

Exploring Many-Body Force Induction in the Similarity Renormalization Group in 1 Dimension

Matthias Heinz

The Ohio State University

Apr 11, 2018

Thesis Committee: Prof. Richard Furstahl, Prof. Robert Perry, Prof. P Sadayappan

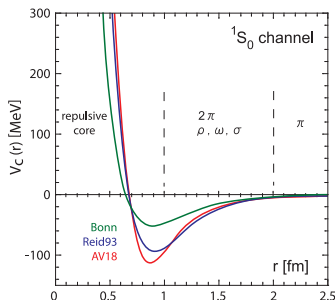
Goals of Low-Energy Nuclear Theory

- Model atomic nuclei and calculate observables like ground state and excited state energies, nuclear radii, half-lives for different decays
- Model nuclear matter to better understand the structure of astrophysical systems like neutron stars
- Use accurate models of nuclear systems to aid in the search for beyond Standard Model physics
- Leverage improved understanding of nuclear physics in a variety of applications

Challenge: The Interaction

The first challenge of low-energy nuclear theory is due to the nature of inter-nucleon forces, which are given by the strong interaction:

- Underlying theory, quantum chromodynamics, cannot be solved in closed form at low energies
- Modern 2-body and 3-body potentials are determined from scattering experiments and few-body nuclei
- Hard repulsive core couples low and high-energy parts of Hamiltonian

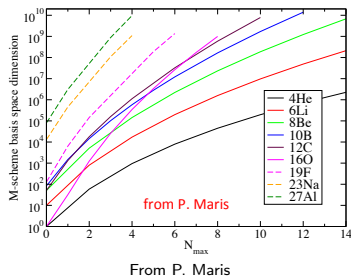


From R.J. Furnstahl, Nucl. Phys. Proc. Suppl. 228 (2012)

Challenge: The Problem Size

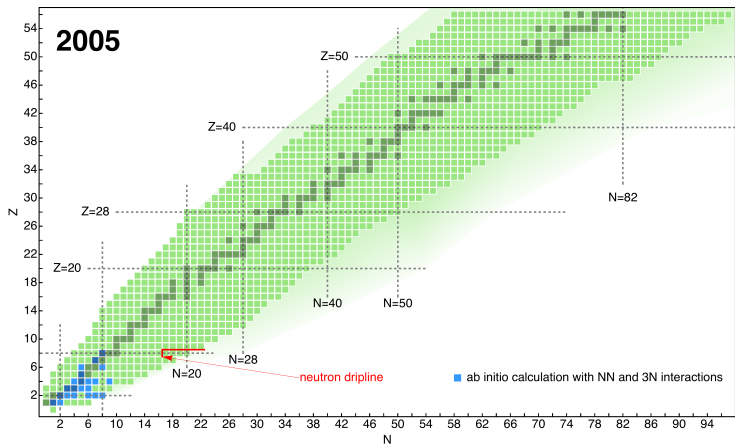
The second challenge of low-energy nuclear theory is that naive approaches quickly become intractable because of the rapid growth of the problem size:

- Basis size grows combinatorially with respect to A , the number of particles
- Sets limit on what nuclei can be modeled, even when taking advantage of the most modern parallel computing clusters
- Strong off-diagonal couplings prevent significant basis truncation



Recent Ab-Initio Explosion

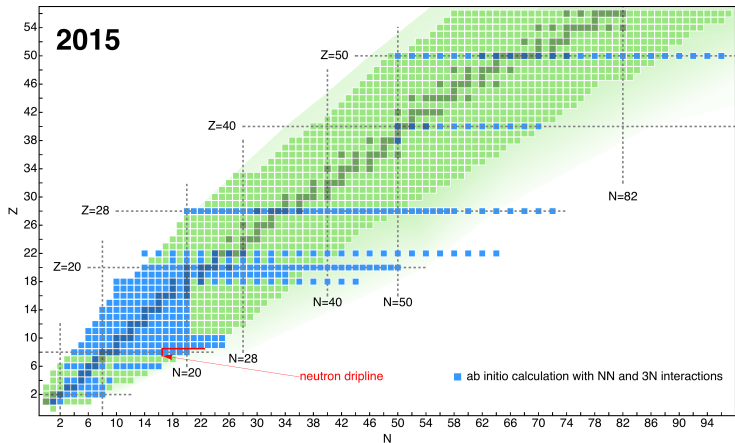
Range of nuclei able to be modeled via ab-initio methods (starting from inter-nucleon forces) has rapidly expanded due to effective field theory (EFT) and renormalization group (RG) methods:



