TBA

Heiko Hergert
Facility for Rare Isotope Beams
& Department of Physics and Astronomy
Michigan State University
Topological Blocking Algorithm

Heiko Hergert
Facility for Rare Isotope Beams
& Department of Physics and Astronomy
Michigan State University
Two-Body Anomaly

Heiko Hergert
Facility for Rare Isotope Beams
& Department of Physics and Astronomy
Michigan State University
Three-Body Anomaly

Heiko Hergert
Facility for Rare Isotope Beams
& Department of Physics and Astronomy
Michigan State University
An Update on IMSRG Developments
Representing the Hamiltonian

- reference state: single Slater determinant
• reference state: **single Slater determinant**
Single-Reference Case

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

\[
\begin{align*}
\langle p \mid H \mid \Phi \rangle & \sim \tilde{n}_p n_s f_s^p, \sum_{kl} f_l^k \lambda_{pl}^k, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pmn}^{skl}, \ldots \\
\langle pq \mid H \mid \Phi \rangle & \sim \tilde{n}_p \tilde{n}_q n_s n_t \tilde{n}_t^{pq}, \sum_{kl} f_{pq}^k \lambda_{kl}^p, \sum_{kl} f_{st}^k \lambda_{ijkl}^{pq}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pqmn}^{stkl}, \ldots \\
\langle pqr \mid H \mid \Phi \rangle & \sim \ldots \\
\end{align*}
\]

- **reference state:** arbitrary
Multi-Reference Case

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

\[
\begin{align*}
\langle p_s | H | \phi \rangle & \sim \bar{n}_p n_s f^p_s, \sum_{kl} f_i^k \lambda^s_{p l}, \sum_{klmn} \Gamma^{k l}_{m n} \lambda^{s k l}_{p m n}, \ldots \\
\langle pq_{st} | H | \phi \rangle & \sim \bar{n}_p \bar{n}_q n_s n_t \Gamma^{pq}_{st}, \sum_{kl} \Gamma^{p k}_{s l} \lambda^t_{q l}, \sum_{kl} f_i^k \lambda^{stk}_{p q l}, \sum_{klmn} \Gamma^{k l}_{m n} \lambda^{stk}_{p q m n}, \ldots \\
\langle pqr_{stu} | H | \phi \rangle & \sim \ldots
\end{align*}
\]
Multi-Reference Case

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

\[ \langle p_s | H | \Phi \rangle \sim \bar{n}_p n_s f_{ps}^p, \sum_{kl} f_{il}^k \lambda_{pl}^k, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pmn}^{skl}, \ldots \]

\[ \langle pq_{st} | H | \Phi \rangle \sim \bar{n}_p \bar{n}_q n_s n_t \Gamma_{pq_{st}}^{ps}, \sum_{kl} \Gamma_{pl}^{k} \lambda_{ql}^t, \sum_{kl} f_{il}^k \lambda_{pql}^{st}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pqmn}^{stkl}, \ldots \]

\[ \langle pqr_{stu} | H | \Phi \rangle \sim \ldots \]

\[ \rho_{mn}^{kl} = \lambda_{mn}^{kl} + \lambda_{m}^{k} \lambda_{n}^{l} - \lambda_{n}^{k} \lambda_{m}^{l} \]

\[ \rho_{lmn}^{ijk} = \lambda_{lmn}^{ijk} + \lambda_{l}^{i} \lambda_{mn}^{jk} + \lambda_{l}^{i} \lambda_{m}^{j} \lambda_{n}^{k} + \text{permutations} \]
Multi-Reference Case

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

\[ \langle p_s | H | \Phi \rangle \sim \tilde{n}_p n_s f^p_s, \sum_{kl} f^k_l \lambda^{sk}_p, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{skl}_{pmn}, \cdots \]

\[ \langle pq_{st} | H | \Phi \rangle \sim \tilde{n}_p \tilde{n}_q n_s n_t f^p_s, \sum_{kl} f^p_{kl} \lambda^{tk}_{ql}, \sum_{kl} f^k_{kl} \lambda^{stkl}_{pqmn}, \cdots \]

\[ \langle pqr_{stu} | H | \Phi \rangle \sim \cdots \]

Irreducible density matrices encode correlations
Decoupling in A-Body Space

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

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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

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

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

$^{40}$Ca

$E$ [MeV]

$E + \text{MBPT}(2)$

$10^{-5}$ $10^{-4}$ $10^{-3}$ $10^{-2}$ $10^{-1}$ $10^0$ $10^1$

$s$

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

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Decoupling

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

$^{40}\text{Ca}$

- $E$ (blue dots)
- $E + \text{MBPT}(2)$ (red squares)

$E [\text{MeV}]$

$V [\text{MeV fm}^3]$

$s$ (horizontal axis)

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

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Decoupling

\[ 40^{\text{Ca}} \]

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

$^{40}$Ca

$E \ [\text{MeV}]$

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

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Decoupling

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

\[ \lambda = 2.0 \text{ fm}^{-1}, e_{\text{Max}} = 8 \]
Decoupling

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

$40^{\text{Ca}}$

$E$ [MeV]

$10^{-5}$ $10^{-4}$ $10^{-3}$ $10^{-2}$ $10^{-1}$ $10^{0}$ $10^{1}$

$s$

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

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Decoupling

\[ E \ \text{[MeV]} \]

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Decoupling

$^{40}\text{Ca}$

$E$ [MeV]

$E + \text{MBPT}(2)$

$s$

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

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Decoupling

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

off-diagonal couplings are rapidly driven to zero.
Decoupling

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

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

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Decoupling

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

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

\[
U(s)HU^\dagger(s)U(s) |\psi_n\rangle = E_n U(s) |\psi_n\rangle
\]
• absorb correlations into \textbf{RG-improved Hamiltonian}

