Low-lying Spectra from the Equation-of-Motion IMSRG

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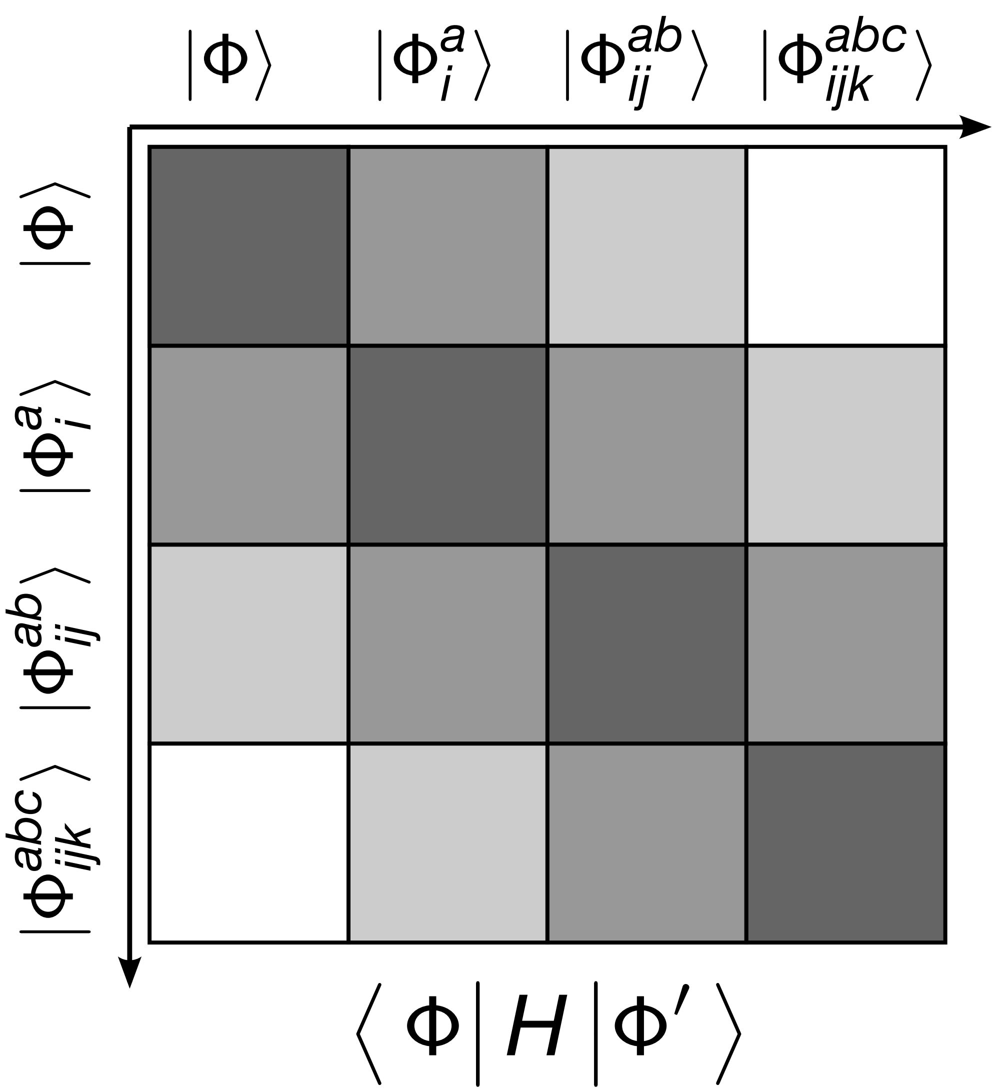
In-Medium SRG

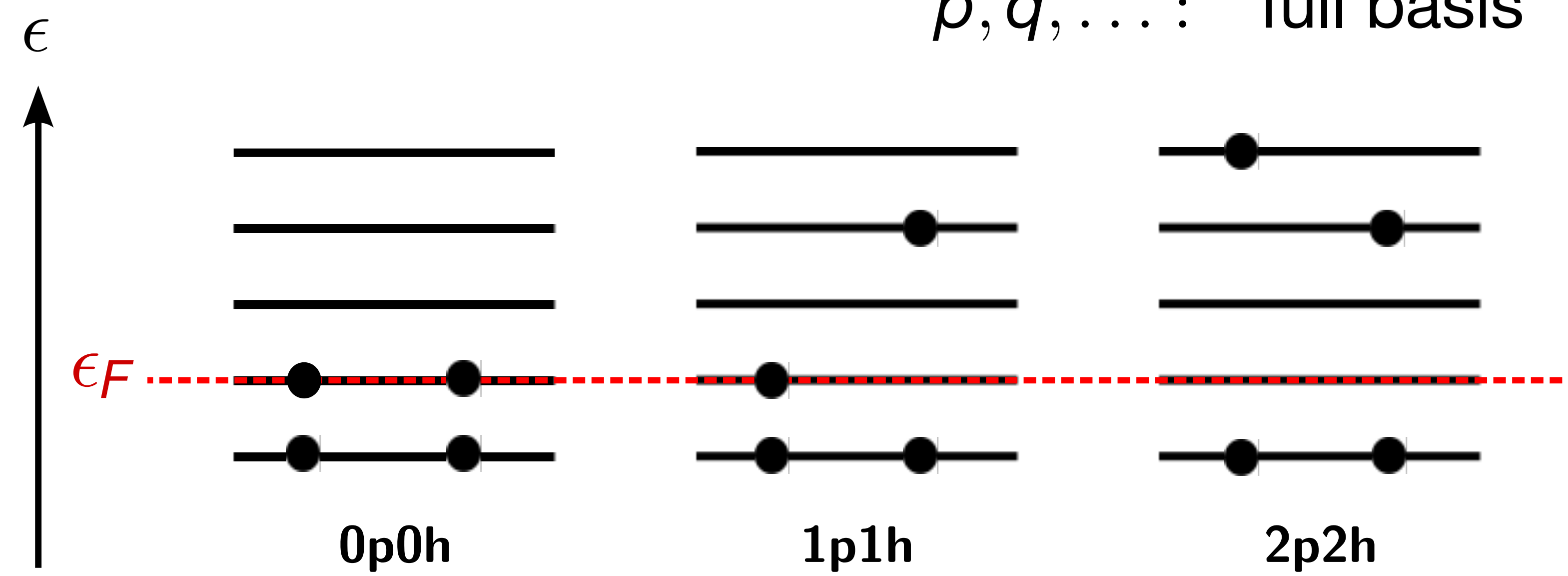
Transforming the Hamiltonian



$a, b, \ldots : \quad \epsilon > \epsilon_F$

$i, j, \ldots : \quad \epsilon \leq \epsilon_F$

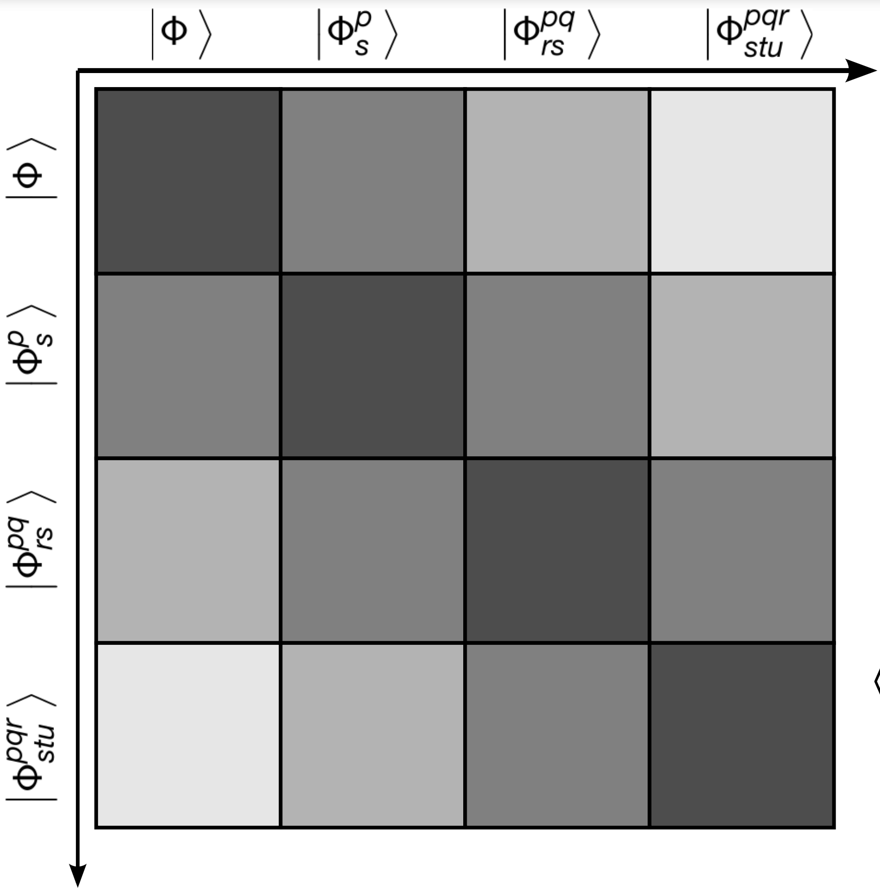
$p, q, \ldots : \quad$ full basis



- reference state: **single Slater determinant**

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

Multi-Reference Case



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

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

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

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

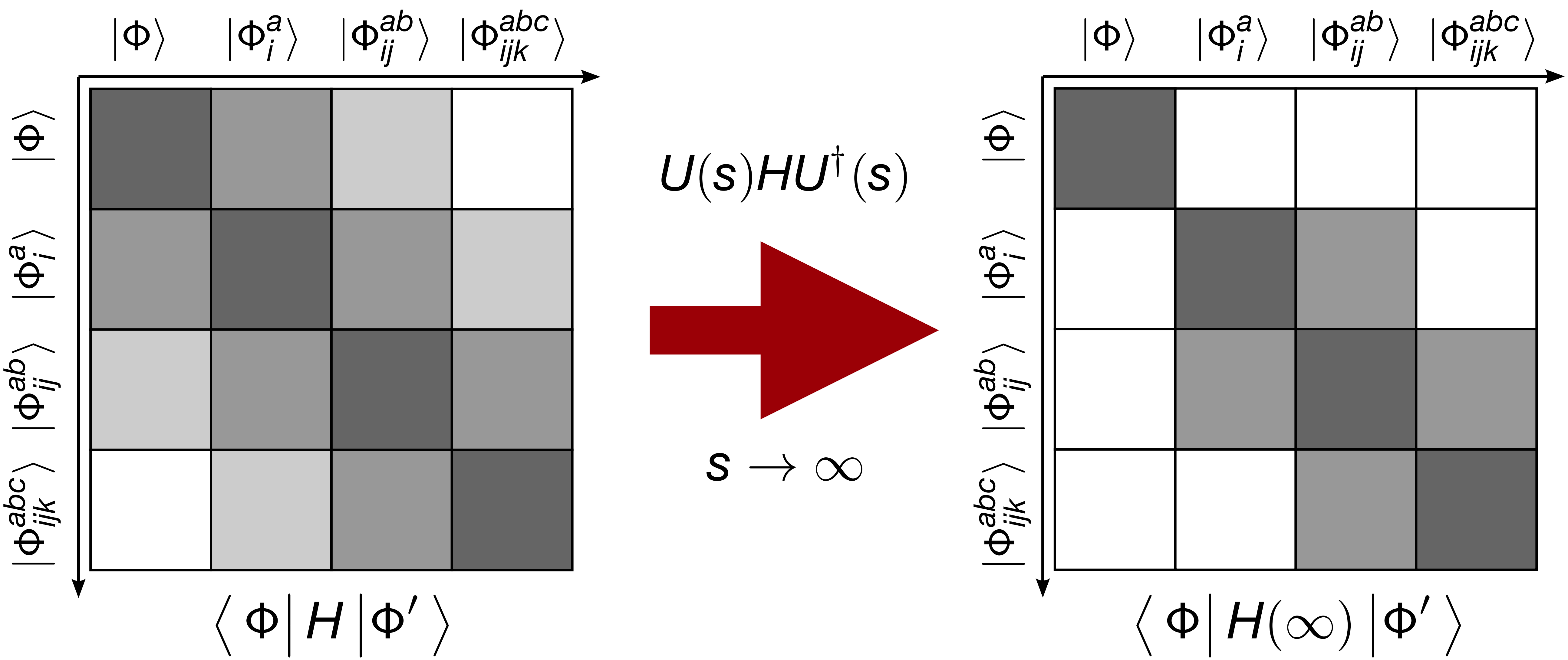
$$\rho^{kl}_{mn} = \lambda^{kl}_{mn} + \lambda^k_m \lambda^l_n - \lambda^k_n \lambda^l \dots$$

$$\rho^{ijk}_{lmn} = \lambda^{ijk}_{lmn} + \lambda^i_l \lambda^{jk}_{mn} + \lambda^i_l \lambda \dots$$

$$\dots$$

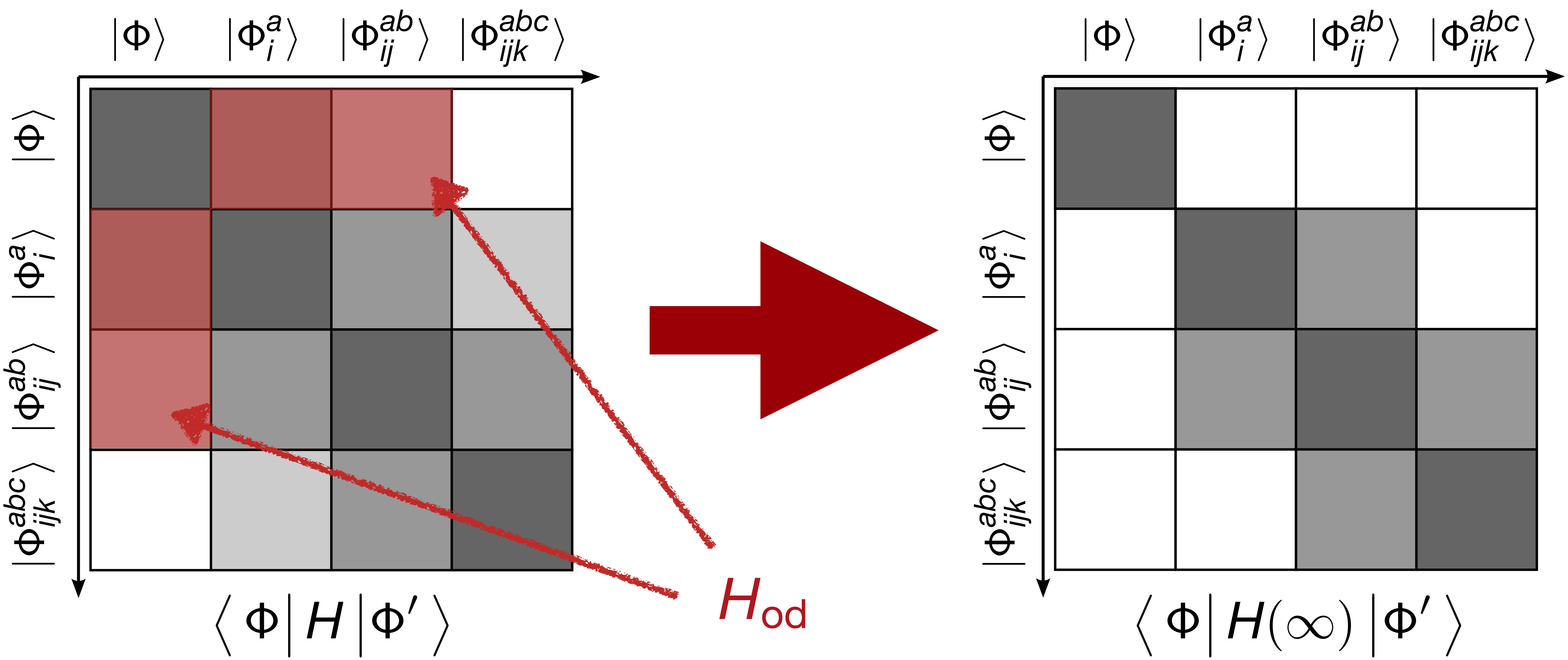
irreducible density matrices encode correlations

