Novel *Ab Initio* Methods for Deformed Nuclei
Progress in *Ab Initio* Calculations

* but current chiral NN+3N forces have deficiencies, are largest source of uncertainty
(Multi-Reference) In-Medium Similarity Renormalization Group

Large-Scale Diagonalization

- basis-size “explosion”: factorial growth
- importance truncation etc. cannot fully compensate this growth as $A$ increases

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

- reference state: single Slater determinant

\[ |\Phi\rangle, |\Phi_i\rangle, |\Phi_{ij}\rangle, |\Phi_{ijk}\rangle \]

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

\[ \epsilon, \epsilon_F \]

\[ a, b, \ldots : \epsilon > \epsilon_F \]
\[ i, j, \ldots : \epsilon \leq \epsilon_F \]
\[ p, q, \ldots : \text{full basis} \]

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

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

$$U(s) H U^\dagger(s)$$

$s \to \infty$
Flow Equation

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

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

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

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero
Decoupling

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

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

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

\[ U(s) |\psi_n\rangle \overset{!}{=} |\Phi\rangle \]
Correlated Reference States

“standard” IMSRG: build correlations on top of Slater determinant (=independent-particle state)
Correlated Reference States

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

“standard” IMSRG
Slater determinant

IMSRG(2)  IMSRG(3)  IMSRG(4)  IMSRG(5)
MR-IMSRG: build correlations on top of already correlated state (e.g., from a method that describes static correlation well)
IMSRG-Improved Methods

XYZ define reference

IMSRG evolve operators

XYZ extract observables

Could add self-consistency.
IMSRG-Improved HF and PHFB

**HF / PHFB**
- define reference
- closed shell: HF Slater determinant
- open shell: number-projected HFB state

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

**HF / PHFB**
- extract observables
- calculation is trivial, energy can be directly read off the evolved Hamiltonian
Oxygen Isotopes

For an approximate or complete implementation of MR-
triples approaches like the completely renormalized CR-CC
expansion for low-momentum Hamiltonians

tainty, and indicating the rapid convergence of the many-body
gains about 2% of additional binding energy compared to
observables.

Illustrate below that this tuning does not hold for general
energy of Green
ately truncated methods, i.e., MR-IMSRG

NCSM results, on the level of 1% 

is very weak, at least in the range 

Note that the ADC
and optimal

were obtained for
and other many-body approaches, using the

and ADC

as well as

, updating earlier

1

for


H. Hergert - INPC 2019, Glasgow, July 30, 2019
Valence-Space IMSRG

- **HF**
  - define reference
  - defines meaning of $P$ (=valence) and $Q$ (=core + non-valence excitation) spaces

- **IMSRG**
  - evolve operators
  - evolve Hamiltonian and observables
  - decouple $P$ and $Q$ spaces
  - determines core part of w.f.

- **Valence CI**
  - extract observables
  - determines valence part of w.f.
Ground-State Energies

Valence-Space IMSRG

Non-Empirical Interactions for the Nuclear Shell Model: An Update

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Abstract

The nuclear shell model has been perhaps the most important conceptual and computational paradigm for the understanding of the structure of atomic nuclei. While the shell model has been predominantly used in a phenomenological context, there have been efforts stretching back over a half century to derive shell model parameters based on a realistic interaction between nucleons. More recently, several ab initio many-body methods—in particular many-body perturbation theory, the no-core shell model, the in-medium similarity renormalization group, and coupled cluster theory—have developed the capability to provide effective shell model Hamiltonians. We provide an update on the status of these methods and investigate the connections between them and potential strengths and weaknesses, with a particular focus on the in-medium similarity renormalization group approach. Three-body forces are demonstrated to be an important ingredient in understanding the modifications needed in phenomenological treatments. We then review some applications of these methods to comparisons with recent experimental measurements, and conclude with some remaining challenges in ab initio shell model theory.

(cf. talk by J. Holt, Fundamental Symmetries & Interactions in Nuclei, Thursday, 3:40pm)
Calcium Isotopes

(cf. talk by V. Somà, Nuclear Structure A, Monday, 1:30pm)

\[ R_{ch}[\text{fm}] \]

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

\[ A_{\text{Ca}} \]

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Calcium Isotopes

$A_{\text{Ca}}$

$R_{\text{ch}} [\text{fm}]$

- Garcia–Ruiz et al., Nat. Phys. 12, 594
- $\text{NNLO}_{\text{sat}}$

“parabola” explained by sd-pf configuration mixing in Shell model: static correlation
• **B(E2) much too small**: effect of intermediate 3p3h, … states that are truncated in IMSRG evolution
Capturing Collective Correlations: IMSRG+Generator Coordinate Method


In-Medium GCM

- no-core (or valence space) GCM calculation to prepare reference state

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

- no-core GCM calculation using evolved Hamiltonian
  - calculate GCM wave functions, observables
Collectivity in $^{A}$Mg

- significantly increased $B(E2)$ values for $^{32,34}$Mg compared to GCM calculation or VS-IMSRG calculations: **dynamical and static correlations**!

- **induced 2B quadrupole operator is small**, contrary to typical VS-IMSRG findings: NO with respect to GCM states equips operator basis with better capability to describe collectivity
Collectivity in $^{\text{A}}$Mg

- **Caution:** occupation numbers are **not observables**, interpret with care!