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

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

\[ U(s)H_{\text{MBPT}}U^\dagger(s)U(s) \left| \psi_n \right\rangle = E_n U(s) \left| \psi_n \right\rangle \]

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

\[ U(s) \left| \psi_n \right\rangle \overset{!}{=} \left| \Phi \right\rangle \]
“standard” IMSRG: build correlations on top of Slater determinant (=independent-particle state)
Correlated Reference States

ε

IMSRG(2)  IMSRG(3)  IMSRG(4)  IMSRG(5)

“standard” IMSR
Slater determinant

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

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**Correlated Reference States**

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

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Correlated Reference States

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

use generalized normal ordering with 2B,… 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.

see talk by K. Vobig
MR-IMSRG References States

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Titanium Isotopes

E. Leistenschneider et al., arXiv:1710.08537

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The graphs depict the neutron number and mass number for titanium isotopes. The plots show the energy levels $S_{2n}$ and $\Delta_{2n}$ as functions of the mass number. The left graph (b) illustrates $S_{2n}$ with data points and lines representing different models and calculations, while the right graph (c) shows $\Delta_{2n}$ with similar models and data points. The models include AME16, TITAN + AME16, 1.8/2.0(EM) VS-IMSRG, NN+3N(lnl) GGF, $N^2$LO sat, GGF, and $N^2$LO sat MR-IMSRG.
Titanium Isotopes

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E. Leistenschneider et al., arXiv:1710.08537
Titanium Isotopes

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

HH, in preparation

$R_{ch}[fm]$ vs $A$

- Open red circles: Garcia–Ruiz et al., Nat. Phys. 12, 594
- Red square: NN+3N(400), $\lambda=2.24$ fm$^{-1}$
- Orange diamond: NN+3N(400), $\lambda=1.88$ fm$^{-1}$
- Blue filled circle: NNLO$_{\text{sat}}$
Calcium Isotopes

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

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MR-IMSRG References States

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Example: $^{20}$Ne

- reference: particle-number & angular-momentum projected HFB

$\beta = 0.0$
$\beta = 0.1$
$\beta = 0.2$
$\beta = 0.3$
$\beta = 0.4$

SM ($0^+_2$): -33.735 MeV

SM ($0^+_1$): -40.491 MeV

Example: $^{20}\text{Ne}$

- reference: particle-number & angular-momentum projected HFB
- range of deformed reference states flow to the $^{20}\text{Ne}$ ground state
Example: $^{20}\text{Ne}$

- reference: particle-number & angular-momentum projected HFB
- range of deformed reference states flow to the $^{20}\text{Ne}$ ground state
- deviation from Shell model result: correlations beyond MR-IMSRG(2)


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Approximate MR-IMSRG(3)


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Approximate MR-IMSRG(3)

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

• size will be **reference-state dependent**
• **ground-state decoupled** Hamiltonians as input for many-body calculations
RG-Improved Hamiltonians

- **ground-state decoupled** Hamiltonians as input for many-body calculations

- In-Medium No-Core Shell Model

  E. Gebrerufael, K. Vobig, HH, R. Roth, PRL 118, 152503 (2017)
- **ground-state decoupled** Hamiltonians as input for many-body calculations

- In-Medium No-Core Shell Model
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- Equation-of-Motion methods
• **ground-state decoupled** Hamiltonians as input for many-body calculations

• In-Medium No-Core Shell Model
  E. Gebrerufael, K. Vobig, HH, R. Roth, PRL 118, 152503 (2017)

• Equation-of-Motion methods

• **decouple valence space** (cf. nuclear CI/Shell Model)
**RG-Improved Hamiltonians**

- **ground-state decoupled** Hamiltonians as input for many-body calculations
- In-Medium No-Core Shell Model  
  E. Gebrerufael, K. Vobig, HH, R. Roth, PRL 118, 152503 (2017)
- Equation-of-Motion methods  

- **decouple valence space** (cf. nuclear CI/Shell Model)
- VS-IMSRG: define off-diagonal Hamiltonian

\[
\{ H^{od} \} = \{ f_{h'}, f_{p'}, f_h, f_v, \Gamma_{hh'}, \Gamma_{hv}, \Gamma_{vv'} \} \quad \text{& H.c.}
\]
• **ground-state decoupled** Hamiltonians as input for many-body calculations

• In-Medium No-Core Shell Model
  
  E. Gebrerufael, K. Vobig, HH, R. Roth, PRL 118, 152503 (2017)

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• **decouple valence space** (cf. nuclear CI/Shell Model)

• VS-IMSRG: define off-diagonal Hamiltonian

\[
\begin{align*}
\left\{ H^{od} \right\} &= \left\{ f^h_{h'}, f^p_{p'}, f^p_{h}, f^q_{v'}, \Gamma_{hh'}, \Gamma_{hp'}, \Gamma_{hv}, \Gamma_{vv'} \right\} \quad \text{& H.c.}
\end{align*}
\]

• (initial) normal ordering and IMSRG decoupling in the target nucleus
(initial) normal ordering and IMSRG decoupling in the target nucleus

consistent with (MR-)IMSRG ground state energies (and CC, SCGF, …) for the same Hamiltonian
Oxygen Spectra

<table>
<thead>
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<th></th>
<th>CCEI</th>
<th>IM-SRG</th>
<th>USDB</th>
<th>Exp.</th>
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</thead>
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<tr>
<td>$^20\text{Ne}$</td>
<td>$^8+$</td>
<td>$^8+$</td>
<td>$^8+$</td>
<td>$^8+$</td>
</tr>
<tr>
<td>$^24\text{Mg}$</td>
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</tbody>
</table>

S. R. Stroberg et al., *PRC* 93, 051301(R) (2016)
N. M. Parzuchowski, S. R. Stroberg et al., PRC96, 034324;
N. M. Parzuchowski et al., PRC95, 044304

