Extensions of the No-Core Shell Model

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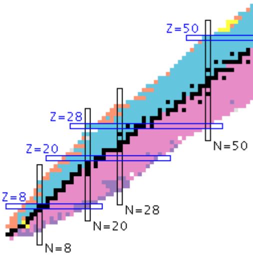
Motivations

- ab initio many-body method for the description of ground and excited states in open-shell nuclei

- No-Core Shell Model (NCSM)
  ⇝ limited by basis dimension, scaling with particle number

- medium-mass methods:
  - In-Medium Similarity Renormalization Group (IM-SRG)
  - Coupled Cluster
  - Perturbation Theory (PT)
  - ...

  ⇝ basic formulations limited to ground states



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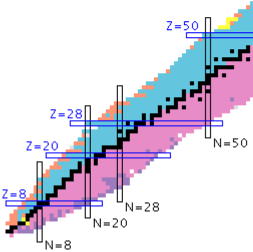
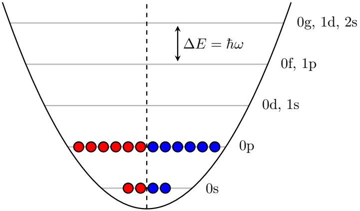
  ⇝ basic formulations limited to ground states

- our approach for overcoming limitations:
  No-Core Shell Model based hybrid methods

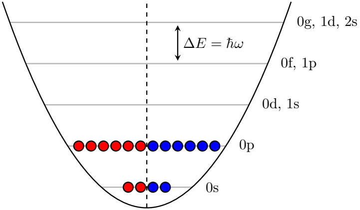


No-Core Shell Model



- use harmonic-oscillator states with given $\hbar\Omega$ as single-particle basis

No-Core Shell Model



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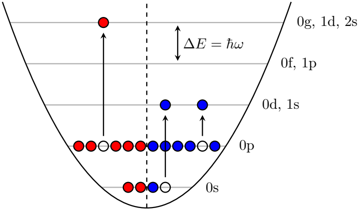
- construct Slater-determinant(s) from single-particle states

No-Core Shell Model



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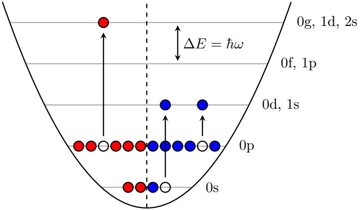

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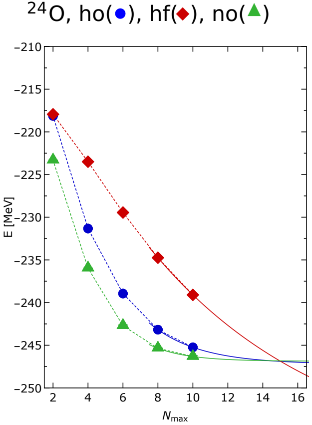
No-Core Shell Model



NN at N^{3}LO, $\alpha = 0.08\ \mathrm{fm}^4$

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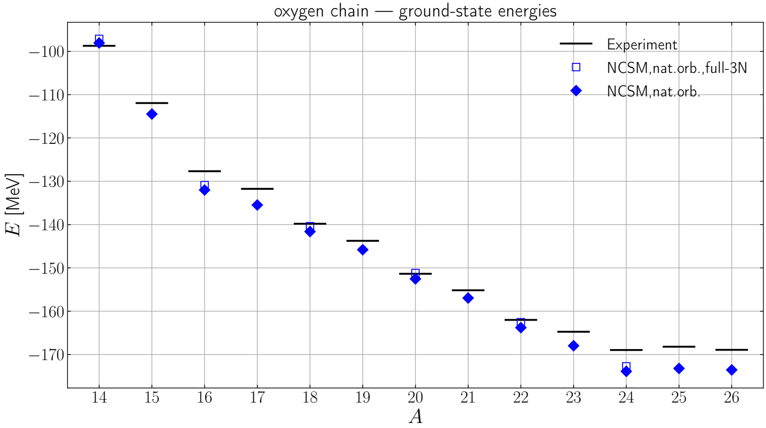
- represent and diagonalize Hamiltonian in this model space

- use of natural-orbital basis
  ⇝ eigenbasis of one-body density from, e.g., second-order Perturbation Theory
- boost N_{max} convergence and eliminate $\hbar\Omega$ dependency

No-Core Shell Model: Oxygen Chain



NN at N^{3}LO, (D. R. Entem et al., PRC 68, 041001 (2003))

3N at N^{2}LO with $\Lambda = 400$ MeV, (R. Roth et al., PRL 109, 052501 (2012))

free-space SRG $\alpha_{2B} = \alpha_{3B} = .08\,\mathrm{fm}^4$

NCSM-PT: NCSM + Perturbation Theory

NCSM

- NCSM reference state from diagonalization in a small model space $\mathcal{M}_{\text{ref}}$ (typically $N_{\text{max}} = 2$)

$$|\Psi\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} c_\nu \, |\phi_\nu\rangle$$

