

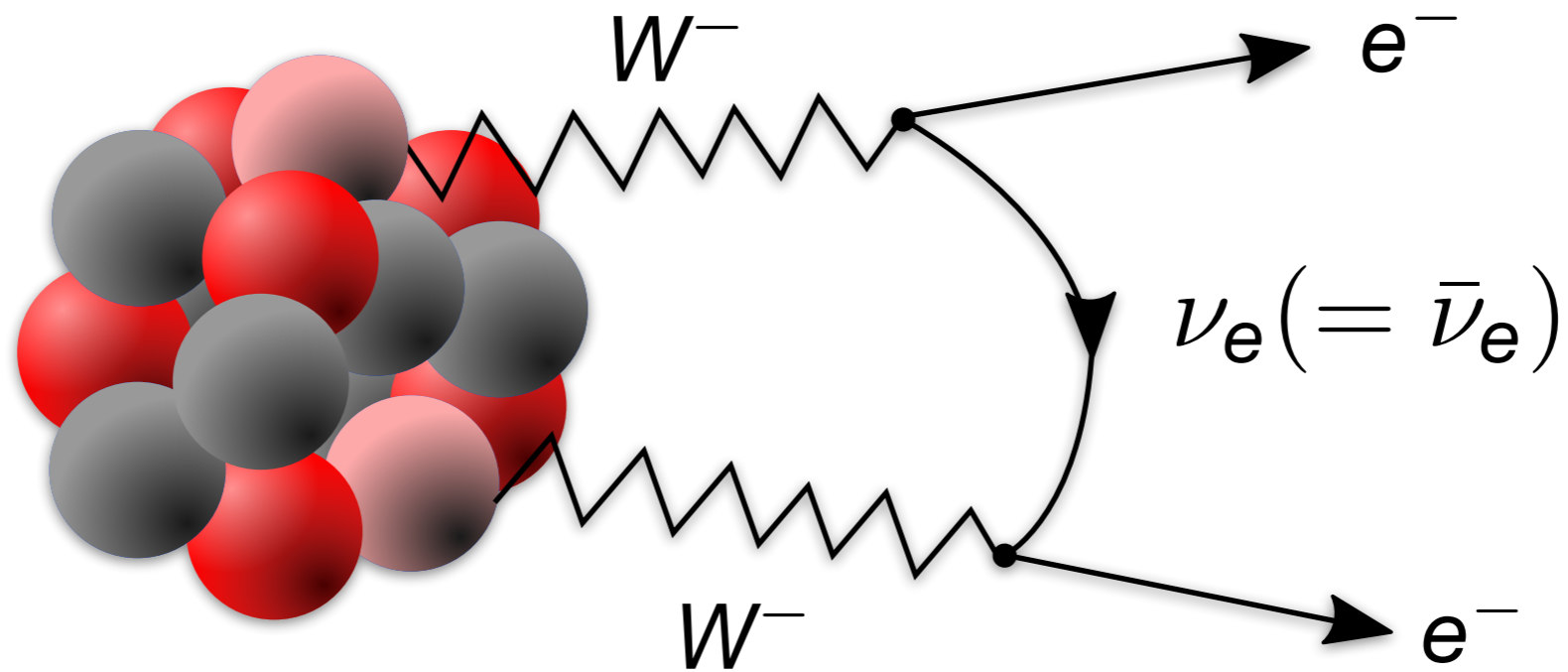
Describing $\beta\beta$ Decay Processes in the In-Medium SRG Framework

Heiko Hergert

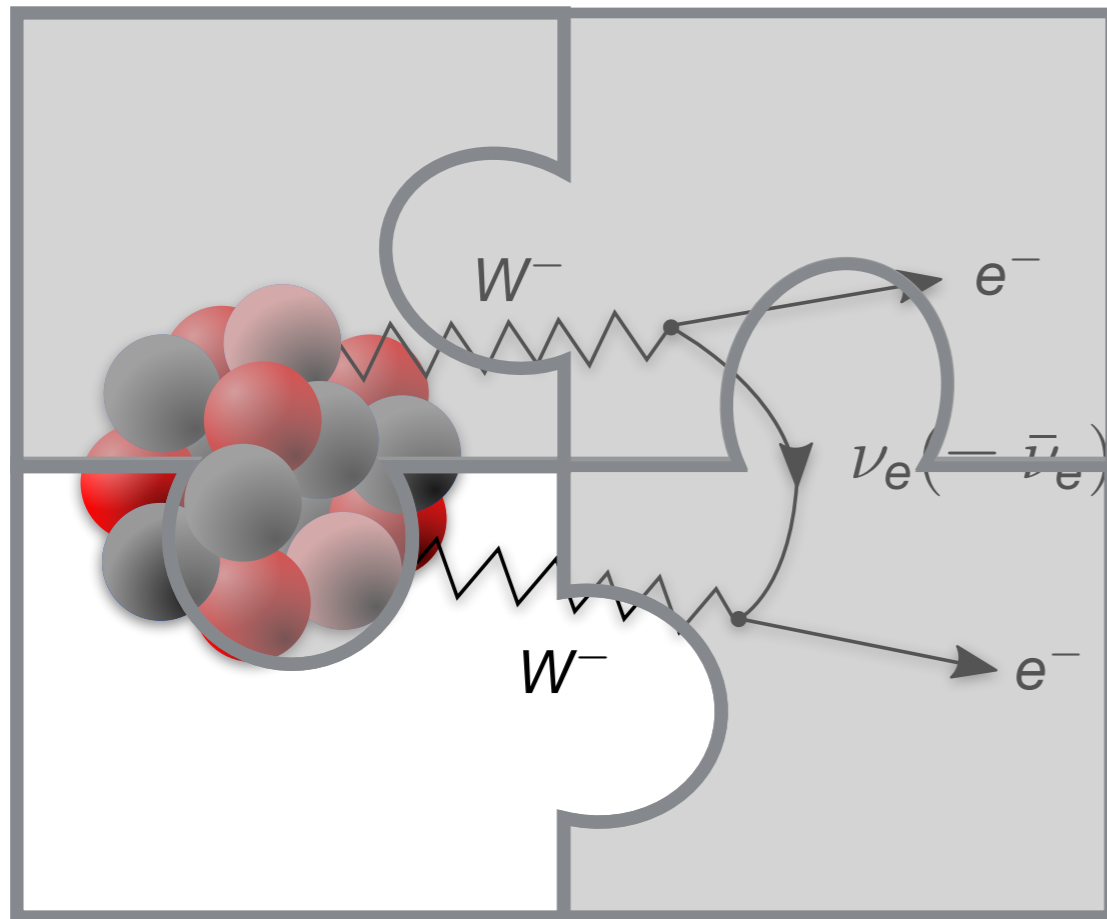
National Superconducting Cyclotron Laboratory
& Department of Physics and Astronomy
Michigan State University



Neutrinoless Double Beta Decay



Neutrinoless Double Beta Decay



- **interactions and transition operators** from Chiral EFT, **including currents**
(cf. talks by S. Pastore and A. Schwenk)
- tune **resolution scale** of the Hamiltonian / Hilbert space
(cf. talk by P. Navrátil, also M. Horoi)
- **(MR-)IM-SRG**: calculate ground (and excited) states or derive Shell Model interaction
(also see talk by R. Stroberg)
- evaluate **1B, 2B** (, 3B,...) **transition operator**

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

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 $H(\mathbf{s}) = U(\mathbf{s})H U^\dagger(\mathbf{s})$:

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

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

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

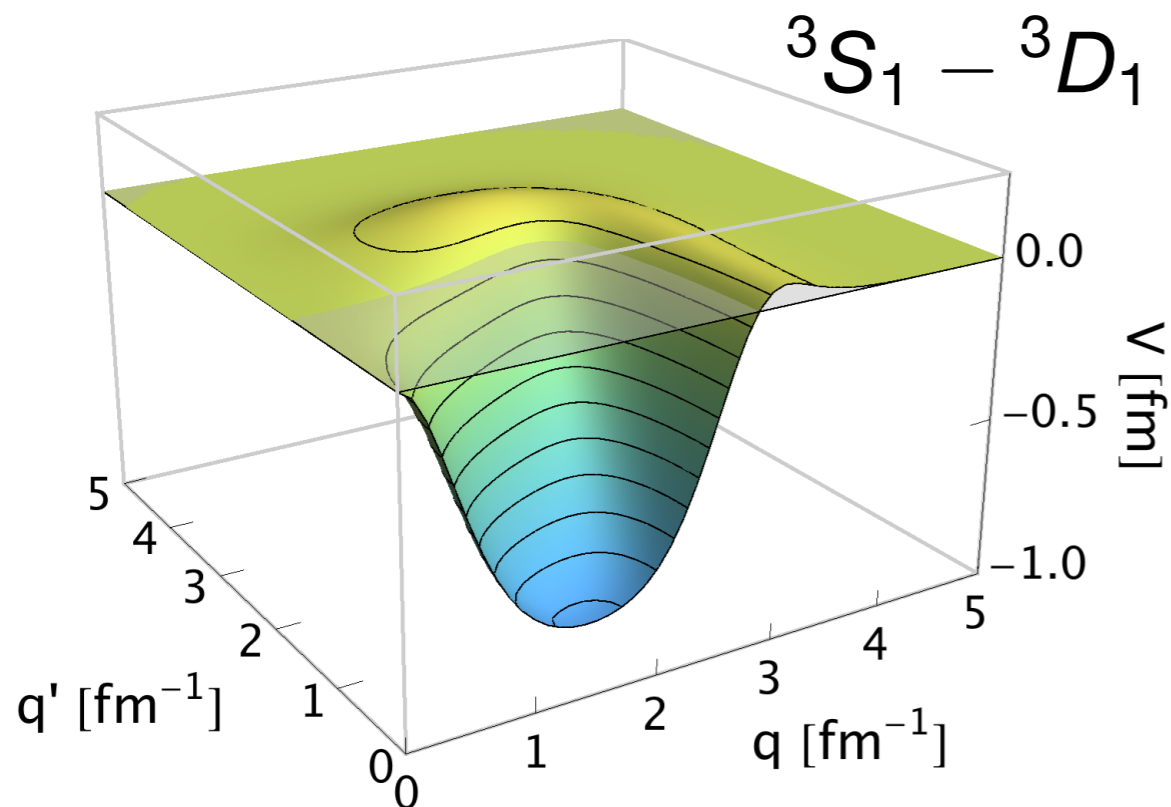
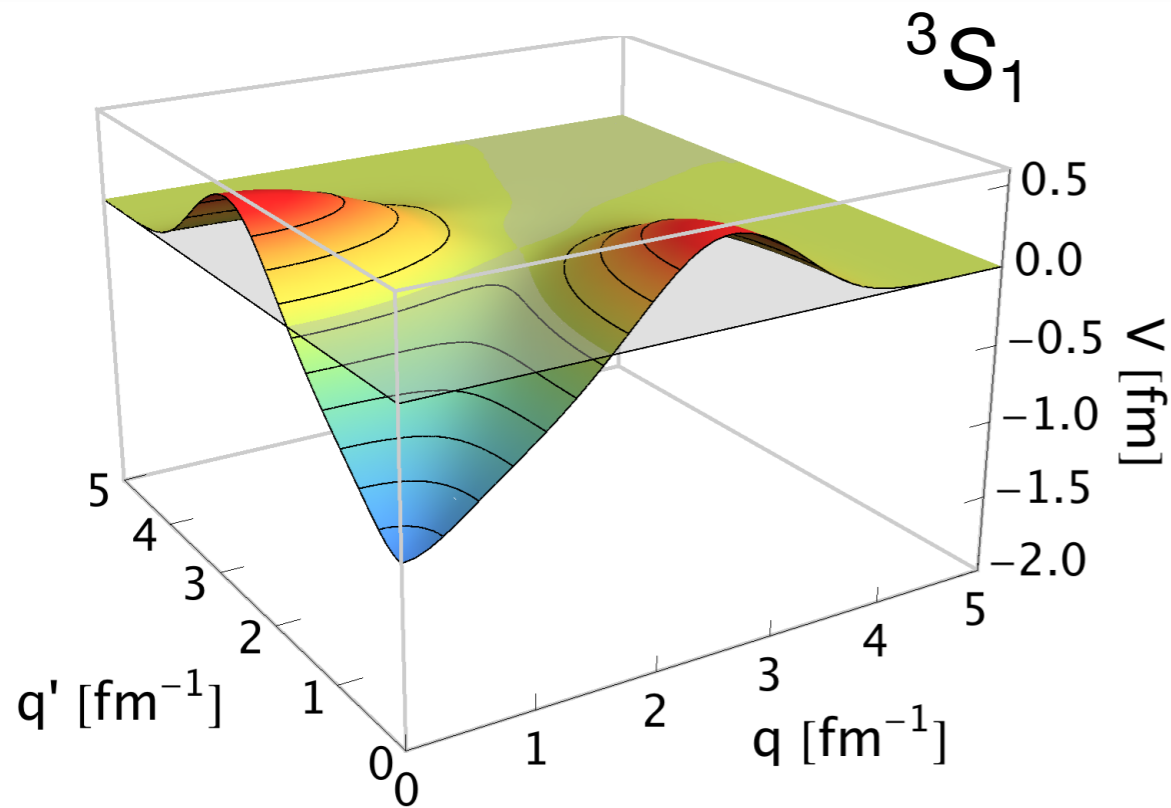
to **suppress** (suitably defined) **off-diagonal Hamiltonian**

