The In-Medium Similarity Renormalization Group: Applications and Perspectives

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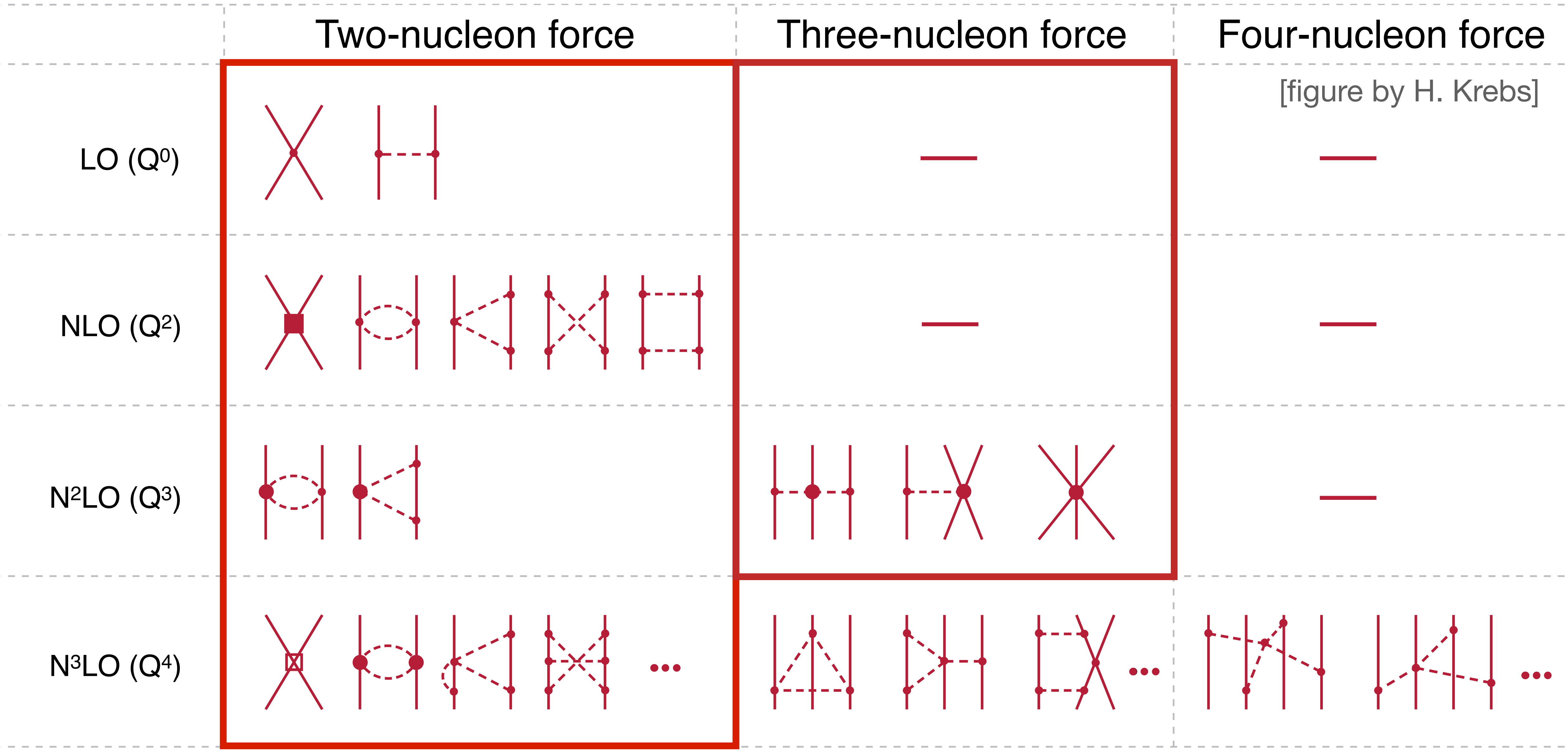
Interactions from Chiral EFT



- organization in powers $(Q/\Lambda_\chi)^\nu$ allows systematic improvement
- low-energy constants fit to NN, 3N data (future: from Lattice QCD (?))
- consistent NN, 3N, ... interactions & operators (**electroweak transitions!**)

The 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

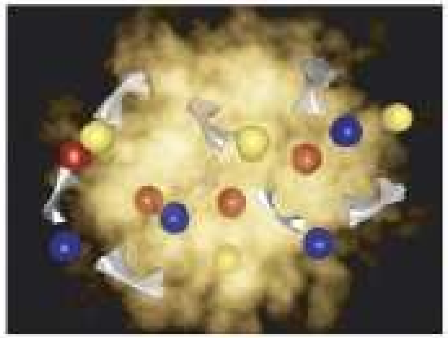
H. H. and R. Roth, Phys. Rev. C75 (2007), 051001

Scales of the Strong Interaction

momentum transfer (resolution)

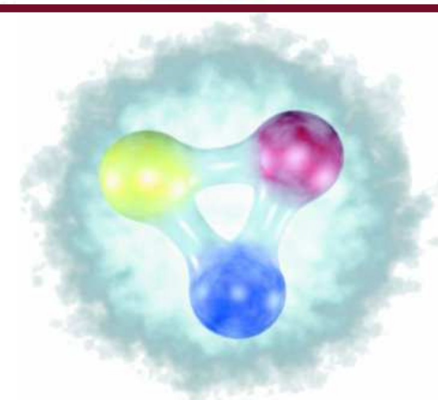
QCD

Chiral EFT

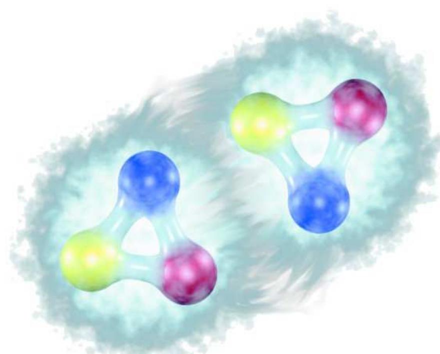


- quarks, gluons

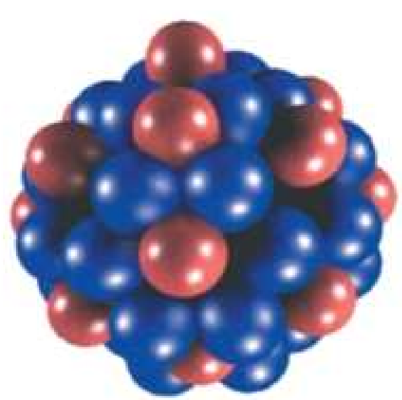
chiral symmetry



- pions, nucleons, ...
  - nuclear interactions
  - few-nucleon systems



(Which) Details necessary?



- finite nuclei
  - nuclear structure & reactions

Similarity Renormalization Group

Basic Idea

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

- flow equation for Hamiltonian $H(s) = U(s)HU^\dagger(s)$:

$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \eta(s) = \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s)$$

- choose $\eta(s)$ to achieve desired behavior, e.g.,

$$\eta(s) = \left[H_d(s), H_{od}(s)\right]$$

  to suppress (suitably defined) off-diagonal Hamiltonian

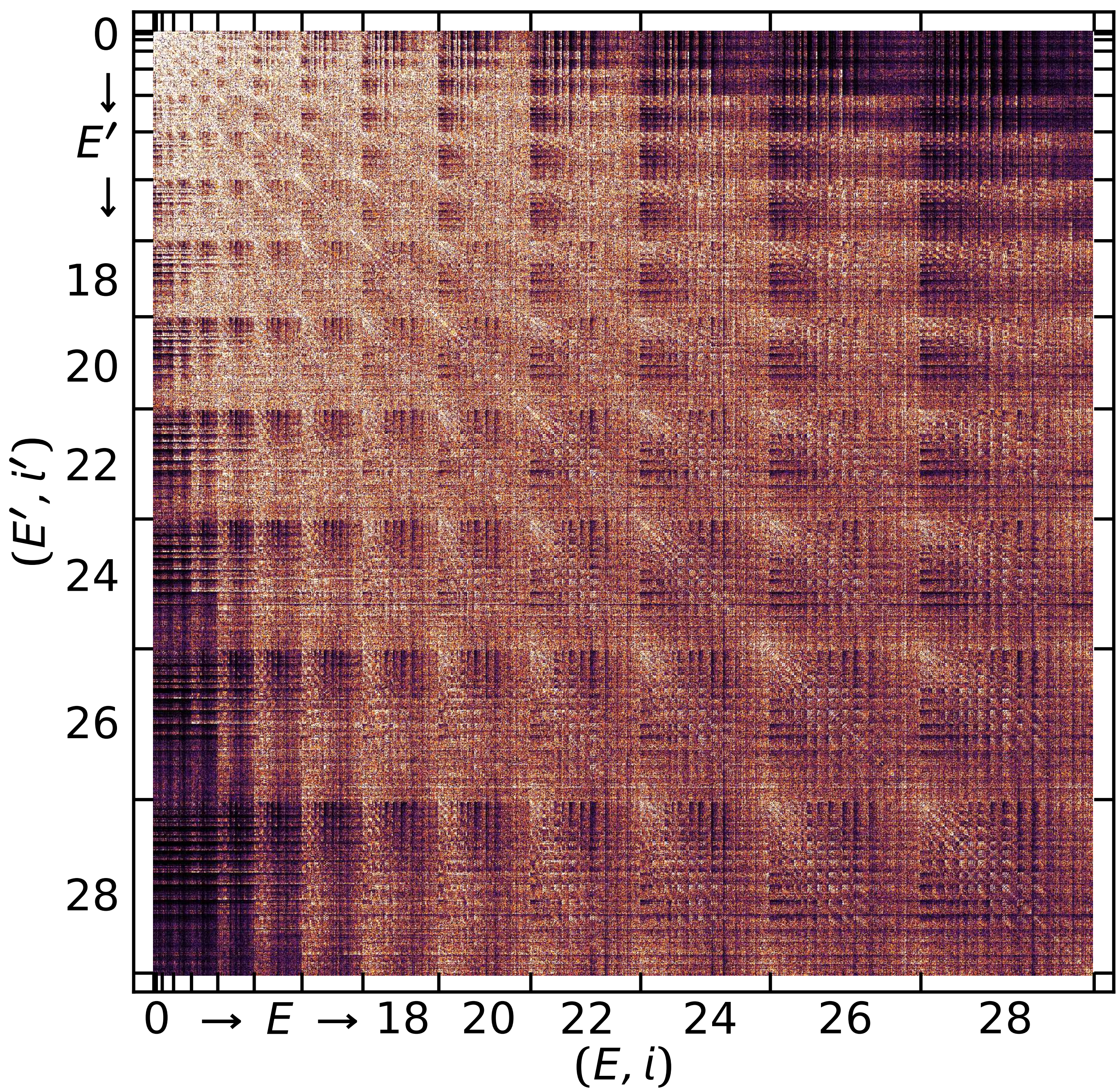
- consistent evolution for all observables of interest

SRG in Three-Body Space

[figures by R. Roth, A. Calci, J. Langhammer]

3B Jacobi-HO Matrix Elements

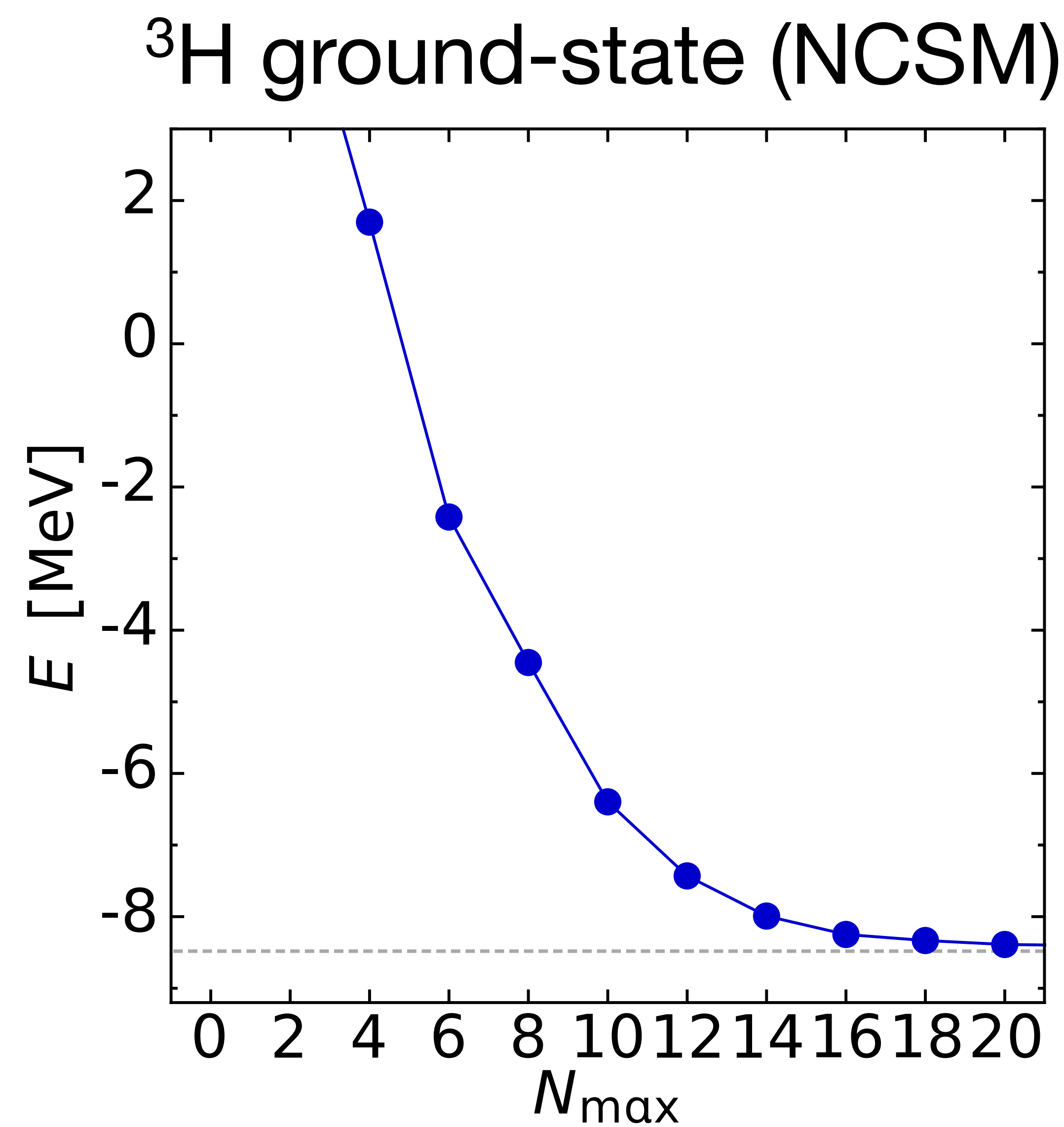
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



chiral NN + 3N

N^{3}LO + N^{2}LO (^{3}H fit)

^{3}H ground-state (NCSM)



SRG in Three-Body Space

[figures by R. Roth, A. Calci, J. Langhammer]

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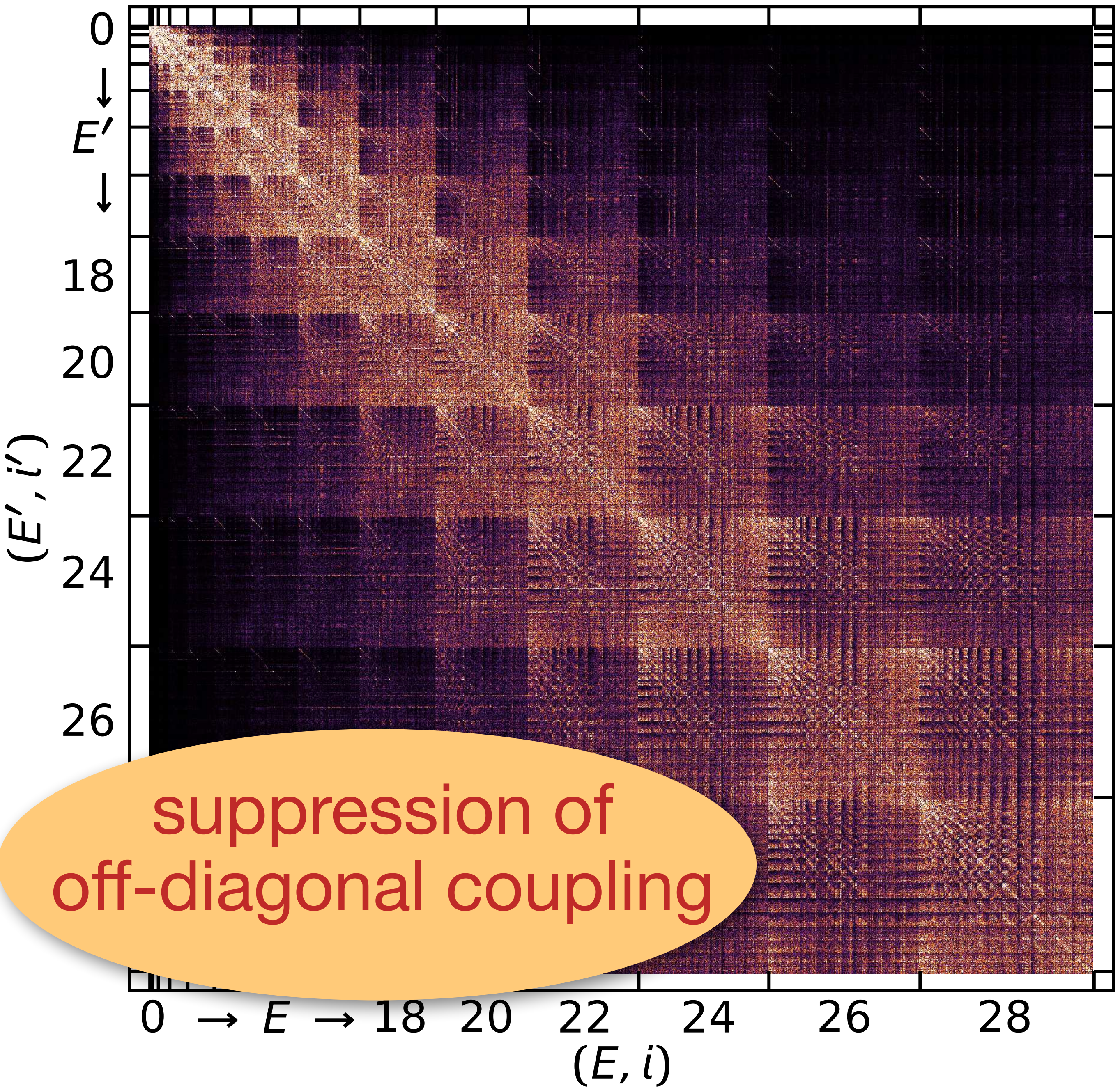
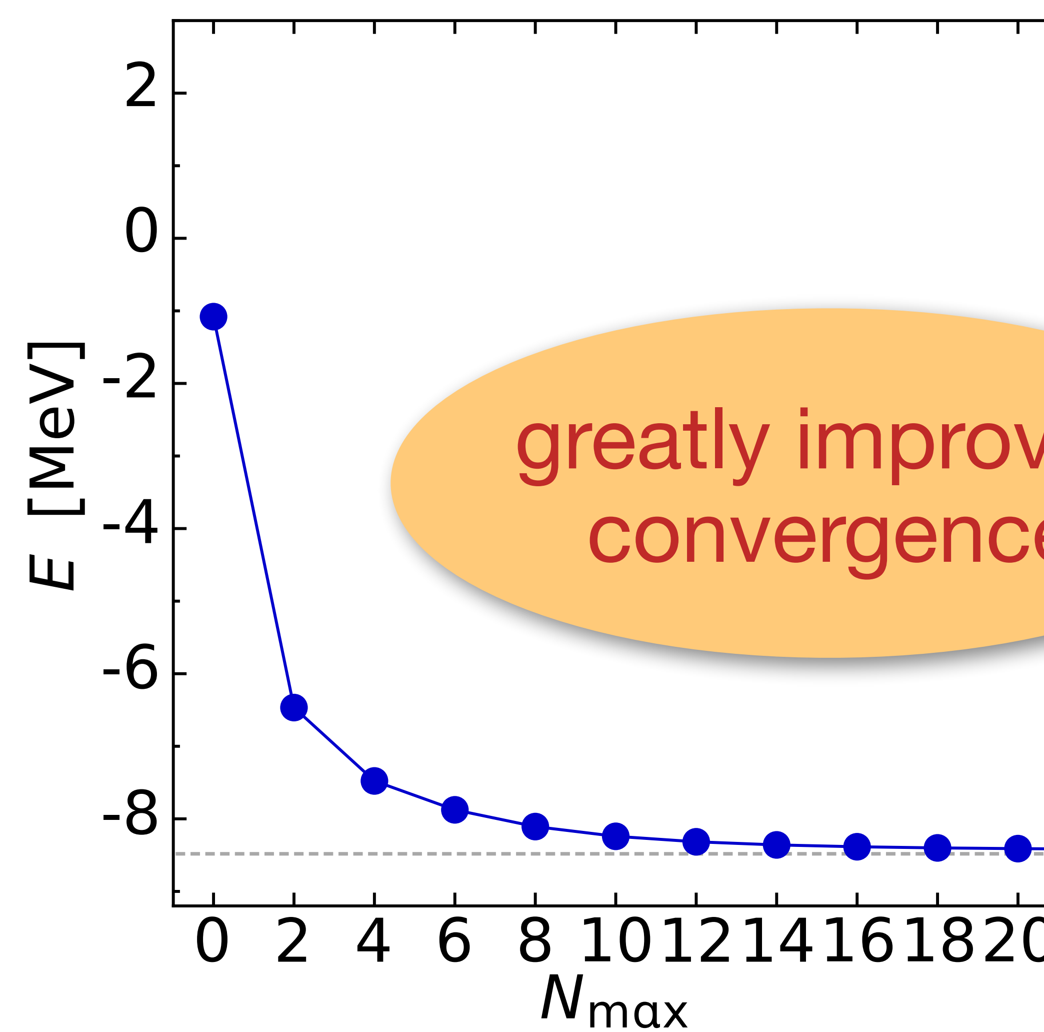


