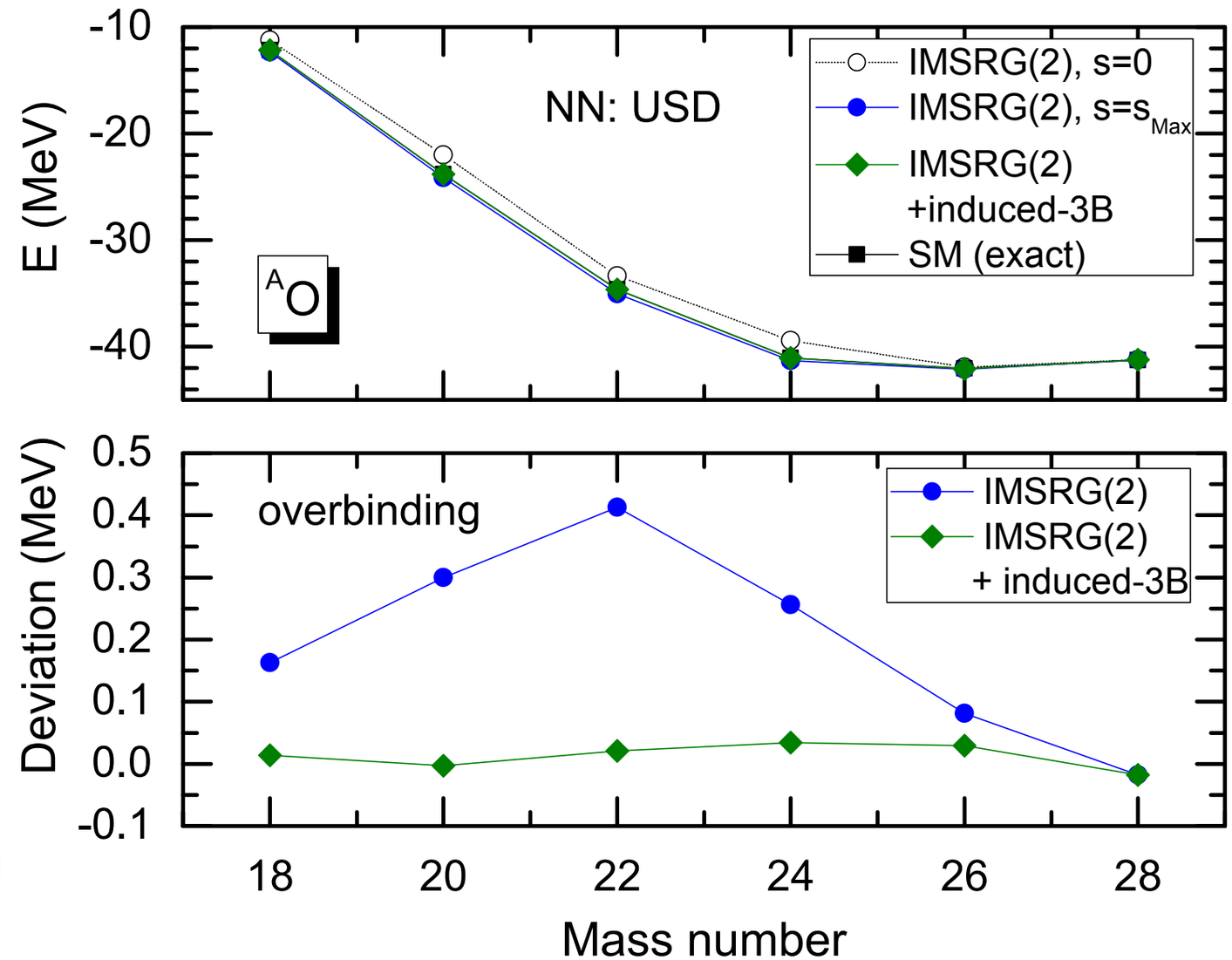

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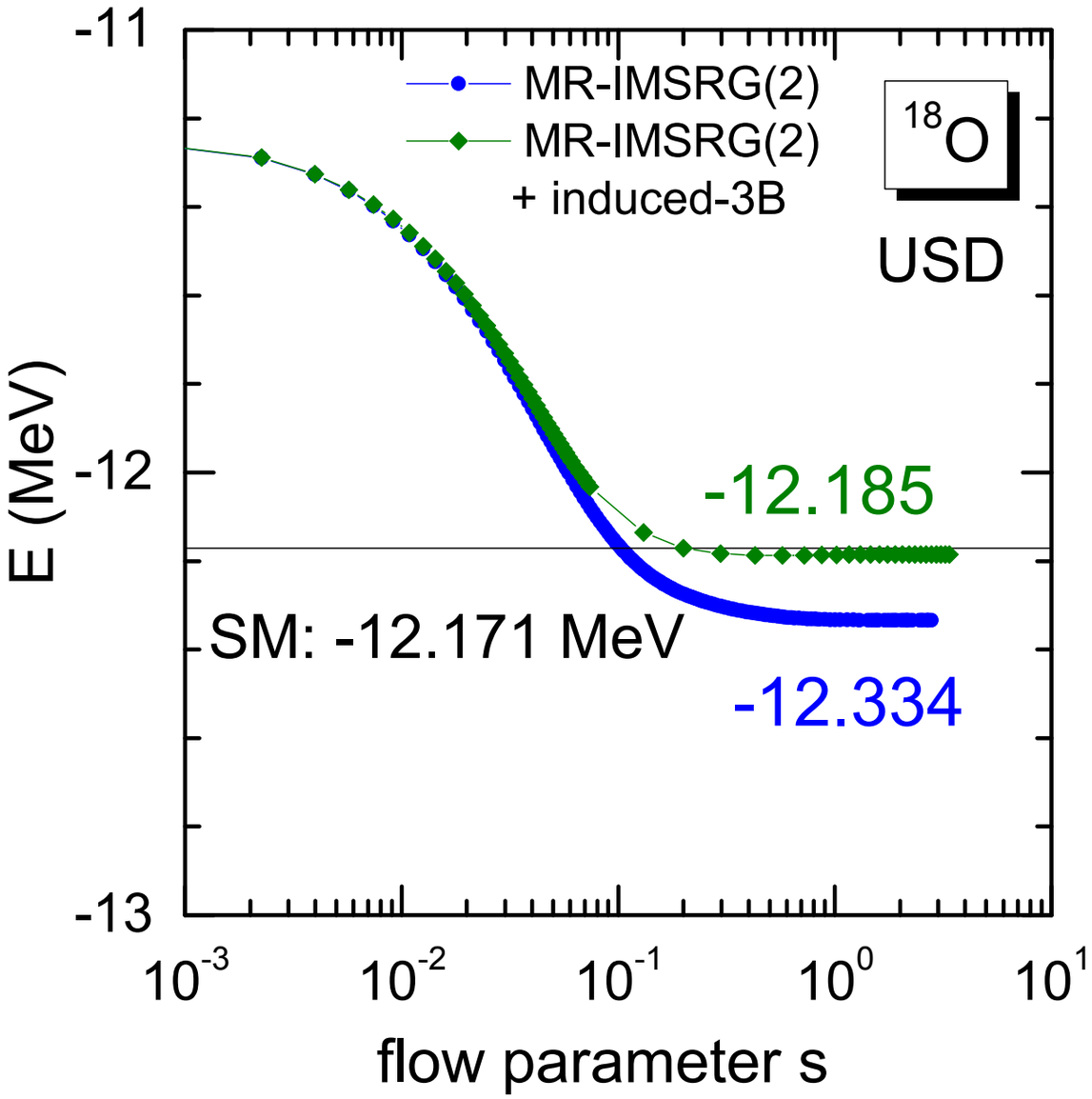

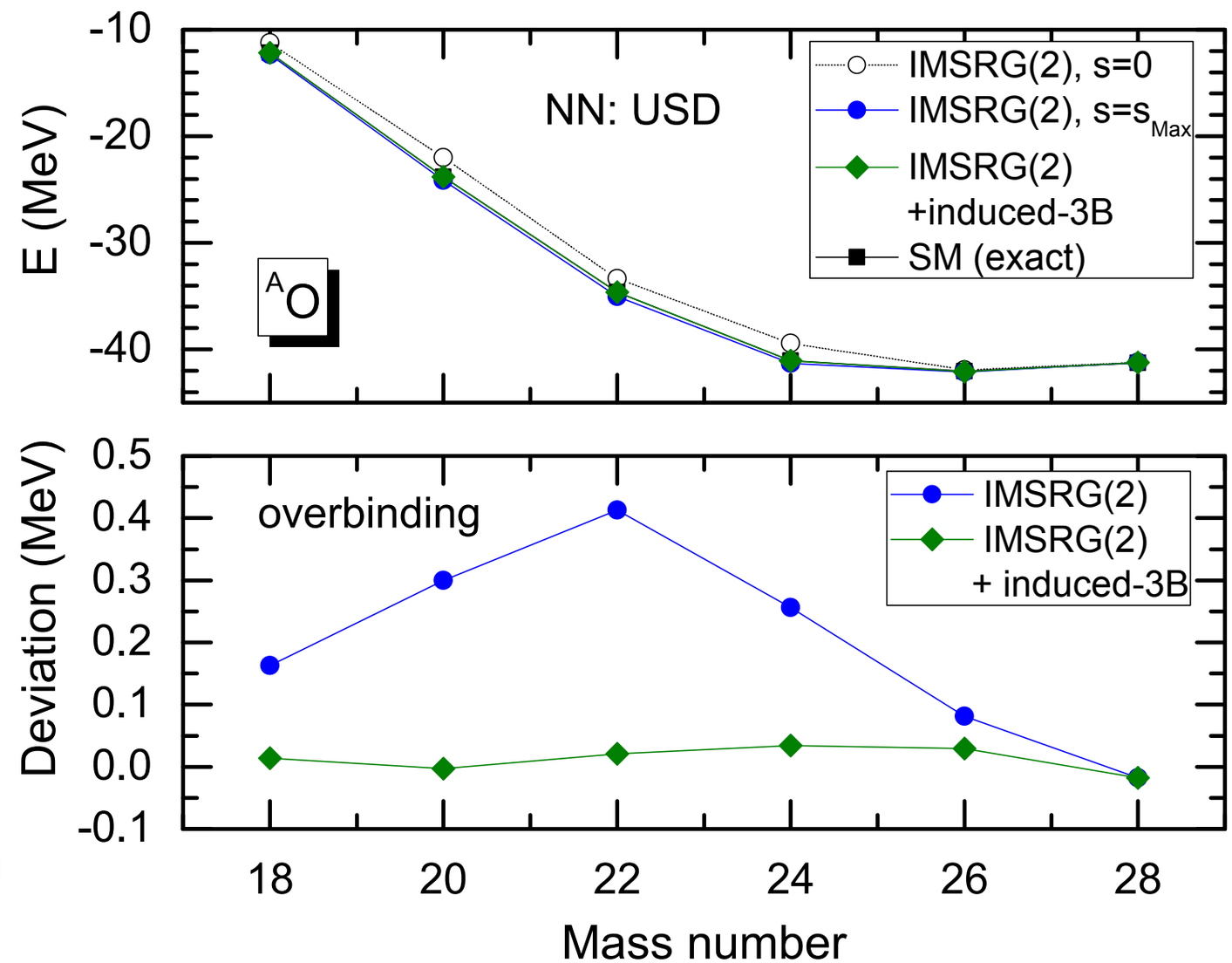

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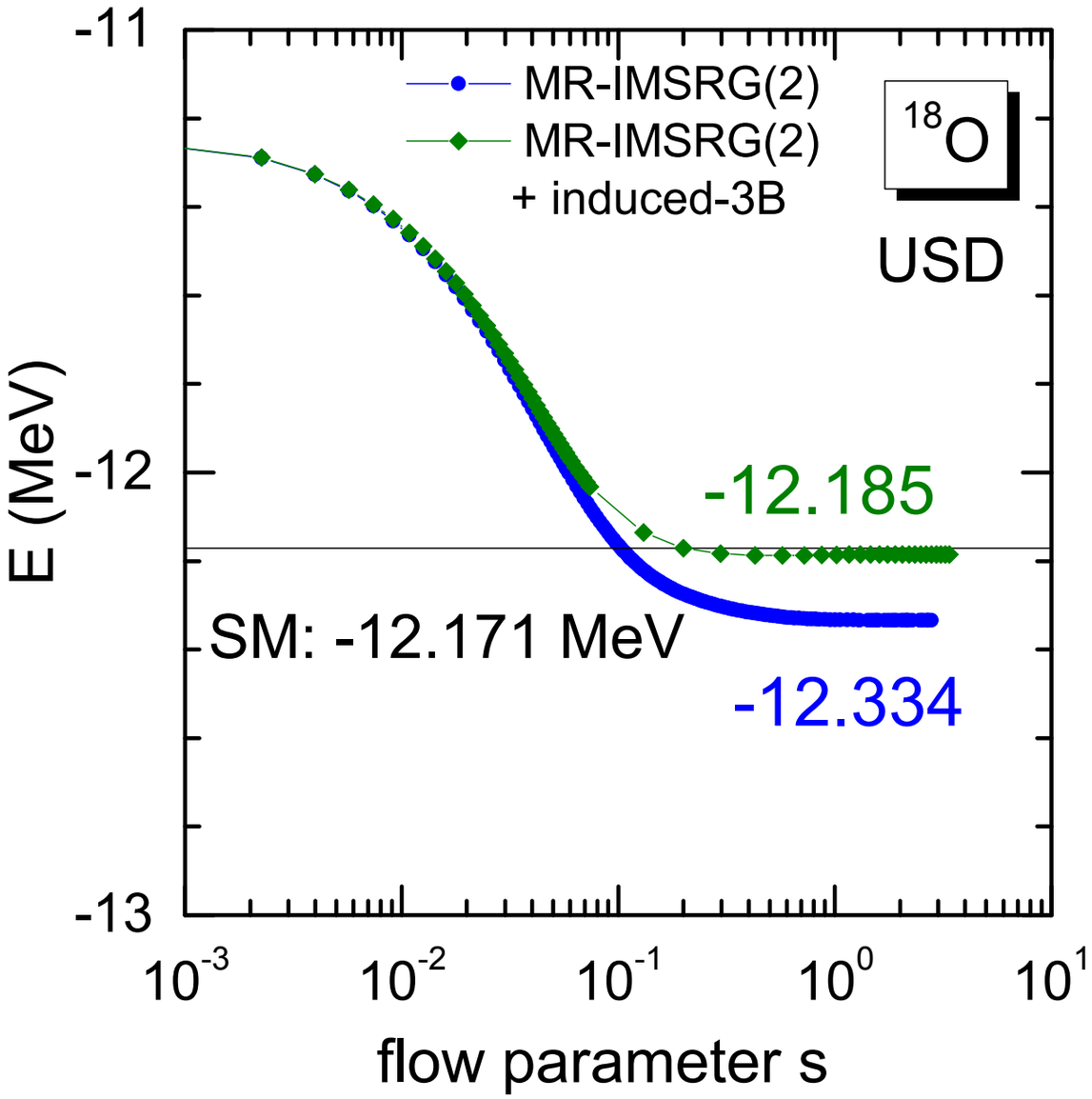
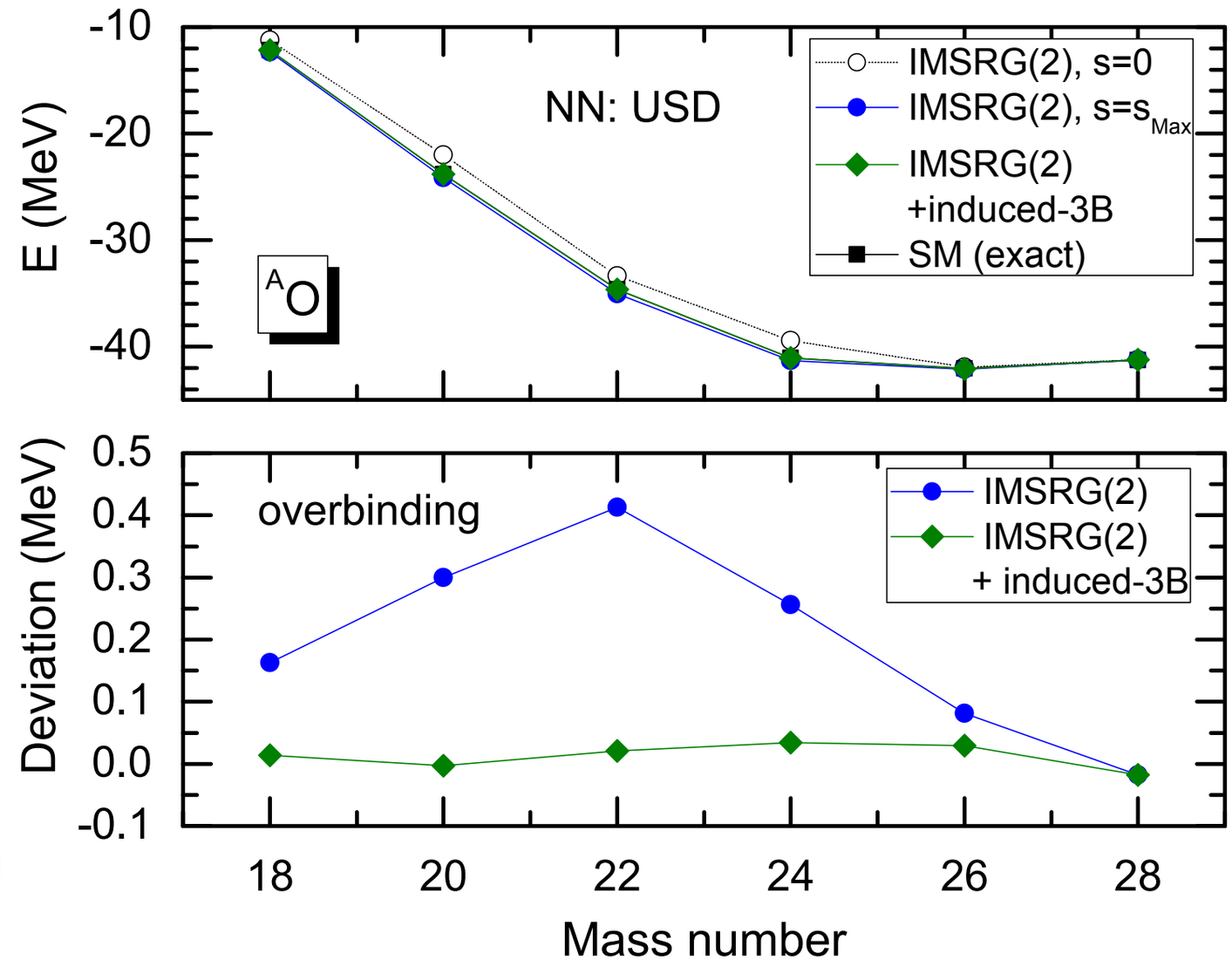
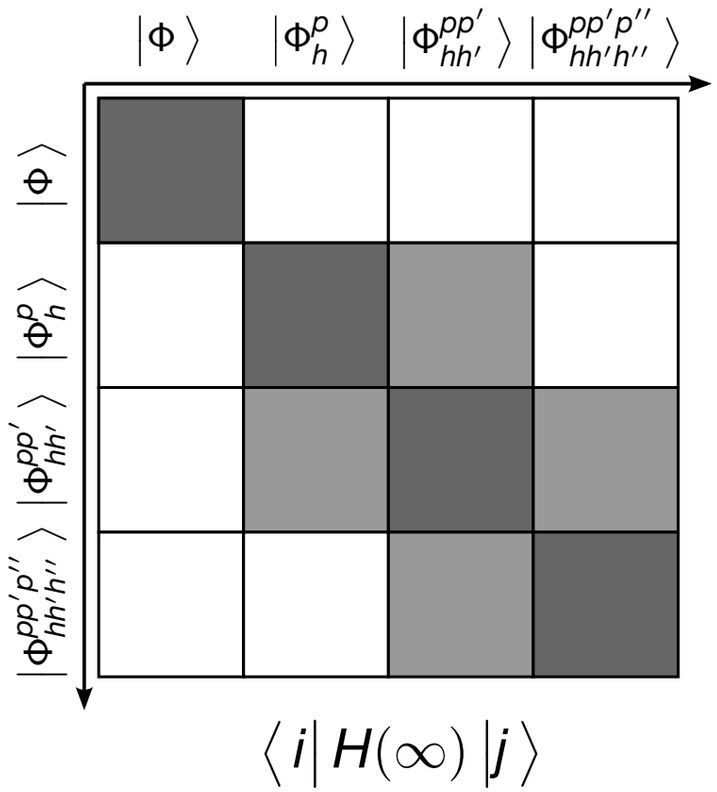




- **approximate MR-IMSRG(3):** induced 3B terms recover bulk of missing correlation energy
- size will be **reference-state dependent**

RG-Improved Hamiltonians



- **ground-state decoupled** Hamiltonians as input for many-body calculations

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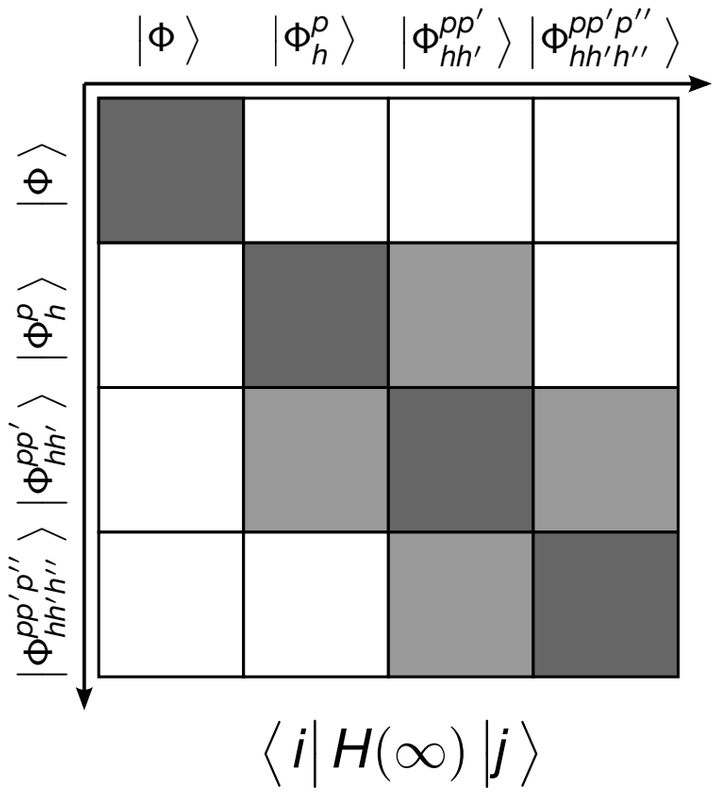

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    E. Gebrerufael, **K. Vobig**, HH, R. Roth, PRL 118, 152503 (2017)

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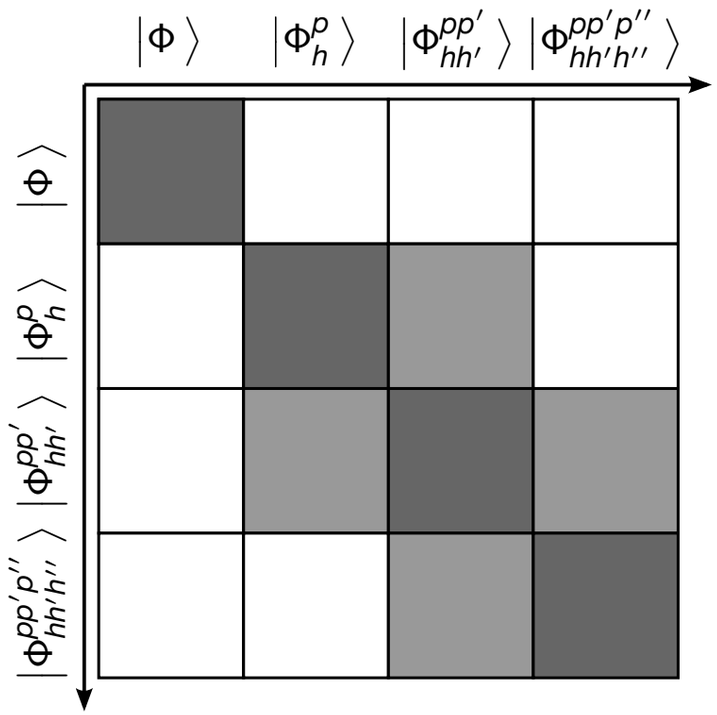

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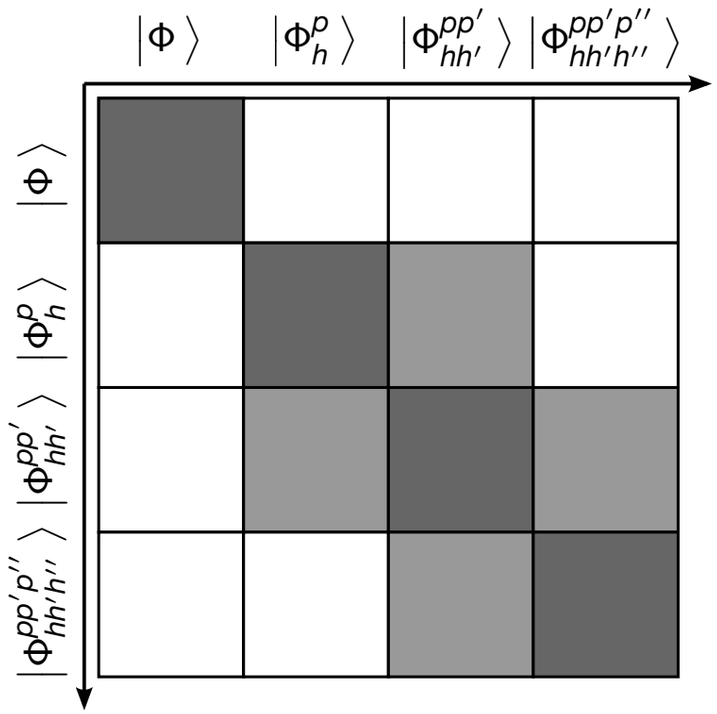

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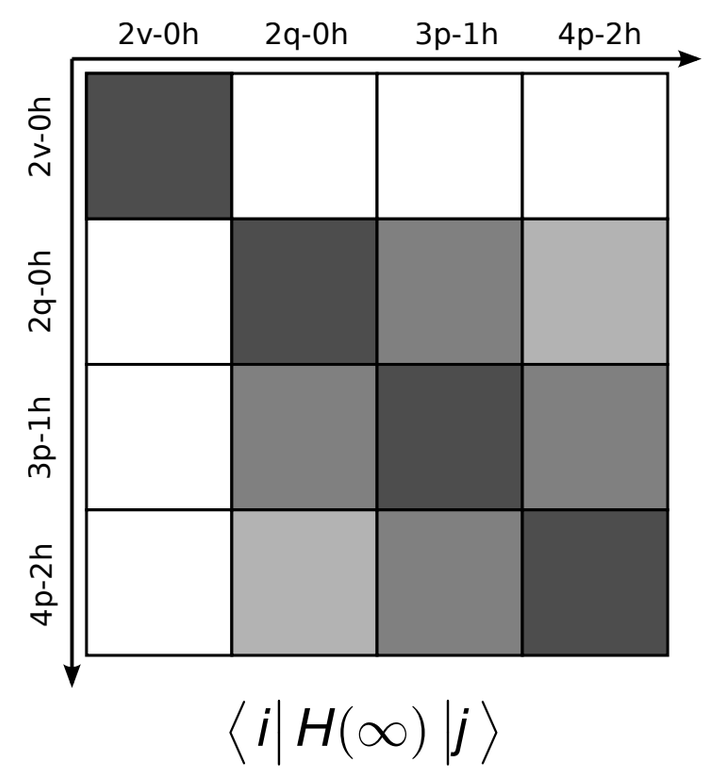

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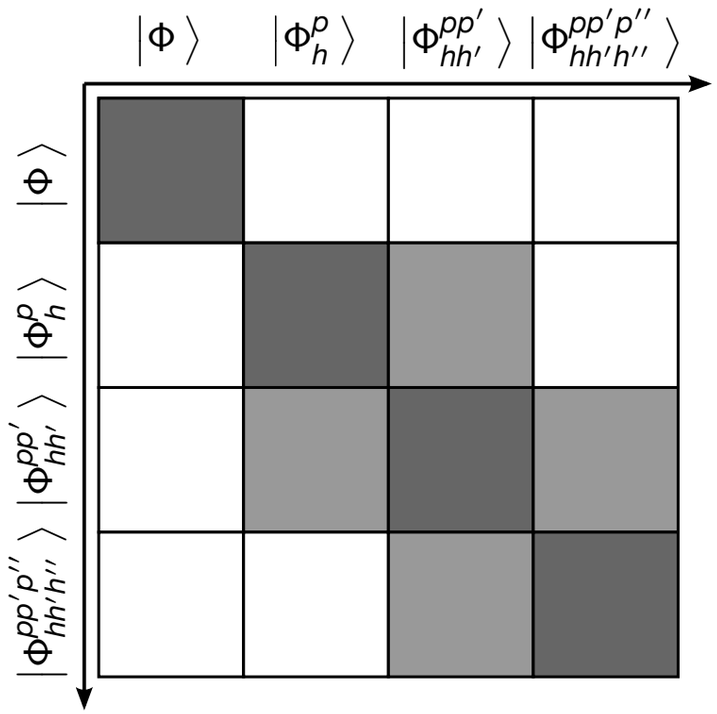