- **consistent evolution** for all **observables** of interest

SRG in Two-Body Space



momentum space matrix elements

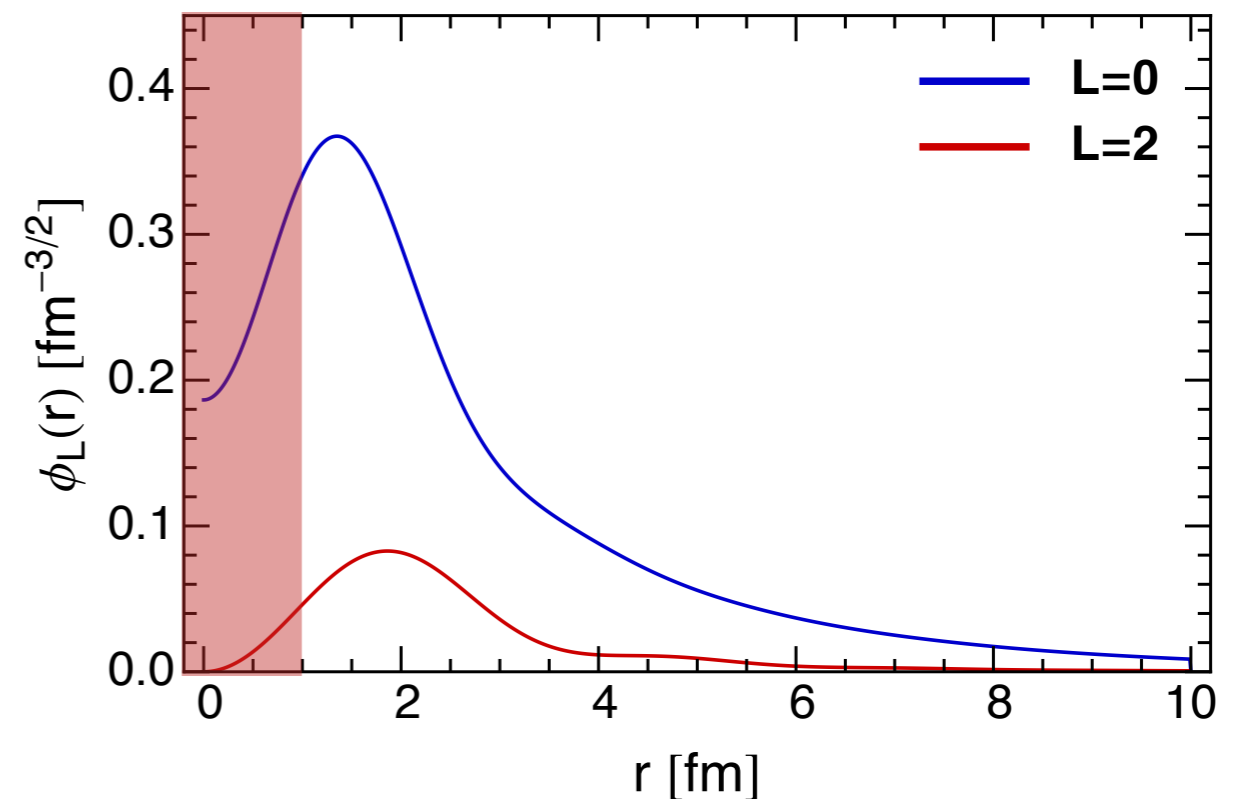


chiral NN
Entem & Machleidt, N3LO

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

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

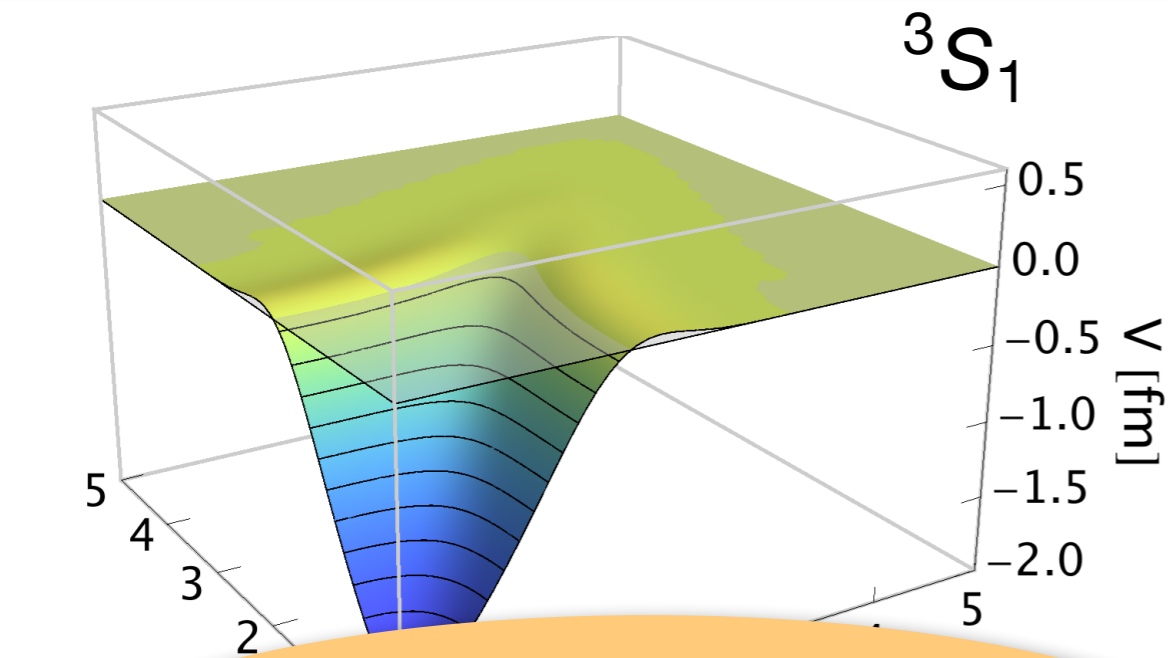
deuteron wave function



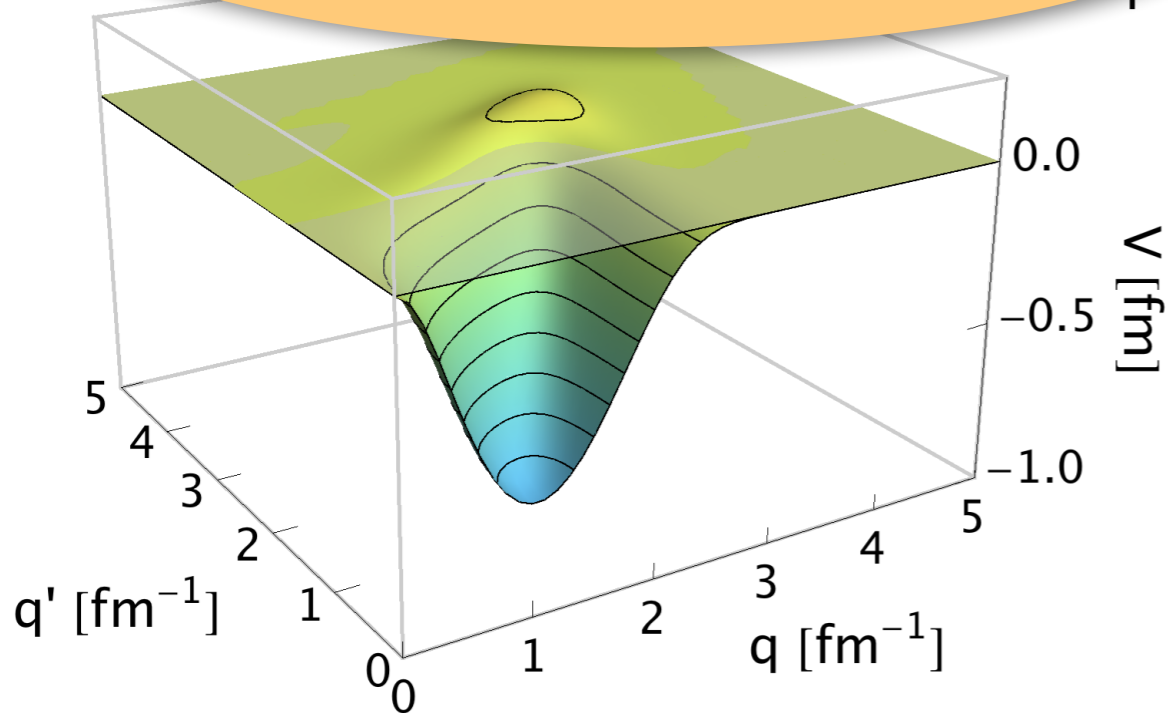
SRG in Two-Body Space



momentum space matrix elements



lowering resolution scale λ
 \Leftrightarrow decoupling of low and high momenta

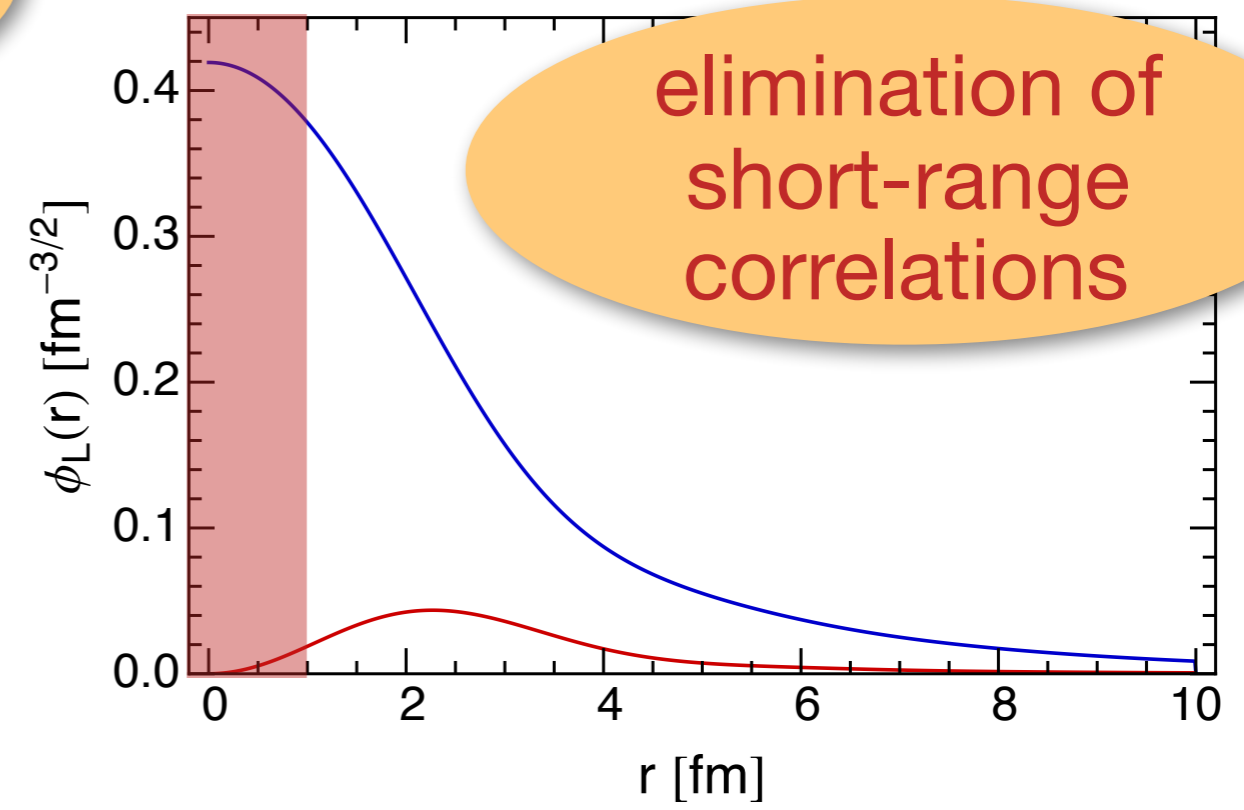


$$\lambda = 1.8 \text{ fm}^{-1}$$

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

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

deuteron wave function



elimination of short-range correlations

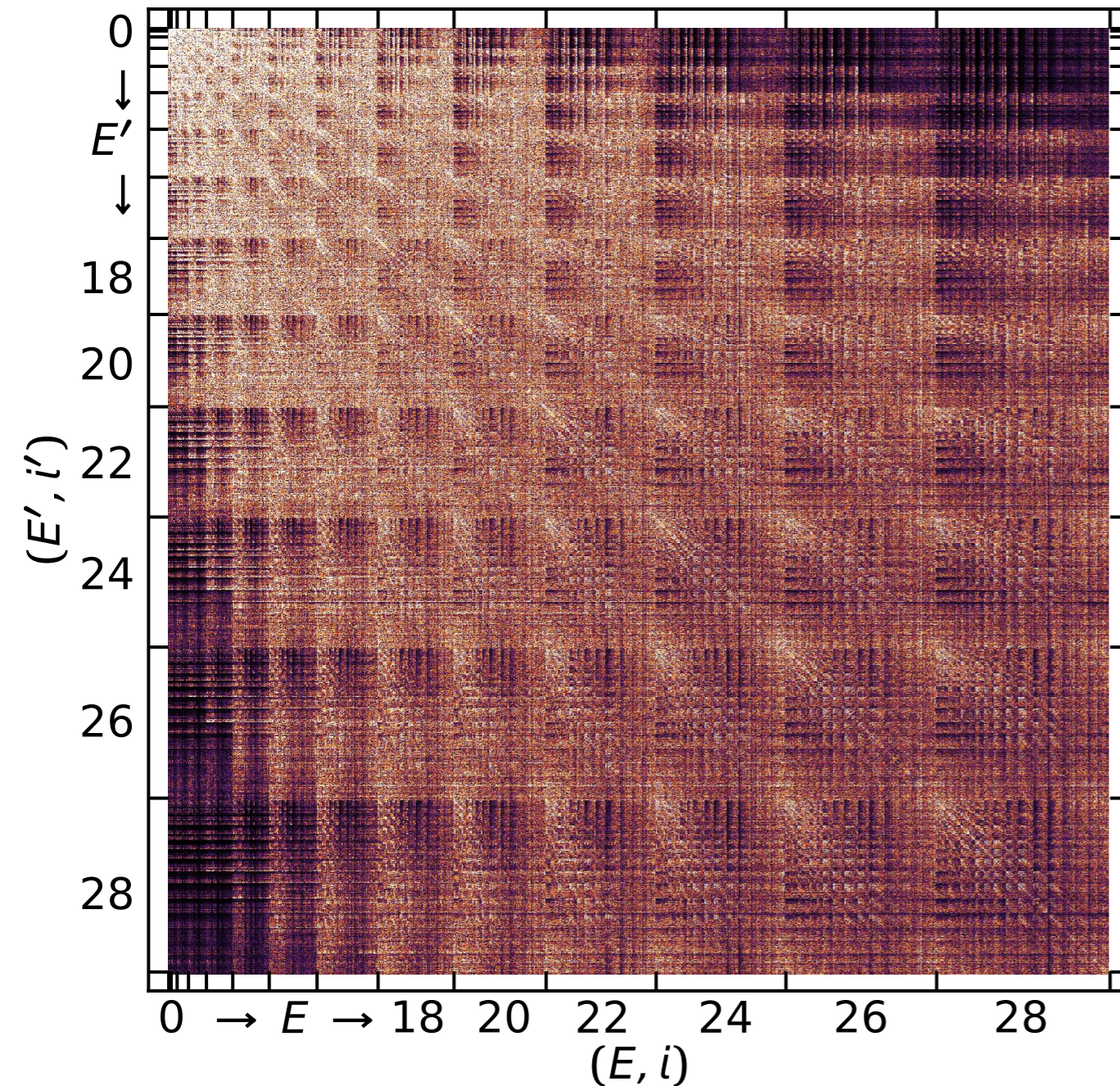
SRG in Three-Body Space



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

3B Jacobi-HO Matrix Elements

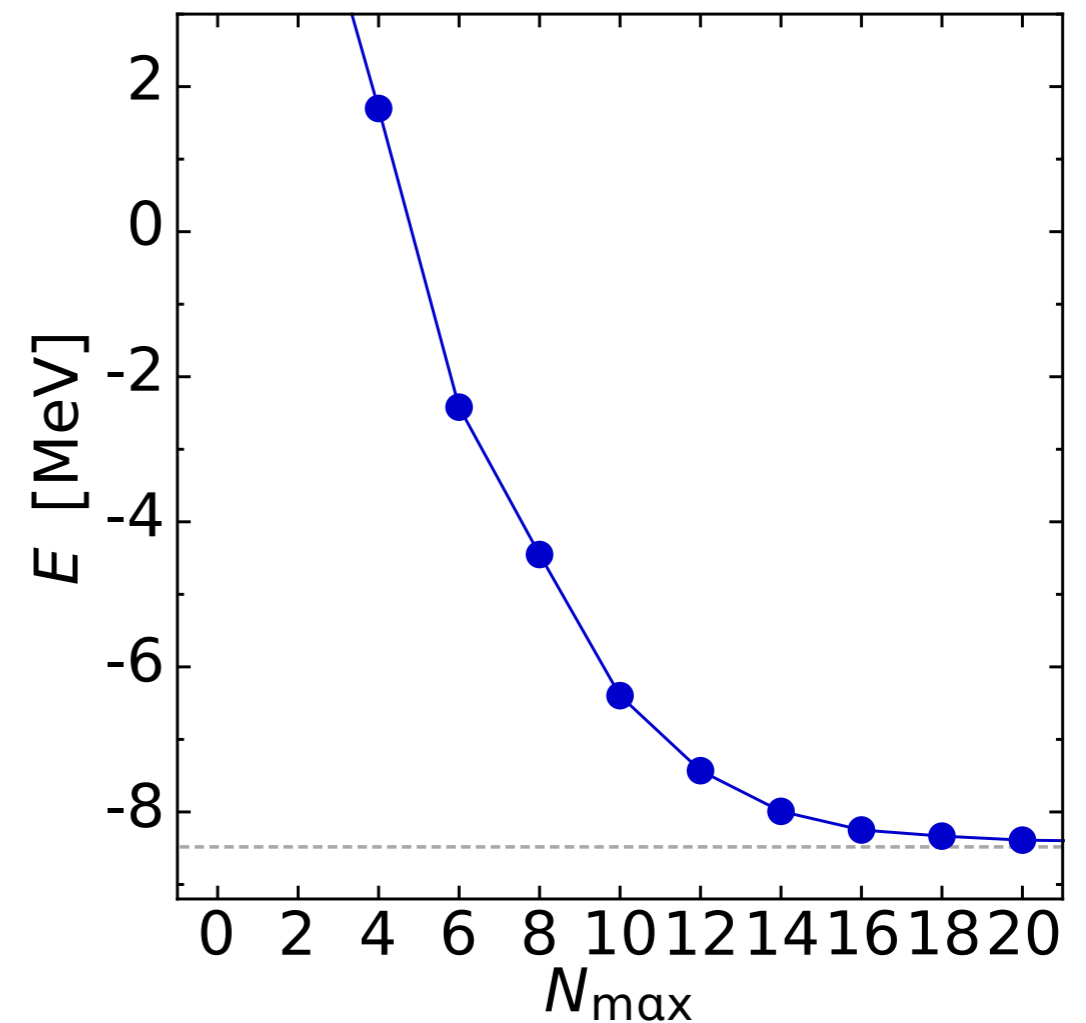
$$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28 \text{ MeV}$$



chiral NN + 3N

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

^3H ground-state (NCSM)



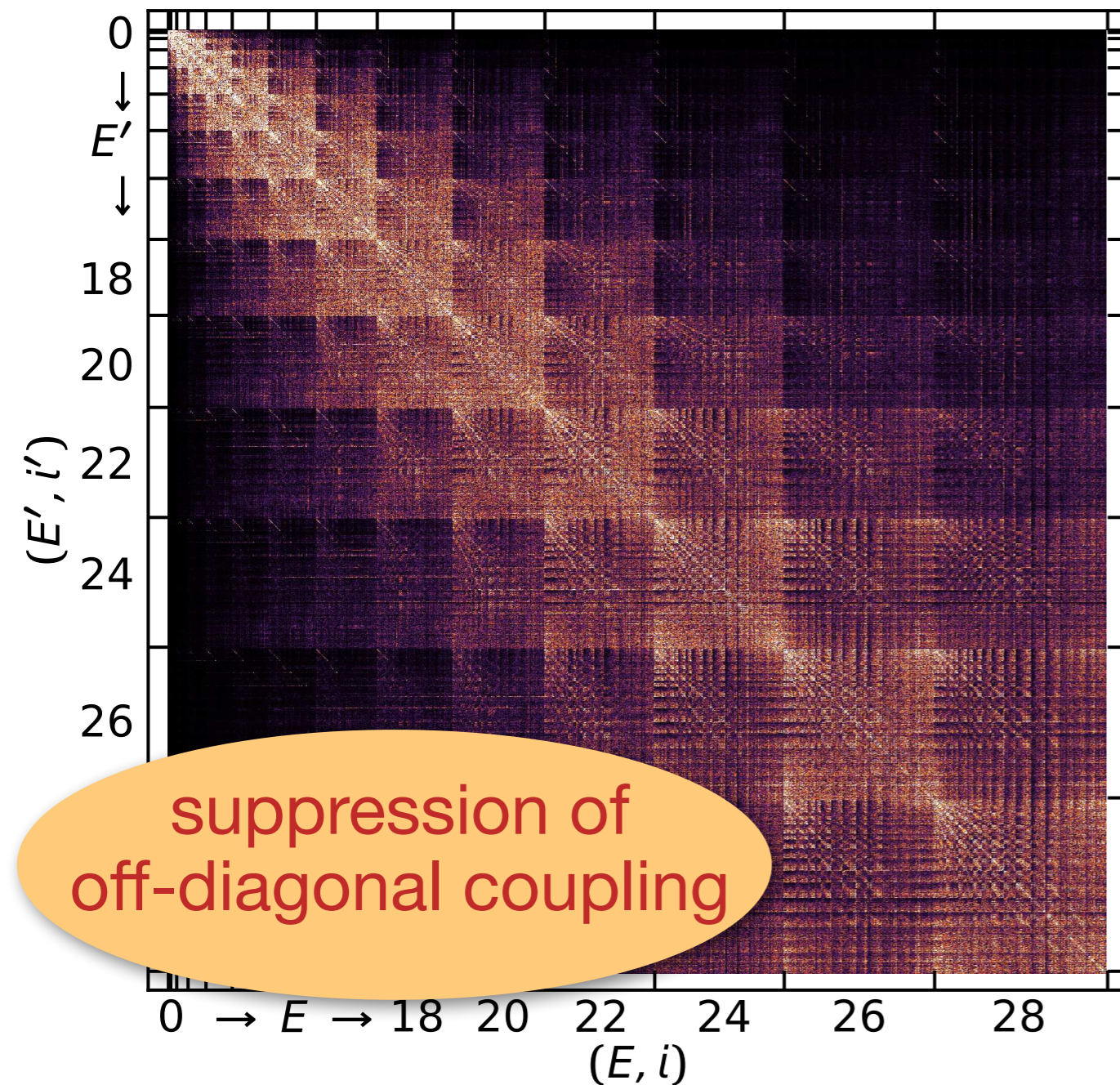
SRG in Three-Body Space



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

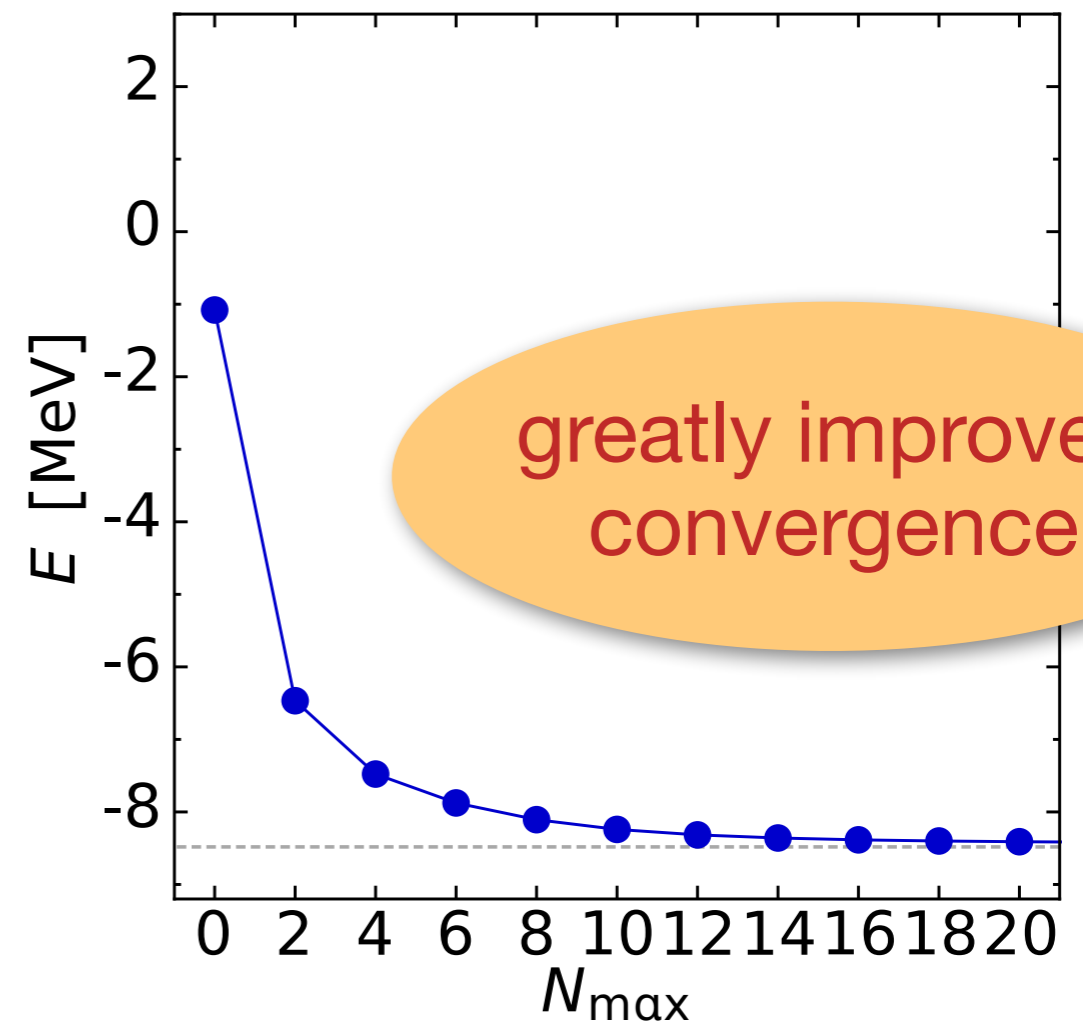
3B Jacobi-HO Matrix Elements

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



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

^3H ground-state (NCSM)



(Multi-Reference) In-Medium SRG

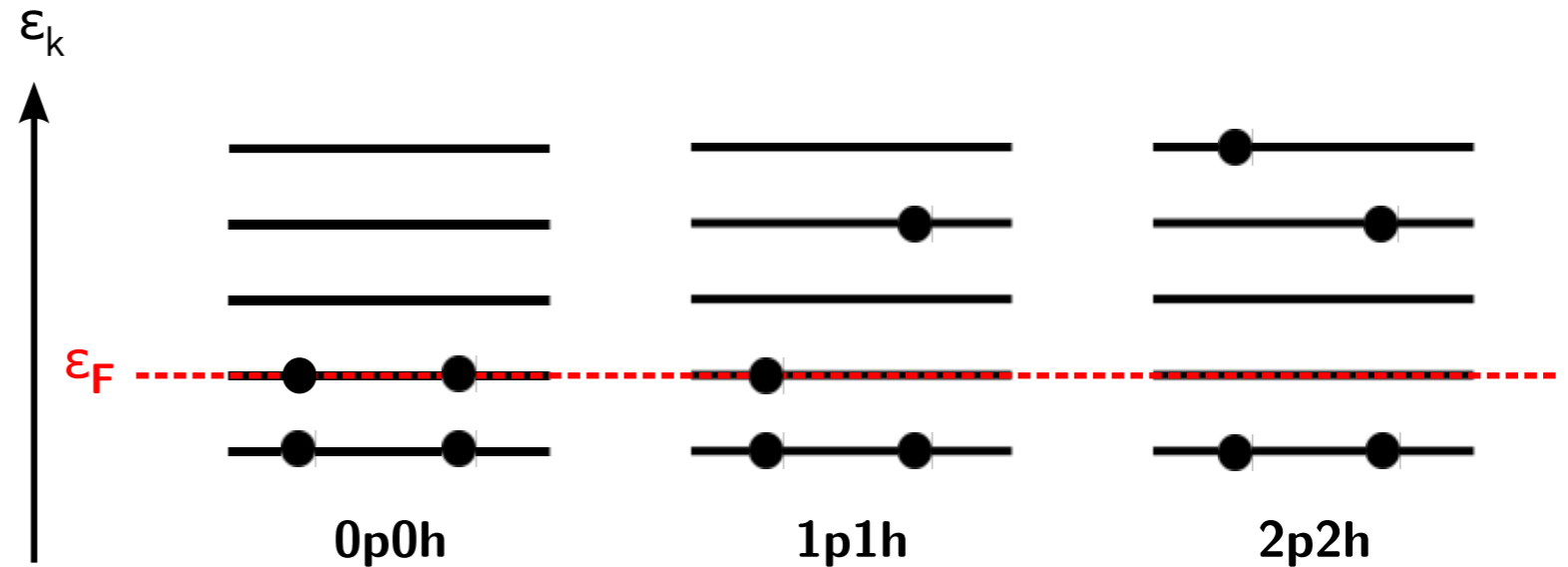
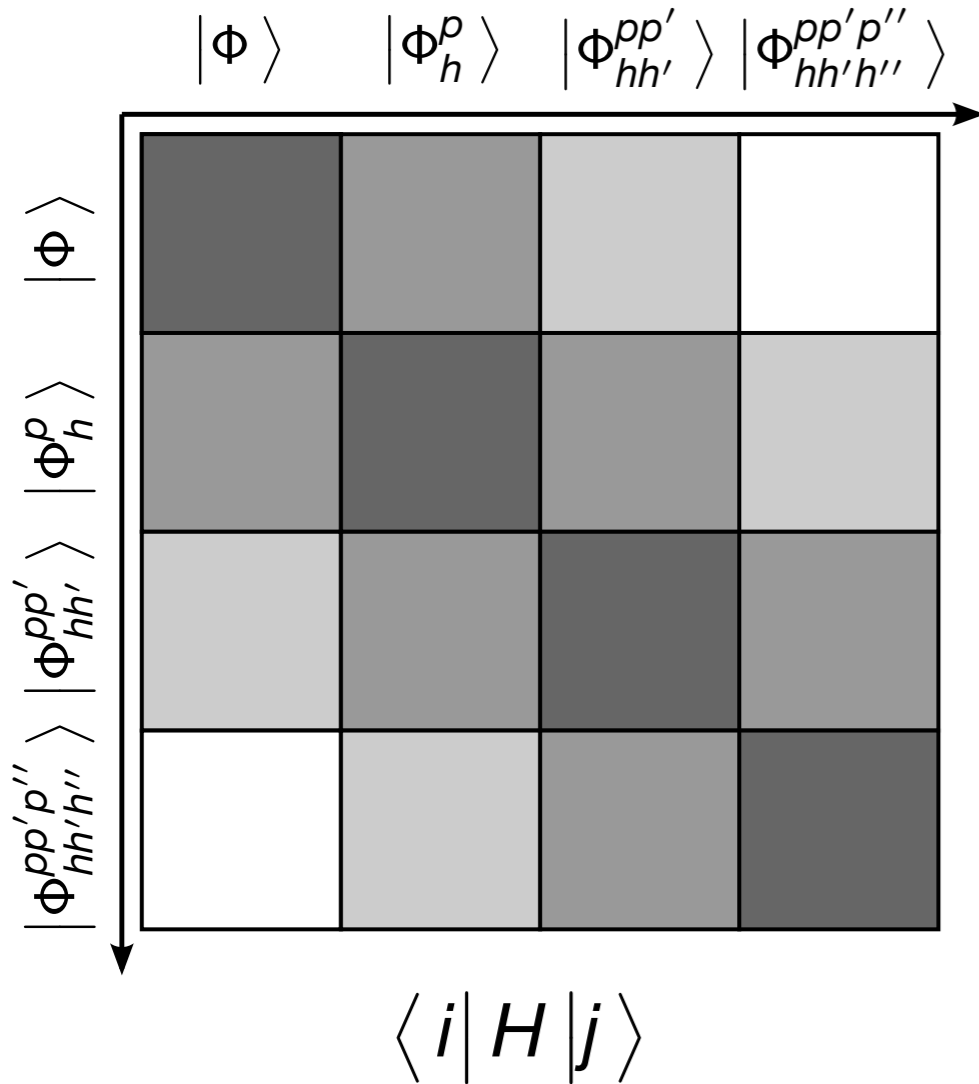
H. H., in preparation

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)

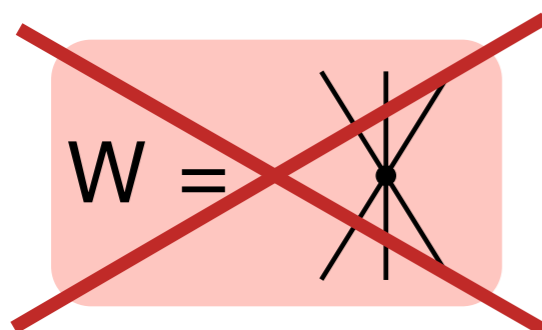
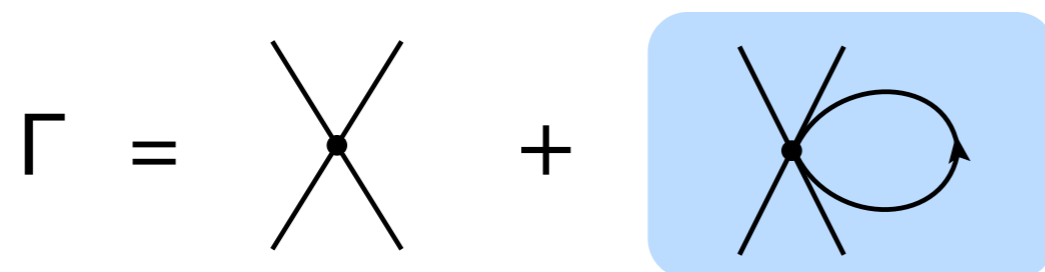
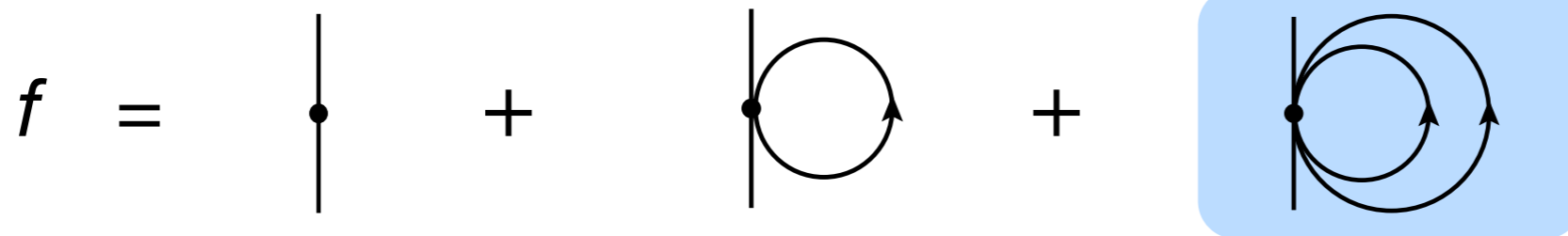
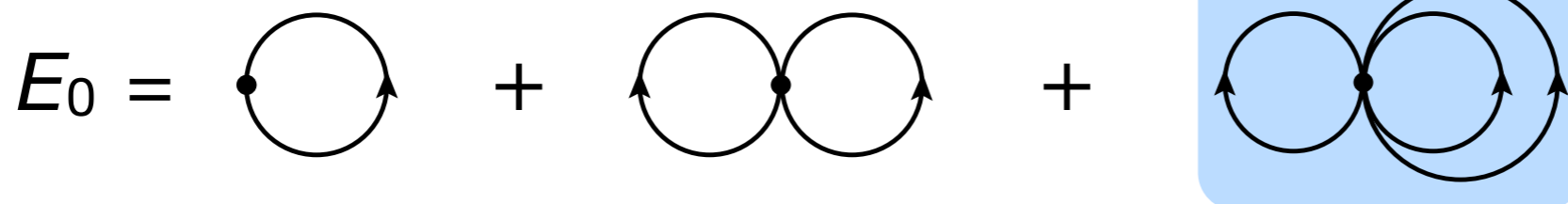
Ground-State Decoupling



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

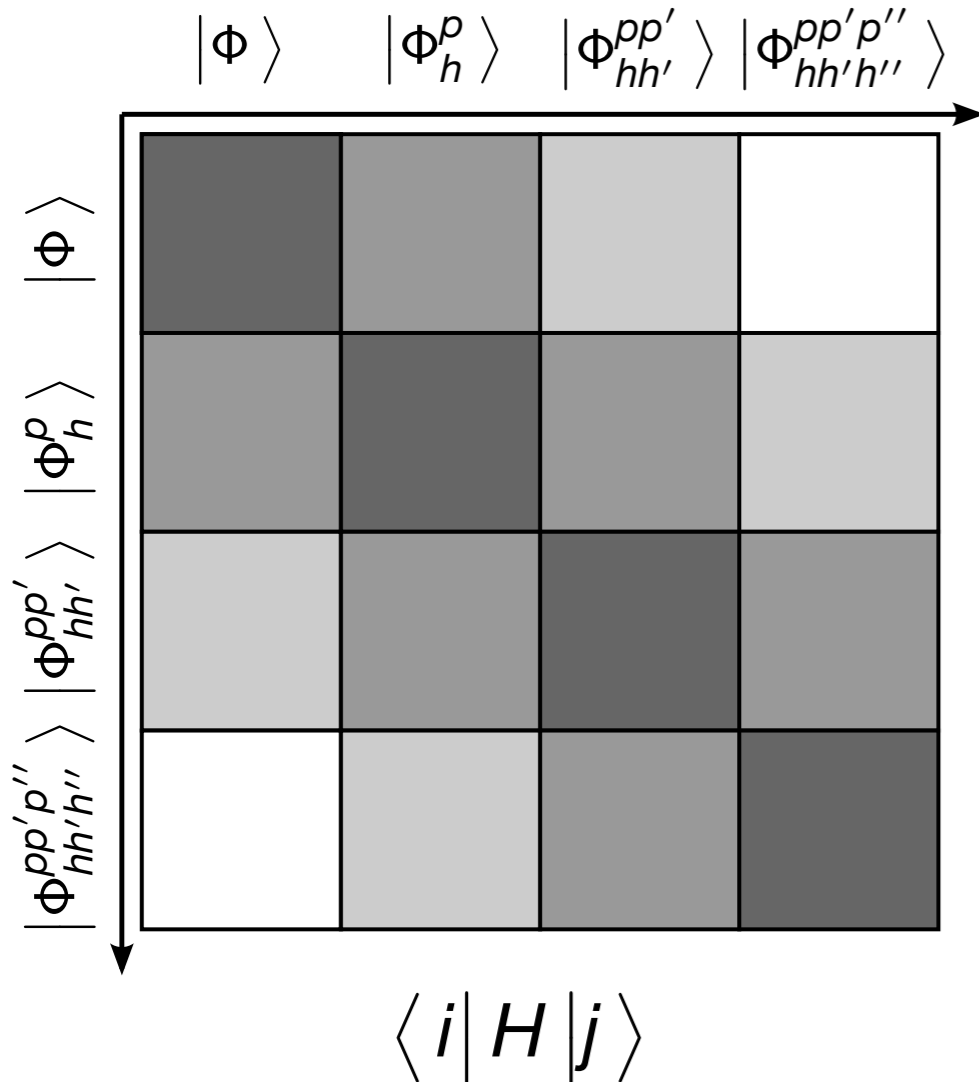
Normal-Ordered Hamiltonian

$$H = E_0 + \sum_{kl} f_l^k : A_l^k : + \frac{1}{4} \sum_{klmn} \Gamma_{mn}^{kl} : A_{mn}^{kl} : + \frac{1}{36} \sum_{ijklmn} W_{lmn}^{ijk} : A_{lmn}^{ijk} :$$



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

Single-Reference Case



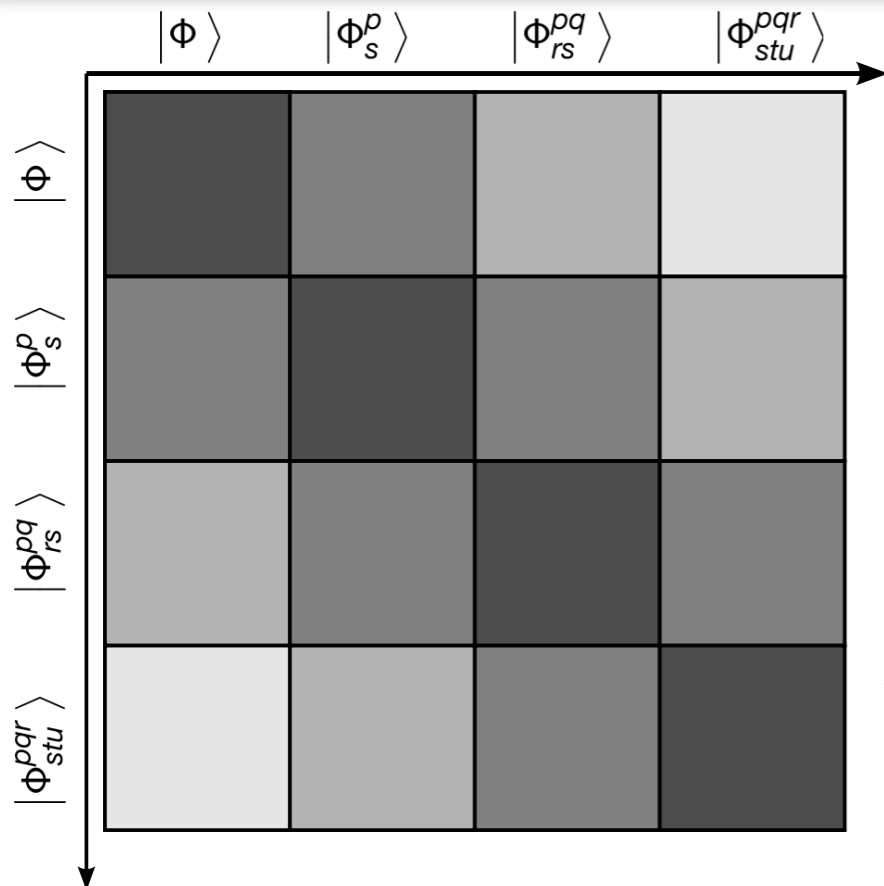
$$A_{j_1 \dots j_N}^{i_1 \dots i_N} \equiv a_{i_1}^\dagger \dots a_{i_N}^\dagger a_{j_N} \dots a_{j_1}$$

$$\langle \begin{smallmatrix} p \\ h \end{smallmatrix} | H | \Psi \rangle = \sum_{kl} f_l^k \langle \Psi | : A_p^h :: A_l^k : | \Psi \rangle = -n_h \bar{n}_p f_h^p$$

$$\langle \begin{smallmatrix} pp' \\ hh' \end{smallmatrix} | H | \Psi \rangle = \sum_{klmn} \Gamma_{mn}^{kl} \langle \Psi | : A_{pp'}^{hh'} :: A_{mn}^{kl} : | \Psi \rangle \sim \Gamma_{hh'}^{pp'}$$

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

Multi-Reference Case



$$\langle \begin{matrix} p \\ s \end{matrix} | H | \Phi \rangle \sim \bar{n}_p n_s f_s^p, \sum_{kl} f_l^k \lambda_{pl}^{sk}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pmn}^{skl}, \dots$$

$$\langle \begin{matrix} pq \\ st \end{matrix} | H | \Phi \rangle \sim \bar{n}_p \bar{n}_q n_s n_t \Gamma_{st}^{pq}, \sum_{kl} \Gamma_{sl}^{pk} \lambda_{ql}^{tk}, \sum_{kl} f_l^k \lambda_{pq}^{stk}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pqmn}^{stkl}, \dots$$

$$\langle \begin{matrix} pqr \\ stu \end{matrix} | H | \Phi \rangle \sim \dots$$

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

$$\rho_{mn}^{kl} = \lambda_{mn}^{kl} + \lambda_m^k \lambda_n^l - \lambda_n^k \lambda_m^l$$

$$\rho_{lmn}^{ijk} = \lambda_{lmn}^{ijk} + \lambda_l^i \lambda_{mn}^{jk} + \lambda_l^i \lambda_m^j \lambda_n^k + \text{permutations}$$

...