suppression of off-diagonal coupling

$\lambda = 1.33\ \mathrm{fm}^{-1}$

^{3}H ground-state (NCSM)



greatly improved convergence

(Multi-Reference) In-Medium SRG

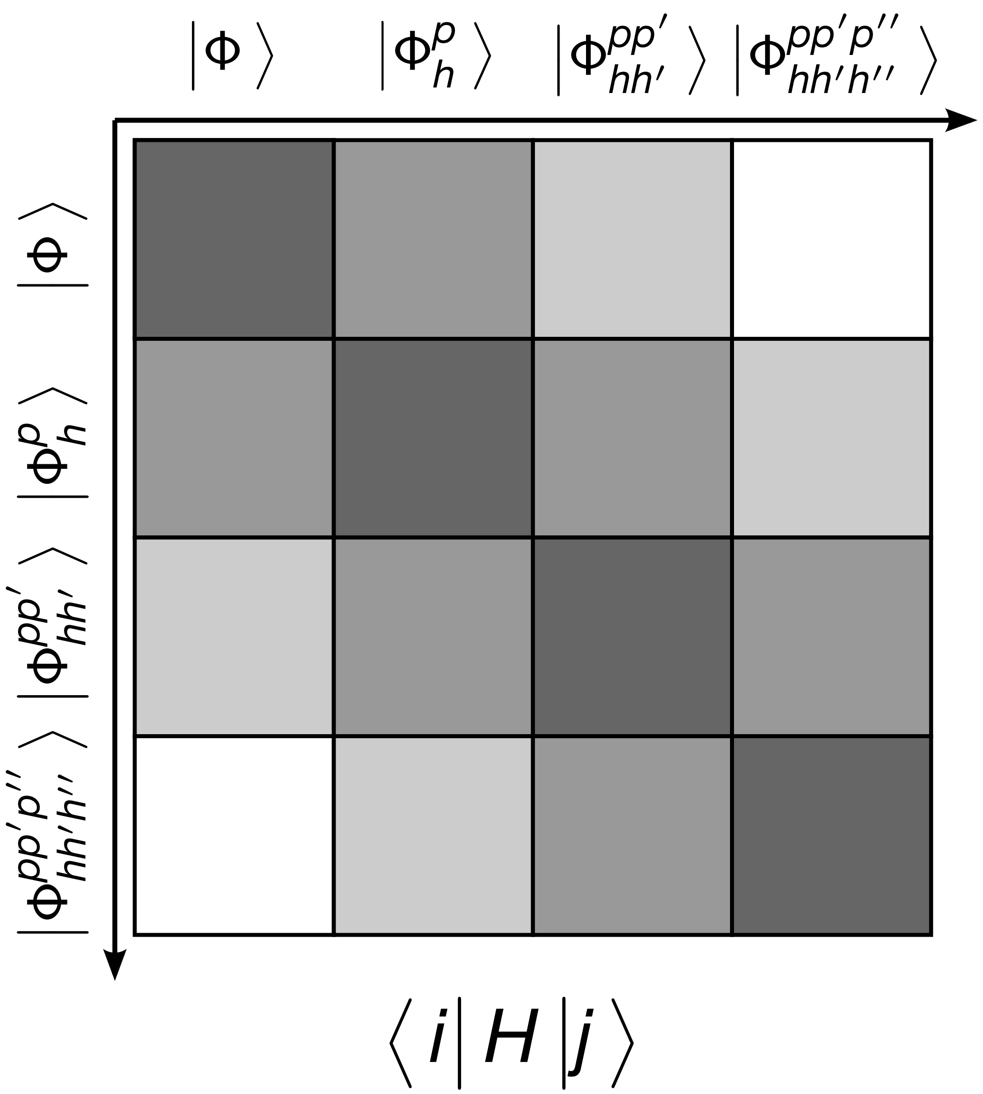
H. H., in preparation

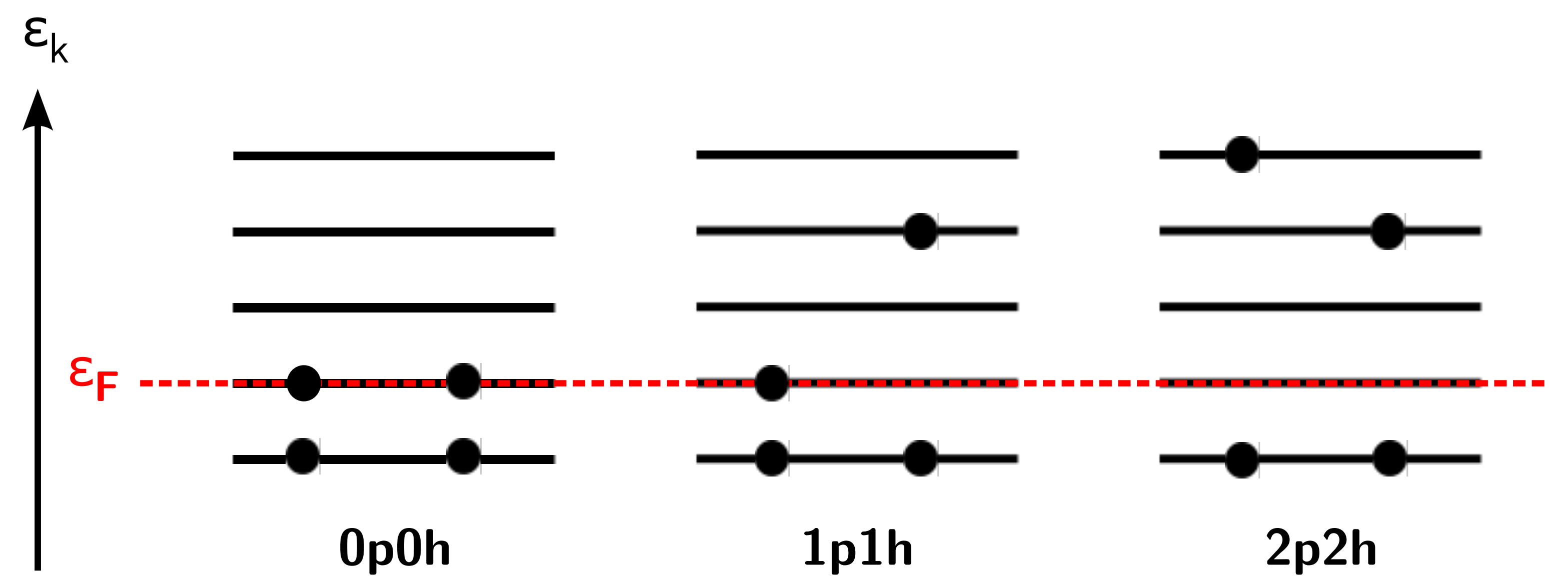
H. H., S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

H. H., S. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

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

Ground-State Decoupling

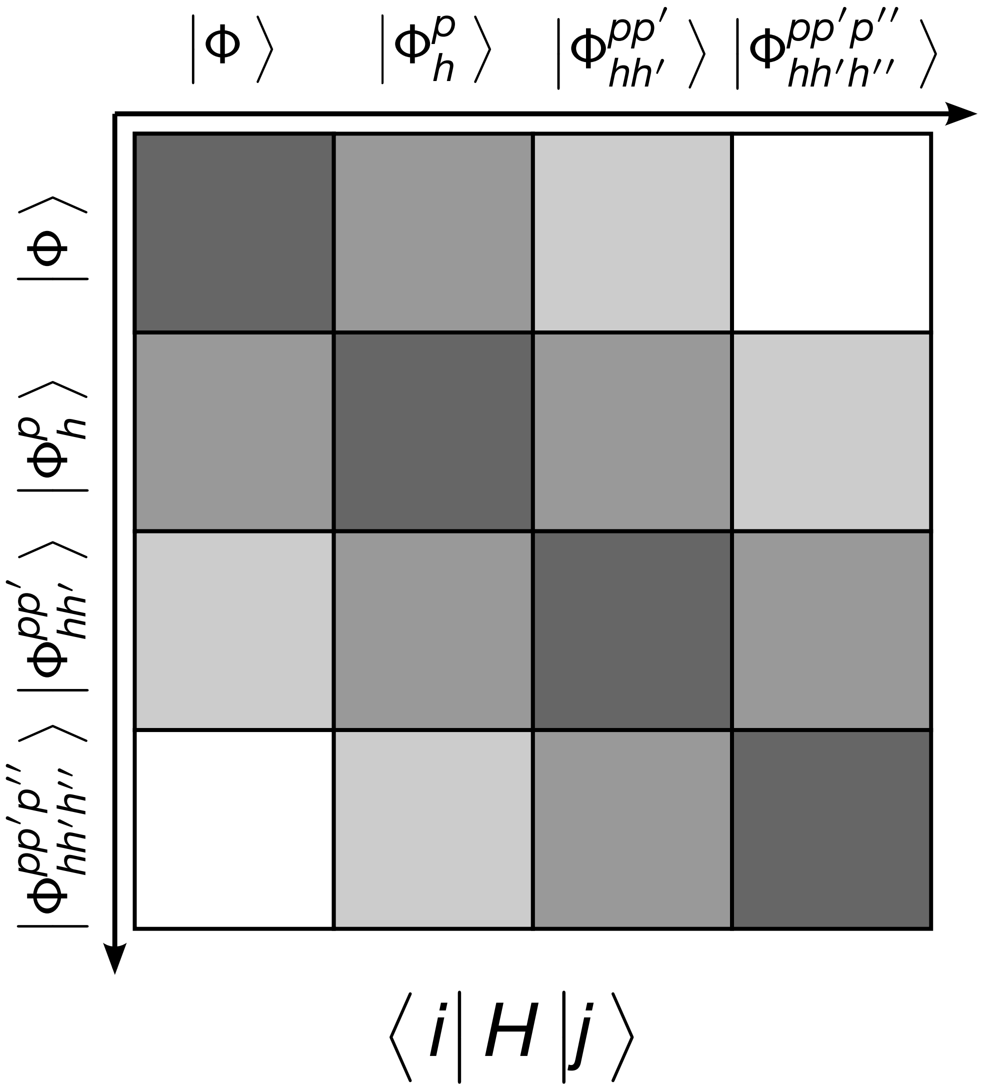




- reference state: **single Slater determinant**

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

Single-Reference Case



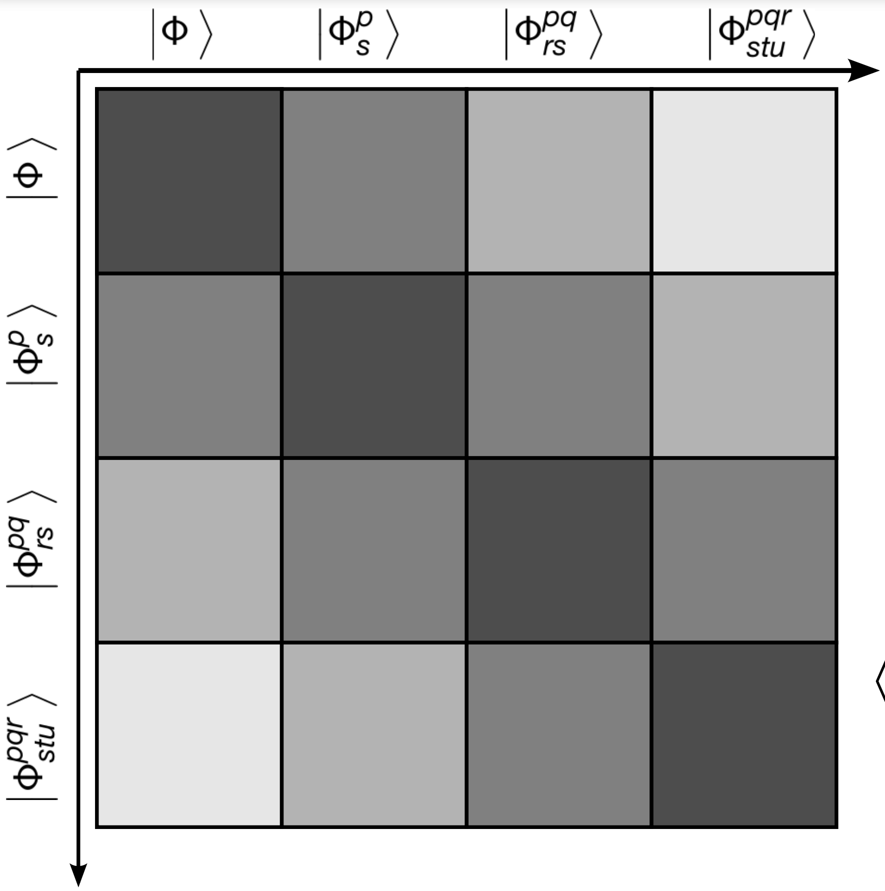
$$A^{i_1\dots i_N}_{j_1\dots j_N} \equiv a^{\dagger}_{i_1}\dots a^{\dagger}_{i_N} a_{j_N}\dots a_{j_1}$$

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

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

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

Multi-Reference Case



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

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

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

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

$$\rho^{kl}_{mn} = \lambda^{kl}_{mn} + \lambda^{k}_{m}\lambda^{l}_{n} - \lambda^{k}_{n}\lambda^{l}_{m}$$

$$\rho^{ijk}_{lmn} = \lambda^{ijk}_{lmn} + \lambda^{i}_{l}\lambda^{jk}_{mn} + \lambda^{i}_{l}\lambda^{j}_{m}\lambda^{k}_{n} + \text{permutations}$$

$$\ldots$$

MR-IM-SRG References States

available

- **number-projected Hartree-Fock Bogoliubov** vacua:

$$\left|\Phi_{ZN}\right\rangle = \frac{1}{(2\pi)^2}\int d\phi_p \int d\phi_n\, e^{i\phi_p(\hat{Z}-Z)} e^{i\phi_n(\hat{N}-N)} \left|\Phi\right\rangle$$

- small-scale (e.g., $0\hbar\Omega$, $2\hbar\Omega$) **No-Core Shell Model**:

$$\left|\Phi\right\rangle = \sum_{N=0}^{N_{\max}} \sum_{i=1}^{\dim(N)} C_i^{(N)} \left|\Phi_i^{(N)}\right\rangle$$

future

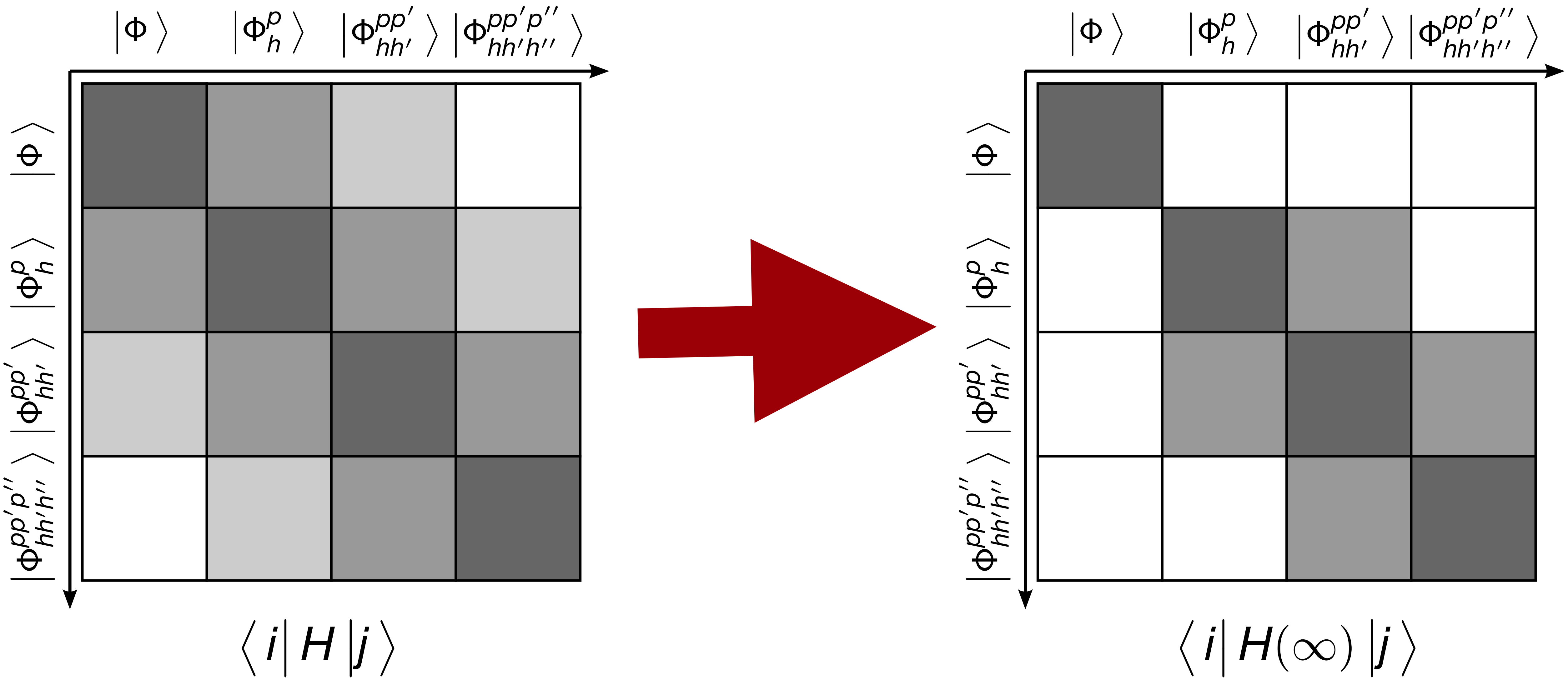
- **Generator Coordinate Method** (w/projections):

$$\left|\Phi\right\rangle = \int dq\, f(q)\, P_{J=0M=0} P_Z P_N \left|q\right\rangle$$

- Density Matrix Renormalization Group, Te... States, …

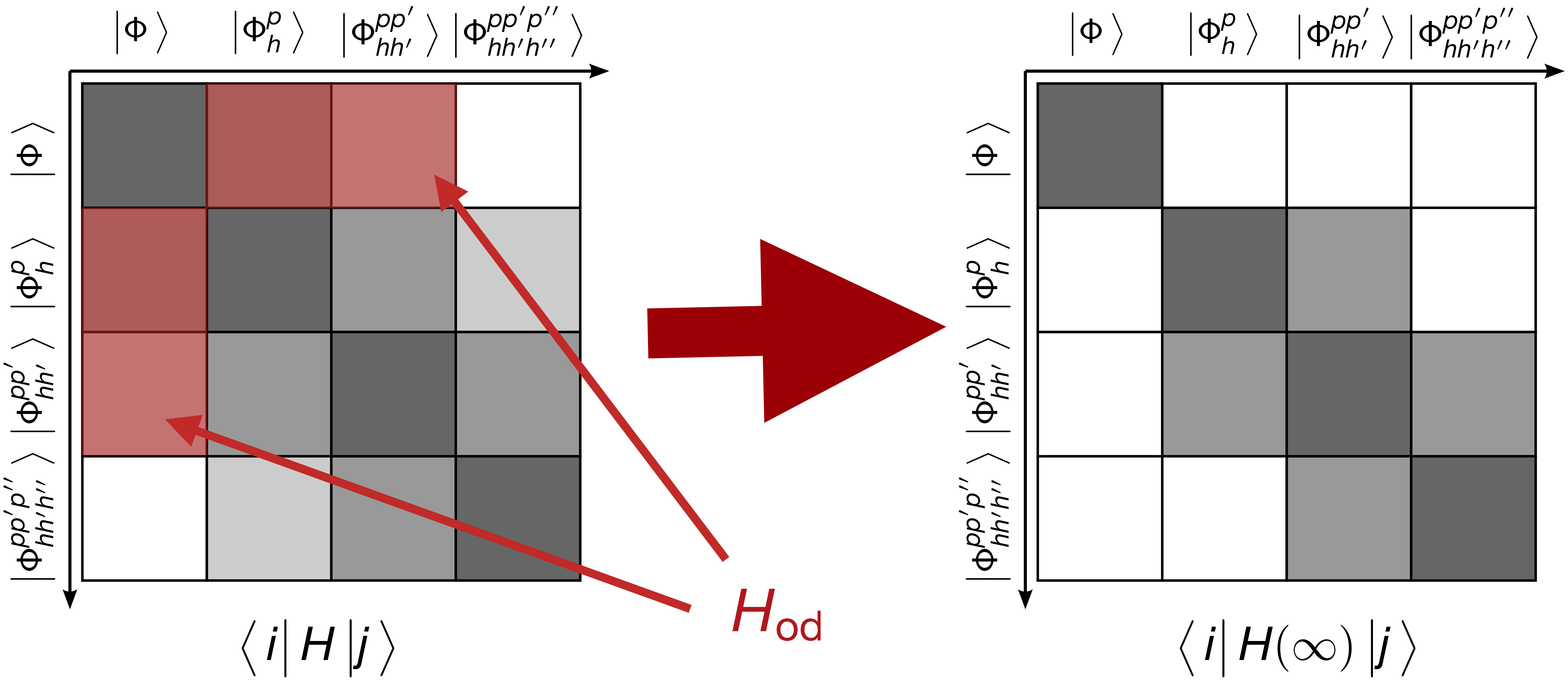
complement particle-hole type correlations