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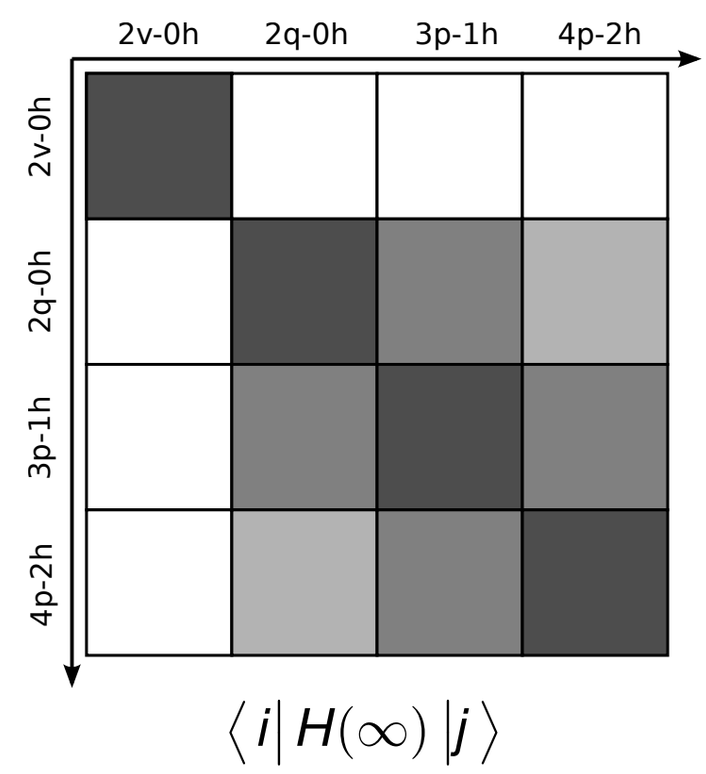
$$\left\{H^{od}\right\} = \{f_{h'}^{h}, f_{p'}^{p}, f_{h}^{p}, f_{v}^{q}, \Gamma_{hh'}^{pp'}, \Gamma_{hv}^{pp'}, \Gamma_{vv'}^{pq}\} \text{ \& H.c.}$$



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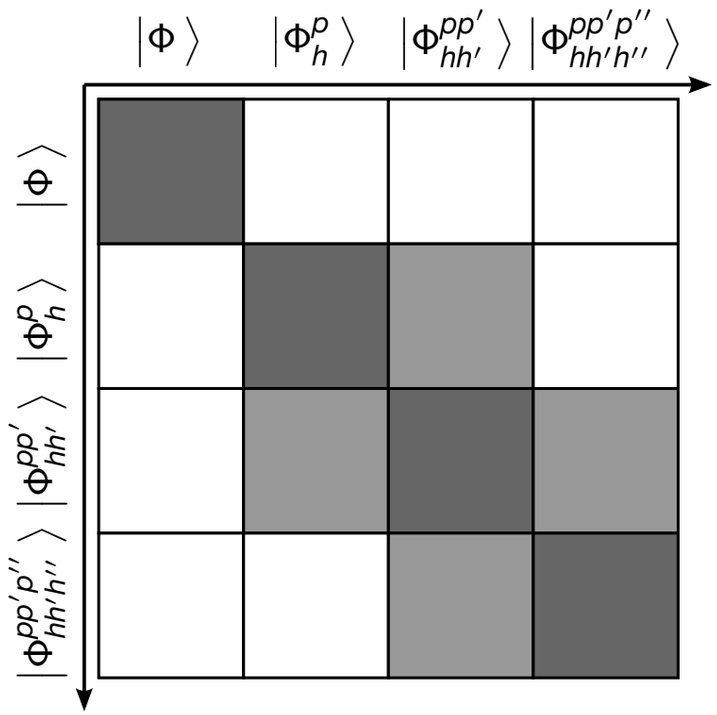

$\langle i | H(\infty) | j \rangle$

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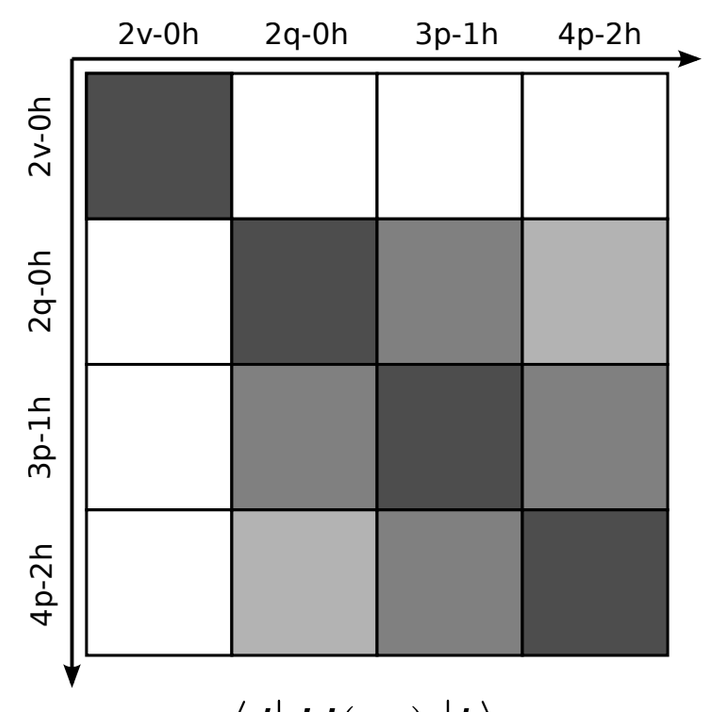
S. R. Stroberg, A. Calci, HH., J. D. Holt, S. K. Bogner, R. Roth, A. Schwenk, PRL 118, 032502 (2017); **S. R. Stroberg**, HH., J. D. Holt, S. K. Bogner, A. Schwenk, PRC 93, 051301(R) (2016)



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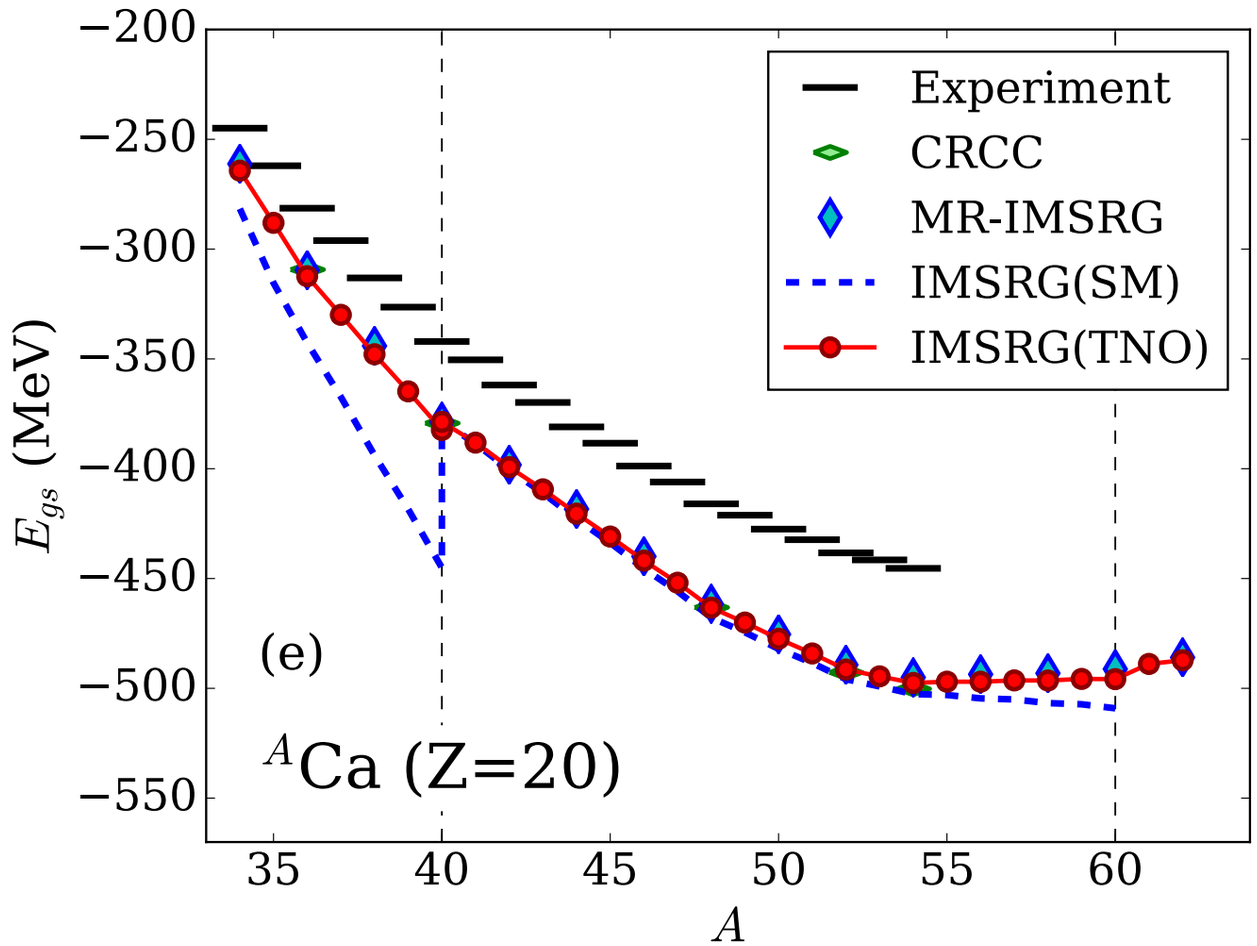
Ground-State Energies

S. R. Stroberg, *A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL* ***118****, 032502 (2017)*



- (initial) normal ordering and IMSRG decoupling in the **target nucleus**

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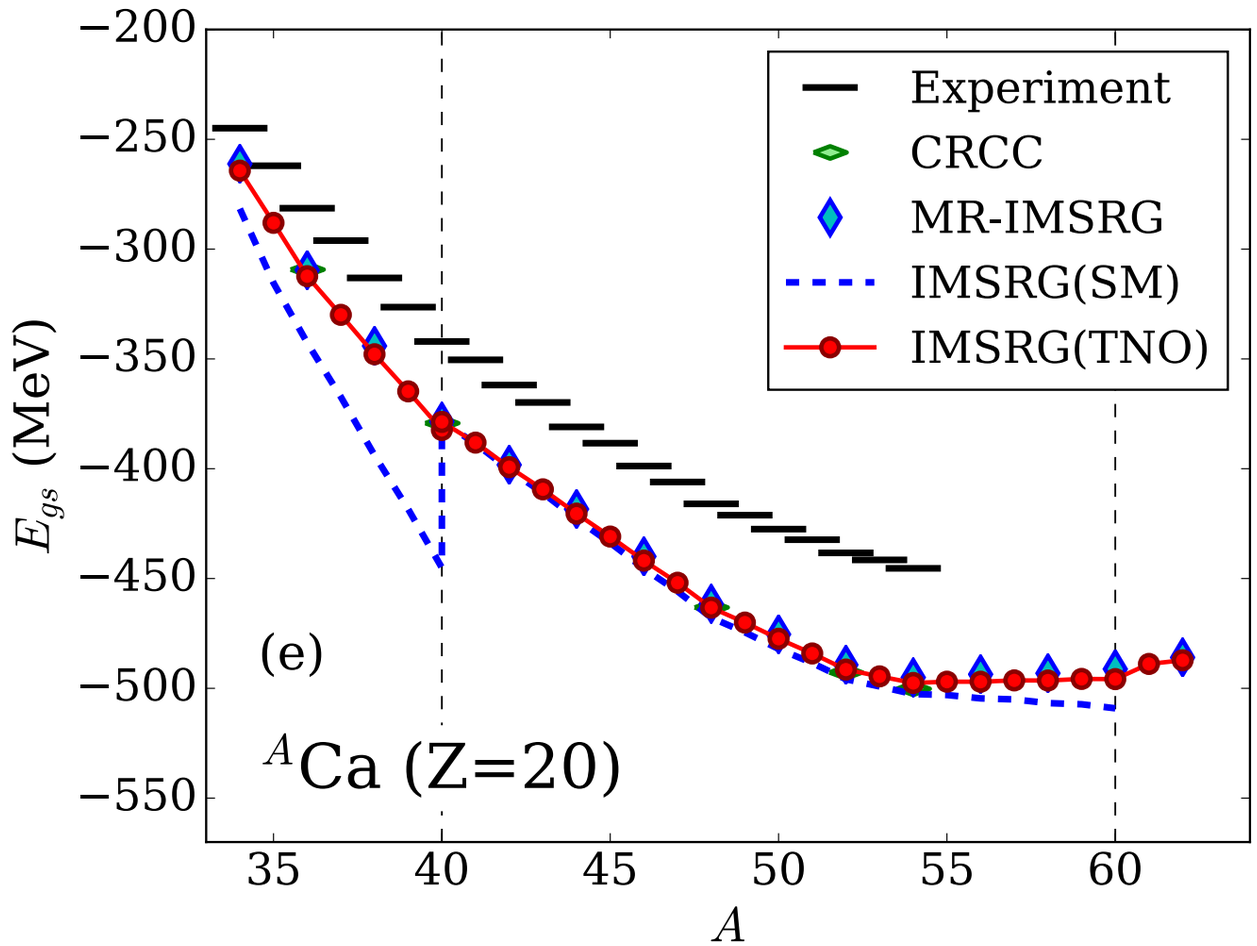
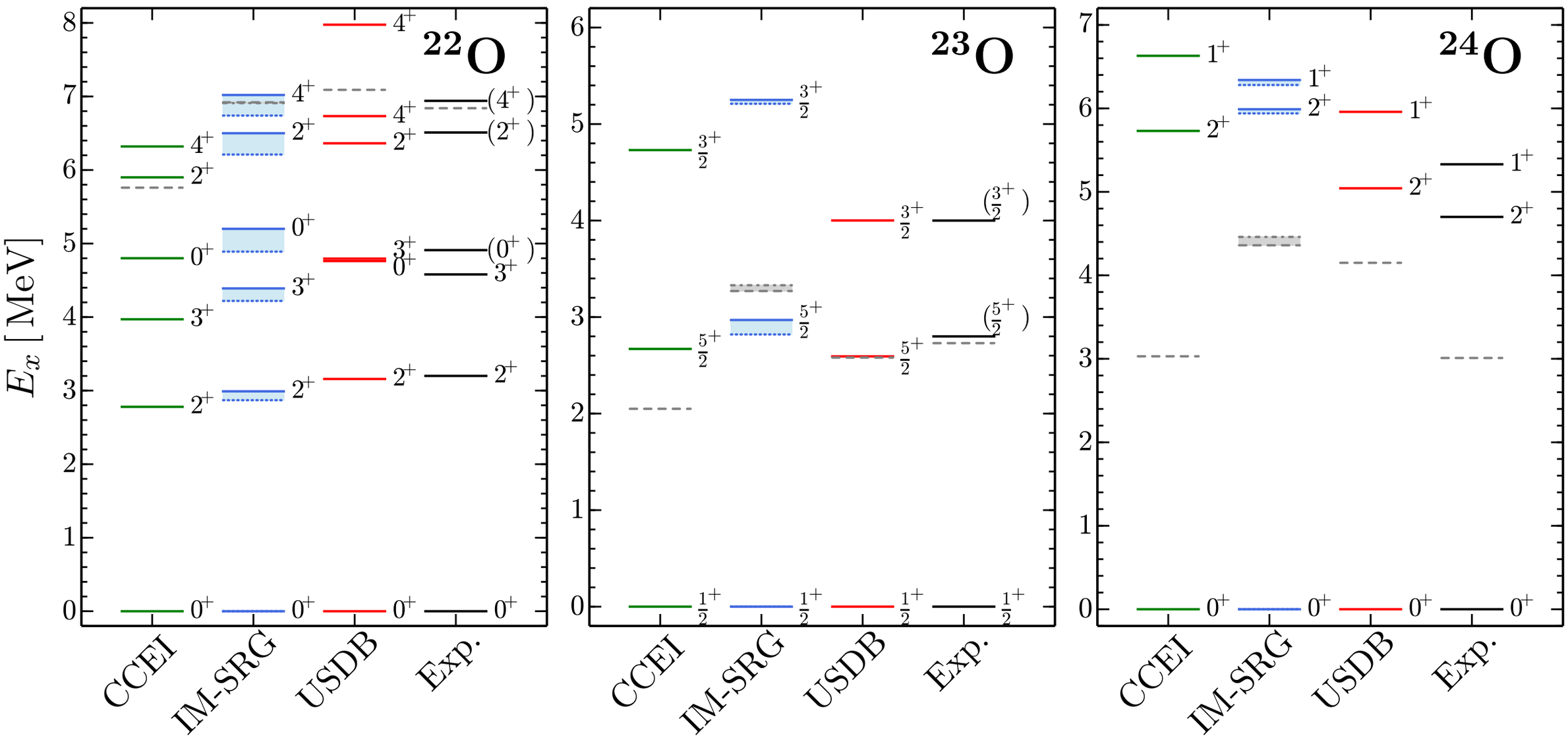


- (initial) normal ordering and IMSRG decoupling in the **target nucleus**
- **consistent with (MR-)IMSRG ground state energies** (and CC, SCGF, …) for the **same Hamiltonian**

Oxygen Spectra

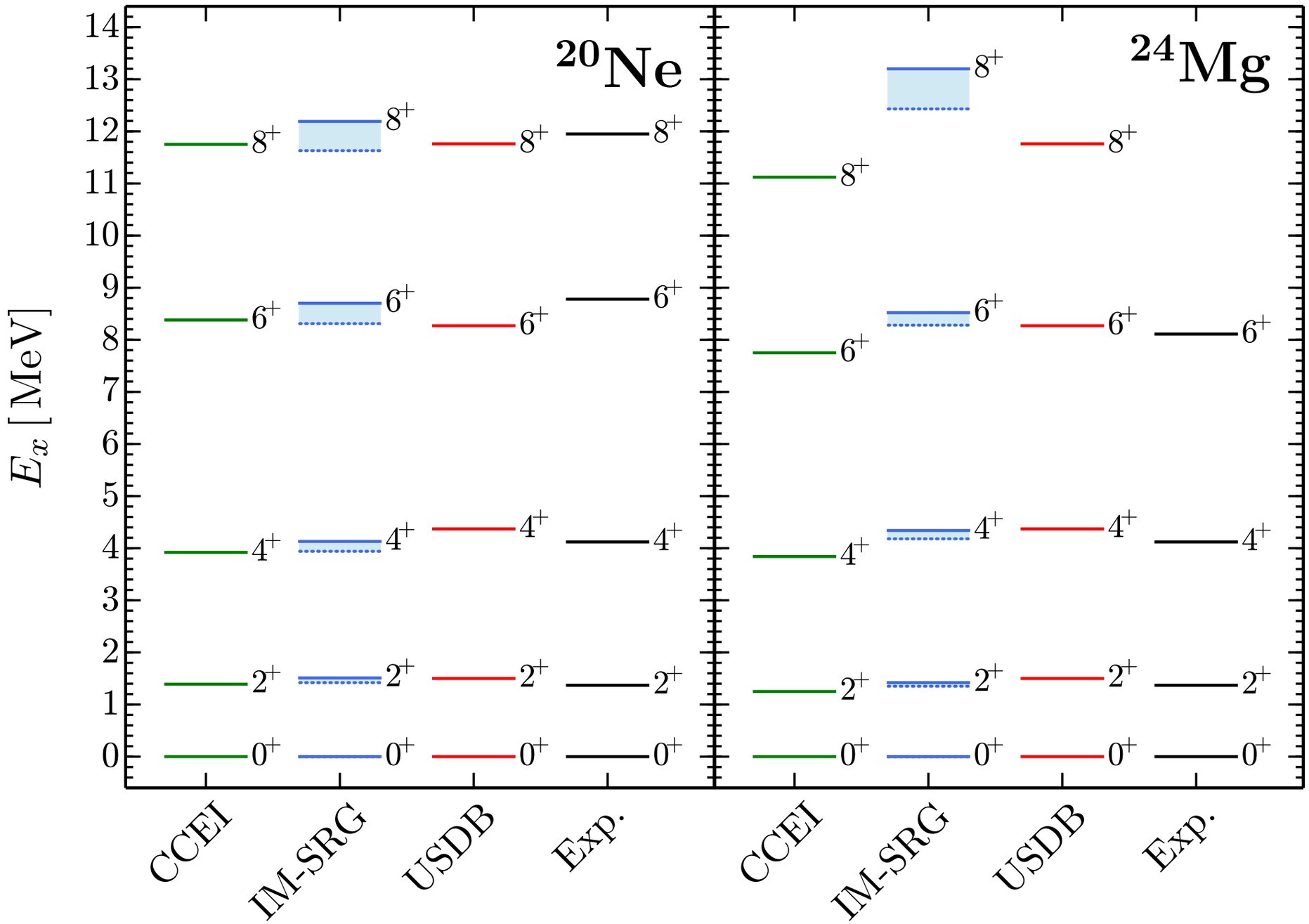
*S. K. Bogner et al., PRL **113**, 142501 (2014)*

NN + 3N(400)



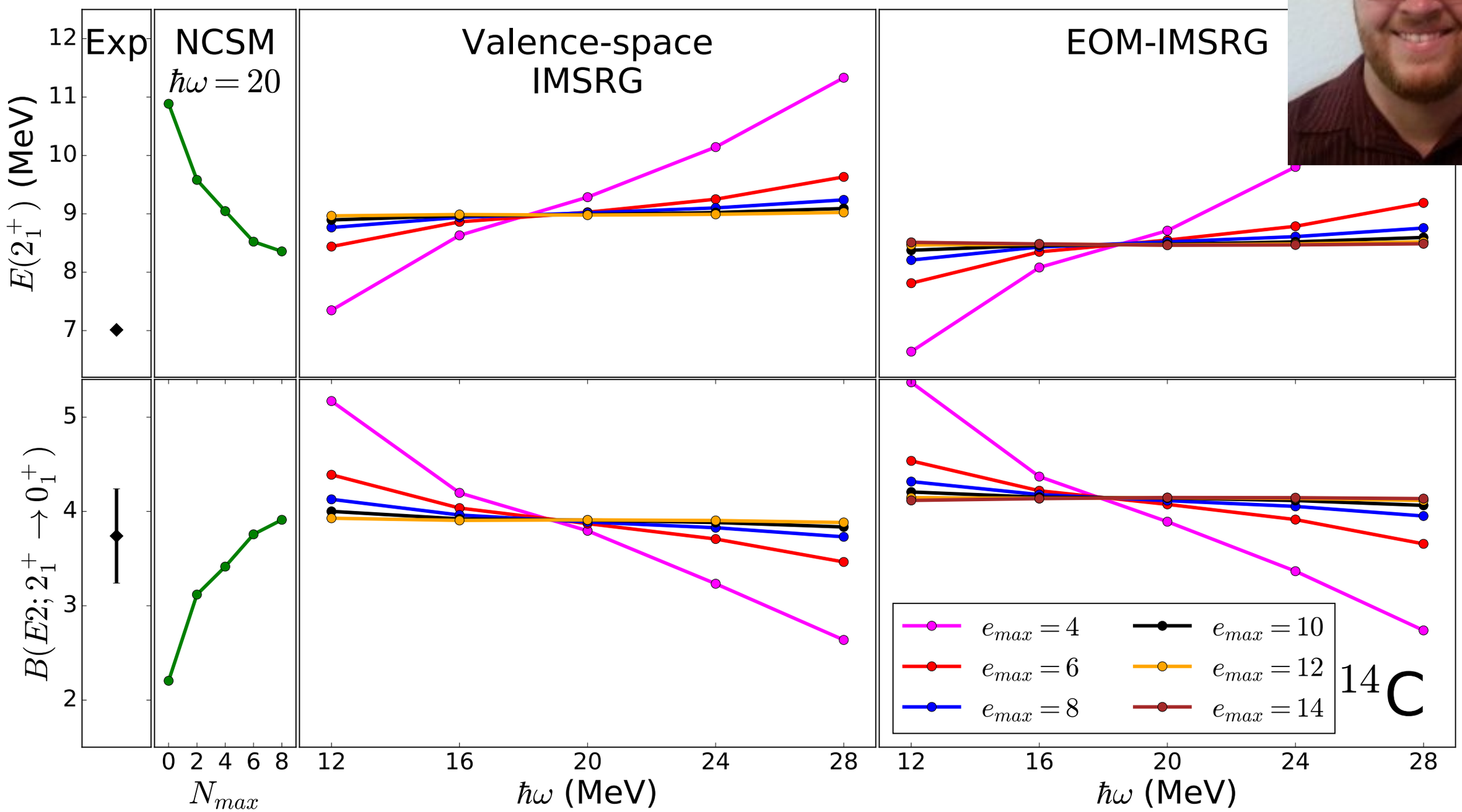
Rotational Bands

*S. R. Stroberg et al., PRC **93**, 051301(R) (2016)*



Transitions

N. M. Parzuchowski, *S. R. Stroberg et al., PRC96, 034324;*
N. M. Parzuchowski *et al., PRC95, 044304*



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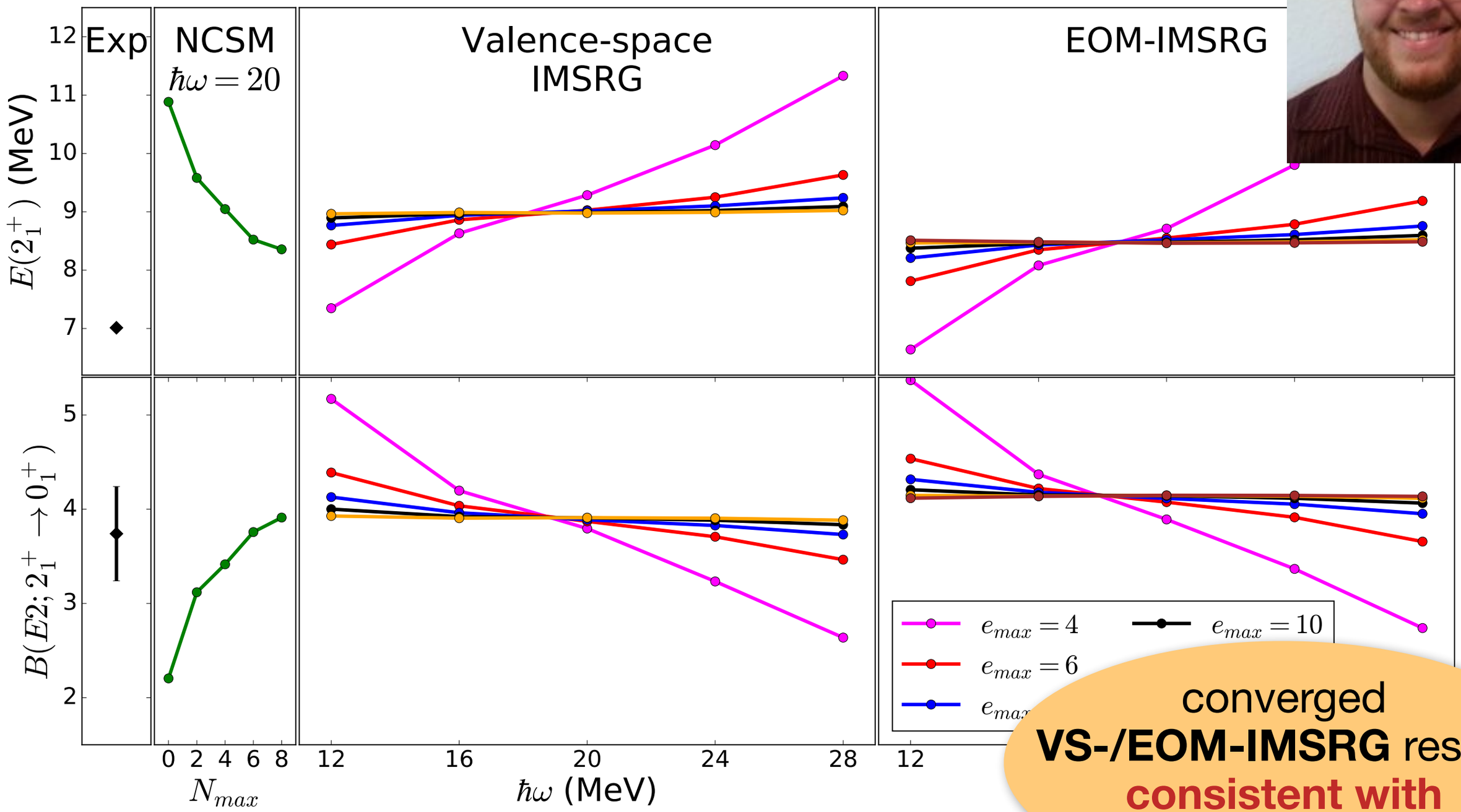

converged **VS-/EOM-IMSRG** results **consistent with NCSM**

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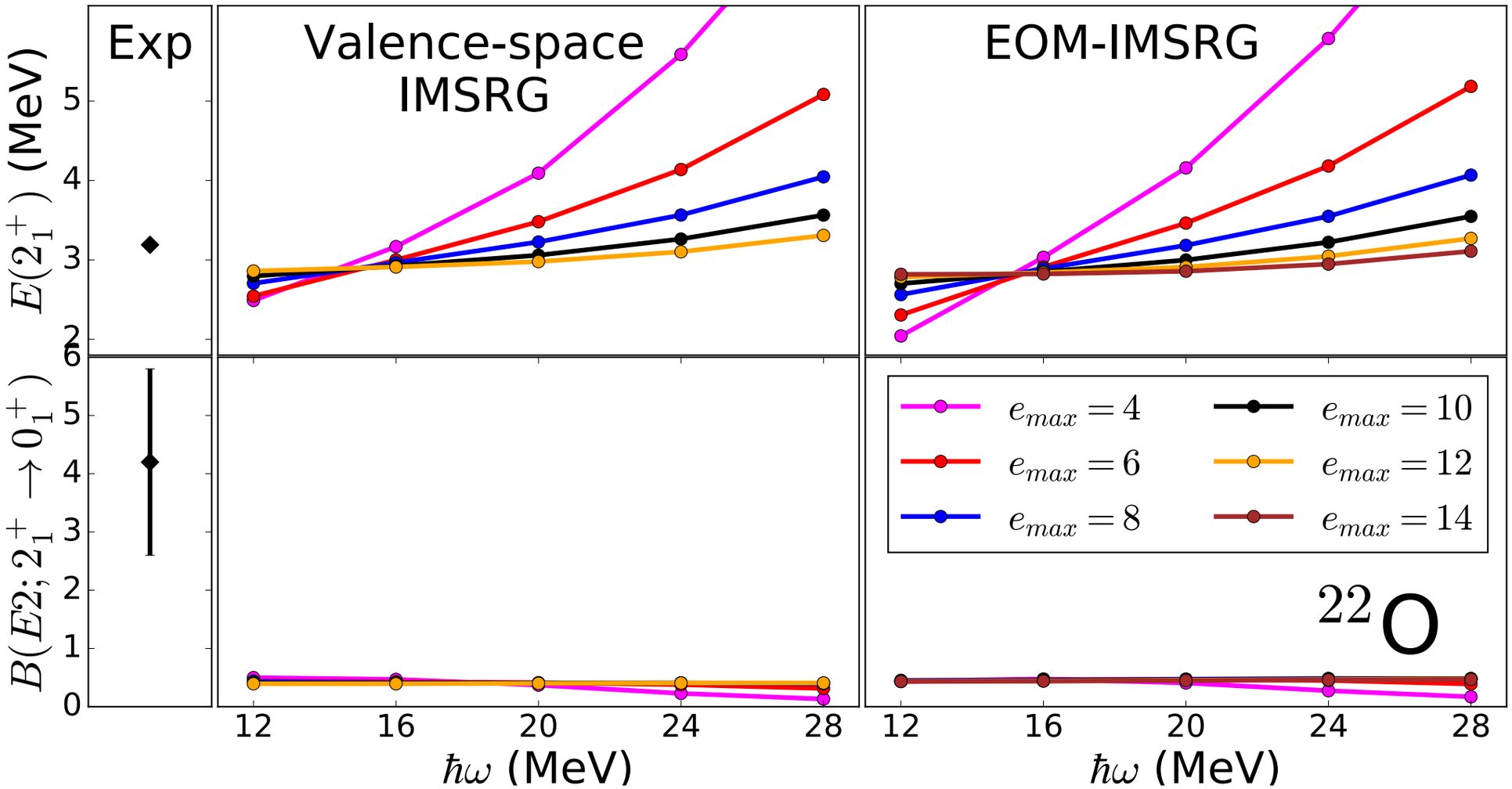