**Transitions**

Converged VS-/EOM-IMSRG results consistent with NCSM
Transitions

N. M. Parzuchowski, S. R. Stroberg et al., PRC96, 034324; N. M. Parzuchowski et al., PRC95, 044304

$\Delta^2_i (\text{MeV})$ vs. $\hbar \omega$ (MeV)

- **Exp**
- **Valence-space IMSRG**
- **EOM-IMSRG**

- $e_{\text{max}} = 4$
- $e_{\text{max}} = 6$
- $e_{\text{max}} = 8$
- $e_{\text{max}} = 10$
- $e_{\text{max}} = 12$
- $e_{\text{max}} = 14$

$^{22}O$
Transitions

- non-zero $B(E2)$ from Shell model: **VS-IMSRG induces effective neutron charge**
Transitions

- 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

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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

---

see talks by K. Vobig, G. Hagen, K. Launey
Epilogue

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• expanding IMSRG capabilities:
Epilogue

- expanding IMSRG capabilities:
  - continuum coupling (with K. Fossez)
Epilogue

- expanding IMSRG capabilities:
  - continuum coupling (with K. Fossez)
  - intrinsic deformation (with J. Yao)
• expanding IMSRG capabilities:
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  • electroweak transitions, response (with R. Stroberg, J. Yao, …)
Epilogue

• expanding IMSRG capabilities:
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• further challenges and opportunities:
Epilogue

- expanding IMSRG capabilities:
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- further challenges and opportunities:
  - treatment of general static (collective) correlations

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Epilogue

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  - novel computational techniques for memory management, scaling, …
Epilogue

• expanding IMSRG capabilities:
  • continuum coupling (with K. Fossez)
  • intrinsic deformation (with J. Yao)
  • electroweak transitions, response (with R. Stroberg, J. Yao, …)

• further challenges and opportunities:
  • treatment of general static (collective) correlations
  • novel computational techniques for memory management, scaling, …
  • coherent uncertainty quantification & propagation
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Supplements
IM-SRG(2) Flow Equations

0-body Flow

\[ \frac{dE}{ds} = \]

1-body Flow

\[ \frac{df}{ds} = \]

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

0-body Flow

\[
\frac{dE}{ds} = \begin{array}{c}
\text{Diagram 1}
\end{array} + \begin{array}{c}
\text{Diagram 2}
\end{array}
\]

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

1-body Flow

\[
\frac{df}{ds} = \begin{array}{c}
\text{Diagram 3}
\end{array} + \begin{array}{c}
\text{Diagram 4}
\end{array} + \begin{array}{c}
\text{Diagram 5}
\end{array} + \begin{array}{c}
\text{Diagram 6}
\end{array}
\]

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

2-body Flow

\[ \frac{d\Gamma}{ds} = \]

\[ + \]

\[ - \]

\[ + \]

\[ + \]

\[ - \]

s channel

ladders

t channel

rings

u channel
2-body Flow

\[ \frac{d\Gamma}{ds} = \]

\[ + \]

\[ - \]

\[ + \]

\[ + \]

\[ - \]

\[ + \]

\[ \text{s channel} \]

\[ \text{t channel} \]

\[ \text{u channel} \]

\[ \text{ladders} \]

\[ \text{rings} \]

\[ O(N^6) \text{ scaling} \]

(before particle/hole distinction)
In-Medium SRG Flow: Diagrams

\[ \Gamma(\delta s) \sim \]

\[ \Gamma(2\delta s) \sim \]
In-Medium SRG Flow: Diagrams

\[ \Gamma(\delta s) \sim \]

\[ \Gamma(2\delta s) \sim \]

& many more...

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In-Medium SRG Flow: Diagrams

\[ \Gamma(\delta s) \sim \]

\[ \Gamma(2\delta s) \sim \]

non-perturbative resummation

& many more...

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0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) r_b^a f_a^b + \frac{1}{2} \sum_{abcd} \eta_{cd}^{ab} \Gamma_{ab}^{cd} n_a n_b \bar{n}_c \bar{n}_d \\
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{cd}^{ab} + \frac{1}{4} \sum_{abcdklm} \left( \eta_{cd}^{kl} \Gamma_{am}^{kl} - \Gamma_{cd}^{kl} \eta_{am}^{kl} \right) \lambda_{cdm}^{bkl}
\]

1-body flow:

\[
\frac{d}{ds} f_2^1 = \sum_{a} \left( \eta_{a}^{1} f_{2}^{a} - f_{a}^{1} \eta_{2}^{a} \right) + \sum_{ab} \left( \eta_{b}^{a} \Gamma_{a2}^{b1} - f_{b}^{a} \eta_{a2}^{b1} \right) \left( n_{a} - n_{b} \right) \\
+ \frac{1}{2} \sum_{abc} \left( \eta_{bc}^{1} \Gamma_{2a}^{b} - \Gamma_{bc}^{1} \eta_{2a}^{b} \right) \left( n_{a} \bar{n}_{b} \bar{n}_{c} + \bar{n}_{a} n_{b} n_{c} \right) \\
+ \frac{1}{4} \sum_{abcde} \left( \eta_{bc}^{1} \Gamma_{2a}^{de} - \Gamma_{bc}^{1} \eta_{2a}^{de} \right) \lambda_{de}^{bc} + \sum_{abcde} \left( \eta_{bc}^{1} \Gamma_{2d}^{be} - \Gamma_{bc}^{1} \eta_{2d}^{be} \right) \lambda_{cd}^{bc} \\
- \frac{1}{2} \sum_{abcde} \left( \eta_{2b}^{1} \Gamma_{a+e}^{cd} - \Gamma_{2b}^{1} \eta_{ae}^{cd} \right) \lambda_{de}^{bc} + \frac{1}{2} \sum_{abcde} \left( \eta_{2b}^{1} \Gamma_{de}^{bc} - \Gamma_{2b}^{1} \eta_{de}^{bc} \right) \lambda_{de}^{ac}
\]
MR-IM-SRG Flow Equations

