

Precision nuclear structure in the in-medium similarity renormalization group

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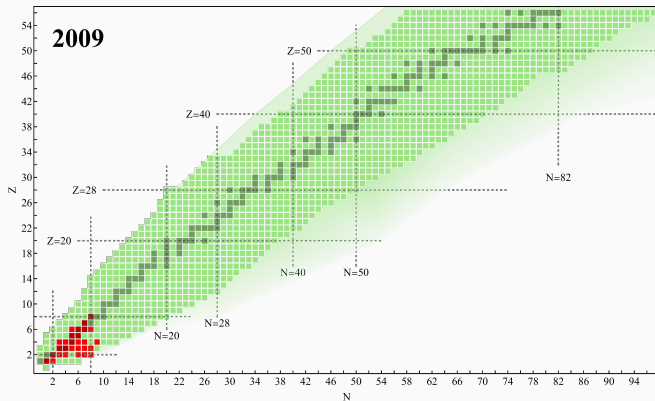
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Ab initio nuclear structure

- Nuclei as made up of A interacting nucleons
- Input (chiral) NN and 3N interactions
into (in limit) exact many-body method
- Advantages:
 - General approach with large range of applicability
 - Systematically improvable
 - Rigorous estimation of uncertainties is possible

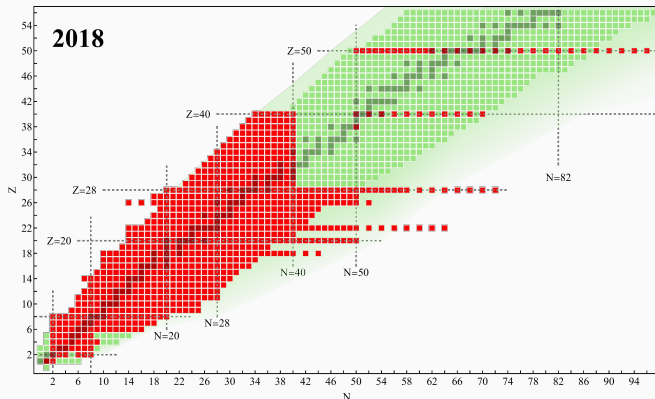
Ab initio explosion



Hebeler 2020, figure by Hergert

- Low resolution interactions for low-energy physics
- Developments in many-body methods

Ab initio explosion



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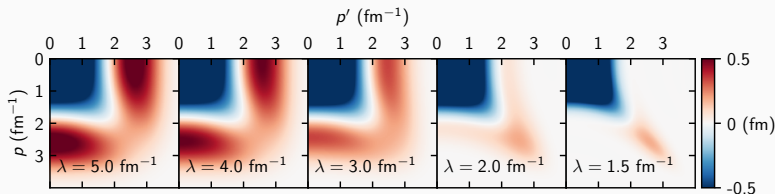
- Low resolution interactions for low-energy physics
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Current state of ab initio theory

- Exact diagonalization (NCSM)
 - Factorial scaling
 - Only modelspace truncation
- Many-body expansion methods
 - MBPT, CC, IM-SRG, SCGF
 - Single-particle basis truncation
and truncation in many-body method
 - Going to higher orders in many-body method
is a substantial amount of work
 - IM-SRG current status: IM-SRG(2)

Target: **IM-SRG(3)**

Similarity renormalization group



Continuous unitary transformation:

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

Flow equation:

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

SRG evolution induces many-body forces over the course of the flow

Normal ordering

Reference state to approximate A -body state:

$$|\Phi\rangle = \prod_i^A a_{p_i}^\dagger |0\rangle$$

Normal ordering w.r.t. $|\Phi\rangle$ pulls out $\langle\Phi|H|\Phi\rangle = \bar{H}^{(0)} = E$ such that

$$\langle\Phi|\bar{H}^{(1)}|\Phi\rangle = 0$$

$$\langle\Phi|\bar{H}^{(2)}|\Phi\rangle = 0$$

$$\langle\Phi|\bar{H}^{(3)}|\Phi\rangle = 0$$

$H^{(3)}$ gives normal-ordered zero- through three-body operators:

$$\bar{H}_{pqrs}^{(2)} = H_{pqrs}^{(2)} + \sum_{ij} \rho_{ij} H_{pqirsj}^{(3)} \quad \bar{H}_{pqrst}^{(3)} = H_{pqrst}^{(3)}$$

Wick's theorem to normal order operators

and simplify products of normal-ordered operators

Normal order Hamiltonian w.r.t. A -body reference state $|\Phi\rangle$:

$$H = H^{(1)} + H^{(2)} + H^{(3)} = \bar{H}^{(0)} + \bar{H}^{(1)} + \bar{H}^{(2)} + \bar{H}^{(3)}$$

