Precision nuclear structure in the in-medium similarity renormalization group

Matthias Heinz

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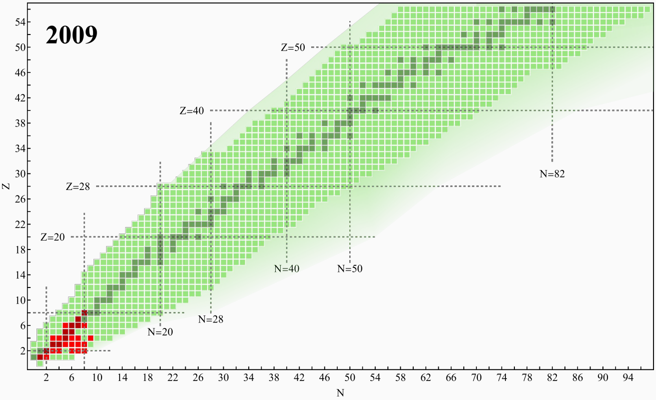
Institut für Kernphysik, TU Darmstadt

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

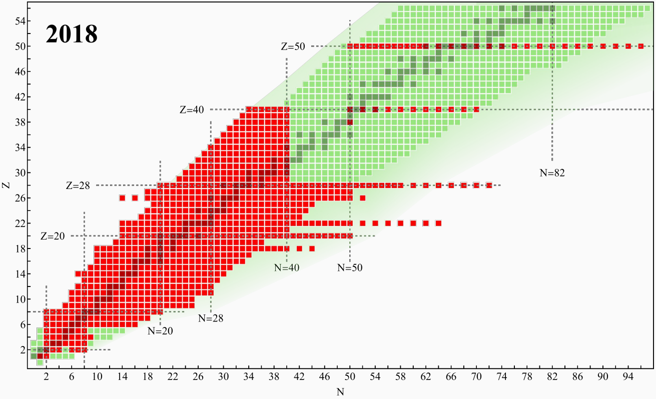
Ab initio explosion



Hebeler 2020, figure by Hergert

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

Ab initio explosion



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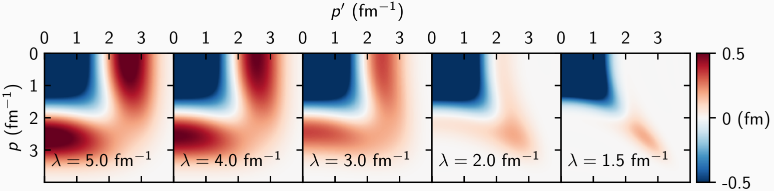
- Low resolution interactions for low-energy physics
- Developments in many-body methods

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:

$$H(s) = U(s)HU^{\dagger}(s)$$

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:

$$|\Phi\rangle = \prod_i^A a^\dagger_{p_i} |0\rangle$$

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:

$$\bar{H}^{(2)}_{pqrs} = H^{(2)}_{pqrs} + \sum_{ij} \rho_{ij} H^{(3)}_{pqirsj} \qquad \bar{H}^{(3)}_{pqrstu} = H^{(3)}_{pqrstu}$$

Wick's theorem to normal order operators

and simplify products of normal-ordered operators

In-medium similarity renormalization group Tsukiyama, Bogner, Schwenk 2012

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 $s \to \infty$

- 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):

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

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

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

$$C^{(2)}_{ijkl} = \sum_{ab} \Big\{ \frac{1}{2}(A_{ijab}B_{abkl} - B_{ijab}A_{abkl})(1 - n_a - n_b) + (n_a - n_b)(1 - P_{ij})(1 - P_{kl})A_{aibk}B_{bjal} \Big\}$$

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$$C^{(3)}_{ijklmn} = \sum_{a} P(ij/k)P(l/mn)(A_{ijla}B_{akmn} - B_{ijla}A_{akmn})$$