0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \eta_{ba} f_a + \frac{1}{2} \sum_{abcd} \eta_{cd} \Gamma_{ab} n_a n_b \bar{n}_c \bar{n}_d
\]

\[
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{cd} \right) \lambda_{cd} + \frac{1}{4} \sum_{abcdklm} \left( \eta_{cd} \Gamma_{kl} n_a - \Gamma_{cd} \eta_{am} \right) \lambda_{cdm}
\]

1-body flow:

\[
\frac{df_1}{ds} = \sum_a \left( \eta_{a2} f_a - f_a \eta_{a2} \right) + \sum_{ab} \left( \eta_{ba} \Gamma_{a2} - f_b \eta_{a2} \right) (n_a - n_b)
\]

\[
+ \frac{1}{2} \sum_{abc} \left( \eta_{bc} \Gamma_{a2} - \Gamma_{bc} \eta_{a2} \right) (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)
\]

\[
+ \frac{1}{4} \sum_{abcde} \left( \eta_{bc} \Gamma_{d2} - \Gamma_{bc} \eta_{d2} \right) \lambda_{de} + \sum_{abcde} \left( \eta_{bc} \Gamma_{d2} - \Gamma_{bc} \eta_{d2} \right) \lambda_{cd}
\]

\[
- \frac{1}{2} \sum_{abcde} \left( \eta_{2b} \Gamma_{d2} - \Gamma_{2b} \eta_{d2} \right) \lambda_{de} + \frac{1}{2} \sum_{abcde} \left( \eta_{2b} \Gamma_{d2} - \Gamma_{2b} \eta_{d2} \right) \lambda_{cd}
\]

\[O(N^5)\]
MR-IM-SRG Flow Equations

0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \eta^{a}_{b} f^{a}_{c} + \frac{1}{2} \sum_{abcd} \eta^{ab}_{cd} \Gamma^{cd}_{ab} n_a n_b \bar{n}_c \bar{n}_d
\]
\[
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma^{ab}_{cd} \right) \lambda^{ab}_{cd} + \frac{1}{4} \sum_{abcdklm} \left( \eta^{ab}_{cd} \Gamma^{kl}_{am} - \Gamma^{ab}_{cd} \eta^{kl}_{am} \right) \lambda^{bkl}_{cdm}
\]

1-body flow:

\[
\frac{d}{ds} f_2^1 = \sum_{a} \left( \eta_{a}^{1} f_{a}^{1} - f_{a}^{1} \eta_{a}^{2} \right) + \sum_{ab} \left( \eta_{b}^{a} \Gamma_{a2}^{b1} - f_{b}^{a} \eta_{a2}^{b1} \right) (n_a - n_b)
\]
\[
+ \frac{1}{2} \sum_{abc} \left( \eta_{bc}^{1} \Gamma_{2a}^{bc} - \Gamma_{bc}^{1a} \eta_{2a}^{bc} \right) (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)
\]
\[
+ \frac{1}{4} \sum_{abcde} \left( \eta_{bc}^{1a} \Gamma_{2a}^{de} - \Gamma_{bc}^{1a} \eta_{2a}^{de} \right) \lambda^{de}_{bc} + \sum_{abcde} \left( \eta_{bc}^{1a} \Gamma_{2d}^{bc} - \Gamma_{bc}^{1a} \eta_{2d}^{bc} \right) \lambda^{ae}_{cd}
\]
\[
- \frac{1}{2} \sum_{abcde} \left( \eta_{2b}^{1a} \Gamma_{ae}^{cd} - \Gamma_{2b}^{1a} \eta_{ae}^{cd} \right) \lambda^{cd}_{be} + \frac{1}{2} \sum_{abcde} \left( \eta_{2b}^{1a} \Gamma_{de}^{bc} - \Gamma_{2b}^{1a} \eta_{de}^{bc} \right) \lambda^{ac}_{de}
\]

O(N^5)  O(N^6)
2-body flow:

\[
\frac{d}{ds} \Gamma_{34}^{12} = \sum_a \left( \eta_a^1 \Gamma_{34}^{a2} + \eta_a^2 \Gamma_{34}^{1a} - \eta_3^a \Gamma_{a4}^{12} - \eta_4^a \Gamma_{3a}^{12} - f_a^1 \eta_{34}^{a2} - f_a^2 \eta_{34}^{1a} + f_3^a \eta_{a4}^{12} + f_4^a \eta_{3a}^{12} \right) \\
+ \frac{1}{2} \sum_{ab} \left( \eta_{ab}^{12} \Gamma_{34}^{ab} - \Gamma_{ab}^{12} \eta_{34}^{ab} \right) (1 - n_a - n_b) \\
+ \sum_{ab} (n_a - n_b) \left( \left( \eta_{3b}^1 \Gamma_{4a}^{2b} - \Gamma_{3b}^{1a} \eta_{4a}^{2b} \right) - \left( \eta_{3b}^2 \Gamma_{4a}^{1b} - \Gamma_{3b}^{2a} \eta_{4a}^{1b} \right) \right)
\]
2-body flow:

\[
\frac{d}{ds} \Gamma_{34}^{12} = \sum_a \left( \eta_a^1 \Gamma_3^{a2} + \eta_a^2 \Gamma_3^{1a} - \eta_3^a \Gamma_{a4}^{12} - \eta_4^a \Gamma_{34}^{12} - f_a^1 \eta_3^{a2} - f_a^2 \eta_3^{1a} + f_3^a \eta_{a4}^{12} + f_4^a \eta_{3a}^{12} \right) \\
+ \frac{1}{2} \sum_{ab} \left( \eta_{ab}^{12} \Gamma_3^{ab} - \Gamma_{ab}^{12} \eta_{34}^{ab} \right) \left( 1 - n_a - n_b \right) \\
+ \sum_{ab} (n_a - n_b) \left( \left( \eta_{3b}^{1a} \Gamma_4^{2b} - \Gamma_{3b}^{1a} \eta_4^{1b} \right) - \left( \eta_{3b}^{2a} \Gamma_4^{1b} - \Gamma_{3b}^{2a} \eta_4^{1b} \right) \right)
\]