MR-IM-SRG References States



available

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

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

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

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

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

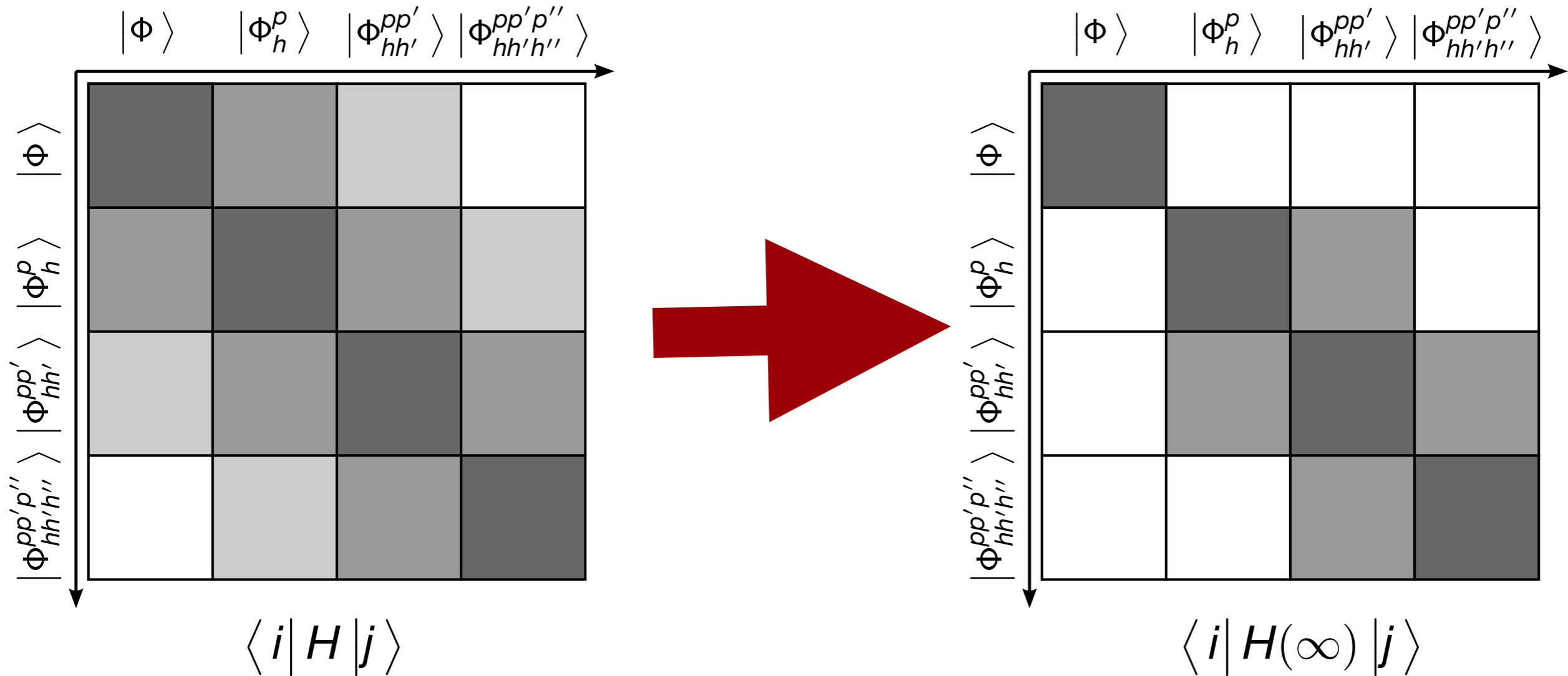
$$|\Phi\rangle = \int dq f(q) P_{J=0M=0} P_Z P_N |q\rangle$$

- Density Matrix Renormalization Group, Tensor Network States, ...

**complement
particle-hole type
correlations**

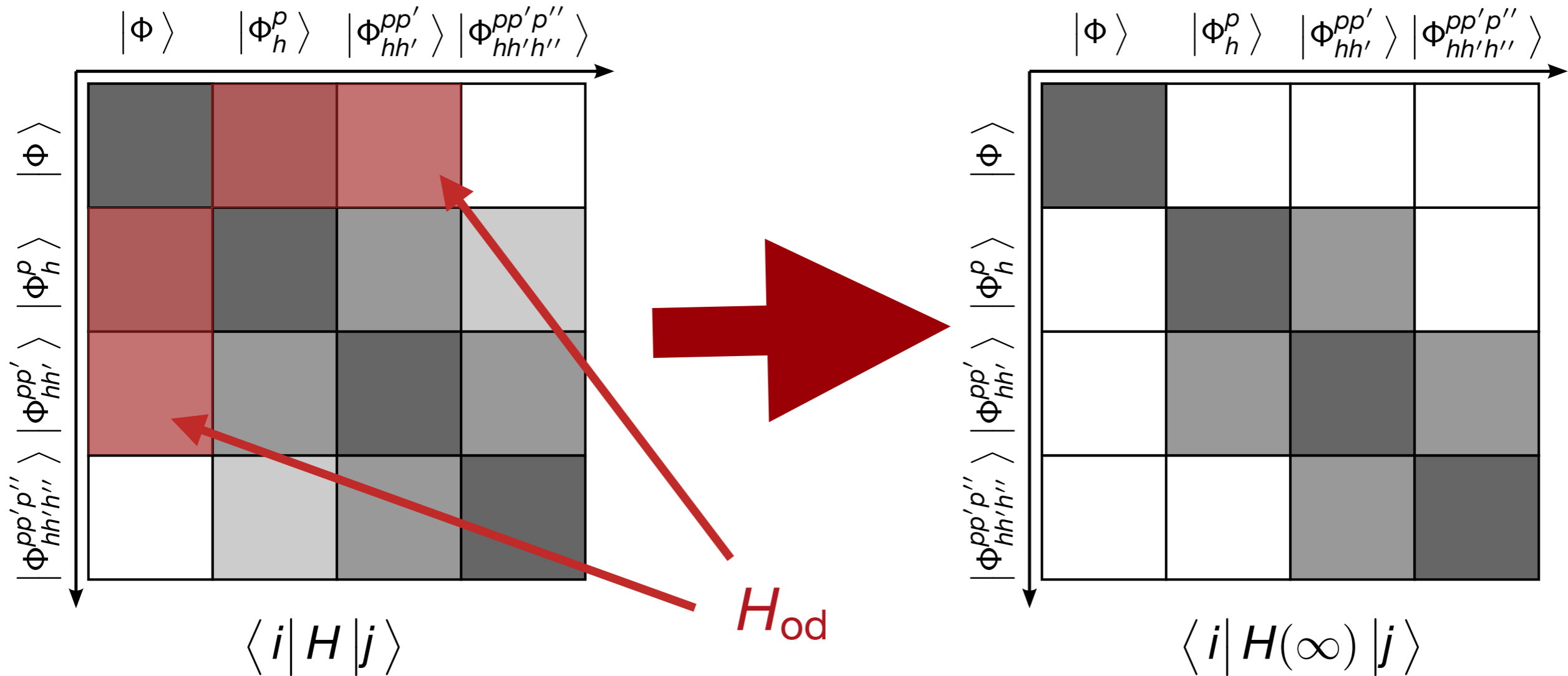
future

Decoupling in A-Body Space



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

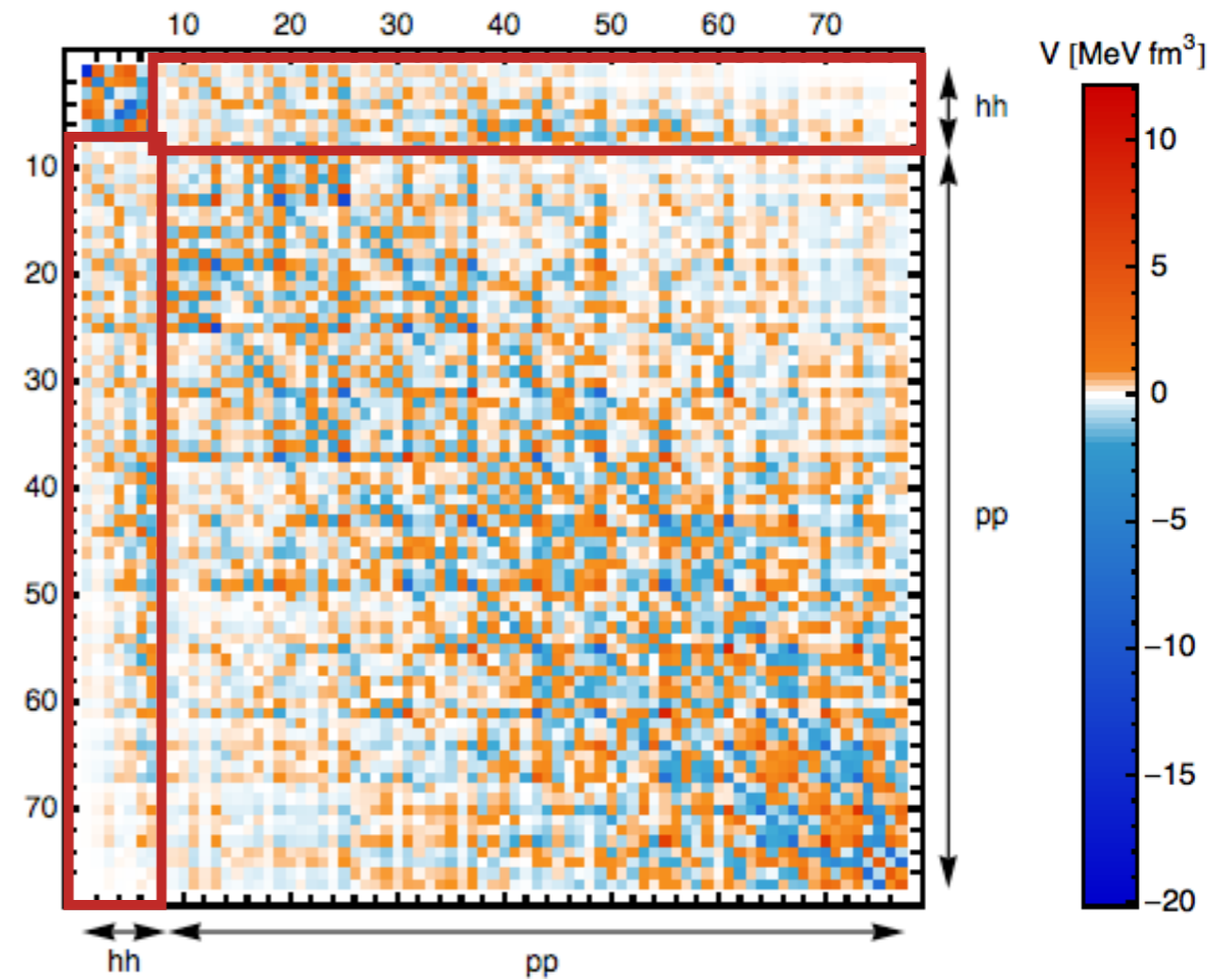
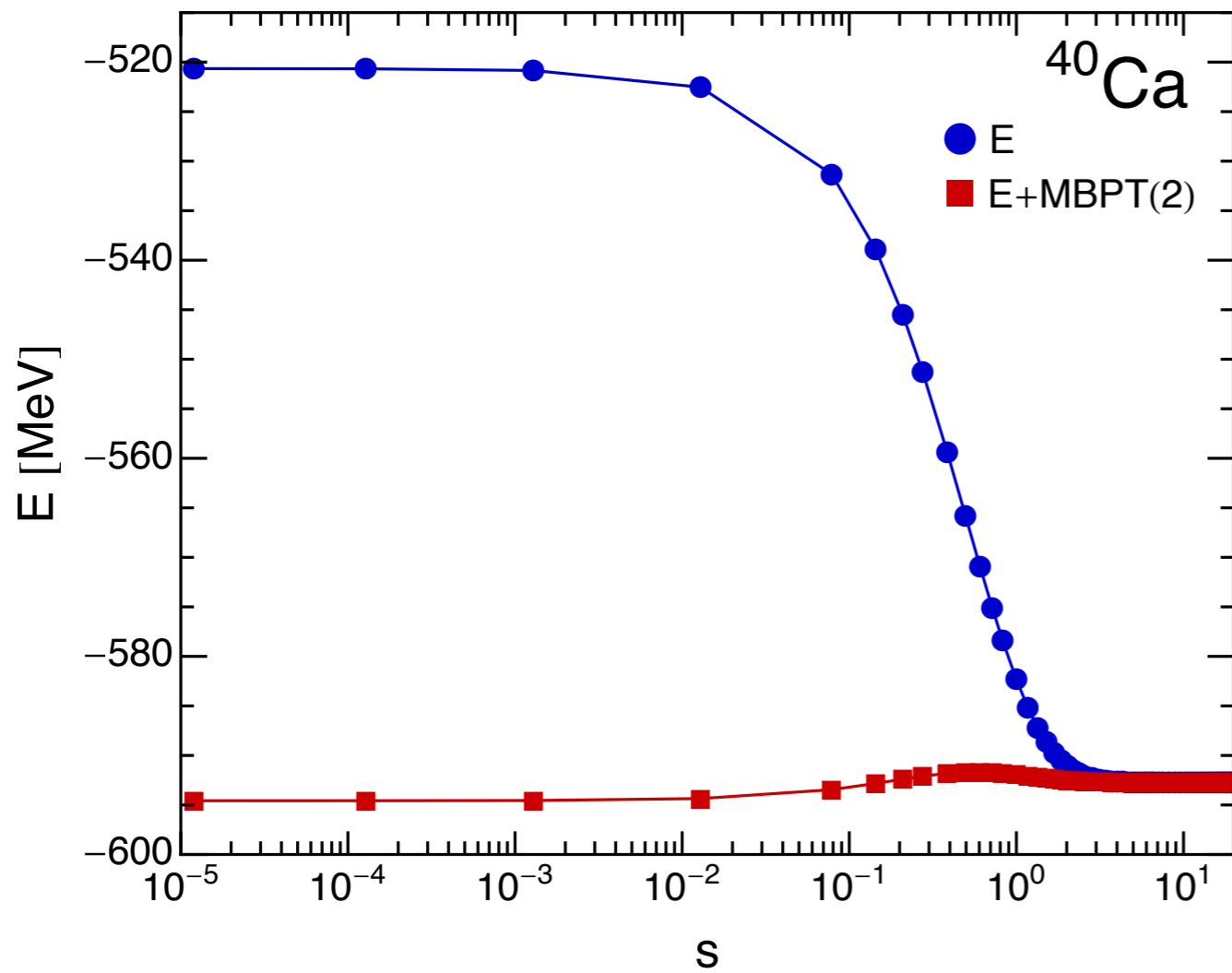
Flow Equation



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

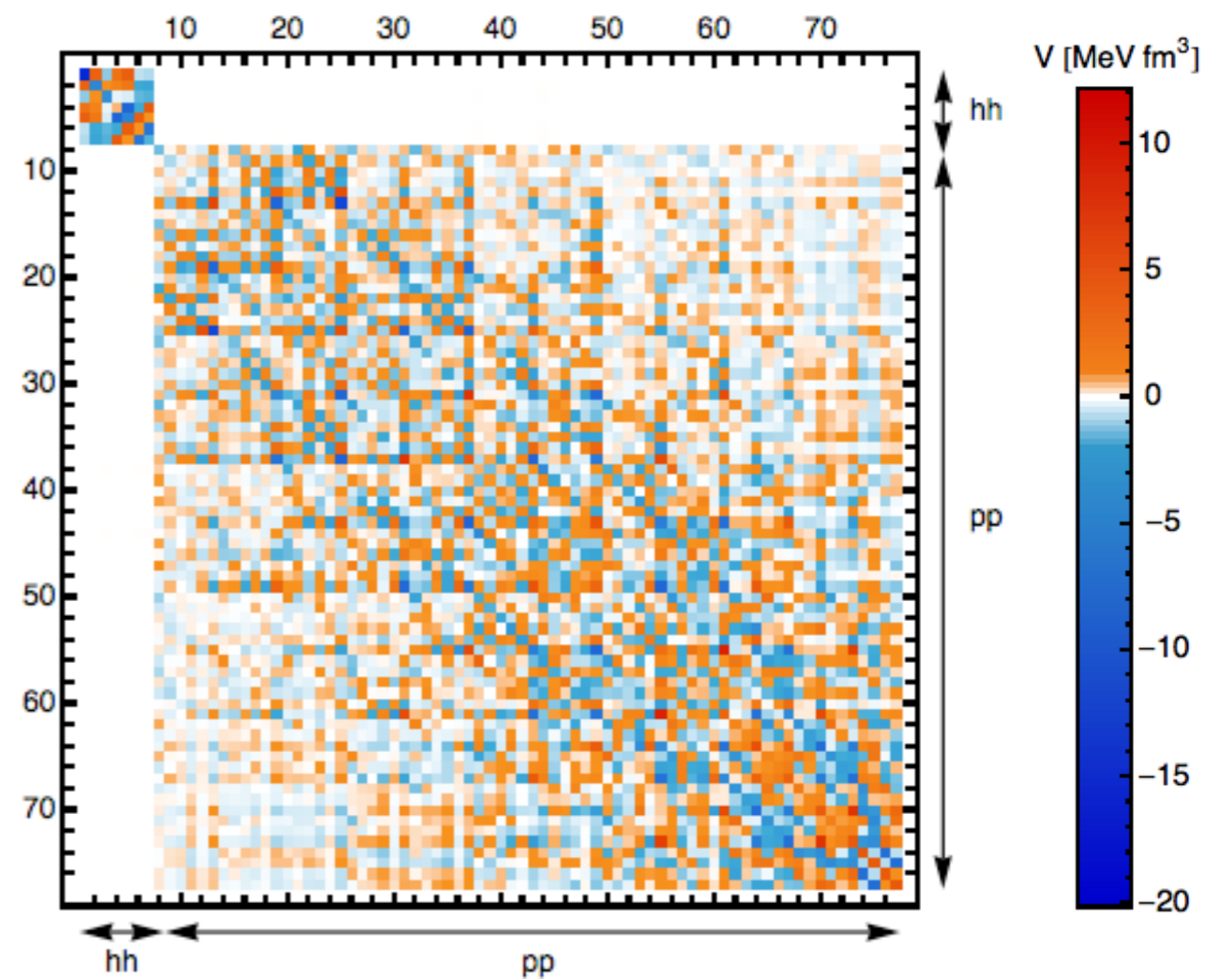
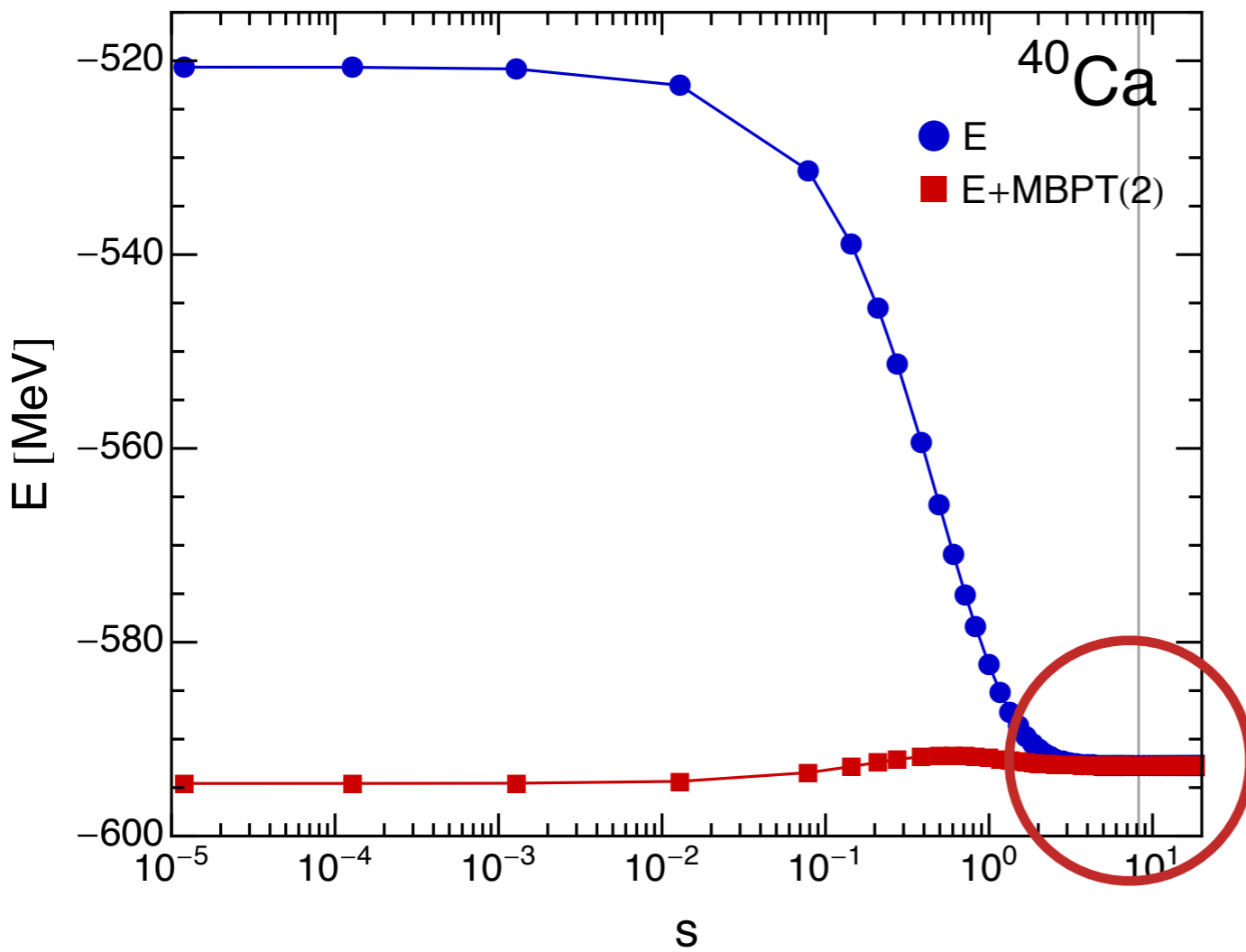
more efficient: solve flow using Magnus methods, **T. D. Morris** et al., PRC **92**, 034331 (2015)