Decoupling in A-Body Space



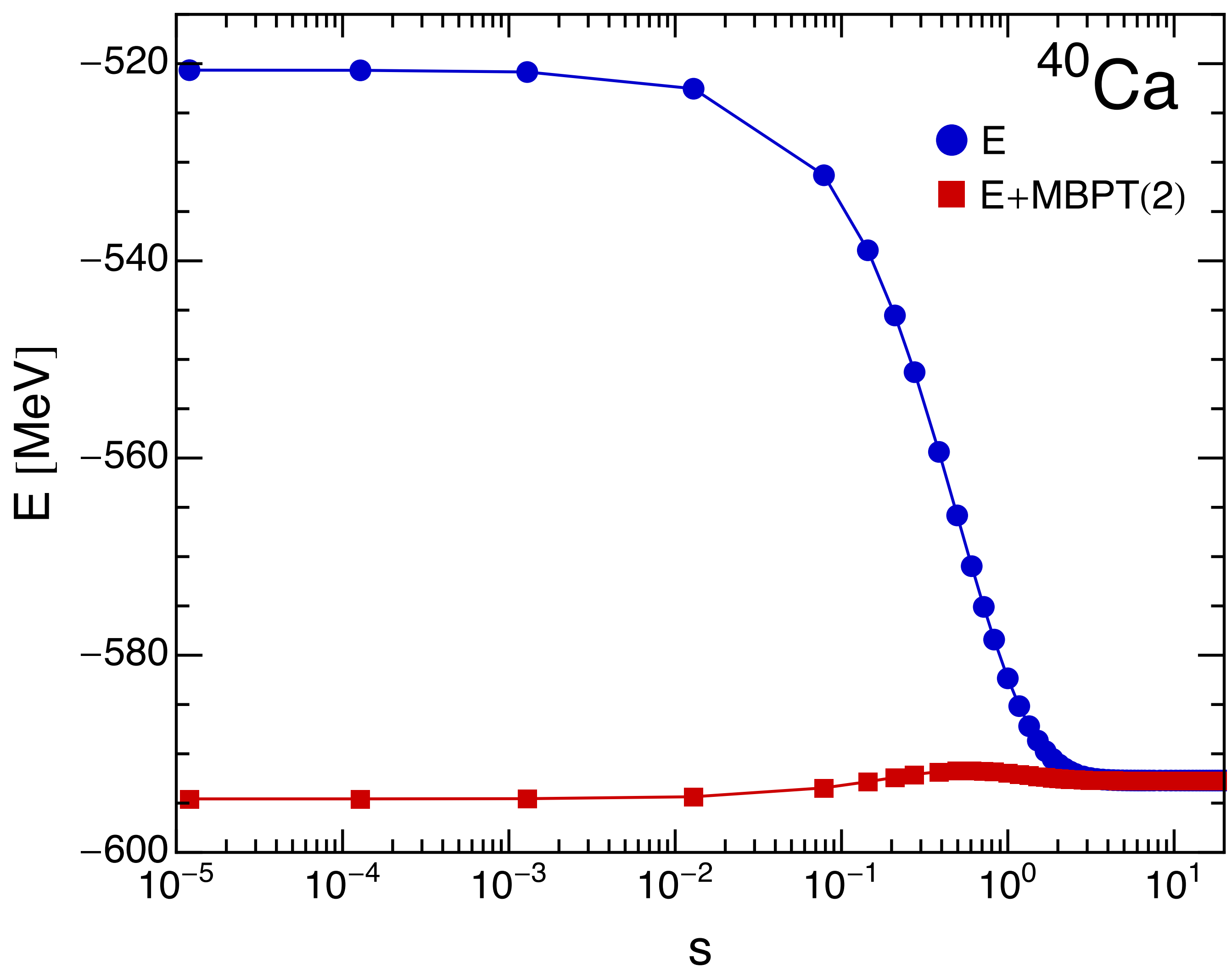
aim: decouple reference state $|\Phi\rangle$
from excitations

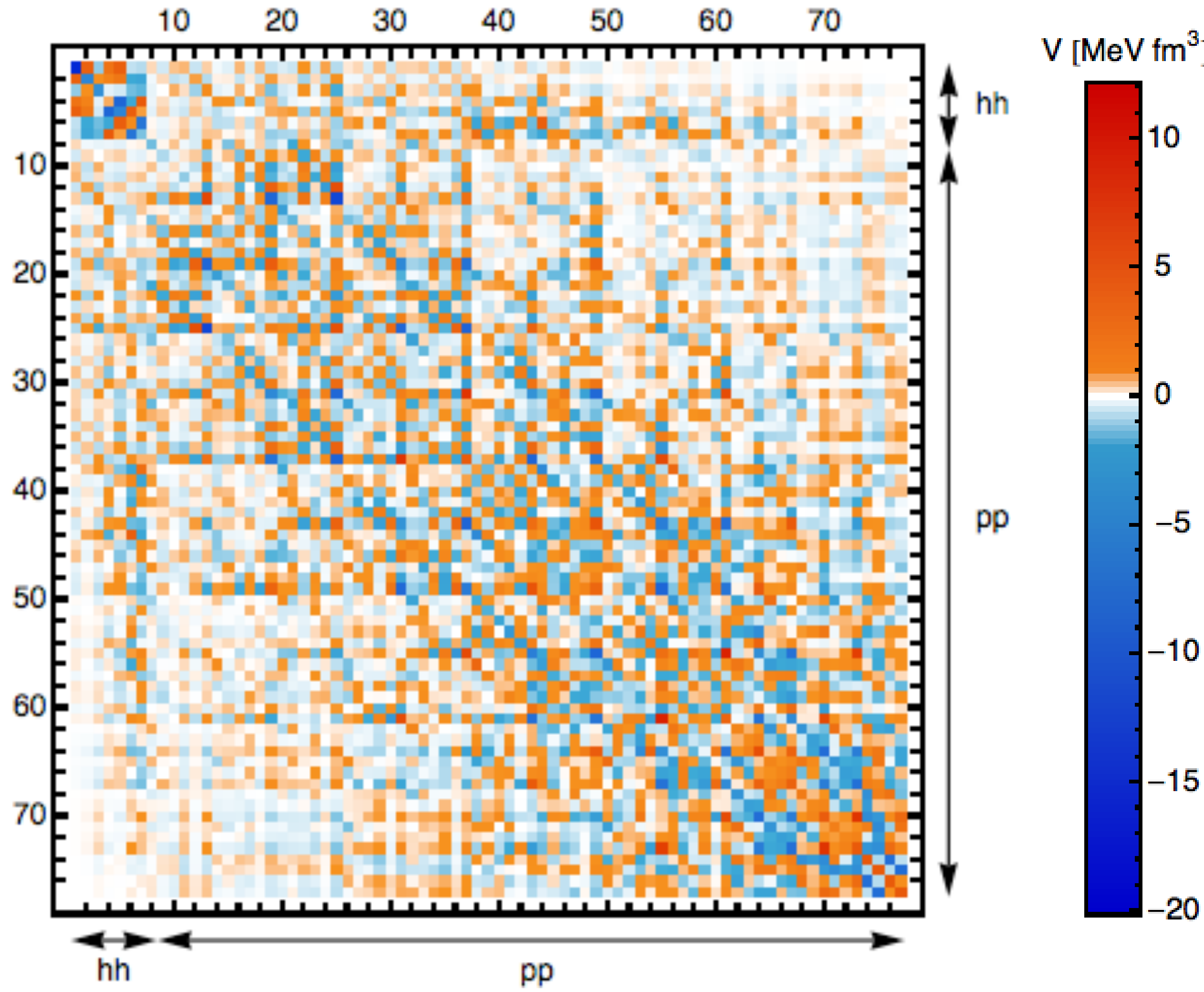
Flow Equation



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

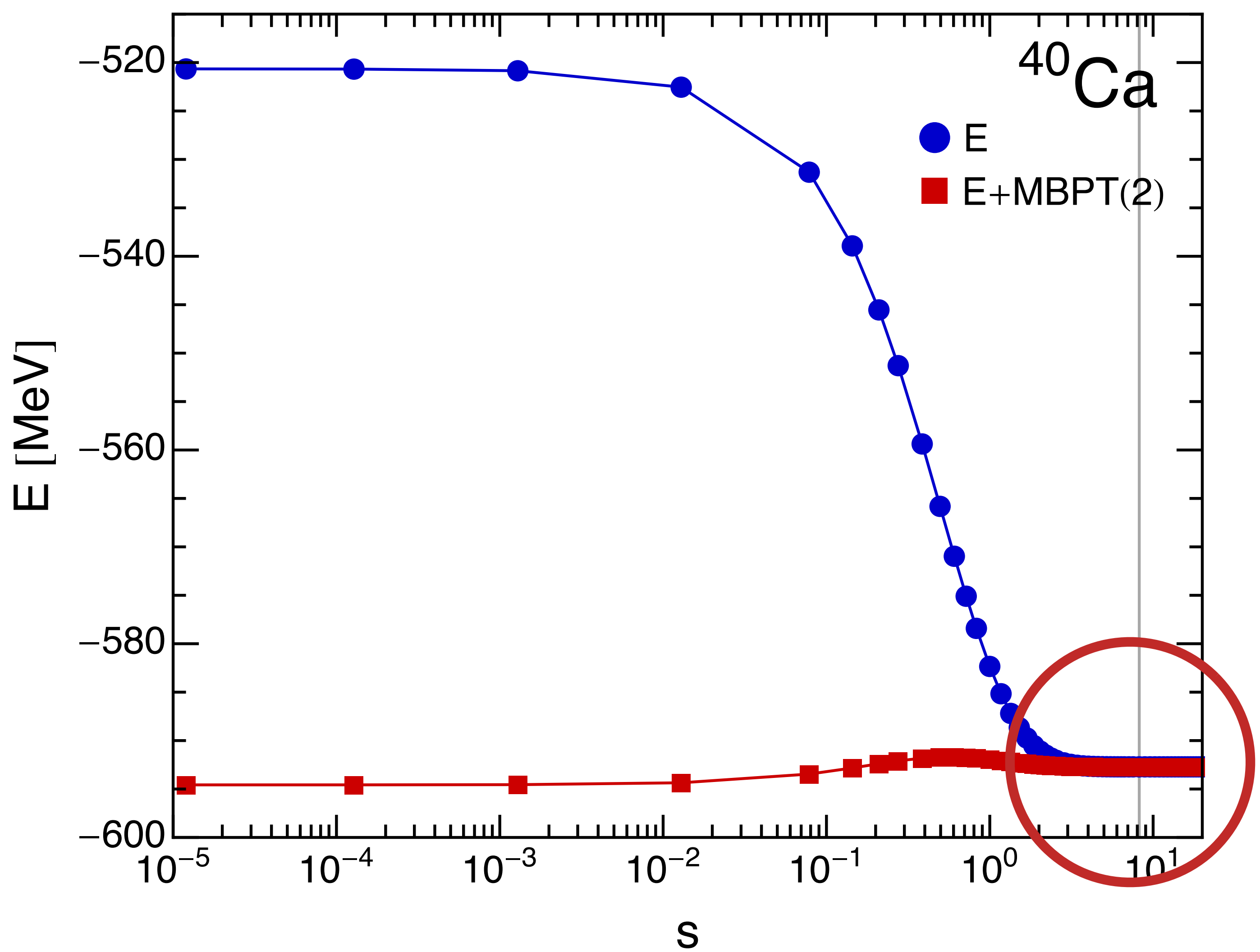
Decoupling

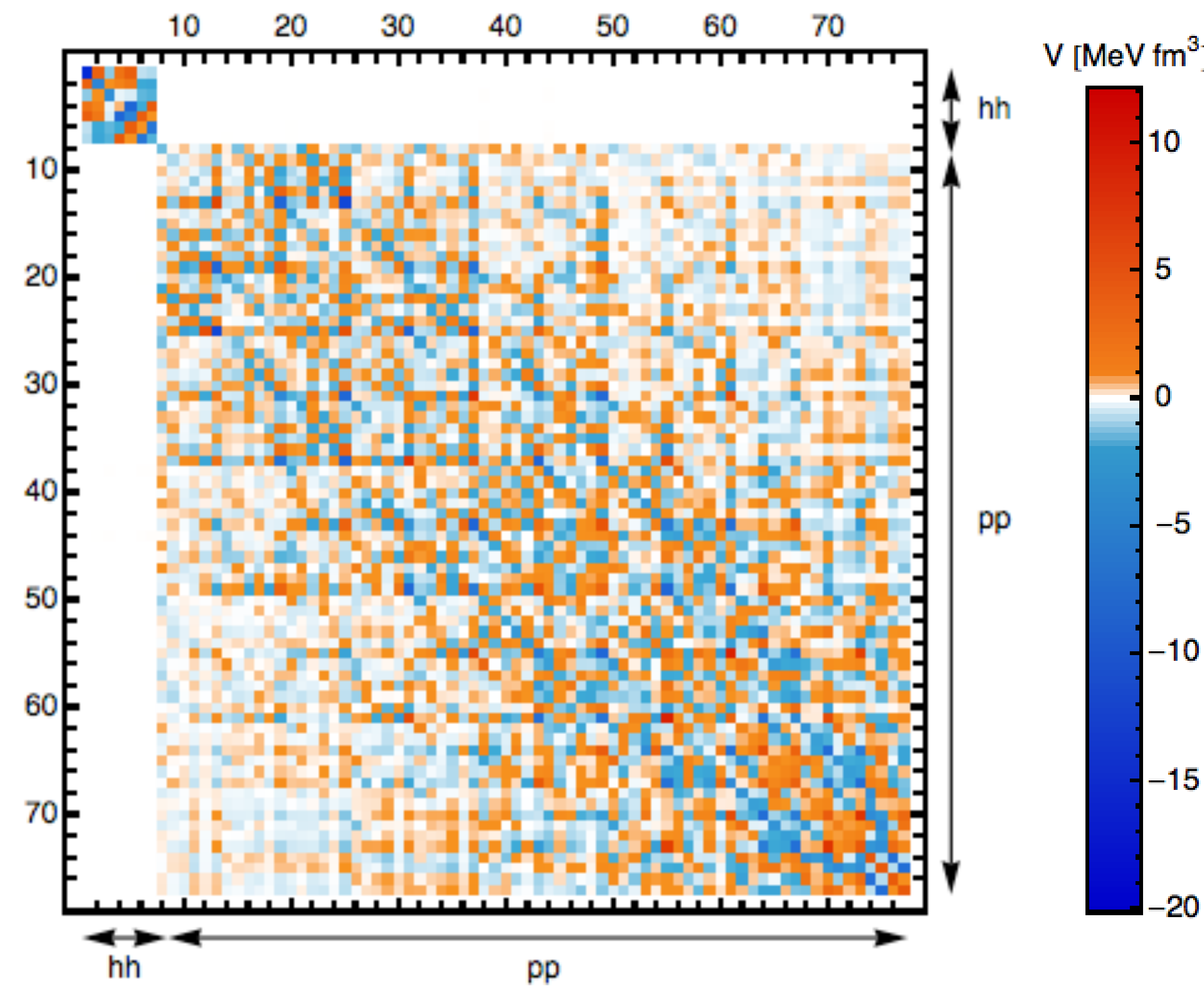




N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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

Ground-State Calculations

H. H., in preparation

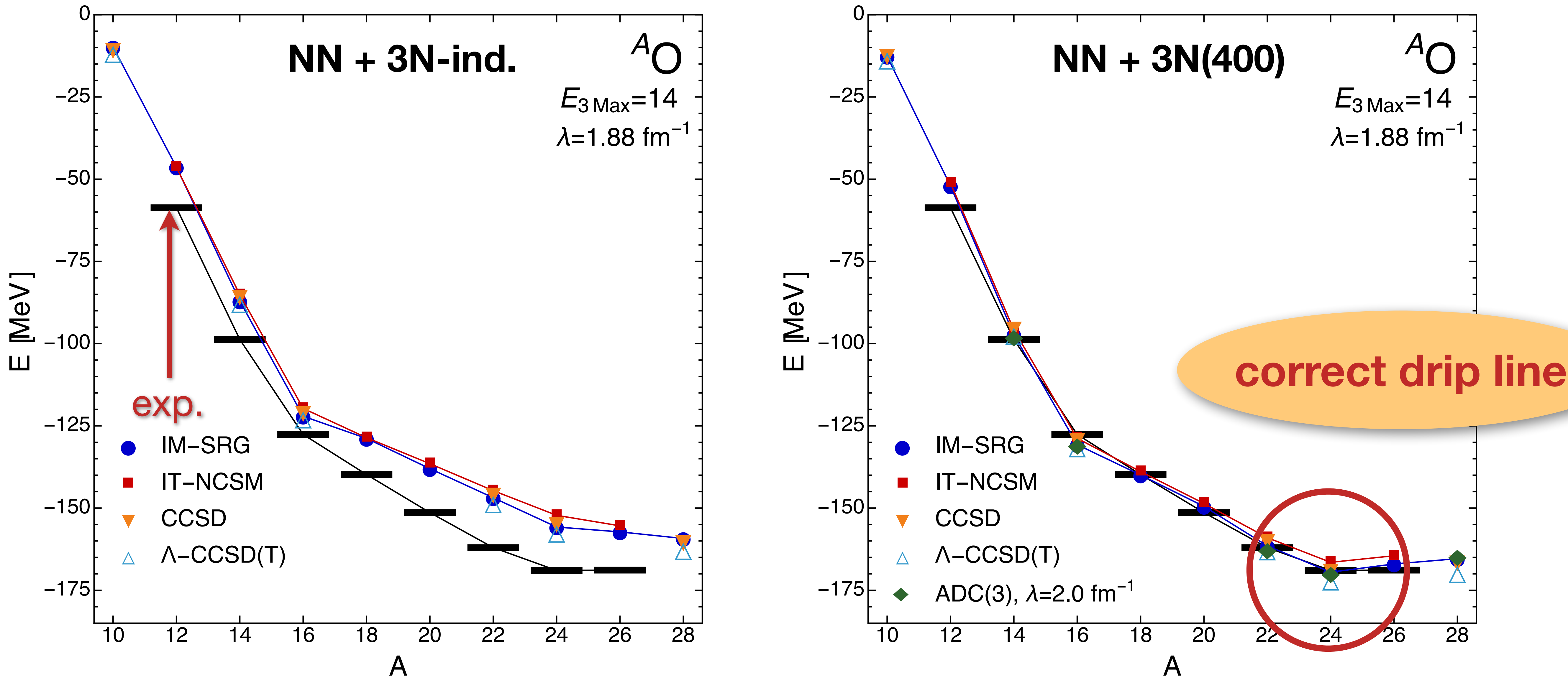
H. H., S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

H. H., S. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

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

Oxygen Isotopes

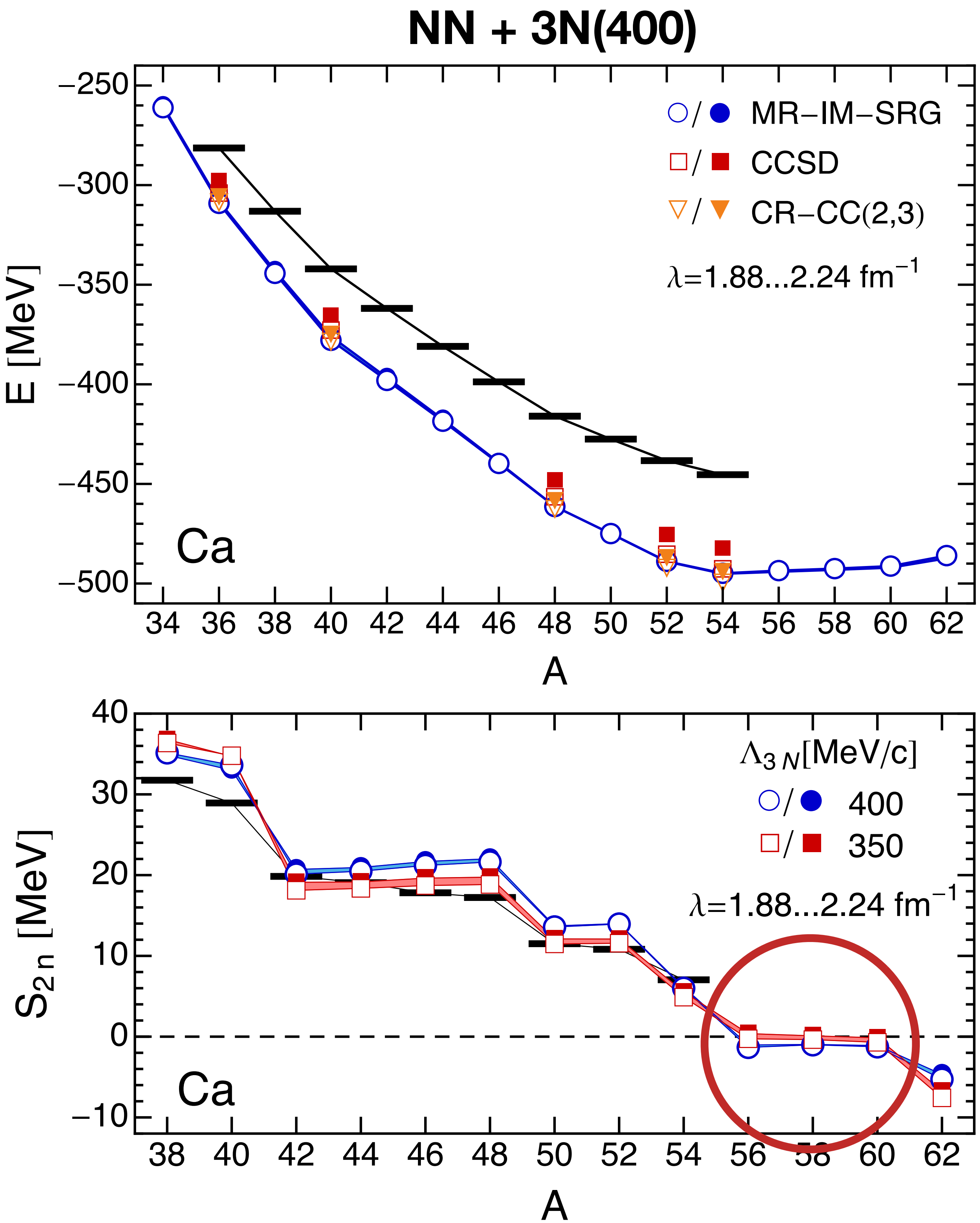
*HH et al., PRL **110**, 242501 (2013), ADC(3): A. Cipollone et al., PRL **111**, 242501 (2013)*