Integrate flow equation

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

with initial condition $H(0) = H$ to $s \rightarrow \infty$

- Up to A -body normal-ordered operators induced by flow
- Approximate evolution of free-space many-body operators through normal ordering

IM-SRG(2)/(3)

IM-SRG(2):

$$H(s) \approx \bar{H}^{(0)}(s) + \bar{H}^{(1)}(s) + \bar{H}^{(2)}(s)$$

$$\eta(s) \approx \cancel{\eta^{(0)}(s)} + \eta^{(1)}(s) + \eta^{(2)}(s)$$

Fundamental commutators:

$$[A^{(1)}, B^{(1)}], [A^{(1)}, B^{(2)}], [A^{(2)}, B^{(2)}],$$

$$[A^{(M)}, B^{(N)}] = \sum_{K=|M-N|}^{M+N-1} C^{(K)}$$

IM-SRG(2)/(3)

IM-SRG(3):

$$H(s) \approx \bar{H}^{(0)}(s) + \bar{H}^{(1)}(s) + \bar{H}^{(2)}(s) + \bar{H}^{(3)}(s)$$

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$$[A^{(1)}, B^{(1)}], [A^{(1)}, B^{(2)}], [A^{(2)}, B^{(2)}], \\ [A^{(1)}, B^{(3)}], [A^{(2)}, B^{(3)}], [A^{(3)}, B^{(3)}]$$

$$[A^{(M)}, B^{(N)}] = \sum_{K=|M-N|}^{M+N-1} C^{(K)}$$

Example: $[2,2] \rightarrow 2/3$

$$[A^{(2)}, B^{(2)}] = \sum_{K=0}^3 C^{(K)}$$

$$C_{ijkl}^{(2)} = \sum_{ab} \left\{ \frac{1}{2} (A_{ijab} B_{abkl} - B_{ijab} A_{abkl}) (1 - n_a - n_b) \right. \\ \left. + (n_a - n_b) (1 - P_{ij}) (1 - P_{kl}) A_{aibk} B_{bjal} \right\}$$

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$$C_{ijklmn}^{(3)} = \sum_a P(ij/k) P(l/mn) (A_{ijla} B_{akmn} - B_{ijla} A_{akmn})$$

Example: $[2,2] \rightarrow 2/3$

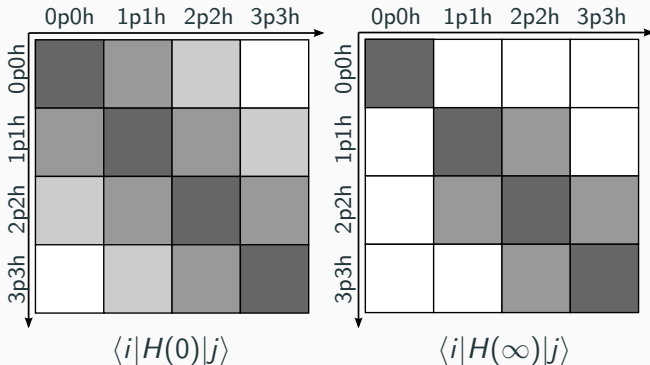
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$$C_{ijklmn}^{(3)} = \sum_a P(ij/k) P(l/mn) (A_{ijla} B_{akmn} - B_{ijla} A_{akmn})$$

$$[A^{(3)}, B^{(3)}]_{ijklmn}^{(3)} \sim \sum_{abc} (\dots) A_{ijkabc} B_{abclmn}$$

IM-SRG: additional considerations



Hergert, 2015

- η chosen so that $|\Phi\rangle$ is decoupled from nph excitations
- MBPT corrections involve $\langle \Phi|H|\Phi_{i,\dots}^a\rangle$ and thus vanish

m-scheme vs. *J*-scheme

For nuclear applications, choose HO-like single-particle basis:

$$|n_a(l_a s_a) j_a m_{j_a} t_a m_{t_a}\rangle \equiv |\alpha_a\rangle \equiv |\alpha_{\tilde{a}} m_{j_{\tilde{a}}}\rangle$$

m-scheme - build antisymmetrized set of 2-body/3-body states:

$$\begin{aligned} |\alpha_a \alpha_b\rangle &\rightarrow O_{pqrs}^{(2)} \\ |\alpha_a \alpha_b \alpha_c\rangle &\rightarrow O_{pqrstu}^{(3)} \end{aligned}$$

J-scheme - couple states to total J/\mathcal{J} :

$$\begin{aligned} |(\alpha_{\tilde{a}} \alpha_{\tilde{b}}) J M_J\rangle &\rightarrow O_{\tilde{p}\tilde{q}\tilde{r}\tilde{s}}^{(2),J} \\ |[(\alpha_{\tilde{a}} \alpha_{\tilde{b}}) J \alpha_{\tilde{c}}] \mathcal{J} M_{\mathcal{J}}\rangle &\rightarrow O_{\tilde{p}\tilde{q}\tilde{r}\tilde{s}\tilde{t}\tilde{u}}^{(3),J_1,J_2,\mathcal{J}} \end{aligned}$$

