Extending the reach of ab initio theory: Valence space IMSRG

Ragnar Stroberg
TRIUMF
ARIS In the Mountains
Keystone, Colorado
May 30, 2017
1. In-medium SRG for a valence space
2. Ensemble normal ordering
3. Selected results
4. Outlook

Similarity renormalization group (SRG)

- $H|\Psi\rangle = E|\Psi\rangle$ is too difficult to solve.
- Perform unitary transformation $\tilde{H} = UHU$ (implicit change of basis) so SE is easier to solve.
- Iterative/guess-and-check approach.
- $U = e^{\Omega} = e^{\Omega_n}e^{\Omega_{n-1}}\ldots e^{\Omega_2}e^{\Omega_1}$
- Alternatively, $\Omega_n \rightarrow \eta ds \Rightarrow$ flow equation
- Computational effort dominated by commutator evaluation.

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

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Many-body forces

\[
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\]

(Two-body) (Two-body) \sim \begin{align*}
&\begin{bmatrix}
1 & 2 \\
1 & 2
\end{bmatrix} \\
&\begin{bmatrix}
1 & 2 \\
1 & 2
\end{bmatrix}
\end{align*}

(Three-body)

(Two-body) (Three-body) \sim \begin{align*}
&\begin{bmatrix}
1 & 2 & 3 \\
1 & 2 & 3
\end{bmatrix} \\
&\begin{bmatrix}
1 & 2 & 3 \\
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\end{bmatrix}
\end{align*}

(Four-body)
What we would like:
Why “in-medium”?

\[ H = E_0 + \sum_{ij} H_{ij} \{ a_i^\dagger a_j \} + \frac{1}{4} \sum_{ijkl} H_{ijkl} \{ a_i^\dagger a_j^\dagger a_l a_k \} + \frac{1}{36} \sum_{ijklmn} H_{ijklmn} \{ a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \} + \ldots \]

- In general, the transformation \( U \) will induce 4-body, 5-body, etc. forces.
- Write \( H \) in terms of excitations out of reference \( |\Phi_0\rangle \).
- Normal ordering: \( \langle \Phi_0 | \{ a_1^\dagger \ldots a_N^\dagger a_N \ldots a_1 \} | \Phi_0 \rangle = 0 \)
- If \( |\Phi_0\rangle \approx |\Psi\rangle \), higher-body terms are negligible.
- Truncate all operators at 2-body level (NO2B).

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Tskukiyma et al (2011)
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Tskukiyama et al (2011)
In-medium SRG

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Tskukiyma et al (2011)

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Solving the many-body problem

- Decouple a $1 \times 1$ sub-block
- Use SRG to suppress excitations out of $|\Phi_0\rangle$
- After decoupling, energy is $E_0 = \langle \Phi_0 | \tilde{H} | \Phi_0 \rangle$
Open shell systems:

- Multiple (quasi-) degenerate configurations ⇒ strong mixing, $|\Phi_0\rangle \not\approx |\Psi\rangle$

- Single Slater determinant may not have good total angular momentum $J$

- Large rotation angle ⇒ induced many-body forces

Strategies:

- Break symmetries and restore afterward
- Construct multi-configuration reference, then decouple (multi-reference IM-SRG)
- Decouple a subset of configurations, then construct state from them using standard shell model machinery, e.g. NuShellX (valence-space IMSRG)

Tsukiyama et al. (2012), Hergert et al. (2013), Bogner et al. (2014)
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Tsukiyama et al. (2012), Hergert et al. (2013), Bogner et al. (2014)
What reference should be used when decoupling a valence space?

(i.e. what is the “medium”?)

Obvious choice: the inert core, e.g. $^{16}\text{O}$. 
Ensemble normal ordering

Experiment
SCGF
GGF
CCSD(T)
IT-NCSM
MR-IMSRG
IMSRG(SM)

Reference: inert core

$\langle \Phi_0 | \{a_i^\dagger \ldots a_N\} | \Phi_0 \rangle = 0$

$\text{Tr} \left( \rho \{a_i^\dagger \ldots a_N\} \right) = 0$

$|\Phi_0\rangle = |^{22}\text{O}\rangle$

$\rho = \sum_\alpha c_\alpha |\Phi_\alpha\rangle \langle \Phi_\alpha|$
Ensemble normal ordering

Reference: inert core

\[ E_{gs} \text{ (MeV)} \]

\( A \)

\( A = 16 \) (\( Z = 8 \))

