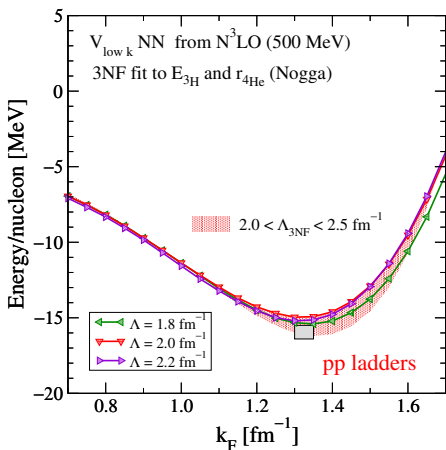
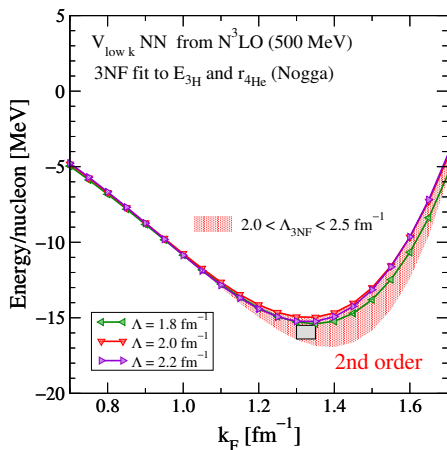


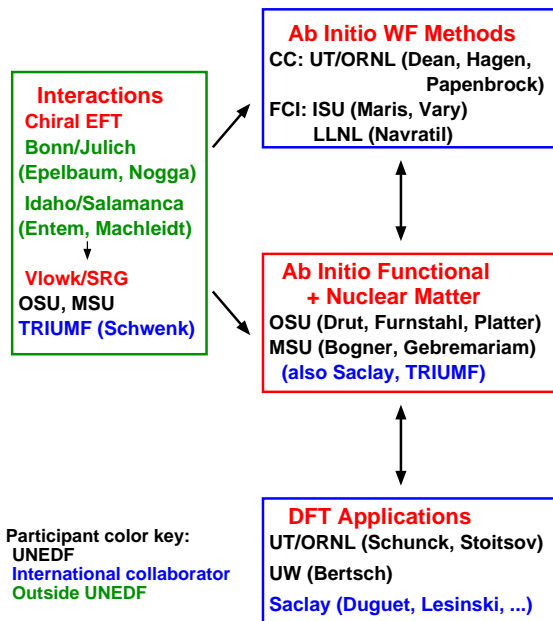
Ab Initio Nuclear DFT Progress Report, Part 2

Short-term gameplan (Progress Report, Part 1):

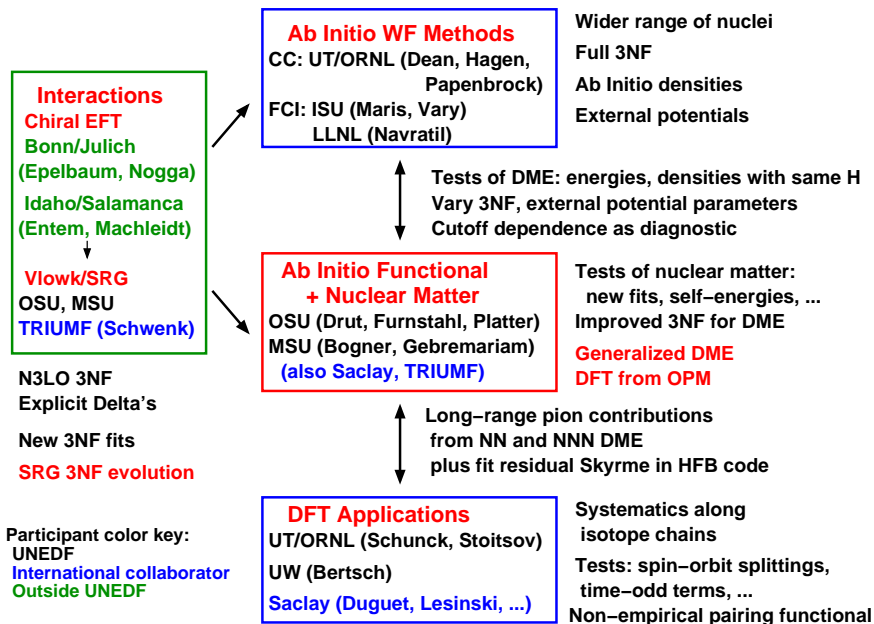
- Use a chiral EFT to a given order (e.g., E/M $N^3\text{LO}$ below); soften with RG (evolve to $\Lambda \approx 2 \text{ fm}^{-1}$ for ordinary nuclei)
 - NN interactions fully, **NNN interactions (3NF) approximately**
- Generate density functional using **NV DME in k -space**