Decoupling in A-Body Space



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

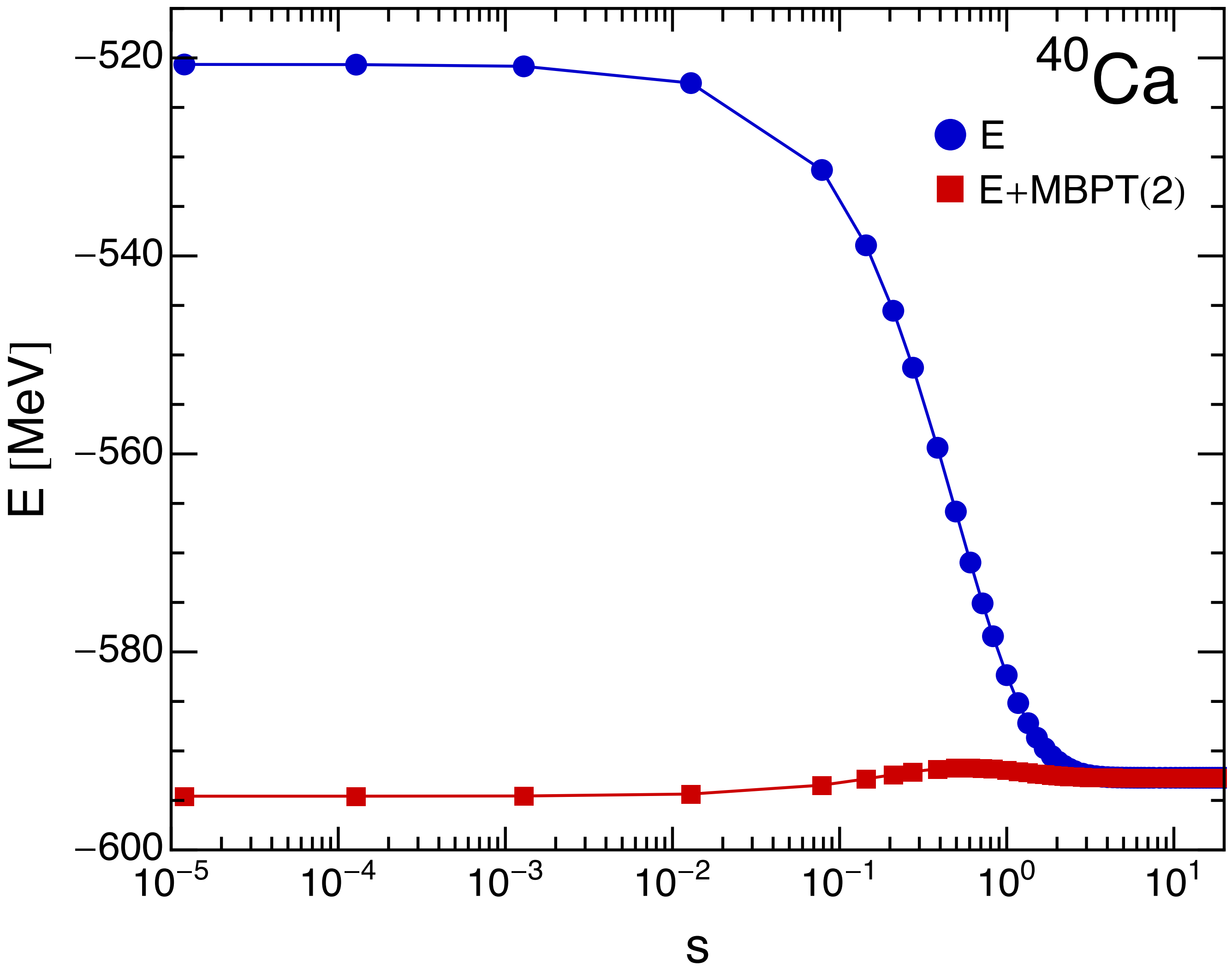
Flow Equation

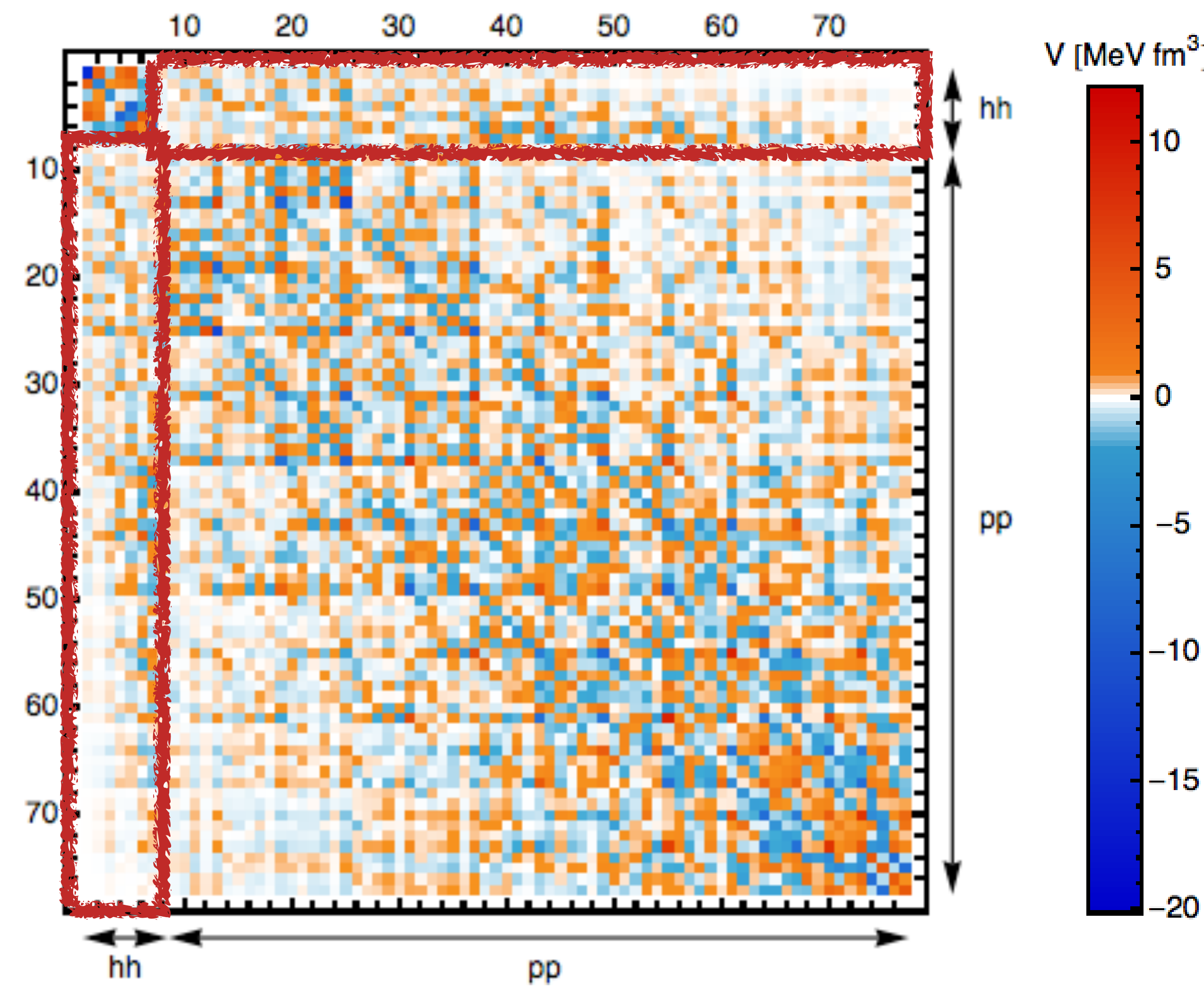


$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right],$$

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

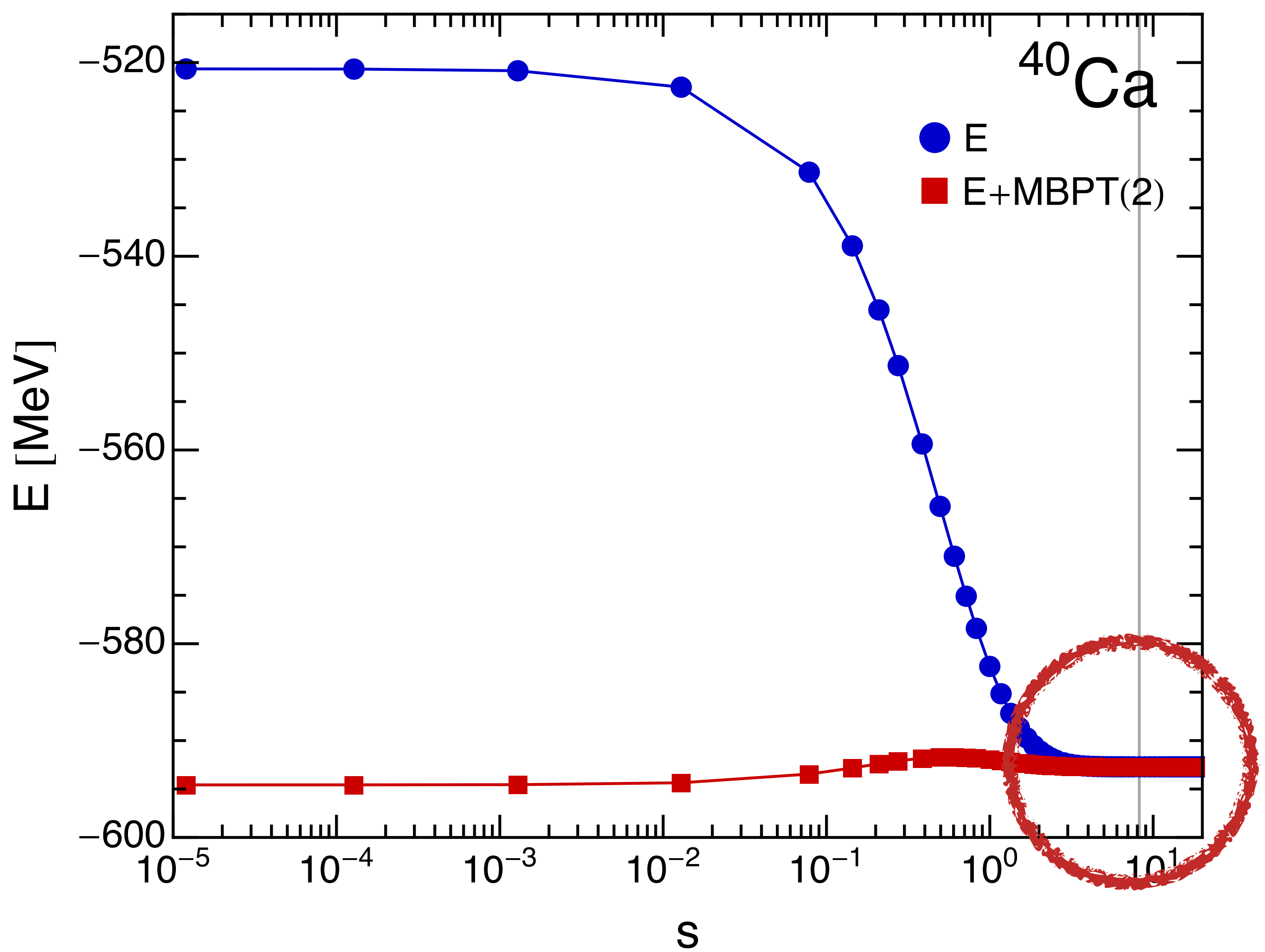
Decoupling

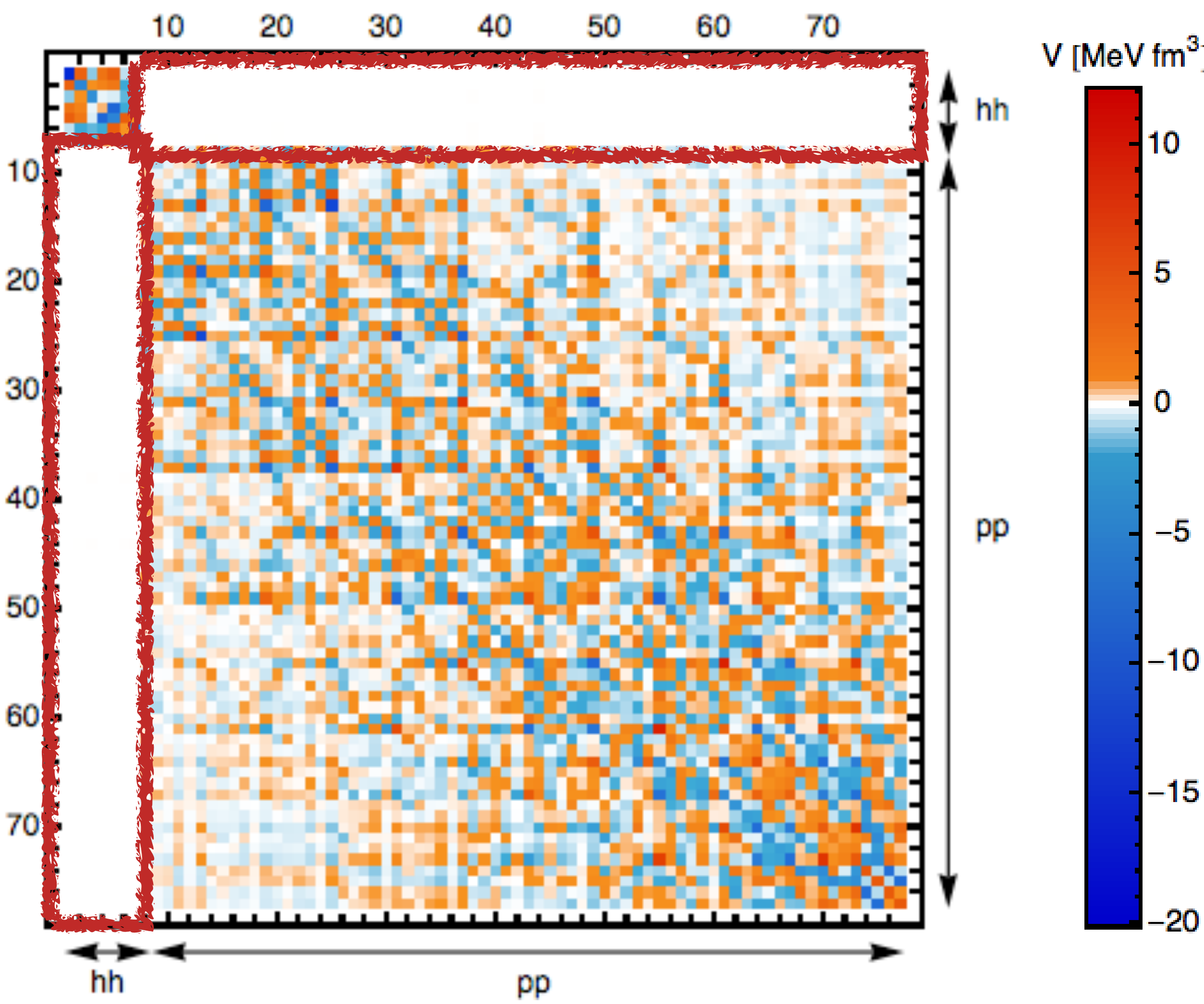




N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

Decoupling



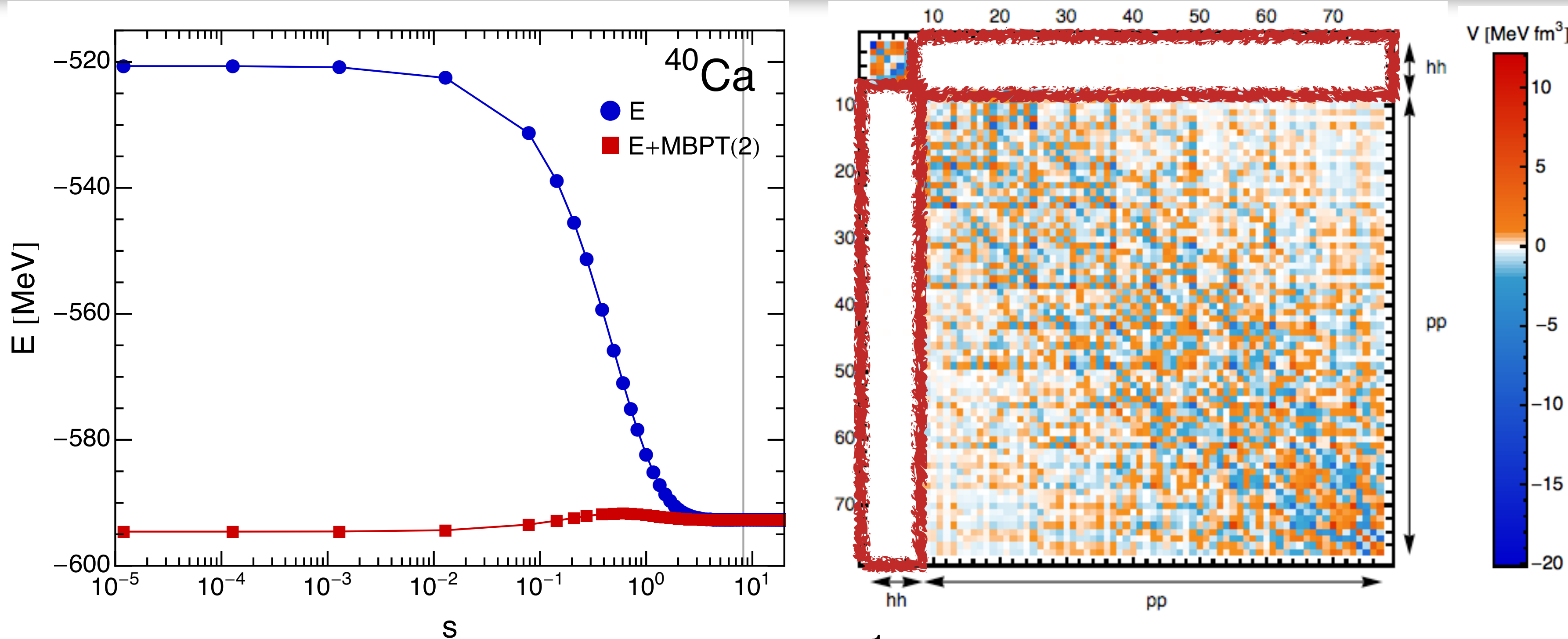


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series **(correlations)**

off-diagonal couplings are rapidly driven to zero

Decoupling



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

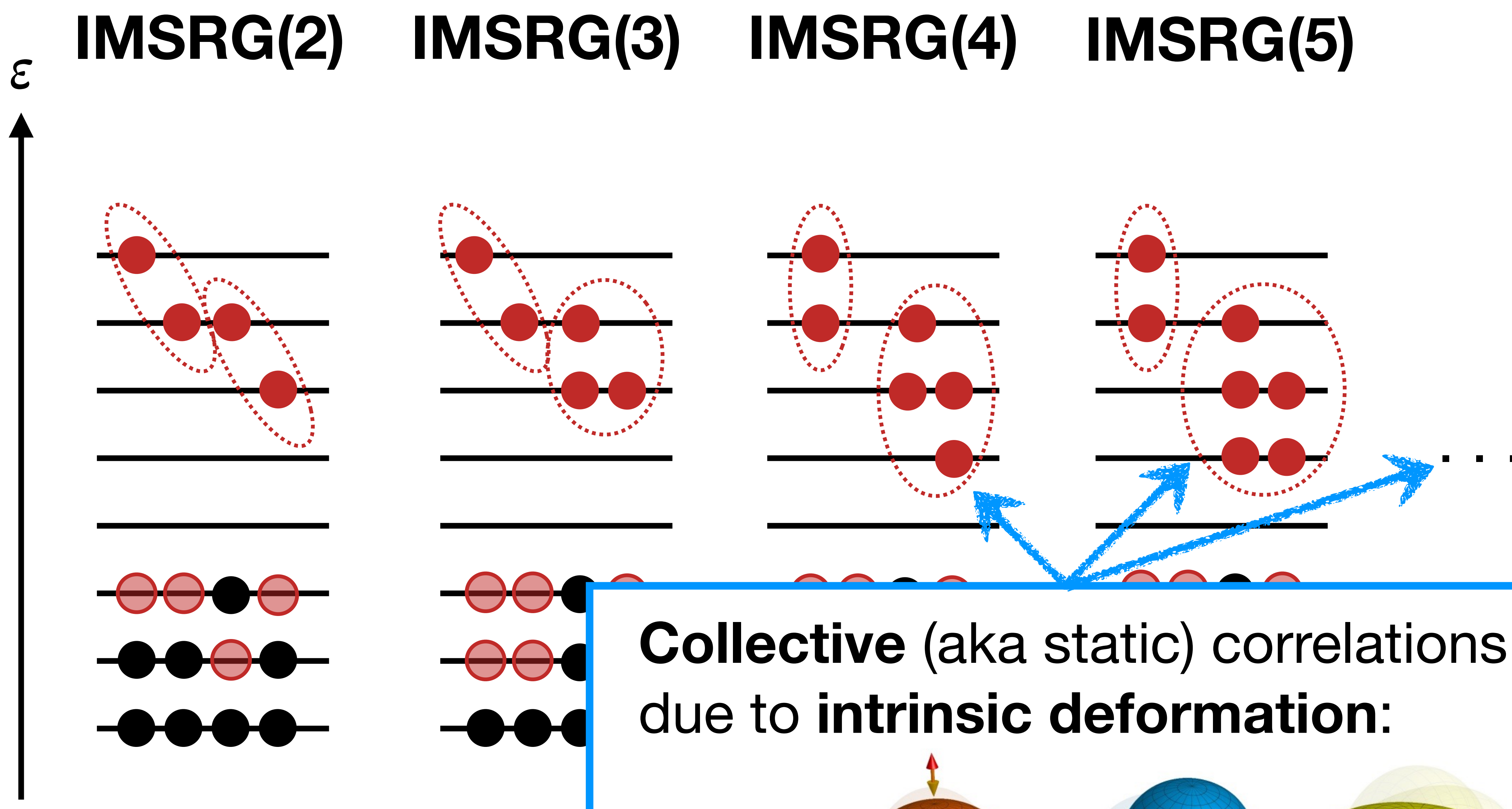
- absorb correlations into **RG-improved Hamiltonian**

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

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

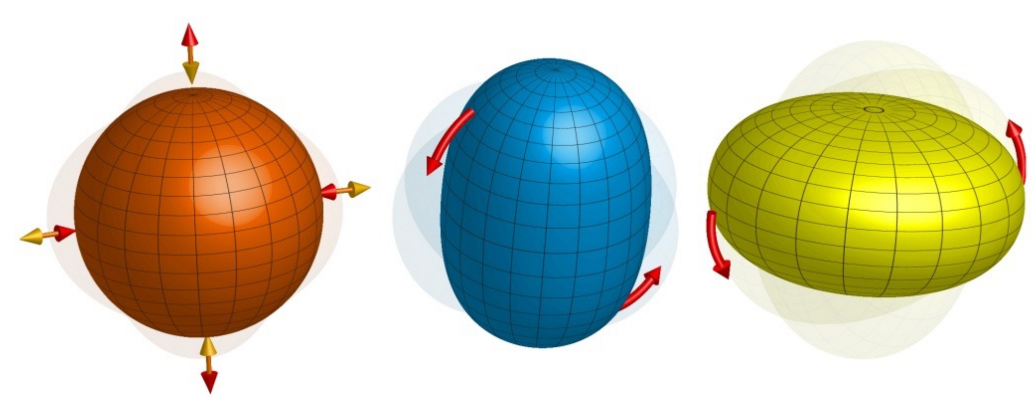