- use these most important multi-particle multi-hole correlations as seed for perturbative improvement

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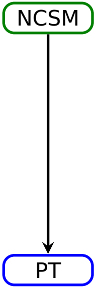

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- use these most important multi-particle multi-hole correlations as seed for perturbative improvement

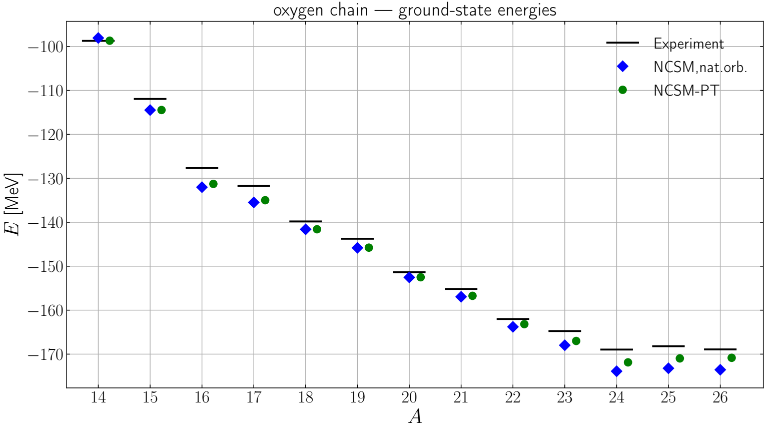
- use second-order multi-configurational PT to capure correlation effects beyond $\mathcal{M}_{\text{ref}}$

$$E^{(2)} = -\sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{|\langle \Psi | W | \phi_\nu \rangle|^2}{E_\nu^{(0)} - E_{\text{ref}}^{(0)}}$$

- evaluate perturbative corrections in large model space (typically single-particle e_{max} truncated)

- convergence booster efficiently accounting for correlation from huge model space

NCSM-PT: Oxygen Chain



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In-Medium No-Core Shell Model: Concept

NCSM

- NCSM calculation in small model space defines reference state

$$|\Psi\rangle = \sum_i c_i \, |\Phi_i\rangle$$

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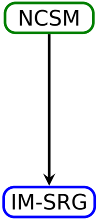

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$$|\Psi\rangle = \sum_i c_i \, |\Phi_i\rangle$$

- perform **multi-reference** IM-SRG aiming at decoupling reference state from generalized ph-excitations $\tilde{a}^{p_1}_{q_1} |\Psi\rangle$, $\tilde{a}^{p_1 p_2}_{q_1 q_2} |\Psi\rangle$, ...

$$\hat{H}(\infty) \; |\Psi\rangle = E(\infty) \; |\Psi\rangle$$

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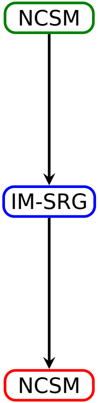

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$$\hat{H}(\infty)\ |\Psi\rangle = E(\infty)\ |\Psi\rangle$$

- use IM-SRG-evolved Hamiltonian $\hat{H}(s)$ as input for subsequent NCSM calculation
- convergence of NCSM calculation massively improved w.r.t. N_{max}

In-Medium No-Core Shell Model: IM-SRG

- use normal-ordered operators truncated at NO2B level throughout evolution

$$\hat{H}(s) \equiv E(s) + \sum_{pq} f^p_q(s)\ \{\hat{p}^\dagger \hat{q}\}_{|\Psi\rangle} + \frac{1}{4}\sum_{pqrs} \Gamma^{pq}_{rs}(s)\,\{\hat{p}^\dagger \hat{q}^\dagger \hat{s}\hat{r}\}_{|\Psi\rangle}$$

- perform unitary transformation via SRG flow equation approach:

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

- generator $\hat{\eta}(s)$ defines decoupling behavior/pattern ⇝ tailor SRG for specific applications

- evaluate commutator ⇝ coupled system of first-order ordinary differential equations