UNEDF Interconnections for Ab Initio Functionals

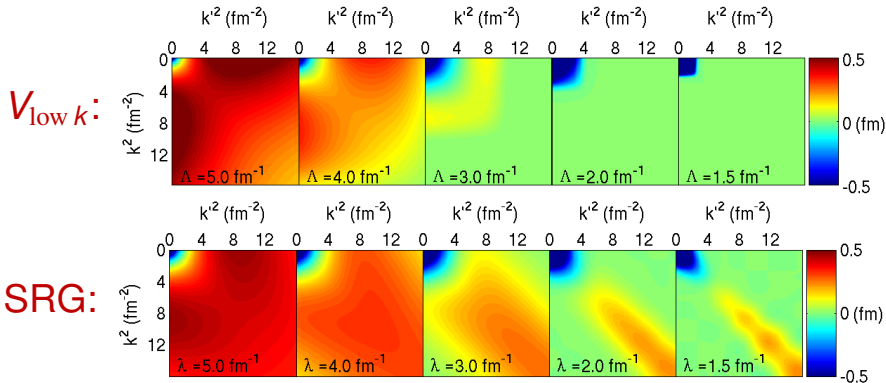


UNEDF Interconnections for Ab Initio Functionals



Progress on $V_{\text{low } k}$ /SRG Interactions (since Aug. 2007)

Bogner, Furnstahl, Perry, Schwenk + OSU students

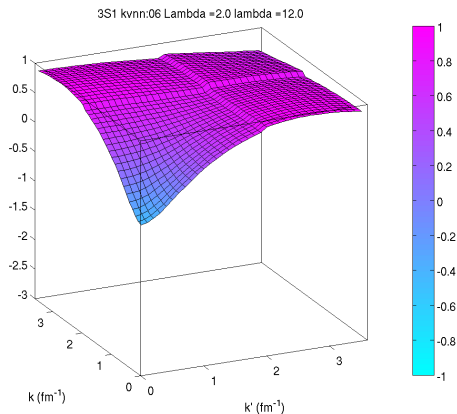
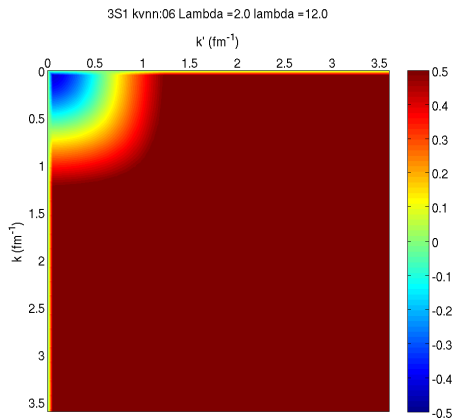


- Website: <http://www.physics.ohio-state.edu/~srg>
- SRG/ $V_{\text{low } k}$ NN computer code upgrades; new NNN fits
- Year 2–3 plan: SRG evolution of NNN (1D \rightarrow 3D). $V_{\text{low } k}$?

Block Diagonalization Via SRG [arXiv:0801.1098]