- two-body flow identical to closed-shell case
2-body flow:

\[
\frac{d}{ds} \Gamma_{34}^{12} = \sum_a \left( \eta_a \Gamma_{34}^{a2} + \eta_a \Gamma_{34}^{1a} - \eta_{3a} \Gamma_{3a}^{12} - \eta_{4a} \Gamma_{3a}^{12} - f_a \eta_{3a}^{12} - f_a \eta_{3a} + f_a \eta_{3a} + f_a \eta_{3a}^{12} \right) \\
+ \frac{1}{2} \sum_{ab} \left( \eta_{ab} \Gamma_{34}^{ab} - \Gamma_{ab} \eta_{34}^{ab} \right) \left( 1 - n_a - n_b \right) \\
+ \sum_{ab} (n_a - n_b) \left( \left( \eta_{3b}^{1a} \Gamma_{4a}^{2b} - \Gamma_{3b} \eta_{4a}^{2b} \right) - \left( \eta_{3b} \Gamma_{4a}^{1b} - \Gamma_{3b} \eta_{4a}^{1b} \right) \right)
\]

- two-body flow identical to closed-shell case
- numerical scaling: \( O(N^6) \)
0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \tau_{ab} \Gamma_{ab}^b + \frac{1}{2} \sum_{abcd} \eta_{ab} \eta_{cd} \Gamma_{ab} n_a n_b n_c n_d \\
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{cd} + \frac{1}{4} \sum_{abcdklm} \left( \eta_{cd} \Gamma_{am}^{kl} - \Gamma_{cd}^{ab} \eta_{am}^{kl} \right) \lambda_{cdlm}
\]
MR-IM-SRG Flow Equations

0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) r_{ab} f_a^b + \frac{1}{2} \sum_{abcd} \eta_{cd} \Gamma_{ab} n_a n_b \tilde{n}_c \tilde{n}_d
\]

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

O(N^4)
MR-IM-SRG Flow Equations

0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) R_{ba} R_{ab} + \frac{1}{2} \sum_{abcd} \eta_{cd} R_{ab} n_a n_b \bar{n}_c \bar{n}_d
\]

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

O(N^4)
0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \tau_{ab} f^b_a + \frac{1}{2} \sum_{abcd} \eta_{cd} \Gamma_{ab} n_a n_b \bar{n}_c \bar{n}_d \\
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{ab}^{cd} + \frac{1}{4} \sum_{abcdklm} \left( \eta_{cd} \Gamma_{am}^{kl} - \Gamma_{cd}^{ab} \eta_{am}^{kl} \right) \lambda_{cdm}^{bk}\]

O(N^4)  
O(N^4)  
O(N^7)
0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \gamma_{ab} f_a^b + \frac{1}{2} \sum_{abcd} \eta_{cd} \Gamma_{ab} n_a n_b \tilde{n}_c \tilde{n}_d \\
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{ab}^{cd} \right) \lambda_{cd}^{ab} + \frac{1}{4} \sum_{abcdklm} \left( \eta_{cd} \Gamma_{am}^{kl} - \Gamma_{cd}^{ab} \eta_{am}^{kl} \right) \lambda_{cdm}^{bl}
\]

O(\(N^4\))

O(\(N^7\))

- storage of full 3B density matrix too expensive in general

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0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \eta^a_b f^b_a + \frac{1}{2} \sum_{abcd} \eta^a_b \Gamma^c_d n_a n_b \bar{n}_c \bar{n}_d
\]

\[
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma^a_b \right) \lambda^a_b + \frac{1}{4} \sum_{abcdklm} \left( \eta^a_b \Gamma^k_l - \Gamma^a_b \eta^k_l \right) \lambda^{bkl}
\]

- storage of full 3B density matrix too expensive in general

exploit structure of specific reference states:
0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) r_{ab} f_a + \frac{1}{2} \sum_{abcd} \eta_{cd} \Gamma_{ab} n_a n_b \bar{n}_c \bar{n}_d \\
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{ab} \right) \lambda_{cd} + \frac{1}{4} \sum_{abcdklm} \left( \eta_{cd} \Gamma_{am} - \Gamma_{cd} \eta_{am} \right) \lambda_{bkl}
\]

\( O(N^4) \) \hspace{2cm} \( O(N^7) \)

- Storage of full 3B density matrix too expensive in general

\[ \lambda_{abc}^{def} = \bar{\lambda}_{abc} \delta_d^a \delta_e^b \delta_f^c + \bar{\lambda}_{a|bc} \delta_d^a \delta_b^b \delta_e^c \delta_f^c + \text{perm.} \]

- Projected HFB: \( O(N^3) \) storage, scaling reduced to \( O(N^4) \)

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MR-IM-SRG Flow Equations

0-body flow:

\[
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \eta_{ab}^{a} f_{a}^{b} + \frac{1}{2} \sum_{abcd} \eta_{cd}^{ab} \Gamma_{ab}^{cd} n_{a} n_{b} \tilde{n}_{c} \tilde{n}_{d} \\
+ \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{cd}^{ab} + \frac{1}{4} \sum_{abcdklm} \left( \eta_{cd}^{ab} \Gamma_{am}^{kl} - \Gamma_{cd}^{ab} \eta_{am}^{kl} \right) \lambda_{cdm}^{bkl}
\]