Images courtesy of Heiko Hergert

Recent Ab-Initio Explosion

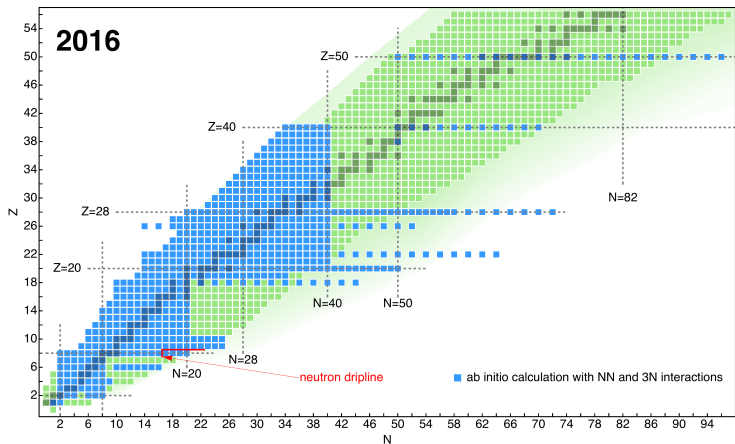
Range of nuclei able to be modeled via ab-initio methods (starting from inter-nucleon forces) has rapidly expanded due to effective field theory (EFT) and renormalization group (RG) methods:



Images courtesy of Heiko Hergert

Recent Ab-Initio Explosion

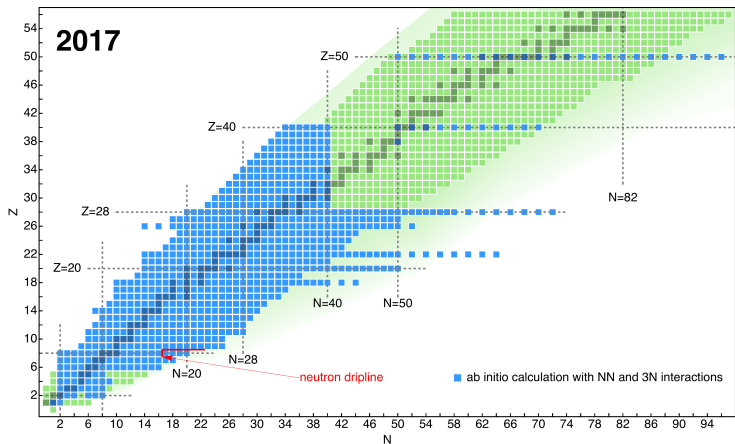
Range of nuclei able to be modeled via ab-initio methods (starting from inter-nucleon forces) has rapidly expanded due to effective field theory (EFT) and renormalization group (RG) methods:



Images courtesy of Heiko Hergert

Recent Ab-Initio Explosion

Range of nuclei able to be modeled via ab-initio methods (starting from inter-nucleon forces) has rapidly expanded due to effective field theory (EFT) and renormalization group (RG) methods:



Images courtesy of Heiko Hergert

The Similarity Renormalization Group

The similarity renormalization group (SRG) is an RG method which performs a continuous unitary transformation on an operator in order to:

- Get rid of coupling between low and high energies
- Preserve low-energy observables (operator eigenvalues)

The Similarity Renormalization Group

The similarity renormalization group (SRG) is an RG method which performs a continuous unitary transformation on an operator in order to:

- Get rid of coupling between low and high energies
- Preserve low-energy observables (operator eigenvalues)

This transformation is given by:

$$\frac{d\hat{H}_s}{ds} = [\hat{\eta}_s, \hat{H}_s] = [[\hat{G}_s, \hat{H}_s], \hat{H}_s] \quad (1)$$

where:

The Similarity Renormalization Group

The similarity renormalization group (SRG) is an RG method which performs a continuous unitary transformation on an operator in order to:

- Get rid of coupling between low and high energies
- Preserve low-energy observables (operator eigenvalues)