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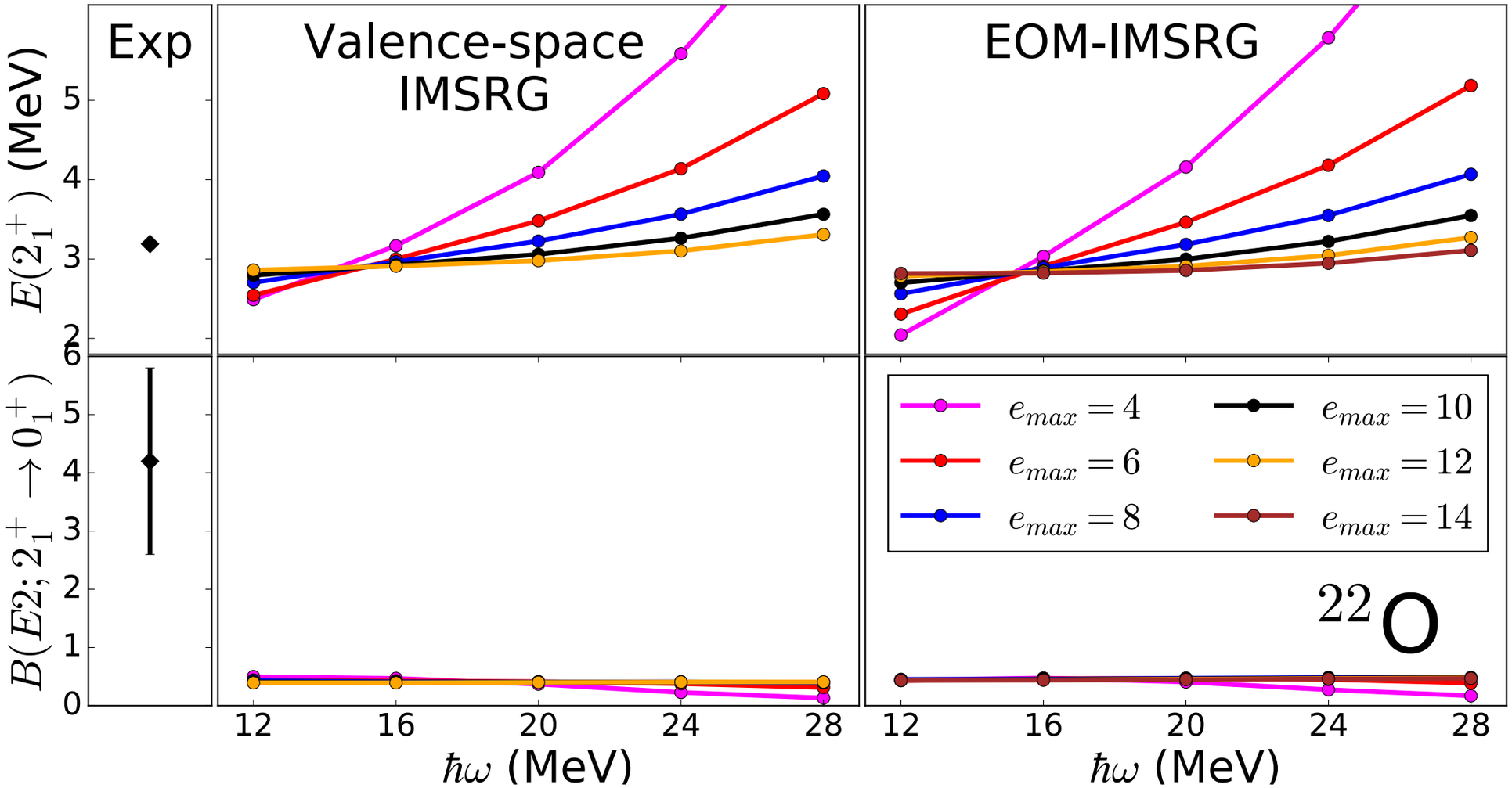

- non-zero B(E2) from Shell model: **VS-IMSRG induces effective neutron charge**

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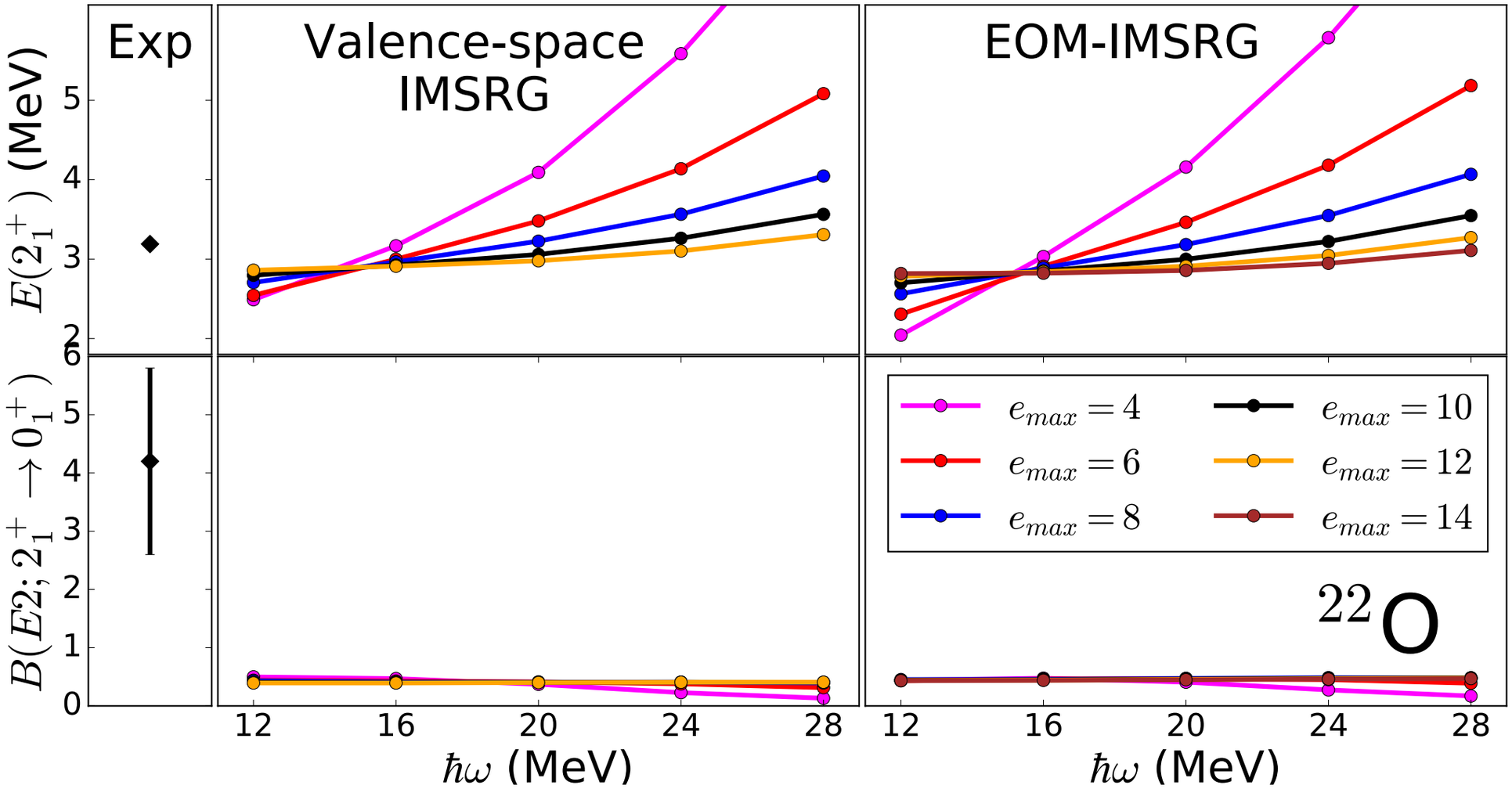

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- **B(E2) much too small:** effect of intermediate 3p3h, … states that are truncated in IMSRG evolution

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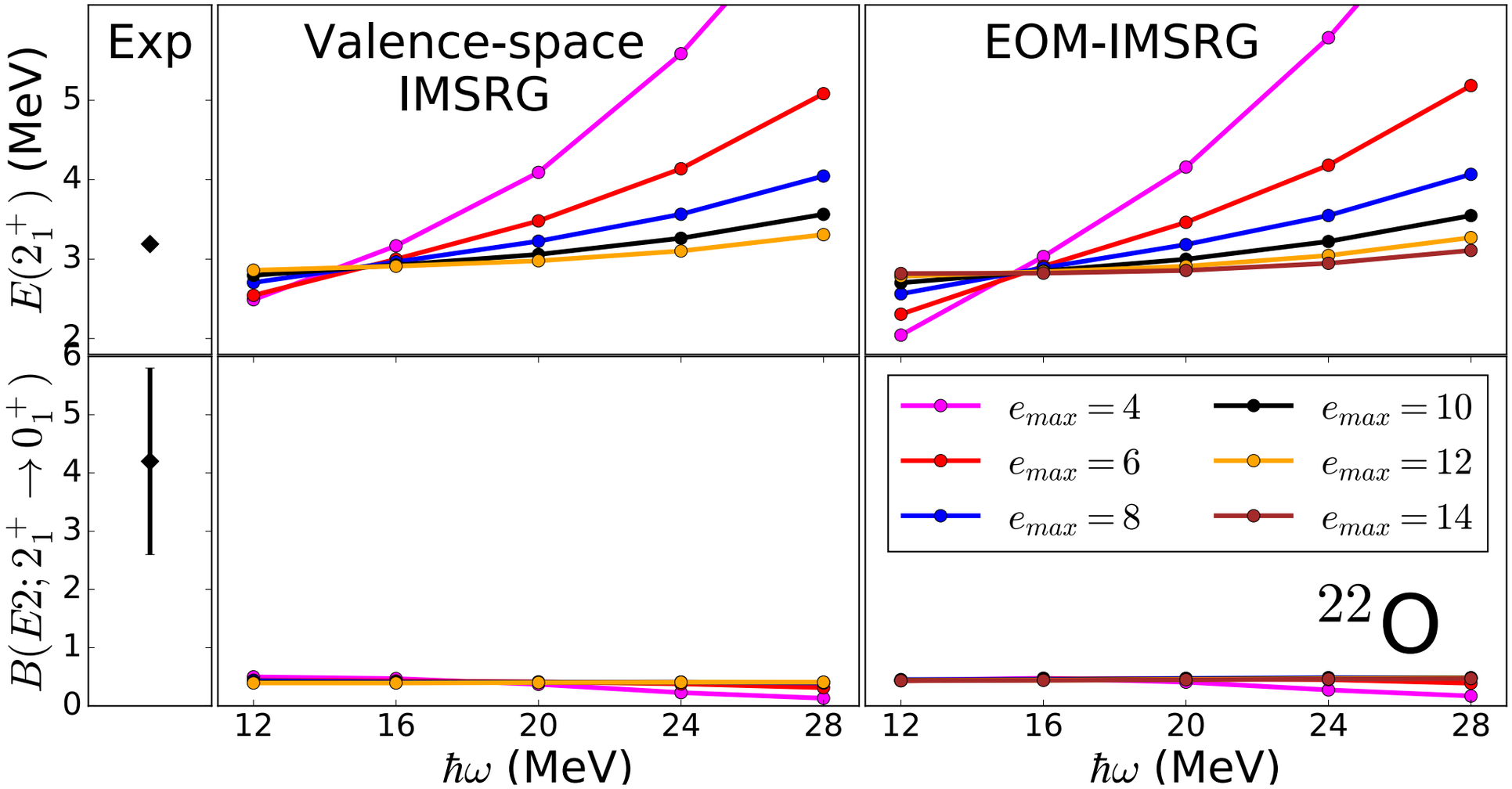

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see talks by **K. Vobig, G. Hagen, K. Launey**

Epilogue

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- **expanding IMSRG capabilities:**

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  - **coherent** uncertainty quantification & propagation

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U. Surrey, UK

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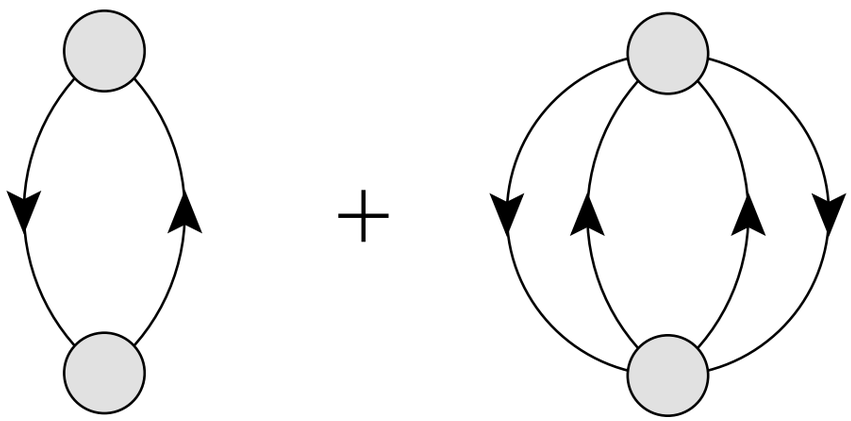
Johannes Gutenberg University of Mainz, Germany

Supplements

IM-SRG(2) Flow Equations

0-body Flow

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



1-body Flow

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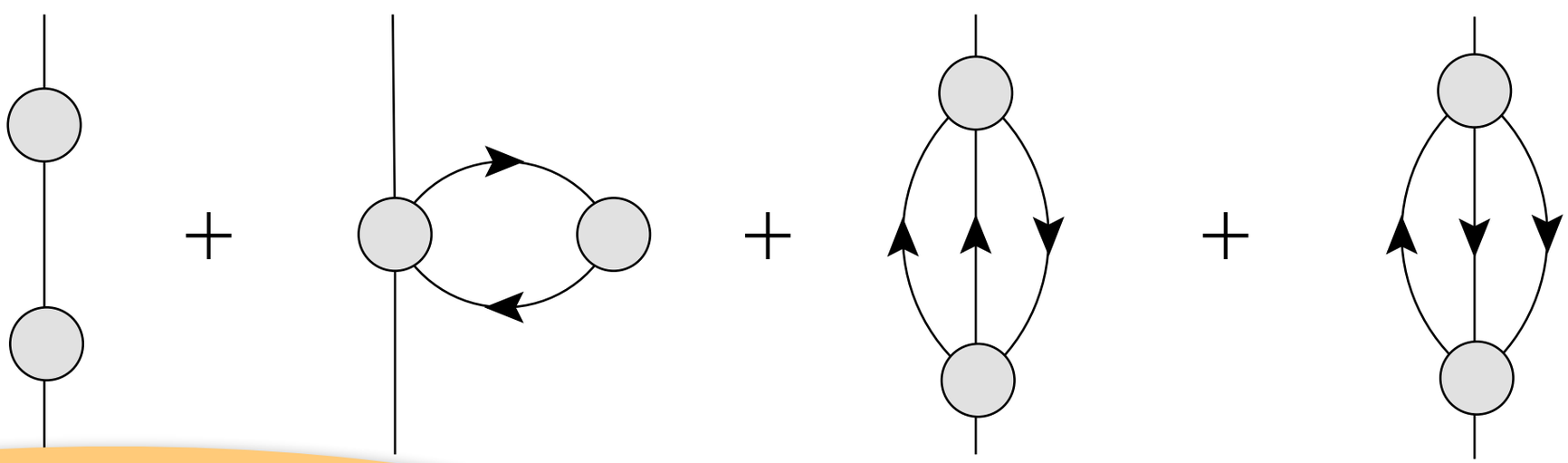


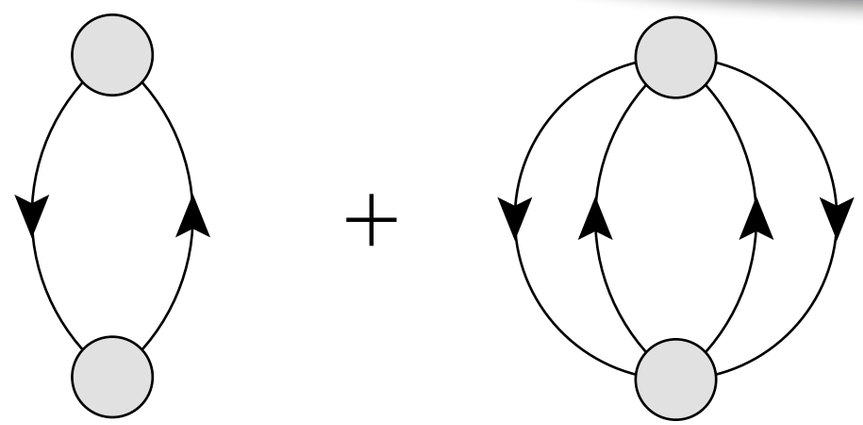
IM-SRG(2): truncate ops. at two-body level

IM-SRG(2) Flow Equations

0-body Flow

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

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



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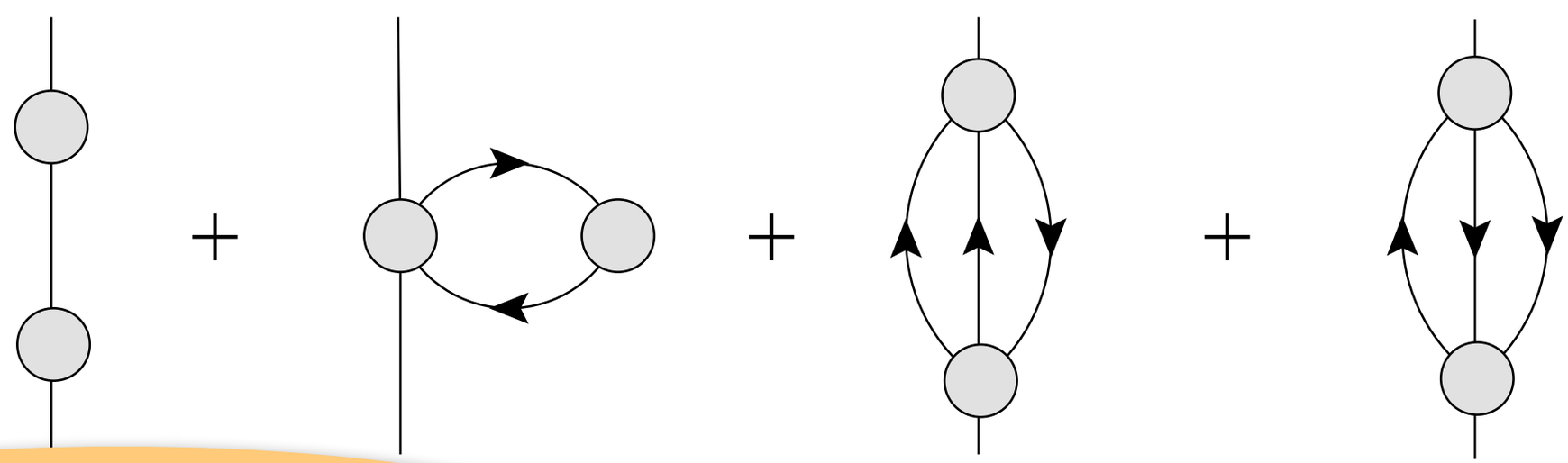
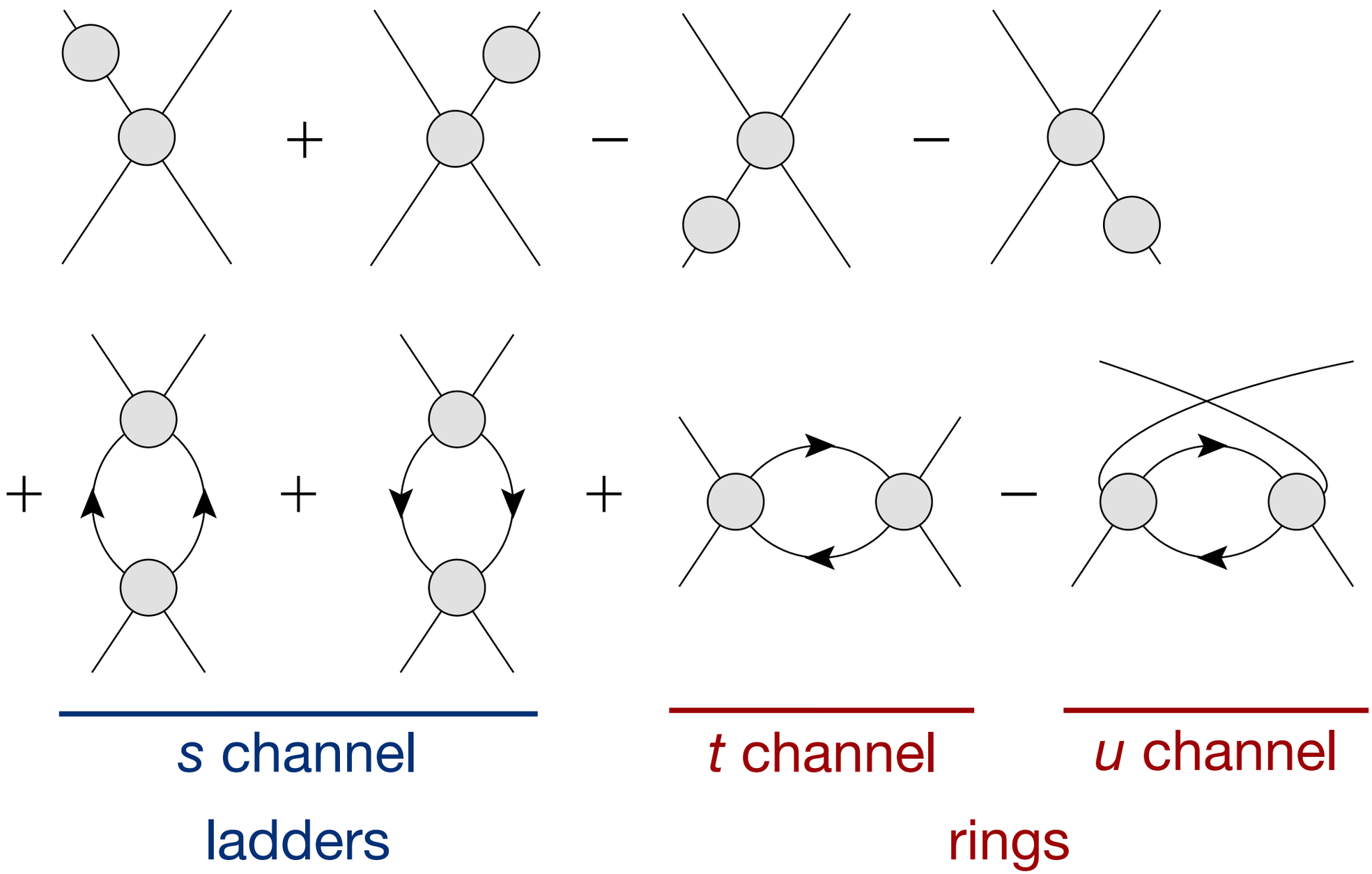