$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

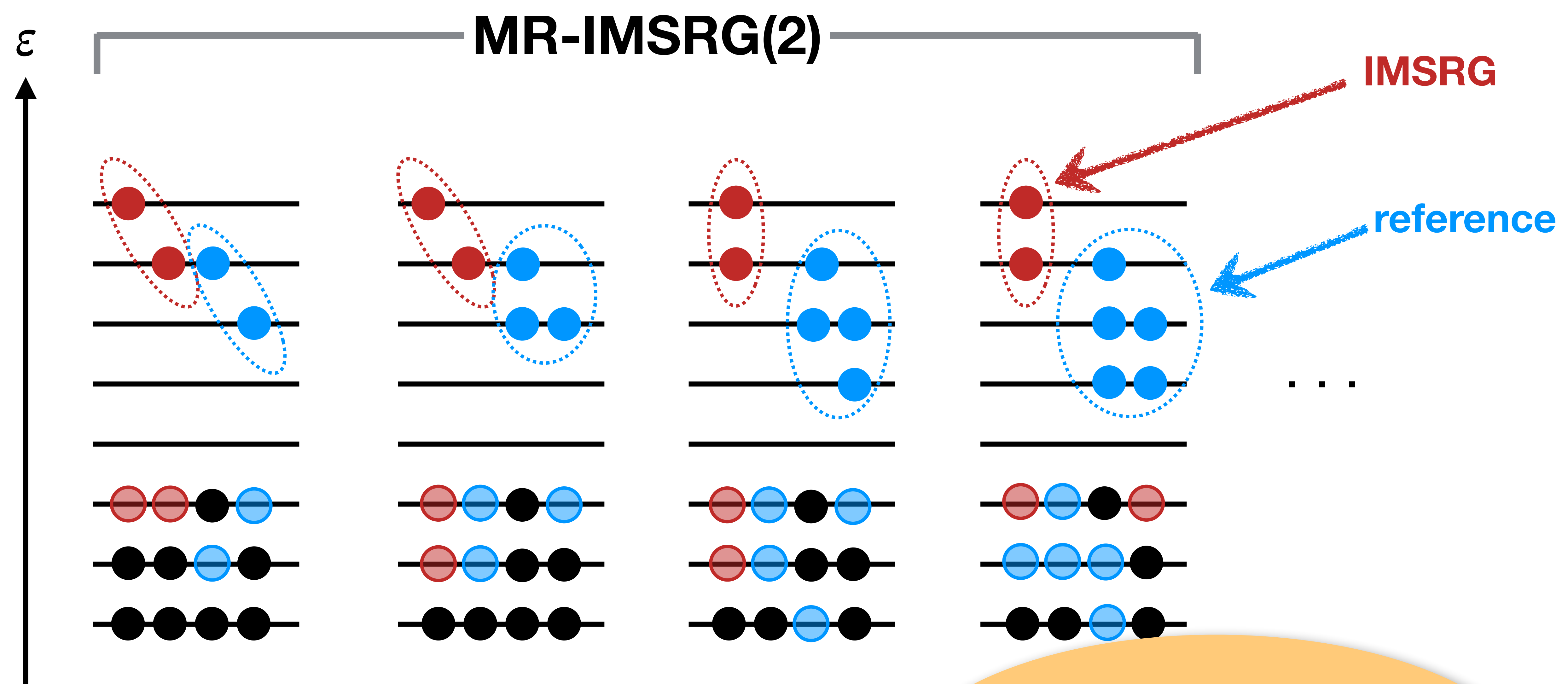


“standard” IMS
Slater determinan

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



Correlated Reference States



MR-IMSRG: build correlation[s on top of]
already correlated state (e.g., fro[m …]
describes static correlation[s]

new contractions (two-body and higher densities), but **scaling remains unchanged**

MR-IMSRG References States

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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**:

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

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

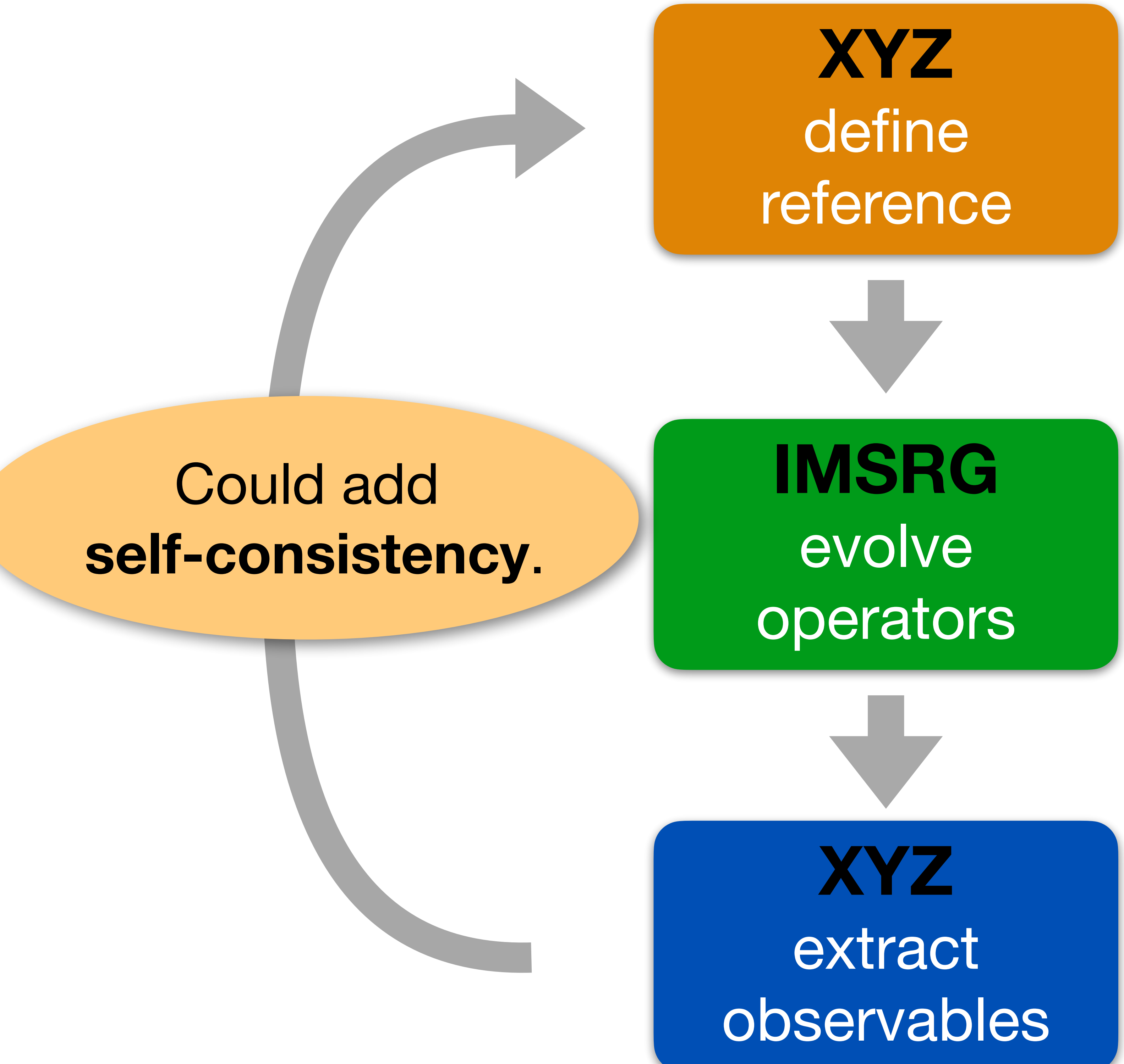
$$\left|\Phi\right\rangle = \int dq\, f(q)\, P_{J=0M=0}P_Z P_N \left|q\right\rangle$$

future

- clustered states, Density Matrix Reno[rmalization Group,] etc.

as long as $|\Phi\rangle$ has $J^\pi = 0^+$, we can use IMSRG evolution for **spherical tensors**