Decoupling



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

Decoupling



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

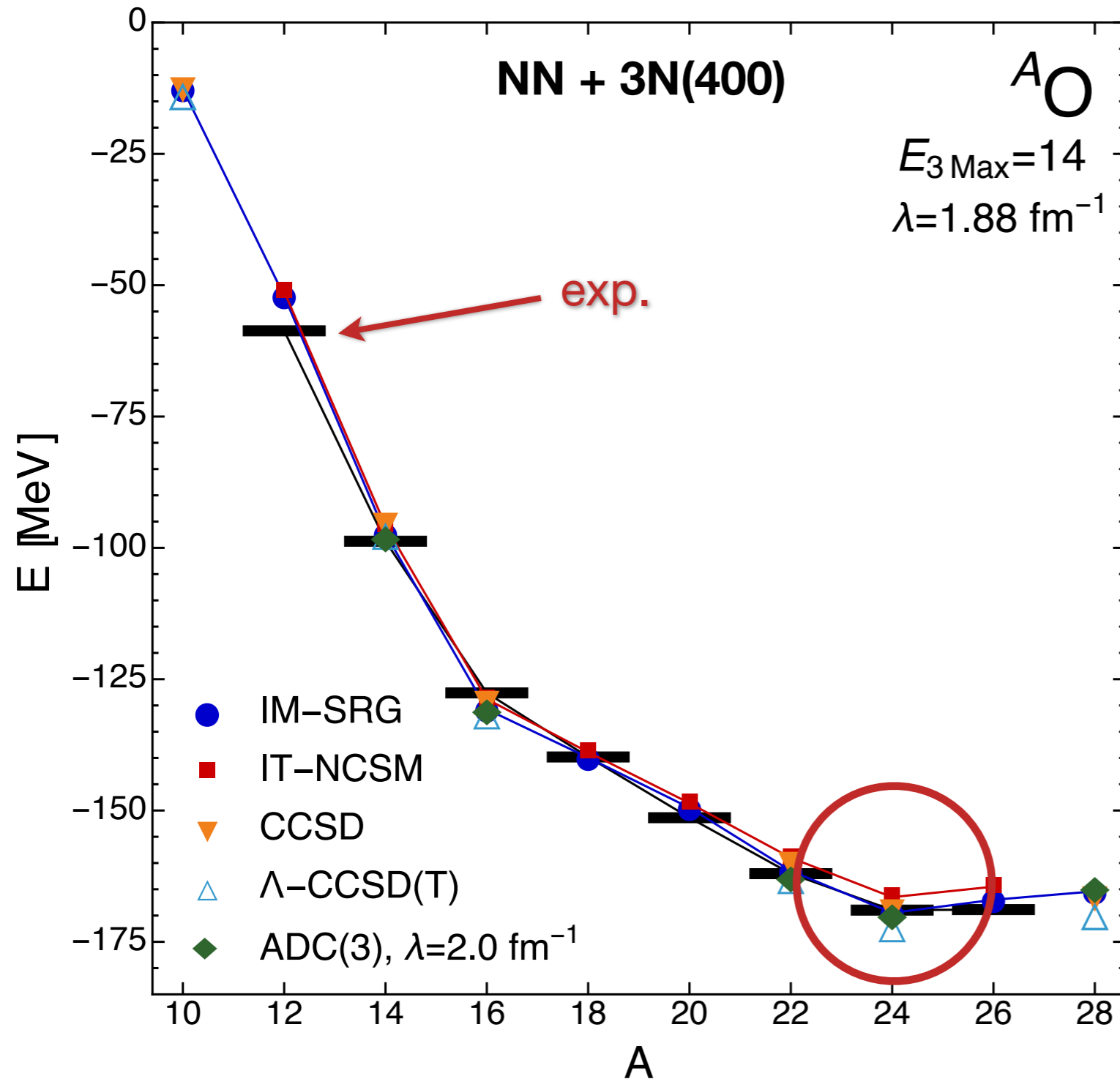
non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Oxygen Isotopes



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



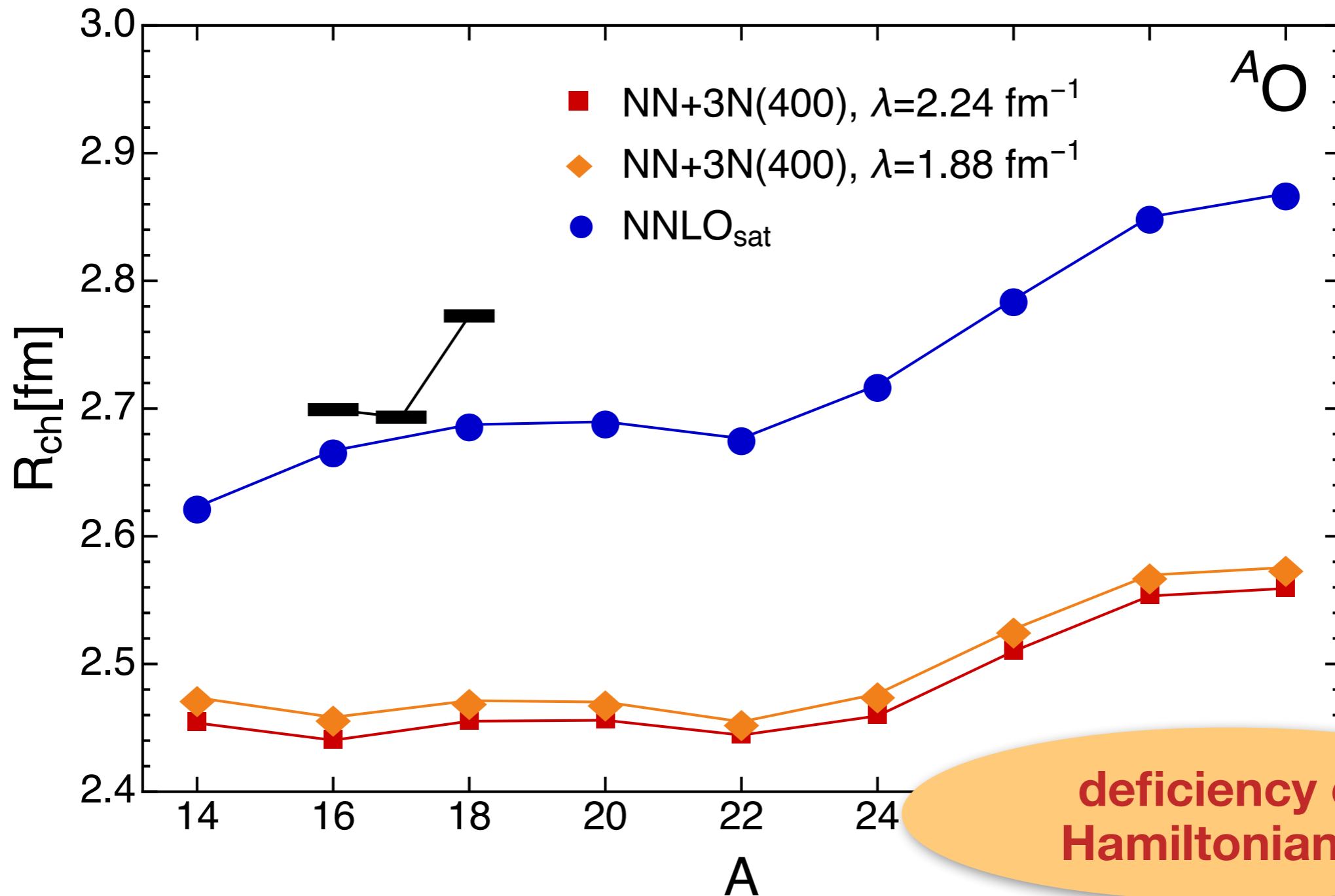
- **Multi-Reference IM-SRG** with number-projected Hartree-Fock-Bogoliubov as reference state
- **consistent results from different many-body methods**

correct drip line

Oxygen Radii



V. Lapoux, V. Somà, C. Barbieri, H. H., J. D. Holt, and S. R. Stroberg, under peer review

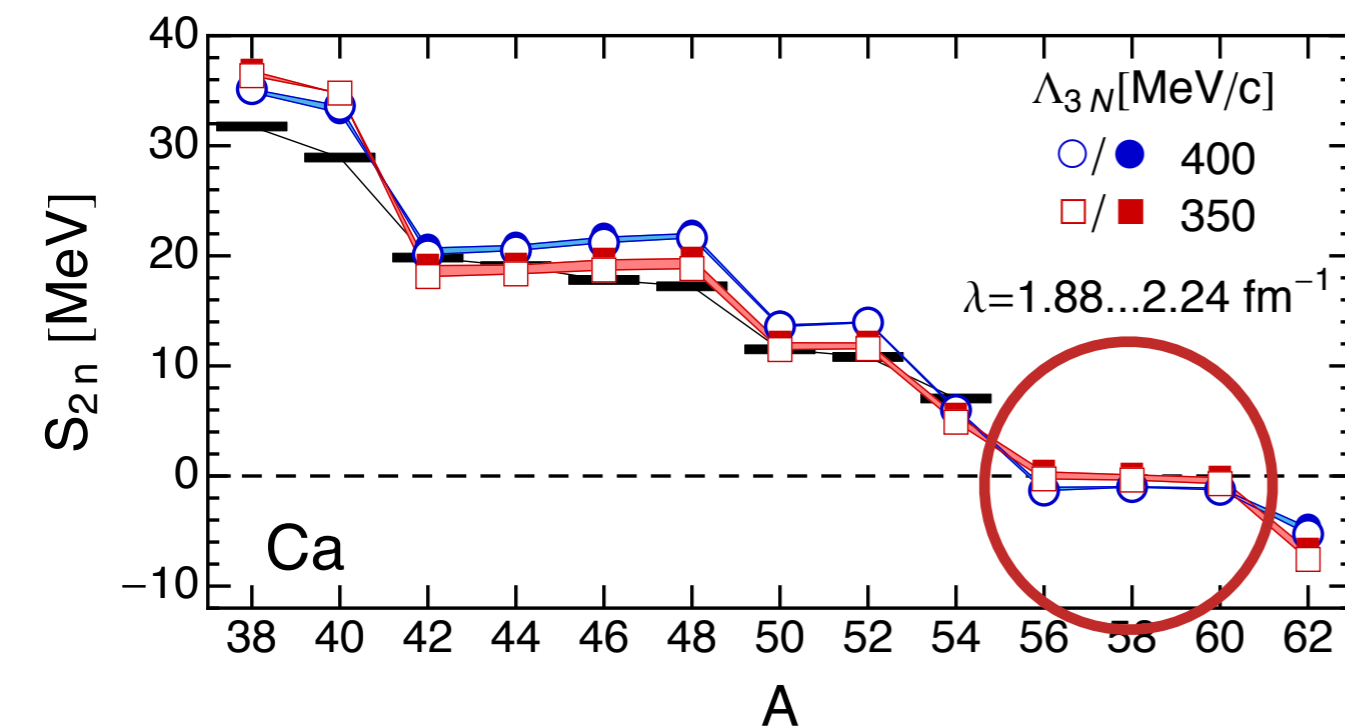
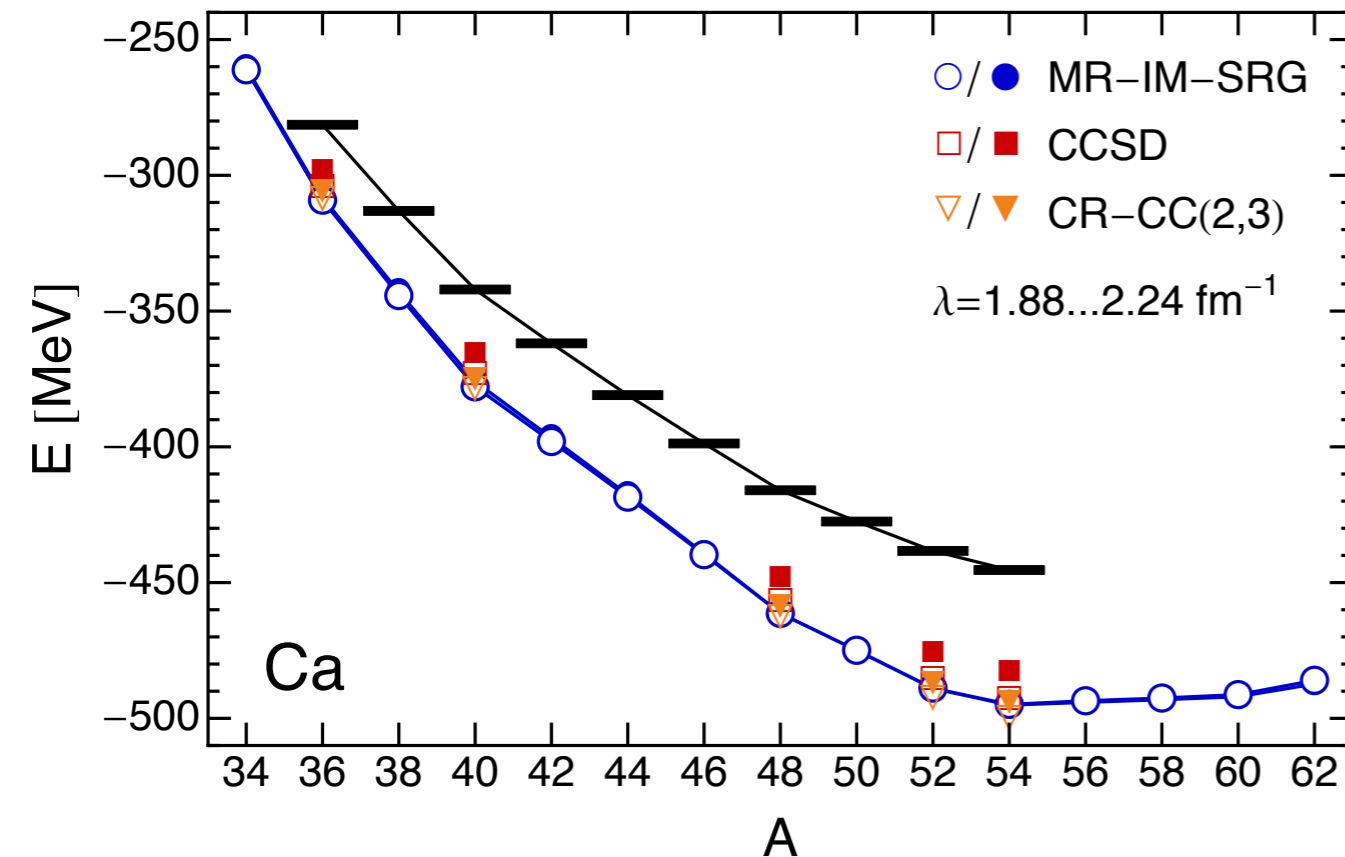


Calcium Isotopes



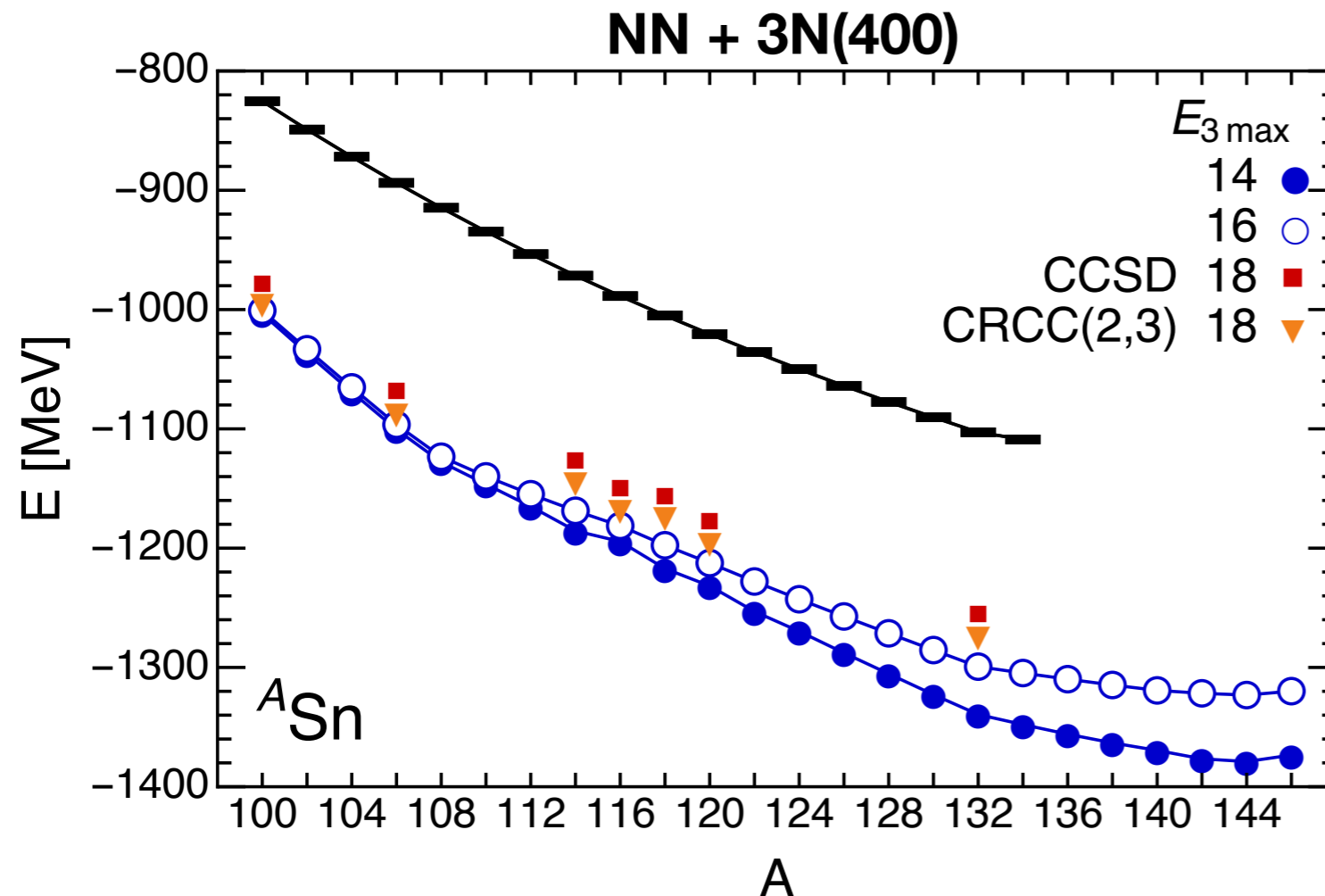
HH et al., PRC 90, 041302(R) (2014)

NN + 3N(400)



- 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 $< 1\text{MeV}$

The Mass Frontier: Tin



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

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

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

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

- need technical improvements to go further

Neutrinoless Double Beta Decay: Ground-State to Ground-State Decay

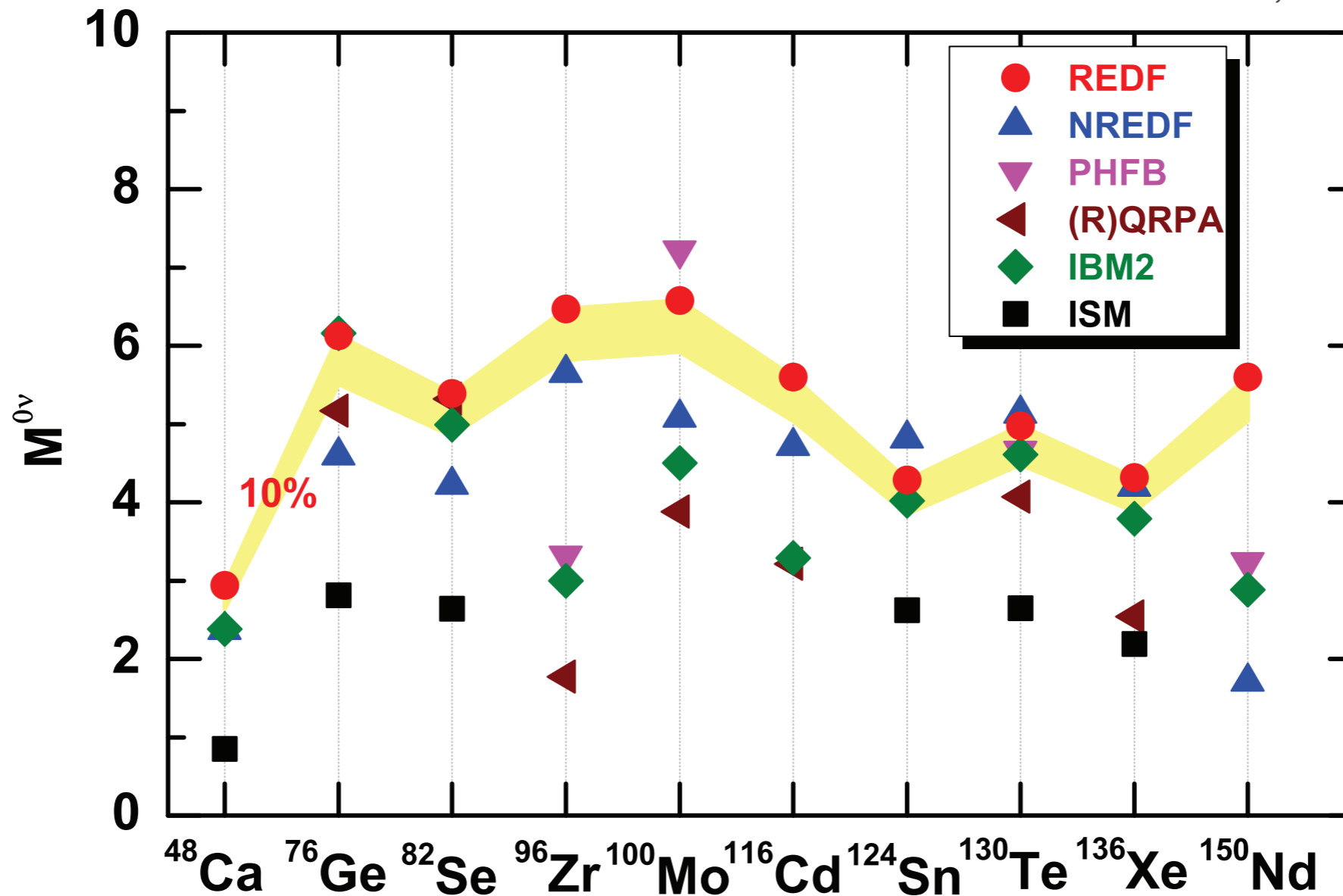
with **J. Yao**, C. Jiao, J. Engel



Nuclear Matrix Elements



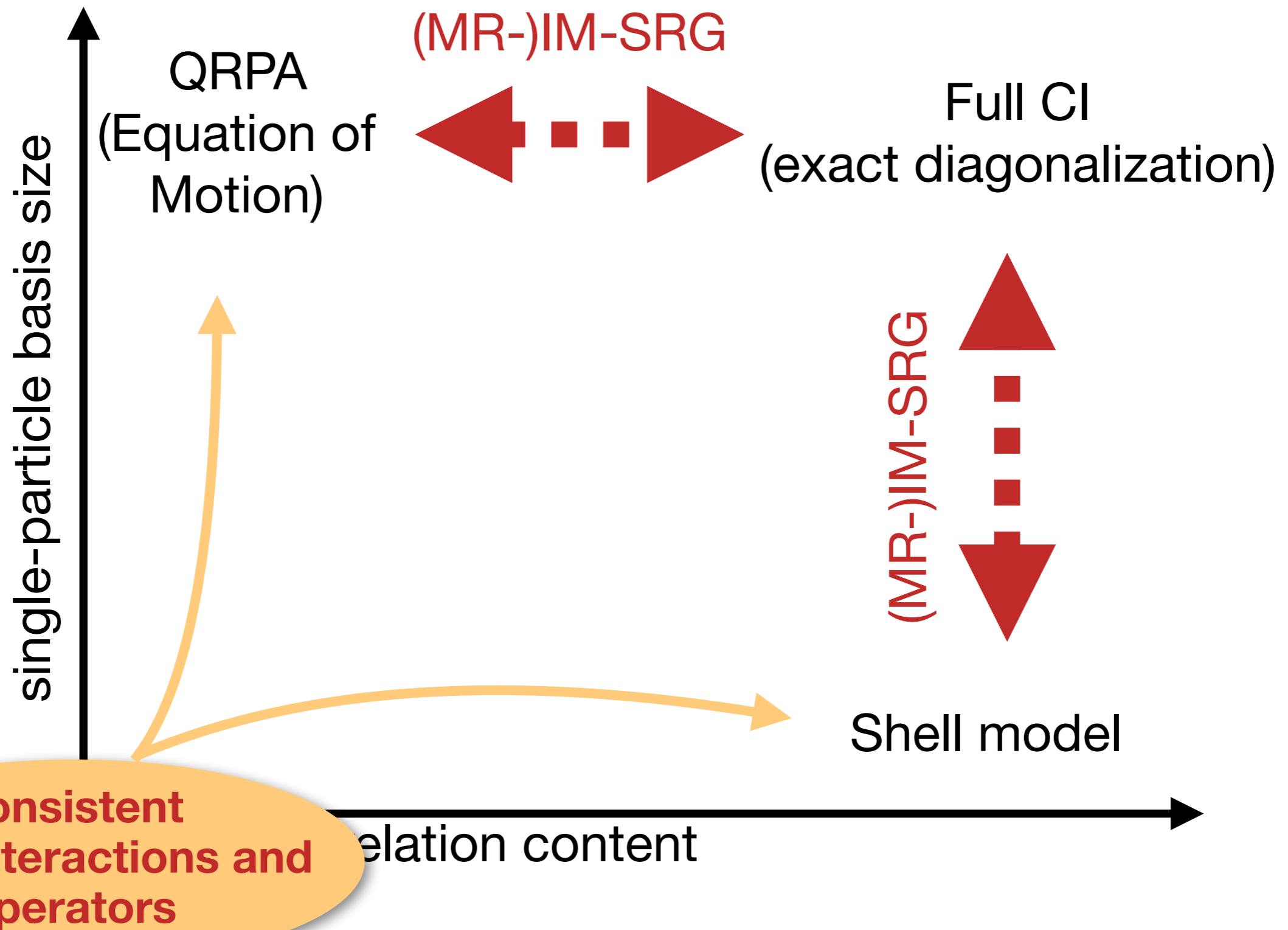
J. Yao et al., PRC 91, 024316 (2015)