Experiment
SCGF
GGF
CCSD(T)
IT-NCSM
MR-IMSRG
IMSRG(SM)
Ensemble normal ordering

Reference: inert core
Reference: nearest closed shell
(Ensemble gives very similar results)
Ground state energies

$E_{gs}$ (MeV)

(a) $^4$C (Z=6)

(b) $^4$N (Z=7)

(c) $^4$O (Z=8)

(d) $^23$Na (Z=11)

(e) $^44$Ca (Z=20)

(f) $^58$Ni (Z=28)

Experiment
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IT-NCSM
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Experiment
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SRS et al. PRL (2017)

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Ground state energies

SRS et al. PRL (2017)

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Saturation and finite nuclei

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Neither interaction is fully consistent however... Saturation properties are important for finite nuclei.


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**Graphs:**

1. **EM 500/400**
   - $^A$Ca (Z=20)

2. **EM 1.8/2.0 Ca**
Saturation and finite nuclei

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EM 1.8/2.0 interaction

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![Graph showing neutron number and proton number relationship](image)

**EM 1.8/2.0 interaction**

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Em 1.8/2.0 Interaction

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AME 2012

EM 1.8/2.0 interaction
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Proton number Z

Neutron number N

Mass Number A

Energy (MeV)

S2n (MeV)

K

N=40

AME 2012

IM-SRG

H

He

Li

Be

B

C

N

O

F

Ne

Na

Al

Si

P

S

Cl

Ar

K

Ca

Sc

Ti

V

Cr

Mn

Fe

Ni

Cu

Zn

Ga

Ge

As

Se

Br

Kr

Rb

Sr

Y

Zr

Nb

Mo

Tc

Ru

Rh

Pd

Ag

Cd

In

Sn

Sb

Te

I

Xe

Cs

Ba

La

Ce

Pr

Nd

Pm

Sm

Eu

Gd

Tb

Dy

Ho

Er

Tm

Yb

Lu

Hf

Ta

W

Re

Os

Ir

Pt

Au

Hg

Tl

Pb

Bi

Po

At

Rn

Fr

Ra

Ac

Cm

Bk

Cf

Es

Fm

Md

No

Lr

Rf

Db

Sg

Bh

Hs

Mt

Ds

Rg

Cn

Nh

Fl

Mc

Lv

Ts

 Og


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Baumann et al. Nature (2007), Möller et al. (1995), Samyn et al. (2004), Holt et al. (in prep.)
A note of caution

- Only difference: choice of initial NN force.
- Identical procedure for fitting 3N contact terms.
- Based on few-body data, all interactions are equally good.
- Big differences for finite nuclei.
- 1.8/2.0 EM interaction is "magic", i.e. lucky.

Simonis et al. arxiv:1704.02915

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The reach of ab initio theory

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Limited by truncation of 3N matrix elements

\[ E_{3 \text{max}} = e_1 + e_2 + e_3 \]
Beyond binding energies

Bogner et al. PRL (2014), SRS et al. PRC(R) (2016),

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Beyond binding energies


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What does the future hold?  
(Technical developments)

- Quantification of many-body uncertainty
  - Perturbative estimation of omitted 3-body terms
  - Invariant trace
  - Full IMSRG(3): Include 3-body terms throughout the calculation

- Heavy-mass frontier
  - Improve handling of 3N forces

- Decoupling arbitrary valence spaces
  - Island(s) of inversion
  - Parity-changing transitions, e.g. $E1$

- Improved basis
  - Two-frequency oscillator basis for halo systems
  - Explicit inclusion of collective modes
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What does the future hold?
(Observables)

- Radii / isotope shifts
- $E^0$ transitions
- Chiral currents for $M1$, Gamow-Teller operators
- Neutrinoless double beta decay
- Structure factors for dark matter detection
- Superallowed Fermi decays
- Suggestions?
Valence space IM-SRG with ensemble normal ordering allows access to all nuclei up to $A \sim 100$.

Reach in $A$ is presently limited by $E_{3\text{max}}$ truncation.

Consistent operators for other observables can be obtained.

Chiral interactions still need work (magic notwithstanding).

Next goal: how to reliably estimate truncation error?

Collaborators:

TRIUMF  A. Calci, J. Holt, P. Navrátil, C. Payne, O. Drozdowski, D. Fullerton, C. Gwak, L. Kemmler, S. Leutheusser, D. Livermore

NSCL/MSU  S. Bogner, H. Hergert, N. Parzuchowski

TU Darmstadt  K. Hebeler, R. Roth, A. Schwenk, J. Simonis, C. Stumpf

ORNL/UT  G. Hagen, T. Morris