IM-SRG(2): truncate ops. at two-body level

IM-SRG(2) Flow Equations

2-body Flow

$$\frac{d\Gamma}{ds} =$$

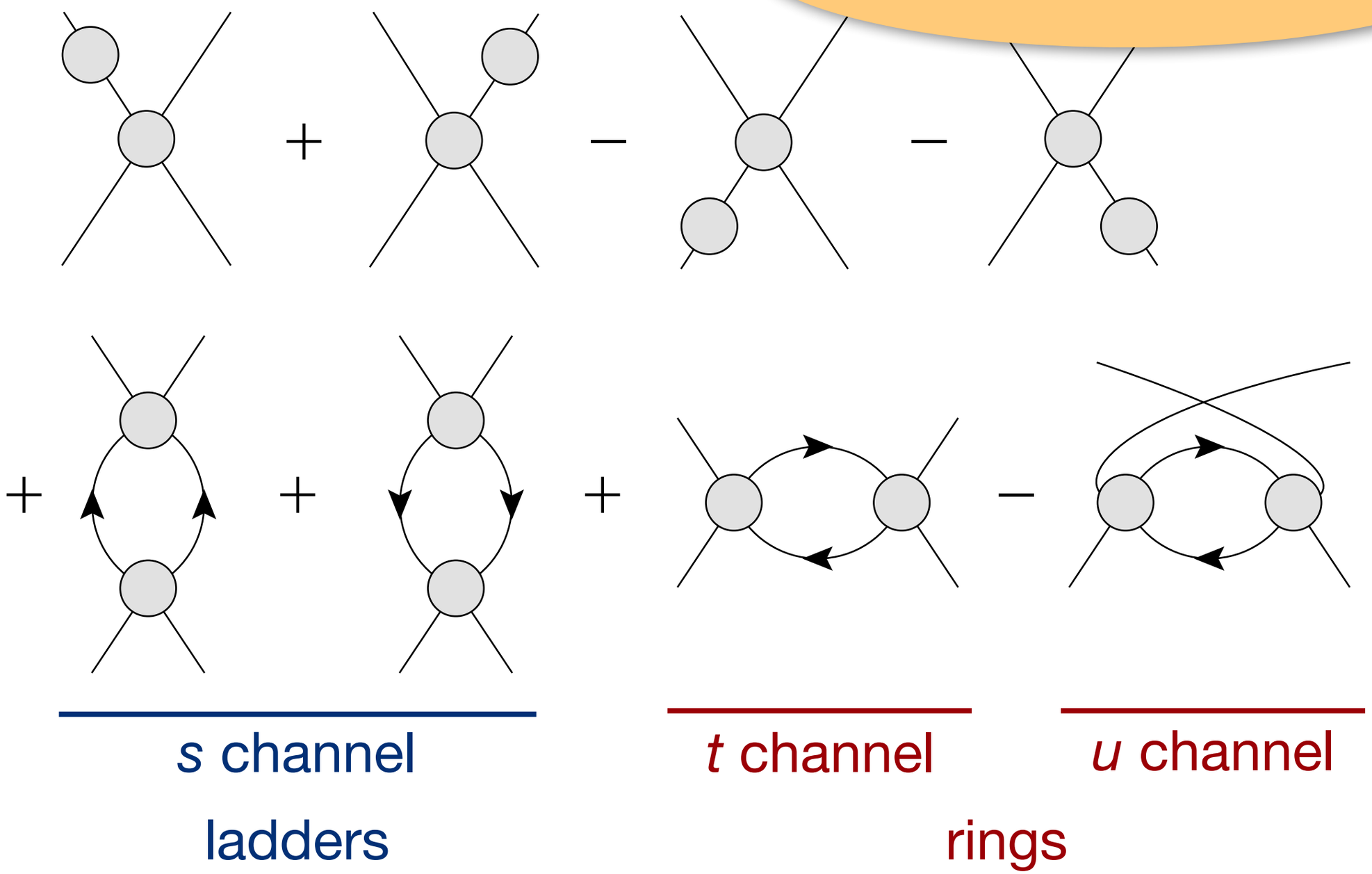


IM-SRG(2) Flow Equations

2-body Flow

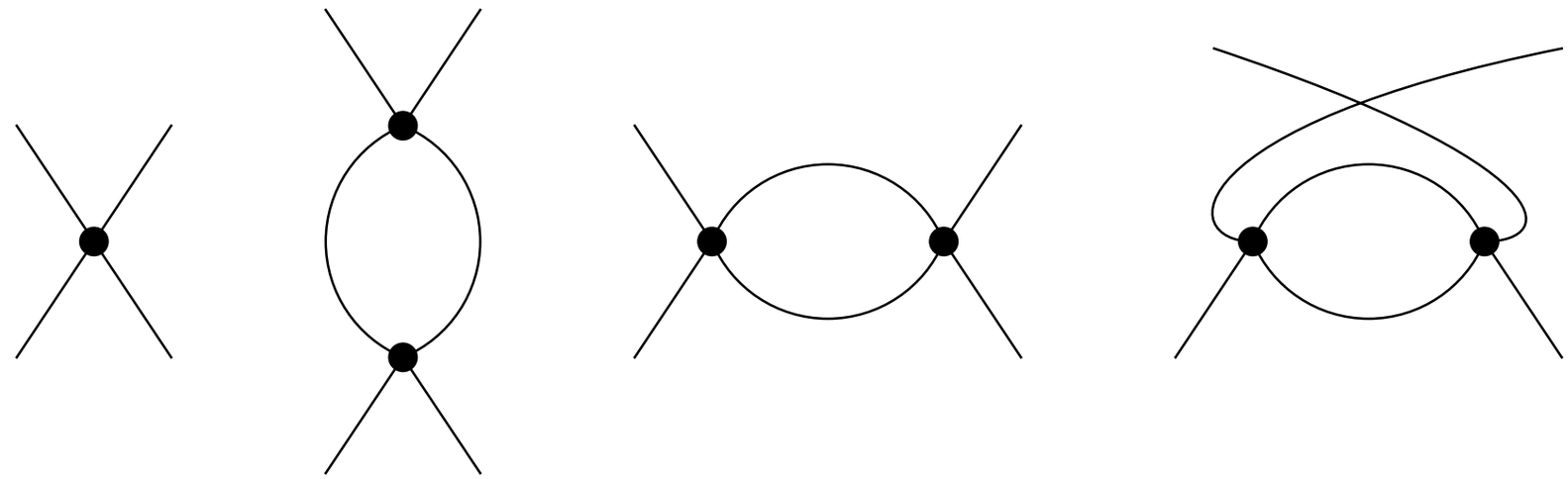
$O(N^6)$ scaling
(before particle/hole distinction)

$$\frac{d\Gamma}{ds} =$$

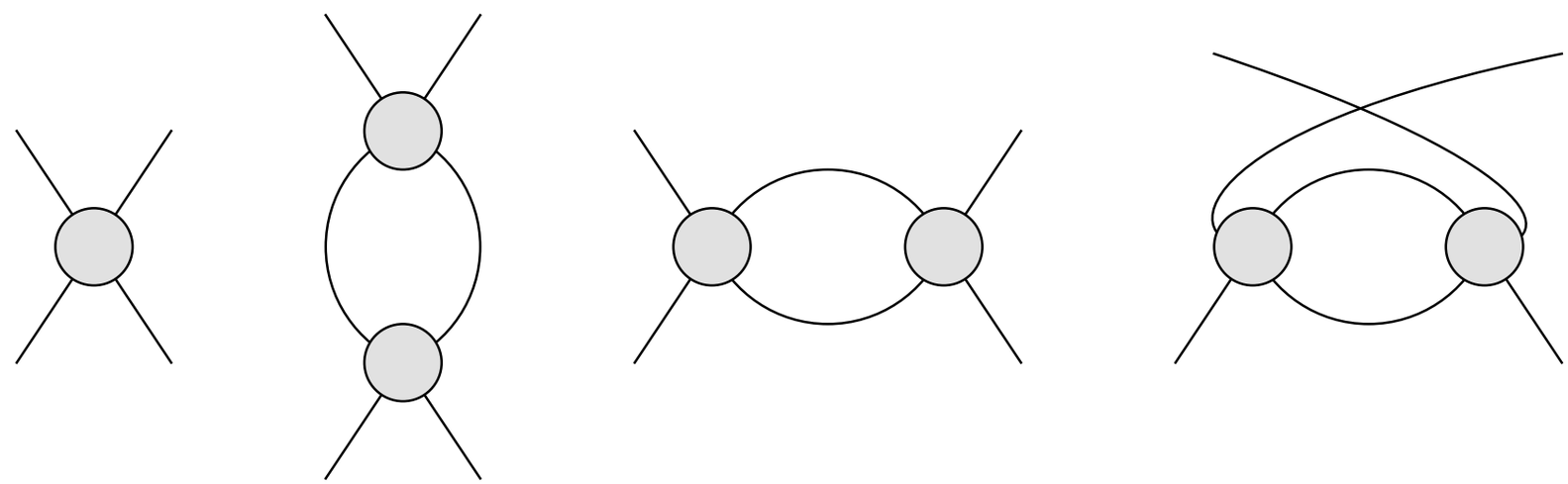


In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$



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



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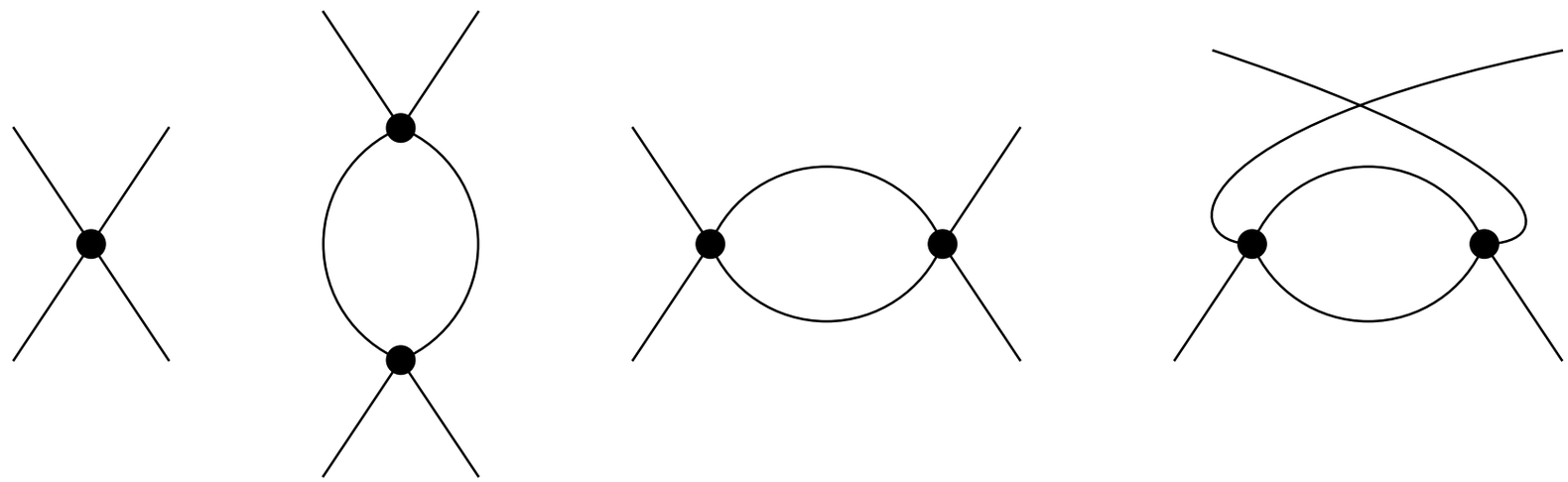

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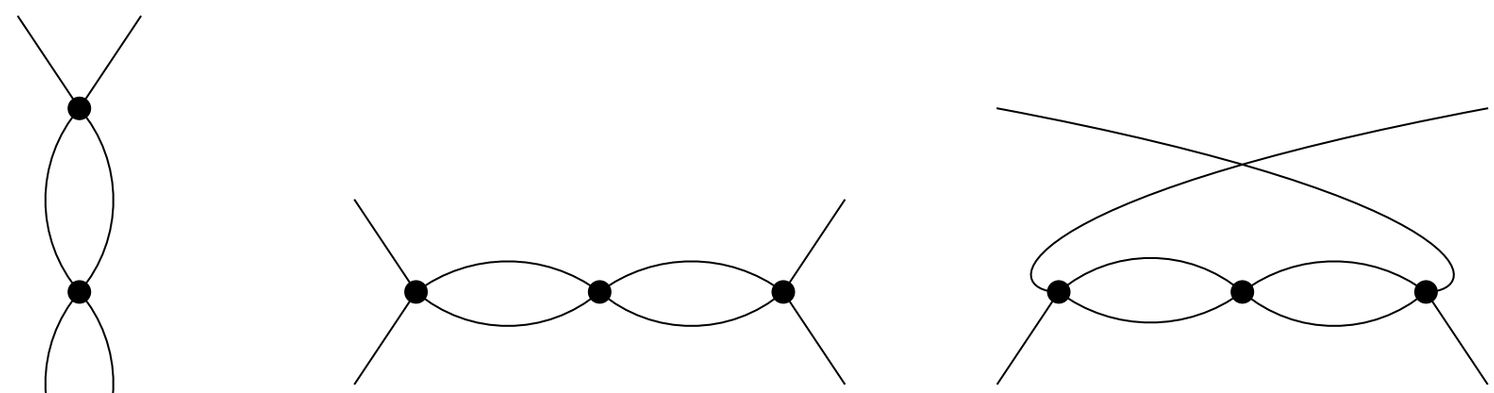

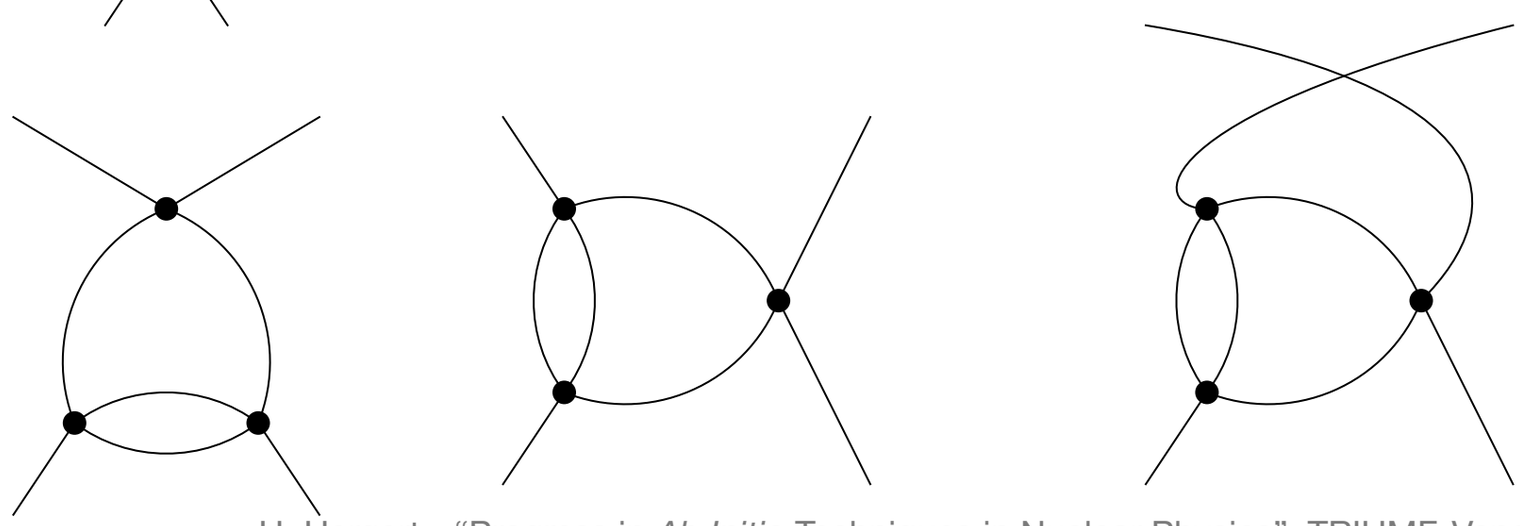

& many more...

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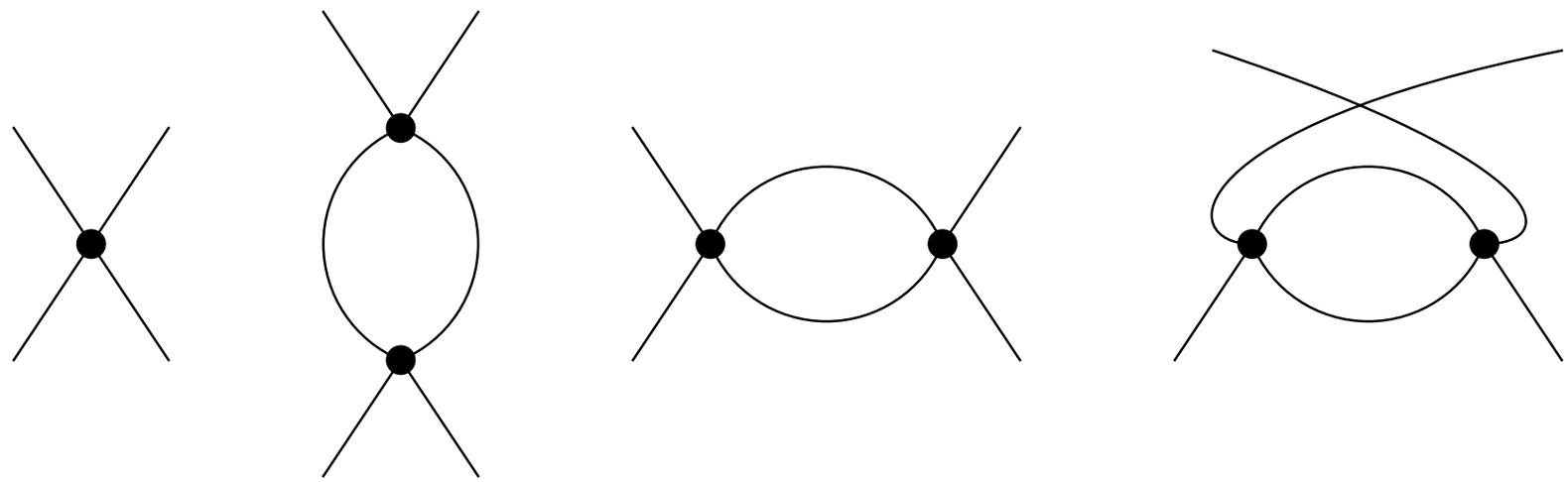

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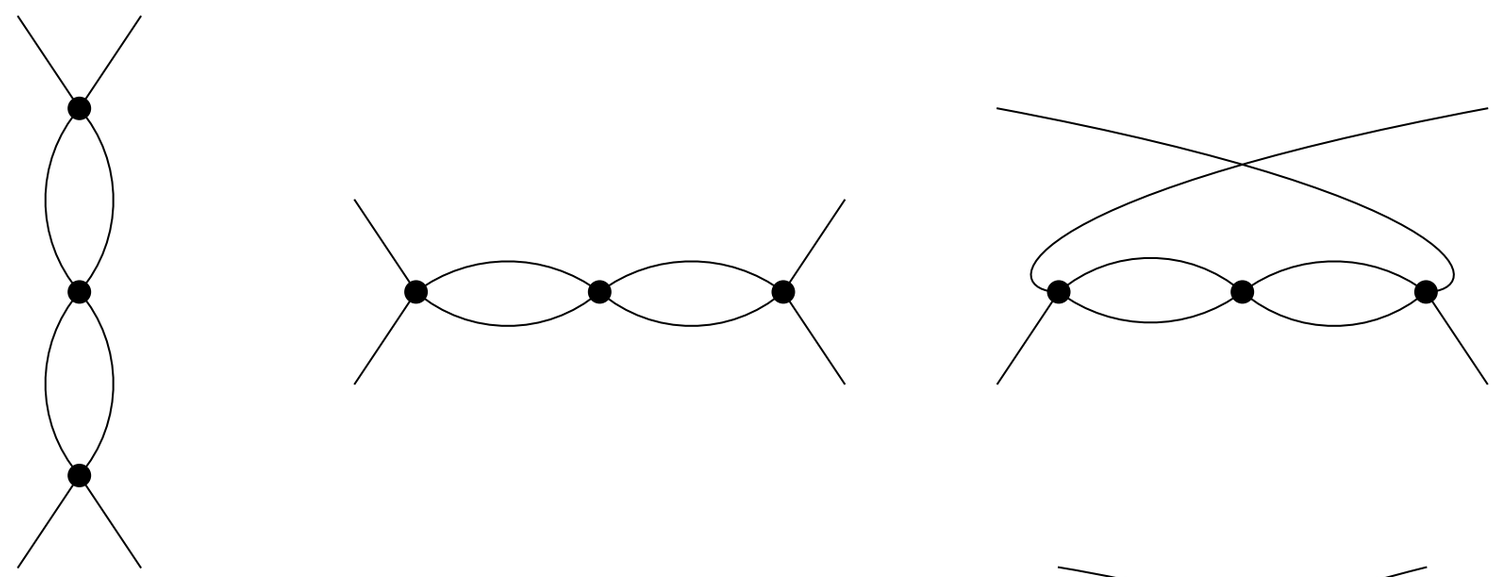
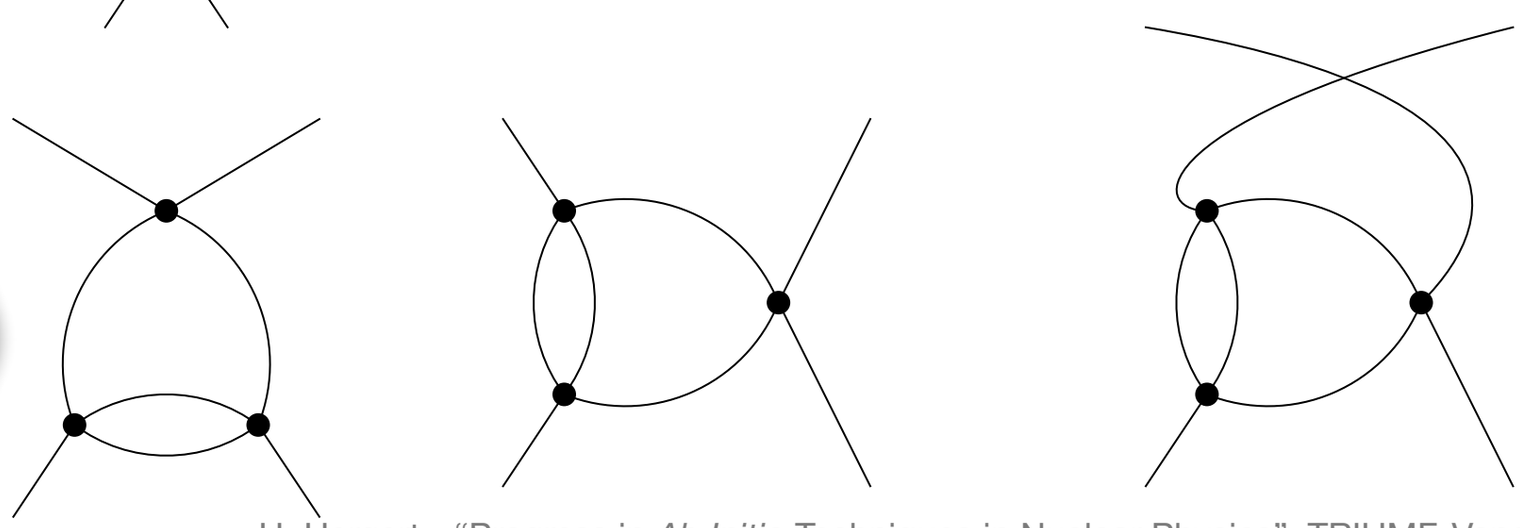


non-perturbative resummation



& many more...

MR-IM-SRG Flow Equations

0-body flow:

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\eta^a_b f^b_a + \frac{1}{2}\sum_{abcd}\eta^{ab}_{cd}\Gamma^{cd}_{ab} n_a n_b \bar{n}_c \bar{n}_d$$
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1-body flow:

$$\frac{d}{ds}f^1_2 = \sum_a\left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b\Gamma^{b1}_{a2} - f^a_b\eta^{b1}_{a2}\right)(n_a - n_b)$$
$$+ \frac{1}{2}\sum_{abc}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a\bar{n}_b\bar{n}_c + \bar{n}_a n_b n_c)$$
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$$-\frac{1}{2}\sum_{abcde}\left(\eta^{1a}_{2b}\Gamma^{cd}_{ae} - \Gamma^{1a}_{2b}\eta^{cd}_{ae}\right)\lambda^{cd}_{be} + \frac{1}{2}\sum_{abcde}\left(\eta^{1a}_{2b}\Gamma^{bc}_{de} - \Gamma^{1a}_{2b}\eta^{bc}_{de}\right)\lambda^{ac}_{de}$$

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$O(N^5)$

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$O(N^6)$

MR-IM-SRG Flow Equations

2-body flow:

$$\frac{d}{ds}\Gamma^{12}_{34} = \sum_a \left(\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\right)$$
$$+ \frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b)$$
$$+ \sum_{ab}(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)$$

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- two-body flow identical to closed-shell case

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- numerical scaling: $O(N^6)$

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$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\eta^a_b f^b_a + \frac{1}{2}\sum_{abcd}\eta^{ab}_{cd}\Gamma^{cd}_{ab} n_a n_b \bar{n}_c \bar{n}_d$$

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O(N^4)

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

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O(N^4) **O(N^7)**

MR-IM-SRG Flow Equations

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$\mathrm{O}(\mathrm{N}^4)$ $\qquad$ $\mathbf{O(N^7)}$

- storage of full 3B density matrix too expensive in general

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➡ exploit structure of specific reference states:

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➡ exploit structure of specific reference states:

- Projected HFB: $\mathrm{O}(\mathrm{N}^3)$ storage, scaling reduced to $\mathrm{O}(\mathrm{N}^4)$

$$\lambda^{abc}_{def} = \bar{\lambda}_{abc}\,\delta^a_d\delta^b_e\delta^c_f + \widetilde{\lambda}_{a|be}\,\delta^a_d\delta^{b\bar{c}}\delta_{e\bar{f}} + \text{perm.}$$

MR-IM-SRG Flow Equations

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- NCSM / active-space CI: small non-zero block only

Magnus Formulation of the In-Medium SRG

T. D. Morris, N. M. Parzuchowski, S. K. Bogner, in preparation

T. D. Morris, N. M. Parzuchowski, S. K. Bogner, PRC **92**, 034331 (2015)

H. H., S. K. Bogner, **T. D. Morris**, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

W. Magnus, Comm. Pure and Appl. Math **VII**, 649-673 (1954)

Magnus Series Formulation

- explicit exponential ansatz for unitary transformation:

$$U(s) = \mathcal{S} \exp \int_0^s ds' \eta(s') \equiv \exp \Omega(s)$$

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$$\frac{d}{ds}\Omega = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_\Omega^k(\eta) \ , \quad \mathrm{ad}_\Omega(O) = [\Omega, O]$$

(B_k: Bernoulli numbers)

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(B_k: Bernoulli numbers)

- construct $O(s) = U(s) O_0 U^\dagger(s)$ using Baker-Campbell-Hausdorff expansion (**Hamiltonian + effective operators**)

Magnus Series Formulation

- explicit exponential ansatz for unitary transformation:

$$U(s) = \mathcal{S} \exp \int_0^s ds' \eta(s') \equiv \exp \Omega(s)$$

- flow equation for **Magnus** operator :

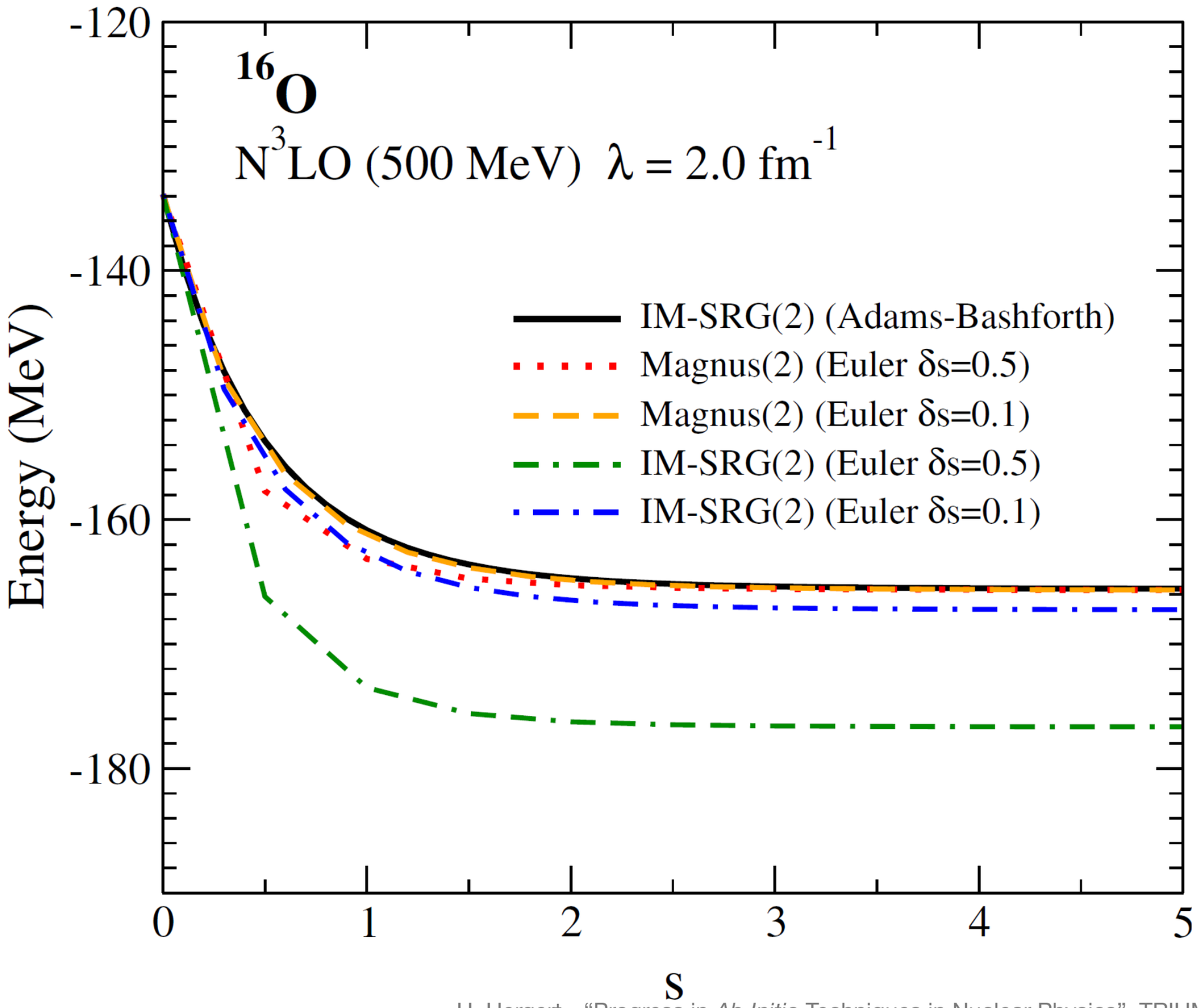
$$\frac{d}{ds}\Omega = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_\Omega^k(\eta) \ , \quad \mathrm{ad}_\Omega(O) = [\Omega, O]$$

(B_k: Bernoulli numbers)

- construct $O(s) = U(s) O_0 U^\dagger(s)$ using Baker-Campbell-Hausdorff expansion (**Hamiltonian + effective operators**)

- MAG(2): **two-body truncation** (as in NO2B, IM-SRG(2))