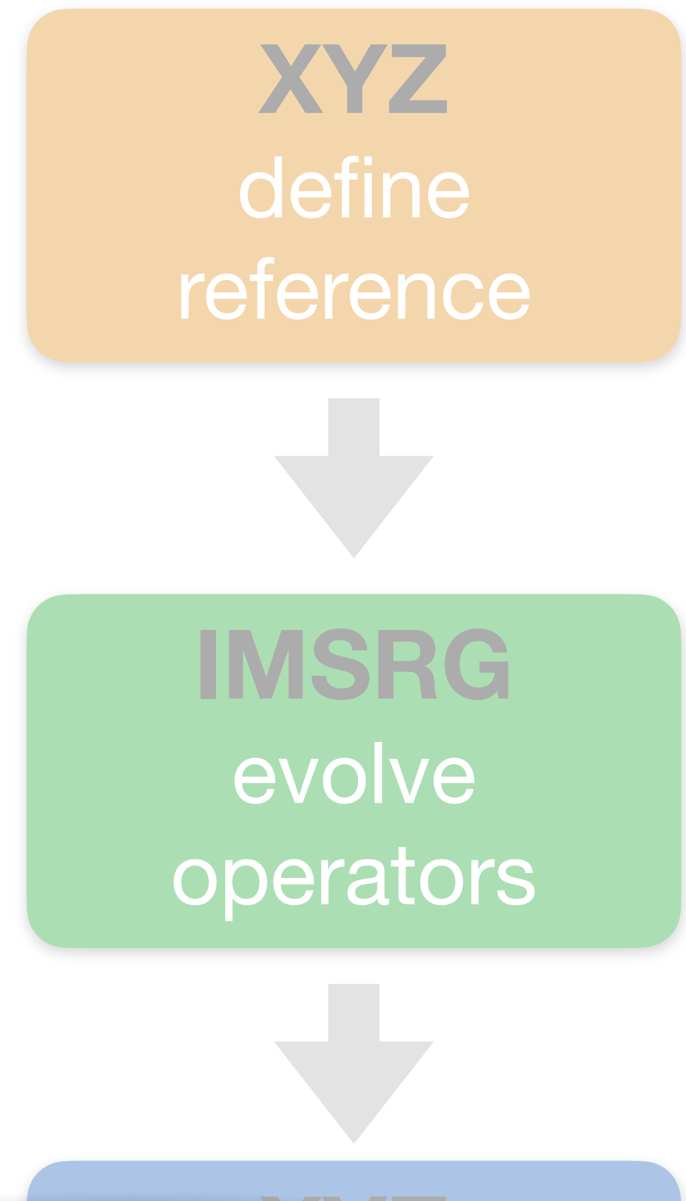
IMSRG-Improved Methods



* mean field or **explicitly correlated**

IMSRG-Improved Methods

- IMSRG for closed and open-shell nuclei: IM-HF and IM-PHFB
  - HH, Phys. Scripta, Phys. Scripta 92, 023002 (2017)
  - HH, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. 621, 165 (2016)
- Valence-Space IMSRG (VS-IMSRG)
  - S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Nucl. Part. Sci. **69**, 165 (2019)
- In-Medium No Core Shell Model (IM-NCSM)
  - E. Gebrerufael, K. Vobig, HH, R. Roth, PRL **118**, 152503 (2017)
- Valence-Space DMRG (VS-DMRG)
  - A. Tichai et al., PLB **845**, 138139 (2023)
- In-Medium Generator Coordinate Method
  - J. M. Yao, J. Engel, L. J. Wang, C. F. Jiao, HH P
  - J. M. Yao et al., PRL 124, 232501 (2020)



more hybrid methods in development (NCSMC, SA-NCSM, DMRG, …)

IMSRG-Improved Methods

XYZ
define
reference

* mean field or **explicitly correlated**

IMSRG
evolve
operators

Could add
self-consistency.

EOM
extract
observables

Equation-of-Motion IMSRG for Closed-Shell Nuclei

Equation-of-Motion Method

N. M. Parzuchowski et al., PRC95, 044304 (2017)

- **Schrödinger equation for excited states:**

$$HQ_k^\dagger |\Psi_0\rangle = E_k Q_k^\dagger |\Psi_0\rangle$$

- Apply **(MR-)IMSRG unitary**:

$$U(s)HU^\dagger(s)U(s)Q_k^\dagger U^\dagger(s)U(s)|\Psi_0\rangle = E_k U(s)Q_k^\dagger U^\dagger(s)U(s)|\Psi_0\rangle$$

- Introduce **transformed operators** and use $U(s)|\Psi_0\rangle = |\Phi_0\rangle$:

$$H(s)Q_k^\dagger(s)|\Phi_0\rangle = E_k Q_k^\dagger(s)|\Phi_0\rangle$$

- Rewrite as **Equation of Motion**:

$$[H(s), Q_k^\dagger(s)]|\Phi_0\rangle = \omega_k Q_k^\dagger(s)|\Phi_0\rangle$$

- **No approximations** so far…

Equation-of-Motion Method

N. M. Parzuchowski et al., PRC95, 044304 (2017)

- write EoM as (generalized) eigenvalue problem

$$\langle\Phi_0|\,[\delta Q(s),[H(s),Q_k^\dagger(s)]]\,|\Phi_0\rangle = \omega_k\langle\Phi_0|\,[\delta Q(s),Q_k^\dagger(s)]\,|\Phi_0\rangle$$

- **ansatz** for excitation operator, e.g., for **closed-shell nuclei,**

$$Q_k^\dagger(s) = \sum_{ai}\left(Q_k\right)^a_i(s) :A^a_i: + \frac{1}{4}\sum_{abij}\left(Q_k\right)^{ab}_{ij}(s) :A^{ab}_{ij}: + \ldots$$

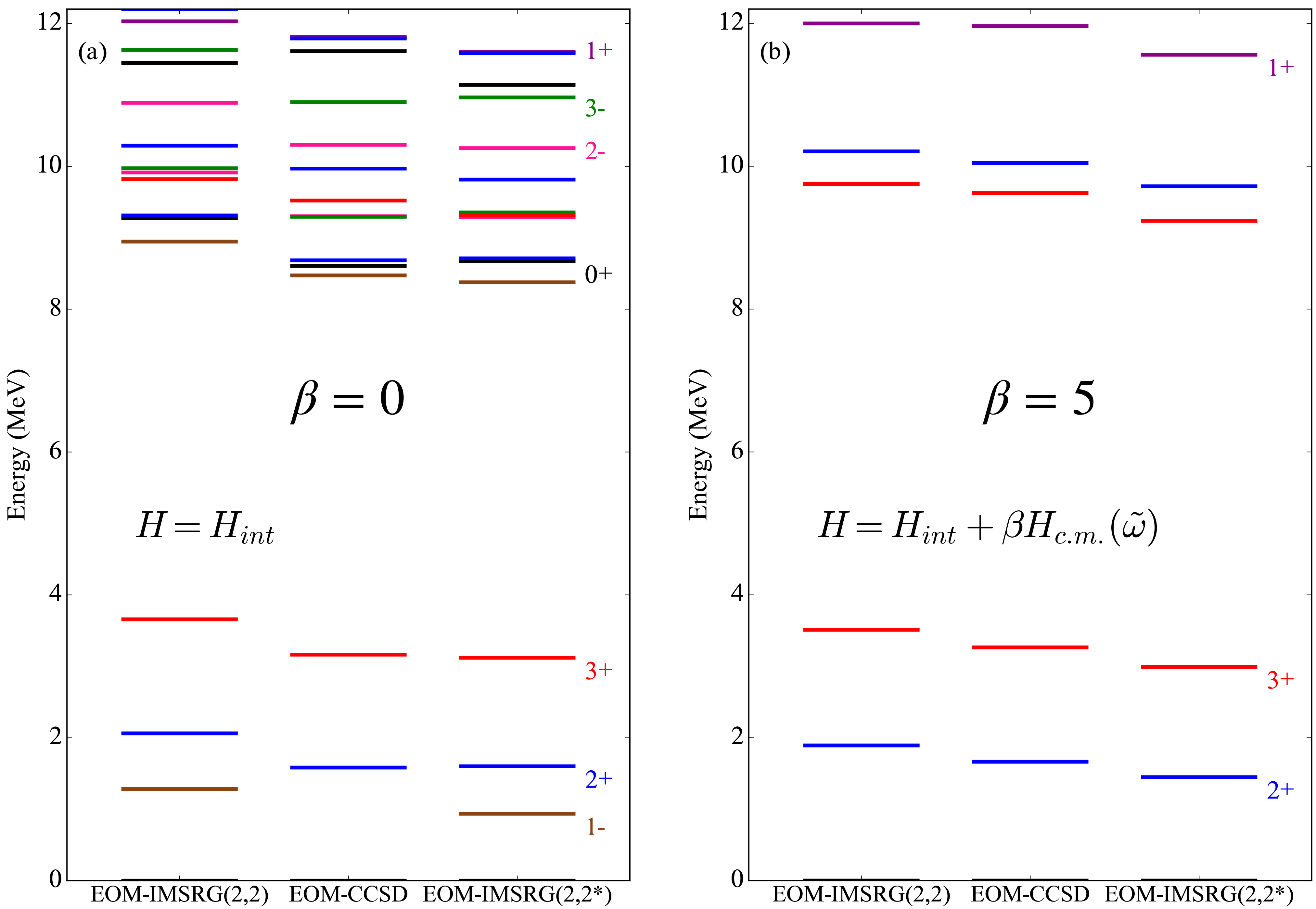
- **only excitations** included - ground-state correlations have been built into Hamiltonian
  - RPA reduces to TDA, etc.

cf. talk by R. Roth

- approximations make $\omega_k(s)$ s**-dependent**

Excitation Spectra

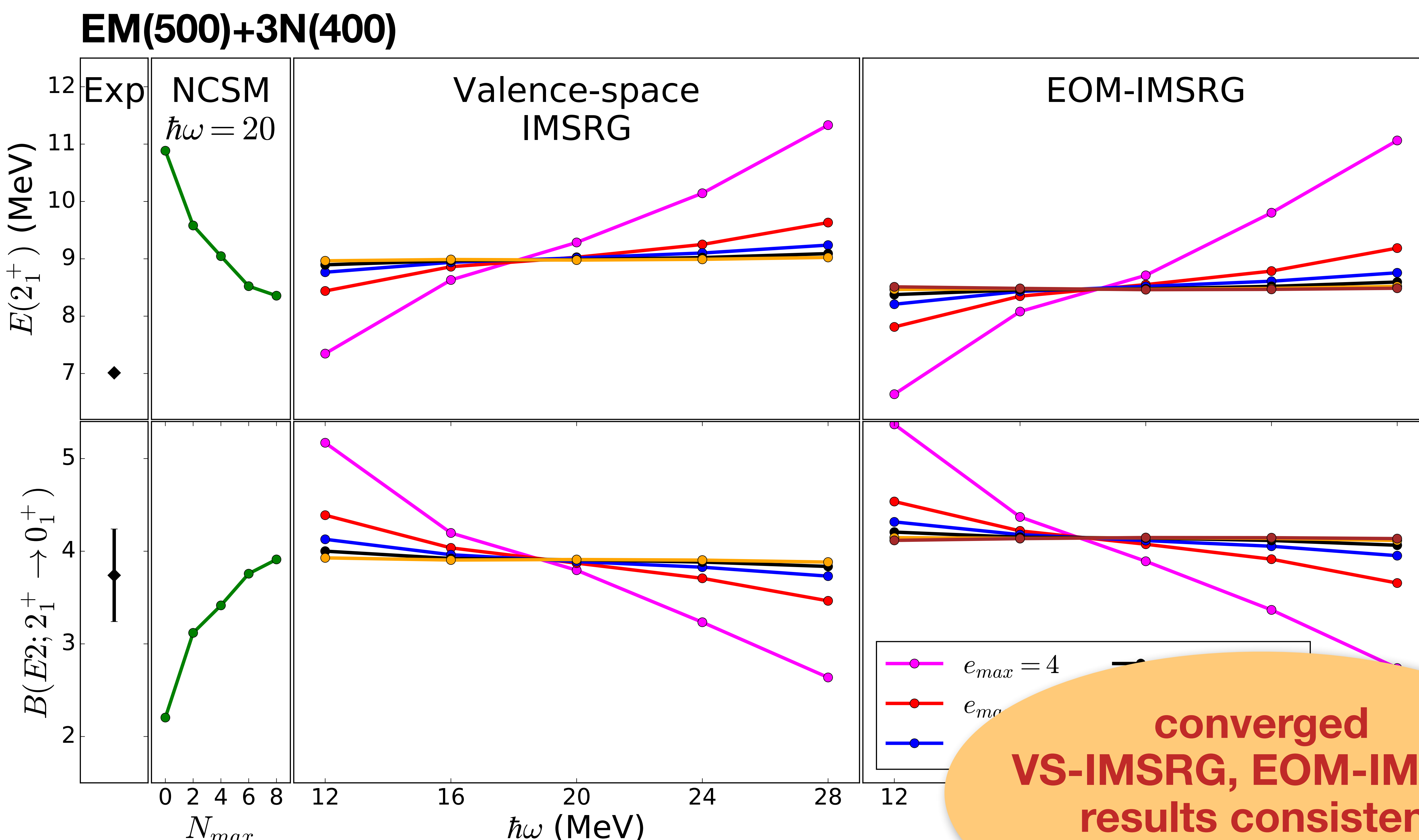
N. M. Parzuchowski et al., PRC95, 044304 (2017)



^{22}O, EM(500) + 3N(400), $\lambda = 2.0\ \text{fm}^{-1}$, $\hbar\omega = 20$ MeV, $e_{\text{Max}} = 11$

Transitions

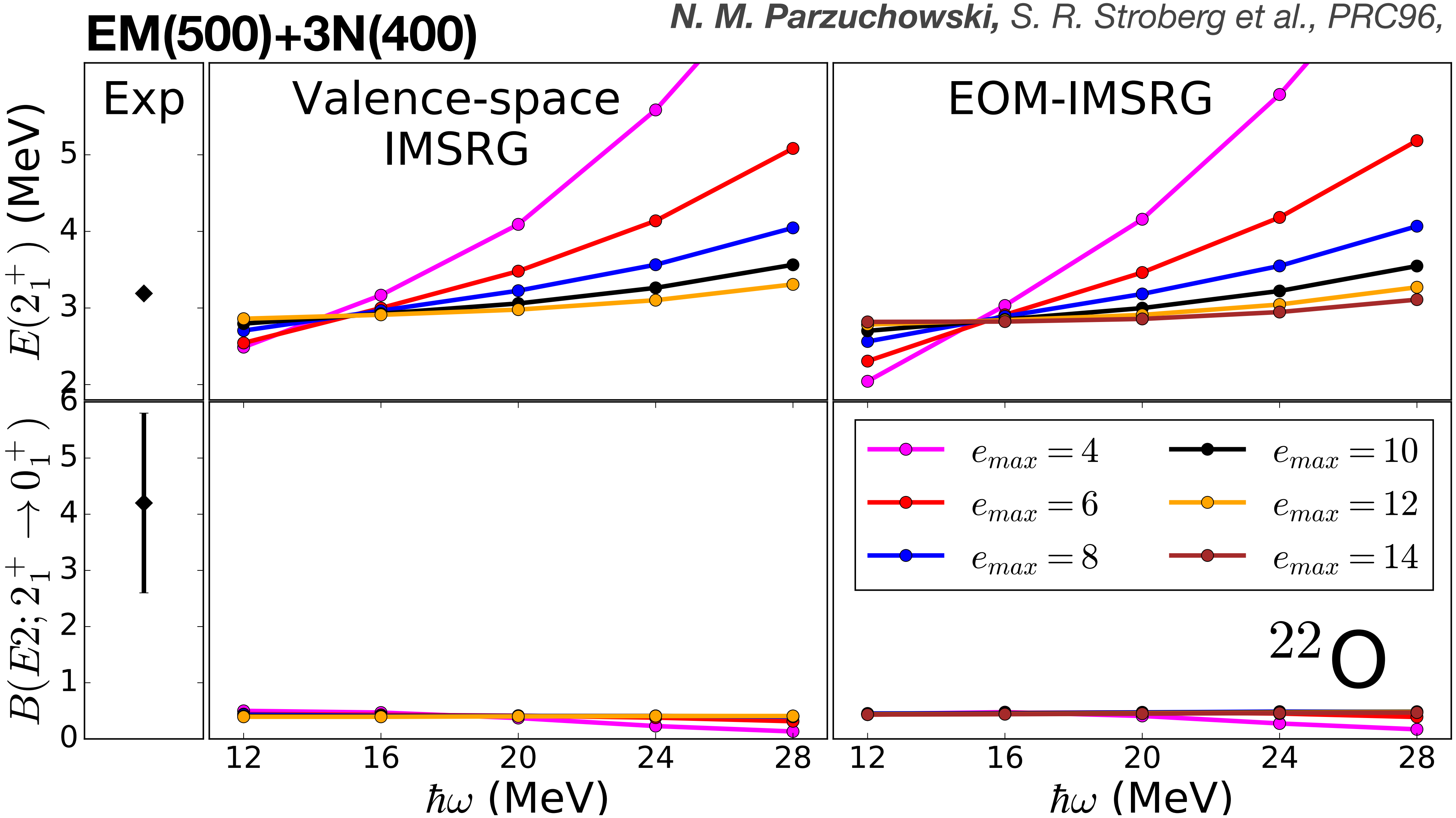
N. M. Parzuchowski, *S. R. Stroberg et al., PRC96, 034324 (2017)*