- Multi-Reference IM-SRG with number-projected Hartree-Fock-Bogoliubov reference state
- consistent results from different many-body methods

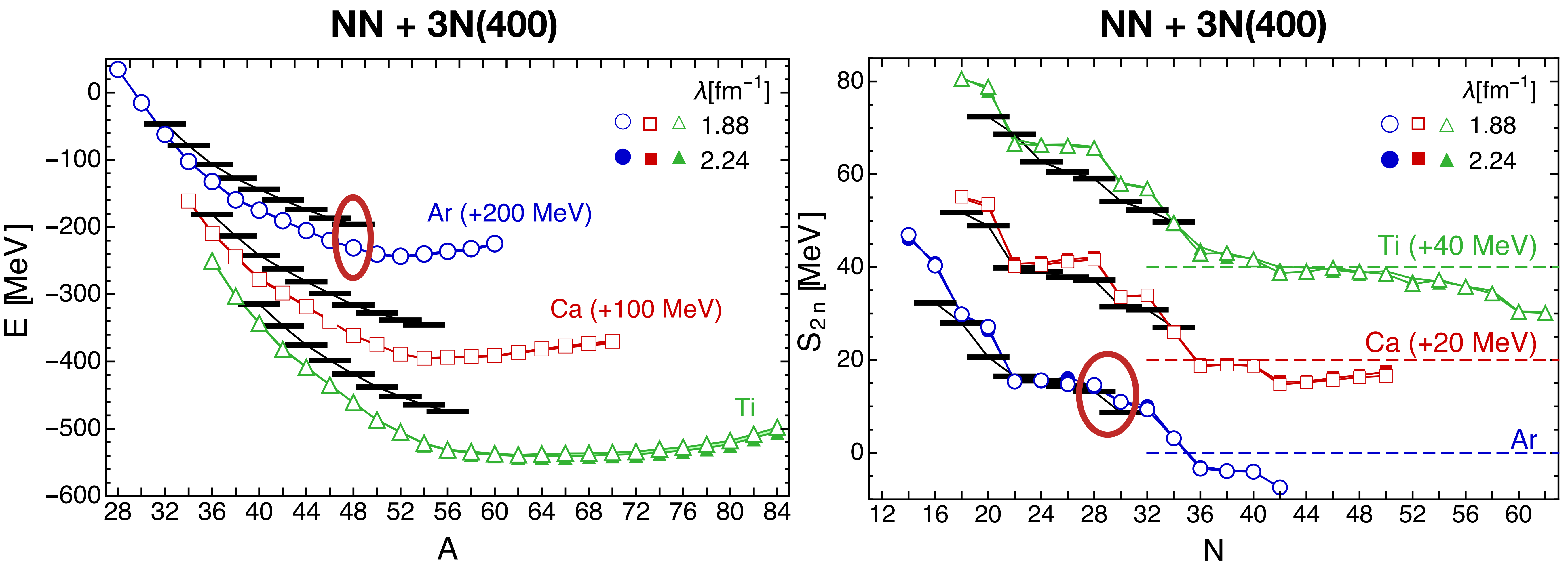
Calcium Isotopes

*HH et al., PRC **90**, 041302(R) (2014)*



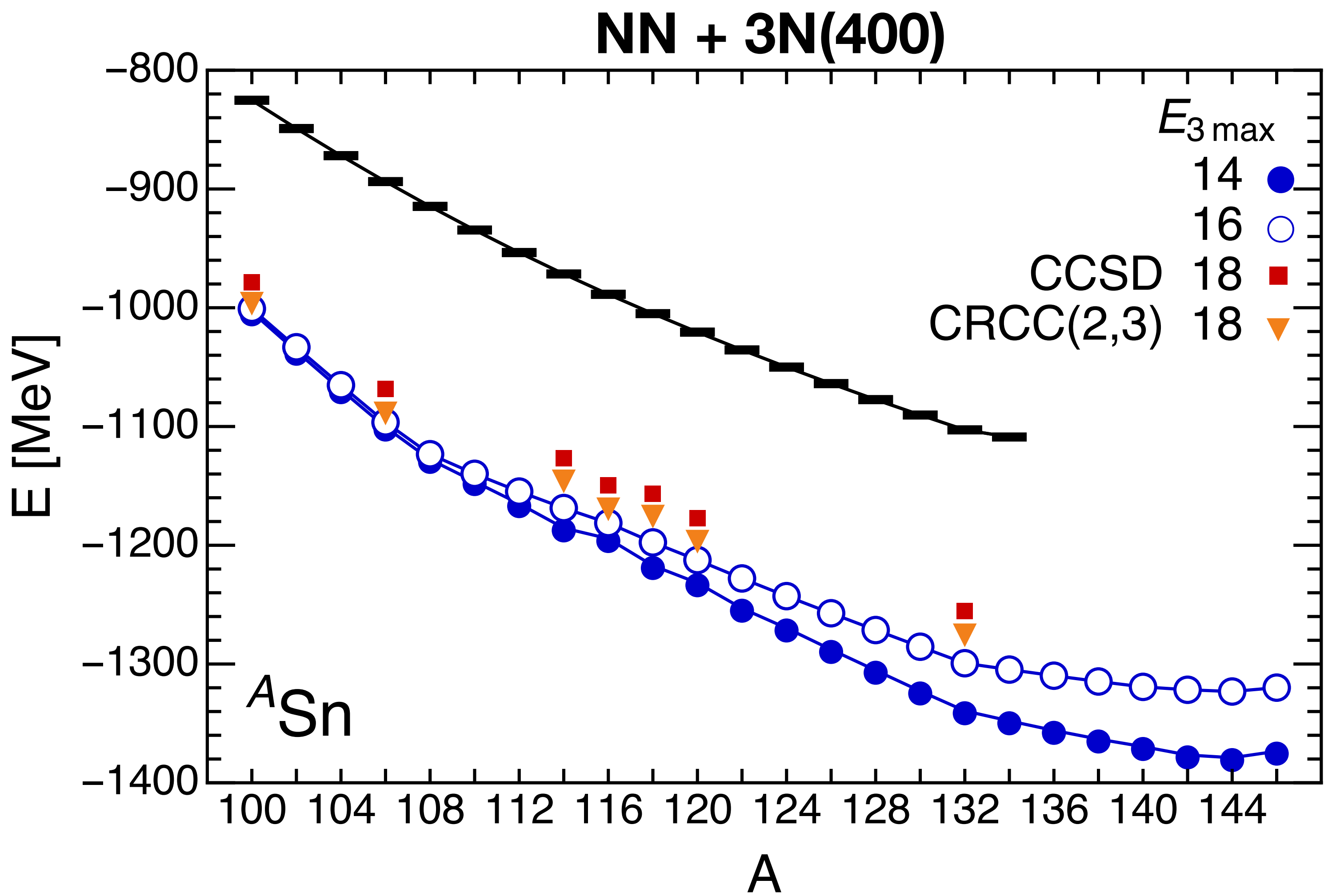
- differential observables (S_{2n}, spectra,...) filter out interaction components that cause overbinding
- predict flat trends for g.s. energies/S_{2n} beyond ^{54}Ca - await experimental data
- ^{52}Ca, ^{54}Ca magic for these NN+3N interactions
- no continuum coupling yet, other S_{2n} uncertainties < 1MeV

Isotopic Chains Around Ca



- S_{2n} consistent with Gor'kov GF, (weak) shell closure predicted in ^{46}Ar
  (Somà et al., PRC 89, 061301(R), 2014)
- ^{48,49}Ar masses measured at NSCL, ^{46}Ar shell closure confirmed
  (Meisel et al., PRL 114, 022501, 2015)

The Mass Frontier: Tin



E_{3max}	memory (float) [GB]
14	5
16	~20
18	100+

- systematics of overbinding similar to Ca (and Ni)
- not converged with respect to 3N matrix element truncation:

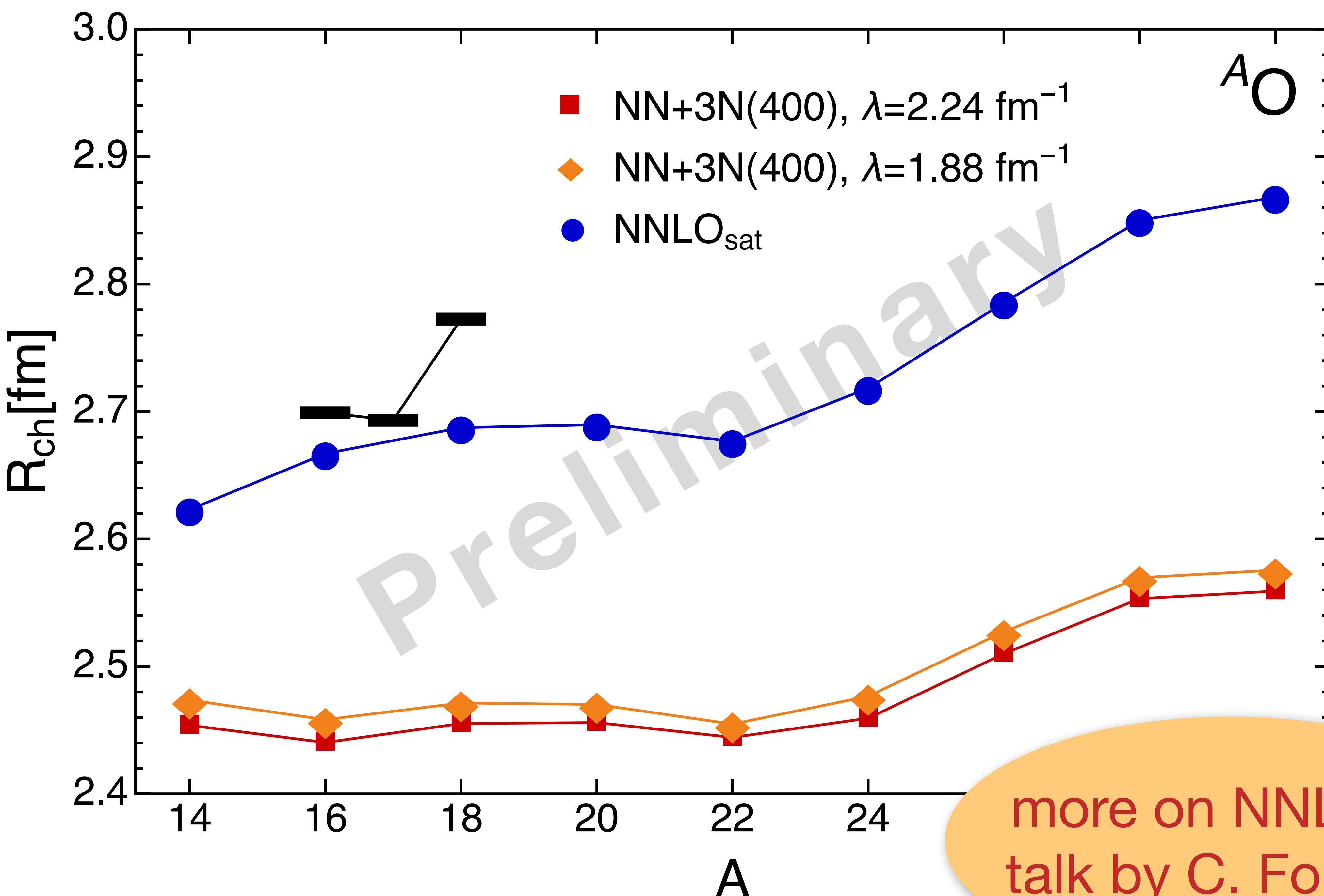
$$e_1 + e_2 + e_3 \leq E_{3max}$$

($e_{1,2,3}$: SHO energy quantum numbers)

- need technical improvements to go further

Oxygen Radii

V. Lapoux, V. Somà, C. Barbieri, H. H., J. D. Holt, and S. R. Stroberg, in preparation



more on NNLO$_{sat}$:
talk by C. Forssén

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)

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

Magnus Series Formulation

- explicit exponential ansatz for unitary transformation:

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

- flow equation for **Magnus** operator :

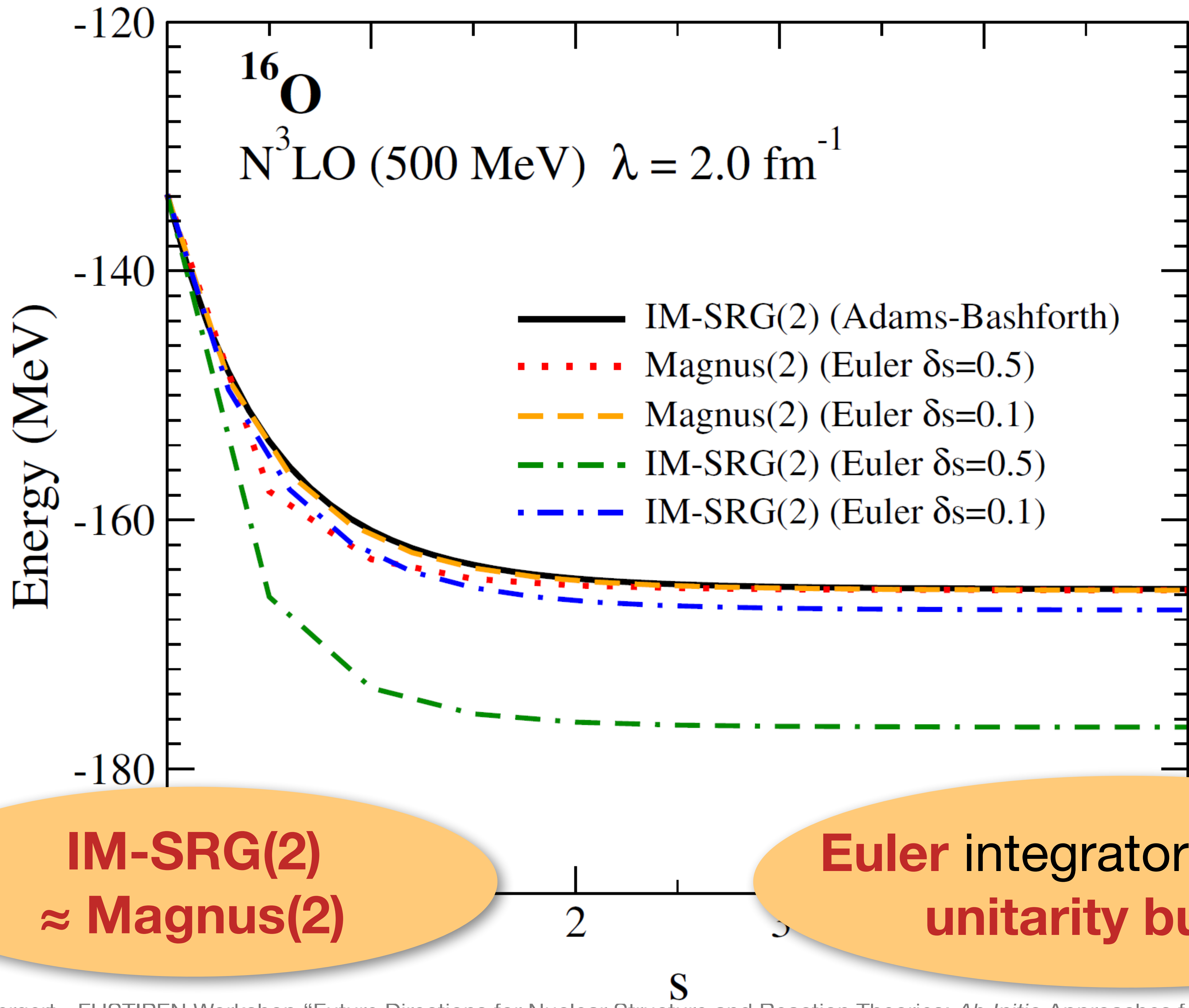
$$\frac{d}{ds}\Omega = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k}(\eta) \;, \quad \mathrm{ad}_{\Omega}(O) = [\Omega, O]$$

(B_k: Bernoulli numbers)

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

- truncate operators to **two-body level** (as in NO2B, IM-SRG(2))

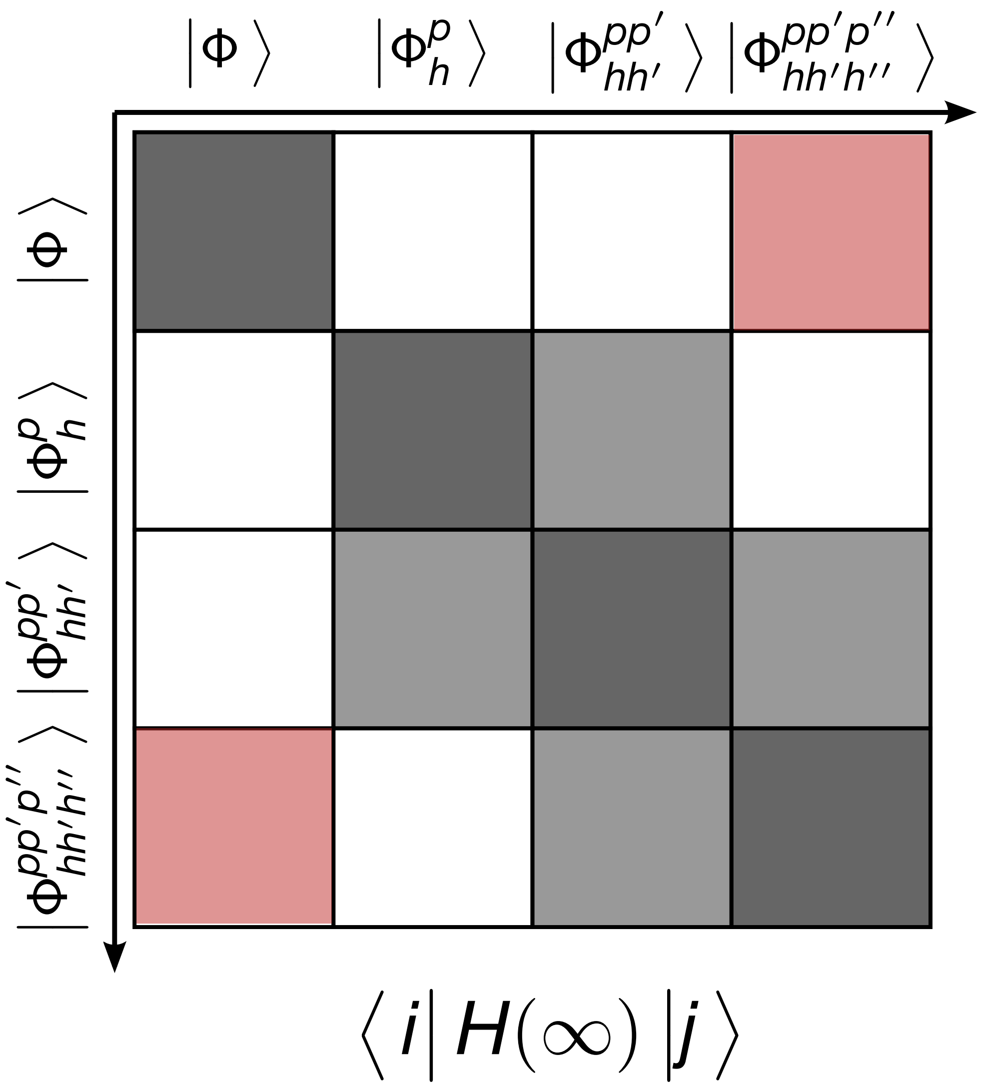
Magnus vs. Direct Integration



IM-SRG(2) ≈ Magnus(2)