Magnus vs. Direct Integration



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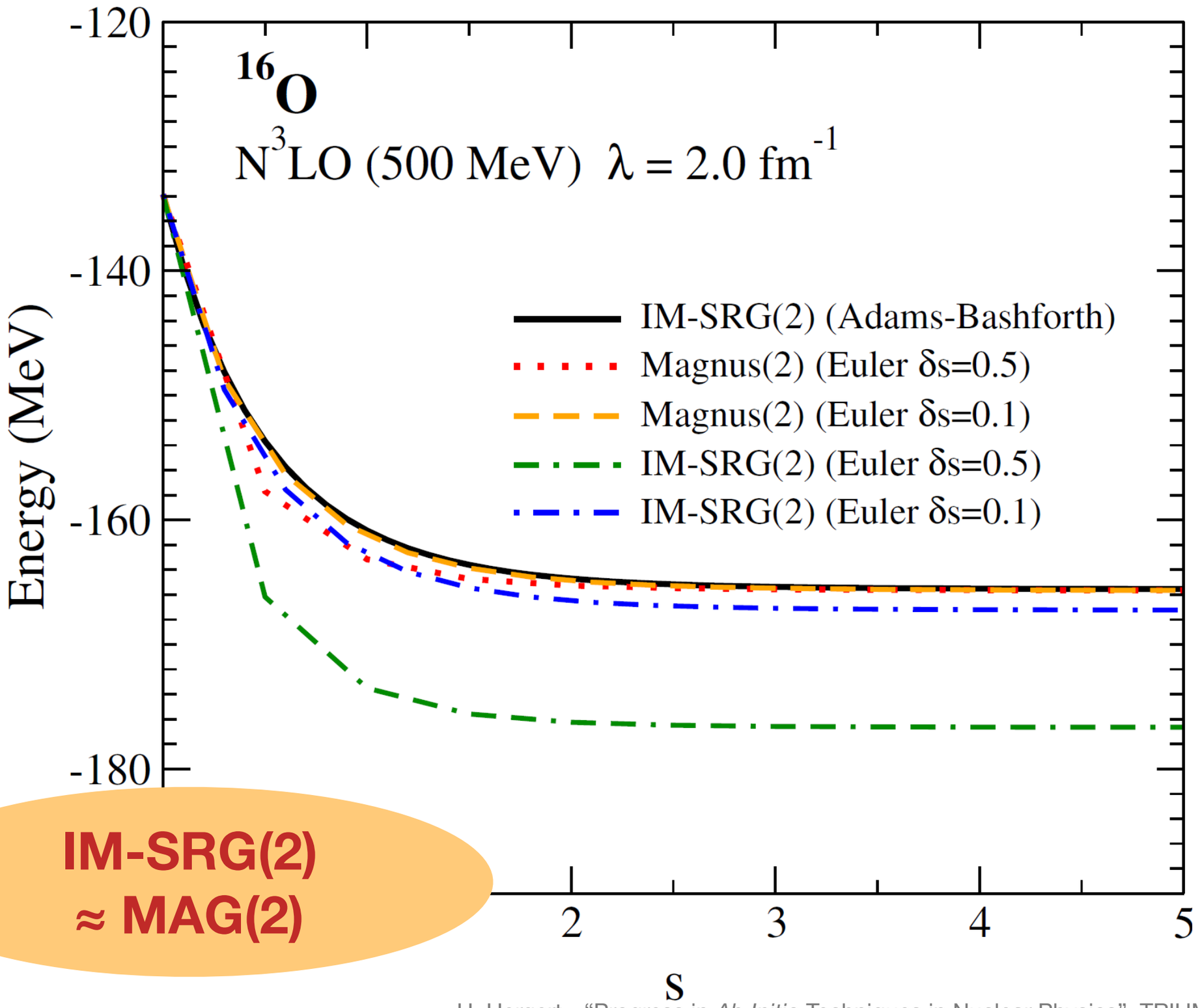

IM-SRG(2) ≈ MAG(2)

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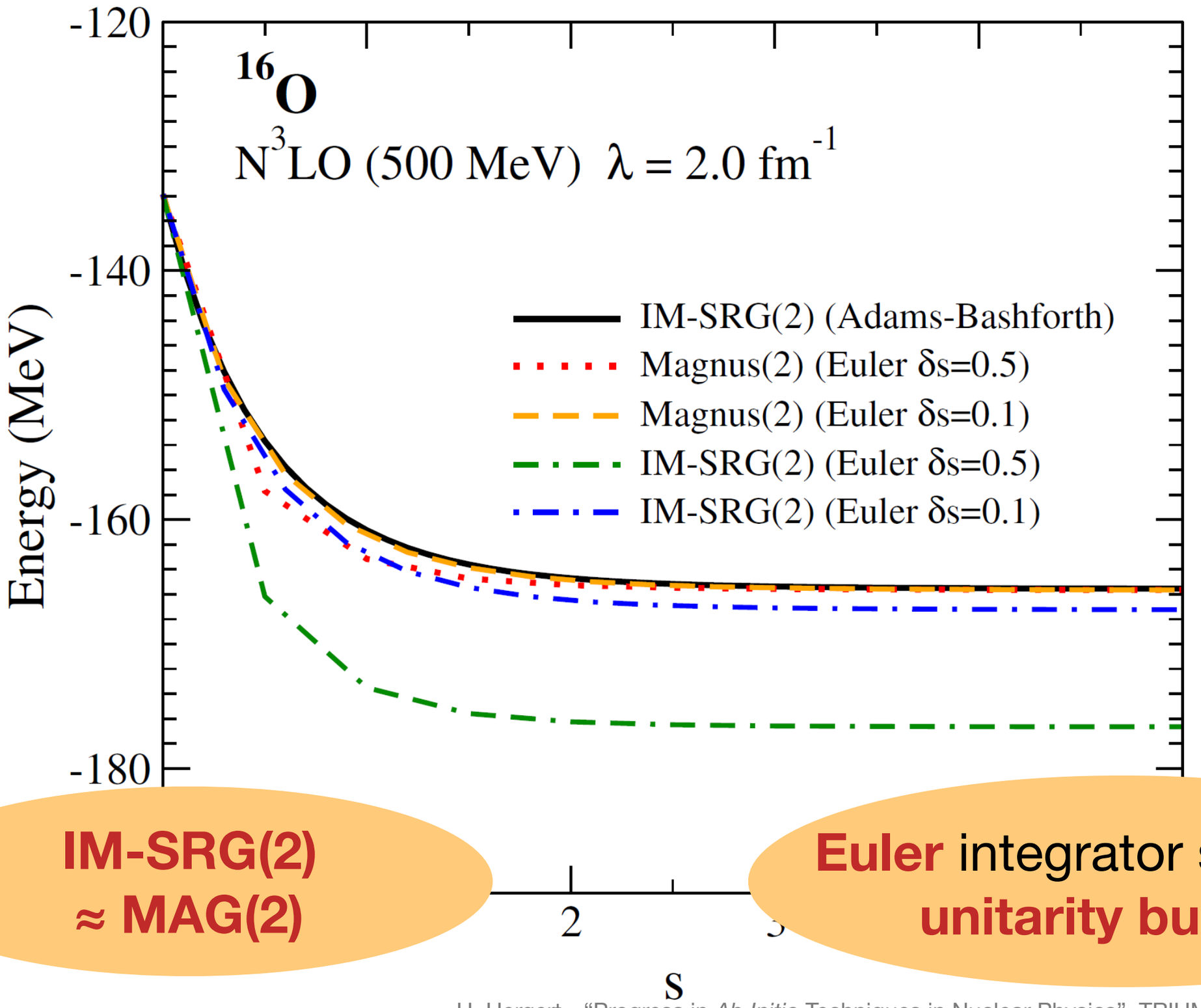

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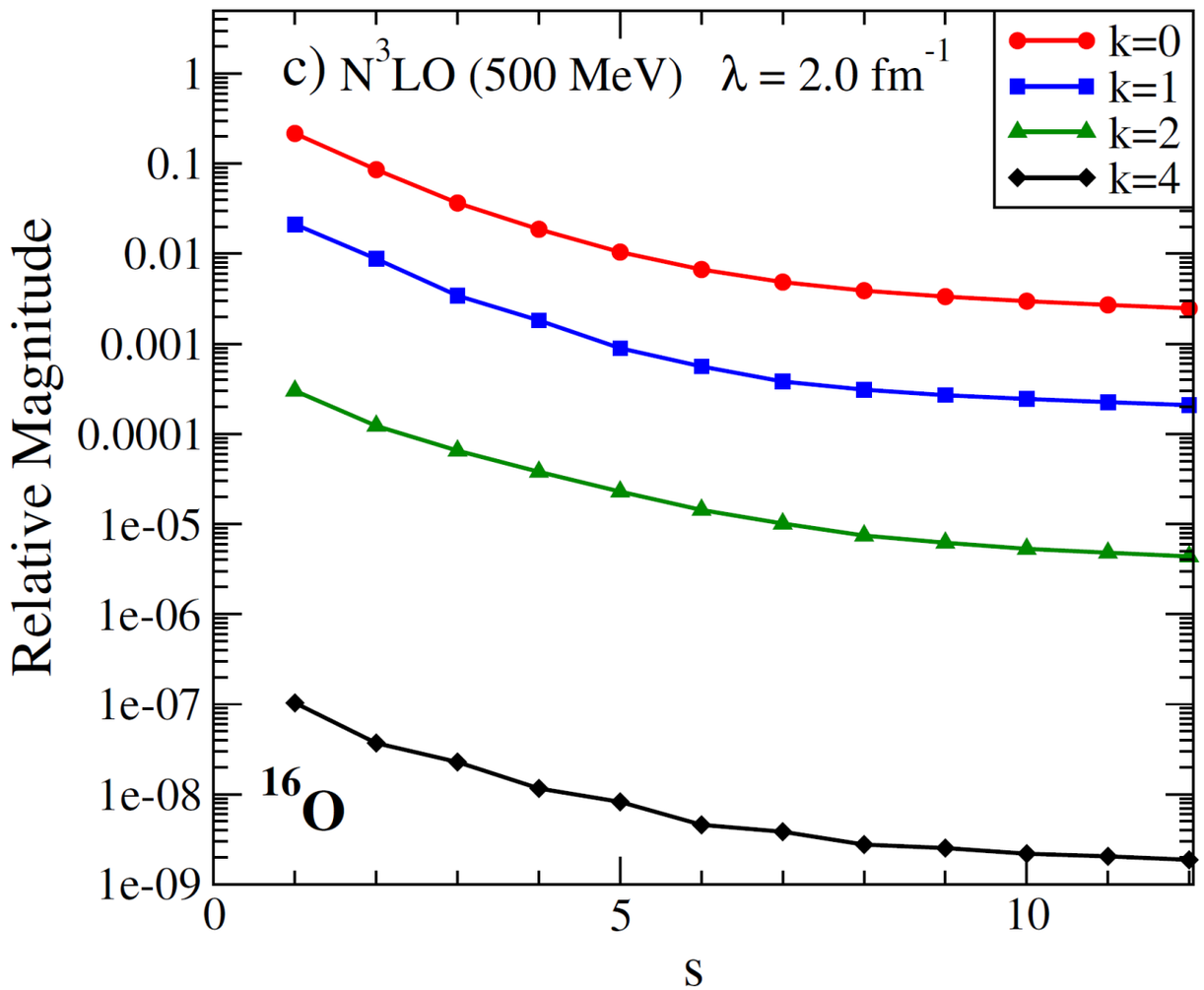
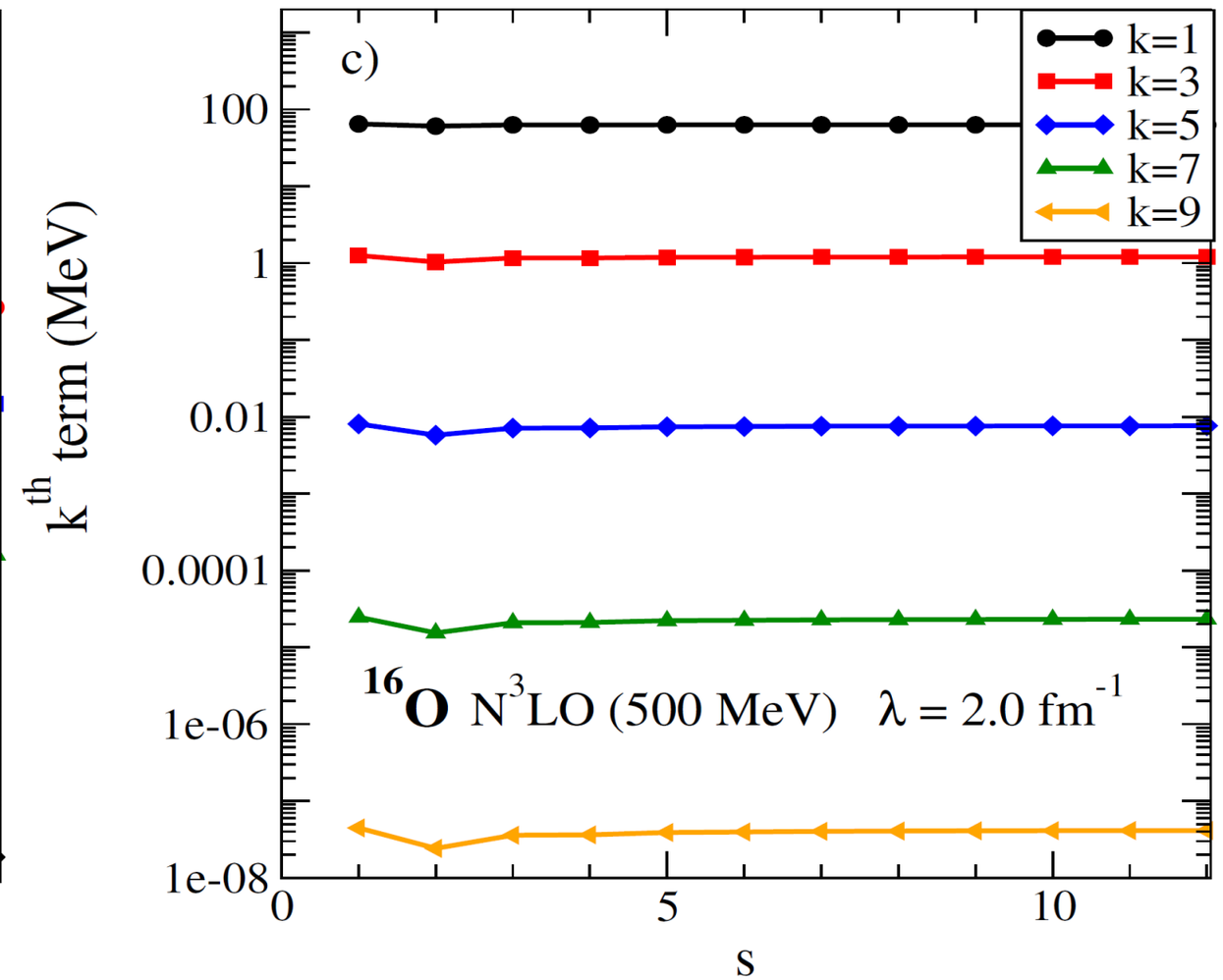
Euler integrator sufficient, **unitarity built in!**

Convergence





$$\frac{d}{ds}\Omega = \sum_k \frac{B_k}{k!} \mathrm{ad}_\Omega^k(\eta)$$

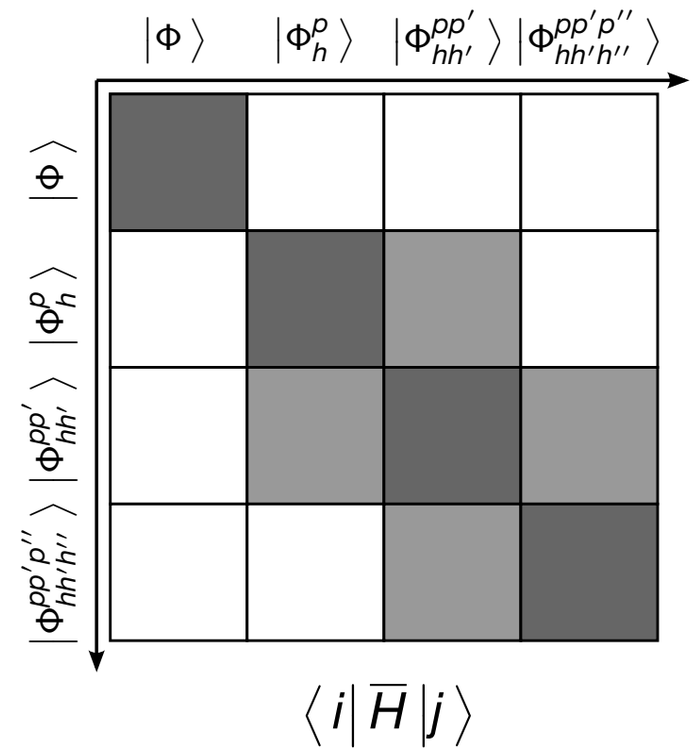
$$H(s) = \sum_k \frac{1}{k!} \mathrm{ad}_\Omega^k(H_0)$$

➡ **ODE and BCH expansions converge rapidly and monotonically**

Approximating IM-SRG(3)

- final Hamiltonian (IM-SRG(A), MAG(A)):

$$\overline{H} = \left(e^{\Omega} H e^{-\Omega}\right) = \overline{H}_{0,1,2} + \overline{H}_3 + \ldots$$



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- final Hamiltonian (IM-SRG(2), MAG(2)):

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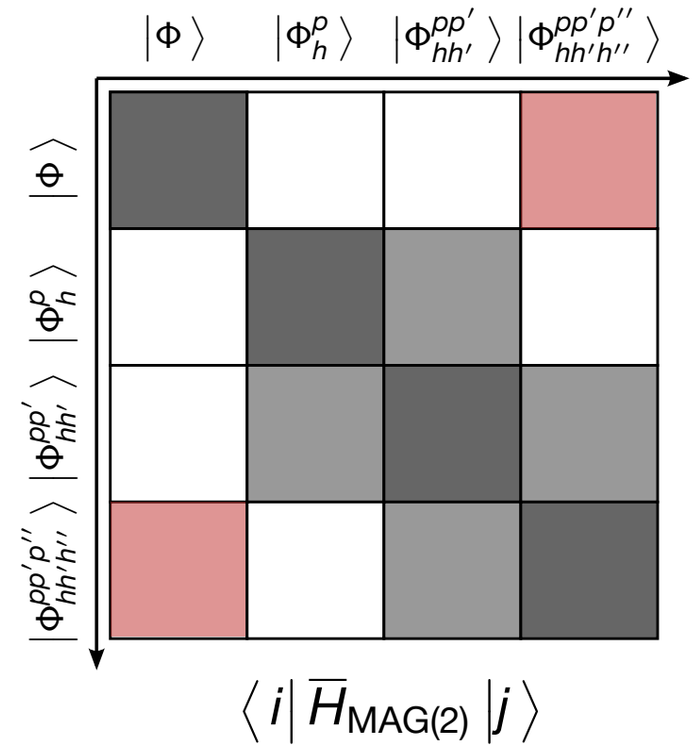

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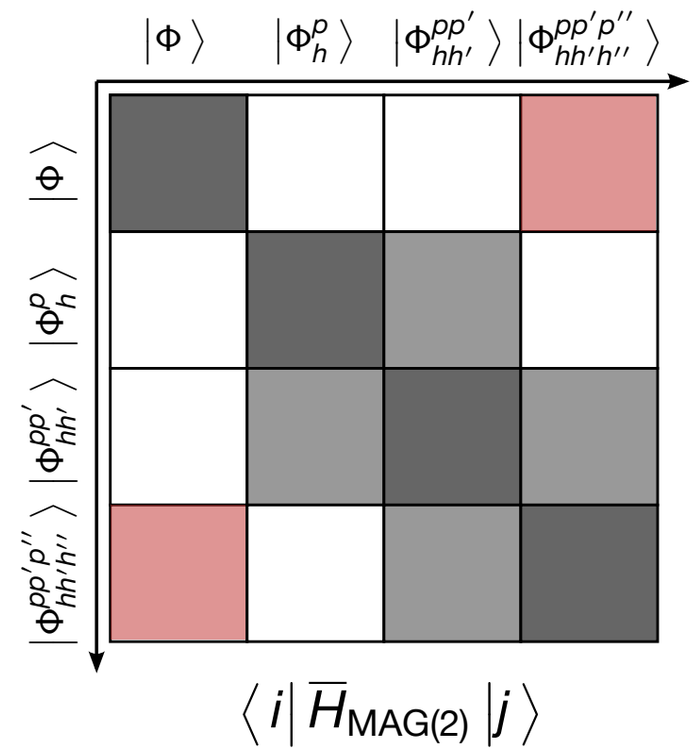

- energy contribution of $\overline{H}_3$ (cf. 0B flow):

$$\Delta E_3 = \frac{1}{36} \sum_{pp'p''hh'h''} \frac{\left|(\overline{H}_3)_{pp'p''hh'h''}\right|^2}{\overline{\Delta}_{pp'p''hh'h''}}$$

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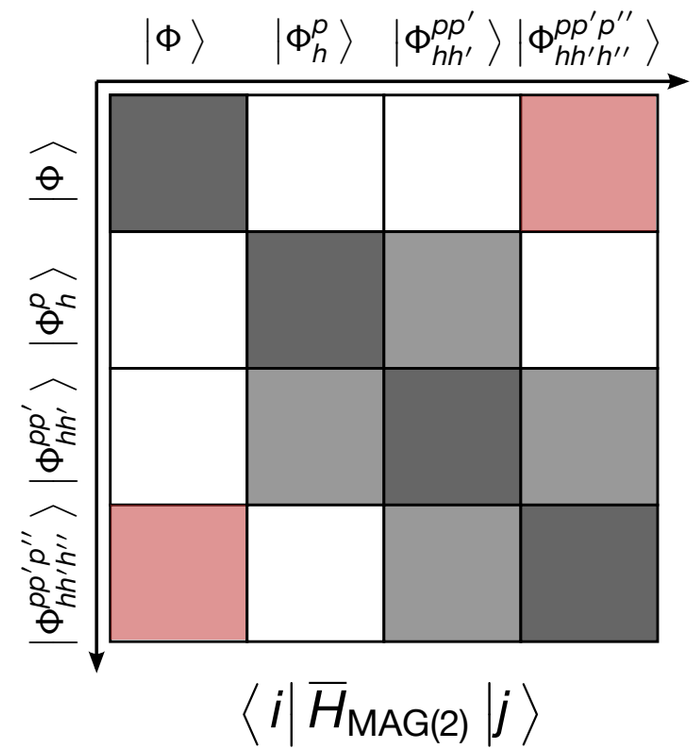

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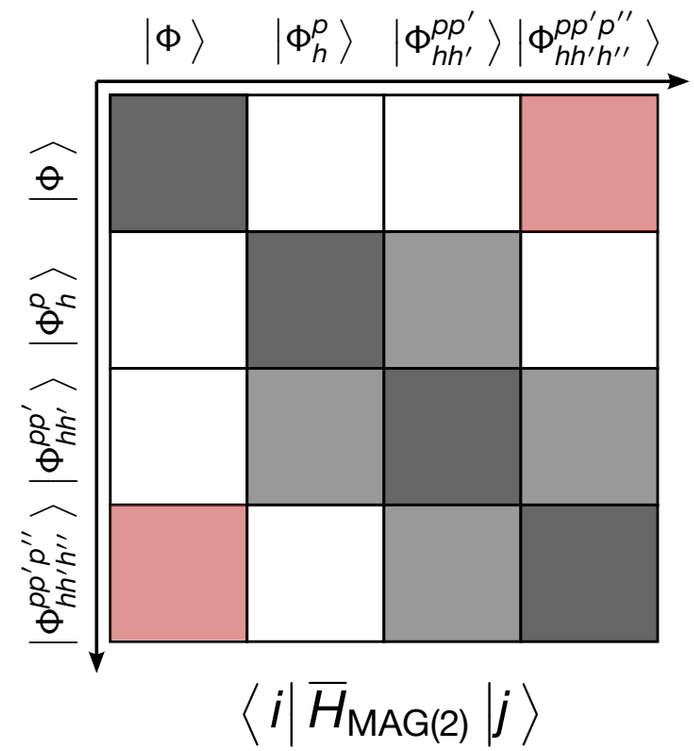

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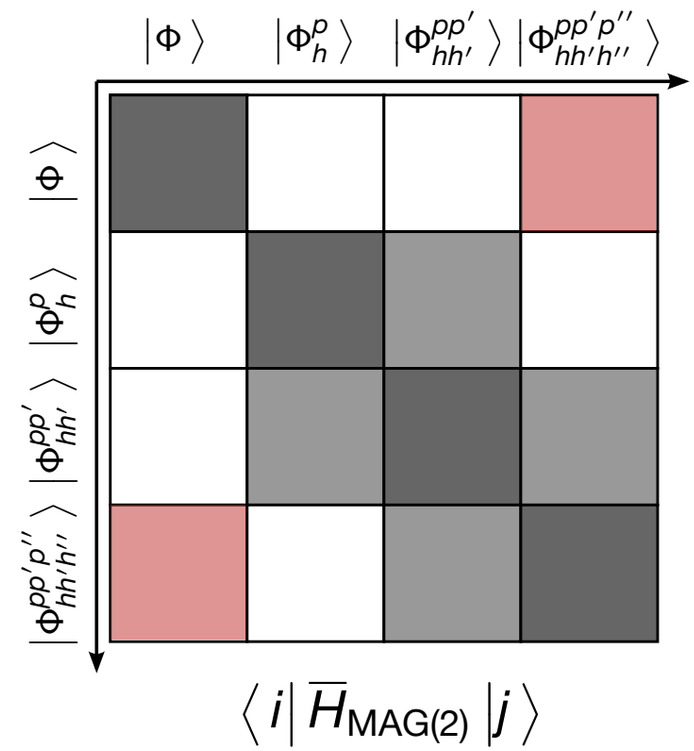

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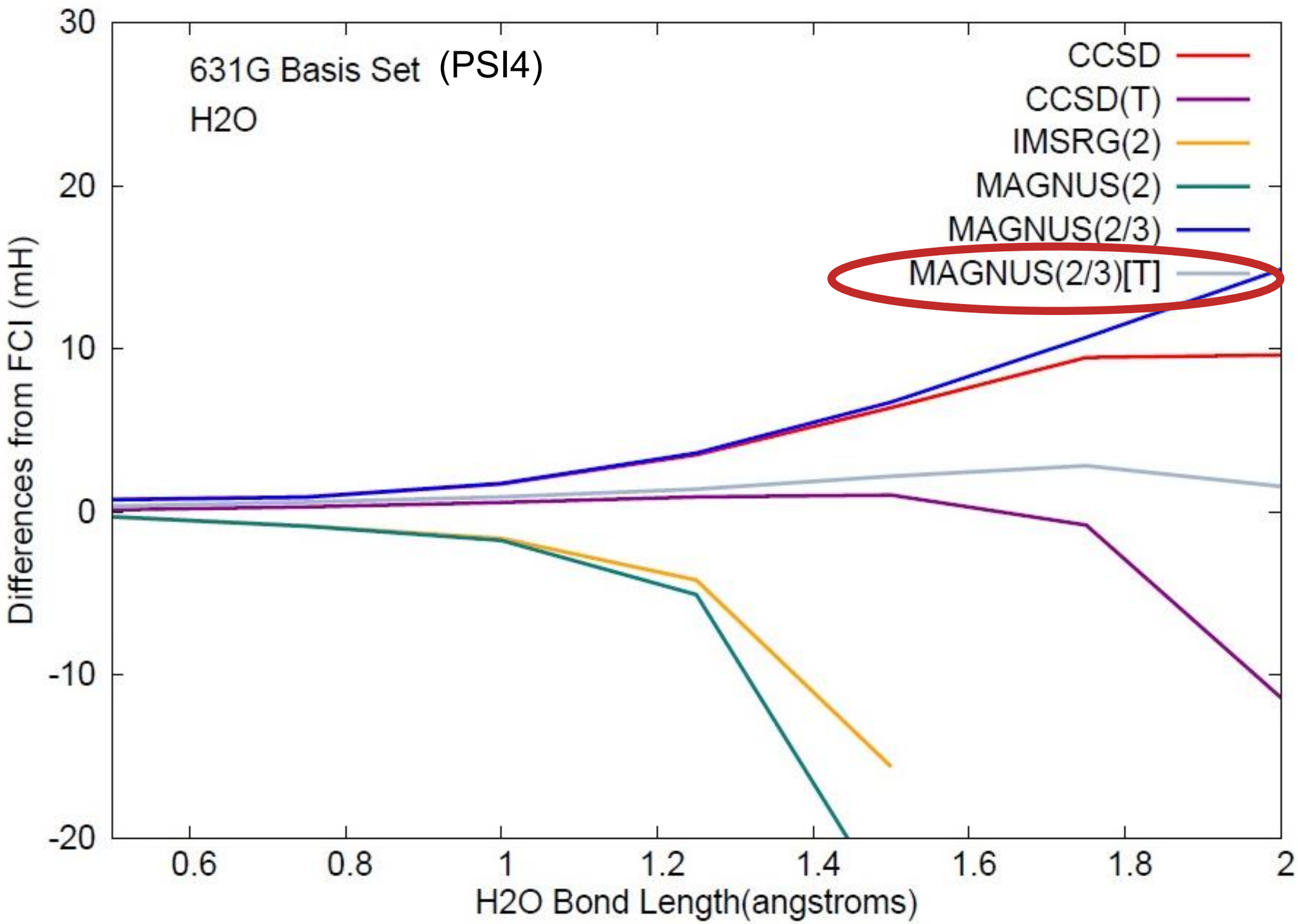
- generalizes to **arbitrary observables, excited states**
- multi-reference variant in development

Example: Bond Breaking in Water



Equation-of-Motion Method

- describe “excited states” based on reference state:

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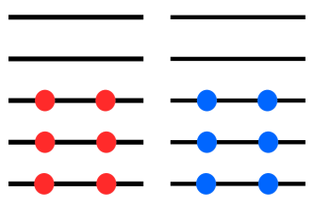
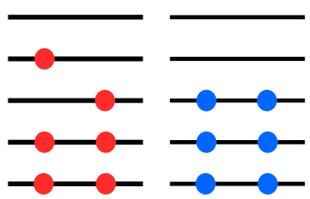
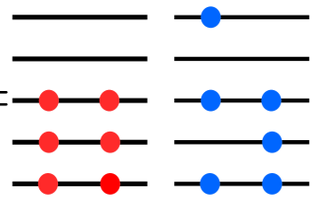
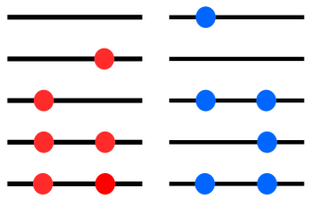
- future: exploit multi-reference capabilities (commutator formulation identical to flow equations)

Full Configuration Interaction

- many-body basis (e.g., Slater determinants)

$|\Phi_1\rangle =$  , $|\Phi_2\rangle =$  , $|\Phi_3\rangle =$  , $|\Phi_4\rangle =$  , $\ldots$

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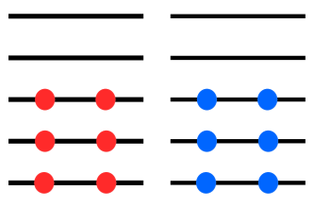
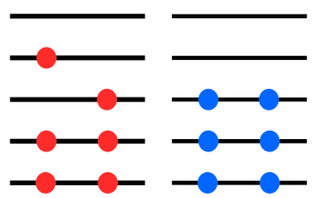
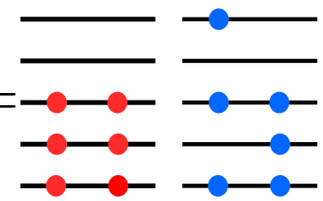
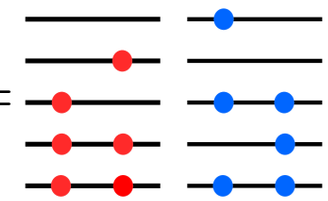
$|\Phi_1\rangle =$  , $|\Phi_2\rangle =$  , $|\Phi_3\rangle =$  , $|\Phi_4\rangle =$  , ...