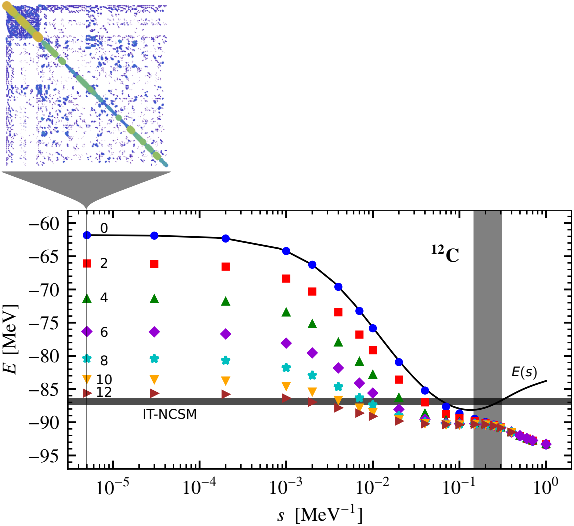
$$\frac{\mathrm{d}}{\mathrm{d}s}E(s) = \sum_{pq}\left(n_p - n_q\right)\ \eta^p_q(s)\ f^q_p(s) + \frac{1}{4}\sum_{pqrs}\left(\eta^{pq}_{rs}(s)\ \Gamma^{rs}_{pq}(s)\ n_p n_q \bar{n}_r \bar{n}_s - [\eta \leftrightarrow \Gamma]\right) + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}f^1_2(s) = \sum_{p}\left(\eta^1_p\ f^p_2\ - [\eta \leftrightarrow f]\right) + \ldots + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Gamma^{12}_{34}(s) = \sum_{p}\left(\left(\eta^1_p\ \Gamma^{p2}_{34} - f^1_p\ \eta^{p2}_{34}\right) - [1 \leftrightarrow 2]\right) + \ldots$$

- coupled formulation restricted to $J = 0$ reference states ⇝ even nuclei

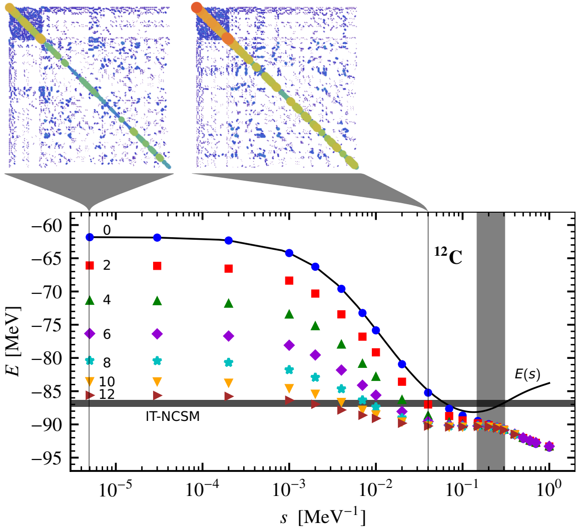
IM-NCSM: Ground State Evolution



$s = 0.00\,\mathrm{MeV}^{-1}$

- eigenvalue = $E(s)$
- strong couplings of N=0 space to basis states at higher N
- high N_{max} necessary for converged results

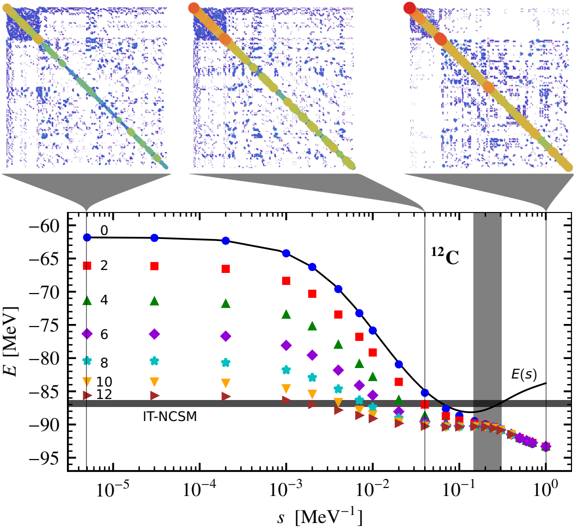
IM-NCSM: Ground State Evolution



$s = 0.04\ \text{MeV}^{-1}$

- coupling of $N = 0$ and higher N basis states partially suppressed
- NCSM convergence accelerated

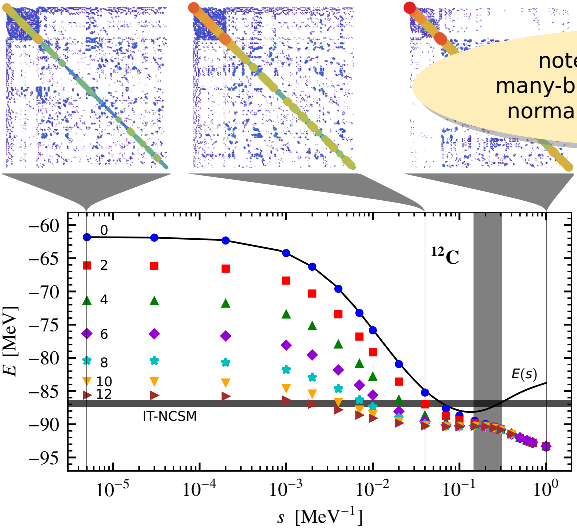
IM-NCSM: Ground State Evolution



$s = 1.00\,\mathrm{MeV}^{-1}$

- $N_{\max} = 0$ space decoupled ⇝ converged results at $N_{\max} = 0$.
- eigenvalue $\neq E(s)$
- reference state $|\Psi\rangle$ not $N_{\max} = 0$ eigenstate anymore
- explicit diagonalization necessary