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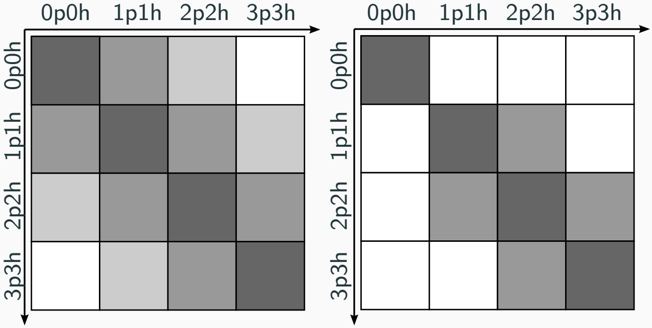
$$[A^{(3)}, B^{(3)}]^{(3)}_{ijklmn} \sim \sum_{abc} (\ldots) A_{ijkabc}B_{abclmn}$$

IM-SRG: additional considerations



$\langle i|H(0)|j\rangle$ $\langle i|H(\infty)|j\rangle$

Hergert, 2015

- η chosen so that $|\Phi\rangle$ is decoupled from *npnh* excitations
- MBPT corrections involve $\langle\Phi|H|\Phi^{a\cdots}_{i\cdots}\rangle$ 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:

$$|\alpha_a \alpha_b\rangle \to O^{(2)}_{pqrs}$$
$$|\alpha_a \alpha_b \alpha_c\rangle \to O^{(3)}_{pqrstu}$$

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

$$|(\alpha_{\tilde{a}} \alpha_{\tilde{b}}) J M_J\rangle \to O^{(2),J}_{\tilde{p}\tilde{q}\tilde{r}\tilde{s}}$$
$$|[(\alpha_{\tilde{a}} \alpha_{\tilde{b}}) J \alpha_{\tilde{c}}] \mathcal{J} M_{\mathcal{J}}\rangle \to O^{(3),J_1,J_2,\mathcal{J}}_{\tilde{p}\tilde{q}\tilde{r}\tilde{s}\tilde{t}\tilde{u}}$$

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): ^{4}He

Start from intrinsic Hamiltonian with only NN force:

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

Work with HO single-particle basis,
and truncate at $e_{\max} = 2 \geq 2n + l$ (N = 40, large-scale N = 1820)

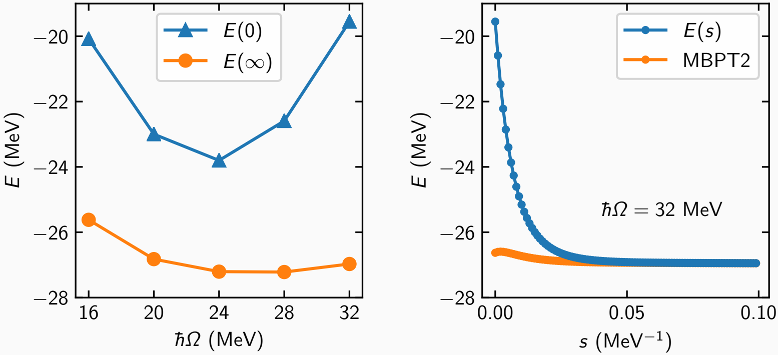
Benchmark: Ragnar Stroberg's IM-SRG(2) implementation

What about IM-SRG(3)?

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

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

IM-SRG(2): ^{4}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:

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

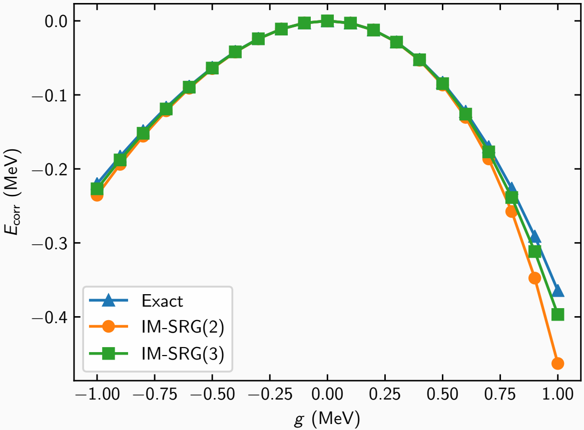
Fix $\delta = 1\,\mathrm{MeV}$, consider 4 particles in 4 levels

Choose reference state with 2 lowest levels filled:

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

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

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