- inputs tailored to specific methods: phenomenological interactions, EDFs, Shell Model interactions, ...
- quenched g_A , “renormalization” of operators,

comparing apples and oranges

Many-Body Approaches



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

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

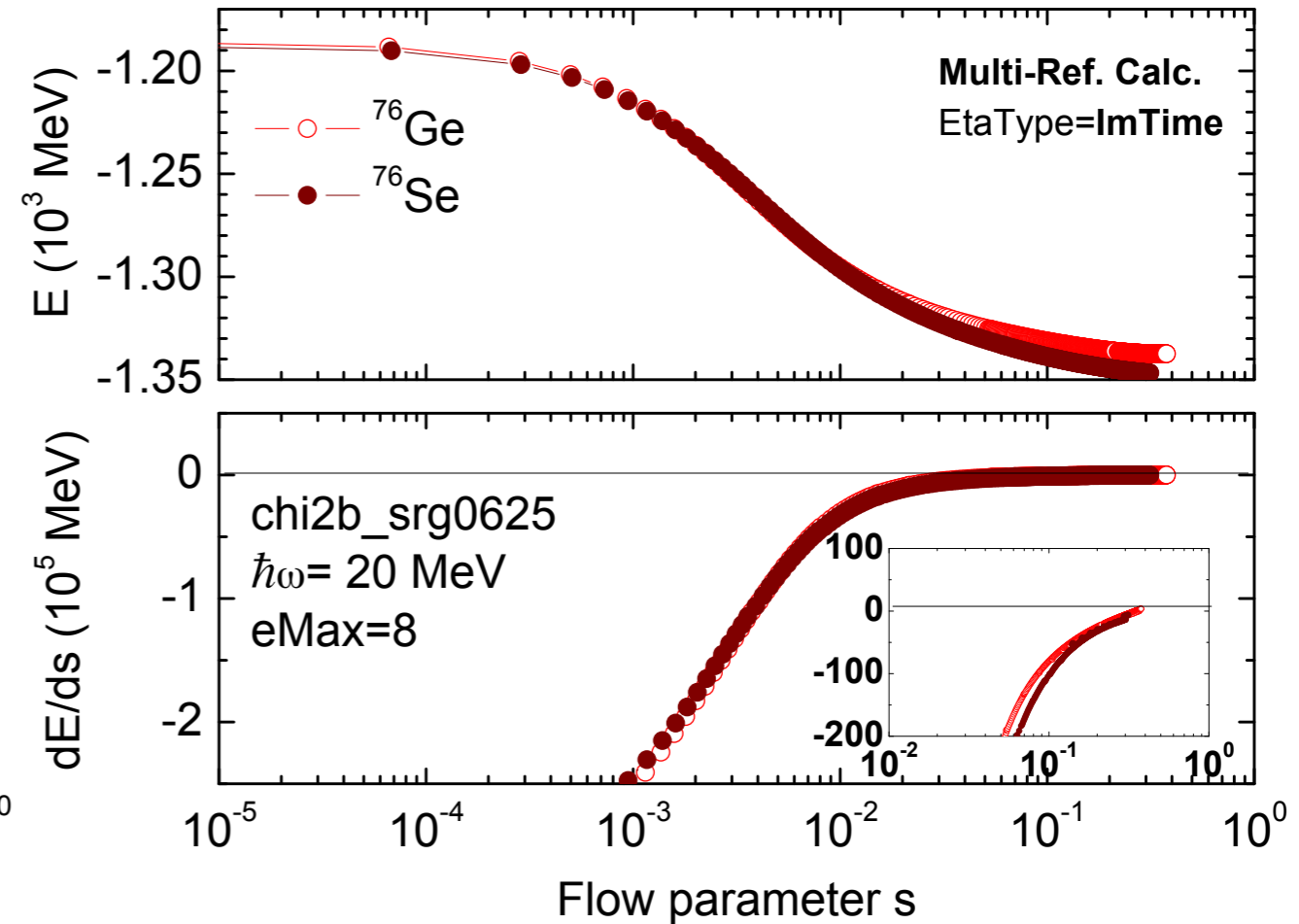
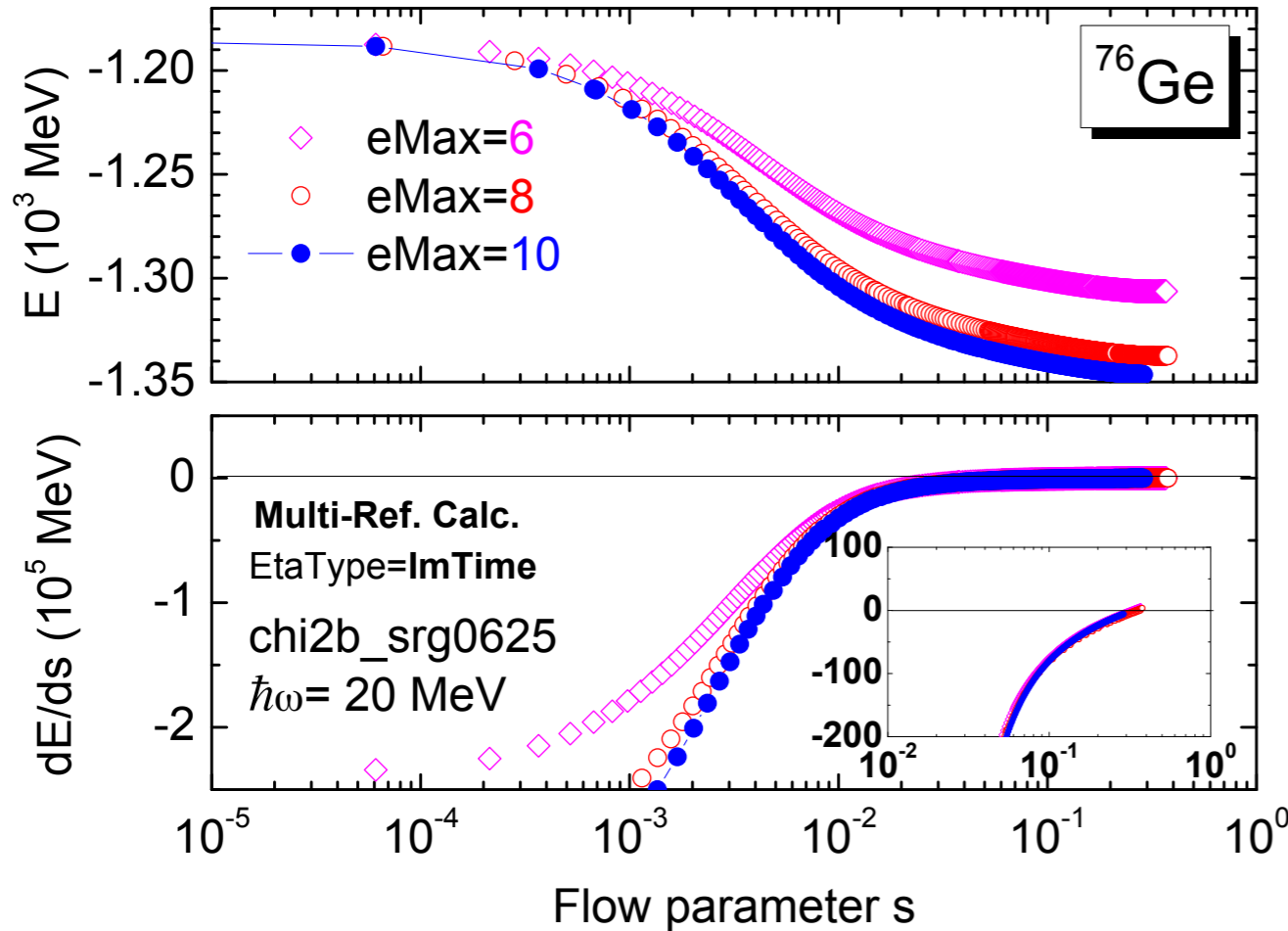
- small-scale (e.g., $0\hbar\Omega$, $2\hbar\Omega$) **No-Core Shell Model**:

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

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

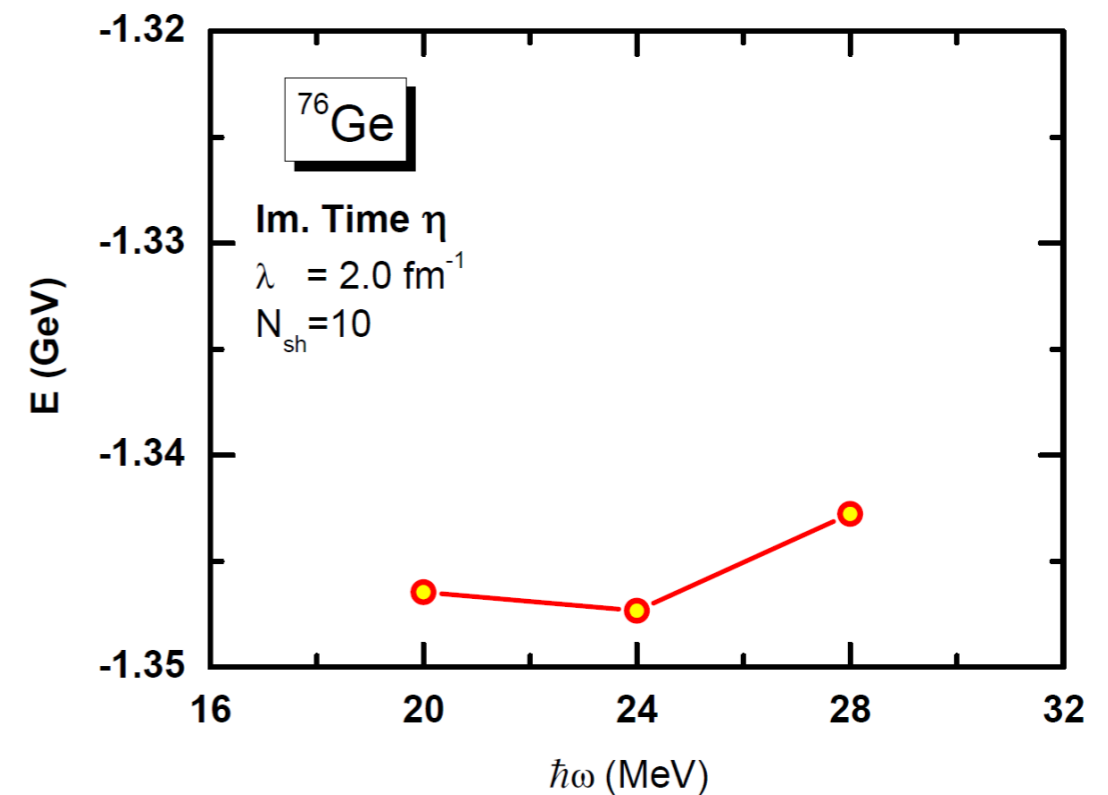
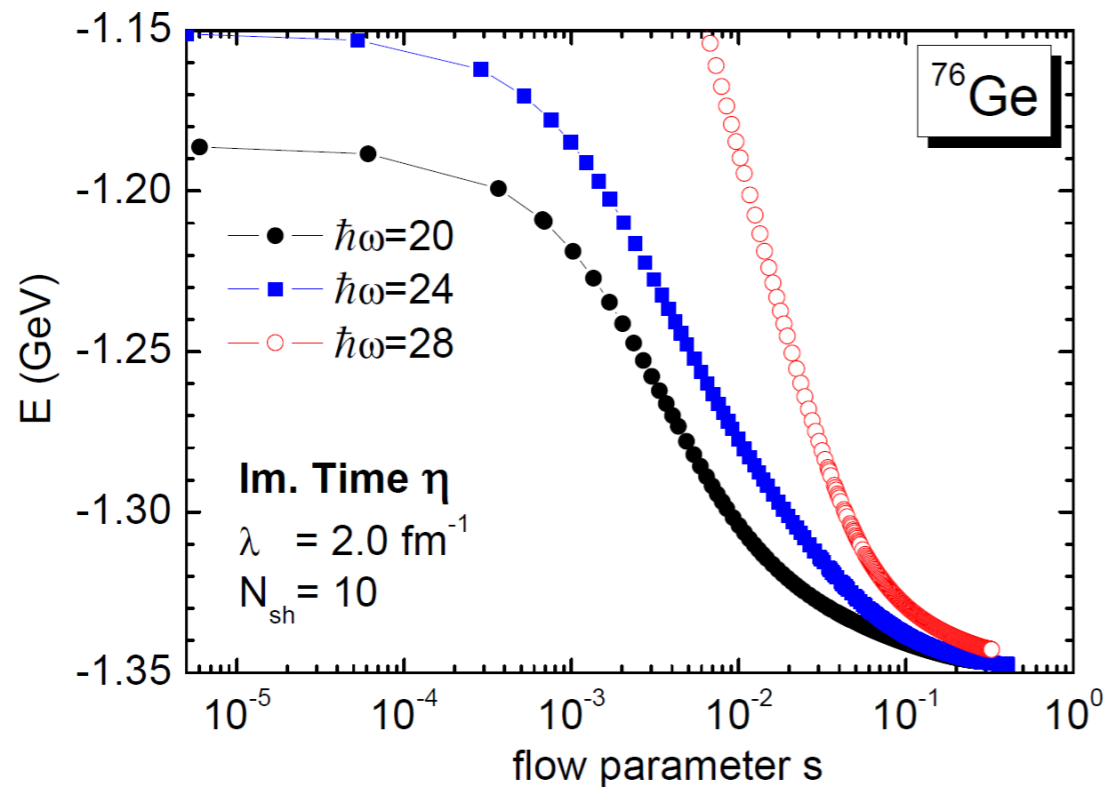
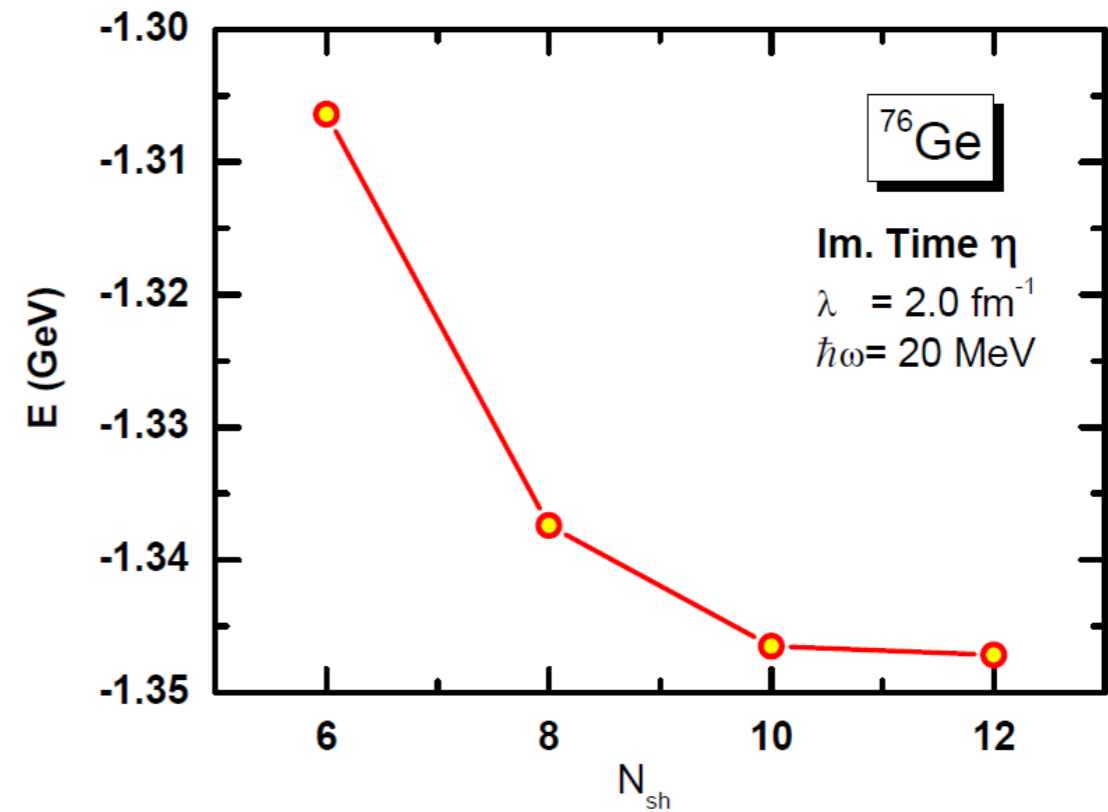
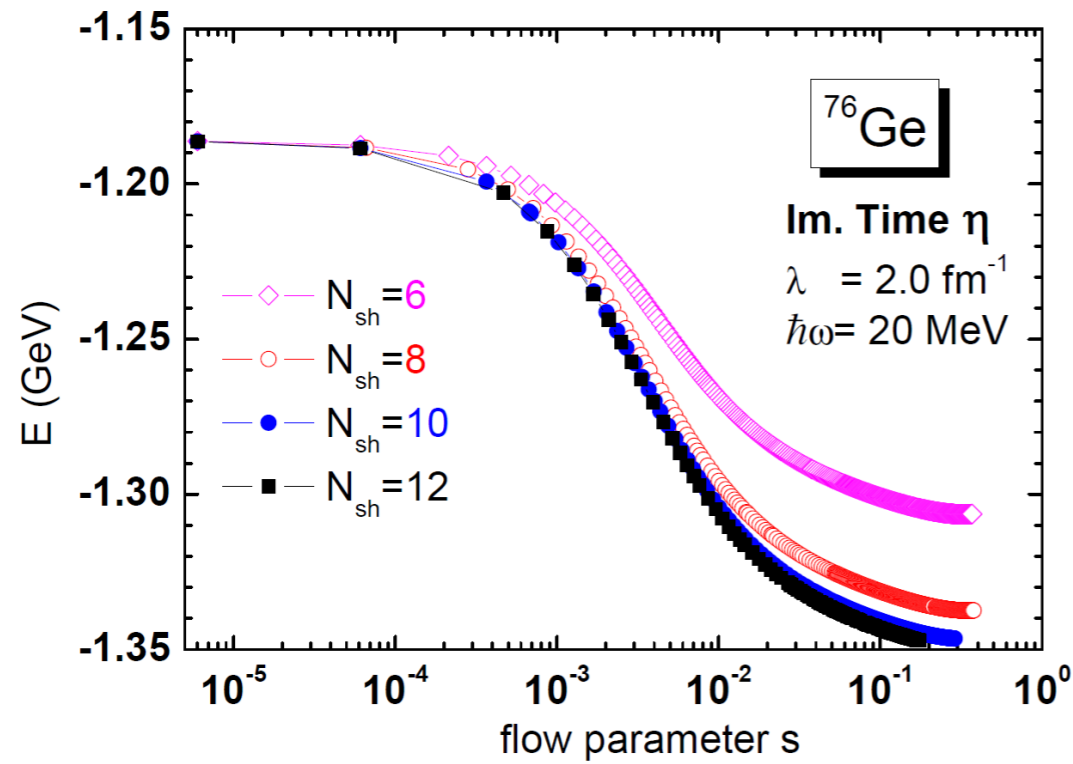
$$|\Phi\rangle = \int dq f(q) P_{J=0M=0} P_Z P_N |q\rangle$$

- Density Matrix Renormalization Group, Tensor Network States, ...



proof of principle: MR-IM-SRG based on **(intrinsically deformed) GCM state converges** ${}^{76}\text{Ge}, {}^{76}\text{Se}$ ground-state energies

$^{76}\text{Ge} \rightarrow ^{76}\text{Se}$



Direct DBD Calculation



- **direct** MR-IM-SRG (Magnus) calculation of **initial and final states**:

$$|\Psi_{I,F}\rangle = e^{\bar{\Omega}_{I,F}} |\Phi_{I,F}\rangle$$

- evaluate NME for transition operator in **closure approximation**:

$$M_{0\nu\beta\beta} = \langle \Phi_F | e^{-\bar{\Omega}_F} O_{0\nu\beta\beta} e^{\bar{\Omega}_I} | \Phi_I \rangle$$

- explore possible expansions and check consistency, e.g.,

$$e^{-\bar{\Omega}_F} = e^{-(\bar{\Omega}_I + \delta\bar{\Omega})} = e^{-\delta\bar{\Omega}} e^{-\bar{\Omega}_I} + \dots$$

in progress

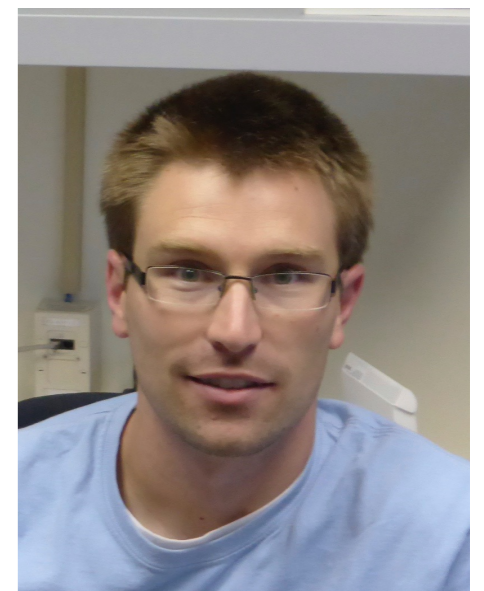
Neutrinoless Double Beta Decay: Explicit Treatment of Excited States

N. M. Parzuchowski, S. K. Bogner, in preparation

S. R. Stroberg, H. H., J. D. Holt, S. K. Bogner, A. Schwenk, PRC93, 051301(R) (2016)

S. K. Bogner, H. H., J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. Lett. 113, 142501 (2014)

K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)



- describe “excited states” based on reference state:

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

- **(MR-)IM-SRG effective Hamiltonian** in EOM approach:

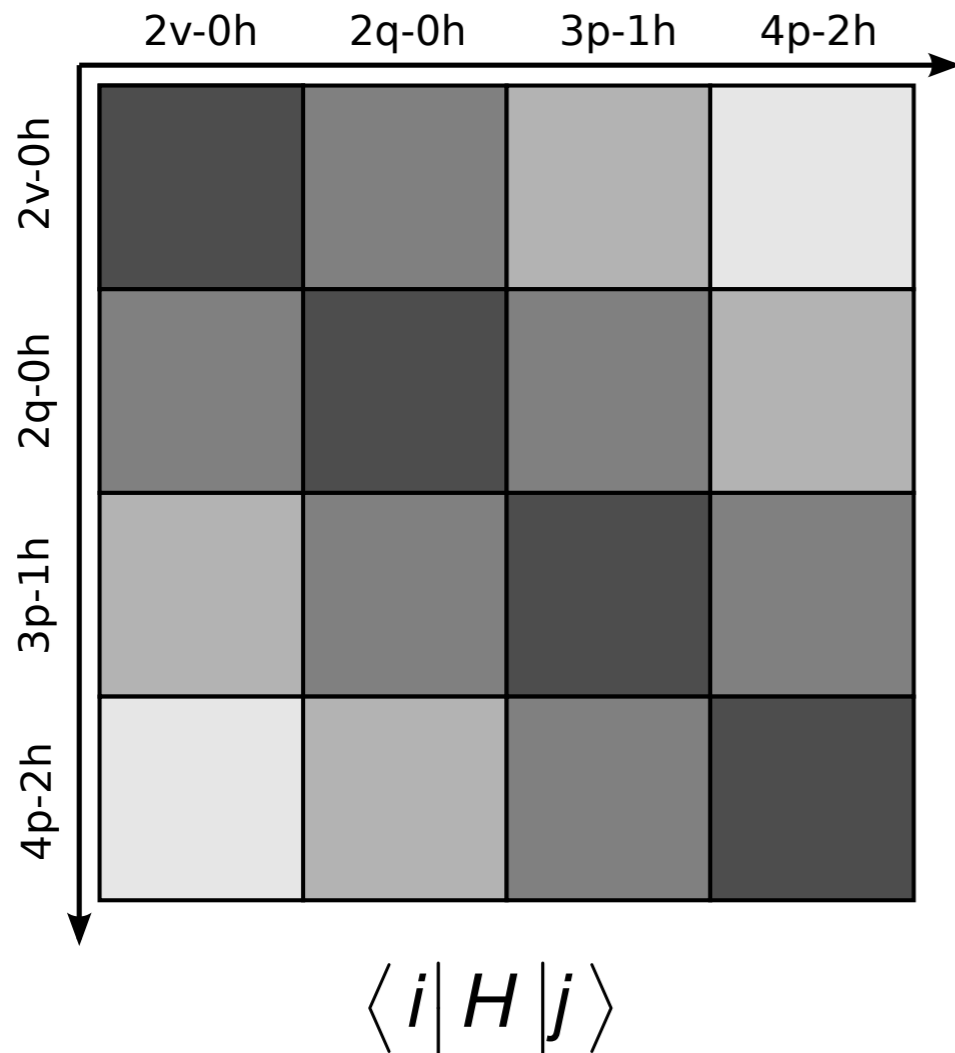
$$[H(s), Q_k^\dagger(s)] = \omega_k(s) Q_k^\dagger(s), \quad \omega_k(s) = E_k(s) - E_0(s)$$

- 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
- **can exploit multi-reference capabilities** (commutator formulation identical to flow equations)

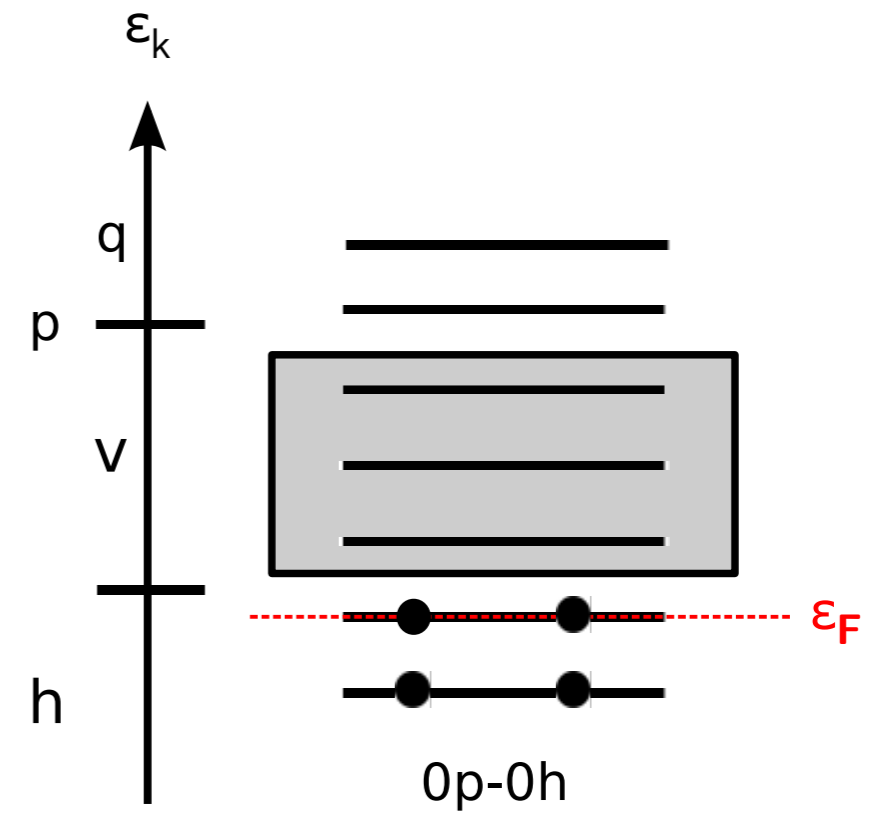
Valence Space Decoupling



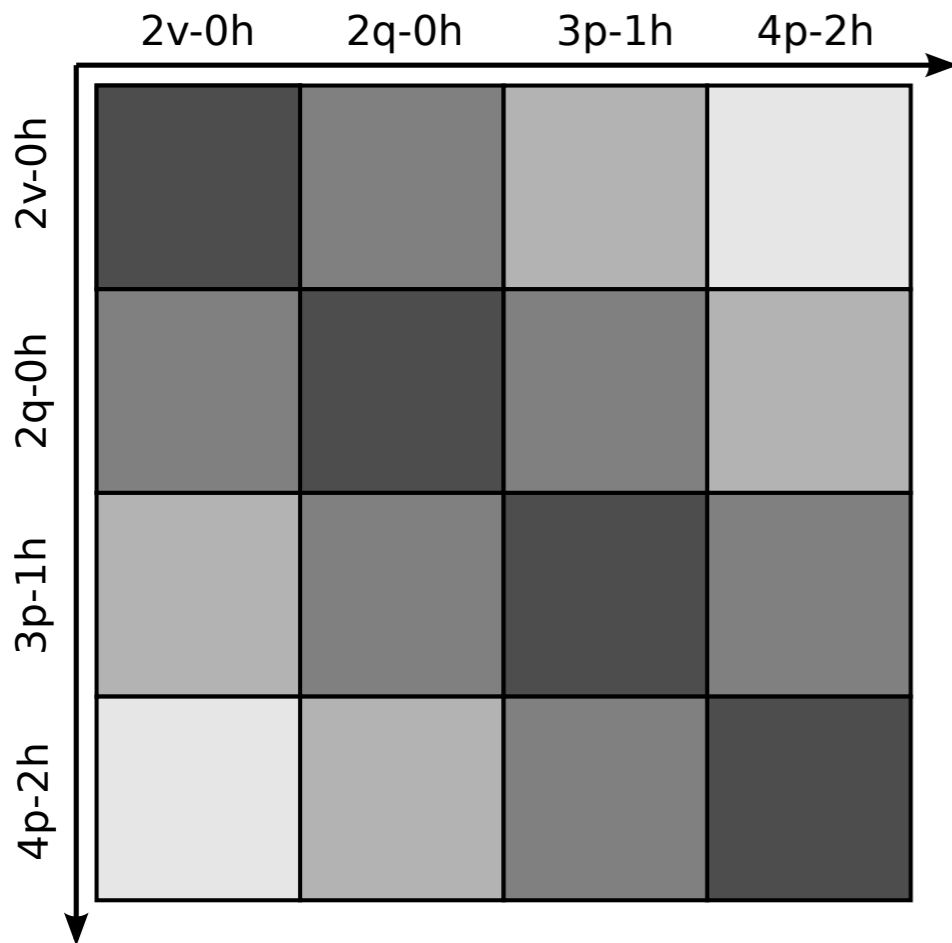
non-valence
particle states

valence
particle states

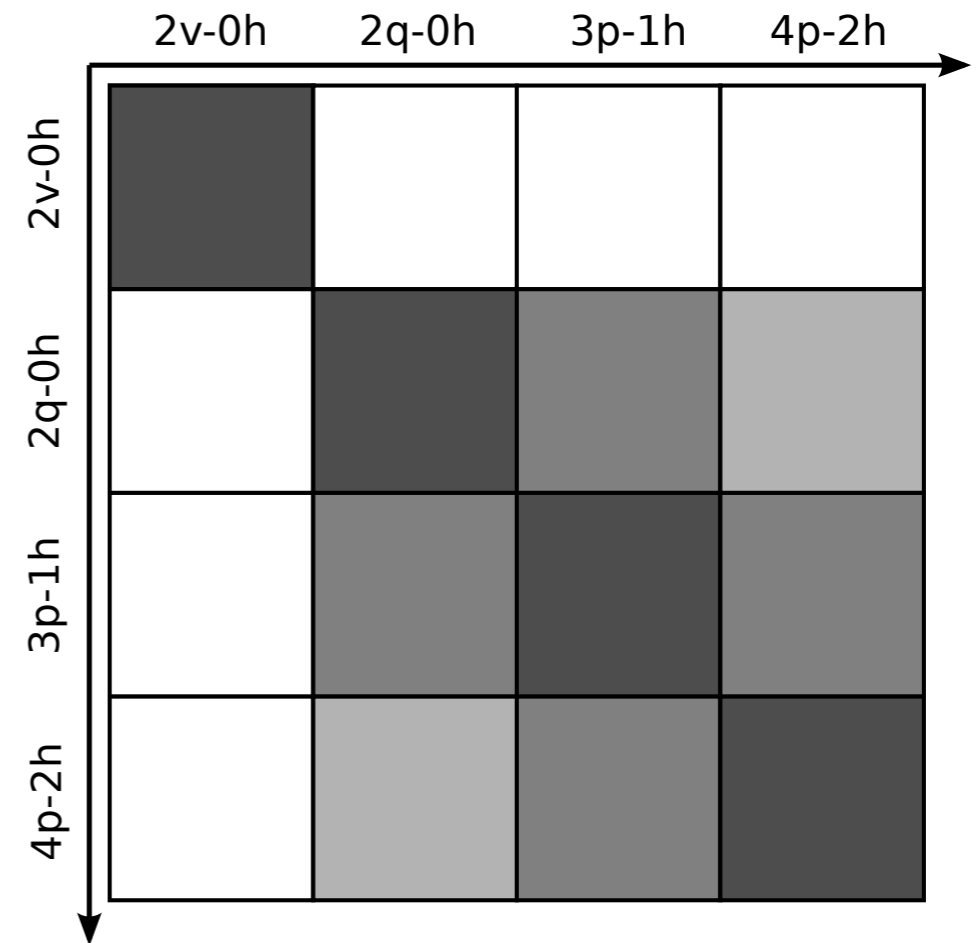
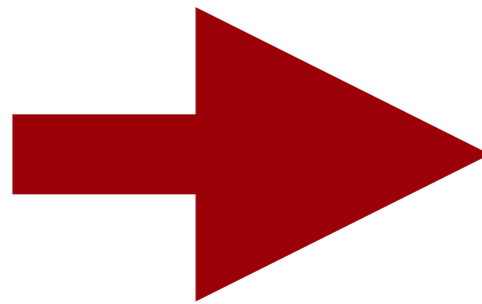
hole states
(core)