- For **low-resolution interactions**, the no-core GCM and Shell Model interpretations of $^{32}$Mg are (at least qualitatively) the same: two neutrons are excited from the sd- into the pf shell.
• VAPNP-HFB potential energy surface for IMSRG-evolved H
• provides basis configurations for IM-GCM
• reasonable reproduction of low-lying states and transitions in $^{48}\text{Ti}$

• consistency between IM-GCM and IM-No Core CI

• adding correlations in IM-NCCI stretches spectrum
The neutron-proton isoscalar pairing fluctuation quenches \( \sim 17\% \) further, which might be canceled out partially by the isovector pairing fluctuation.

- **tentative** value: \( M^{0v} = 0.61(5) \)
- consistent with tentative VS-IMSRG result \( M^{0v} \approx 0.58 \) (cf. J. Holt’s talk, Fundamental Symmetries…, Thursday, 3:40pm)
- comparison with CC (S. Novario, G. Hagen) in progress
- **next steps**: improve IMSRG truncations, include currents, \(^{76}\text{Ge}\)
Cluster Structures: $^8\text{Be}$

HFB potential energy surface

CHiral Interaction: SRG softened NN from Entem & Machleidt with 3NF from chiral EFT.

J. M. Yao et al PRC (2011)
Cluster Structures: $^8$Be

- Spherical and prolate references flow towards **different 0$^+$ states**.

- Consistent with IM-NCSM:
  - **prolate reference**: ground state and excited 2$^+$ state
  - **spherical reference**: first excited 0$^+$
The Shape of Things to Come
Coming Attractions

• approximate (MR-)IMSRG(3) for no-core and valence-space applications (validation in progress)

• towards quantification of many-body truncation errors

• automated code generation (cf. talk by P. Arthuis, Nuclear Structure C, Friday, 11:40am)

• IM-GCM applications for clustered states, Mg isotopes, neutrinoless double beta decay, …

• Multireference EOM-IMSRG based on intrinsically deformed states (with R. Wirth)

• excitations and odd nuclei

• explore additional IM-XYZ approaches…
Acknowledgments

S. K. Bogner, M. Hjorth-Jensen, R. Wirth, J. M. Yao
NSCL/FRIB, Michigan State University

K. Fossez
Argonne National Laboratory

S. R. Stroberg
U Washington

G. Hagen, T. D. Morris, S. Novario
UT Knoxville & Oak Ridge National Laboratory

E. Gebrerufael (*), K. Hebeler, S. König, R. Roth, A. Schwenk, K. Vobig (*)
TU Darmstadt, Germany

R. J. Furnstahl, N. M. Parzuchowski (*)
The Ohio State University

J. D. Holt, P. Navrátil
TRIUMF, Canada

B. Bally, J. Engel
University of North Carolina - Chapel Hill

T. Duguet, V. Somà, A. Tichai
CEA Saclay, France

C. Barbieri
U. Surrey, UK

J. Simonis
Johannes Gutenberg University Mainz, Germany
Supplements
SRG in a Nutshell

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

- choose \( \eta(s) \) to achieve desired behavior, e.g.,
  \[
  \eta(s) = \{H_d(s), H_{od}(s)\}
  \]
  to suppress (suitably defined) off-diagonal Hamiltonian

- **consistent evolution** for all observables of interest
Operator Bases for the RG Flow

• **choose a basis of operators** to represent the flow (make an educated guess about physics):

\[
H(s) = \sum_i c_i(s)O_i, \quad \eta(s) = \sum_i f_i(\{c(s)\})O_i
\]

• **close algebra by truncation**, if necessary:

\[
[O_i, O_j] = \sum_k g_{ijk}O_k
\]

• **flow equations** for the coefficient *(coupling constants)*:

\[
\frac{d}{ds}c_k = \sum_{ij} g_{ijk} f_i(\{c\}) c_j
\]

• “obvious” choice for many-body problems:

\[
\{O_{pq}, O_{pqrs}, \ldots\} = \{a_p^\dagger a_q, a_p^\dagger a_q^\dagger a_s a_r, \ldots\}
\]
Normal-Ordered Hamiltonian

\[ H = E_0 + \sum_{pq} f_q^p \tilde{A}_q^p + \frac{1}{4} \sum_{pqrs} \Gamma_{rs}^{pq} \tilde{A}_{rs}^{pq} + \frac{1}{36} \sum_{pqrsstu} W_{stu}^{pq} \tilde{A}_{stu}^{pq} \]

- \( E_0 = \) [diagram showing components]
- \( f = \) [diagram showing components]
- \( \Gamma = \) [diagram showing components]
- \( W = \) [diagram showing components]

**NO2B approximation:**
2B Hamiltonian with in-medium contributions from 3B interactions
Single-Reference Decoupling

- reference state: **Slater determinant**
- normal-ordered operators and their products **depend on occupation numbers** (one-body density)
Multi-Reference Decoupling

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

\[
\begin{align*}
\langle p_s | H | \Phi \rangle & \sim \bar{n}_p n_s f^p_s, \sum_{kl} f^k_l \lambda^{sk}_p, \sum_{klm} \Gamma^{kl}_{mn} \lambda^{skl}_p, \cdots \\
\langle pq_{st} | H | \Phi \rangle & \sim \bar{n}_p \bar{n}_q n_s n_t f^{pq}_{st}, \sum_{kl} f^k_l \lambda^{tk}_{pq}, \sum_{kl} \Gamma^{kl}_{pqml} \lambda^{stkl}_{pq}, \cdots \\
\langle pqr_{stu} | H | \Phi \rangle & \sim \cdots
\end{align*}
\]

irreducible density matrices encode correlations
Approximate MR-IMSRG(3)

- **approximate MR-IMSRG(3):** induced 3B terms recover bulk of missing correlation energy

- size will be **reference-state dependent**