This transformation is given by:

$$\frac{d\hat{H}_s}{ds} = [\hat{\eta}_s, \hat{H}_s] = [[\hat{G}_s, \hat{H}_s], \hat{H}_s] \quad (1)$$

where:

- $\hat{\eta}_s$ is the generator of the transformation

The Similarity Renormalization Group

The similarity renormalization group (SRG) is an RG method which performs a continuous unitary transformation on an operator in order to:

- Get rid of coupling between low and high energies
- Preserve low-energy observables (operator eigenvalues)

This transformation is given by:

$$\frac{d\hat{H}_s}{ds} = [\hat{\eta}_s, \hat{H}_s] = [[\hat{G}_s, \hat{H}_s], \hat{H}_s] \quad (1)$$

where:

- $\hat{\eta}_s$ is the generator of the transformation
- \hat{G}_s is the flow operator, given by the user, which dictates the form to which the operator evolves

The Similarity Renormalization Group

The similarity renormalization group (SRG) is an RG method which performs a continuous unitary transformation on an operator in order to:

- Get rid of coupling between low and high energies
- Preserve low-energy observables (operator eigenvalues)

This transformation is given by:

$$\frac{d\hat{H}_s}{ds} = [\hat{\eta}_s, \hat{H}_s] = [[\hat{G}_s, \hat{H}_s], \hat{H}_s] \quad (1)$$

where:

- $\hat{\eta}_s$ is the generator of the transformation
- \hat{G}_s is the flow operator, given by the user, which dictates the form to which the operator evolves
- s is the flow parameter, which goes from $s = 0$ towards $s = \infty$ over the course of an SRG evolution

Benefits of SRG

A typical example of an application of the SRG to a calculation looks like:

- 1 Start with 2-body or 3-body operator in a large basis
- 2 Apply SRG to drive operator towards the diagonal
- 3 Truncate basis, keeping low-energy sector and discarding high-energy sector
- 4 Embed 2-body or 3-body operator in A -body
- 5 Compute desired A -body observable

Benefits of SRG

A typical example of an application of the SRG to a calculation looks like:

- 1 Start with 2-body or 3-body operator in a large basis
- 2 Apply SRG to drive operator towards the diagonal
- 3 Truncate basis, keeping low-energy sector and discarding high-energy sector
- 4 Embed 2-body or 3-body operator in A -body
- 5 Compute desired A -body observable

Problem Size Reduction

Truncating the basis in the 2-body or 3-body space greatly reduces the size of the resulting A -body space, thus making calculations of A -body observables feasible.

Limits of SRG

While the SRG evolution of an A -body operator is unitary when done in the A -body space, it induces many-body forces that are seen when embedding the A -body operator in the basis for a larger system. These many-body forces:

- Change the eigenvalues of the operator
- Are in general not possible to fully account for
- Show up as an error in the computed observables
- Scale with the size of the full system, limiting the application of SRG to small and medium systems

Limits of SRG

While the SRG evolution of an A -body operator is unitary when done in the A -body space, it induces many-body forces that are seen when embedding the A -body operator in the basis for a larger system. These many-body forces:

- Change the eigenvalues of the operator
- Are in general not possible to fully account for
- Show up as an error in the computed observables
- Scale with the size of the full system, limiting the application of SRG to small and medium systems

Alternative Flow Operators

Currently, the kinetic energy, \hat{T} , is used as the flow operator, \hat{G}_s , for nearly all SRG calculations. Alternative choices for \hat{G}_s many induce fewer many-body forces, extending the range of SRG to heavier isotopes.

1-Dimensional Setting

SRG was originally explored in the context of low-energy nuclear physics in a 1-dimensional system:

- System of A bosons
- Factor out center-of-mass behavior and focus on behavior relative to center-of-mass
- 2-body local potential, $V(p, p')$, given in terms of relative Jacobi momenta
- Transform to discrete harmonic oscillator basis to embed 2-body potential in A -body system