IM-NCSM: Ground State Evolution



note effects of neglected many-body contributions beyond normal-ordered two-body level

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- eigenvalue $\neq E(s)$
- reference state $|\Psi\rangle$ not $N_{max} = 0$ eigenstate anymore
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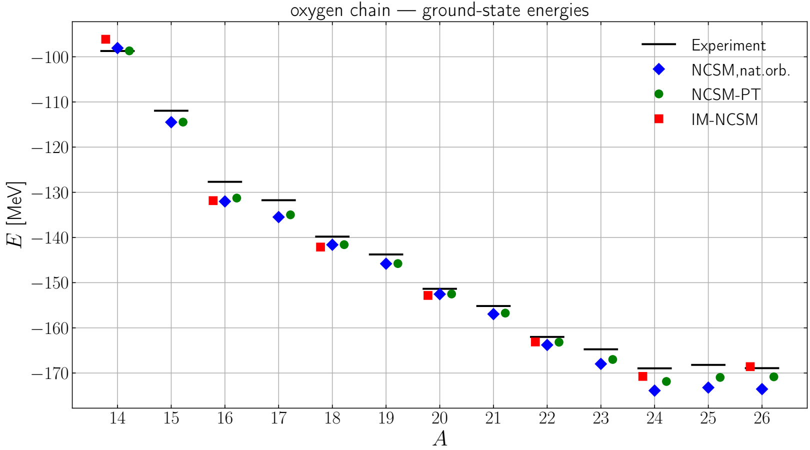
IM-NCSM: Oxygen Chain



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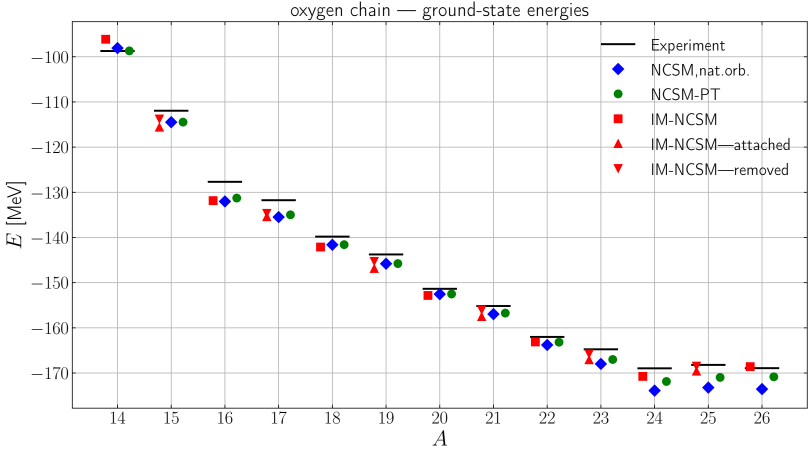
IM-NCSM: Particle-Attached Particle Removed



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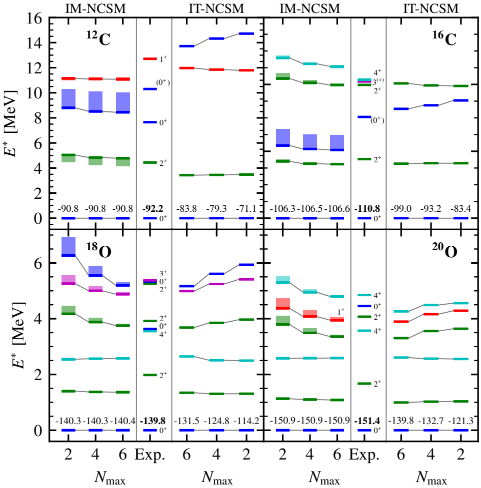
Applications: Spectra

E. Gebrerufael et al, Phys. Rev. Lett. 118, 152503 (2017)



- good agreement for well converged states
- slow convergence w.r.t. N_{max}
  ⇝ dominant contributions from outside $N_{max} = 0$ space

IM-NCSM bands: uncertainty estimate

Epilogue

- **Thanks to my group**
  - S. Alexa, **E. Gebrerufael**, T. Hüther, J. Müller, R. Roth, S. Schulz, C. Stumpf, **A. Tichai**, R. Wirth
    Institut für Kernphysik, TU Darmstadt

- **Thank you for your attention!**

COMPUTING TIME

JURECA	LOEWE-CSC	LICHTENBERG
JÜLICH FORSCHUNGSZENTRUM	CSC Center for Scientific Computing Frankfurt	HRZ Hochschulrechenzentrum