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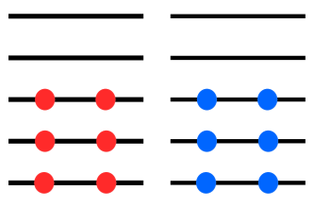
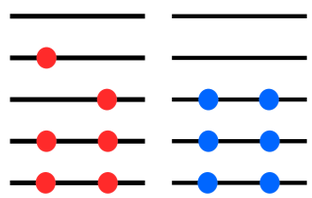
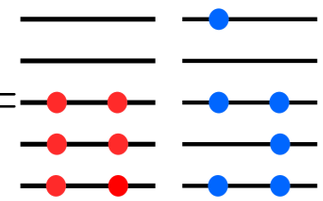
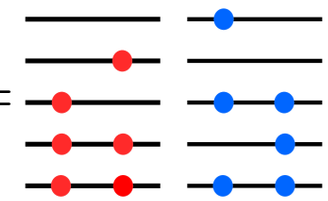
$|\Phi_1\rangle =$  , $|\Phi_2\rangle =$  , $|\Phi_3\rangle =$  , $|\Phi_4\rangle =$  , ...

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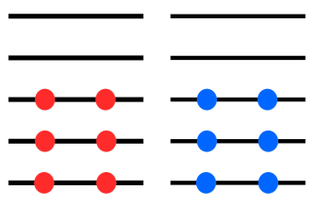
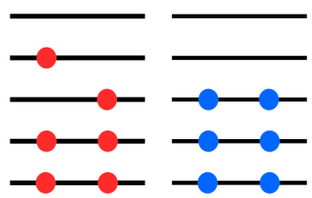
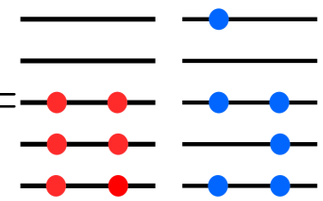
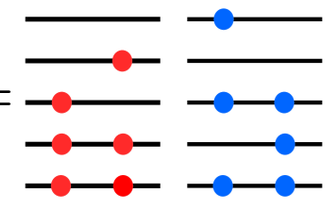
$|\Phi_1\rangle =$  , $|\Phi_2\rangle =$  , $|\Phi_3\rangle =$  , $|\Phi_4\rangle =$  , ...

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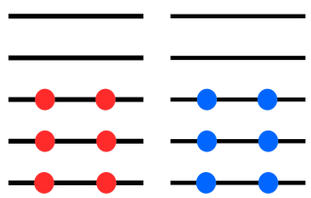
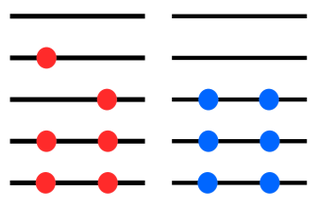
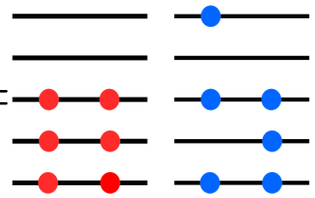
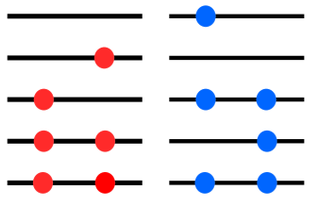
$|\Phi_1\rangle =$  , $|\Phi_2\rangle =$  , $|\Phi_3\rangle =$  , $|\Phi_4\rangle =$  , ...

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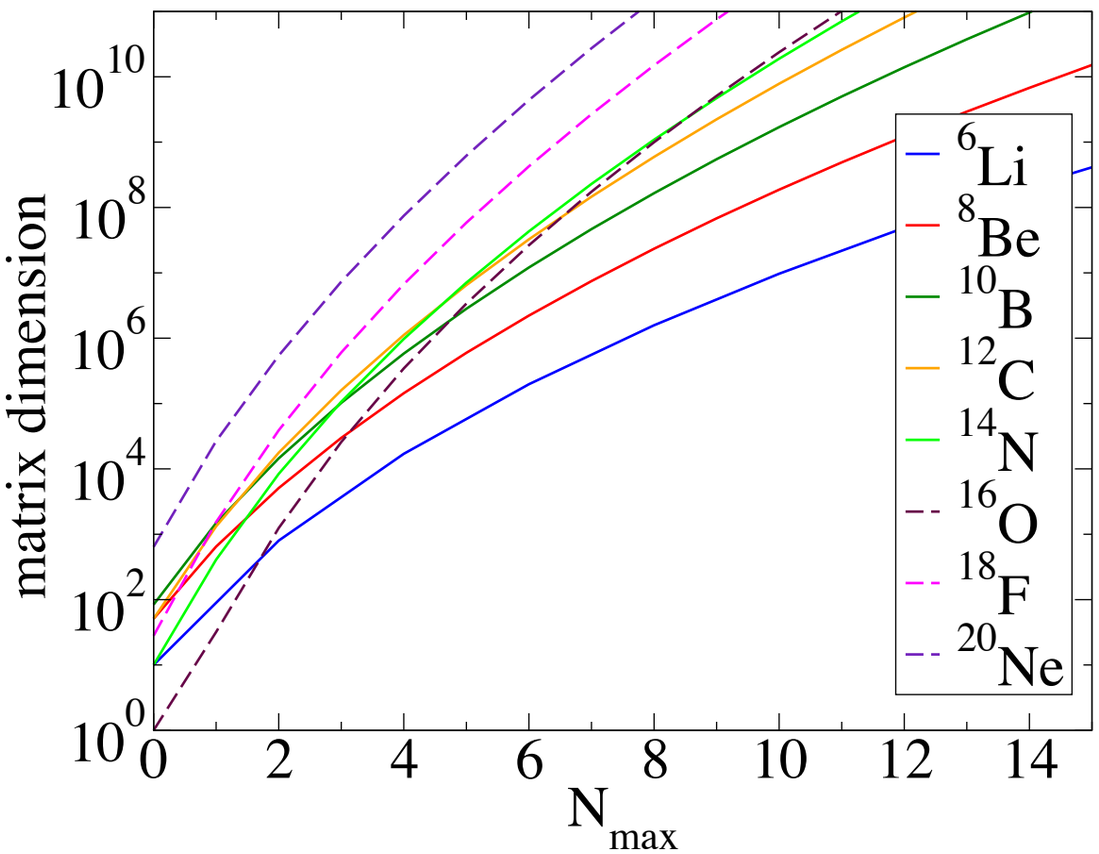
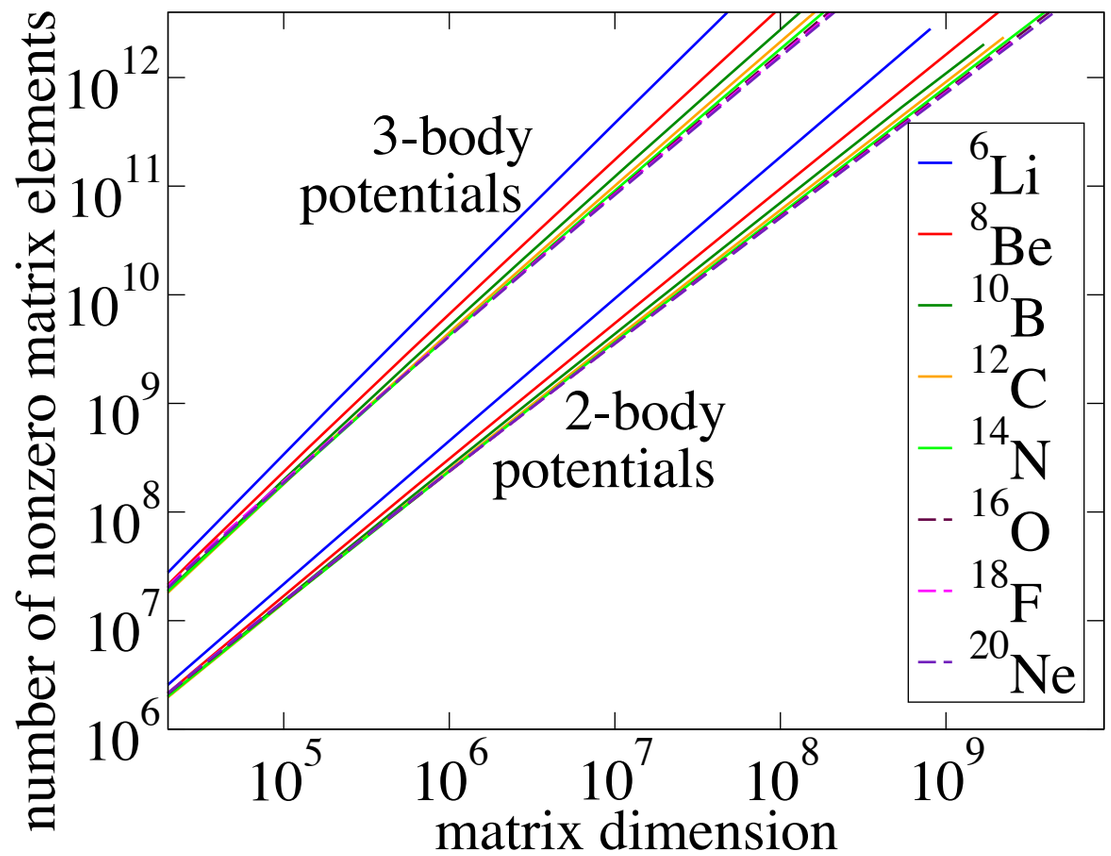
Basis Size "Explosion"





from: C. Yang, H. M. Aktulga, P. Maris, E. Ng, J. Vary, Proceedings of NTSE-2013

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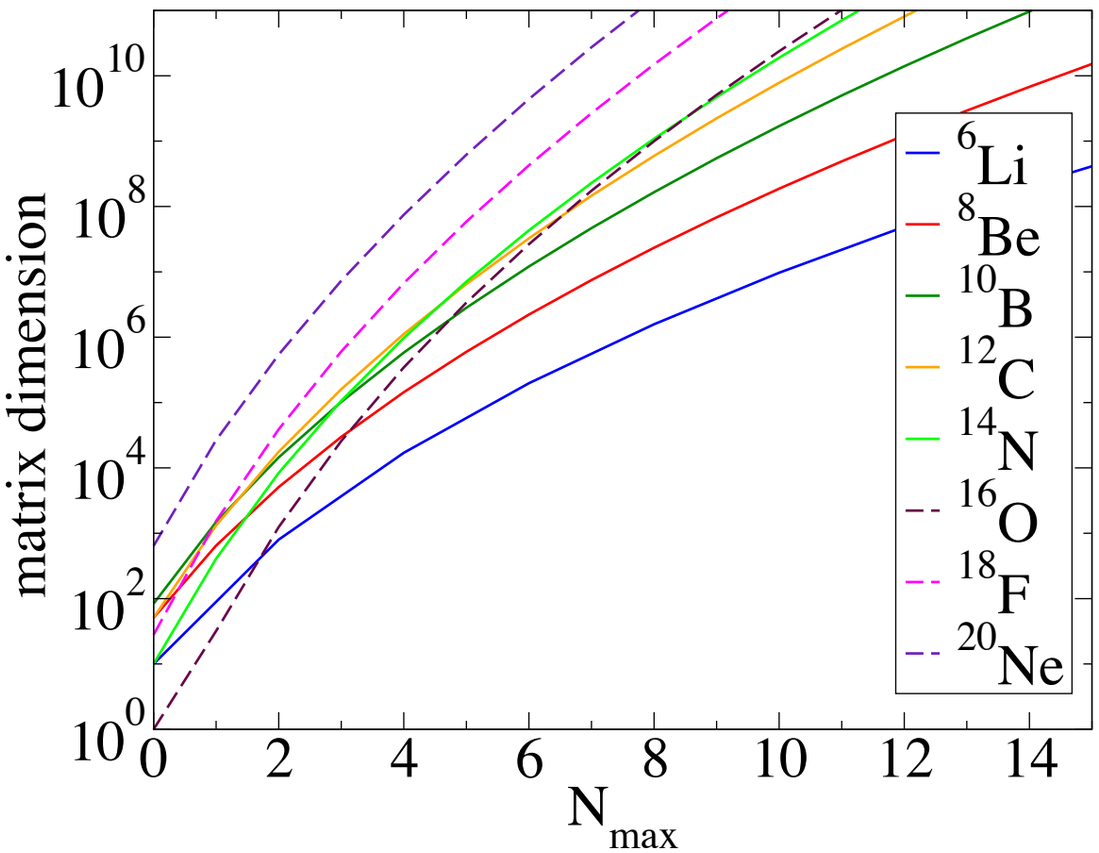

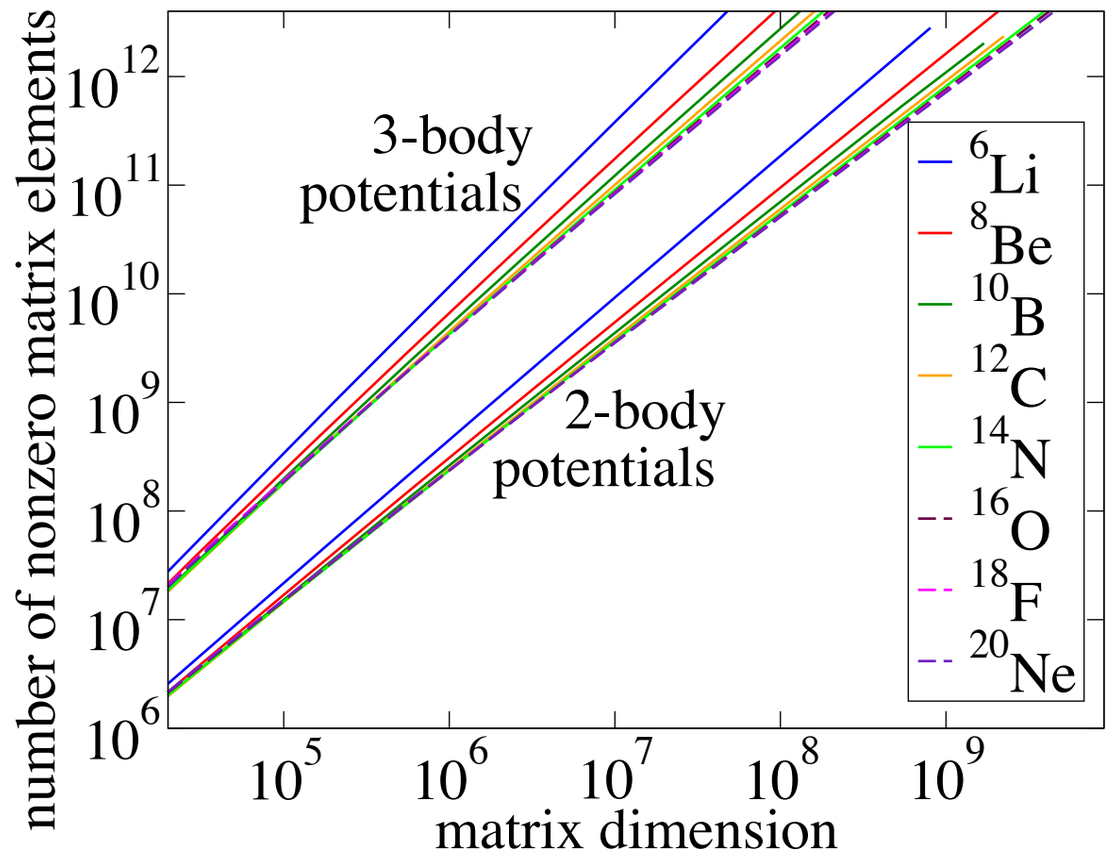

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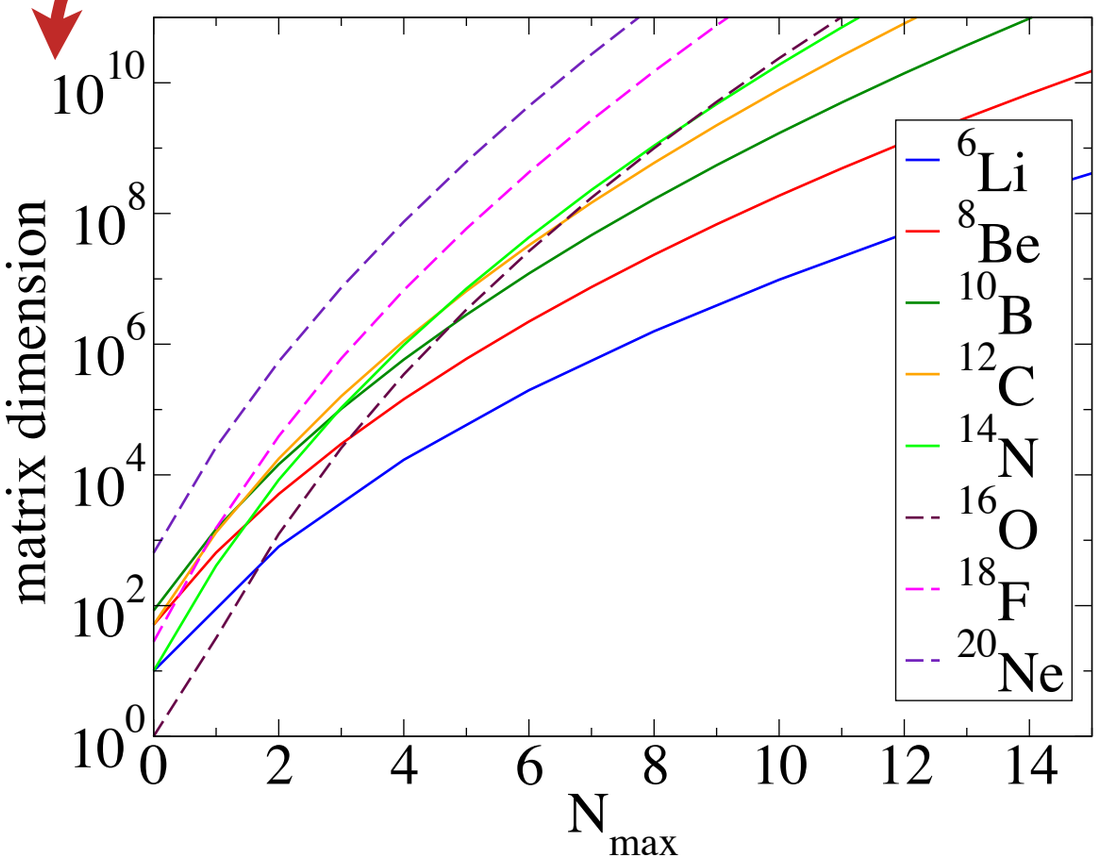
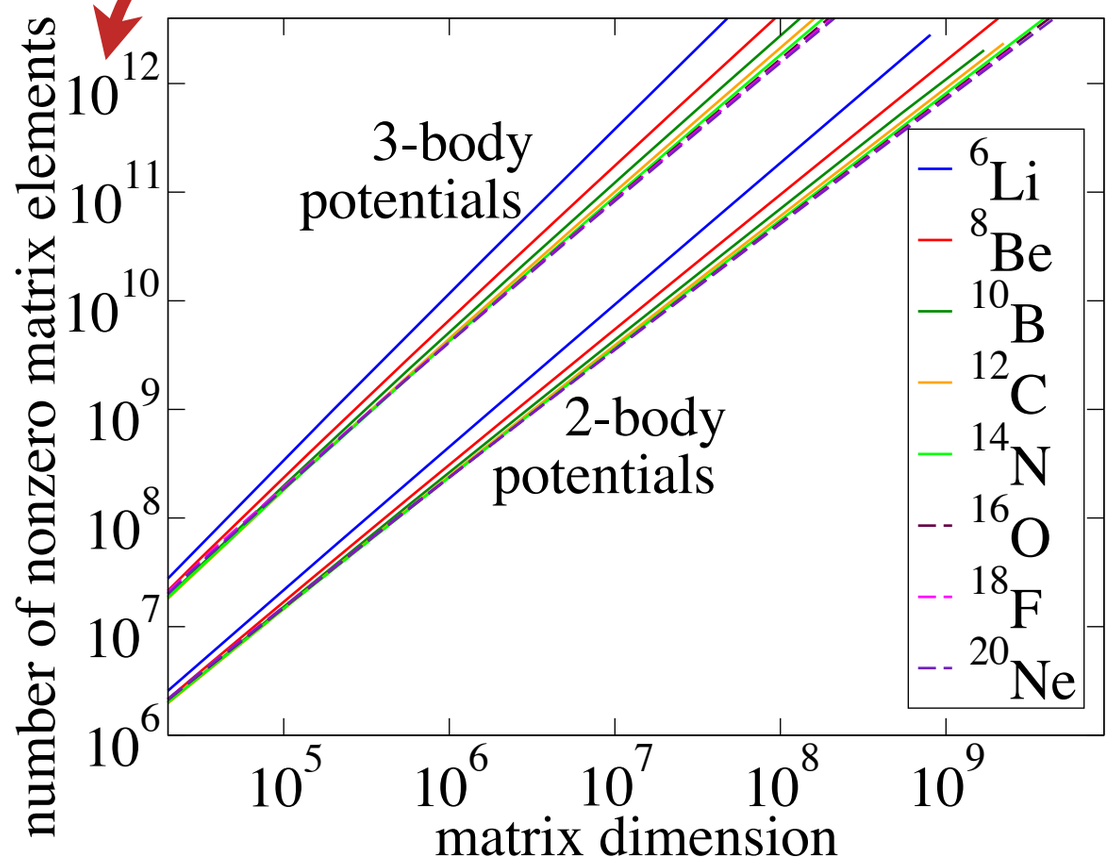
Basis Size "Explosion"

75 GB per vector



7.5 TB



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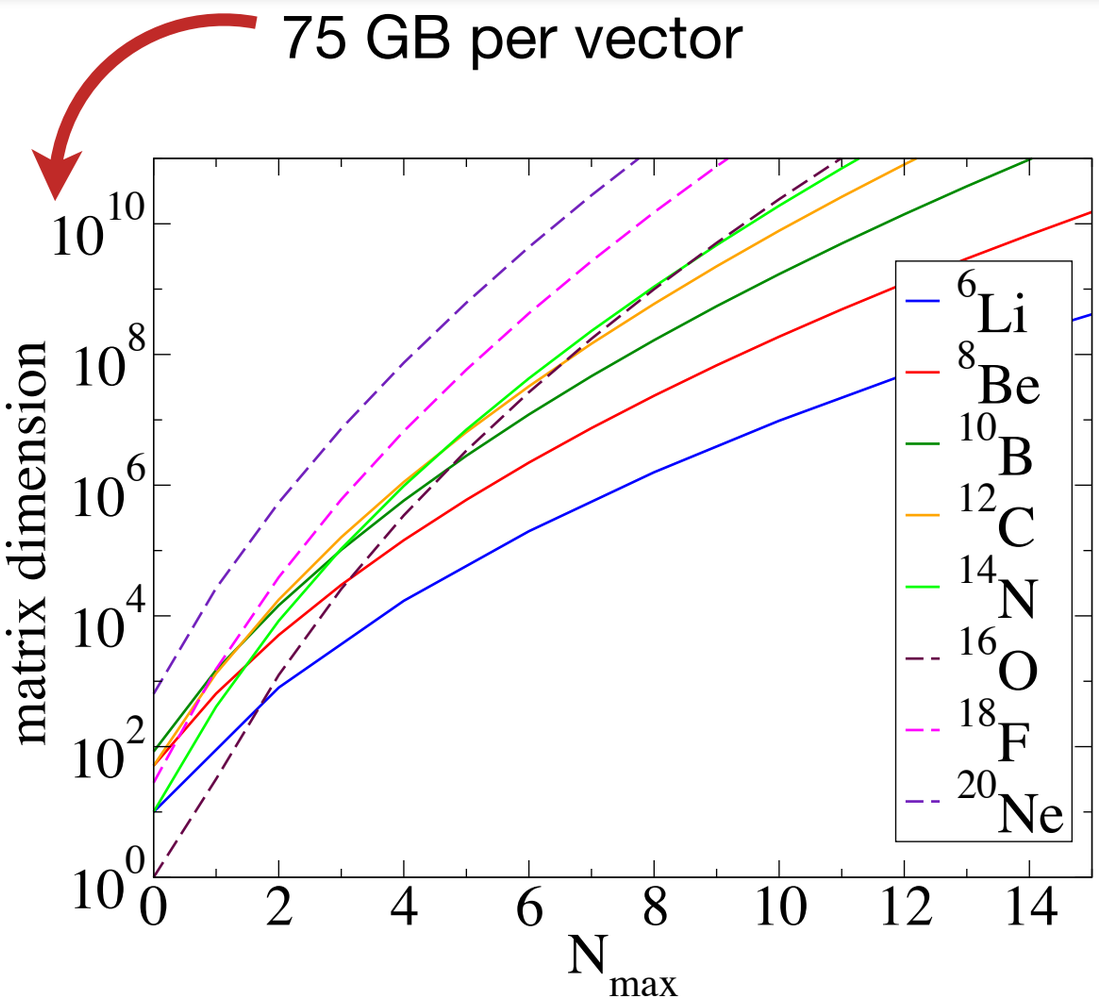
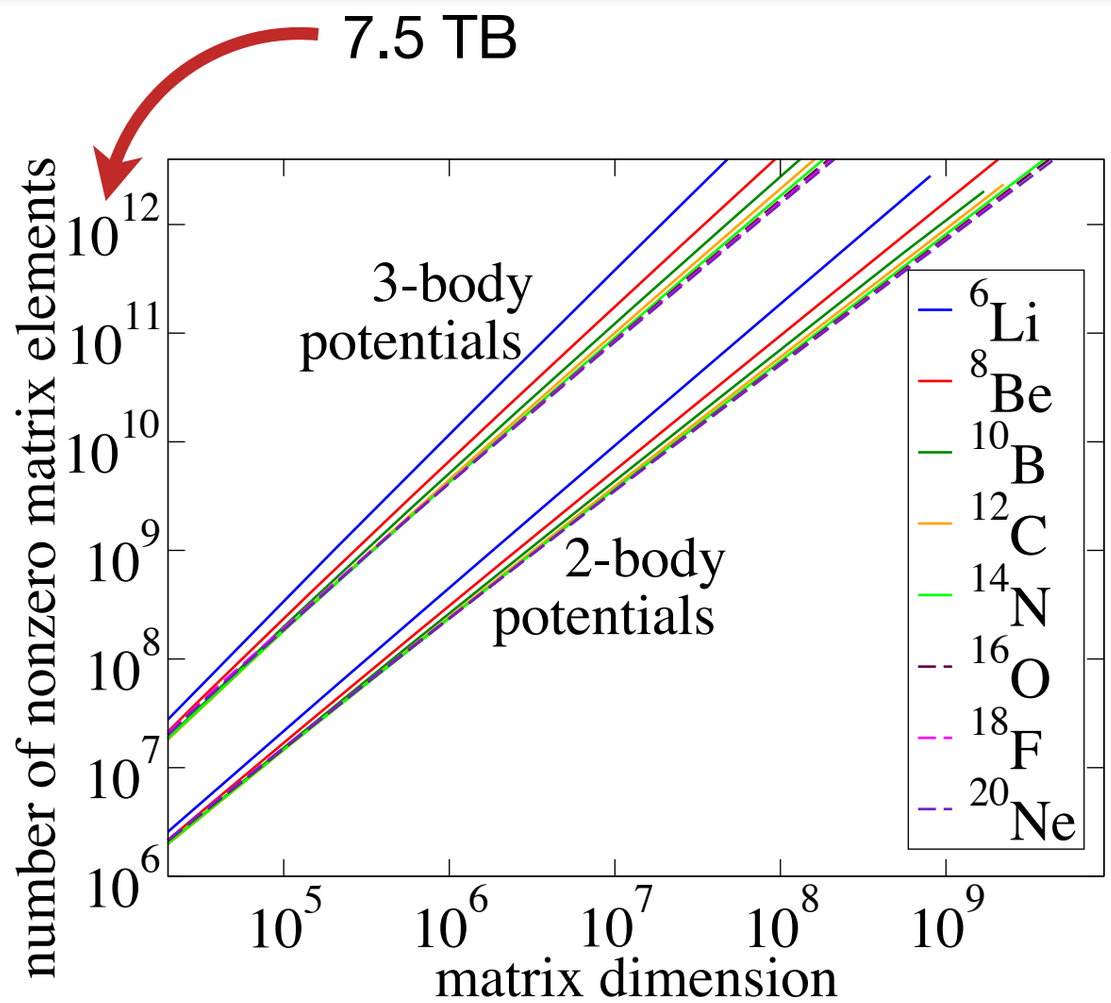
Basis Size "Explosion"