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

Approximate IM-SRG(3)/Magnus(3)



approximate **restoration of induced 3N terms**:

$$W(\infty) = \sum_{k=1}^{\infty} \frac{1}{k!} \mathrm{ad}^{k}_{\Omega}\left(H_0\right)_{3B}$$

$$\approx \left[\Omega, \widetilde{H}(\infty)\right]_{3B}$$

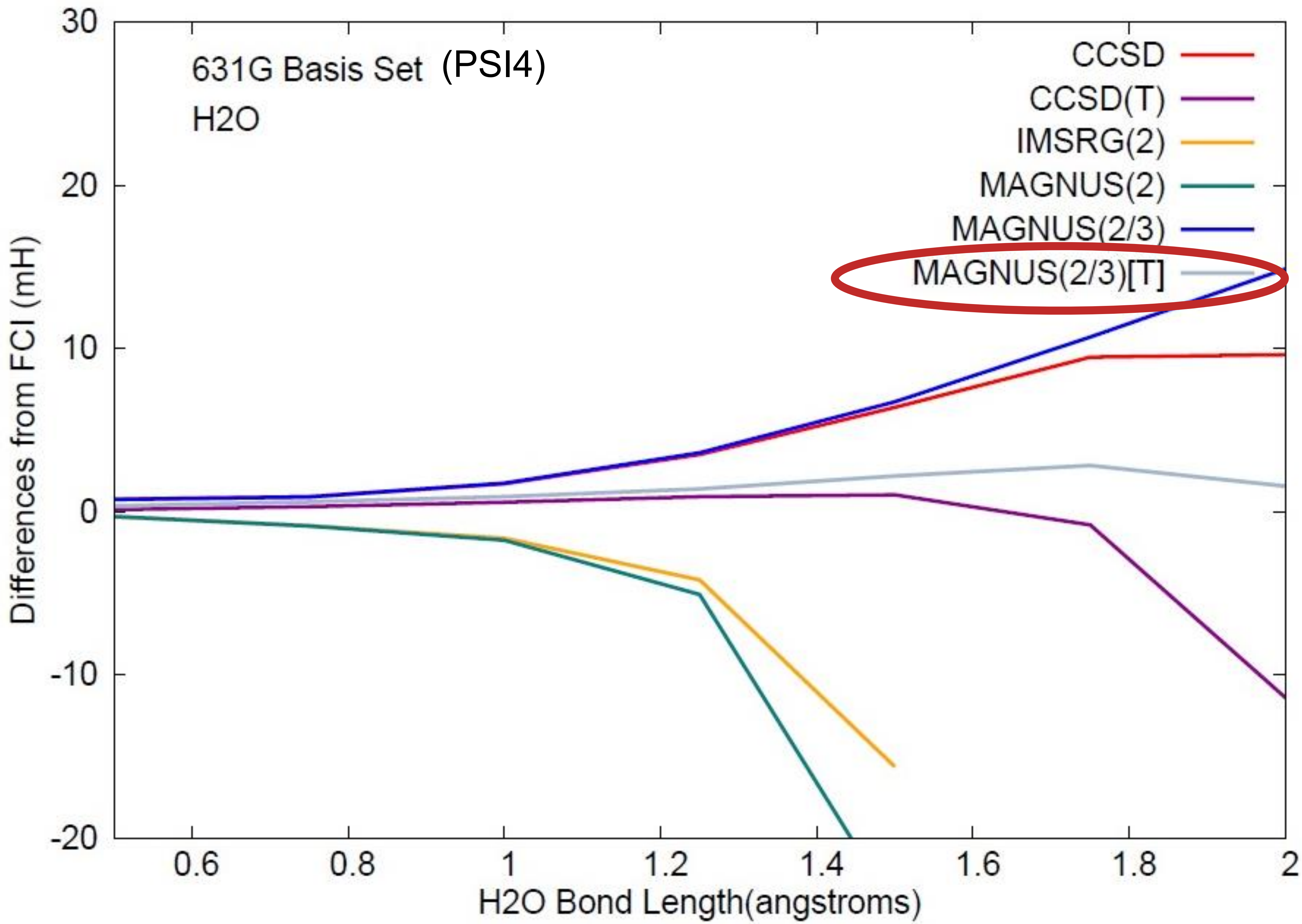
where

$$\widetilde{H}(\infty) = \sum_{k=1}^{\infty} \frac{1}{(k+1)!} \mathrm{ad}^{k}_{\Omega}\left(H_0\right)_{2B}$$

➡ **energy correction** (dressed ~ CR-CC(2,3)):

$$\Delta E = -\frac{1}{36} \sum_{p_1 p_2 p_3 h_1 h_2 h_3} \frac{\left|W_{p_1 p_2 p_3 h_1 h_2 h_3}(\infty)\right|^2}{\Delta_{p_1 p_2 p_3 h_1 h_2 h_3}(\infty)}$$

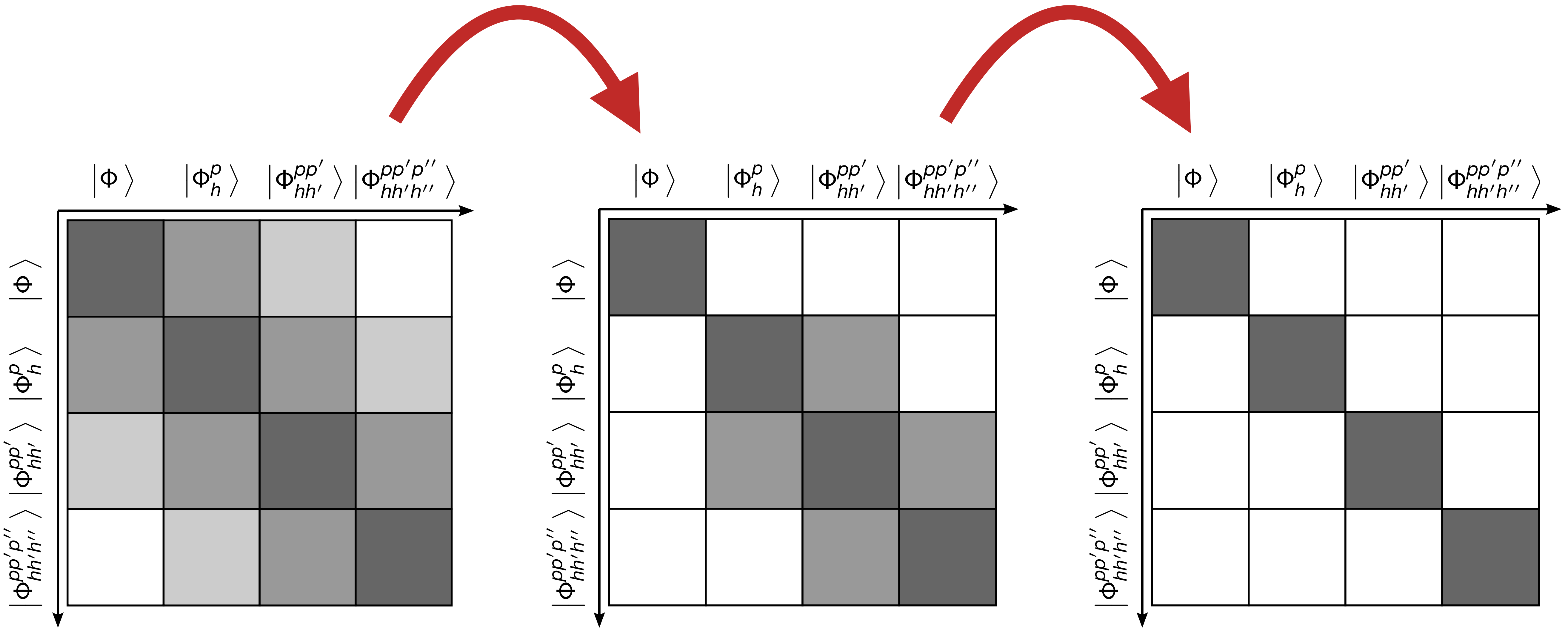
Stretched Water



IM-SRG for Excited States

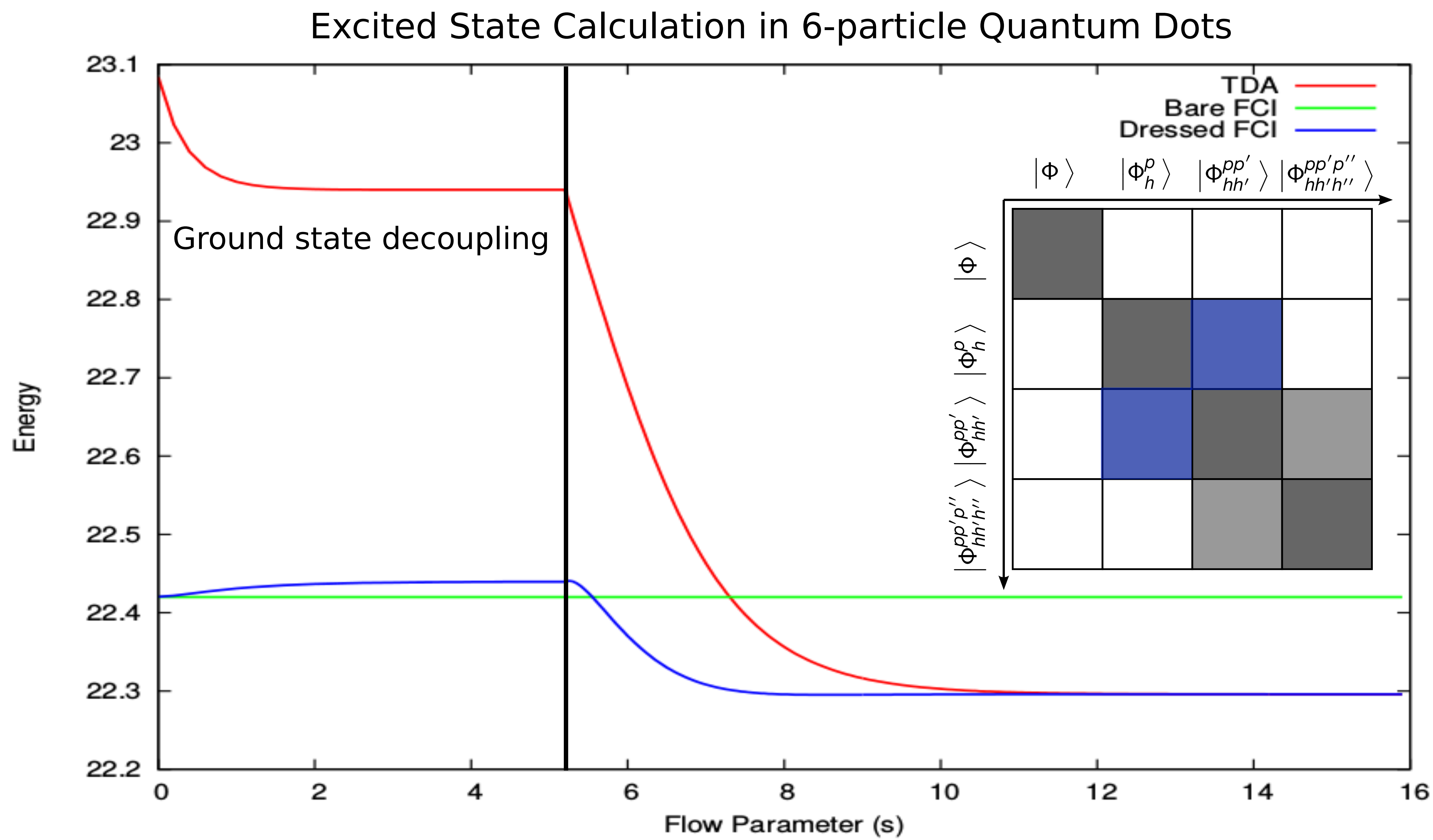
N. M. Parzuchowski, T. D. Morris, S. K. Bogner, in preparation

Excited State Decoupling



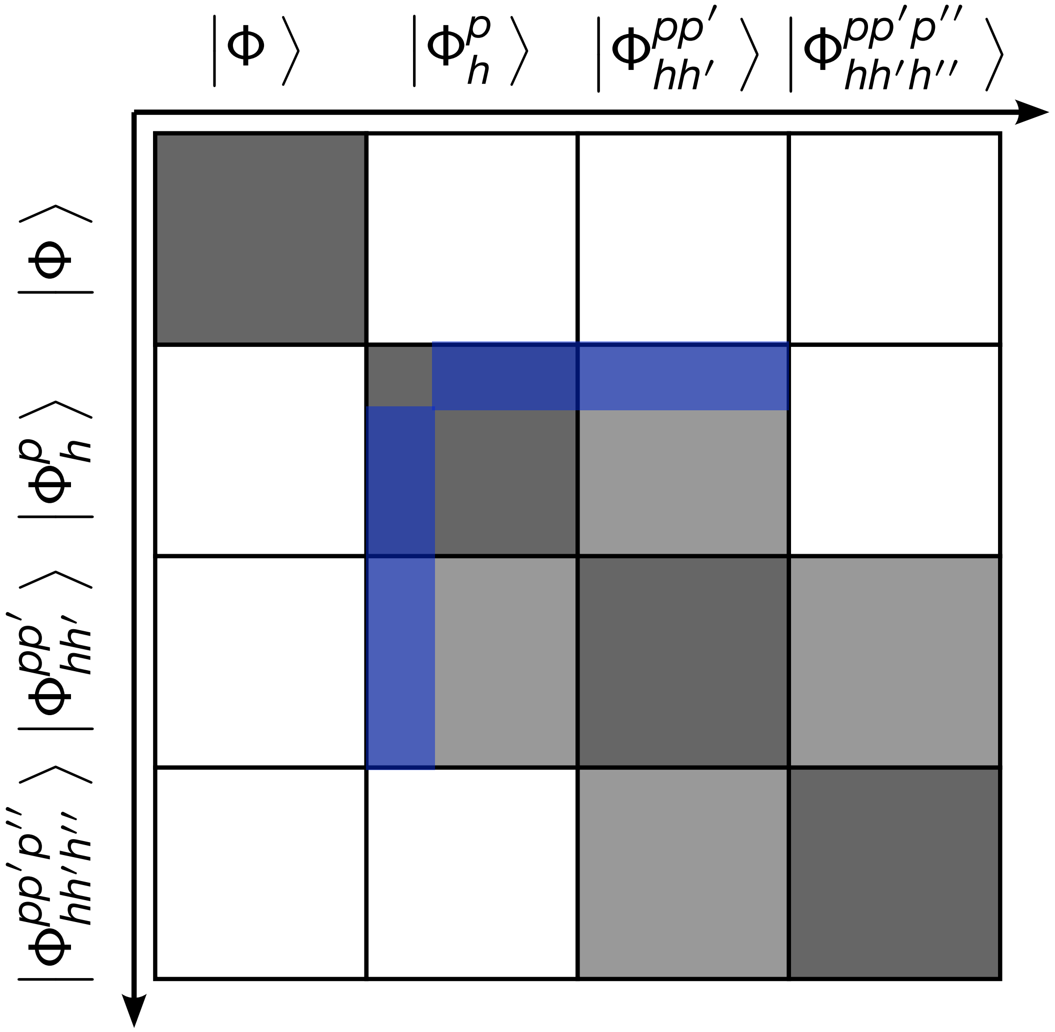
Can we decouple multiple states simultaneously? Maybe entire blocks?

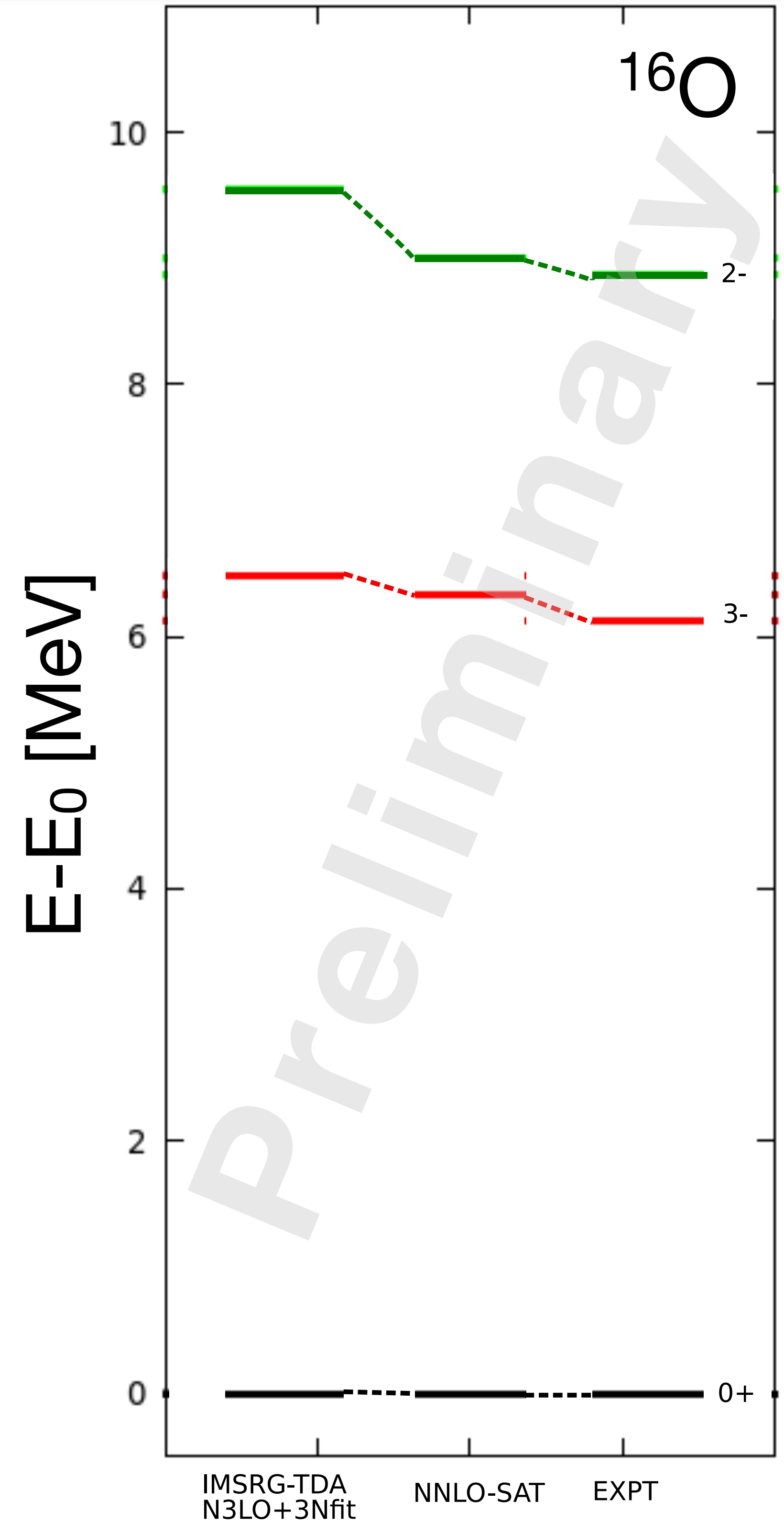
Quantum Dots



➡ **Multi-state decoupling can generate sizable induced forces…**

Sub-Block Decoupling





control induced forces by only **decoupling a 1p-1h ("valence") sub-block**

Equation-of-Motion Method

- describe "excited states" based on reference state:

$$\left|\Phi_k\right\rangle = Q_k^\dagger \left|\Phi_0\right\rangle$$

- **IM-SRG effective Hamiltonian** in EOM approach:

$$\left[H(s), Q_k^\dagger(s)\right] = \omega_k(s) Q_k^\dagger(s), \quad \omega_k(s) = E_k(s) - E_0(s)$$

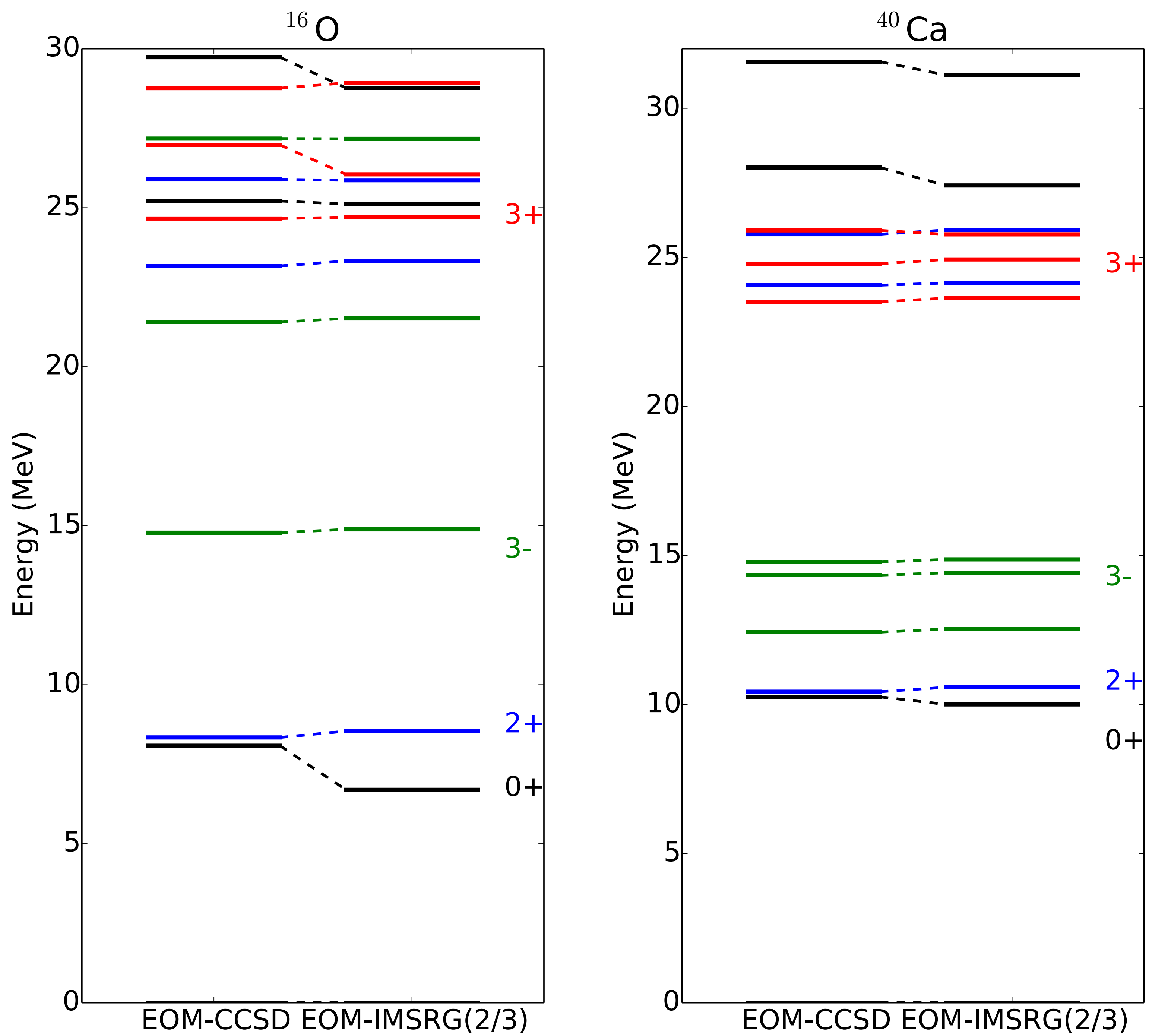
- ansatz for excitation operator (g.s. correlations built into Hamiltonian):

$$Q_k^\dagger(s) = \sum_{ph} q_h^p(s) :A_h^p: + \frac{1}{4}\sum_{pp'hh'} q_{hh'}^{pp'}(s) :A_{hh'}^{pp'}:$$