SFB 1245

Deutsche Forschungsgemeinschaft
DFG

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung

BACKUP

SRG: Basic Concept & Formalism

- transformation towards diagonal form w.r.t. specific basis

- unitary transformation $\leftrightsquigarrow$ SRG flow equation

$$\hat{H}(s) \equiv \hat{U}^{\dagger}(s)\hat{H}(0)\hat{U}(s) \quad \leftrightsquigarrow \quad \frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s), \hat{H}(s)\right], \quad \hat{\eta}(s) \equiv -\hat{U}^{\dagger}(s)\frac{\mathrm{d}}{\mathrm{d}s}\hat{U}(s)$$

- observables have to be evolved simultaneously (if $\hat{\eta}(s)$ depends on $\hat{H}(s)$)

$$\frac{\mathrm{d}}{\mathrm{d}s}\hat{O}(s) = \left[\hat{\eta}(s), \hat{O}(s)\right]$$

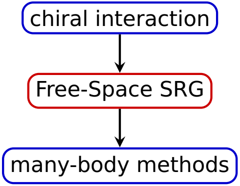
- choice of generator $\hat{\eta}$ $\longleftrightarrow$ desired behavior

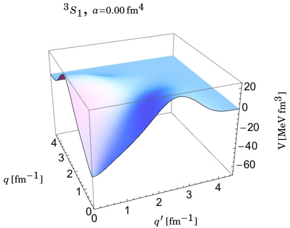
- antihermitian generator $\hat{\eta}(s)$ determines decoupling behavior and decoupling pattern
$\rightsquigarrow$ tailor SRG for specific applications

- SRG induces many-body terms up to the A-body level

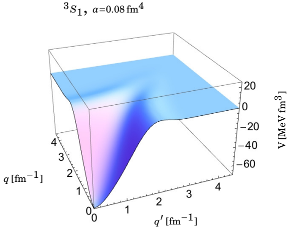
$$\hat{H}(s) = \hat{H}^{[0]}(s) + \hat{H}^{[1]}(s) + \ldots + \hat{H}^{[A]}(s)$$

SRG-based Many-Body Methods

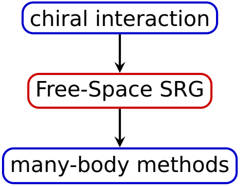




- tame strong short-range correlations
- "generic" decoupling of high- and low momenta in two- and three-body momentum space
- "softer" interaction with improved convergence properties in many-body calculations



SRG-based Many-Body Methods



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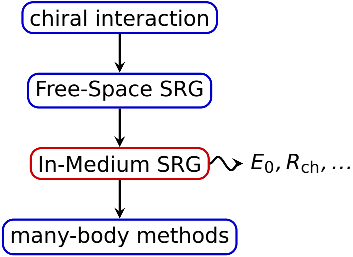


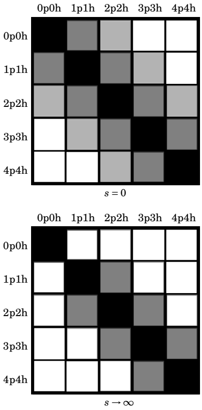
- decoupling of reference state of specific A-body system
- even further acceleration of model-space convergence
- new opportunities, e.g., valence-space interactions from ab initio treatment

IM-SRG and Reference-State Decoupling

- decouple reference state $|\Phi\rangle$ from its ph-excitations $|\Phi^{p_1}_{q_1}\rangle, |\Phi^{p_1 p_2}_{q_1 q_2}\rangle, \ldots$
- partition Hamiltonian $\hat{H} = \hat{H}^{\mathrm{d}} + \hat{H}^{\mathrm{od}}$, suppress "off-diagonal" part
- reference state $|\Phi\rangle$ becomes ground-state of $\hat{H}(\infty)$ with eigenvalue $\langle\Phi|\hat{H}(\infty)|\Phi\rangle$
- achieved, e.g., via Wegner generator

$$\hat{\eta}(s) \equiv \left[\hat{H}^{\mathrm{d}}(s), \hat{H}(s)\right]$$

- improved numerical characteristics and efficiencies: White and imaginary-time generator



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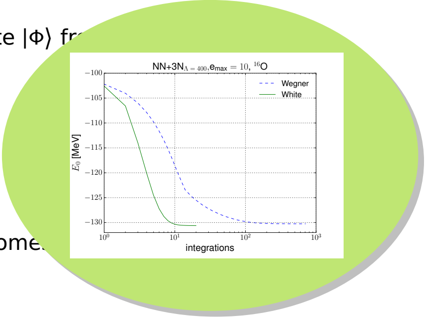