converged VS-IMSRG, EOM-IMSRG results consistent with NCSM

Transitions

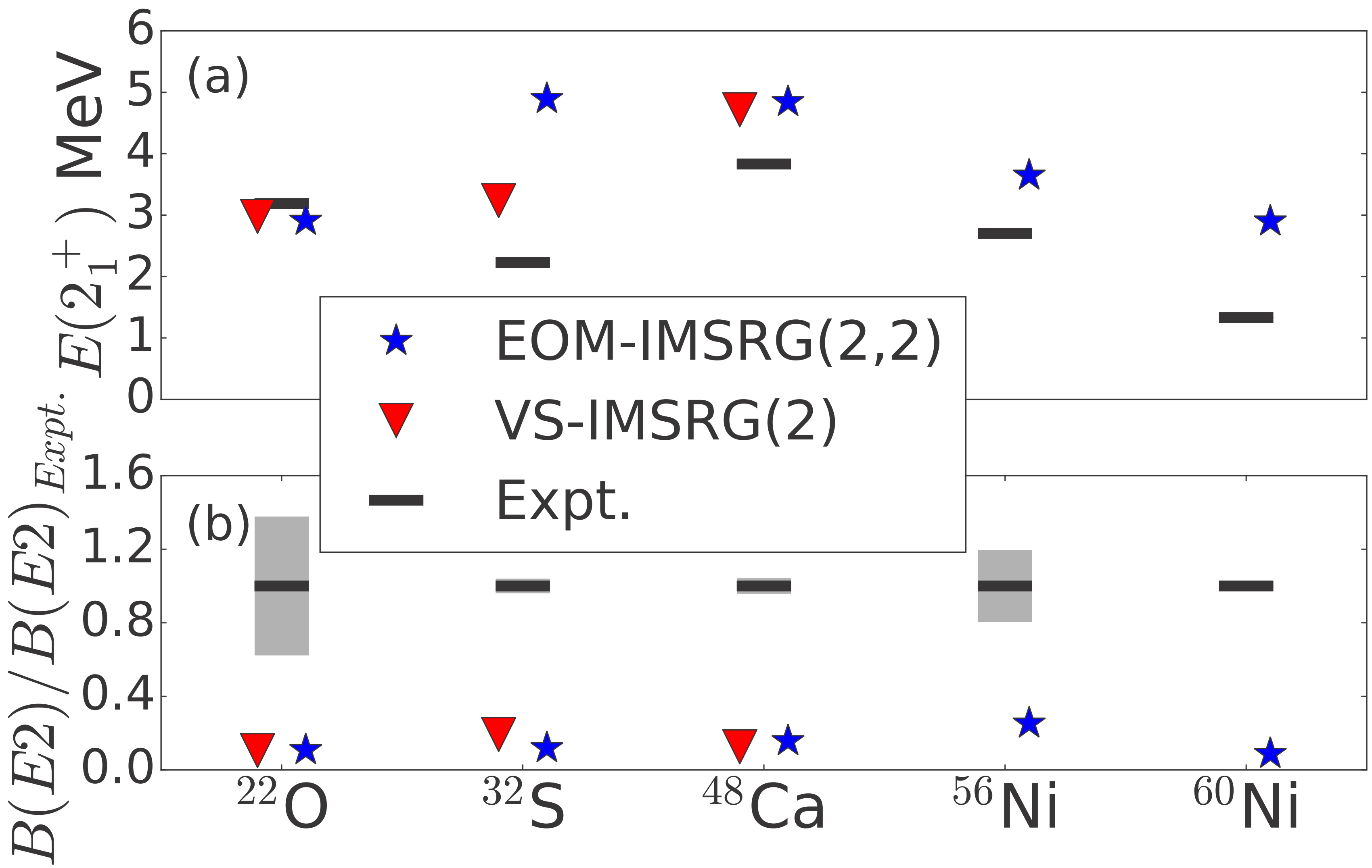
N. M. Parzuchowski, S. R. Stroberg et al., PRC96, 034324 (2017)



- non-zero B(E2) from Shell model: **VS-IMSRG induces effective neutron charge**
- **B(E2) much too small:** effect of intermediate 3p3h, … states that are truncated in IMSRG evolution

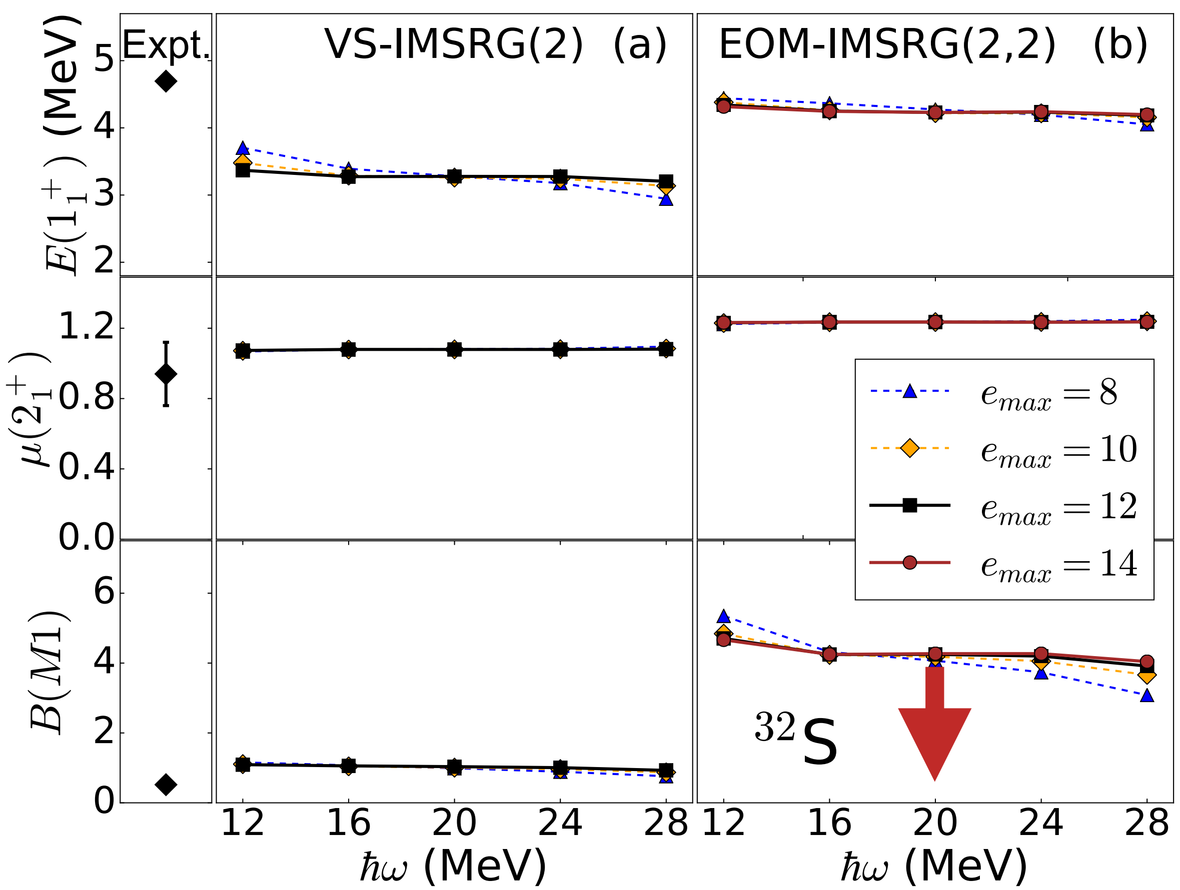
Transitions

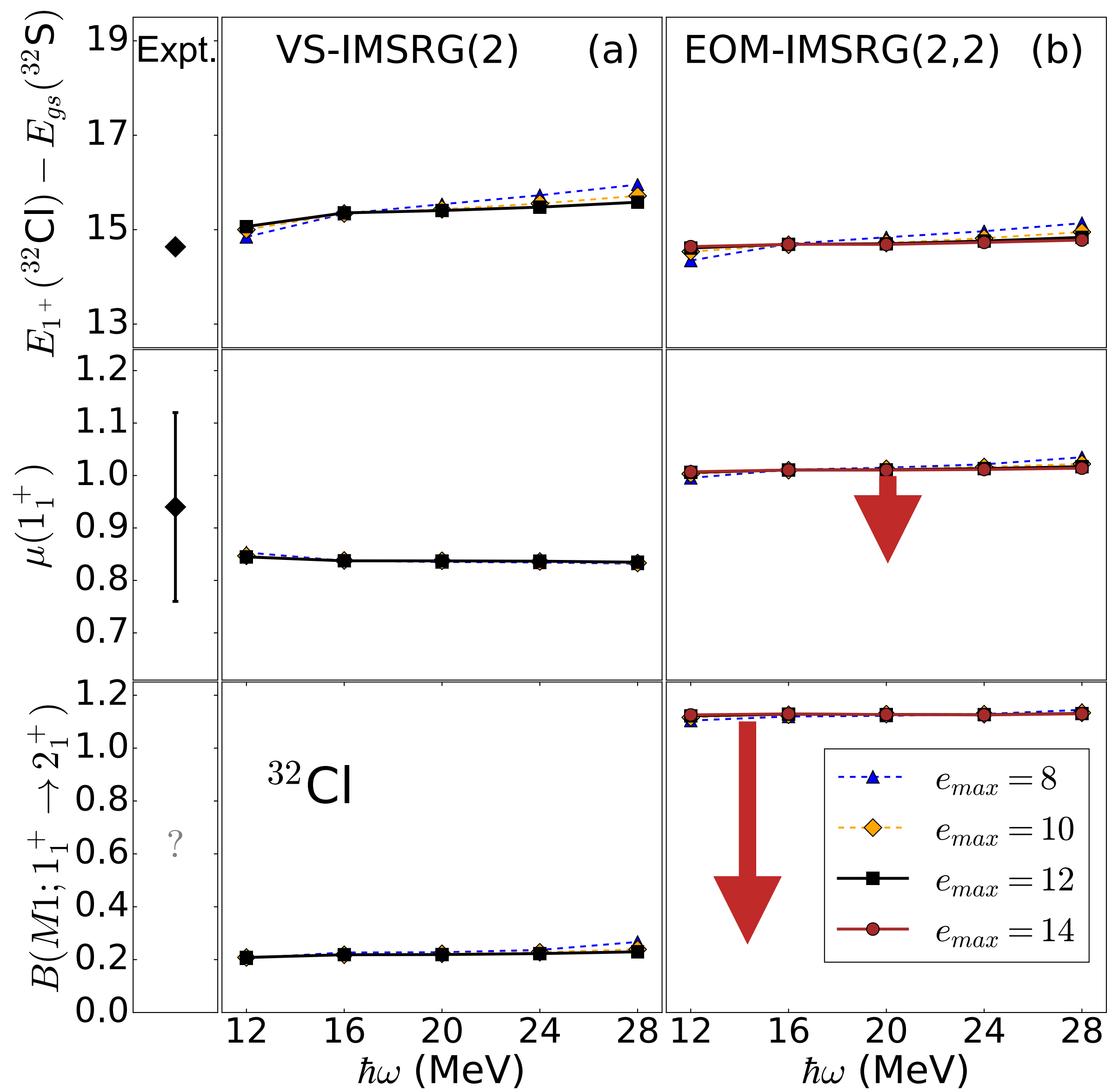
*N. M. Parzuchowski, S. R. Stroberg et al., PRC **96**, 034324 (2017)*
*S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 307 (2019)*
*S. R. Stroberg et al. PRC **105**, 034333 (2022)*



- **B(E2) much too small:** missing collectivity due to intermediate 3p3h, … states that are truncated in IMSRG evolution (**static correlation**)

Charge-Exchange EOM-IMSRG





- ^{32}Cl via **charge-exchange EOM** from ^{32}S
- discrepancy between EOM-IMSRG and VS-IMSRG from npnh correlations **within the valence shell**

Multireference EOM-IMSRG

Multireference EOM

Parzuchowski, Wirth, Hergert

- generalized eigenvalue problem:

$$\langle \Phi_0 | [\delta Q(s), [H(s), Q_n^\dagger(s)]] | \Phi_0 \rangle = \omega_n(s) \langle \Phi_0 | [\delta Q(s), Q_n^\dagger(s)] | \Phi_0 \rangle$$

- ansatz for **excitation operator**:

$$Q_k^\dagger(s) = \sum_{pq} \left(Q_k\right)^p_q(s) : A^p_q : + \frac{1}{4} \sum_{pqrs} \left(Q_k\right)^{pq}_{rs}(s) : A^{pq}_{rs} : + \dots$$

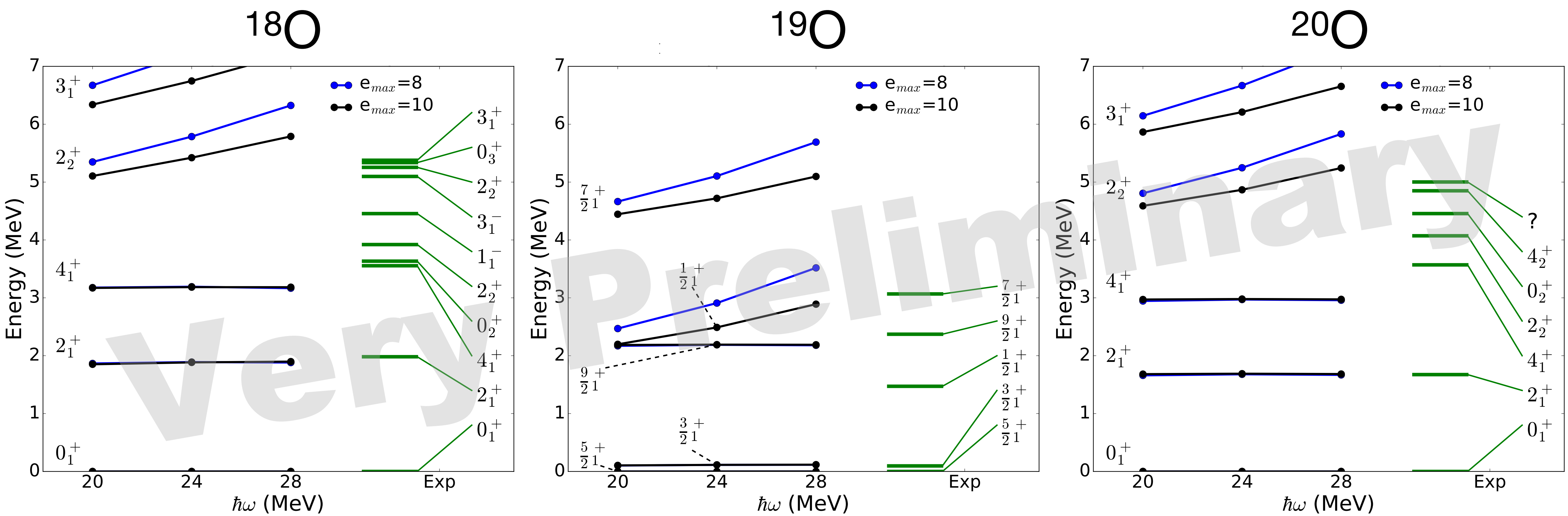
- indices run over **entire single-particle basis**

- basis of excitations is **nonorthogonal, overcomplete** - overlap matrix on RHS is **singular**

- N**-body excitation operator,** A**-body Hamiltonian:** up to $\lambda^{(\mathbf{2N-1})}$ in overlap, LHS might require up to $\lambda^{(\mathbf{A+2N-1})}$