J-scheme matrix elements independent of $M_J/M_{\mathcal{J}}$

Outline of project

- Reimplement IM-SRG(2) and extend implementation to IM-SRG(3) in m -scheme
- Validate m -scheme implementation
- Implement IM-SRG(3) in J -scheme
- Validate J -scheme implementation against m -scheme implementation
- Study IM-SRG(3) contributions to ground-state properties of medium-mass nuclei

IM-SRG(2): ^4He

Start from intrinsic Hamiltonian with only NN force:

$$H = T_{\text{int}} + V^{(2)}$$

Work with HO single-particle basis,

and truncate at $e_{\text{max}} = 2 \geq 2n + l$ ($N = 40$, large-scale $N = 1820$)

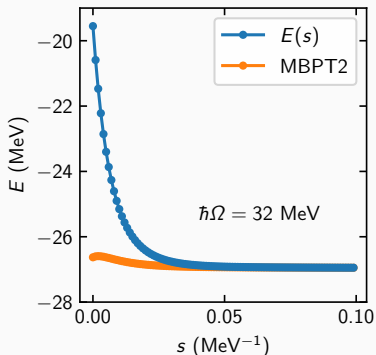
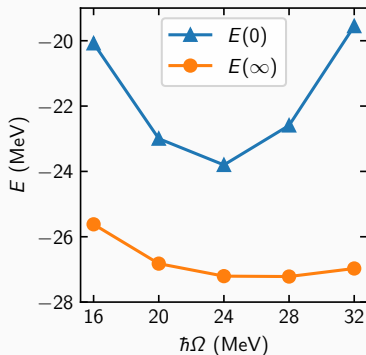
Benchmark: Ragnar Stroberg's IM-SRG(2) implementation

What about IM-SRG(3)?

- $\mathcal{O}(N^6)$ storage resources ~ 10 GB ($40^6 \times 8$ bytes)
- $\mathcal{O}(N^9)$ compute resources ~ 100 TFLOPs (40^9 operations)

Comparison: CCSD-T1 has $\mathcal{O}(N^7)$ computational cost

IM-SRG(2): ${}^4\text{He}$ results



- Second- and third-order MBPT corrections absorbed into E
- Agreement with Stroberg up to 10^{-5} MeV

IM-SRG(3): pairing Hamiltonian

Hamiltonian with 2-fold degenerate levels
with (attractive) pairing interaction:

$$H = \delta \sum_{p\sigma} (p - 1) a_{p\sigma}^\dagger a_{p\sigma} - \frac{g}{2} \sum_{pq} a_{p+}^\dagger a_{p-}^\dagger a_{q-} a_{q+}$$

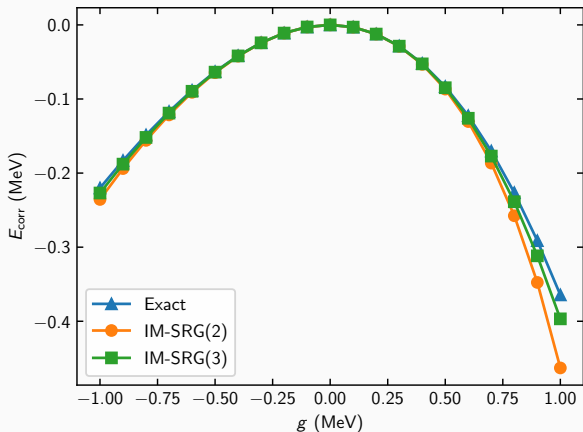
Fix $\delta = 1$ MeV, consider 4 particles in 4 levels

Choose reference state with 2 lowest levels filled:

- Reference state is the Hartree-Fock Slater determinant
- Has Hartree-Fock energy $E_{\text{HF}} = 2 - g$ (for $A = 4$)
- IM-SRG needs to bring in correlation effects

$$E_{\text{corr}} = E_{\text{exact}} - E_{\text{HF}} = E(\infty) - E(0)$$

IM-SRG(3): pairing Hamiltonian results



- See systematic improvement in correlation energy
- IM-SRG(3) helps with expansion convergence for large g

Outlook

Accomplished so far:

- Implemented general (m -scheme) IM-SRG(2)/(3)
- Validated implementation against previous calculation and exactly solvable pairing Hamiltonian

Next steps:

- Implement J -scheme IM-SRG(3) commutators
- Validate implementation against m -scheme commutators
- Optimize performance to extend basis truncation
- Study medium-mass closed-shell nuclei (^{40}Ca)

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Thank you for your attention