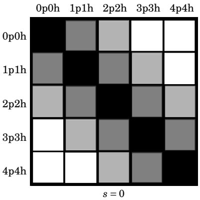

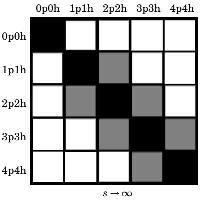

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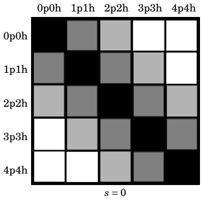
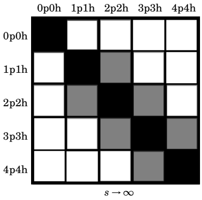
other decoupling patterns possible
(e.g. valence-space decoupling)

- impro… …ciencies: White and imaginary-time generator





In-Medium SRG: Key Ingredients

- determine reference state $|\Phi\rangle$ of A-body system (HF,NCSM,HFB,...)

- use normal-ordered form of operators throughout the evolution

$$\hat{H}(s) = E(s) + \sum_{pq} f^p_q(s) \, \{\hat{p}^\dagger \hat{q}\}_{|\Phi\rangle} + \frac{1}{4} \sum_{pqrs} \Gamma^{pq}_{rs}(s) \{\hat{p}^\dagger \hat{q}^\dagger \hat{s} \hat{r}\}_{|\Phi\rangle} + \dots$$

$$\hat{\eta}(s) = \sum_{pq} \eta^p_q(s) \, \{\hat{p}^\dagger \hat{q}\}_{|\Phi\rangle} + \frac{1}{4} \sum_{pqrs} \eta^{pq}_{rs}(s) \{\hat{p}^\dagger \hat{q}^\dagger \hat{s} \hat{r}\}_{|\Phi\rangle} + \dots$$

$\rightsquigarrow$ reference state $|\Phi\rangle$ of A-body system defines form of operators

- IMSRG(2): truncate operators at normal-ordered two-body level

- derive flow equations for $E(s)$, $f^p_q(s)$ and $\Gamma^{pq}_{rs}(s)$ from

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

note difference to free-space SRG!

- choose and construct appropriate generator

- solve ODE system

Reference states

- type of reference state determines IM-SRG "flavor"
- Single-Reference IM-SRG (SR-IM-SRG):
  - reference state is single Slater determinant from, e.g., Hartree-Fock calculation

    $$|\Phi\rangle = |i_1 \ldots i_A\rangle$$

  - applicable to closed-shell nuclei
- Multi-Reference IM-SRG (MR-IM-SRG):
  - reference state from previous NCSM or Hartree-Fock-Bogoliubov calculation

    $$|\Phi\rangle = \sum_k |\phi_k\rangle$$

  - applicable to open-shell nuclei
  - emergence of additional terms involving irreducible density matrices $\lambda^{(2)}, \lambda^{(3)}, \ldots$

Commutator Evaluation

- evaluation of $\frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s), \hat{H}(s)\right]$ via (generalized) Wick's theorem

$$\{\hat{A}_1 \ldots\}\{\hat{B}_1 \ldots\} = \sum_{\text{ext. contr.}} \{\hat{A}_1 \ldots \hat{B}_1 \ldots\}$$

- single-particle transformed into natural-orbital basis (eigenbasis of $\gamma^{(1)}$, $\gamma^p_q \to n_p \delta_{pq}$)

- result: coupled system of first-order ordinary differential equations

$$\frac{\mathrm{d}}{\mathrm{d}s}E(s) = \sum_{pq} (n_p - n_q)\ \eta^p_q(s)\ f^q_p(s) + \frac{1}{4}\sum_{pqrs}\left(\eta^{pq}_{rs}(s)\ \Gamma^{rs}_{pq}(s)\ n_p n_q \bar{n}_r \bar{n}_s - [\eta \leftrightarrow \Gamma]\right) + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}f^1_2(s) = \sum_p \left(\eta^1_p\ f^p_2\ - [\eta \leftrightarrow f]\right) + \ldots + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Gamma^{12}_{34}(s) = \sum_p \left(\left(\eta^1_p\ \Gamma^{p2}_{34} - f^1_p\ \eta^{p2}_{34}\right) - [1 \leftrightarrow 2]\right) + \ldots$$

- neglection of $\lambda^{(3)}$, only scalar part of $\lambda^{(2)}$ considered ($\rightsquigarrow$ restriction to even nuclei)

- express in terms of reduced matrix elements ($\leftrightsquigarrow$ rank of spherical tensor operators)

- implemented in C, using BLAS, exploitation of physical symmetries (parity,...)