Very Early Application

Parzuchowski, Wirth, Hergert

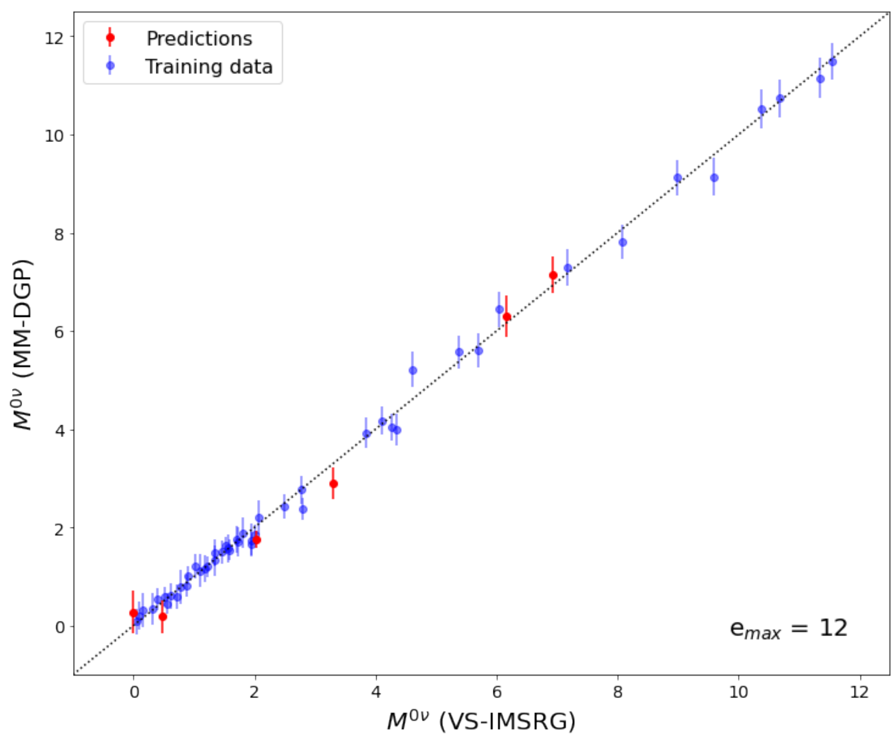


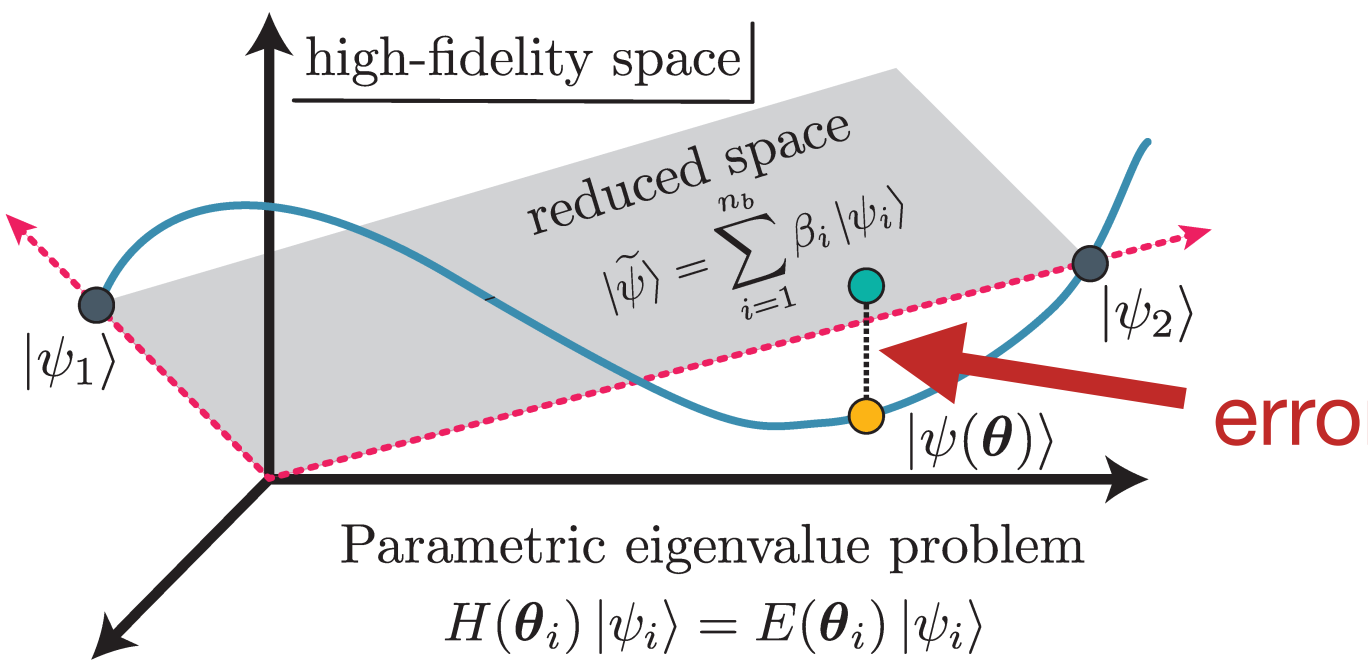
- PNP reference: $\lambda^{(3)}$ included in construction of overlap
- **treatment of small/zero overlaps under control?**
- **particle-attachment/removal** for odd mass
- future: de-normal operators?

Two More Things…

Emulators

J. Melendez et al., JPG 49, 102001 (2022), C. Drischler et al., Front. Phys. 10, 1092931 (2023)
E. Bonilla et al., PRC 106, 054322 (2022), P. Giuliani et al., Front. Phys. 10, 1054524 (2023)
J. Pitcher, A. Belley et al., in preparation, A. Belley et al., arXiv:2308.15643 (v2)





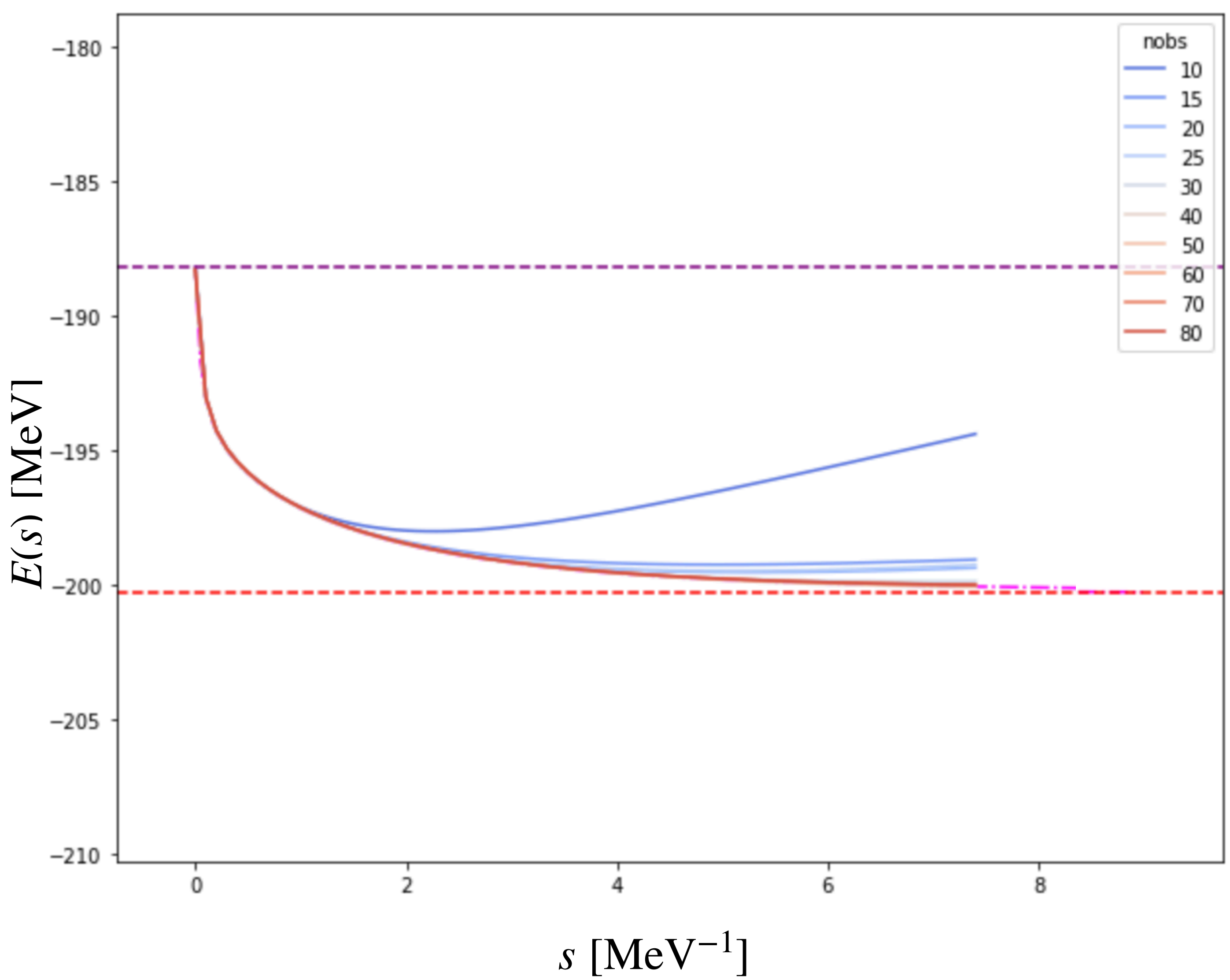
- **Data driven** (only expectation values)
- E.g. Multi-output, Multi-fidelity **Deep Gaussian Processes** (MM-DGP)

- **Physics driven** reduced-order models (ROMs)
- E.g., **Galerkin projection** for bound-state or scattering wave functions

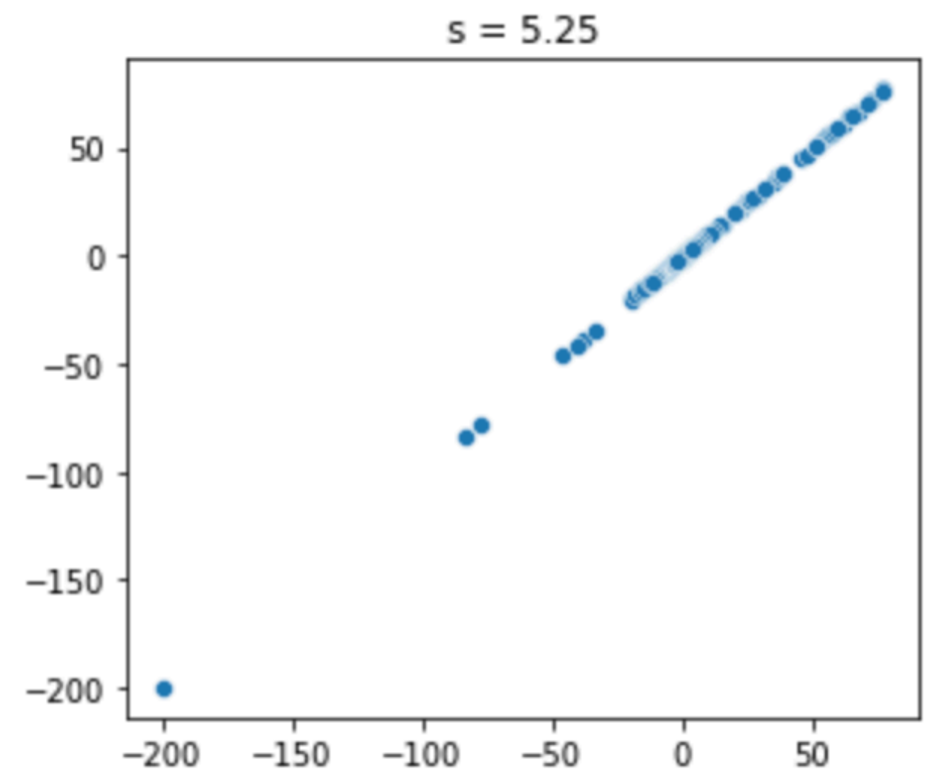
Emulating IMSRG Flows

J. Davison, HH, *J. Crawford, S. Bogner, in preparation*

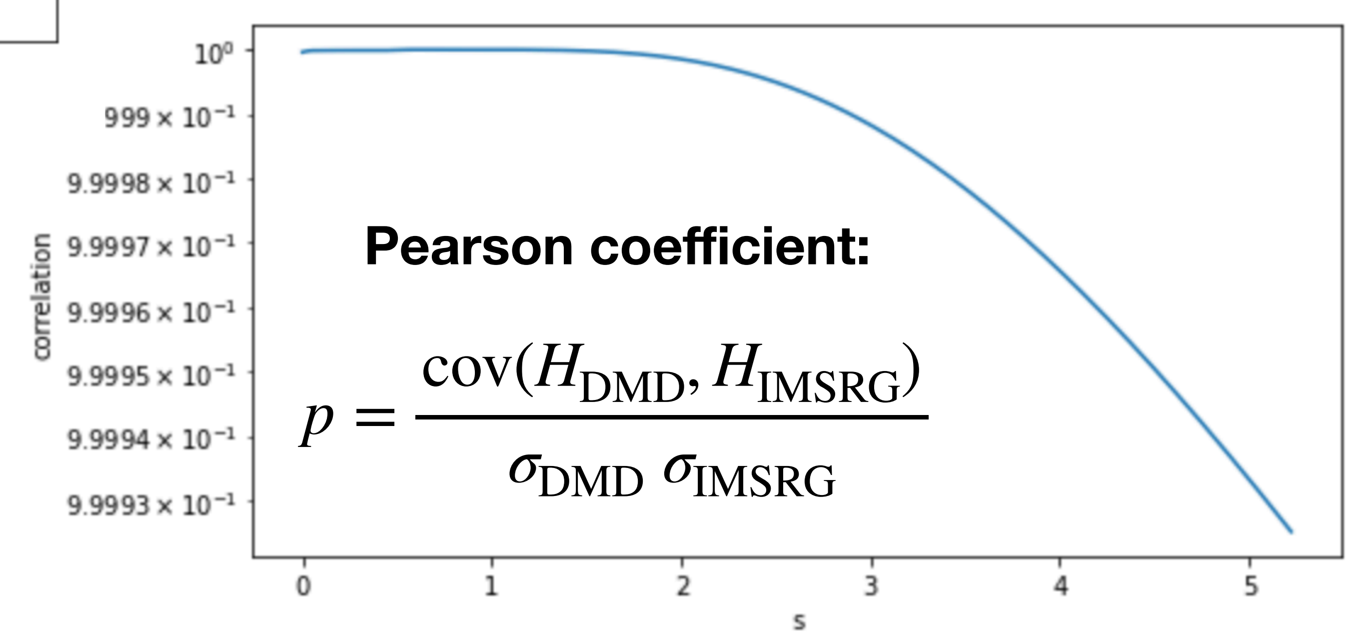
EM(500) N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$



$H_{\mathrm{DMD}}(s)$ vs. $H_{\mathrm{IMSRG}}(s)$



Dynamic Mode Decomposition **emulator** "learns" **all flowing operator coefficients** from snapshots!