- **polynomial** effort vs. factorial scaling of Shell Model

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

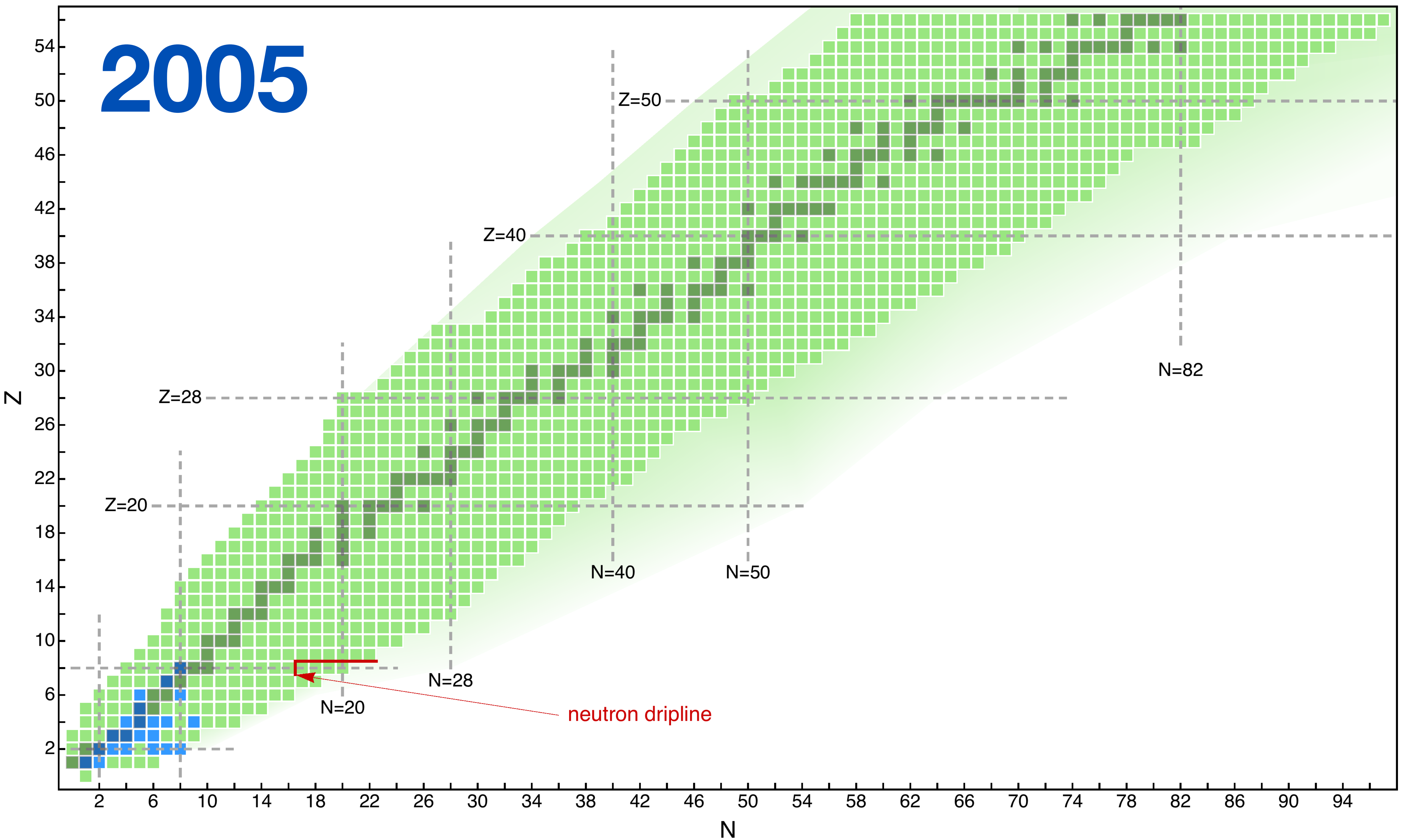
Spectra of Closed-Shell Nuclei



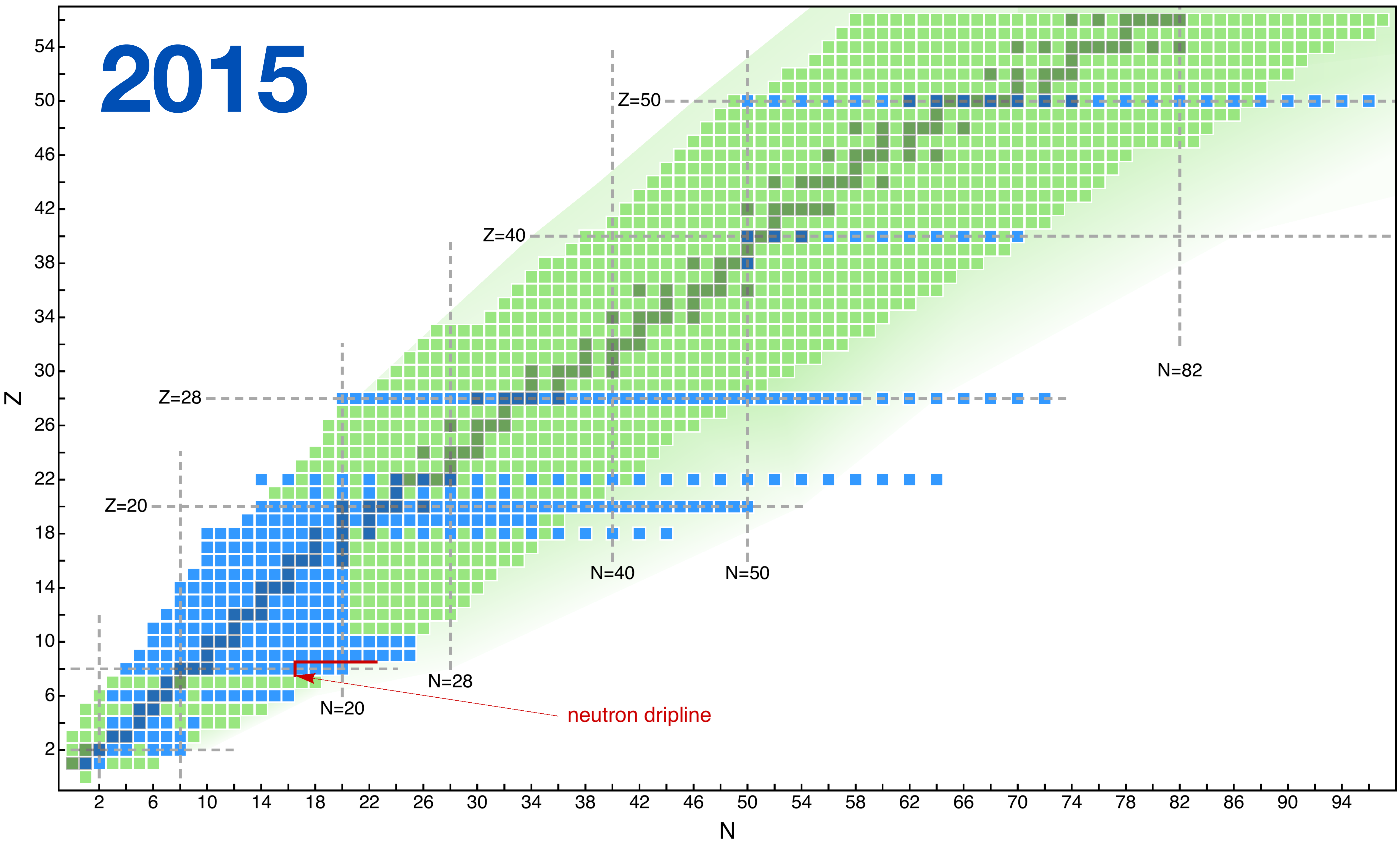
EOM-CCSD results courtesy of G. Hagen

Epilogue

Progress in *Ab Initio* Calculations



Progress in *Ab Initio* Calculations



Summary

- **predictive theory:** interaction, operators, many-body method with systematic uncertainties & convergence to exact result
- enormous progress in *ab initio* nuclear structure and reactions
- rapidly **growing capabilities**: g.s. energies, spectra, radii, transitions, etc. for **increasingly heavy nuclei**
- new generation of chiral Hamiltonians, **greatly improved optimization** - also **more accurate (?)**
    - $\mathrm{NNLO}_{\mathrm{sat}}$, $\mathrm{NNLO}_{\mathrm{sim}}$
    - EKM / LENPIC interactions
    - local NNLO

IM-SRG+
Shell Model:
talk by J. D. Holt

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J. Engel, J. Yao
University of North Carolina - Chapel Hill

NERSC

NSF

DEPARTMENT OF ENERGY UNITED STATES OF AMERICA

NUCLEI
Nuclear Computational Low-Energy Initiative

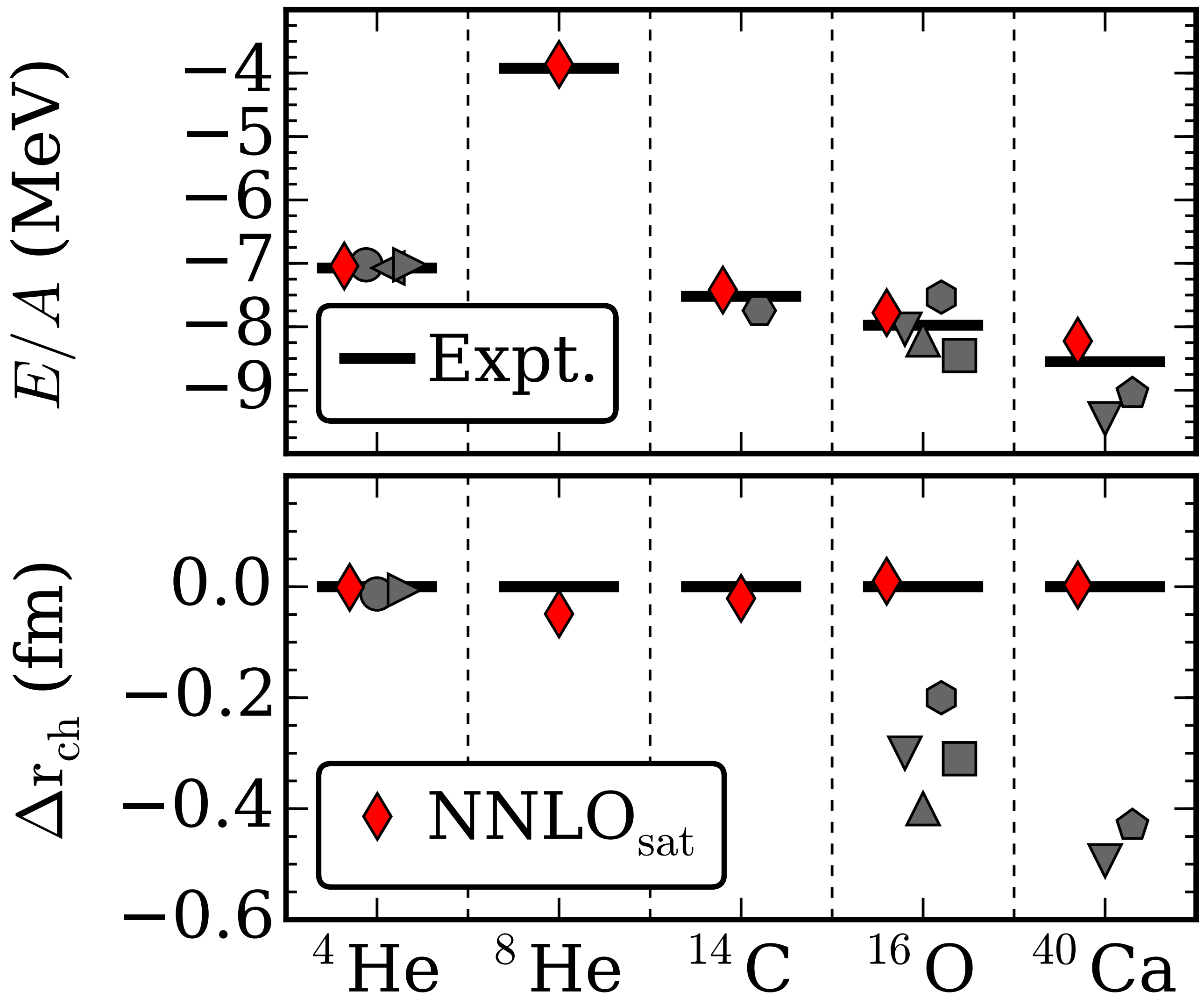
Ohio Supercomputer Center

ICER

Supplements

NNLO$_{sat(uration)}$

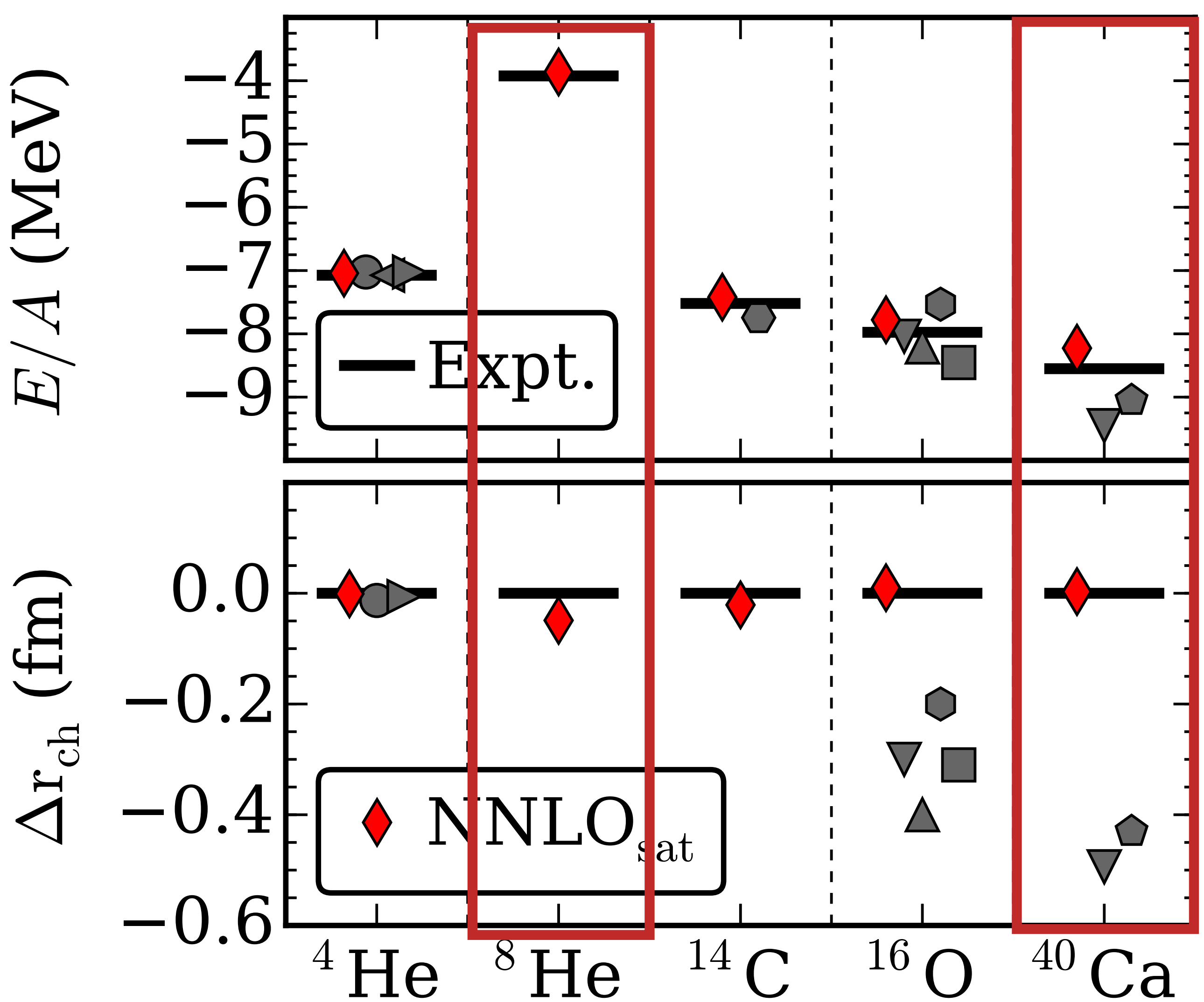
A. Ekström et al., PRC **91**, 051301(R) (2015)



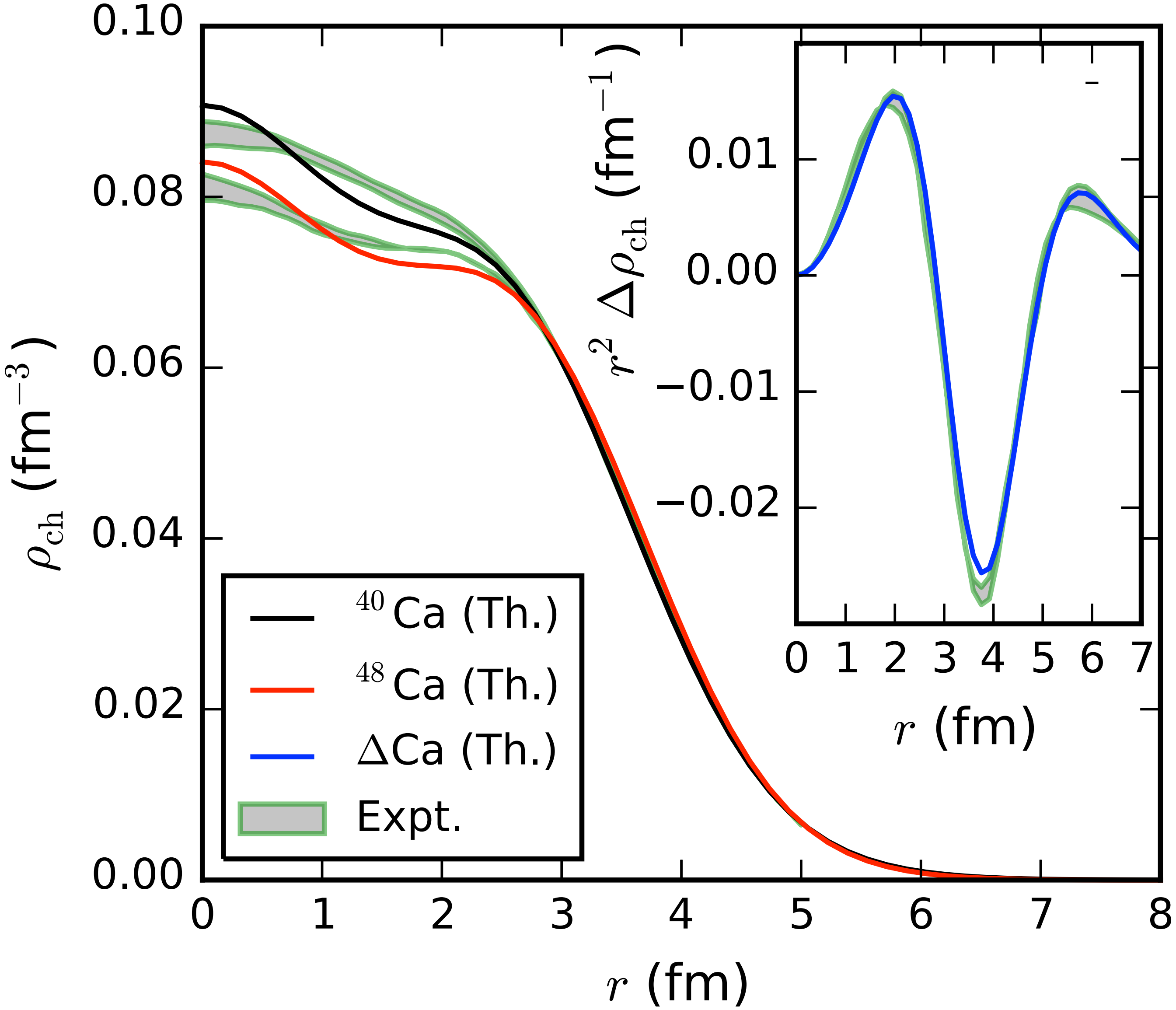
- simultaneous optimization of NN and 3N interaction
- inputs:
  - phase shifts ($E_{lab} \leq 35$ MeV)
  - ^{3}H, ^{3}He, ^{4}He g.s. energies & radii (s-shell)
  - ^{14}C, ^{16}O g.s. energies & radii (p-shell)
  - ^{22,24,25}O g.s. energies (sd-shell)