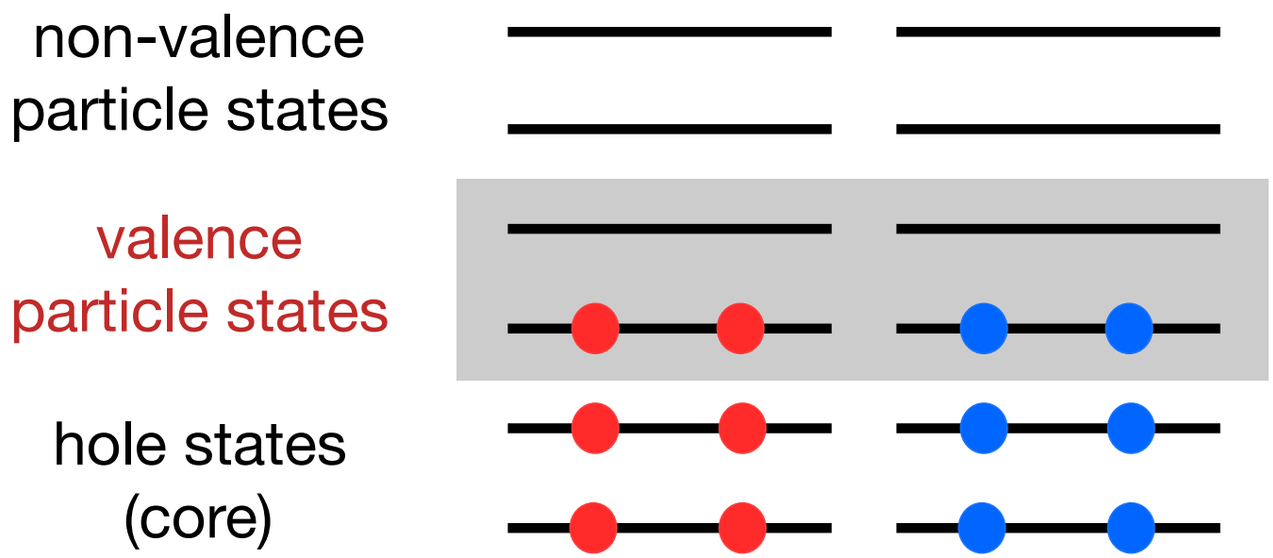




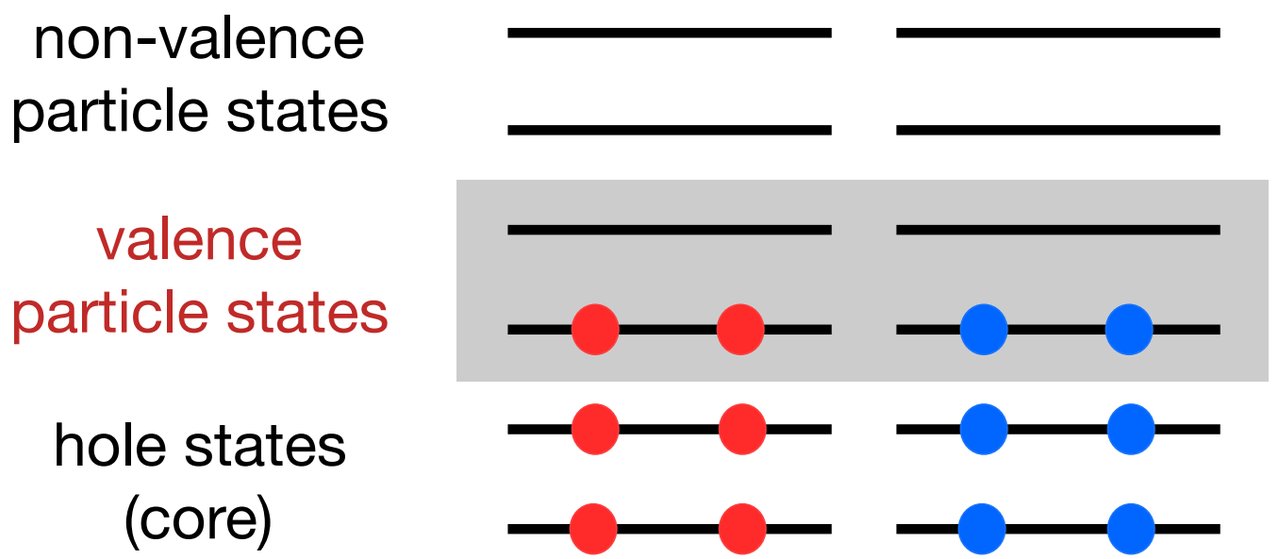
from: C. Yang, H. M. Aktulga, P. Maris, E. Ng, J. Vary, Proceedings of NTSE-2013

- **constructing and storing full *H* matrix is impossible**
- can exploit **matrix sparseness**, but problem is still very **hard**

Core and Valence Spaces



Core and Valence Spaces



- introduce an **inert core:** restrict states to the form

$$\left|\Psi_i\right\rangle = \left|\overline{\Psi}_i\right\rangle \otimes \left|\text{core}\right\rangle$$

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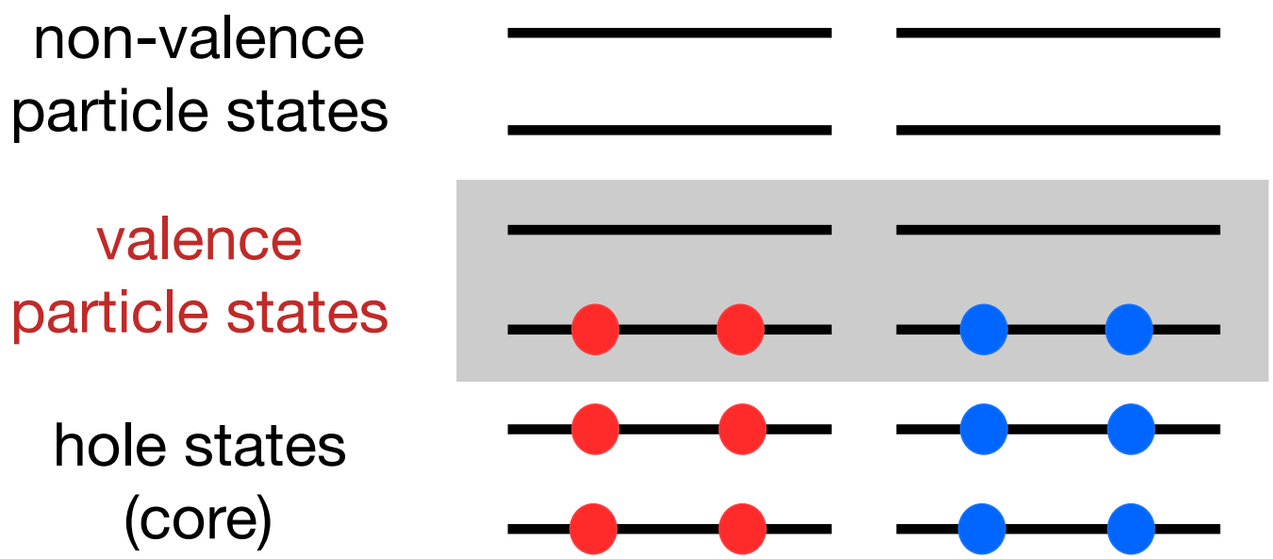

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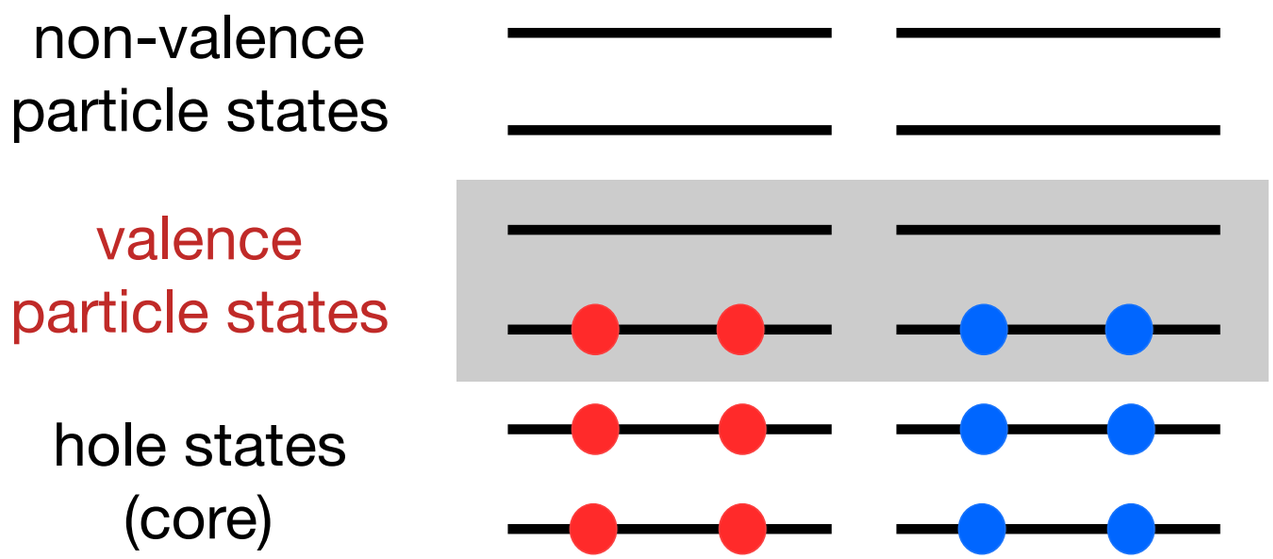

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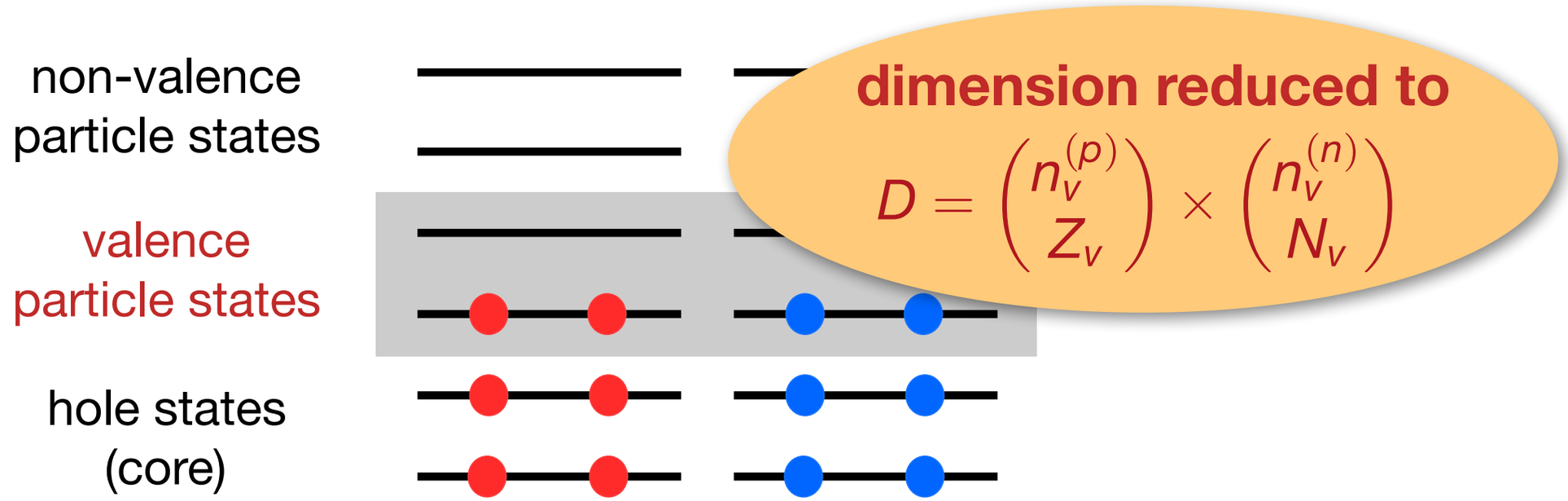

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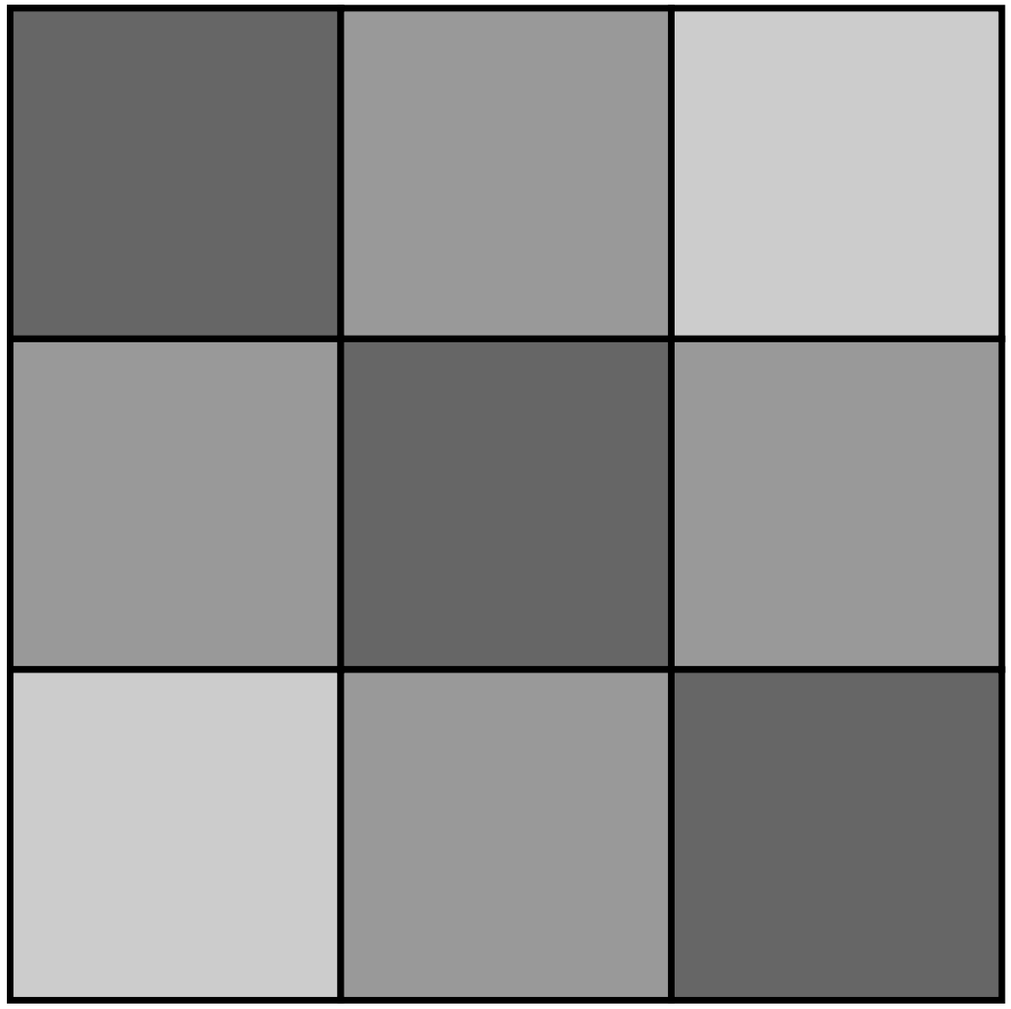
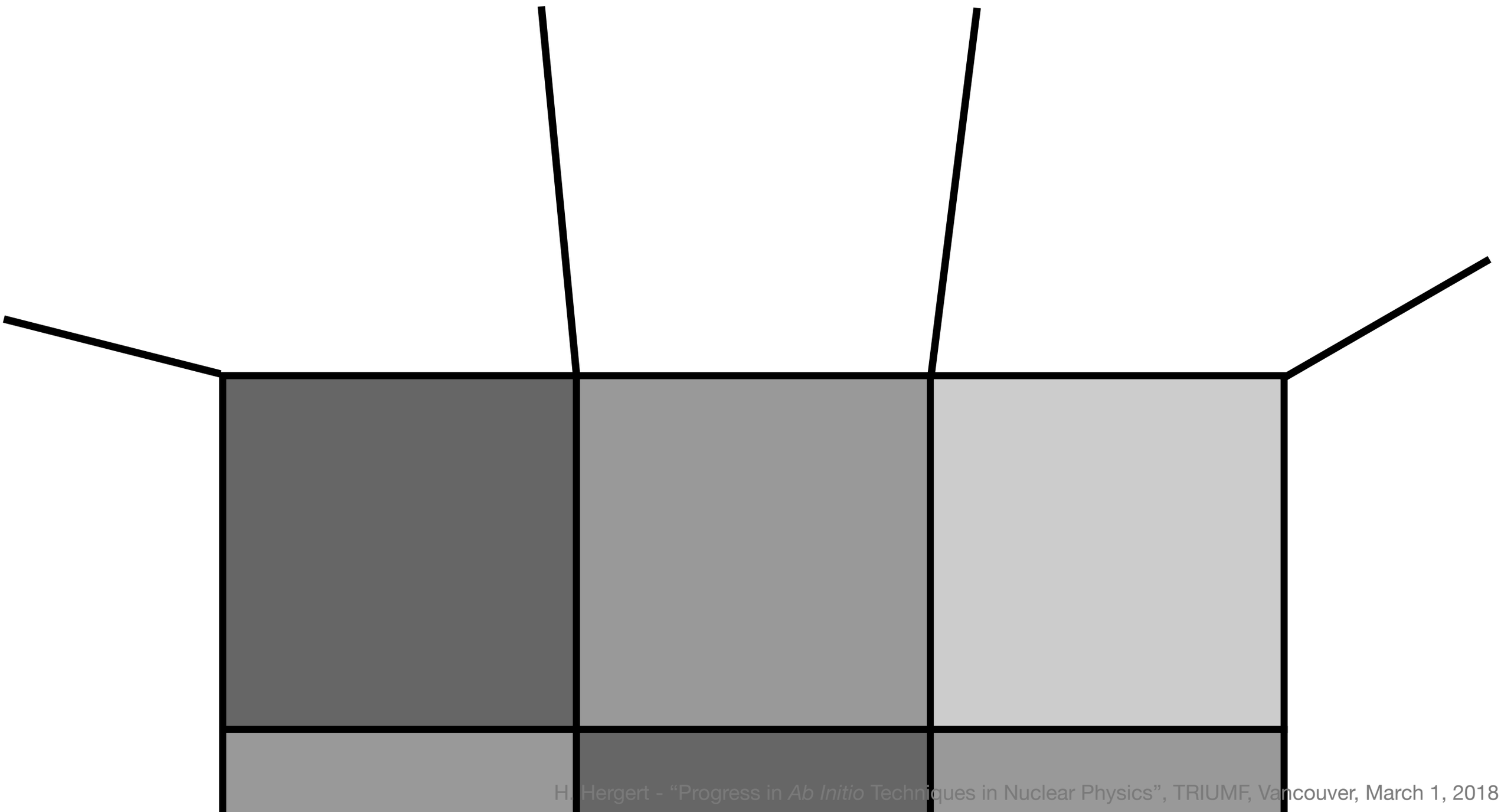
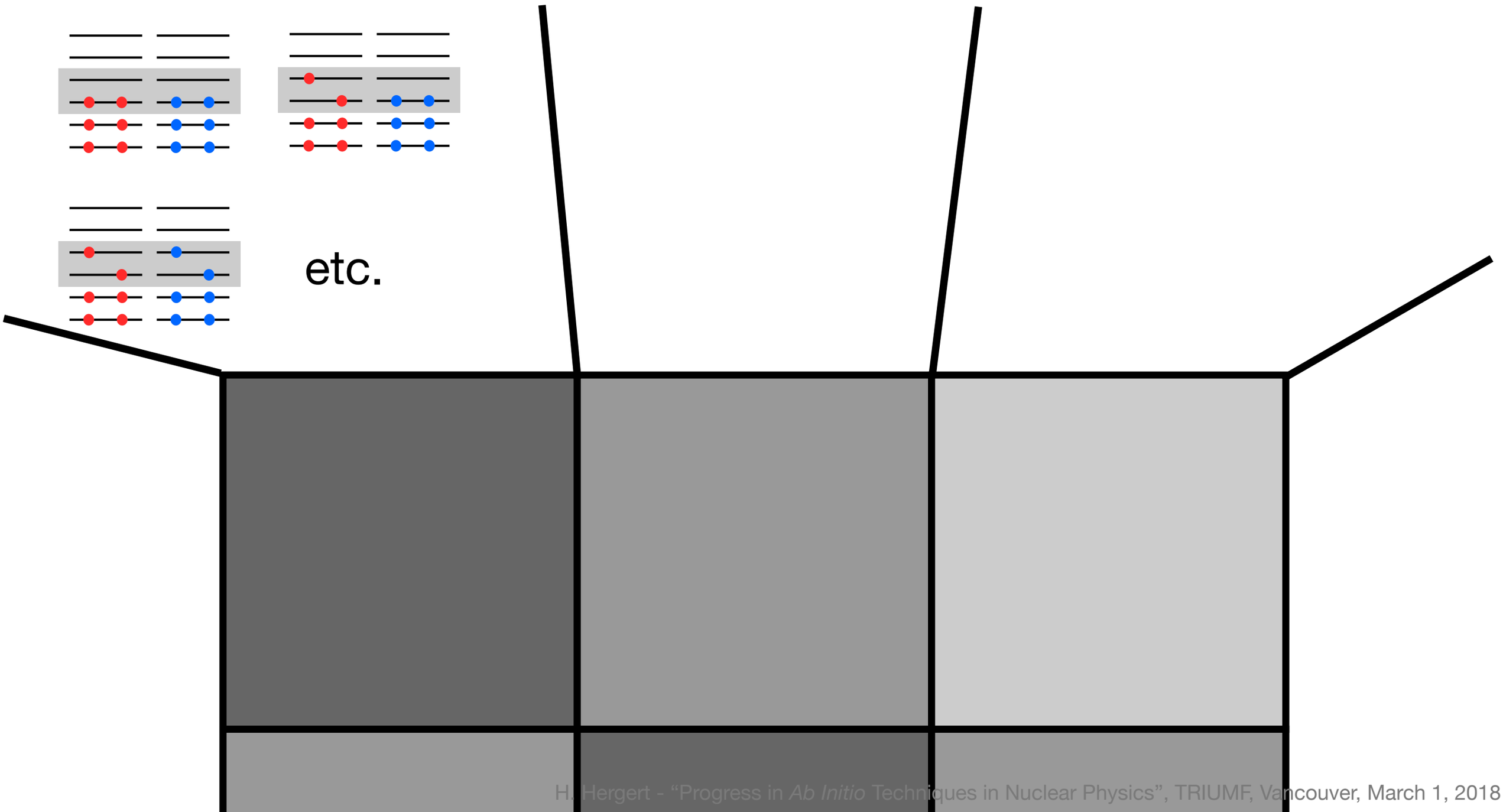
Effective Hamiltonian