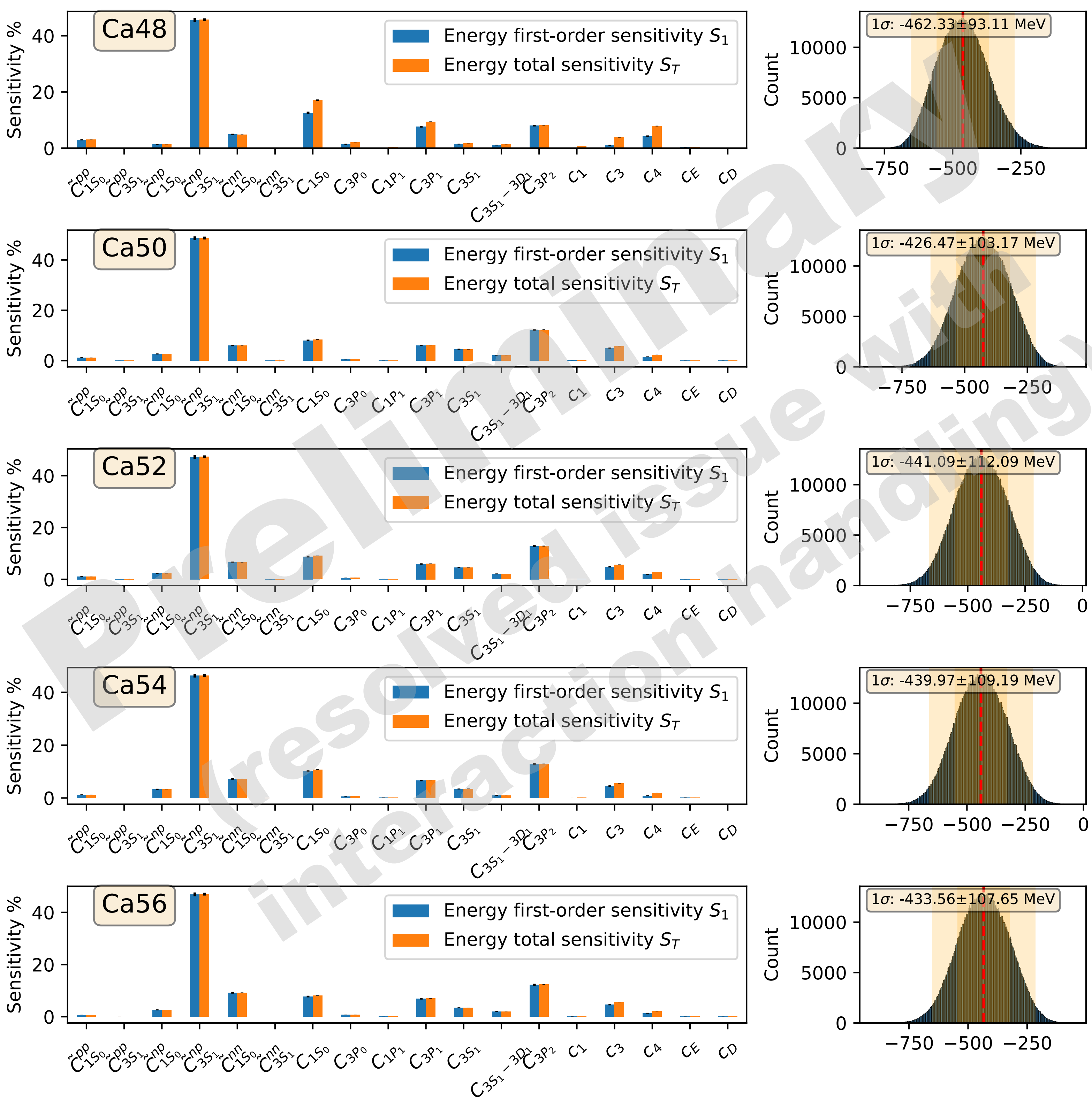


Pearson coefficient:

$$p = \frac{\mathrm{cov}(H_{\mathrm{DMD}}, H_{\mathrm{IMSRG}})}{\sigma_{\mathrm{DMD}}\,\sigma_{\mathrm{IMSRG}}}$$

Emulation for Operators (IMSRG)

J. Davison, HH, *J. Crawford, S. Bogner, in preparation*

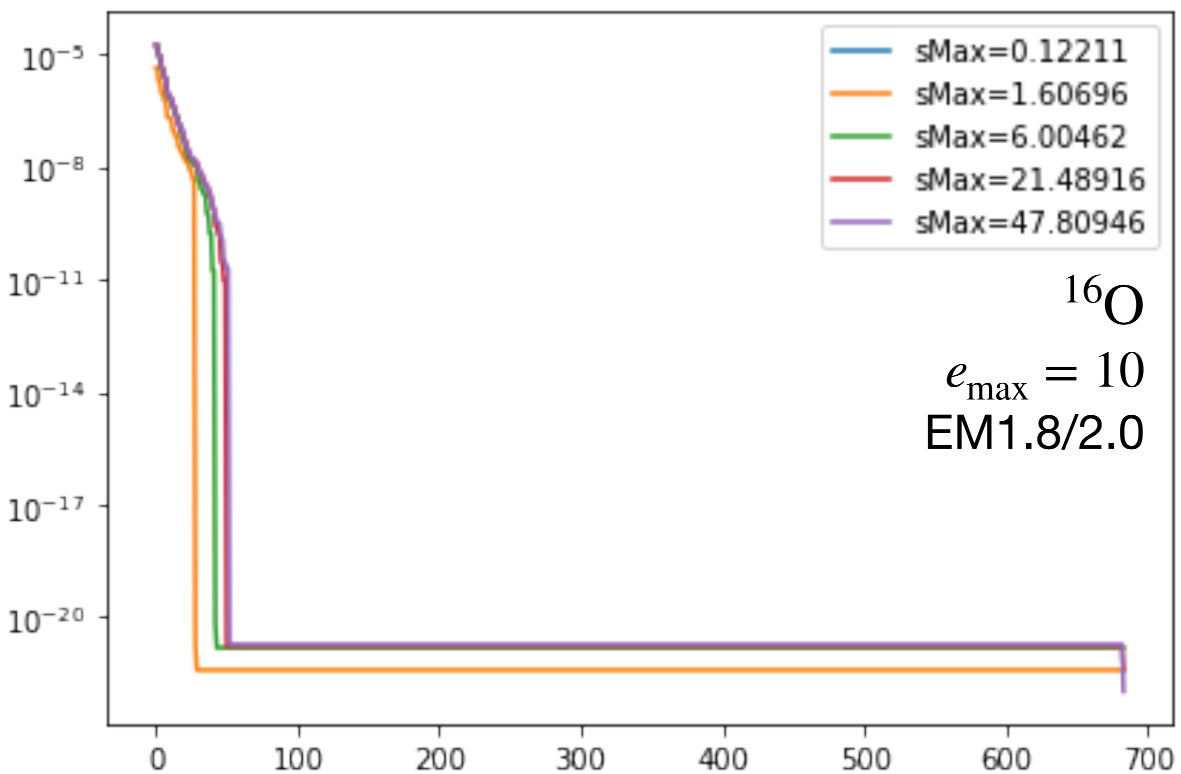


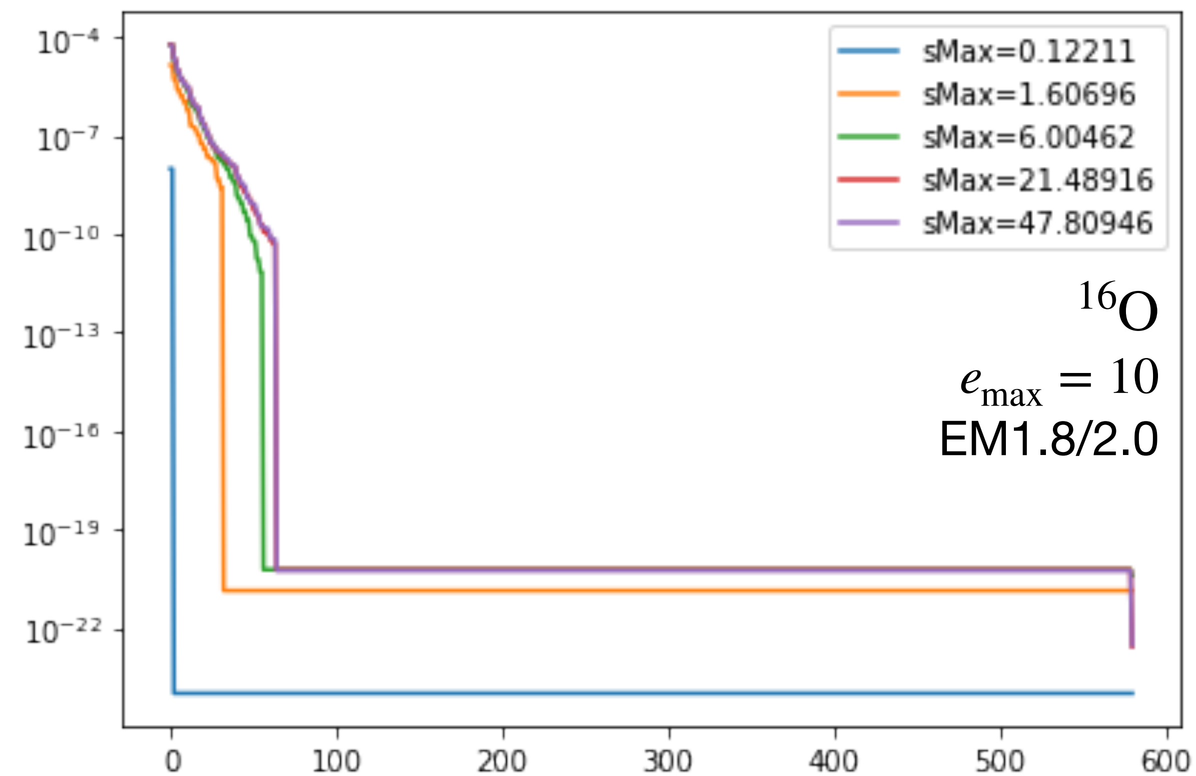
- non-invasive **ROM emulator** based on Dynamic Mode Decomposition
- ΔNNLO$_{GO}$, NN+3N, $e_{max} = 12, E_{3max} = 14$
- O(10M) samples
- **computational effort reduced by 5+ orders of magnitude**

Low-Rank Structures in IMSRG

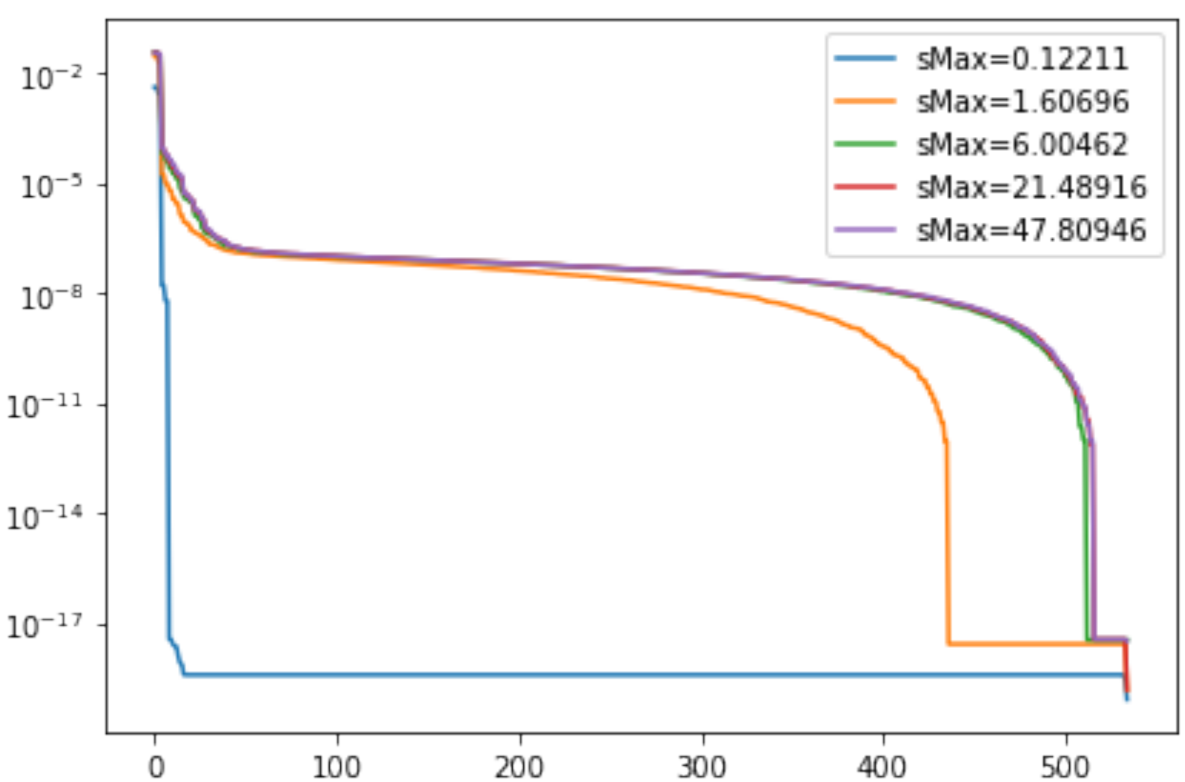
FRIB

***B. Zhu,** dissertation (2023)*





^{16}O, $e_{\max} = 10$, EM1.8/2.0



- **Magnus-IMSRG:**

$$U(s) = e^{\Omega(s)}$$

- SVD reveals that $\Omega(s)$ **has a low rank**

Epilogue

Conclusions & Outlook

- **EOM-IMSRG for closed-shell** nuclei performs as expected
  - e.g., in comparison with EOM-CCSD, VS-IMSRG, …
- **MR-EOM-IMSRG** implemented for **normal ordered operators**
  - **challenges:** need (at least) **irreducible three-body densities**, **overcompleteness** of basis, …
  - alternative pathways through de-normal ordering?
- future: **complement / interface with other approaches**
- progress in **emulation of IMSRG evolution** (applicable to SRG evolution?)
- ongoing: **identification of exploitable low-rank structures**

Acknowledgments

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and everyone I forgot to list…

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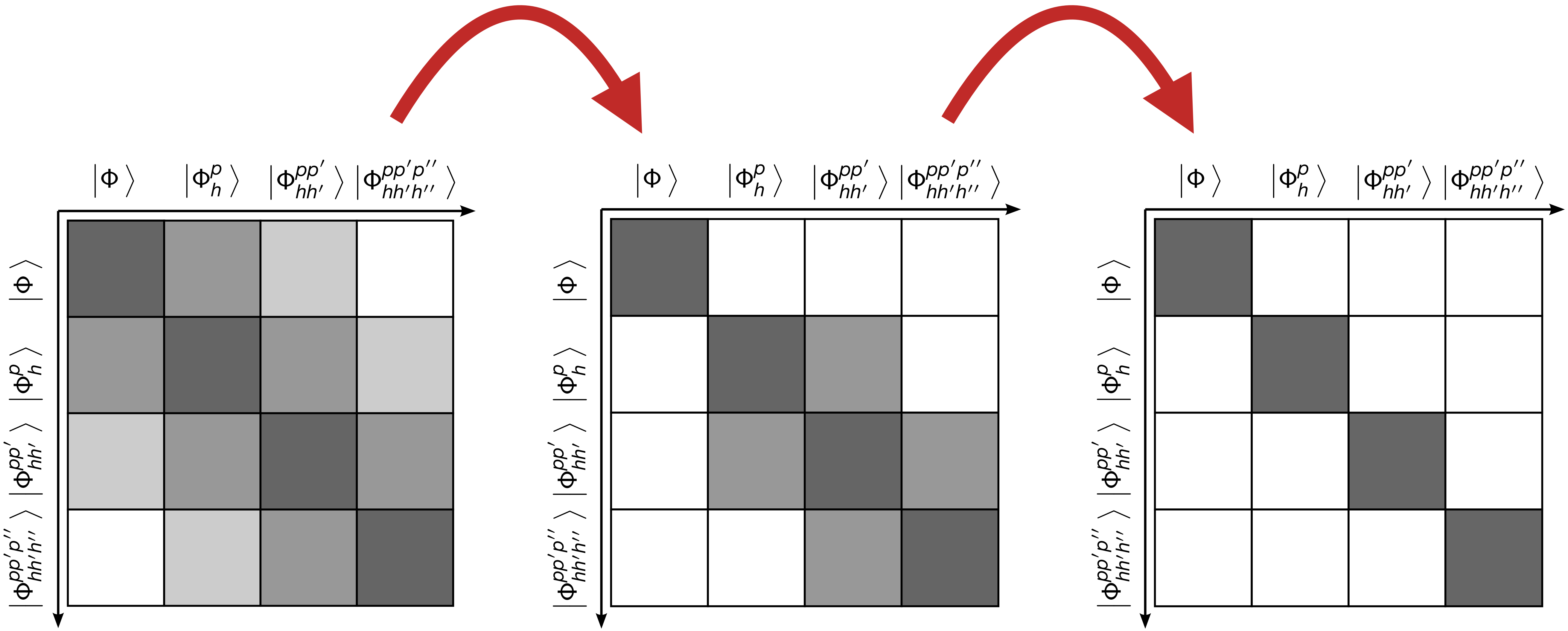
Supplements