Valence Space Decoupling



$$\langle i | H | j \rangle$$



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

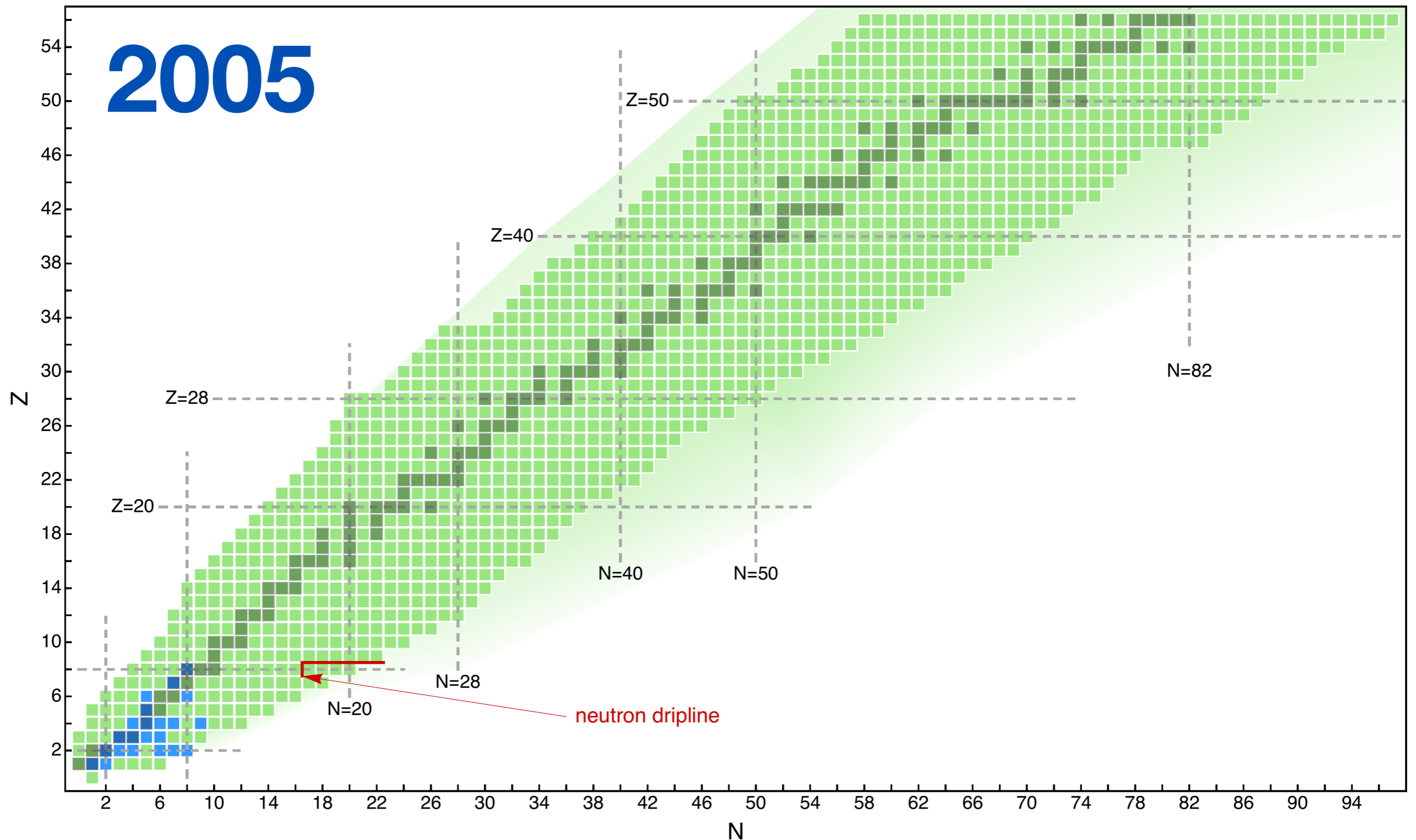
off-diagonal Hamiltonian:

$$\{ H^{od} \} = \{ f_{h'}^h, f_{p'}^p, f_h^p, f_v^q, \Gamma_{hh'}^{pp'}, \Gamma_{hv}^{pp'}, \Gamma_{vv'}^{hh'} \}$$

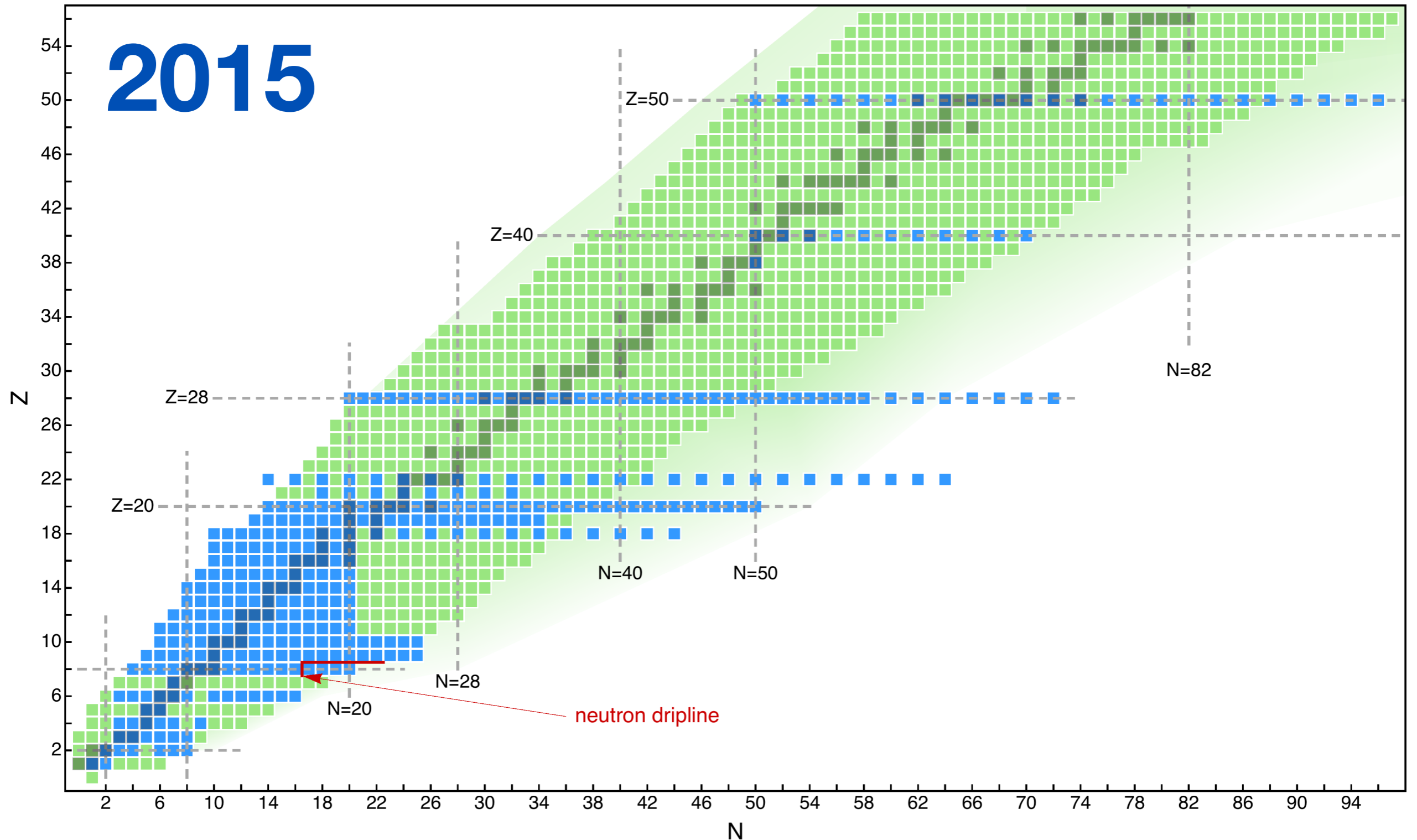
consistent interaction and DBD operator for Shell Model
(talk by R. Stroberg)

Epilogue

Progress in *Ab Initio* Calculations



Progress in *Ab Initio* Calculations



- towards ***ab initio* NMEs**: interaction, operators, many-body method with **systematic uncertainties** & convergence to exact result
- rapidly **growing capabilities**: g.s. energies, spectra, radii, transitions, ...
- ➔ **ingredients for NME calculation, plus validation through other observables**
- test new generation of chiral Hamiltonians, **greatly improved optimization** - also **more accurate (?)**
- NNLO_{sat}, NNLO_{sim}, EKM / LENPIC interactions, local NNLO, etc.

Acknowledgments



S. K. Bogner, M. Hjorth-Jensen, T. D. Morris, N. M. Parzuchowski, F. Yuan
NSCL, Michigan State University

E. Gebrerufael, K. Hebel, R. Roth, A. Schwenk, J. Simonis, C. Stumpf, K. Vobig, K. Wendt
TU Darmstadt, Germany

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Supplements

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. Tuskijama, 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:

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

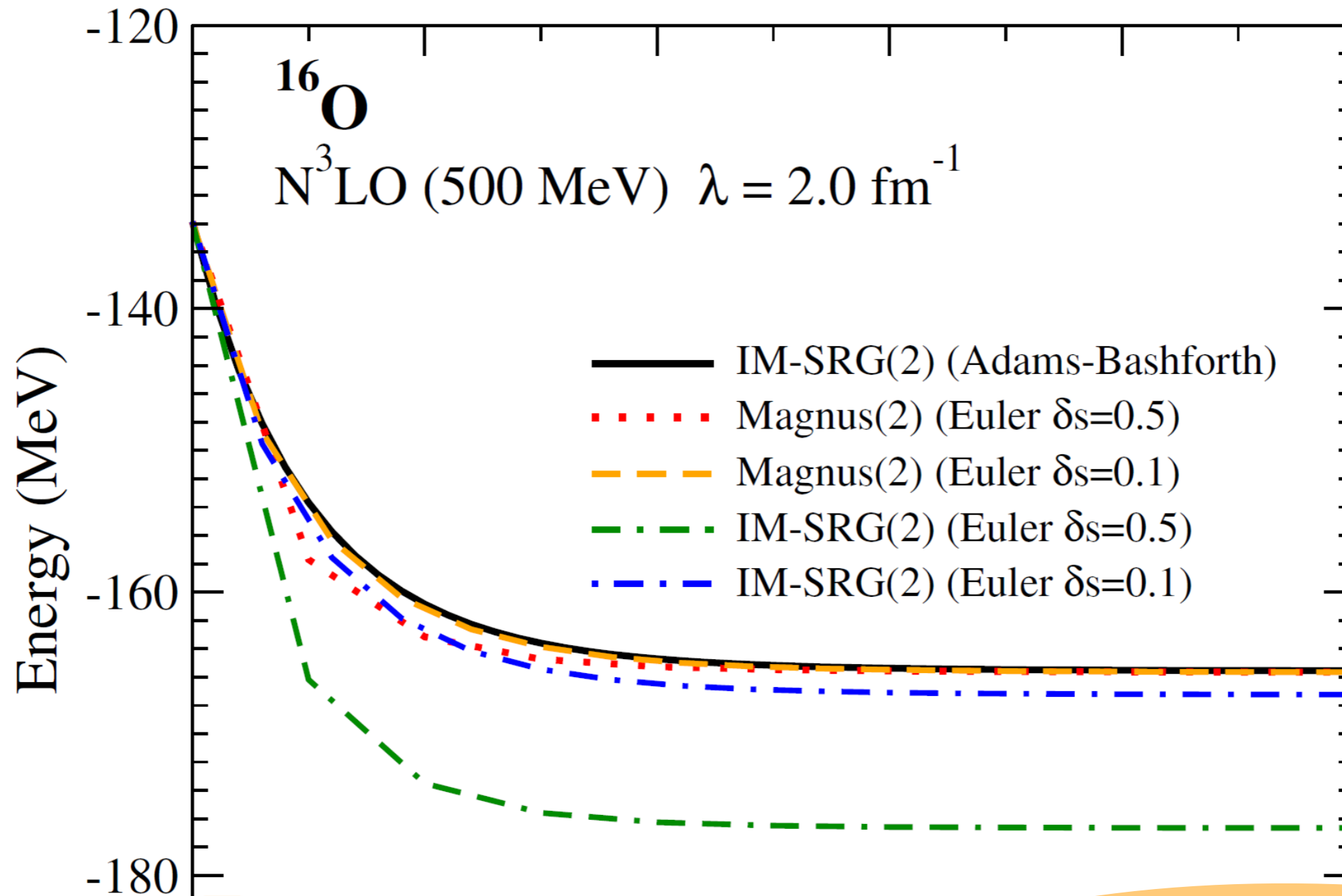
- flow equation for **Magnus** operator :

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

(B_k : Bernoulli numbers)

- construct $O(s) = U(s)O_0U^\dagger(s)$ using Baker-Campbell-Hausdorff expansion (**Hamiltonian + effective operators**)
- MAG(2): **two-body truncation** (as in NO2B, IM-SRG(2))

Magnus vs. Direct Integration



**IM-SRG(2)
 \approx MAG(2)**

Euler integrator sufficient,
unitarity built in!

s

Approximating IM-SRG(3)



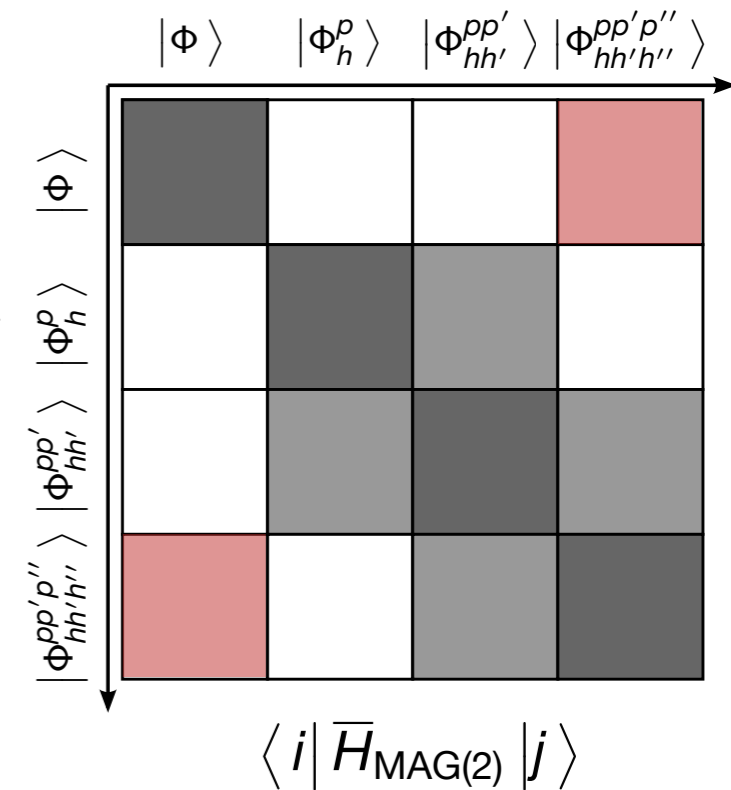
- final Hamiltonian (IM-SRG(2), MAG(2)):

$$\bar{H}_{\text{MAG}(2)} = \left(e^{\Omega_{1,2}} H e^{-\Omega_{1,2}} \right) = \bar{H}_{0,1,2} + \bar{H}_3 + \dots$$

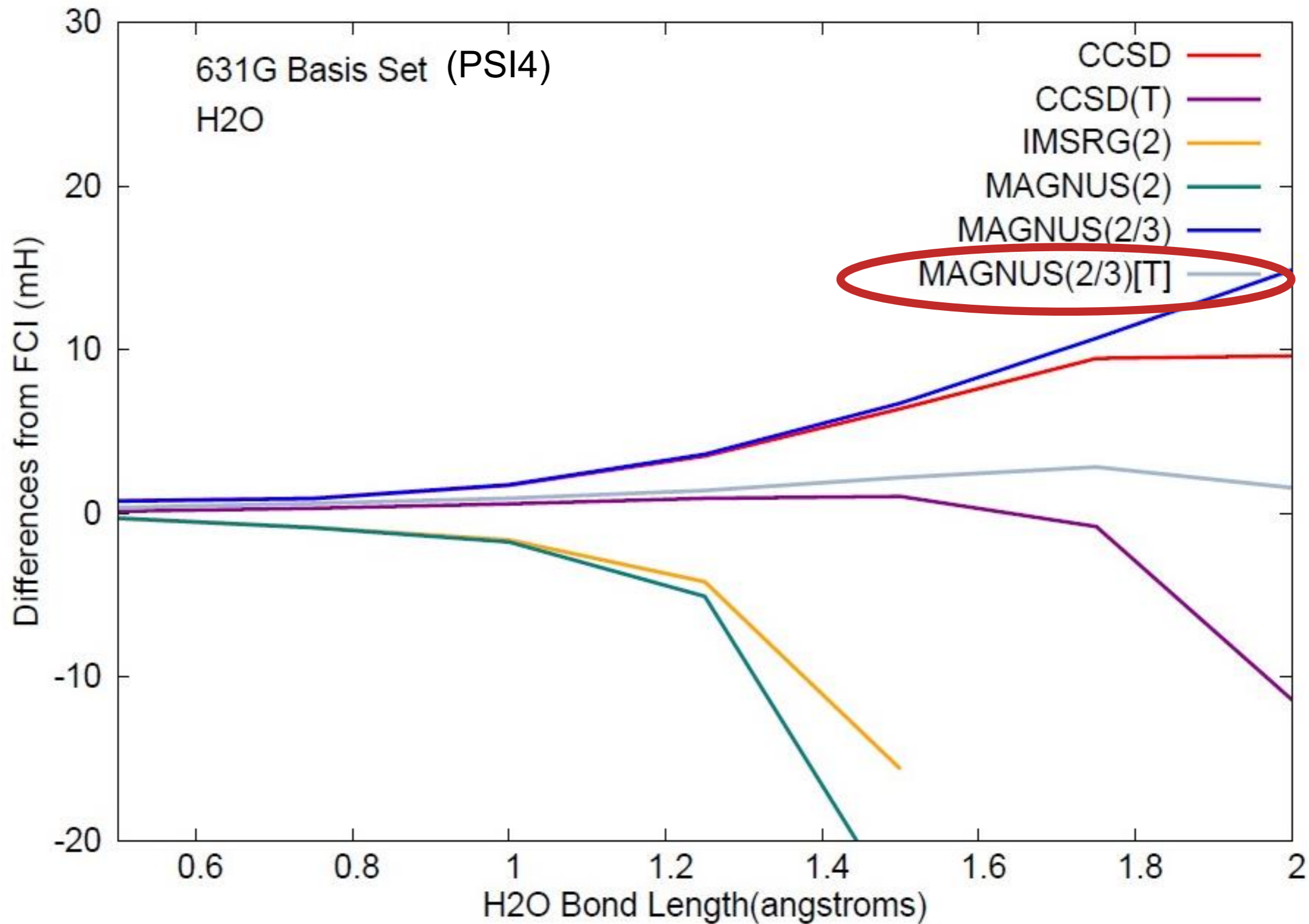
- energy contribution of \bar{H}_3 (cf. 0B flow):

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

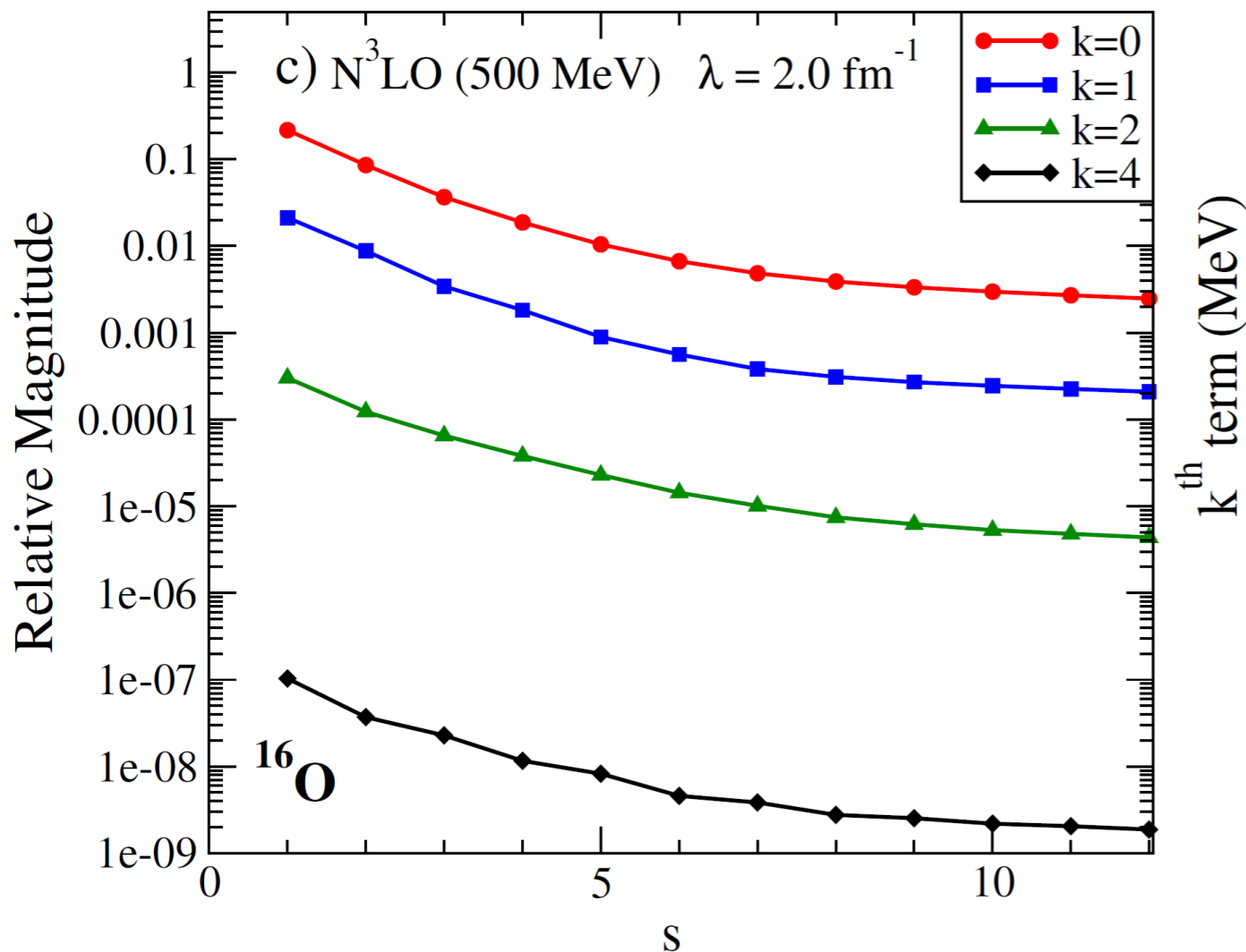
- **family of non-iterative methods**: level of approximation for \bar{H}_3 and energy denominator $\bar{\Delta}$
- generalizes to **arbitrary observables, excited states**
- multi-reference variant in development