$NNLO_{sat}$

*A. Ekström et al., PRC **91**, 051301(R) (2015)*



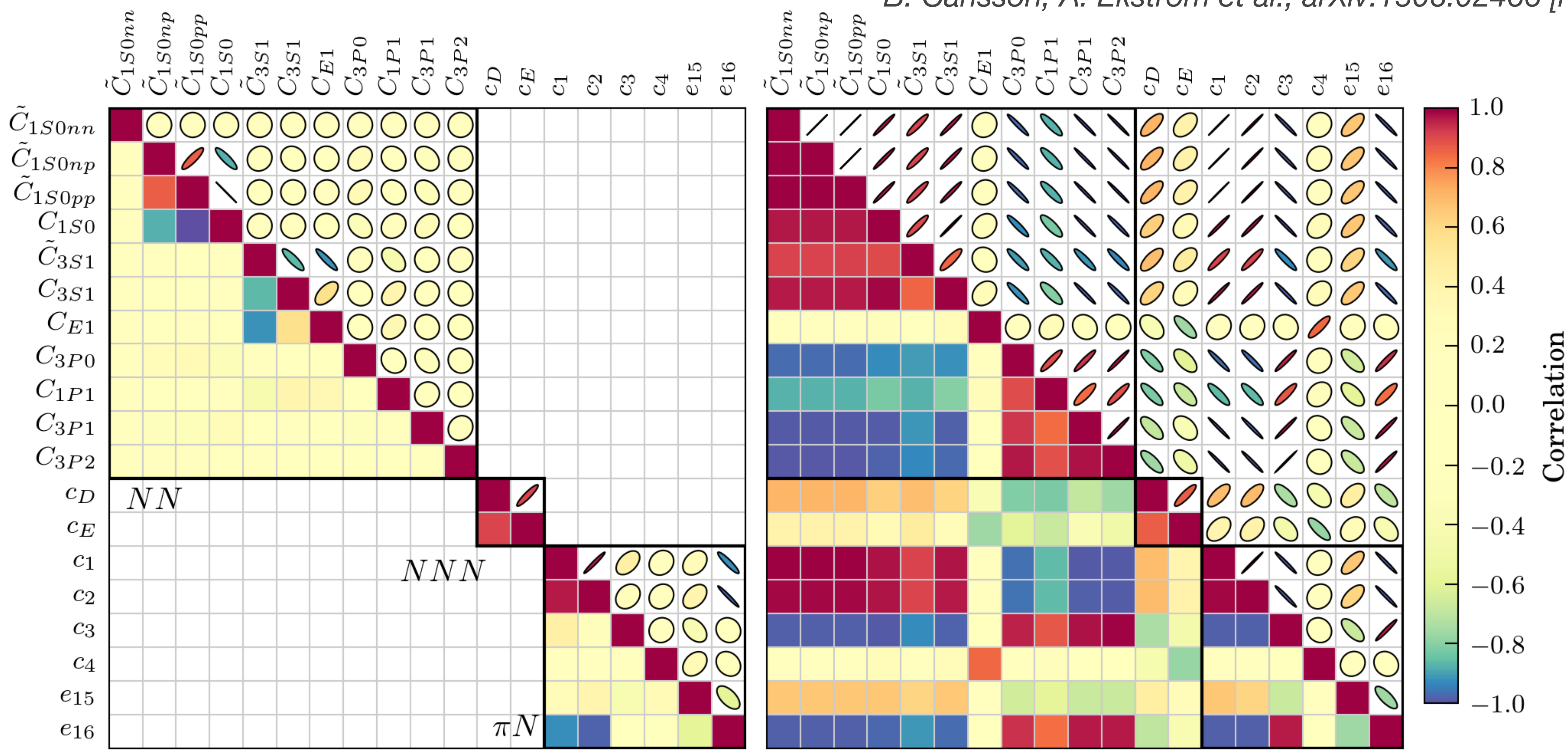
*G. Hagen et al., Nature Physics **12**, 186 (2015)*



- accurate description of ^{8}He, ^{40,48}Ca g.s. energies & radii, ^{40,48}Ca charge distributions
- predictions for electric dipole polarizability, neutron skin, weak form factor of ^{48}Ca

Optimization of Correlated LECs

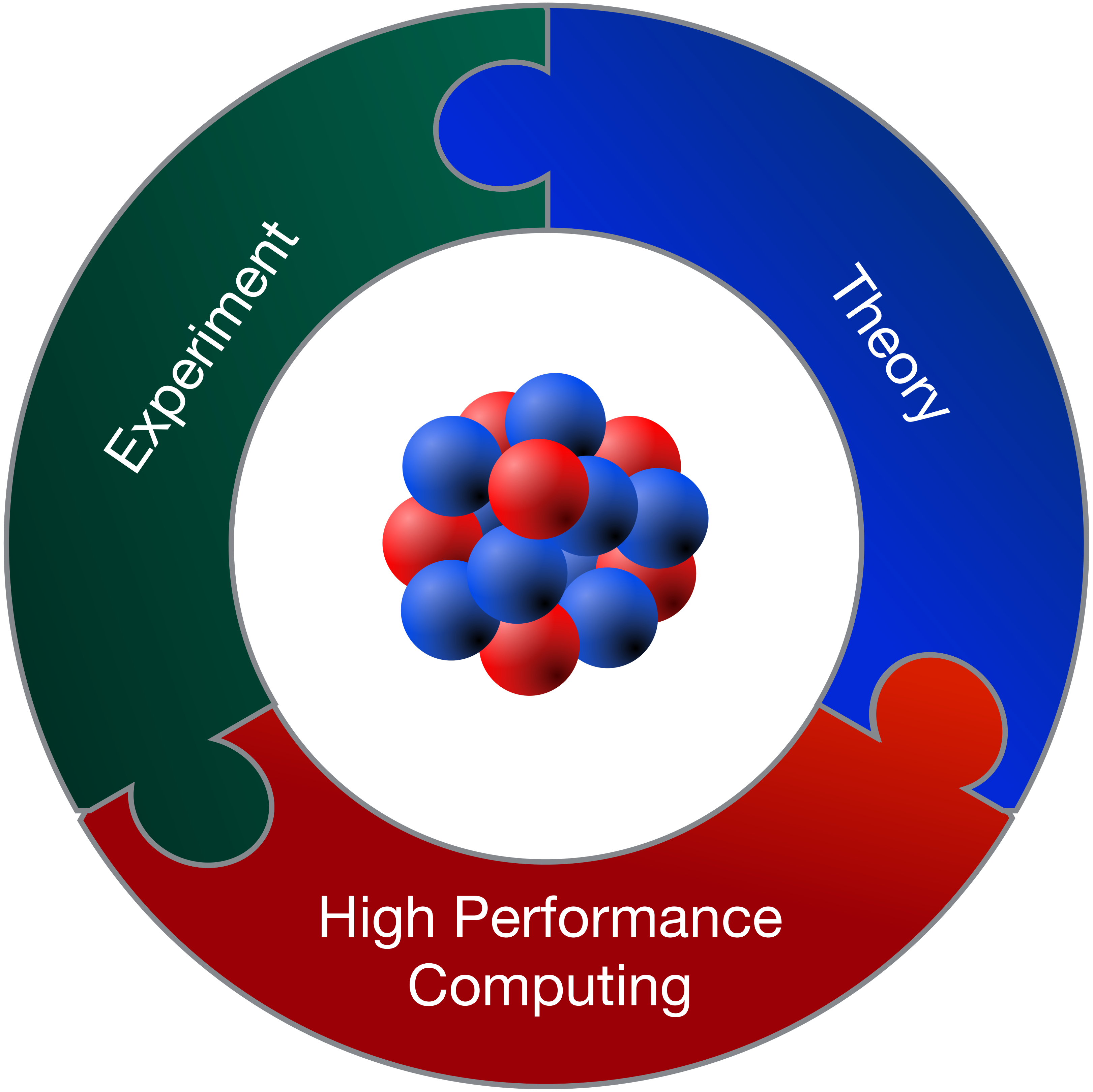
B. Carlsson, A. Ekström et al., arXiv:1506.02466 [nucl-th]



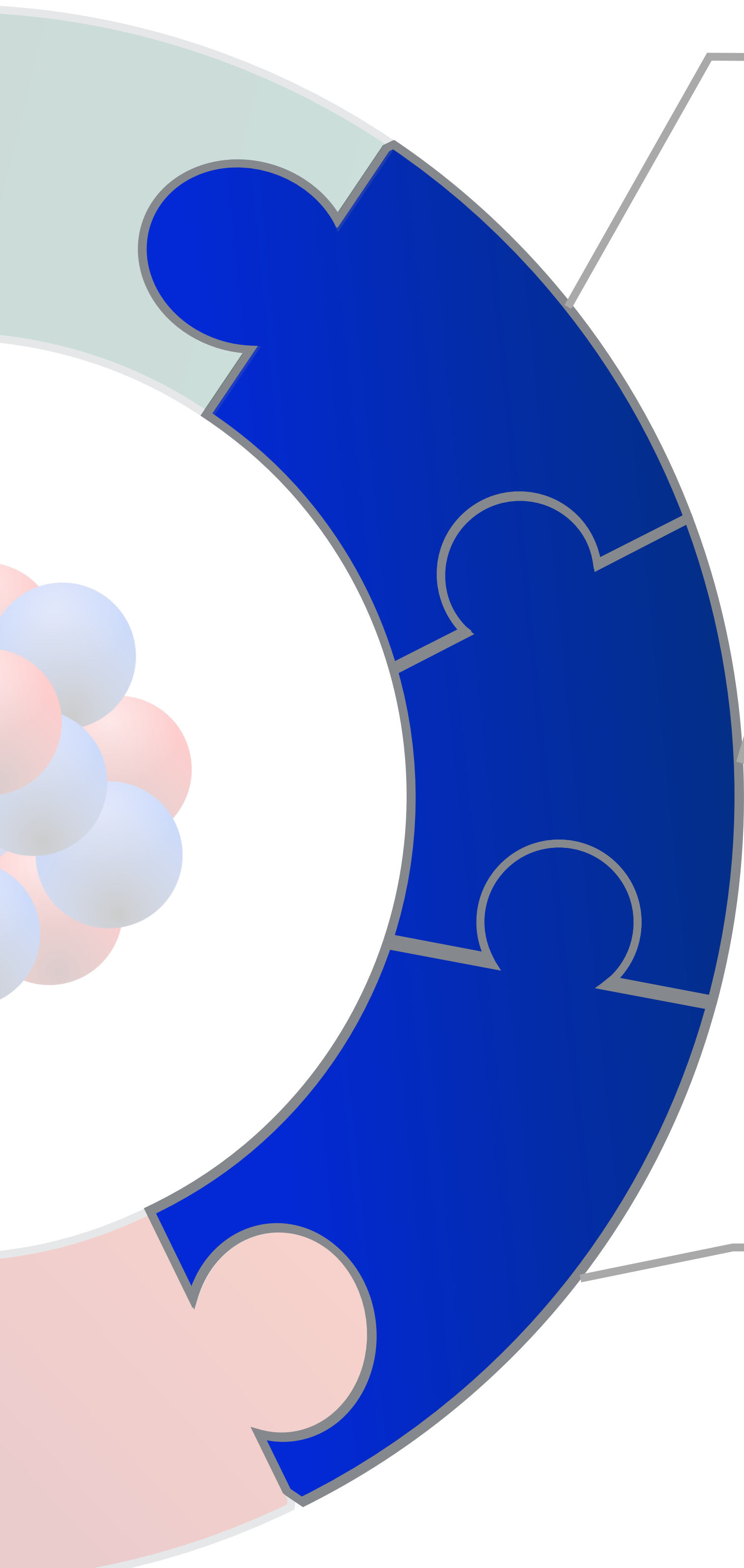
- chiral LECs in NN, 3N, πN sectors are correlated
- sequential vs. simultaneous optimization, NNLO, NN+3N:

$$E(^4\text{He}) = 28^{+8}_{-18}\ \text{MeV} \quad \text{vs.} \quad E(^4\text{He}) = 28.26^{+4}_{-5}\ \text{MeV}$$

The Nuclear Many-Body Problem

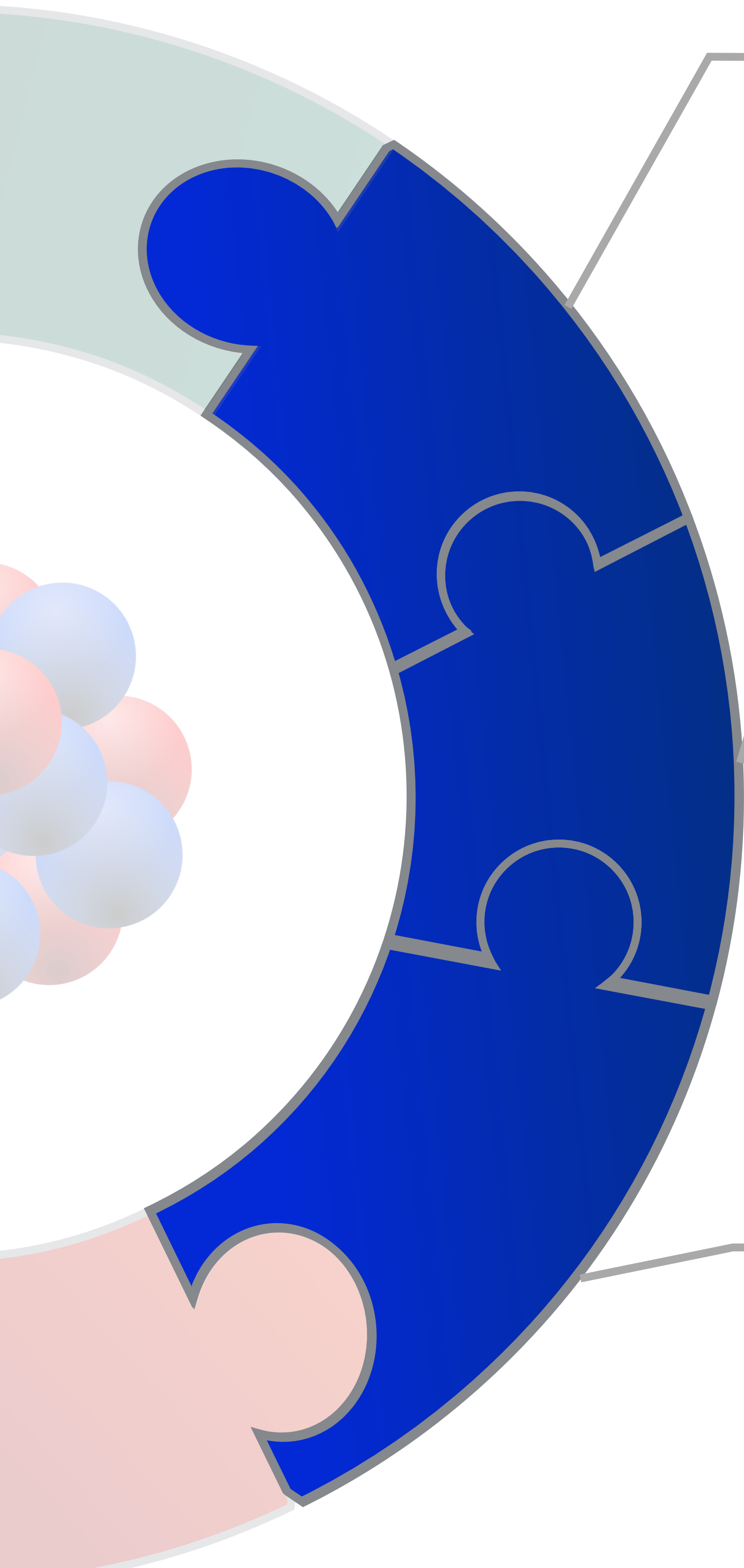


Theory Ingredients



- **Interactions (& Operators) from Chiral EFT**
    - symmetries of low-energy QCD
    - power counting
- **Similarity Renormalization Group**
    - systematically dial resolution scales (cutoffs) of theory
    - trade-off: enhanced convergence & accuracy of many-body methods vs. omitted induced 4N, …, AN forces
- ***Ab Initio* Many-Body Method**
    - systematically improvable towards exact solution

Uncertainty Quantification



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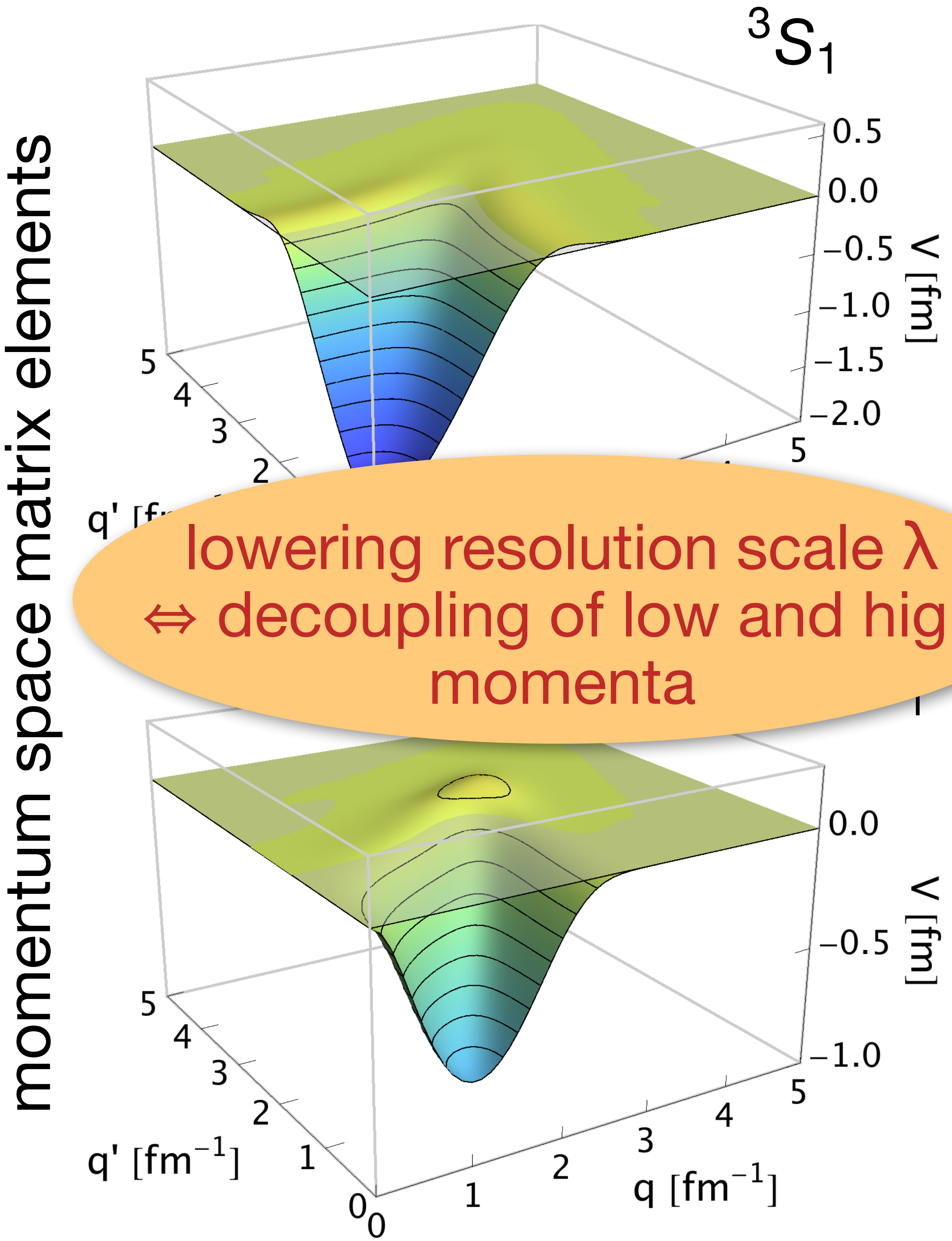
SRG in Two-Body Space