Excited State Decoupling

N. Parzuchowski, *S. K. Bogner, T. D. Morris*

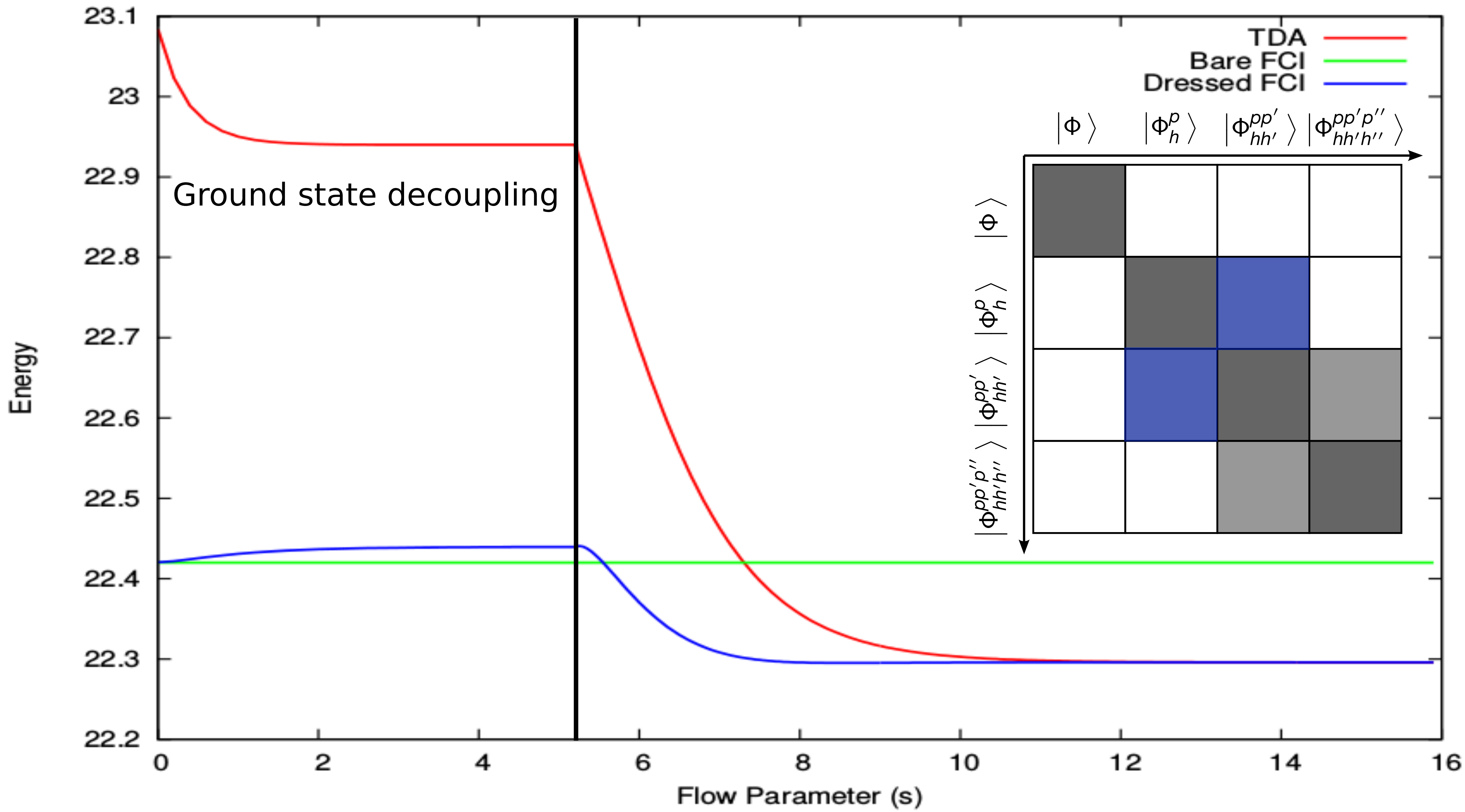


Can we decouple multiple states simultaneously? Maybe entire blocks?

Quantum Dots

N. Parzuchowski, *Dissertation, 2018*

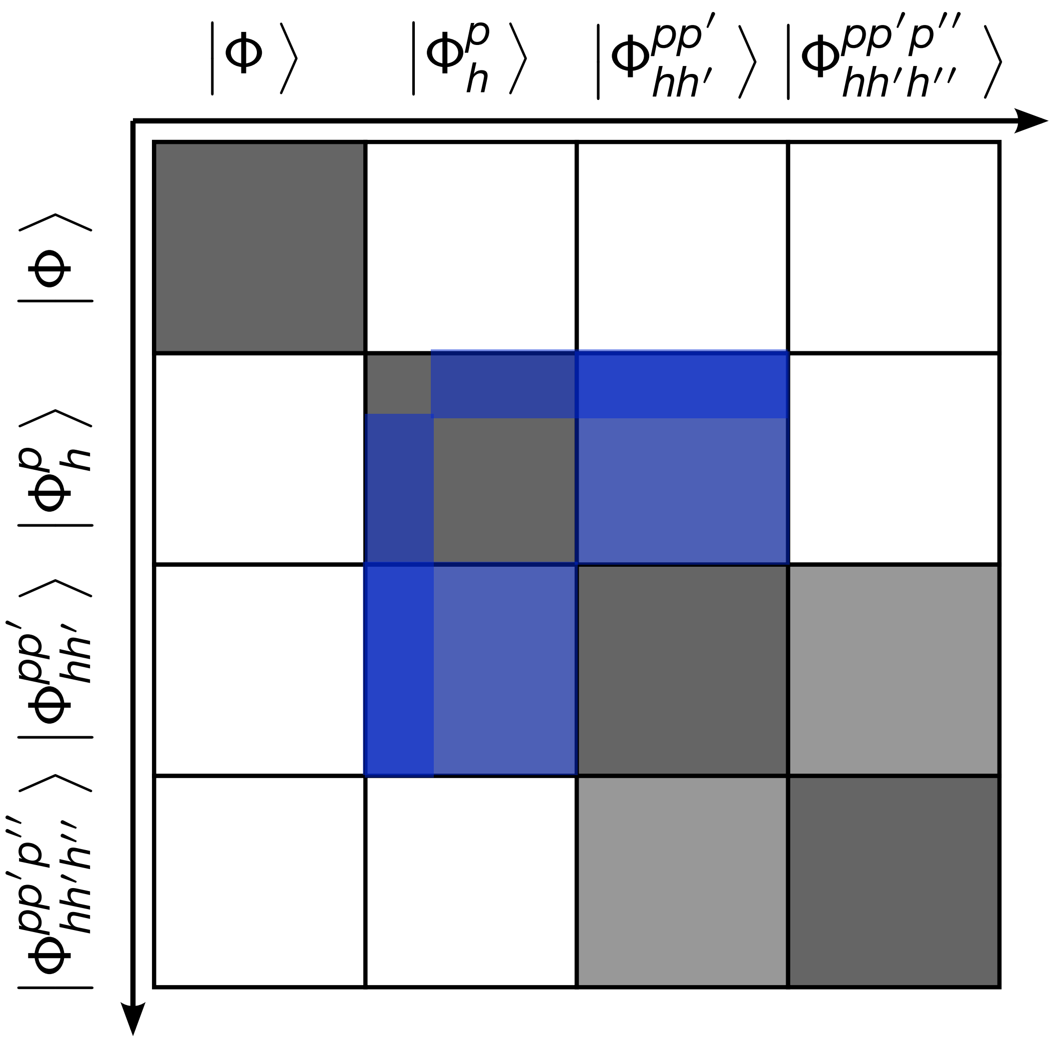
Excited State Calculation in 6-particle Quantum Dots

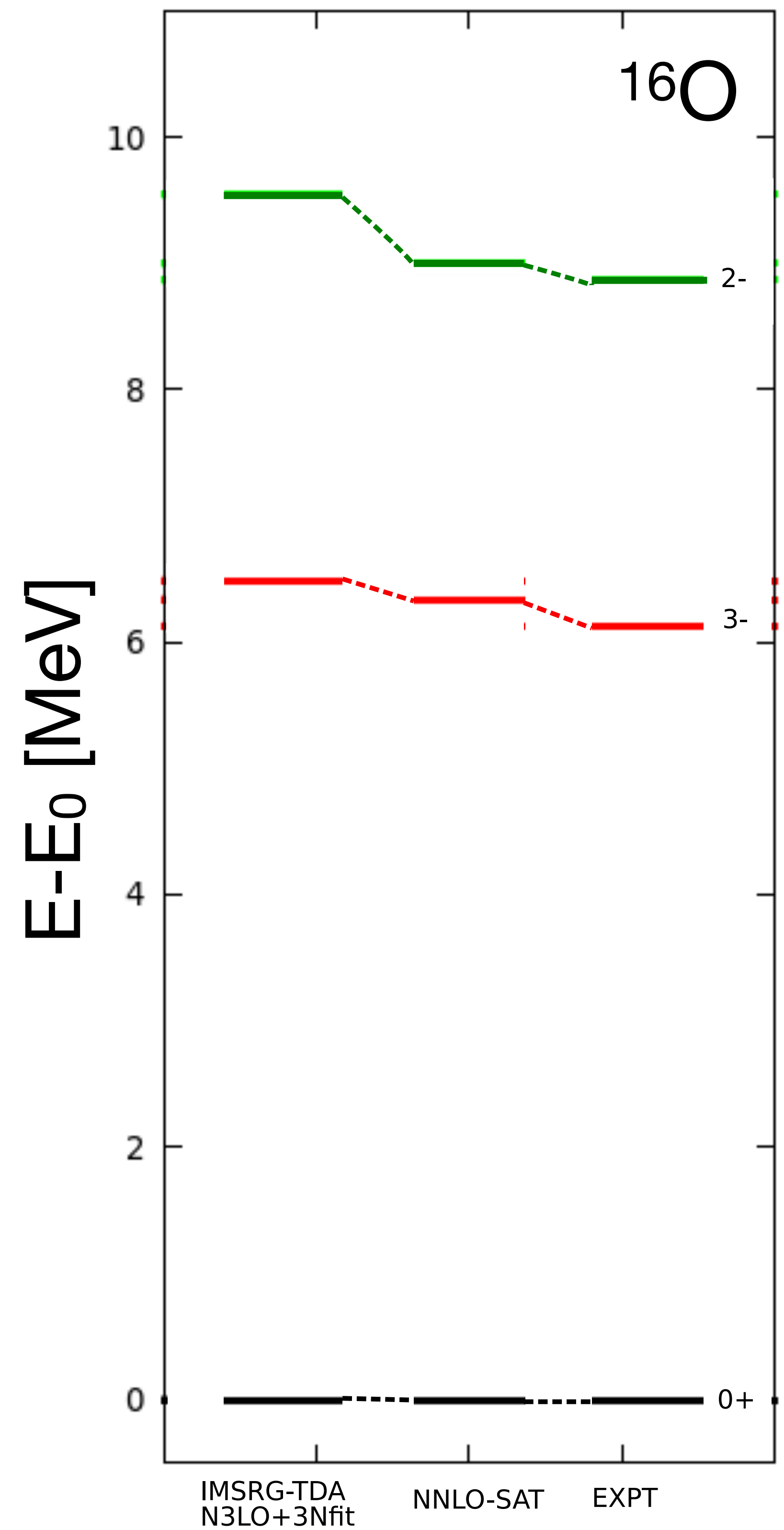


➡ **Multi-state decoupling can generate sizable induced forces…**

Sub-Block Decoupling

N. Parzuchowski, Dissertation, 2018





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

Koopman Operator Theory

- **nonlinear** dynamical system:
  - $\mathbf{x} \in X \subseteq \mathbb{R}^n\,, \quad \mathbf{F}^t : X \to X\,, \qquad \mathbf{x}(t) = \mathbf{F}^t(\mathbf{x}(0))$
  - flow map $\mathbf{F}^t$ propagates $\mathbf{x}(0)$ forward in time
- define a set $\mathscr{G}(X)$ of **observables or measurement functions** $g : X \to \mathbb{C}$
- define the semi-group of **Koopman operators** by
  - $K^t : \mathscr{G}(X) \to \mathscr{G}(X), \qquad K^t g(\mathbf{x}) = g(F^t(\mathbf{x}))$
  - K^t is **linear** if $\mathscr{G}(X)$ is a **linear** function space, e.g., $L^2(\mathbb{R})$
- Describe **nonlinear dynamics** through a generally **infinite-dimensional linear operator** that acts on **measurements**!

Koopman Operators & IMSRG

Review: S. L. Brunton et al., arXiv:2102.12086

- IMSRG flow is a **nonlinear** "dynamical" system
- Hamiltonian in (NO2B) operator algebra:

$$H \equiv E_0 + \sum_{pq} f_{pq} : a_p^\dagger a_q : + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} : a_p^\dagger a_q^\dagger a_s a_r :$$

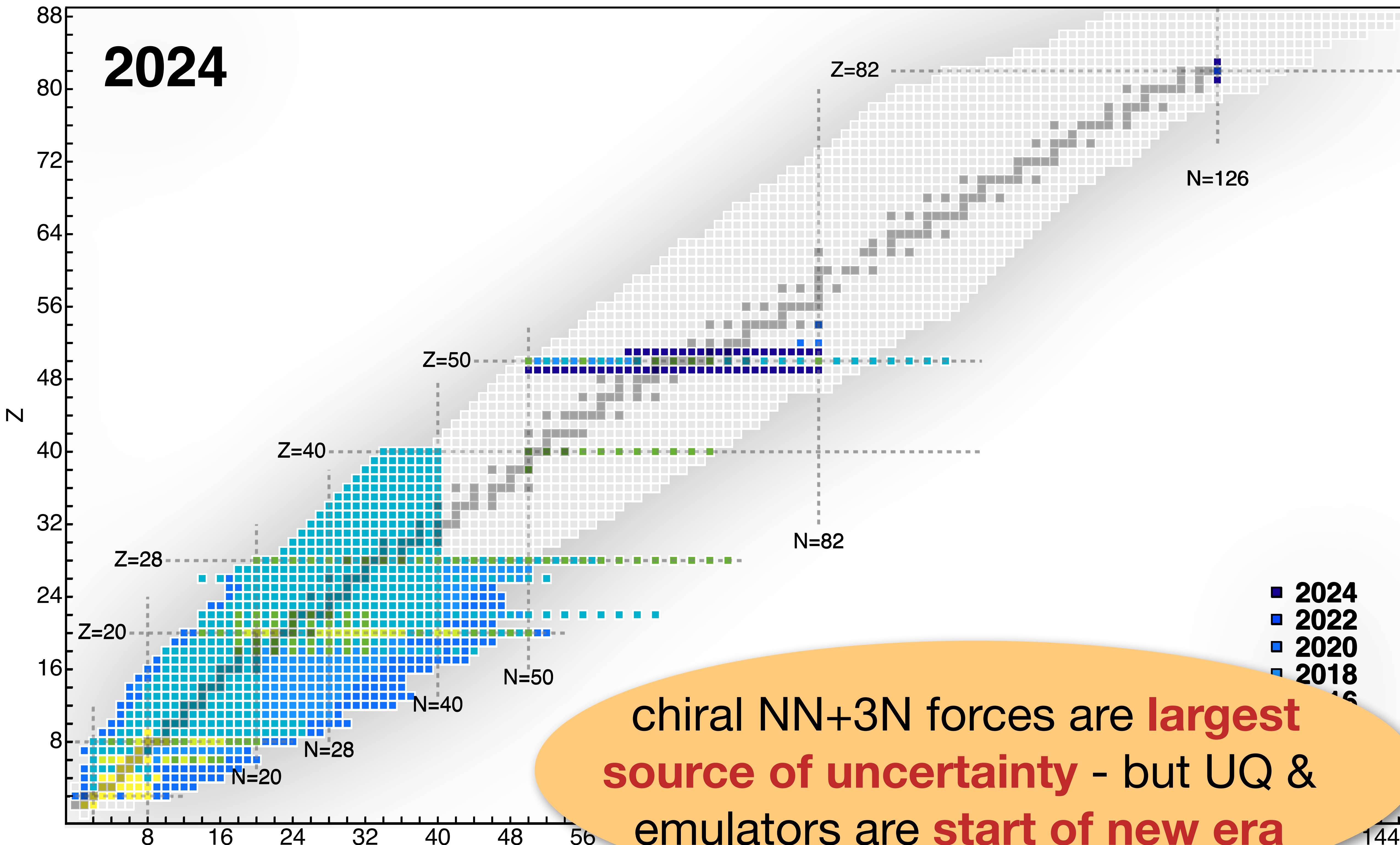
- define $\mathbf{h} \equiv \begin{pmatrix} E_0 & \cdots & f_{pq} & \cdots & \Gamma_{pqrs} & \cdots \end{pmatrix}^T \ldots$
- … and write the evolution in **Koopman operator form:**

$$K^{\bar{s}} \mathbf{h} = \begin{pmatrix} (U_{\bar{s}} H U_{\bar{s}}^\dagger)_0 & \cdots & (U_{\bar{s}} H U_{\bar{s}}^\dagger)_{pq} & \cdots & (U_{\bar{s}} H U_{\bar{s}}^\dagger)_{pqrs} & \cdots \end{pmatrix}^T$$

- **What have we gained compared to other approaches? We can construct Koopman operators from "observations"!**

Progress in *Ab Initio* Calculations

[cf. HH, Front. Phys. **8**, 379 (2020)]



chiral NN+3N forces are **largest source of uncertainty** - but UQ & emulators are **start of new era**