**O(N^4)**

storage of full 3B density matrix too expensive in general

exploit structure of specific reference states:

- Projected HFB: \(O(N^3)\) storage, scaling reduced to \(O(N^4)\)
  \[
  \lambda_{def}^{abc} = \tilde{\lambda}_{abc} \delta_{d}^{a} \delta_{e}^{b} \delta_{f}^{c} + \tilde{\lambda}_{a|be} \delta_{d}^{a} \delta_{bc}^{b} \delta_{ef}^{c} + \text{perm.}
  \]

- NCSM / active-space CI: small non-zero block only
Magnus Formulation of the In-Medium SRG


Magnus Series Formulation

- explicit exponential ansatz for unitary transformation:

\[ U(s) = S \exp \int_0^s ds' \eta(s') \equiv \exp \Omega(s) \]
• explicit exponential ansatz for unitary transformation:

\[ U(s) = S \exp \int_0^s ds' \eta(s') \equiv \exp \Omega(s) \]

• flow equation for **Magnus** operator:

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

\( (B_k: \text{Bernoulli numbers}) \)
Magnus Series Formulation

- explicit exponential ansatz for unitary transformation:

\[ U(s) = S \exp \int_0^s ds' \eta(s') \equiv \exp \Omega(s) \]

- 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<sub>k</sub>: Bernoulli numbers)

- construct \( O(s) = U(s)O_0U^\dagger(s) \) using Baker-Campbell-Hausdorff expansion (**Hamiltonian + effective operators**)
Magnus Series Formulation

• explicit exponential ansatz for unitary transformation:

\[ U(s) = S \exp \int_0^s ds' \eta(s') \equiv \exp \Omega(s) \]

• flow equation for Magnus operator:

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

\((B_k: \text{Bernoulli numbers})\)

• 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

\[ \text{O}^{\text{16}} \]

N^{3\text{LO}} (500 MeV) \( \lambda = 2.0 \text{ fm}^{-1} \)

-120
-140
-160
-180

Energy (MeV)

0 1 2 3 4 5

S

- IM-SRG(2) (Adams-Bashforth)
- Magnus(2) (Euler \( \delta s = 0.5 \))
- Magnus(2) (Euler \( \delta s = 0.1 \))
- IM-SRG(2) (Euler \( \delta s = 0.5 \))
- IM-SRG(2) (Euler \( \delta s = 0.1 \))

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Magnus vs. Direct Integration

$^\text{16}_\text{O}$

$N^3\text{LO} (500 \text{ MeV}) \, \lambda = 2.0 \text{ fm}^{-1}$

- IM-SRG(2) (Adams-Bashforth)
- Magnus(2) (Euler $\delta s=0.5$)
- Magnus(2) (Euler $\delta s=0.1$)
- IM-SRG(2) (Euler $\delta s=0.5$)
- IM-SRG(2) (Euler $\delta s=0.1$)

$\text{IM-SRG}(2) \approx \text{MAG}(2)$
Magnus vs. Direct Integration

$\text{IM-SRG(2)} \approx \text{MAG(2)}$

$\text{Euler integrator sufficient, unitarity built in!}$
Convergence

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

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

\[\rightarrow\text{ODE and BCH expansions converge rapidly and monotonically}\]
• final Hamiltonian (IM-SRG(A), MAG(A)):

\[
\overline{H} = (e^{\Omega}He^{-\Omega}) = \overline{H}_{0,1,2} + \overline{H}_{3} + \ldots
\]
Approximating IM-SRG(3)

- final Hamiltonian (IM-SRG(2), MAG(2)):
  \[
  \bar{H}_{\text{MAG}(2)} = (e^{\Omega_{1,2}}He^{-\Omega_{1,2}}) = \bar{H}_{0,1,2} + \bar{H}_3 + \ldots
  \]
• final Hamiltonian (IM-SRG(2), MAG(2)):

\[ H_{\text{MAG}(2)} = (e^{\Omega_{1,2}} H e^{-\Omega_{1,2}}) = H_{0,1,2} + H_3 + \ldots \]

• energy contribution of \( H_3 \) (cf. 0B flow):

\[ \Delta E_3 = \frac{1}{36} \sum_{pp'p''hh'h''} \frac{|(H_3)_{pp'p''hh'h''}|^2}{\Delta_{pp'p''hh'h''}} \]

\[ \langle i | H_{\text{MAG}(2)} | j \rangle \]
Approximating IM-SRG(3)

- final Hamiltonian (IM-SRG(2), MAG(2)):
  \[
  \overline{H}_{\text{MAG}(2)} = \left(e^{\Omega_{1,2}} He^{-\Omega_{1,2}}\right) = \overline{H}_{0,1,2} + \overline{H}_3 + \ldots
  \]

- energy contribution of \(\overline{H}_3\) (cf. 0B flow):
  \[
  \Delta E_3 = \frac{1}{36} \sum_{pp'p''hh'h''} \frac{|(\overline{H}_3)_{pp'p''hh'h''}|^2}{\overline{\Delta}_{pp'p''hh'h''}}
  \]

- family of non-iterative methods: level of approximation for \(\overline{H}_3\) and energy denominator \(\overline{\Delta}\)
Approximating IM-SRG(3)

- final Hamiltonian (IM-SRG(2), MAG(2)):
  \[
  \overline{H}_{\text{MAG}(2)} = (e^{\Omega_{1,2}}H e^{-\Omega_{1,2}}) = \overline{H}_{0,1,2} + \overline{H}_3 + \ldots
  \]