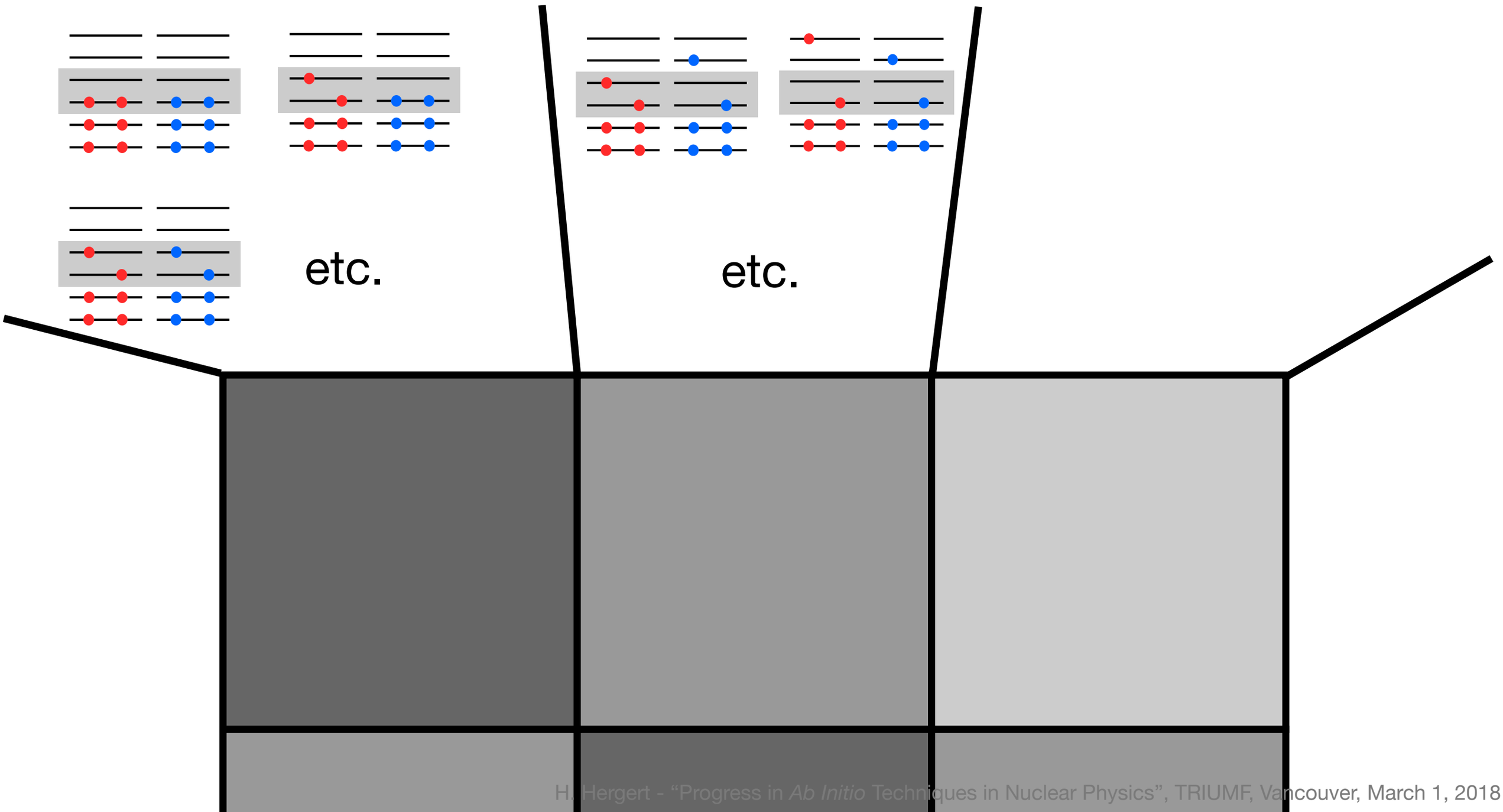
Effective Hamiltonian



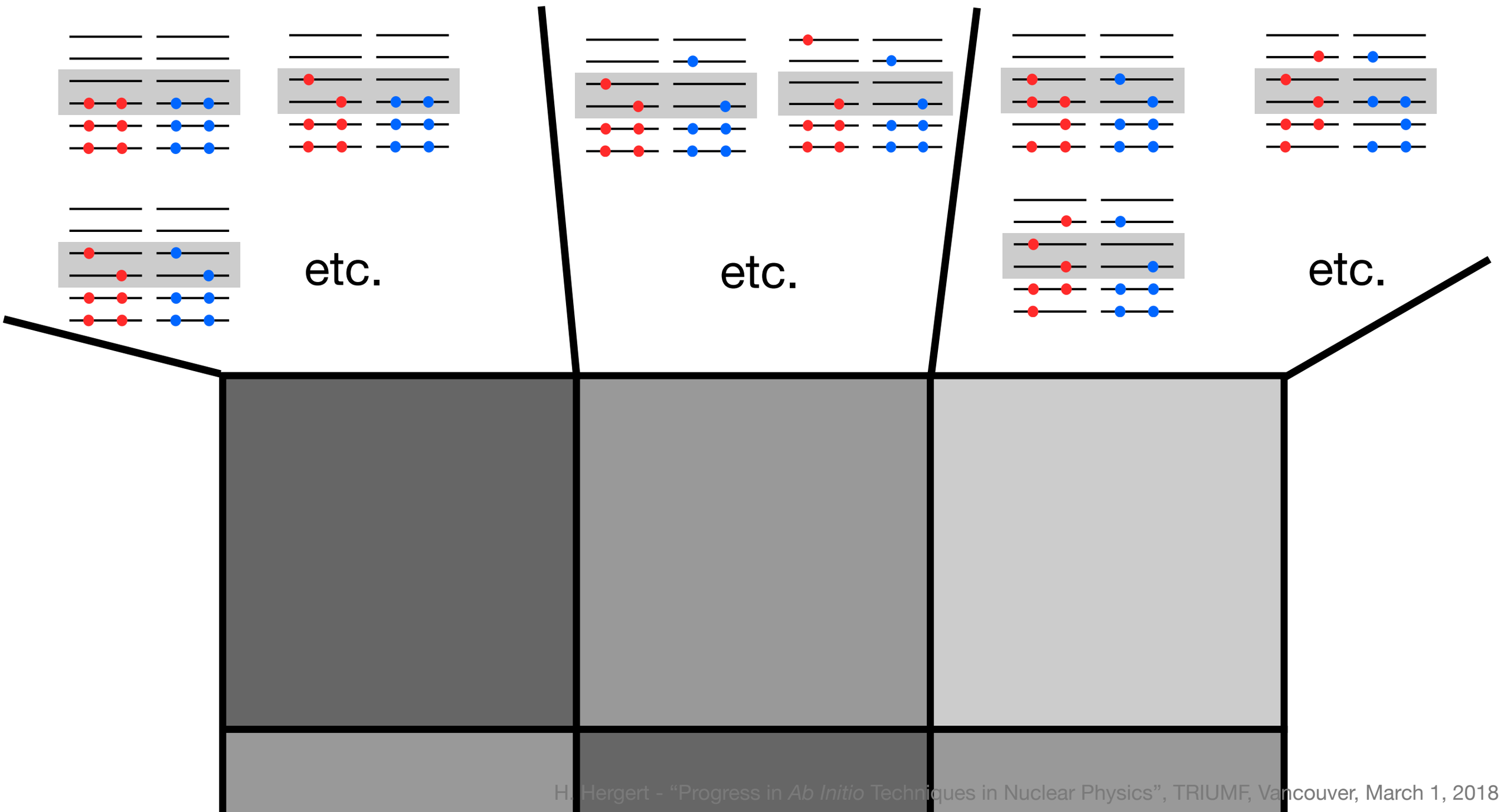
Effective Hamiltonian



Effective Hamiltonian

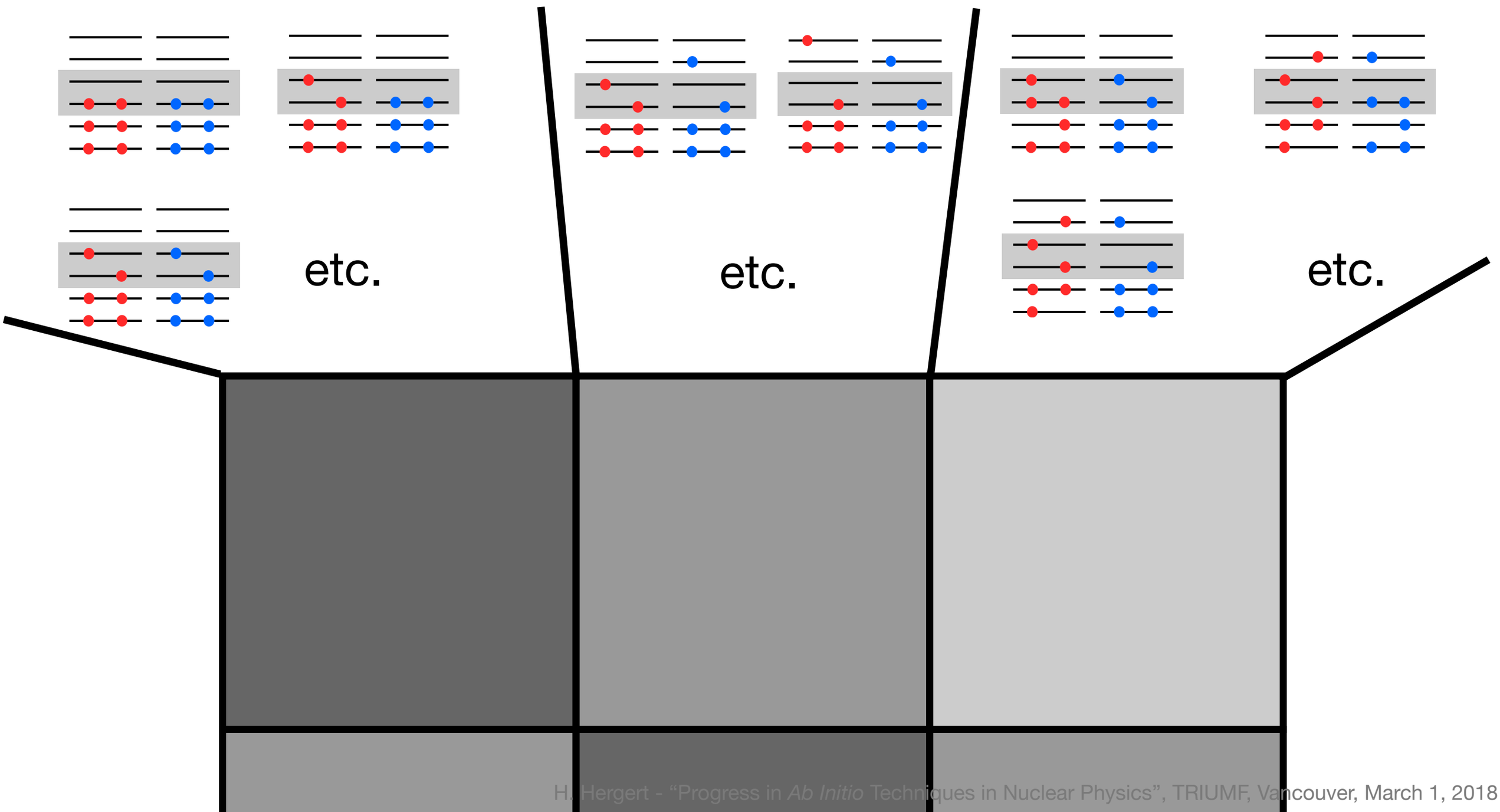


Effective Hamiltonian



Effective Hamiltonian

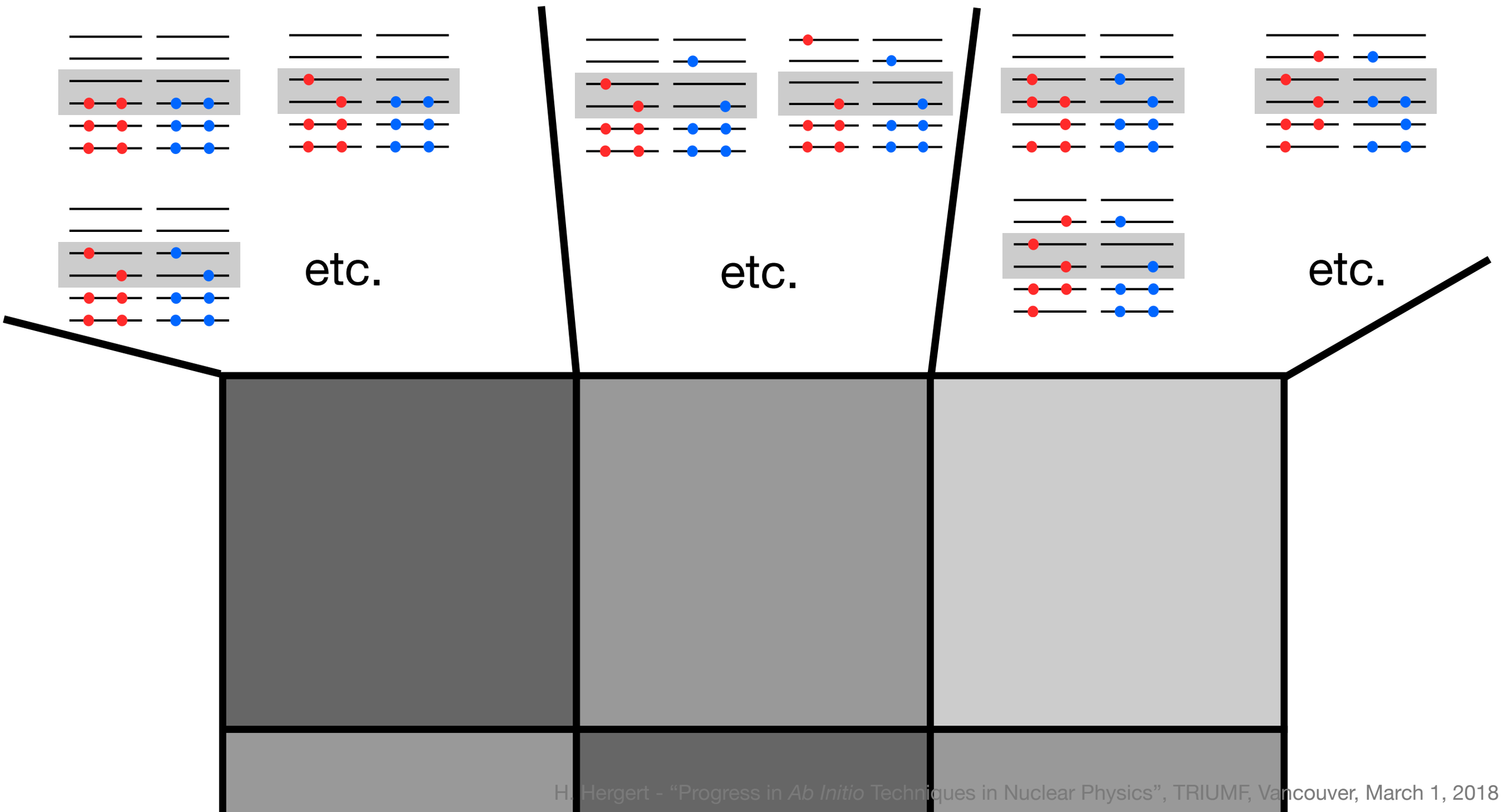
P space
(included configurations)



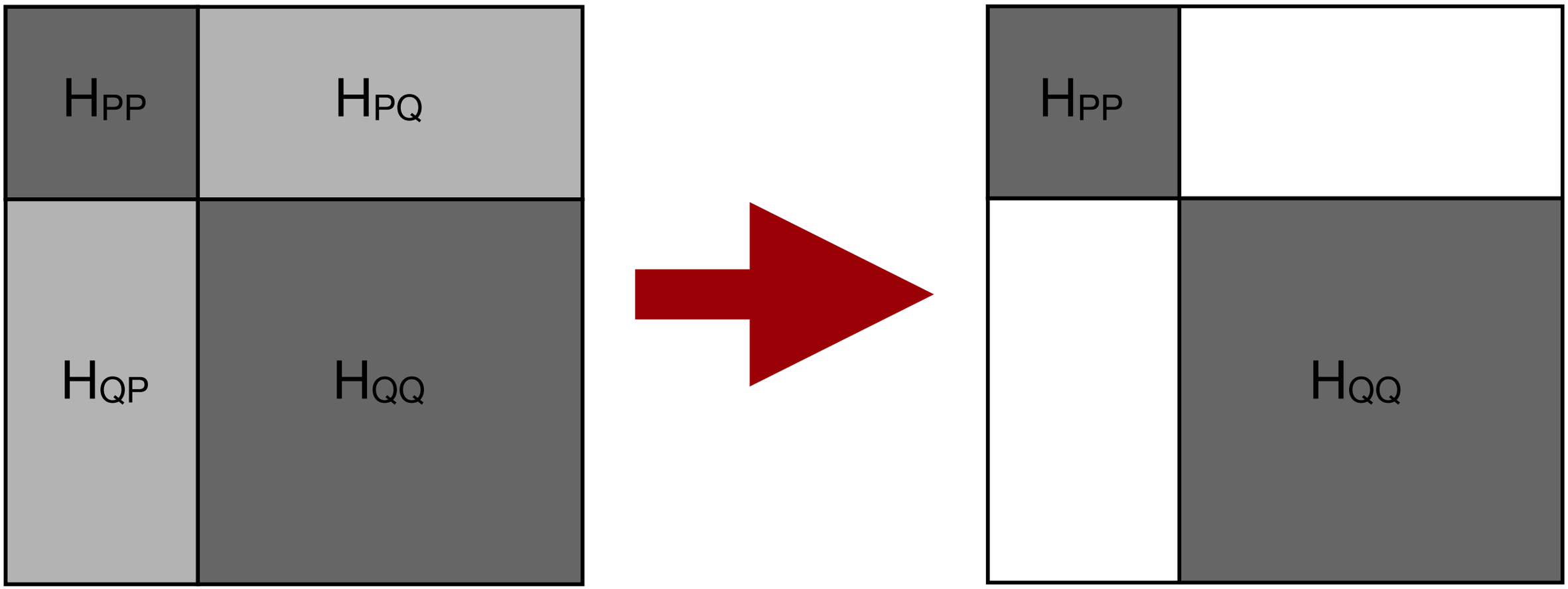
Effective Hamiltonian

P space
(included configurations)

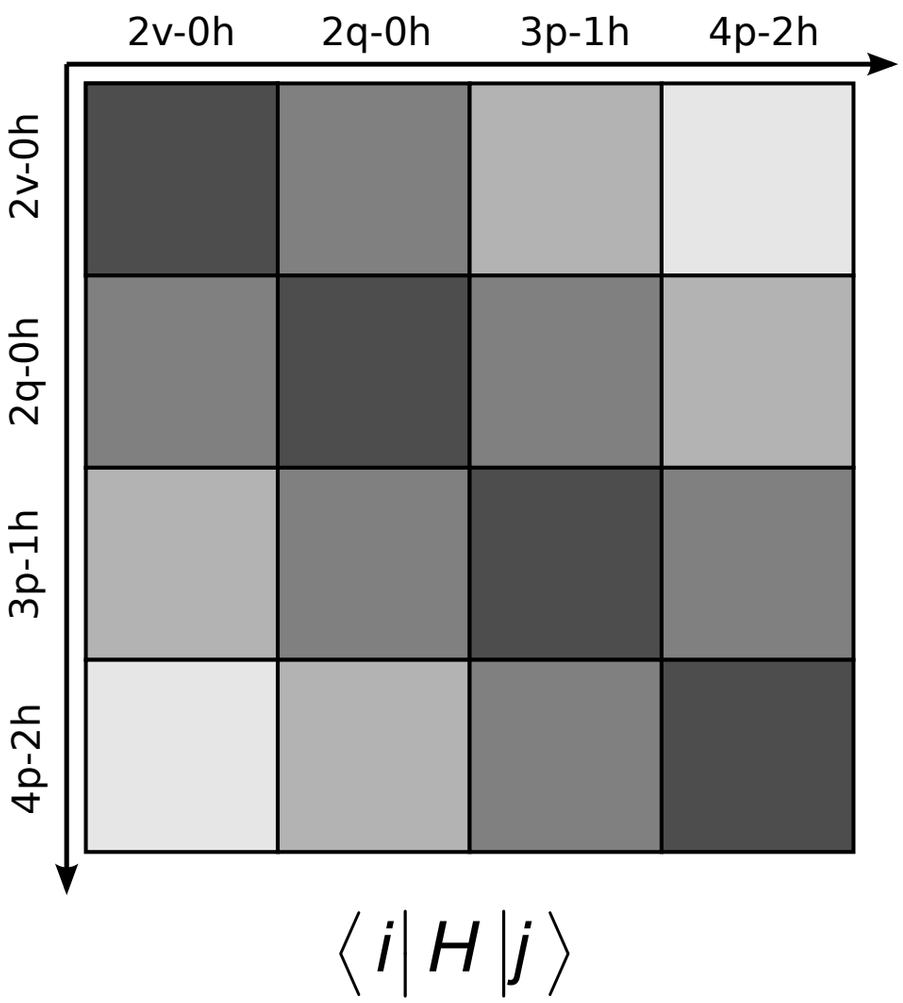
Q space
(excluded configurations)



Effective Hamiltonian



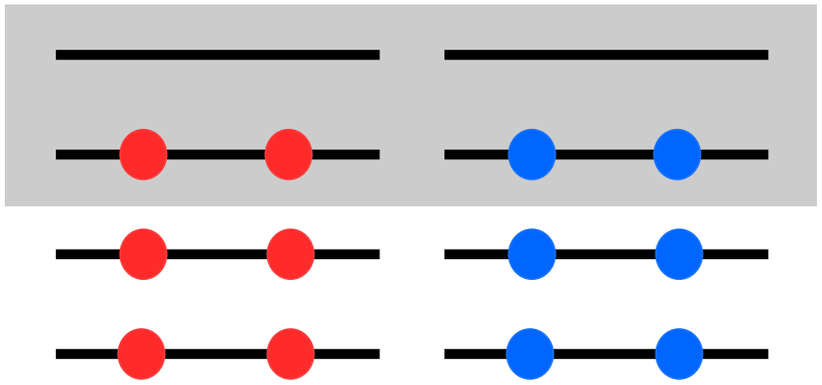
Valence Space Decoupling



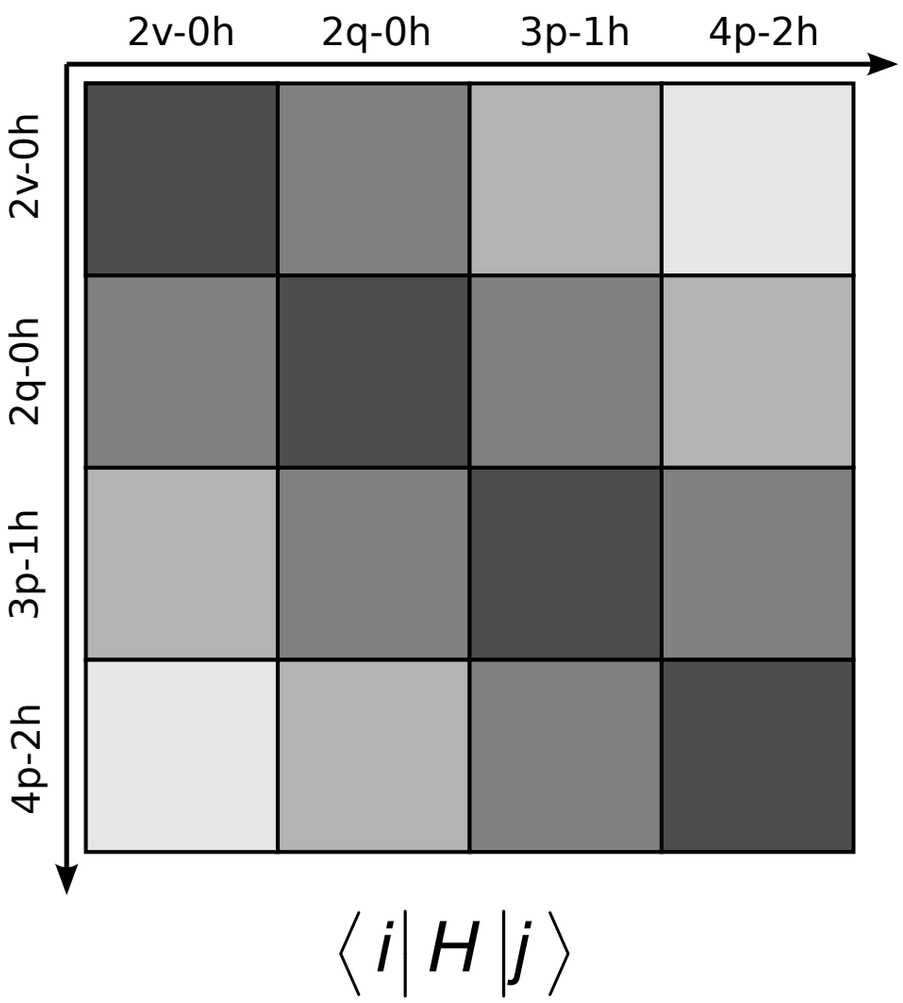
q: non-valence particle states

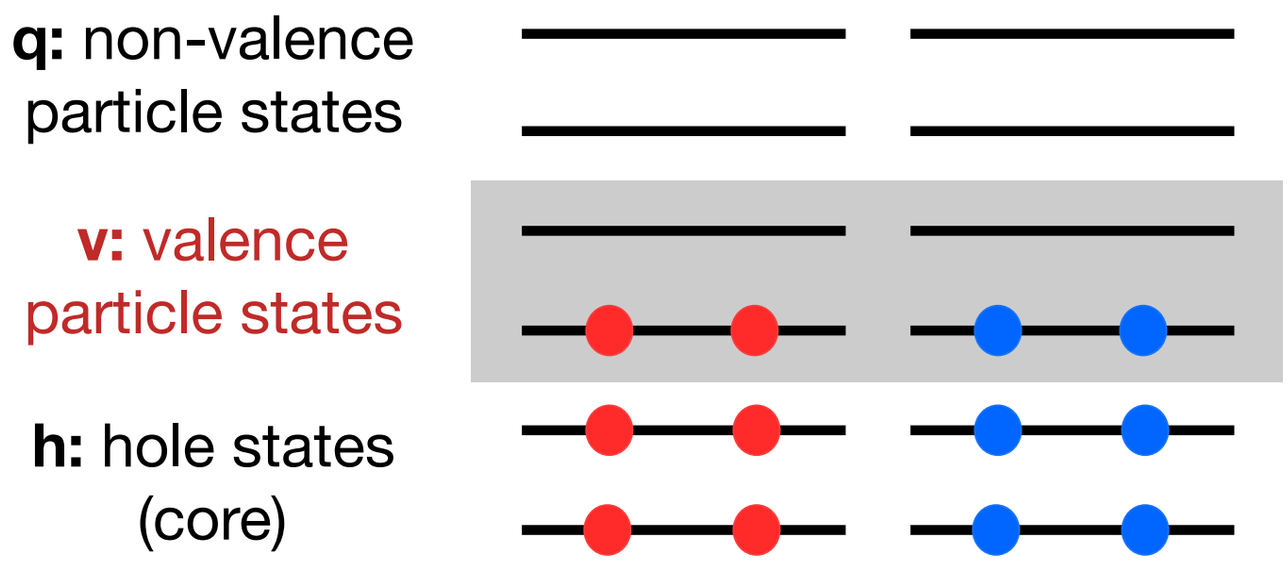
v: valence particle states

h: hole states (core)



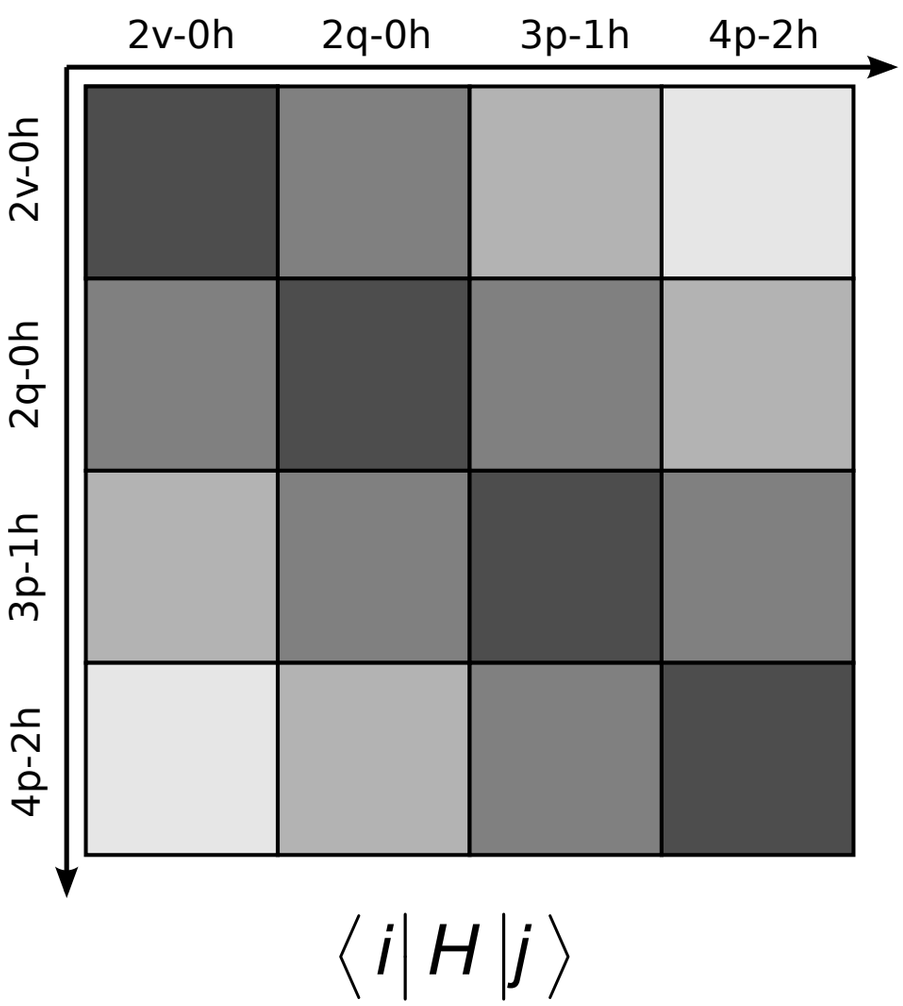
Valence Space Decoupling

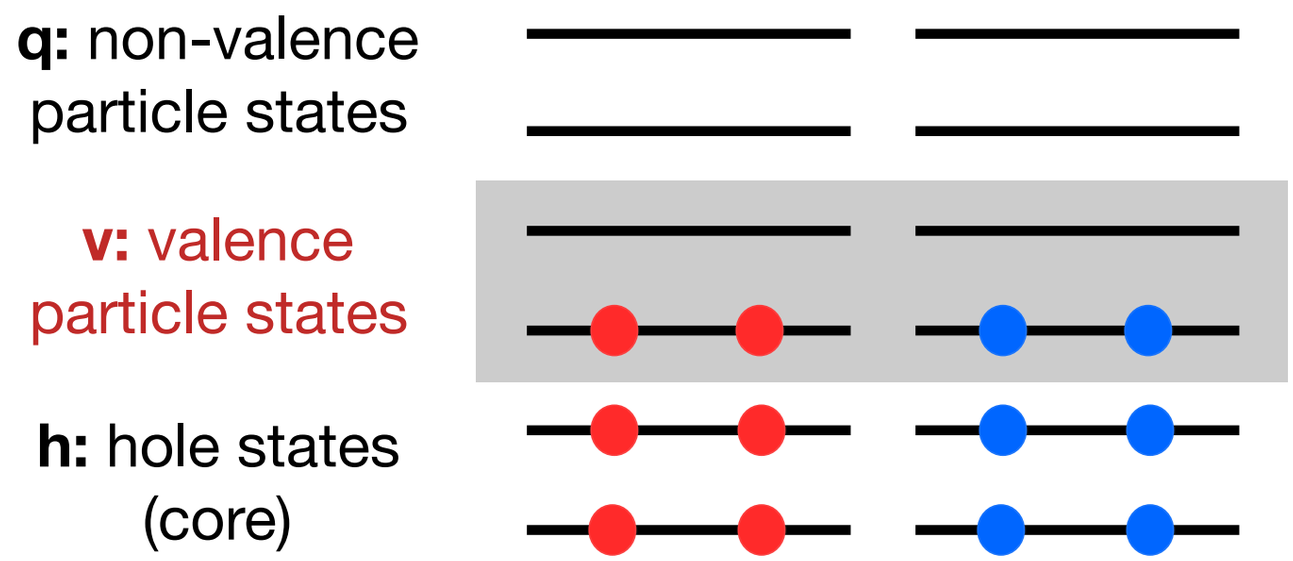




- NN (maybe 3N?) operators can only act on 2 (3) valence nucleons

Valence Space Decoupling





- NN (maybe 3N?) operators can only act on 2 (3) valence nucleons
- remaining core and valence particles are **spectators**