Commutator Evaluation

- evaluation of $\frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s), \hat{H}(s)\right]$ via (generalized) Wick's theorem

$$\{\hat{A}_1\ldots\}\,\{\hat{B}_1\ldots\} = \sum_{\text{ext. contr.}} \{\hat{A}_1\ldots\hat{B}_1\ldots\}$$

- single-particle transformed into natural-orbital basis (eigenbasis of $\gamma^{(1)}$, $\gamma^p_q \rightarrow n_p \delta_{pq}$)

- result: coupled system of first-order ordinary differential equations

$$\frac{\mathrm{d}}{\mathrm{d}s}E(s) = \sum_{pq}\left(n_p - n_q\right)\,\eta^p_q(s)\,f^q_p(s) + \frac{1}{4}\sum_{pqrs}\left(\eta^{pq}_{rs}(s)\,\Gamma^{rs}_{pq}(s)\,n_p n_q \bar{n}_r \bar{n}_s - [\eta \leftrightarrow \Gamma]\right) + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}f^1_2(s) = \sum_p \left(\eta^1_p\, f^p_2 - [\eta \leftrightarrow f]\right) + \ldots + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Gamma^{12}_{34}(s) = \sum_p \left(\left(\eta^1_p\,\Gamma^{p2}_{34} - f^1_p\,\eta^{p2}_{34}\right) - [1 \leftrightarrow 2]\right) + \ldots$$

- neglection of $\lambda^{(3)}$, only scalar part of $\lambda^{(2)}$ considered (⇝ restriction to even nuclei)

- express in terms of reduc… …sor operators)

- imple…

nonlinear algebraic equations for cluster amplitudes (CC)
↕
coupled differential equations for matrix elements (IM-SRG)

ODE Solving

- formally $\frac{\mathrm{d}}{\mathrm{d}s}\vec{x}(s) = \vec{f}(\vec{x}(s))$, with $\vec{x}(s) = (E(s), f_0^0(s), f_1^0(s), \ldots, \Gamma_{00}^{00}(s), \Gamma_{01}^{00}(s), \ldots)$

- flow equations are coupled system of first-order ordinary differential equations

- typically: ~ 60 million coupled differential equations

- numerical integration of ODE system until $\hat{H}^{\mathrm{od}}$ is “sufficiently” suppressed

- ODE solver from gsl with RKF45 algorithm is employed

Magnus Expansion

- IM-SRG unitarily transforms Hamiltonian

$$\hat{H}(s) \equiv \hat{U}^{\dagger}(s)\hat{H}(0)\hat{U}(s) \quad \leftrightsquigarrow \quad \frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s), \hat{H}(s)\right]$$

- unitary transformations can be written as

$$\hat{U}(s) = \exp(\hat{\Omega}(s))$$

- derive differential equation for $\hat{\Omega}(s)$ associated with unitary transformation $\hat{U}(s)$

$$\frac{\mathrm{d}}{\mathrm{d}s}\hat{\Omega}(s) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \left[\hat{\Omega}(s), \hat{\eta}(s)\right]_k \qquad = \sum_{k=0}^{\infty} \frac{B_k}{k!} \underbrace{\left[\hat{\Omega}(s), \left[\hat{\Omega}(s), \left[\ \dots \left[\hat{\Omega}(s), \left[\hat{\Omega}(s)\right.\right.\right.\right.\right.}_{\text{k-times}}, \hat{\eta}(s)\left.\left.\left.\left.\left.\right]\right]\right]\right]\right]$$

- solve flow equations for matrix elements of anti-hermitian $\hat{\Omega}(s)$
- Magnus(2): truncate all operators involved at two-body level
- apply unitary transformation via Baker-Campbell-Hausdorff series

$$\hat{O}(s) = \exp(-\hat{\Omega}(s))\hat{O}(0)\exp(\hat{\Omega}(s)) = \sum_{k=0}^{\infty} \frac{1}{k!} \left[\hat{\Omega}(s), \hat{O}(0)\right]_k$$

Magnus Expansion

- IM-SRG unitarily transforms Hamiltonian

$$\hat{H}(s) \equiv \hat{U}^\dagger(s)\hat{H}(0)\hat{U}(s) \quad \leftrightsquigarrow \quad \frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s), \hat{H}(s)\right]$$

- unitary transformations can be written as

$$\hat{U}(s) = \exp(\hat{\Omega}(s))$$

- derive differential equation for $\hat{\Omega}(s)$ associated with unitary transformation $\hat{U}(s)$

$$\frac{\mathrm{d}}{\mathrm{d}s}\hat{\Omega}(s) = \sum_{k=0}^{\infty} \frac{B_k}{k!}\left[\hat{\Omega}(s), \hat{\eta}(s)\right]_k \qquad = \sum_{k=0}^{\infty} \frac{B_k}{k!} \underbrace{\left[\hat{\Omega}(s), \left[\hat{\Omega}(s), \left[\, \ldots \left[\hat{\Omega}(s), \left[\hat{\Omega}(s),\right.\right.\right.\right.\right.}_{\text{k-times}} \hat{\eta}(s)\left.\left.\left.\left.\left.\right]\right]\right]\right]\right]$$