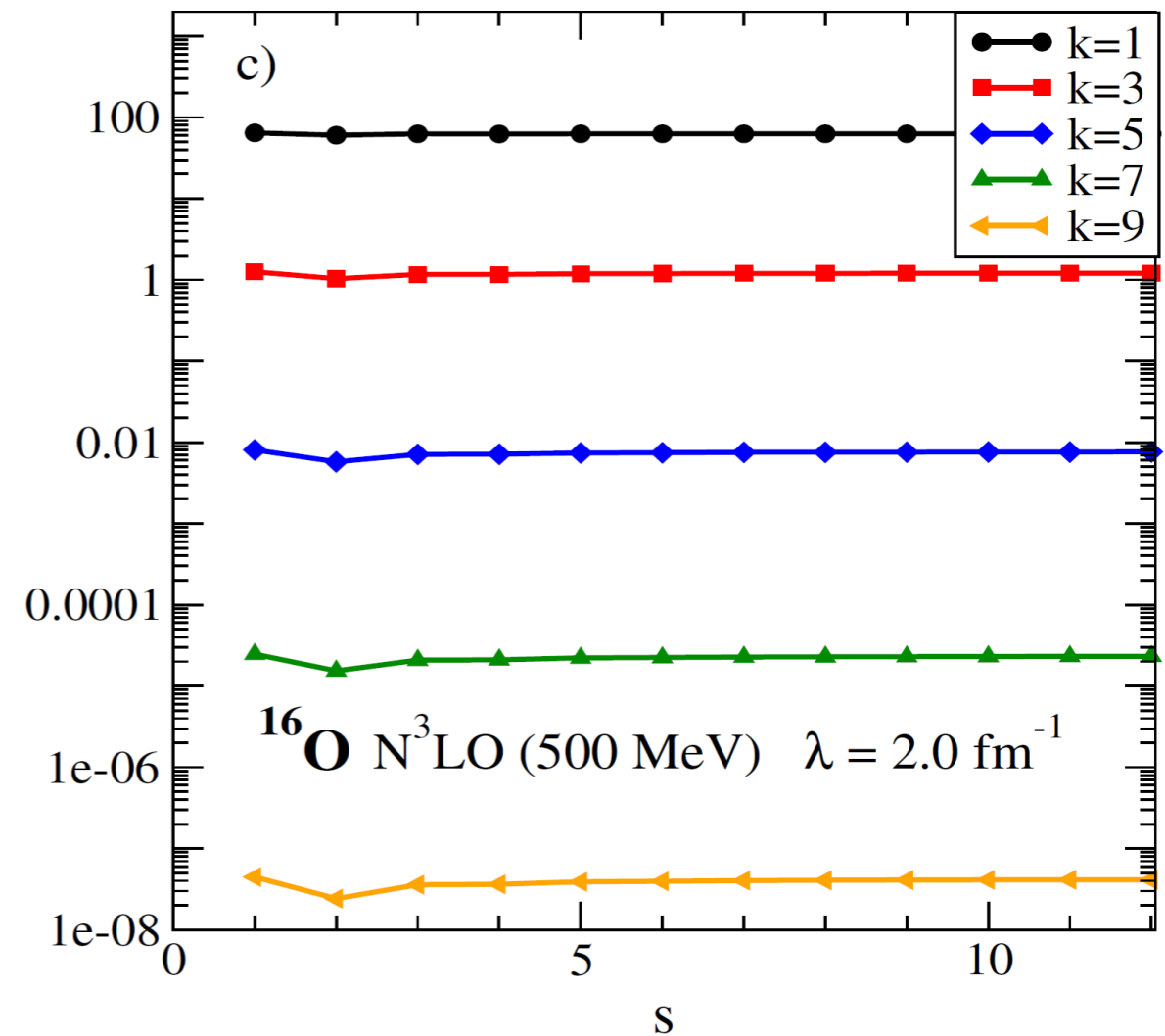
Example: Bond Breaking in Water



Convergence



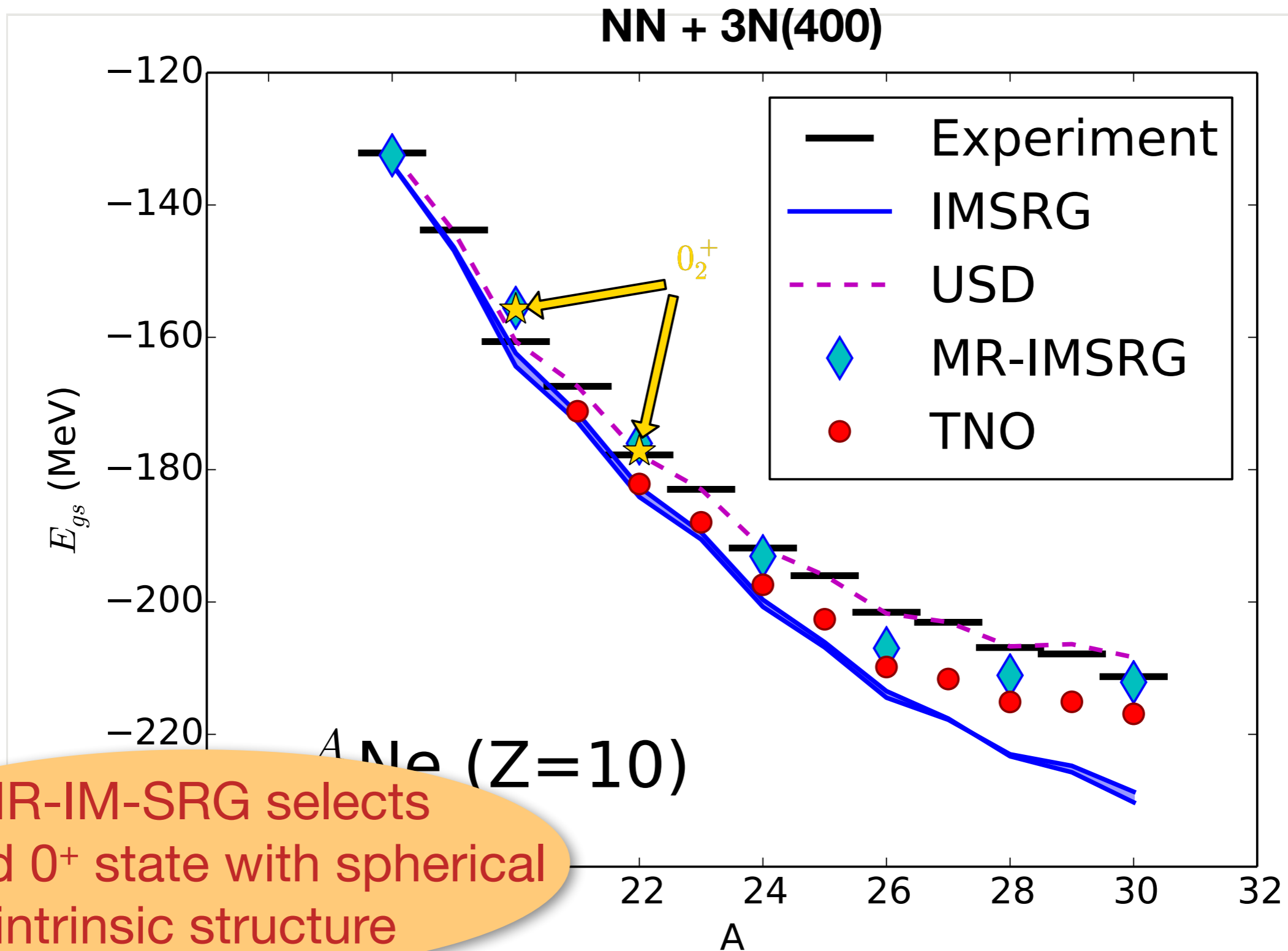
$$\frac{d}{ds}\Omega = \sum_k \frac{B_k}{k!} \text{ad}_{\Omega}^k(\eta)$$



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

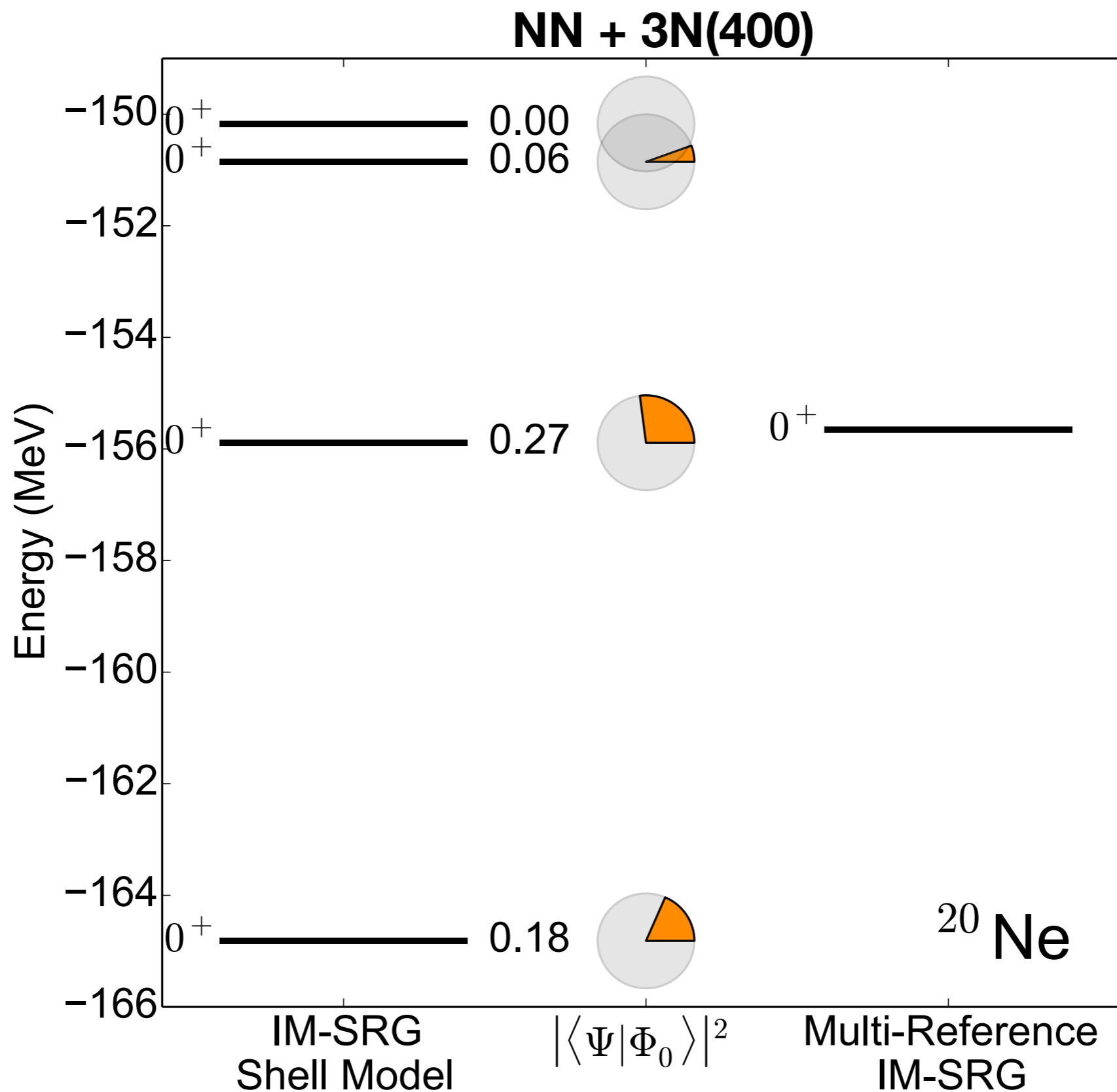
➔ ODE and BCH expansions converge rapidly and monotonically

Neon Isotopes

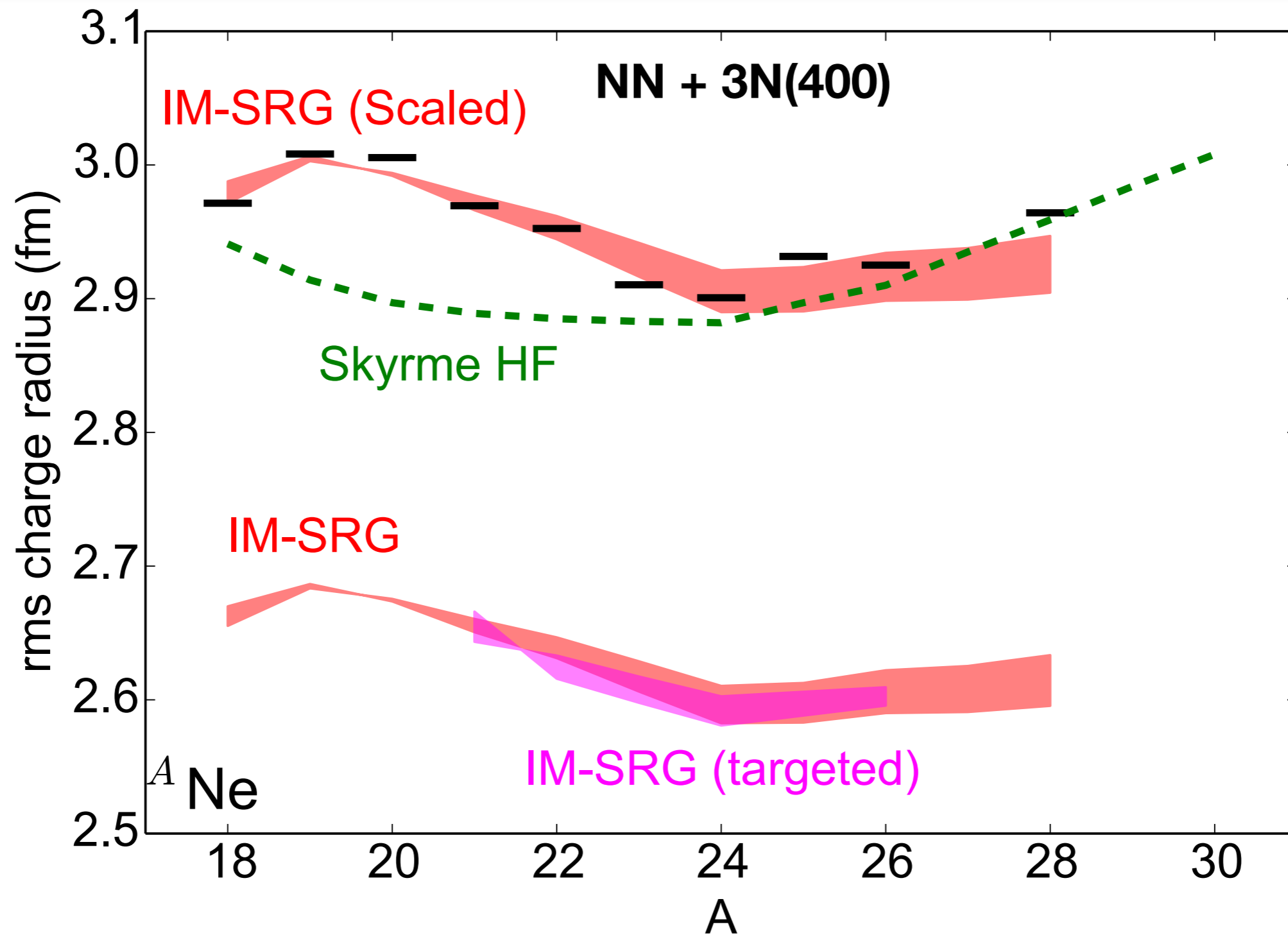


MR-IM-SRG selects excited 0_2^+ state with spherical intrinsic structure

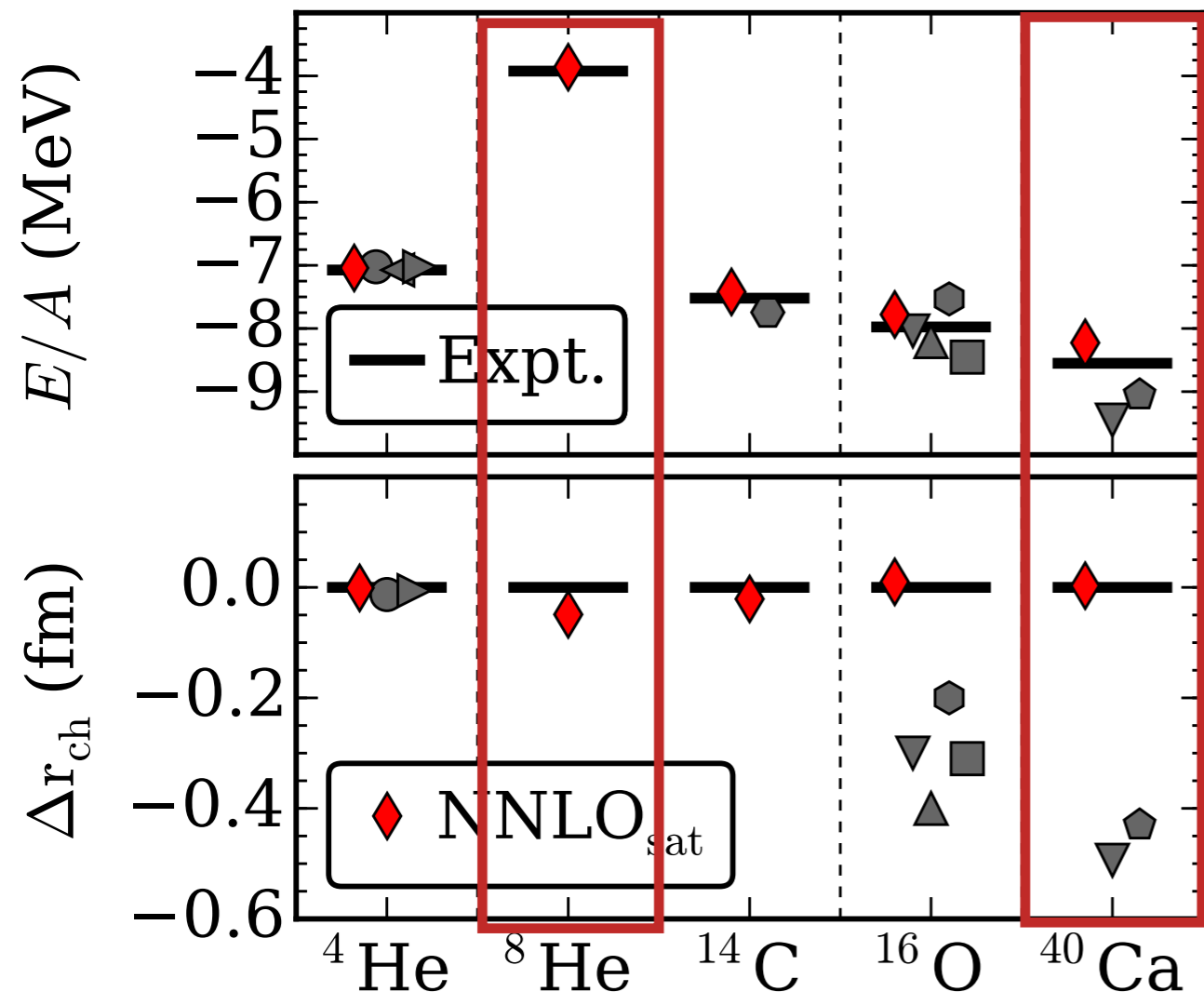
Deformation: ^{20}Ne



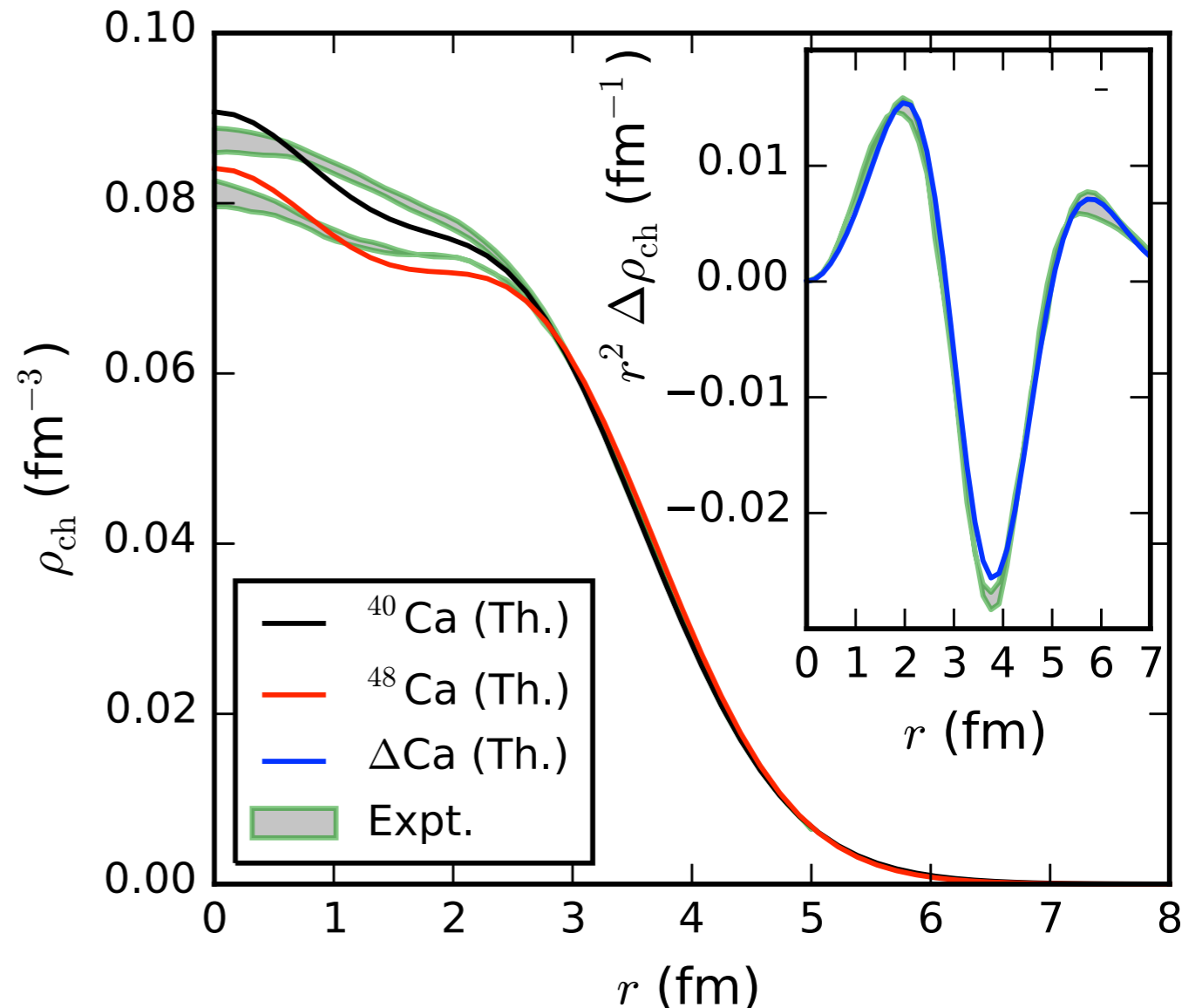
Neon Radii



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



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

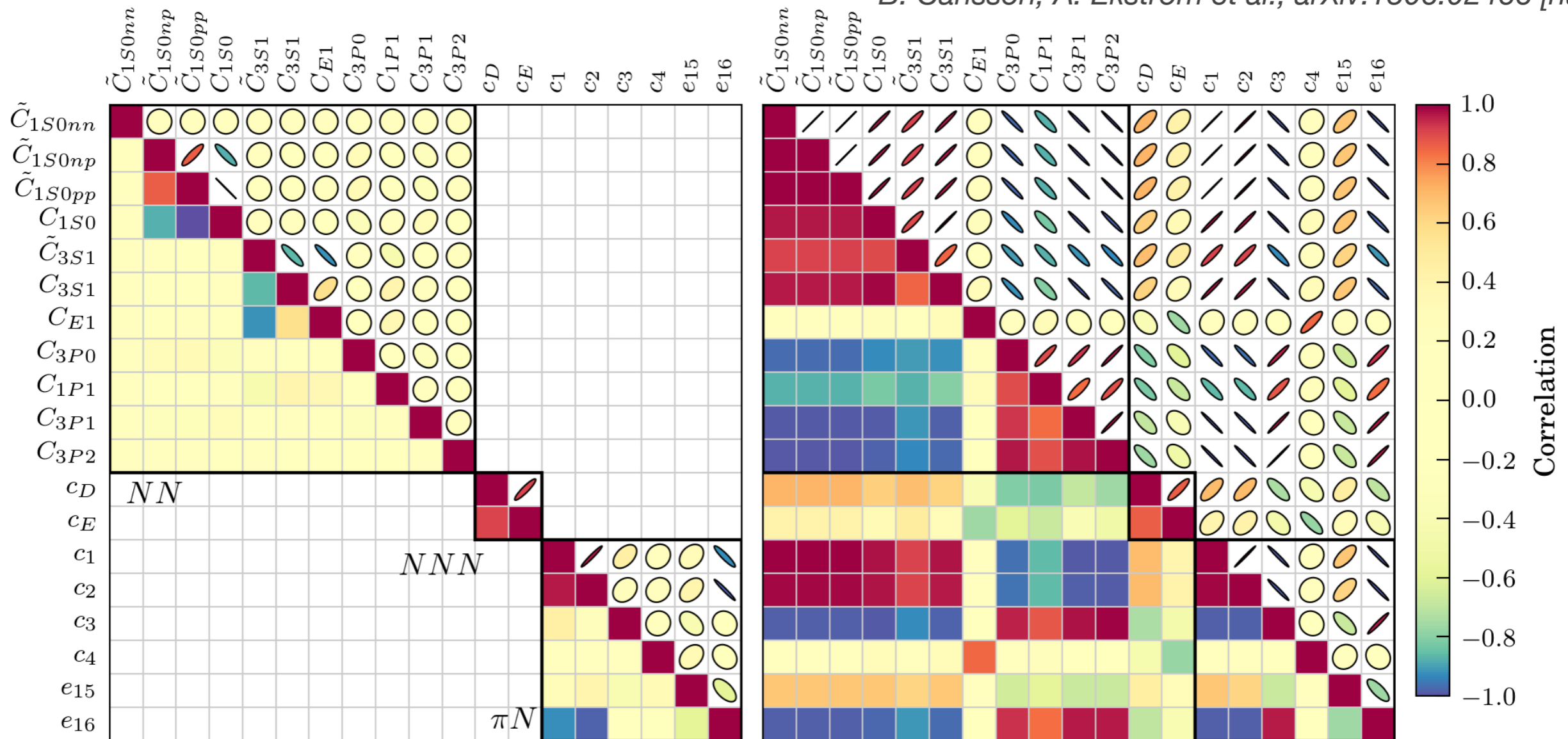


- accurate description of ^8He , $^{40,48}\text{Ca}$ g.s. energies & radii, $^{40,48}\text{Ca}$ charge distributions
- predictions for electric dipole polarizability, neutron skin, weak form factor of ^{48}Ca

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:

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

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

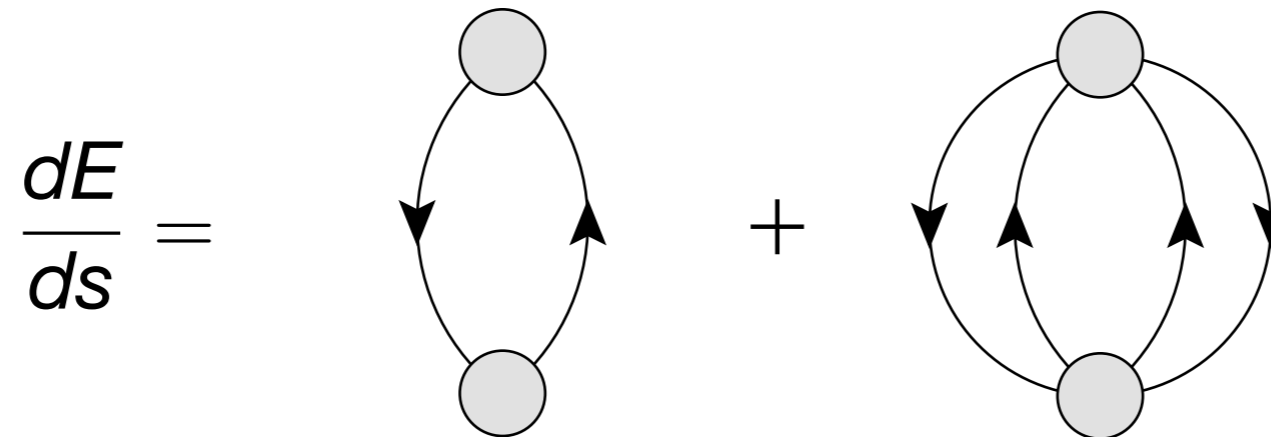
$$\frac{dH}{d\lambda} = \left[\left[\sum a^\dagger a, \underbrace{\sum a^\dagger a^\dagger aa}_{2\text{-body}} \right], \underbrace{\sum a^\dagger a^\dagger aa}_{2\text{-body}} \right] = \dots + \underbrace{\sum a^\dagger a^\dagger a^\dagger aaa}_{3\text{-body}} + \dots$$