Harmonic Oscillator Basis

Harmonic oscillator (HO) states are the eigenstates to the “particle in a 1-dimensional harmonic oscillator potential” problem:

$$\hat{H}_{HO} |n\rangle = E_n |n\rangle \quad (2)$$

Harmonic Oscillator Basis

Harmonic oscillator (HO) states are the eigenstates to the “particle in a 1-dimensional harmonic oscillator potential” problem:

$$\hat{H}_{HO} |n\rangle = E_n |n\rangle \quad (2)$$

For a system of A particles, the general state is a product state of single-particle eigenstates:

$$|n_1, n_2, \dots, n_A\rangle = \prod_{i=1}^A |n_i\rangle \quad (3)$$

Harmonic Oscillator Basis

Harmonic oscillator (HO) states are the eigenstates to the “particle in a 1-dimensional harmonic oscillator potential” problem:

$$\hat{H}_{HO} |n\rangle = E_n |n\rangle \quad (2)$$

For a system of A particles, the general state is a product state of single-particle eigenstates:

$$|n_1, n_2, \dots, n_A\rangle = \prod_{i=1}^A |n_i\rangle \quad (3)$$

When working with relative Jacobi coordinates:

- Define harmonic oscillator states to be with respect to Jacobi momenta
- Require $A - 1$ Jacobi coordinates and thus product states of $A - 1$ HO states

Symmetrizing the HO Basis

Spin-statistics theorem

The state of any system of identical bosons must be symmetric under any permutation of the particles.

Symmetrizing the HO Basis

Spin-statistics theorem

The state of any system of identical bosons must be symmetric under any permutation of the particles.

We can create an A -body basis of HO product states that reflect this condition by:

- Diagonalizing the 2-body symmetrizer, $S = (1 + P_{12})/2$, and selecting the eigenstates with eigenvalue 1 to get our 2-body basis
- Generating a set of A -body product states from the symmetrized $(A - 1)$ -body basis
- Getting the A -body states by diagonalizing the A -body symmetrizer

Symmetrizing the HO Basis

Spin-statistics theorem

The state of any system of identical bosons must be symmetric under any permutation of the particles.

We can create an A -body basis of HO product states that reflect this condition by:

- Diagonalizing the 2-body symmetrizer, $S = (1 + P_{12})/2$, and selecting the eigenstates with eigenvalue 1 to get our 2-body basis
- Generating a set of A -body product states from the symmetrized $(A - 1)$ -body basis
- Getting the A -body states by diagonalizing the A -body symmetrizer

In this work, we do this to get symmetrized 2-body and 3-body bases.

The Negele Potential

Negele Potential

$$\hat{V}(p, p') = \frac{V_1}{2\pi\sqrt{2}} e^{-(p-p')^2\sigma_1^2/8} + \frac{V_2}{2\pi\sqrt{2}} e^{-(p-p')^2\sigma_2^2/8} \quad (4)$$

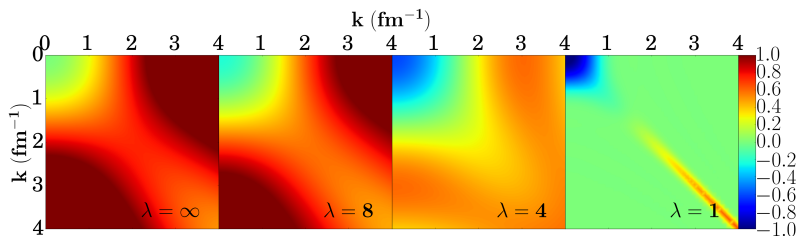
We use two parametrizations of the Negele potential:

- \hat{V}_α is nuclear-like, with a mid-range attractive part and a short-range repulsive part
- \hat{V}_β is purely attractive

2-Body Momentum Space SRG

With both \hat{T} as the flow operator and an alternative block diagonal flow operator, we see SRG achieve the desired decoupling of low and high momenta:

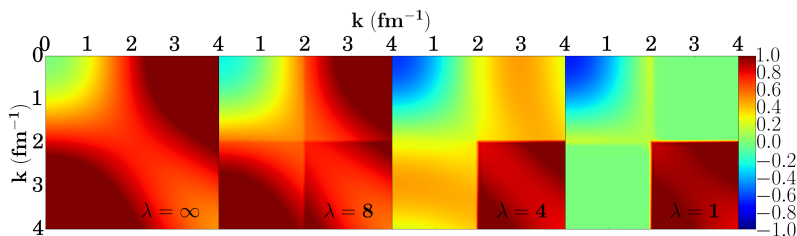
With $\hat{G}_s = \hat{T}$:



2-Body Momentum Space SRG

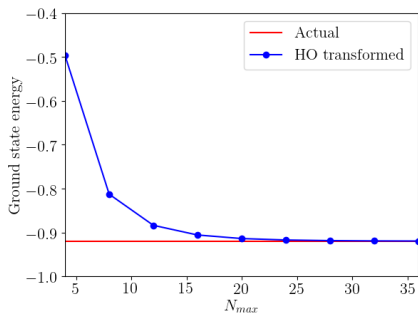
With both \hat{T} as the flow operator and an alternative block diagonal flow operator, we see SRG achieve the desired decoupling of low and high momenta:

With $\hat{G}_s = \hat{H}_{BD}$:

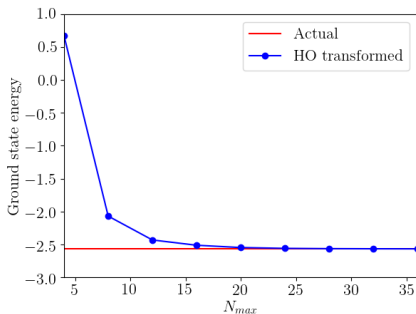


Transformation to HO Space

When transforming operators to HO space, we must pick a value of N_{max} such that our low-energy observables are converged to their true values. These figures focus on \hat{V}_α since \hat{V}_β converges much faster. We find $N_{max} = 28$ to be sufficient for the 2-body and 3-body ground state energies.



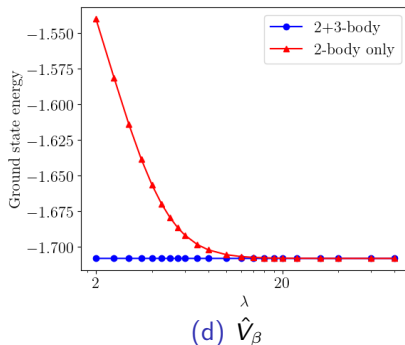
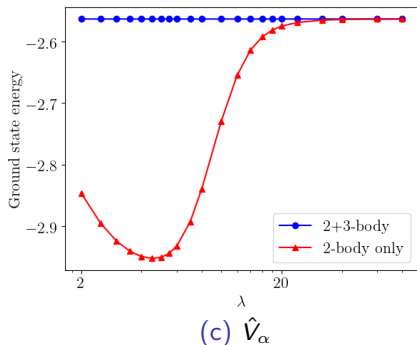
(a) 2-body



(b) 3-body

Induced 3-Body Force with $G_s = T$

We find a large 3-body force induced by the 2-body SRG evolution with $\hat{G}_s = \hat{T}$.



Induced 3-Body Force with Alternative Flow Operator

We define an alternative flow operator, \hat{H}_{BDHO} , that is block-diagonal in HO space:

$$\hat{G}_s = \hat{H}_{BDHO} = \hat{T} + \hat{V}\Theta(N - \Lambda)\Theta(N' - \Lambda), \quad (5)$$

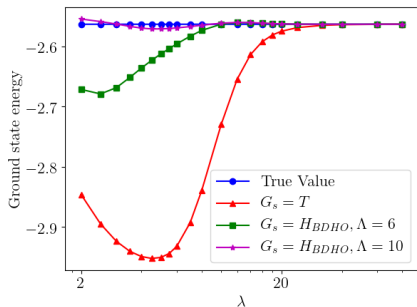
where Λ is the harmonic oscillator cutoff for the low-energy sector.

Induced 3-Body Force with Alternative Flow Operator

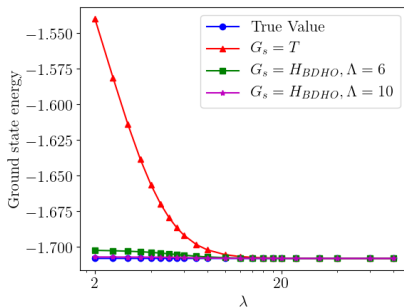
We define an alternative flow operator, \hat{H}_{BDHO} , that is block-diagonal in HO space:

$$\hat{G}_s = \hat{H}_{BDHO} = \hat{T} + \hat{V}\Theta(N - \Lambda)\Theta(N' - \Lambda), \quad (5)$$

where Λ is the harmonic oscillator cutoff for the low-energy sector.