- energy contribution of \( \overline{H}_3 \) (cf. 0B flow):
  \[
  \Delta E_3 = \frac{1}{36} \sum_{pp'p''hh'h''} \left| \frac{(\overline{H}_3)_{pp'p''hh'h''}}{\overline{\Delta}_{pp'p''hh'h''}} \right|^2
  \]

- family of non-iterative methods: level of approximation for \( \overline{H}_3 \) and energy denominator \( \overline{\Delta} \)

- generalizes to arbitrary observables, excited states
Approximating IM-SRG(3)

- final Hamiltonian (IM-SRG(2), MAG(2)):
  \[
  \overline{H}_{\text{MAG}(2)} = (e^{\Omega_{1,2}} He^{-\Omega_{1,2}}) = \overline{H}_{0,1,2} + \overline{H}_3 + \ldots
  \]

- energy contribution of \( \overline{H}_3 \) (cf. 0B flow):
  \[
  \Delta E_3 = \frac{1}{36} \sum_{pp'p''hh'h''} \left| \langle \overline{H}_3 \rangle_{pp'p''hh'h''} \right|^2 \frac{\overline{\Delta}_{pp'p''hh'h''}}{\Delta_{pp'p''hh'h''}}
  \]

- family of non-iterative methods: level of approximation for \( \overline{H}_3 \) and energy denominator \( \overline{\Delta} \)

- generalizes to arbitrary observables, excited states

- multi-reference variant in development

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Example: Bond Breaking in Water

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• describe “excited states” based on reference state:

\[ |\Phi_k\rangle = Q_k^\dagger |\Phi_0\rangle \]
• describe “excited states” based on reference state:

\[ |\Phi_k\rangle = Q_k\dagger |\Phi_0\rangle \]

• \textbf{(MR-)IM-SRG effective Hamiltonian} in EOM approach:

\[ [H(s), Q_k\dagger(s)] = \omega_k(s)Q_k\dagger(s), \quad \omega_k(s) = E_k(s) - E_0(s) \]
Equation-of-Motion Method

- 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):
  \[ Q_k^\dagger(s) = \sum_{ph} q_h^p(s) :A_h^p : + \frac{1}{4} \sum_{pp'h'h'} q_{hh'}^{pp'}(s) :A_{hh'}^{pp'} : \]
Equation-of-Motion Method

• 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
Equation-of-Motion Method

- describe “excited states” based on reference state:

\[ |\Phi_k\rangle = Q^\dagger_k |\Phi_0\rangle \]

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

\[ [H(s), Q^\dagger_k(s)] = \omega_k(s) Q^\dagger_k(s), \quad \omega_k(s) = E_k(s) - E_0(s) \]

- ansatz for excitation operator (g.s. correlations built into Hamiltonian):

\[ Q^\dagger_k(s) = \sum_{ph} q^p_h(s) :A^p_h : + \frac{1}{4} \sum_{pp'hh'} q^{pp'}_{hh'}(s) :A^{pp'}_{hh'} : \]

- polynomial effort vs. factorial scaling of Shell Model

- future: exploit multi-reference capabilities (commutator formulation identical to flow equations)
Full Configuration Interaction

- many-body basis (e.g., Slater determinants)

\[ |\Phi_1\rangle = \begin{array}{cccc}
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
\end{array} \]
\[ |\Phi_2\rangle = \begin{array}{cccc}
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
\end{array} \]
\[ |\Phi_3\rangle = \begin{array}{cccc}
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
\end{array} \]
\[ |\Phi_4\rangle = \begin{array}{cccc}
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
    \bullet & \bullet & \bullet & \bullet \\
\end{array} \], \ldots
• many-body basis (e.g., Slater determinants)

\[ |\Phi_1\rangle = \ldots, |\Phi_2\rangle = \ldots, |\Phi_3\rangle = \ldots, |\Phi_4\rangle = \ldots, \ldots \]

• intrinsic Hamiltonian:

\[ H_{\text{int}} = \left(1 - \frac{1}{A}\right) \sum_i \frac{p_i^2}{2m} - \frac{1}{A} \sum_{i<j} \frac{p_i \cdot p_j}{m} + V^{[2]} + V^{[3]} \]
Full Configuration Interaction

- many-body basis (e.g., Slater determinants)

\[ |\Phi_1\rangle = \psi_1, |\Phi_2\rangle = \psi_2, |\Phi_3\rangle = \psi_3, |\Phi_4\rangle = \psi_4, \ldots \]

- intrinsic Hamiltonian:

\[ H_{\text{int}} = \left(1 - \frac{1}{A}\right) \sum_i \frac{p_i^2}{2m} - \frac{1}{A} \sum_{i<j} \frac{p_i \cdot p_j}{m} + V^{[2]} + V^{[3]} \]

- treat A as particle number operator

(H. H., R. Roth, PLB 682, 27 (2009))
Full Configuration Interaction

- many-body basis (e.g., Slater determinants)

\[
|\Phi_1\rangle = \ldots |\Phi_2\rangle = \ldots |\Phi_3\rangle = \ldots |\Phi_4\rangle = \ldots
\]

- intrinsic Hamiltonian:

\[
H_{\text{int}} = \left(1 - \frac{1}{A}\right) \sum_i \frac{p_i^2}{2m} - \frac{1}{A} \sum_{i<j} \frac{p_i \cdot p_j}{m} + V[2] + V[3]
\]

- treat A as particle number operator
  (H. H., R. Roth, PLB 682, 27 (2009))

- diagonalize Hamiltonian matrix, but dimensions are huge:
Full Configuration Interaction

- many-body basis (e.g., Slater determinants)

\[ |\Phi_1\rangle = \cdot \cdot \cdot , |\Phi_2\rangle = \cdot \cdot \cdot , |\Phi_3\rangle = \cdot \cdot \cdot , |\Phi_4\rangle = \cdot \cdot \cdot , \ldots \]