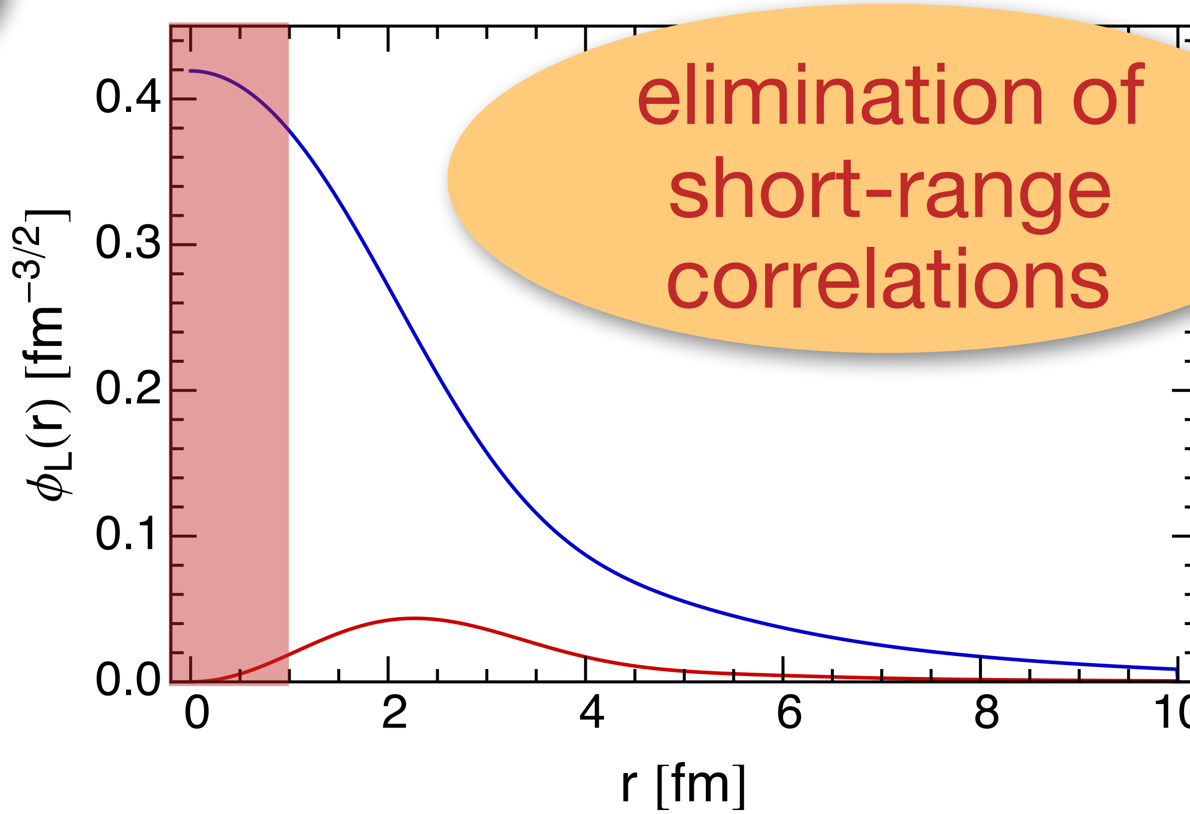
lowering resolution scale λ
⇔ decoupling of low and high momenta

λ = 1.8 fm^{-1}

$$\eta(\lambda) = 2\mu\left[T_{\rm rel}, H(\lambda)\right]$$

$$\lambda = s^{-1/4}$$

deuteron wave function



elimination of short-range correlations

Induced Interactions

- SRG is a unitary transformation in A-body space
- up to A-body interactions are induced during the flow:

$$\frac{dH}{d\lambda} = [[\sum a^\dagger a, \sum \underbrace{a^\dagger a^\dagger a a}_{\text{2-body}}], \sum \underbrace{a^\dagger a^\dagger a a}_{\text{2-body}}] = \ldots + \sum \underbrace{a^\dagger a^\dagger a^\dagger a a a}_{\text{3-body}} + \ldots$$

- state-of-the-art: evolve in three-body space, truncate induced four- and higher many-body forces
(Jurgenson, Furnstahl, Navratil, PRL 103, 082501; Hebeler, PRC 85, 021002; Wendt, PRC 87, 061001)
- λ-dependence of eigenvalues is a diagnostic for size of omitted induced interactions

Normal Ordering

- second quantization: $A^{k_1 \ldots k_N}_{l_1 \ldots l_N} = a^\dagger_{k_1} \ldots a^\dagger_{k_N} a_{l_N} \ldots a_{l_1}$
- particle- and hole density matrices:

$$\lambda^k_l = \langle \Phi | A^k_l | \Phi \rangle \longrightarrow n_k \delta^k_l \,, \quad n_k \in \{0,1\}$$
$$\xi^k_l = \lambda^k_l - \delta^k_l \longrightarrow -\bar{n}_k \delta^k_l \equiv -(1-n_k)\delta^k_l$$

- define normal-ordered operators recursively:

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

- algebra is simplified significantly because

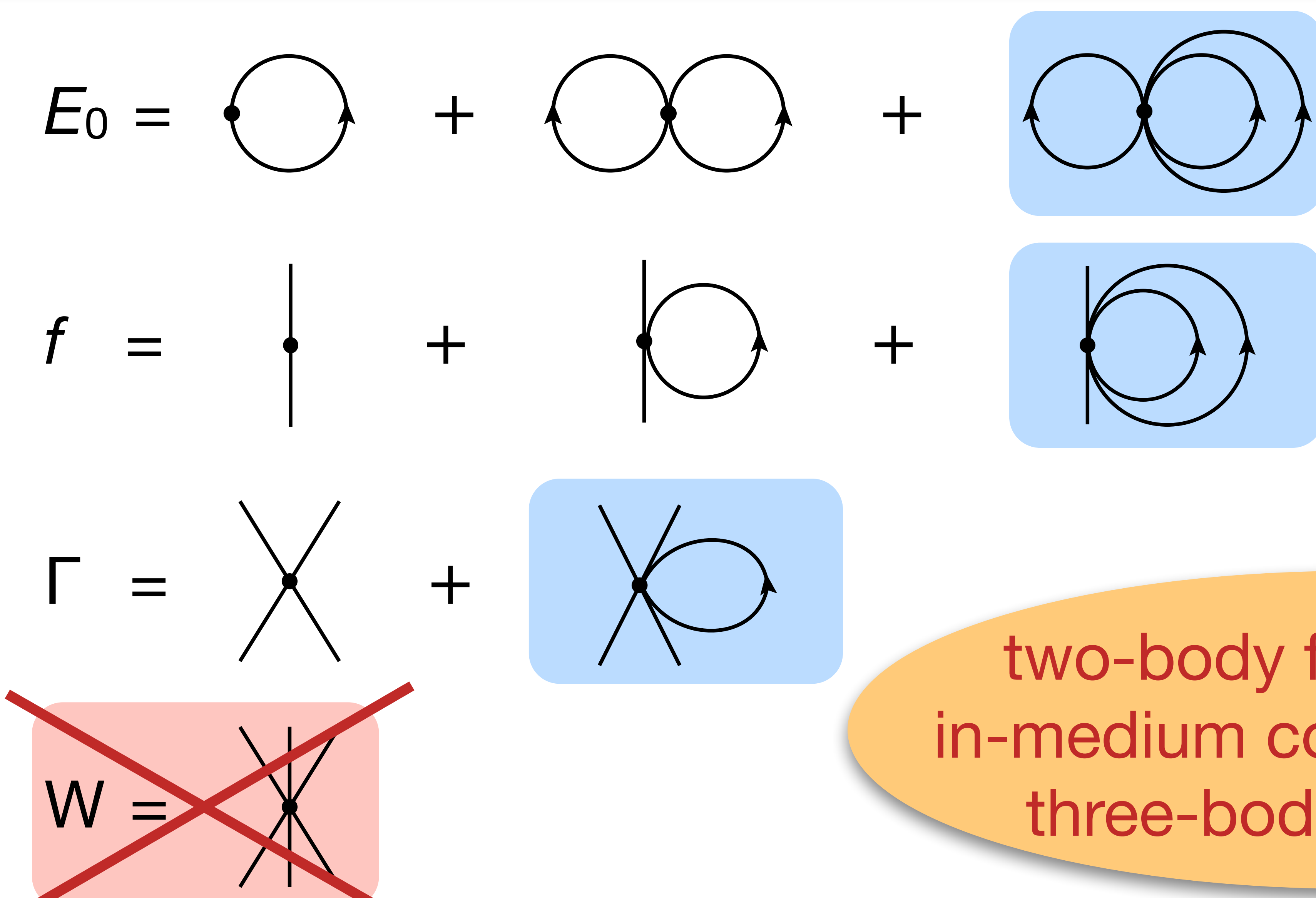
$$\langle \Phi | :A^{k_1 \ldots k_N}_{l_1 \ldots l_N}: | \Phi \rangle = 0$$

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

Normal-Ordered Hamiltonian

Normal-Ordered Hamiltonian

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

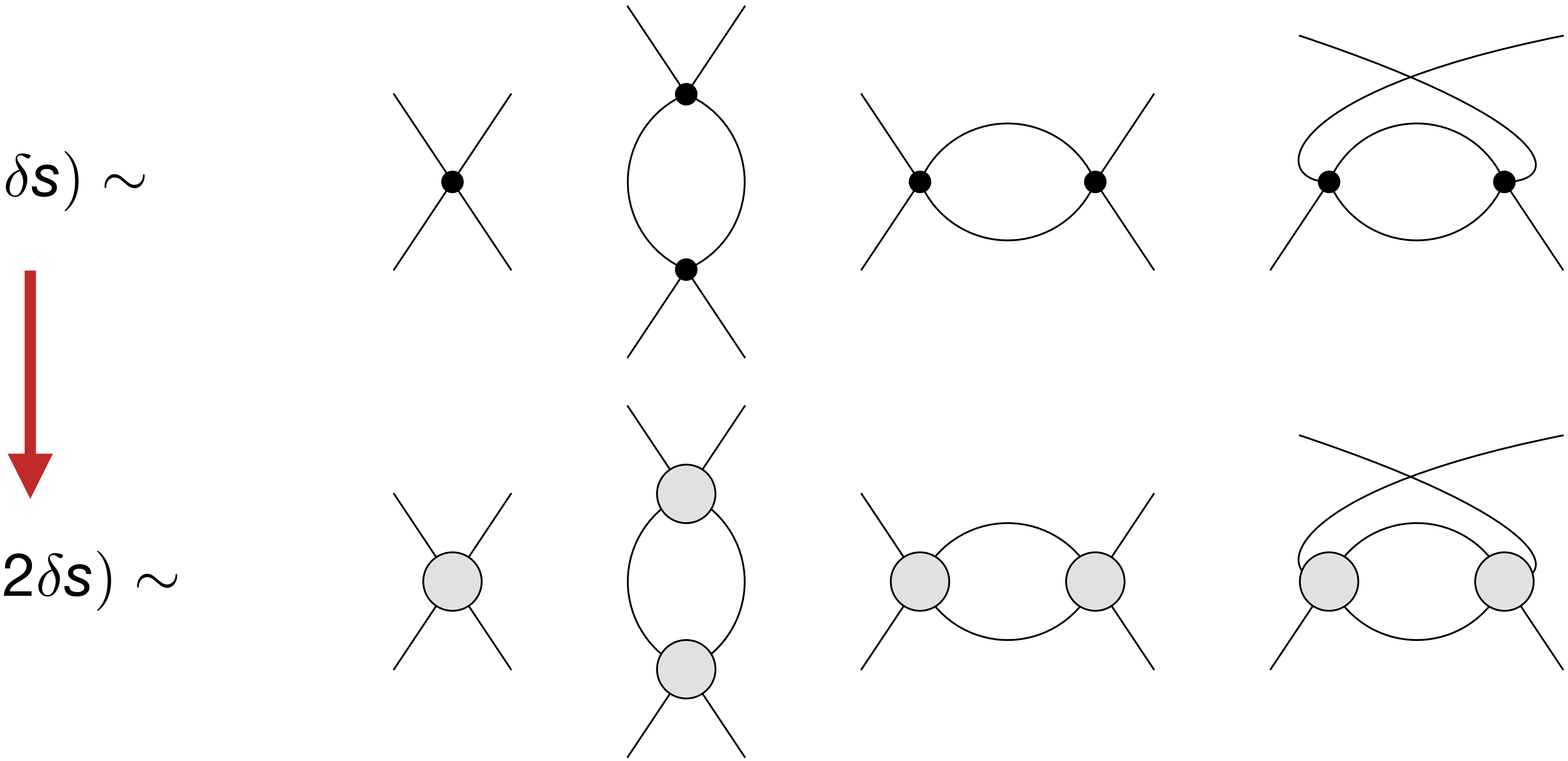


two-body formalism with in-medium contributions from three-body interactions

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

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



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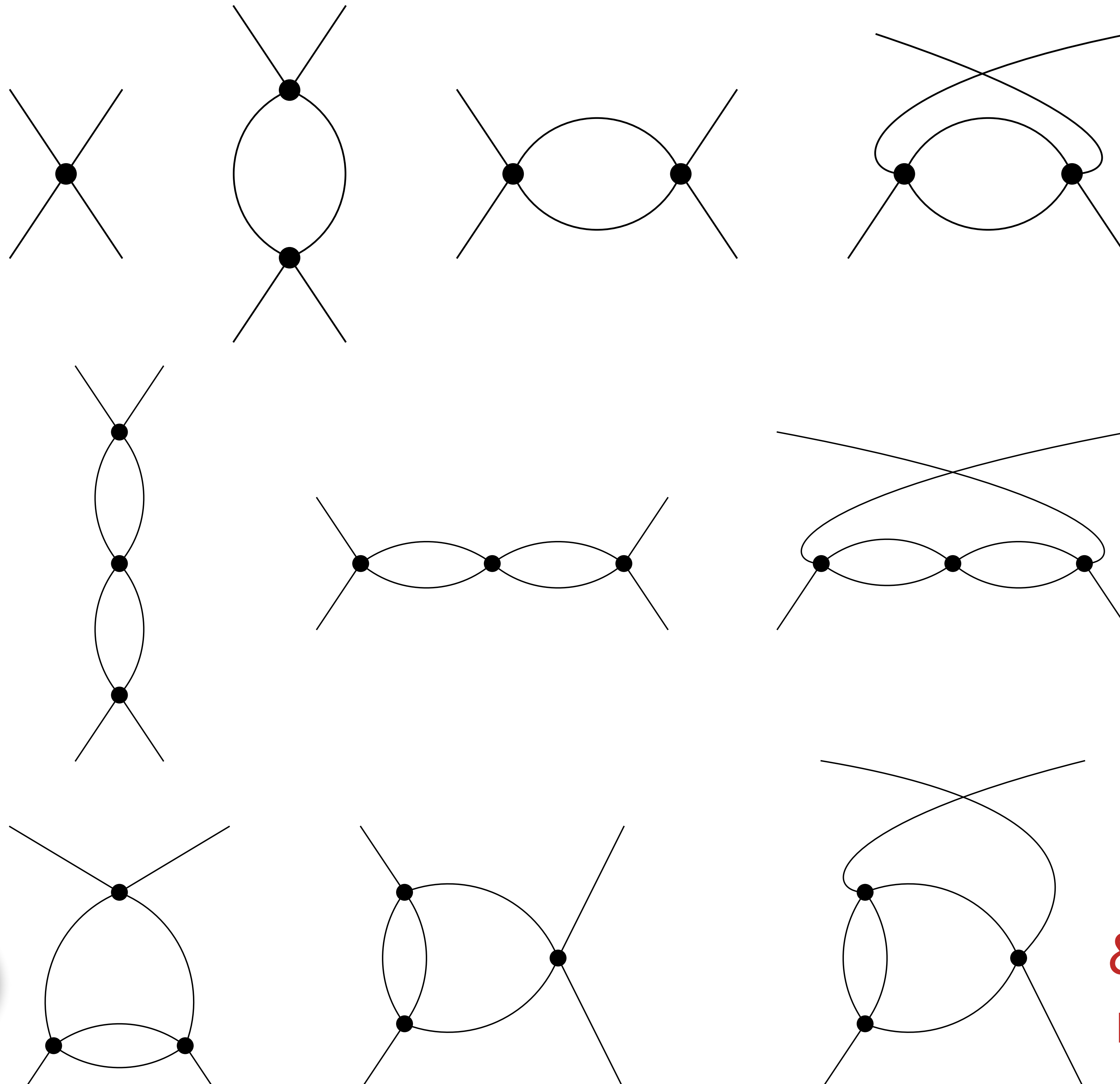


non-perturbative resummation

& many more...

Choice of Generator

- Wegner: $$\eta^{I} = \left[H_d, H_{od}\right]$$

- White: (J. Chem. Phys. 117, 7472)

$$\eta^{II} = \sum_{ph} \frac{f^{p}_{h}}{\Delta^{p}_{h}} :A^{p}_{h}: + \frac{1}{4}\sum_{pp'hh'} \frac{\Gamma^{pp'}_{hh'}}{\Delta^{pp'}_{hh'}} :A^{pp'}_{hh'}: - \text{H.c.}$$

$\Delta^{p}_{h}, \Delta^{pp'}_{hh'}$: approx. 1p1h, 2p2h excitation energies

- "imaginary time": (Morris, Bogner)

$$\eta^{III} = \sum_{ph} \operatorname{sgn}\left(\Delta^{p}_{h}\right) f^{p}_{h} :A^{p}_{h}: + \frac{1}{4}\sum_{pp'hh'} \operatorname{sgn}\left(\Delta^{pp'}_{hh'}\right) \Gamma^{pp'}_{hh'} :A^{pp'}_{hh'}: - \text{H.c.}$$

- 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 $\ll 1\%$

Brillouin Generator

- consider unitary variations of the energy functional

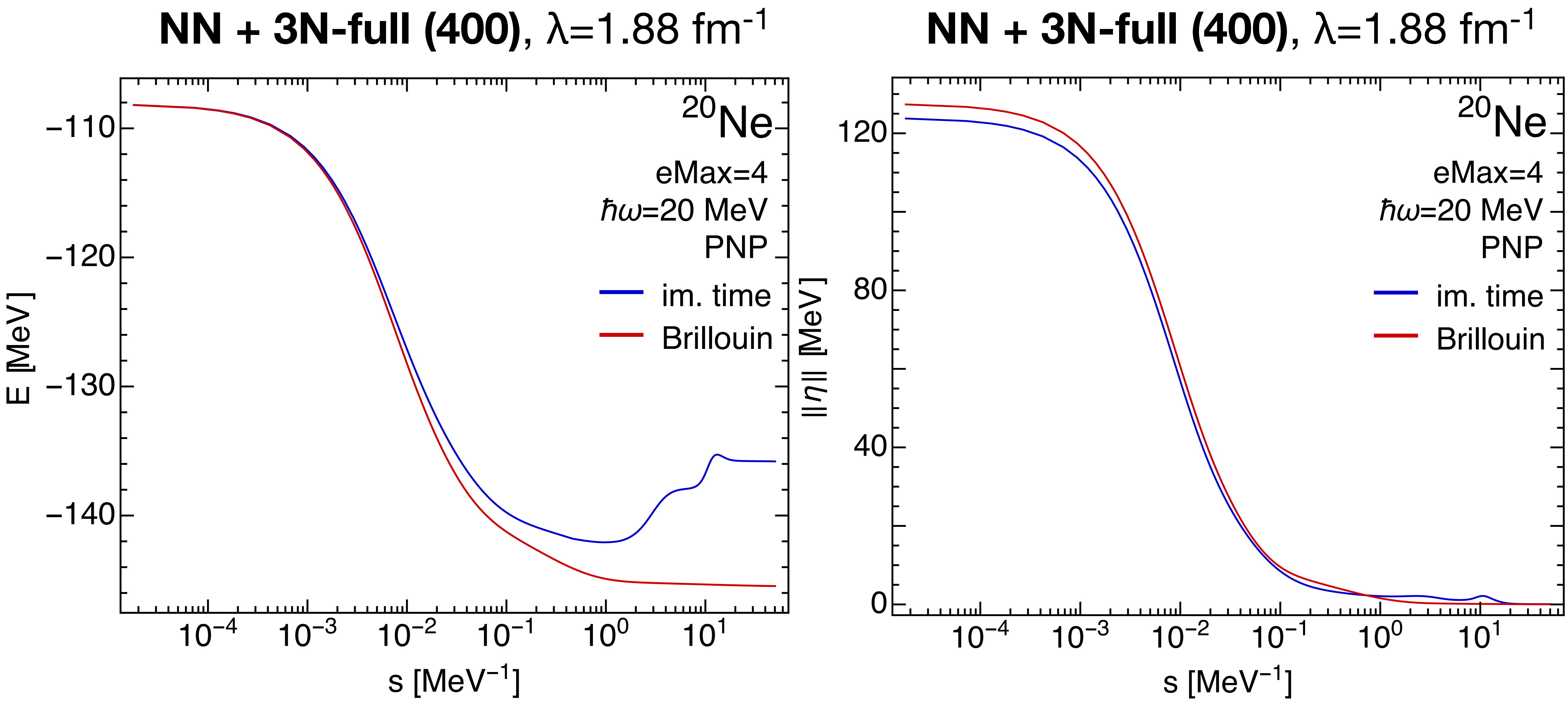
$$E(s) = \left\langle \Phi \right| H(s) \left| \Phi \right\rangle$$

- define generator as the residual of the irreducible Brillouin condition (= gradient of E)

$$\eta^{p}_{r} \equiv \left\langle \Phi \right| \left[:A^{p}_{r}:, H \right] \left| \Phi \right\rangle$$
$$\eta^{pq}_{rs} \equiv \left\langle \Phi \right| \left[:A^{pq}_{rs}:, H \right] \left| \Phi \right\rangle$$

- fixed point ($\eta = 0$) is reached when IBC is satisfied, energy stationary (cf. ACSE approach in Quantum Chemistry)
- Brillouin generator depends linearly on $\lambda^{p}_{s}, \lambda^{pq}_{st}, \lambda^{pqr}_{stu}$, higher irreducible density matrices are not required

Brillouin Generator



- ➡ energy & norm of Brillouin generator decay monotonically
- ➡ Projected HFB: 3B density matrix is (quasi-)diagonal ($O(N^3)$ storage), can be fully included in generator and energy flow

Particle-Number Projected HFB

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

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

- calculate irreducible densities (project only once), e.g.,

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

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

$$\lambda^k_l = n_k\delta^k_l \left(= v^2_k\delta^k_l\right), \quad 0 \leq n_k \leq 1$$

- in NO basis, $\lambda^{kl}_{mn}, \lambda^{klm}_{nop}$ require only $N^2/2$, $N^3/4$ storage