- solve flow equations for ma

- Magnus(2): truncate all

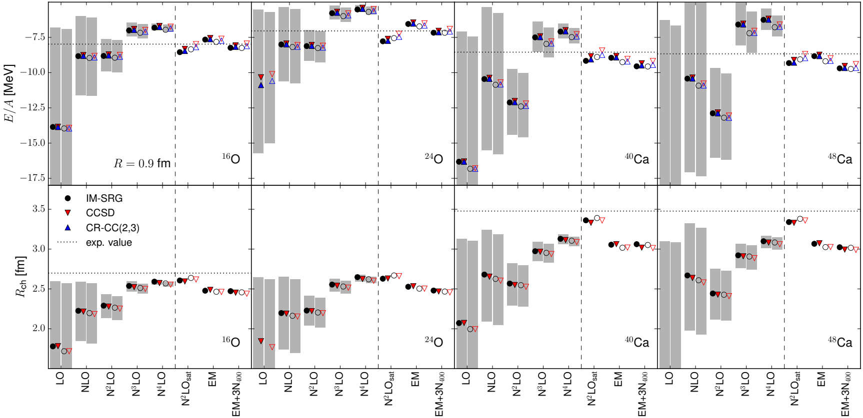
- apply unitary transformation via Baker-Campbell-Hausdorff series

foundation of IM-SRG:
(efficient) commutator evaluation machinery
$$\hat{C}^L_M(s) = \left[\hat{A}^0_0(s), \hat{B}^L_M(s)\right]$$

$$\hat{O}(s) = \exp(-\hat{\Omega}(s))\hat{O}(0)\exp(\hat{\Omega}(s)) = \sum_{k=0}^{\infty} \frac{1}{k!}\left[\hat{\Omega}(s), \hat{O}(0)\right]_k$$

Benchmarks: LENPIC-NN vs. Others

paper in preparation



theoretical error bars in gray

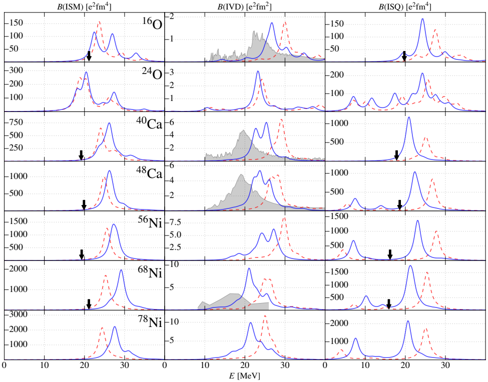
$\alpha = 0.04$ fm^4 (open)

$\alpha = 0.08$ fm^4 (solid)

- characteristic pattern from LO to N^{4}LO
- compared to NN of E. & M.
  - more attractive 3N forces necesssary (N^{3}LO,N^{4}LO)
  - radii improved, still underestimated

IM-SRG & SRPA: Transition Strengths

R. Trippel, doctoral thesis



N^2LO_{sat} (blue line)

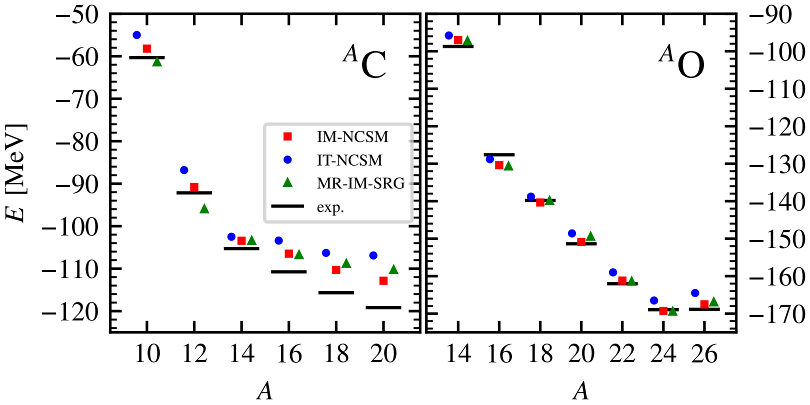
NN_{EM}+$3N_{400}$ (dashed red line)

exp. centroid (arrow) or spectra (gray)

- SRPA: 2p2h EoM approach
  ⇝ description of collective motions
- IM-SRG-evolved Hamiltonian as input
  ⇝ improved physical content of reference state
- transition strengths of high experimental interest
- good qualitiative agreement between experiment and theory
  ⇝ improved via IM-SRG

IM-NCSM: Ground States Carbon & Oxygen Chain

E. Gebrerufael et al, Phys. Rev. Lett. 118, 152503 (2017)



- very good agreement between methods for oxygen (deviations $\sim 2\%$)
- larger method uncertainties for carbon isotopes, especially ^{12}C