- intrinsic Hamiltonian:

\[ H_{\text{int}} = \left( 1 - \frac{1}{A} \right) \sum_i \frac{p_i^2}{2m} - \frac{1}{A} \sum_{i<j} \frac{p_i \cdot p_j}{m} + V^{[2]} + V^{[3]} \]

- treat A as particle number operator
  (H. H., R. Roth, PLB 682, 27 (2009))

- diagonalize Hamiltonian matrix, but dimensions are huge:

\[ D^{(4}\text{He}) = \binom{100}{2}^\text{prot.} \times \binom{100}{2}^\text{neut.} = 2.45 \times 10^7 \]

\[ D^{(16}\text{O}) = \binom{100}{8}^\text{prot.} \times \binom{100}{8}^\text{neut.} = 3.46 \times 10^{22} \]
Basis Size “Explosion”

Figure 1: The characteristics of the CI projected Hamiltonian $\hat{H}$ for a variety of nuclei.

- The growth of the matrix dimension ($|A|$) with respect to $N_{\text{max}}$.
- The growth of the number of nonzero matrix elements in $\hat{H}$ with respect to $|A|$ for both two-body and two-plus-three-body potentials.

To compute the eigenvalues of $\hat{H}$ efficiently on a high performance parallel computer, the following three issues must be addressed carefully:

1. The generation and distribution of the many-body basis states — This step essentially determines how the matrix Hamiltonian $\hat{H}$ or $\hat{H}_Z$ is partitioned and distributed in subsequent calculations.
2. The construction of the sparse matrix Hamiltonian $\hat{H}$ — This step is performed simultaneously on all processors. Each processor will construct its portion of $\hat{H}$ defined by the many-body basis states assigned to it. Because the positions of the nonzero elements of the Hamiltonian is not known a priori, the key to achieving good performance during this step is to quickly identify the locations of these elements without evaluating them numerically first.
3. The calculation of the eigenvalues and eigenvectors using the Lanczos iteration — The major cost of the Lanczos iteration is the computation required to perform sparse matrix-vector multiplications of the form $y \leftarrow \hat{H}x$, where $x$, $y$ are both vectors. Performing efficient orthogonalizations of the Lanczos basis vectors is also an important issue to consider.

Parallel basis generation

Because the rows and columns of $\hat{H}$ are indexed by valid many-body basis states, the first step of the nuclear CI calculation is to generate these states so that they can be used to construct and manipulate matrix elements of $\hat{H}$ in subsequent calculations.

From: C. Yang, H. M. Aktulga, P. Maris, E. Ng, J. Vary, Proceedings of NTSE-2013
Basis Size “Explosion”

- constructing and storing full $H$ matrix is impossible

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Basis Size “Explosion”

Constructing and storing full $H$ matrix is impossible.

- 75 GB per vector
- 7.5 TB

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

- constructing and storing full $H$ matrix is impossible
• constructing and storing full $H$ matrix is impossible
• can exploit matrix sparseness, but problem is still very hard
Core and Valence Spaces

- **Non-valence particle states**
- **Valence particle states**
- **Hole states (core)**
Core and Valence Spaces

- Introduce an inert core: restrict states to the form

\[ |\psi_i\rangle = |\overline{\psi}_i\rangle \otimes |\text{core}\rangle \]
• introduce an inert core: restrict states to the form

$$|\Psi_i\rangle = |\overline{\Psi}_i\rangle \otimes |\text{core}\rangle$$

• basis states:

$$|\Phi_{v_1,\ldots,v_{A_v}}\rangle = a_{v_1}^\dagger \ldots a_{v_{A_v}}^\dagger |\text{core}\rangle$$
Core and Valence Spaces

- introduce an **inert core**: restrict states to the form

\[ |\psi_i\rangle = |\overline{\psi}_i\rangle \otimes |\text{core}\rangle \]

- basis states:

\[ |\phi_{v_1,\ldots,v_{Av}}\rangle = a_{v_1}^\dagger \ldots a_{v_{Av}}^\dagger |\text{core}\rangle \]

- wave functions for \( A_v < A \) (\( A_v \ll A \)) particles (**core implicit**)

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• introduce an **inert core**: restrict states to the form

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• basis states:

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• wave functions for \( A_v < A \) (\( A_v \ll A \)) particles (**core implicit**)
Effective Hamiltonian
Effective Hamiltonian
Effective Hamiltonian

e etc.
Effective Hamiltonian
Effective Hamiltonian

\( P \) space
(included configurations)

etc.

etc.

etc.
Effective Hamiltonian

\( P \) space
(included configurations)

\( Q \) space
(excluded configurations)

etc.

etc.

etc.
Effective Hamiltonian

\[
\begin{array}{ccc}
H_{PP} & H_{PQ} \\
H_{QP} & H_{QQ}
\end{array}
\]

\[
\begin{array}{ccc}
H_{PQ} & \text{white} \\
H_{QQ} & \text{white}
\end{array}
\]
Valence Space Decoupling

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

\(2v-0h\) \(2q-0h\) \(3p-1h\) \(4p-2h\)

\(2v-0h\) \(2q-0h\) \(3p-1h\) \(4p-2h\)

\(3p-1h\) \(2q-0h\) \(2v-0h\)

\(4p-2h\) \(2v-0h\) \(2q-0h\) \(3p-1h\)

\(v\): valence particle states

\(q\): non-valence particle states

\(h\): hole states (core)
Valence Space Decoupling

- NN (maybe 3N?) operators can only act on 2 (3) valence nucleons
Valence Space Decoupling

- NN (maybe 3N?) operators can only act on 2 (3) valence nucleons

- remaining core and valence particles are **spectators**

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