Correlated Reference States and Effective Hamiltonians in the IMSRG Framework
(Multi-Reference) In-Medium Similarity Renormalization Group

Transforming the Hamiltonian

- reference state: single Slater determinant

excitations relative to reference state: normal-ordering
Decoupling in A-Body Space

\[ \langle i | H | j \rangle \]

aim: decouple reference state \( |\Phi\rangle \) from excitations

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

- non-perturbative resummation of MBPT series (correlations)
- off-diagonal couplings are rapidly driven to zero

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Decoupling

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

\[ U(s)H U^\dagger(s)U(s) \left| \psi_n \right\rangle = E_n U(s) \left| \psi_n \right\rangle \]

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

\[ U(s) \left| \psi_n \right\rangle \overset{!}{=} \left| \Phi \right\rangle \]

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Correlated Reference States

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

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

IMSRG(2)  IMSRG(3)  IMSRG(4)  IMSRG(5)
Correlated Reference States

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

use generalized normal ordering with $2B,\ldots$ densities
MR-IMSRG References States

- Slater determinants (uncorrelated)

- number-projected Hartree-Fock Bogoliubov vacua

- Generator Coordinate Method (with projections)

- small-scale No-Core Shell Model

- clustered states, Density Matrix Renormalization Group, tensor networks etc.
MR-IMSRG References States

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Titanium Isotopes

First, we see GGF calculations. Each isotopic chain was shifted by a multiple of to overpredict the

FIG. 4. The mass landscape of titanium isotopes is shown from three perspectives: (a) absolute masses (shown in binding energy format), (b) its first

update values with TITAN data.

Both theoretical calculations (lines) and experimental values (points) are shown. The no-shell hypothesis on

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

- Garcia–Ruiz et al., Nat. Phys. 12, 594
- NN+3N(400), $\lambda=2.24$ fm$^{-1}$
- NN+3N(400), $\lambda=1.88$ fm$^{-1}$
- NNLO$_{\text{sat}}$

\[
R_{ch}[\text{fm}] = \lambda A^{1/3}
\]
Calcium Isotopes

\[ A_{Ca} \]

\[ R_{ch}[fm] \]

- Garcia–Ruiz et al., Nat. Phys. 12, 594
- \( NNLO_{sat} \)

parabola explained by sd-pf configuration mixing in Shell model: static correlation

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Excited States


MR-IMSRG References States

- Slater determinants (uncorrelated)
- number-projected Hartree-Fock Bogoliubov vacua
- Generator Coordinate Method (with projections)
- small-scale No-Core Shell Model
- clustered states, Density Matrix Renormalization Group, tensor networks etc.
- use IMSRG Hamiltonian as input for Equation-of-Motion approach
- all nucleons active
- currently include up to $2p2h$ excitation operators
Valence Space Decoupling

construct **non-empirical interactions**
(and other operators) for use in the nuclear **configuration interaction** method
Valence Space Decoupling

\[ \langle i | H | j \rangle \]

\[ \langle i | H(\infty) | j \rangle \]

**change definition of off-diagonal Hamiltonian:**

\[ \left\{ H^{od} \right\} = \{ f_{h}^{'}, f_{pp}', f_{p}, f_{v}, \Gamma_{hh}', \Gamma_{hv}', \Gamma_{pp}', \Gamma_{vv}' \} \& \text{H.c.} \]
Ground-State Energies

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

sd-shell spectra agree very well with experiment and USDA/B...

... for NN+3N(400) with “wrong” $c_D = -0.2$. 

S. K. Bogner et al., PRL 113, 142501 (2014), S. R. Stroberg et al., PRC 93, 051301(R) (2016)
Transitions

N. M. Parzuchowski, S. R. Stroberg et al., PRC 96, 034324;

Converged VS-/EOM-IMSRG results consistent with NCSM

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• 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

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

MR-IMSRG References States

- Slater determinants (uncorrelated)
- number-projected Hartree-Fock Bogoliubov vacua
- **Generator Coordinate Method (with projections)**
- small-scale No-Core Shell Model
- clustered states, Density Matrix Renormalization Group, tensor networks etc.
Example: $^{20}$Ne

- 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):** induced 3B terms recover bulk of missing correlation energy

• **size will be reference-state dependent**
IMSRG+GCM for $^{20}$Ne

- Rotational band spread out

- $B(E2)$ significantly boosted, but still underestimated (2B part of effective E2 not included yet, spectrum spread out)
Merging IMSRG and NCSM

E. Gebrerufael, K. Vobig, HH and R. Roth, *in preparation*

MR-IMSRG References States

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- clustered states, Density Matrix Renormalization Group, tensor networks etc.
E. Gebrerufael, K. Vobig, HH and R. Roth, PRL 118, 152503 (2017)

**NCSM**
- define reference state

**IMSRG**
- evolve operators
  - evolve Hamiltonian and observables with MR-IMSRG
  - decoupling in A-body space

**NCSM**
- diagonalization in small model space
- use eigenstate as reference
- extract observables
  - diagonalize evolved Hamiltonian
  - calculate eigenstates, observables
$s = 0.00 \text{ MeV}^{-1}$

\[N_{\text{max}} = 0\]
\[N_{\text{max}} = 2\]
\[N_{\text{max}} = 4\]

Slater determinants

Slater determinants

figures by E. Gebrerufael
$^{12}\text{C}$: Hamiltonian Matrix Evolution

$E(s) \quad s = 1.00 \text{ MeV}^{-1}$

- $N_{\text{max}}=0, 2, 4$ eigenvalues (almost) identical due to decoupling…
- … but IMSRG truncation artifacts appear eventually (missing induced 3B+ terms)
Evolution of the Hamiltonian Matrix

• **induced couplings** between reference and $N_{\text{max}}=0$ states

• $E(s)$ does not track lowest eigenvalue

$\Rightarrow$ **diagonalize** $H(s)$
Evolution of Ground-State Energies

- strongly enhanced convergence
- plateau in flow
- identify critical $s_{\text{max}}$ at which induced many-body terms become relevant

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**12C: Excitation Spectra**

**IM-NCSM**

- $s_{max} = 0.3 \text{ MeV}^{-1}$

**NCSM**

- $\hbar \Omega = 16 \text{ MeV}$

- $\hbar \Omega = 20 \text{ MeV}$

- EM 500/400 NO2B

- $\lambda = 1.88 \text{ fm}^{-1}$

- $E_{gs} [\text{MeV}]$
  - $-92.2$

- $N_{max}$
  - $2$
  - $4$
  - $6$

- $E^* [\text{MeV}]$
  - $1^+$
  - $(0^+)$
  - $0^+$
  - $2^+$

**Results**

- „uncertainty band”: **flow parameter variation** from $s_{max}/2$
  to $s_{max}$

- excellent agreement for converged states
• excellent agreement for converged states

• predict **1+ state** that has not yet been observed experimentally
Epilogue
Where Do We Go from Here?

- Revisit **optical potentials** (à la J. Rotureau et al., PRC 95, 024315)
  - MR-EOM / GCM / … to describe **few-particle and collective** correlation
  - **continuum coupling** for exotic nuclei (see K. Fossez)
  - Use **IMSRG-evolved Hamiltonians** in RGM/NCSMC/…)
- **Utopia:** Can we **systematically** connect many-body system to few-body system via IMSRG (or other RG) methods?
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CEA Saclay, France

C. Barbieri
U. Surrey, UK

J. Simonis
Johannes Gutenberg University of Mainz, Germany