(g) \hat{V}_α



(h) \hat{V}_β

srg1d is the Python framework behind this work.

- Validated against previous results for 2-body and 3-body cases
- Abstracts technical details (basis construction and symmetrization, operator embedding, etc.) from user
- Simplifies writing SRG calculations
- Testing a new flow operator requires user to change 2 lines of code in an existing script

With srg1d, further exploration of this 1-dimensional setting is made easy.

Conclusions and Future Work

Conclusions:

- Validated implementation against previous results
- Alternative flow operator results are preliminary
 - Need to compare rate of decoupling between different flow operators
 - Need to explore 4-body and 5-body forces induced to see general trends
- `srg1d` framework makes additional testing easy

Conclusions and Future Work

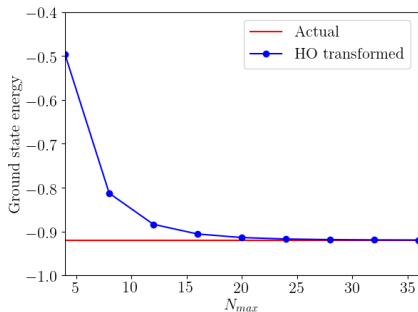
Conclusions:

- Validated implementation against previous results
- Alternative flow operator results are preliminary
 - Need to compare rate of decoupling between different flow operators
 - Need to explore 4-body and 5-body forces induced to see general trends
- `srg1d` framework makes additional testing easy

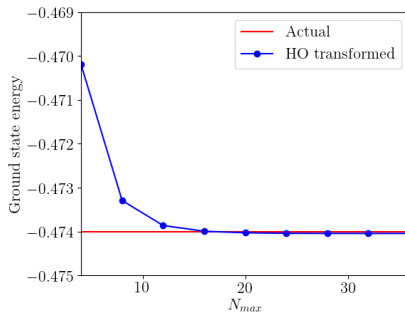
Future Work:

- Test proposed alternative flow operators further
- Formulate new flow operators with different features
- Seek to understand what features of flow operators are desirable

2-Body V_α vs. V_β

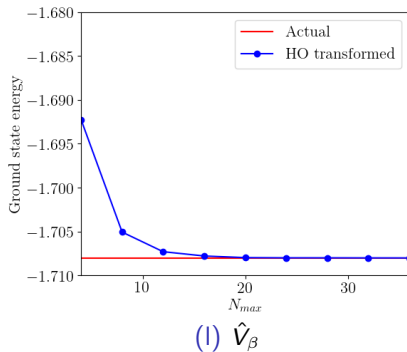
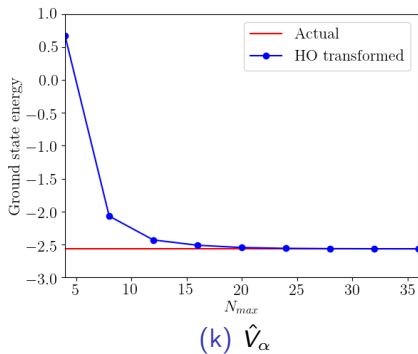


(i) \hat{V}_α

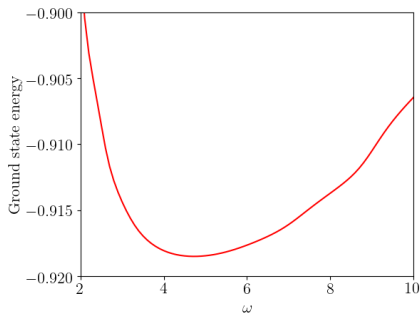


(j) \hat{V}_β

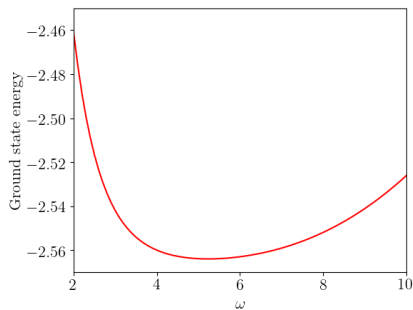
3-Body V_α vs. V_β



ω Optimization



(m) 2-body ground state energy



(n) 3-body ground state energy