- 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

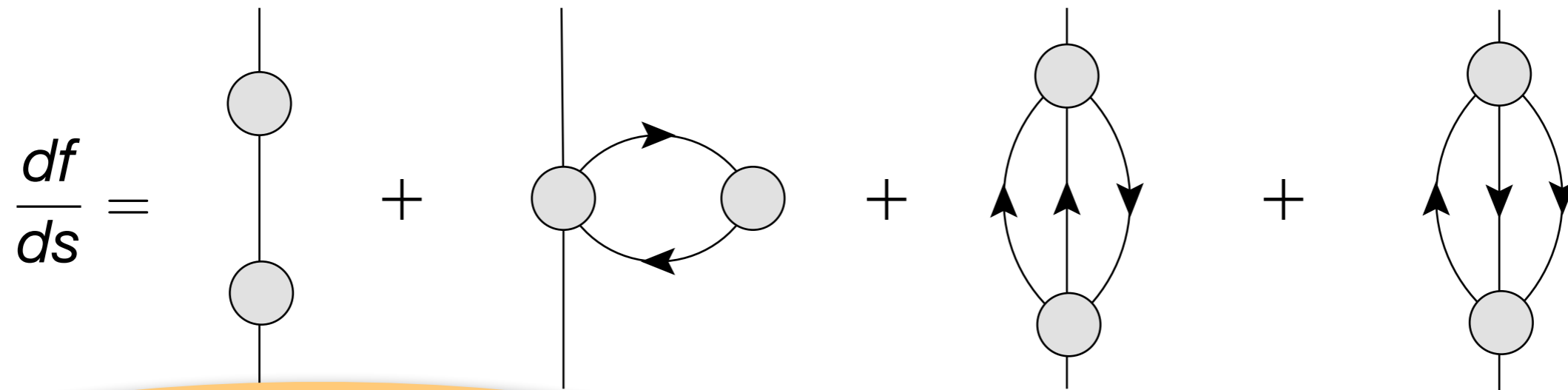
IM-SRG(2) Flow Equations



0-body Flow



1-body Flow



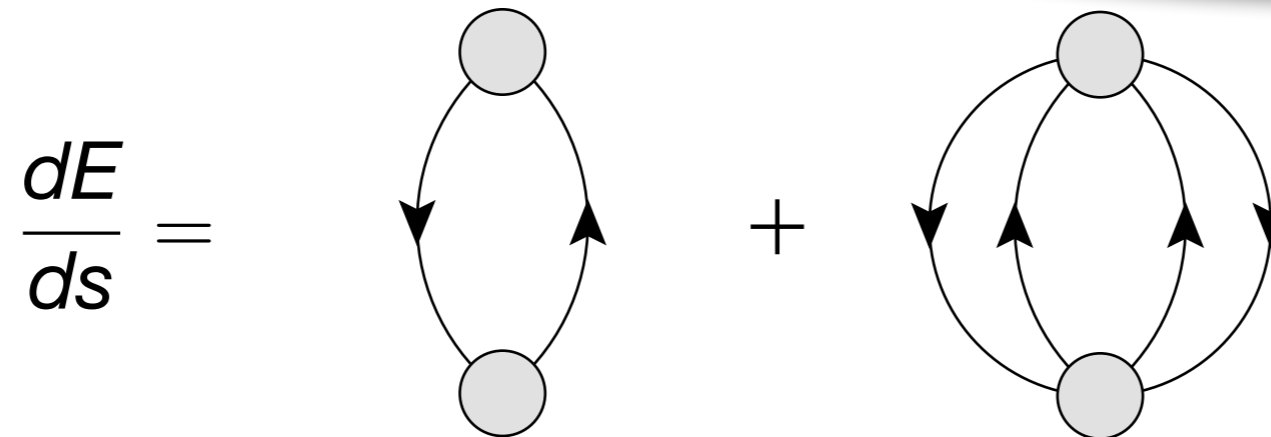
IM-SRG(2): truncate ops.
at two-body level

IM-SRG(2) Flow Equations

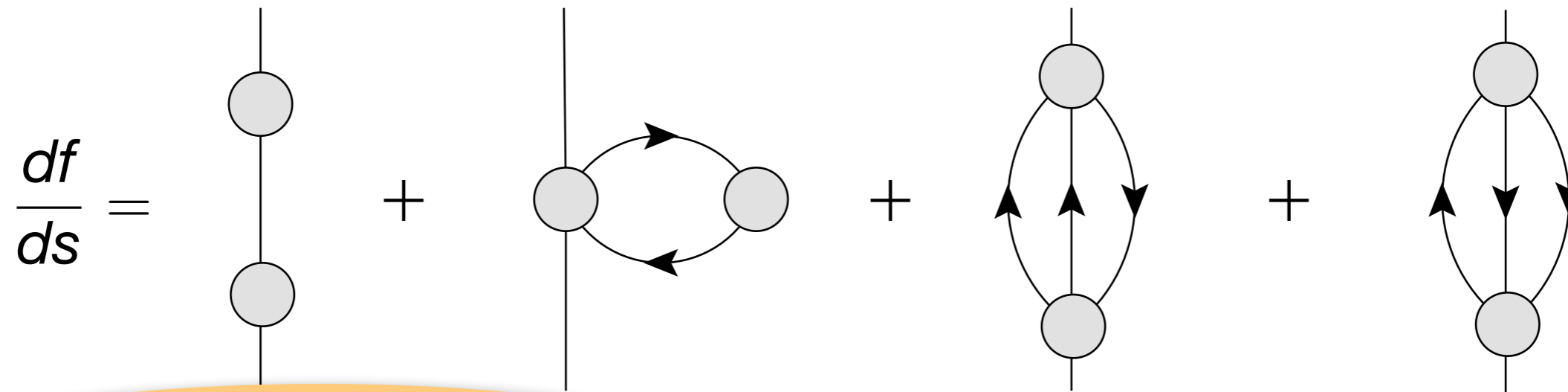


0-body Flow

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



1-body Flow



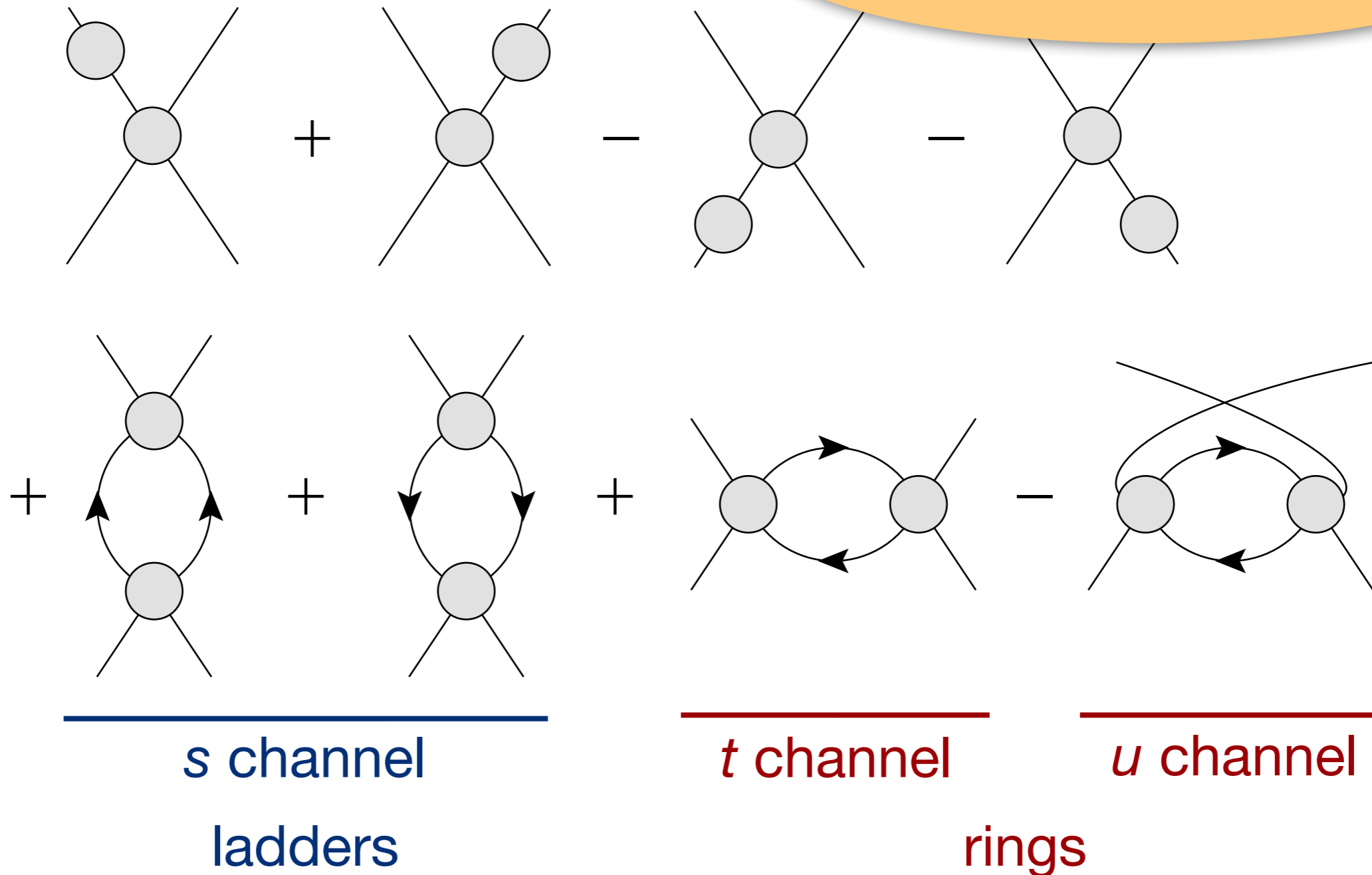
IM-SRG(2): truncate ops. at two-body level

IM-SRG(2) Flow Equations



2-body Flow

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



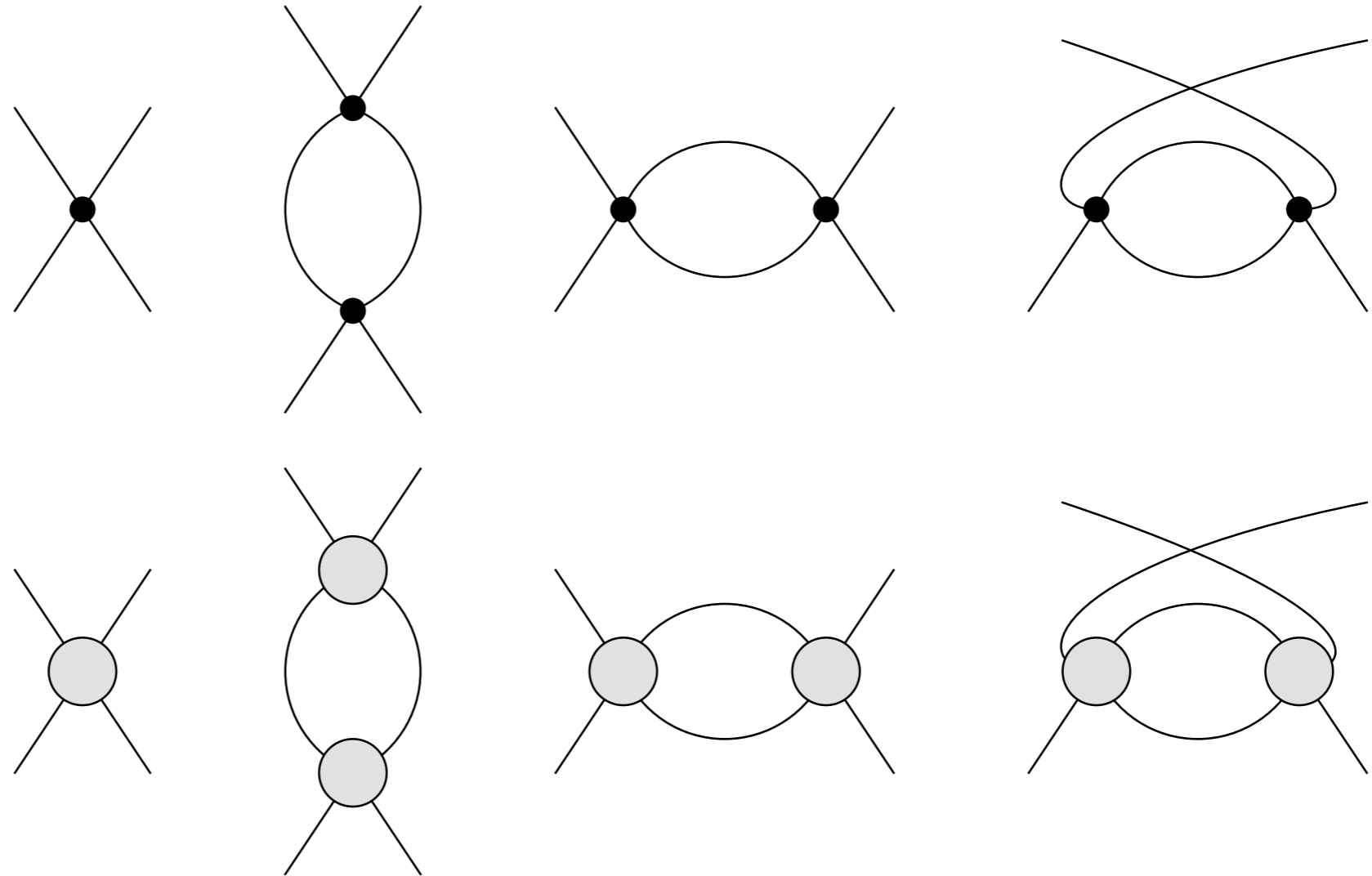
In-Medium SRG Flow: Diagrams



$\Gamma(\delta s) \sim$



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



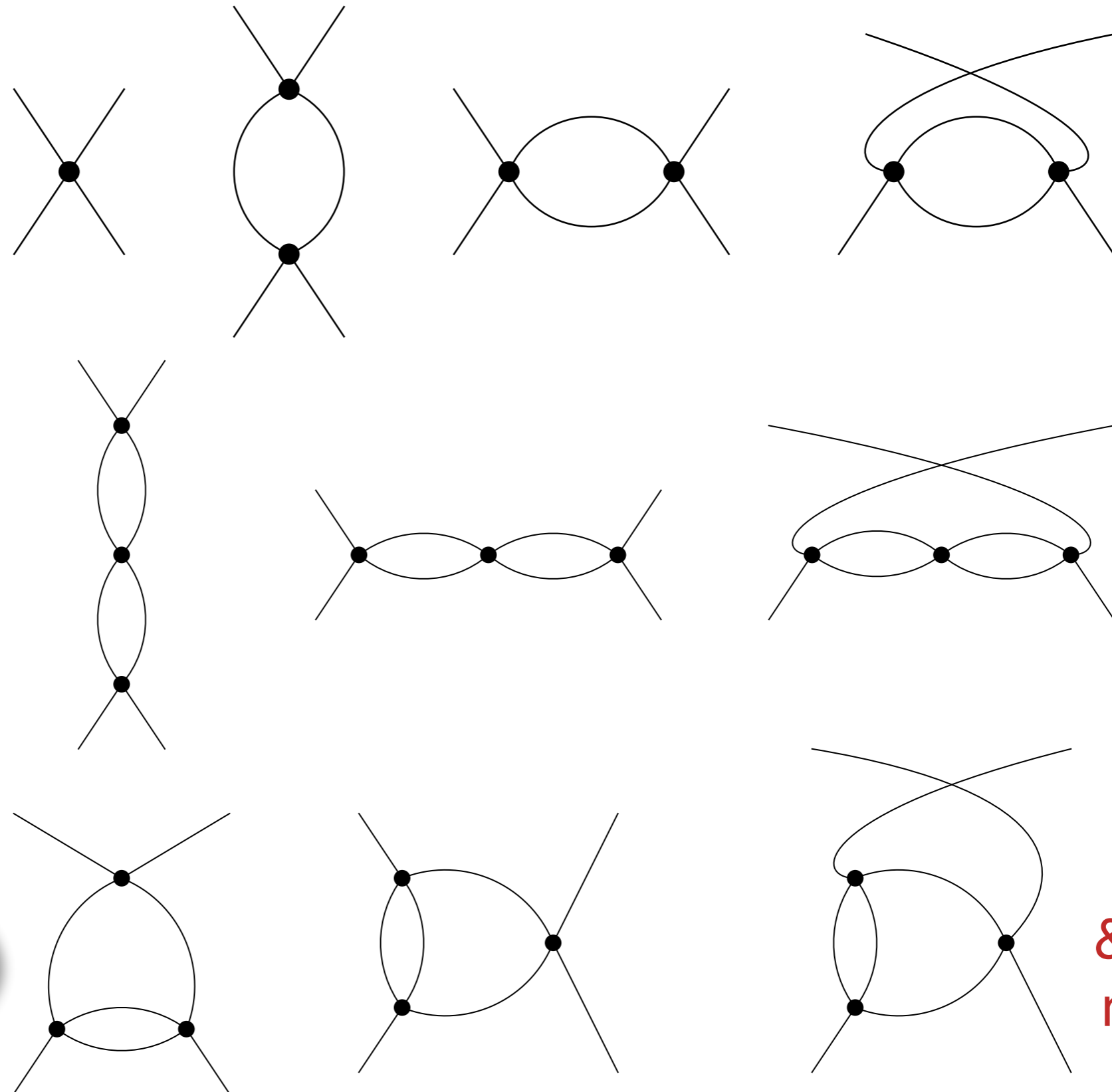
In-Medium SRG Flow: Diagrams



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



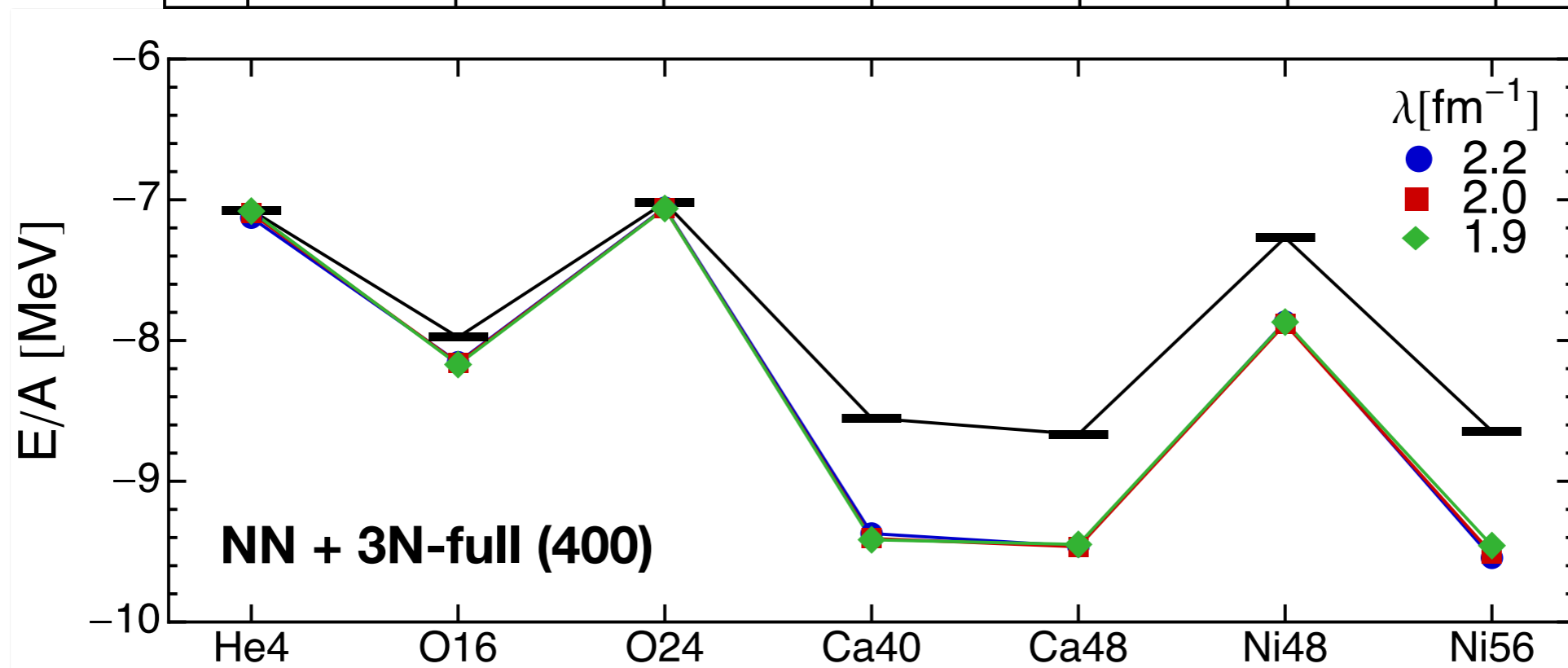
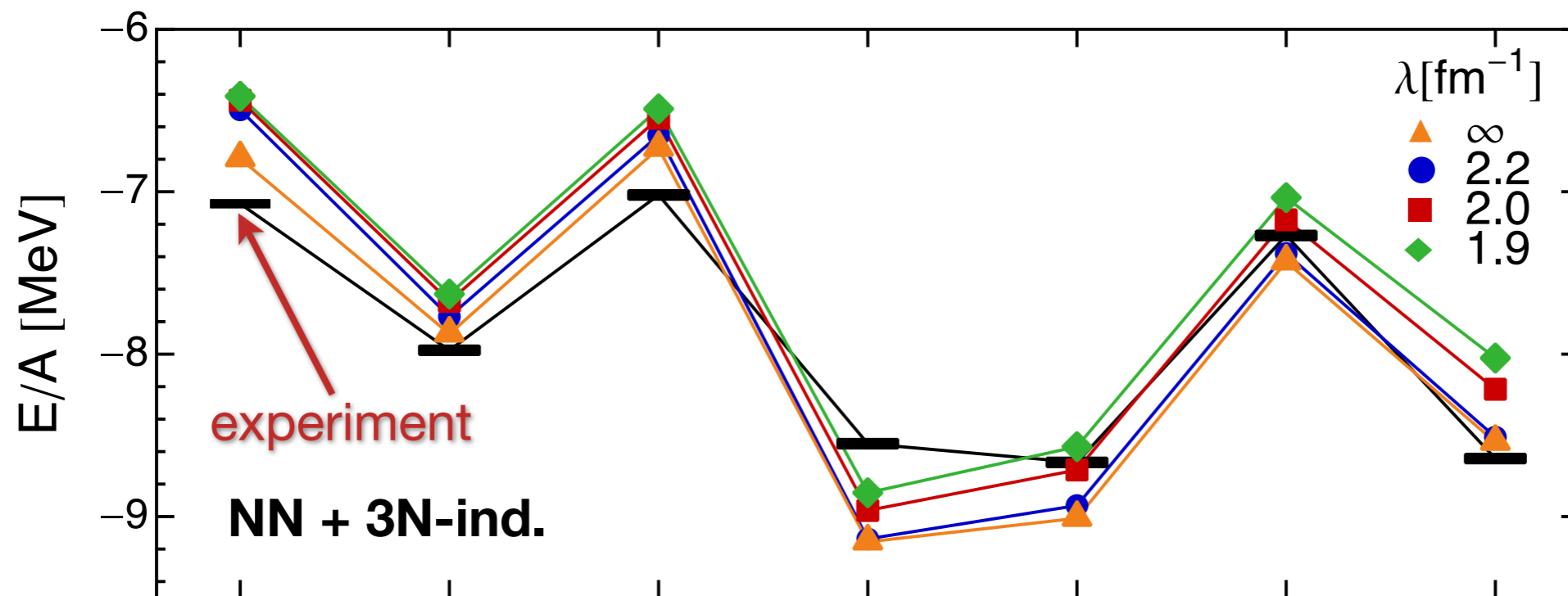
$$\Gamma(2\delta s) \sim$$



non-
perturbative
resummation

& many
more...

Results: Closed-Shell Nuclei



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

Choice of Generator



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

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

$$\eta^{II} = \sum_{ph} \frac{f_h^p}{\Delta_h^p} : A_h^p : + \frac{1}{4} \sum_{pp'hh'} \frac{\Gamma_{hh'}^{pp'}}{\Delta_{hh'}^{pp'}} : A_{hh'}^{pp'} : - \text{H.c.}$$

$\Delta_h^p, \Delta_{hh'}^{pp'}$: approx. 1p1h, 2p2h excitation energies

- **“imaginary time”:** (Morris, Bogner)

$$\eta^{III} = \sum_{ph} \text{sgn}(\Delta_h^p) f_h^p : A_h^p : + \frac{1}{4} \sum_{pp'hh'} \text{sgn}(\Delta_{hh'}^{pp'}) \Gamma_{hh'}^{pp'} : A_{hh'}^{pp'} : - \text{H.c.}$$

- off-diagonal matrix elements are suppressed like $e^{-\Delta^2 s}$ (Wegner), e^{-s} (White), and $e^{-|\Delta|s}$ (imaginary time)

- g.s. energies ($s \rightarrow \infty$) differ by $\ll 1\%$

MR-IM-SRG Flow Equations



0-body flow:

$$\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \eta_b^{af} \eta_a^{fb} + \frac{1}{2} \sum_{abcd} \eta_{cd}^{ab} \Gamma_{ab}^{cd} n_a n_b \bar{n}_c \bar{n}_d \quad \mathcal{O}(N^4)$$

$$+ \frac{1}{4} \sum_{abcd} \left(\frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{cd}^{ab} + \frac{1}{4} \sum_{abcdklm} \left(\eta_{cd}^{ab} \Gamma_{am}^{kl} - \Gamma_{cd}^{ab} \eta_{am}^{kl} \right) \lambda_{cdm}^{bkl}$$

$\mathcal{O}(N^4)$
 $\mathcal{O}(N^7)$

- storage of full 3B density matrix too expensive in general
- ➔ exploit structure of specific reference states:
 - Projected HFB: $\mathcal{O}(N^3)$ storage, scaling reduced to $\mathcal{O}(N^4)$

$$\lambda_{def}^{abc} = \bar{\lambda}_{abc} \delta_d^a \delta_e^b \delta_f^c + \tilde{\lambda}_{a|be} \delta_d^a \delta_e^{b\bar{c}} \delta_{ef} + \text{perm.}$$
 - NCSM / active-space CI: small non-zero block only

Particle-Number Projected HFB



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

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

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

$$\lambda_i^k = \frac{\langle \Psi | A_i^k P_N | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad \lambda_{mn}^{kl} = \frac{\langle \Psi | A_{mn}^{kl} P_N | \Psi \rangle}{\langle \Psi | \Psi \rangle} - \lambda_m^k \lambda_m^l + \lambda_n^k \lambda_m^l$$

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

$$\lambda_i^k = n_k \delta_i^k \quad (= v_k^2 \delta_i^k), \quad 0 \leq n_k \leq 1$$

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