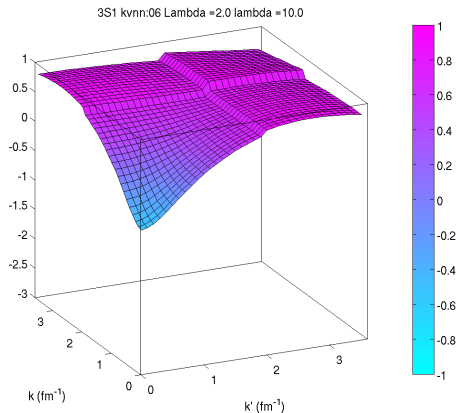
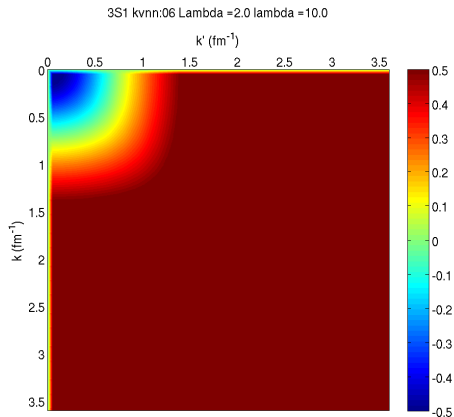
• Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?

• Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$



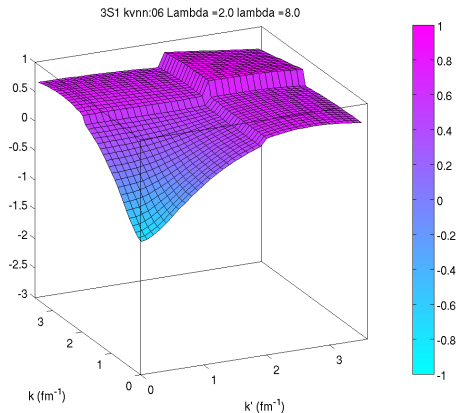
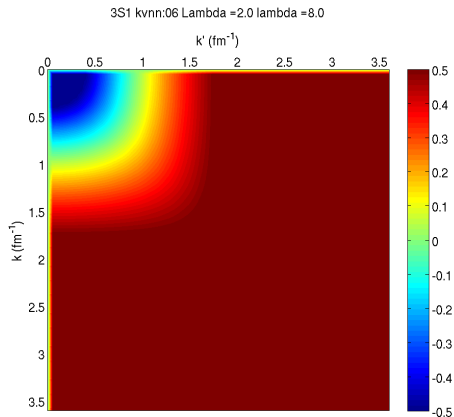
Block Diagonalization Via SRG [arXiv:0801.1098]

- Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?
- Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$



Block Diagonalization Via SRG [arXiv:0801.1098]

- Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?
- Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$

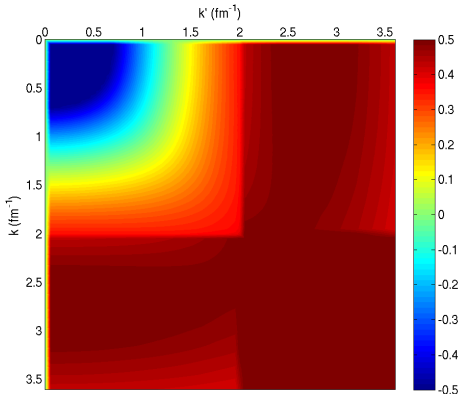


Block Diagonalization Via SRG [arXiv:0801.1098]

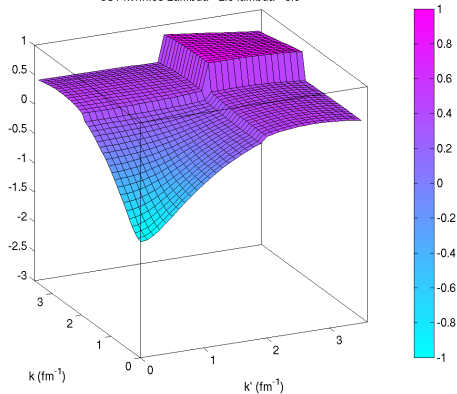
• Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?

• Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$

3S1 kvnn:06 Lambda =2.0 lambda =6.0



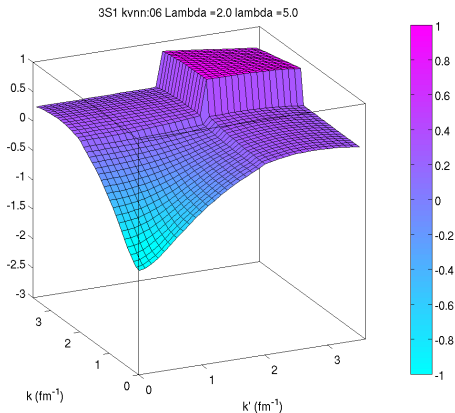
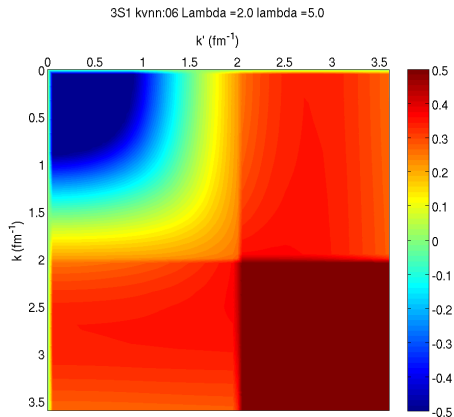
3S1 kvnn:06 Lambda =2.0 lambda =6.0



Block Diagonalization Via SRG [arXiv:0801.1098]

• Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?

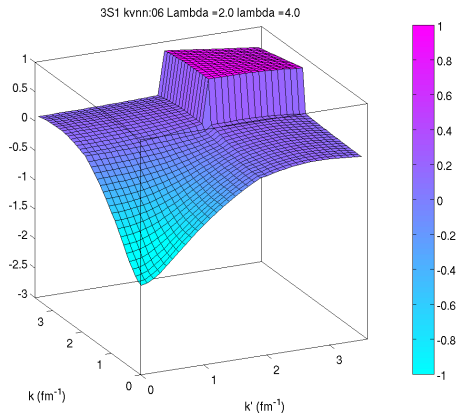
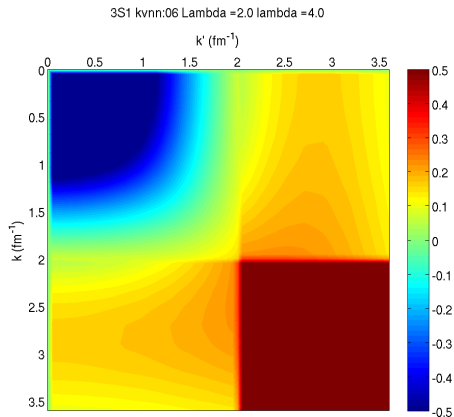
• Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$



Block Diagonalization Via SRG [arXiv:0801.1098]

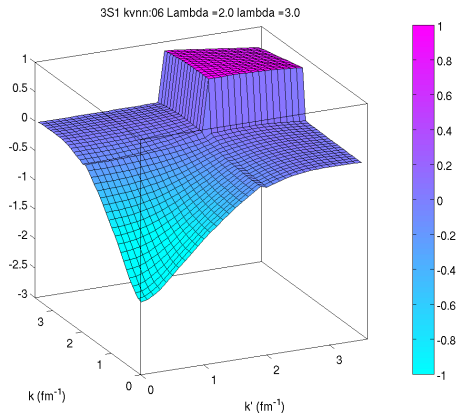
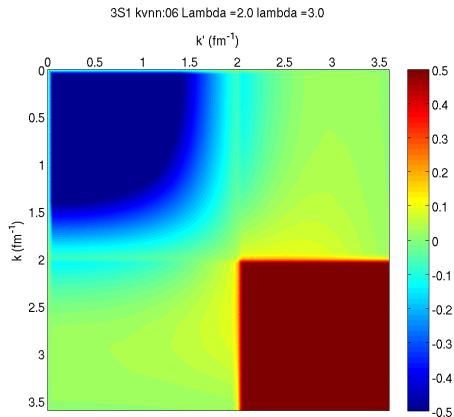
• Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?

• Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$



Block Diagonalization Via SRG [arXiv:0801.1098]

- Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?
- Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$

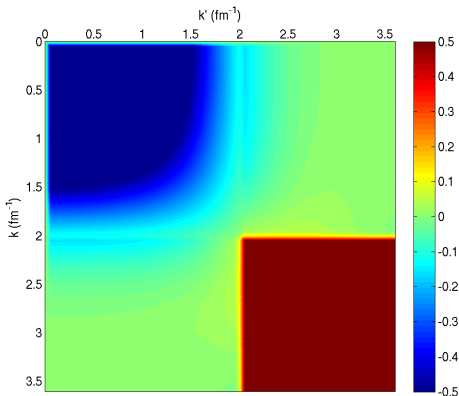


Block Diagonalization Via SRG [arXiv:0801.1098]

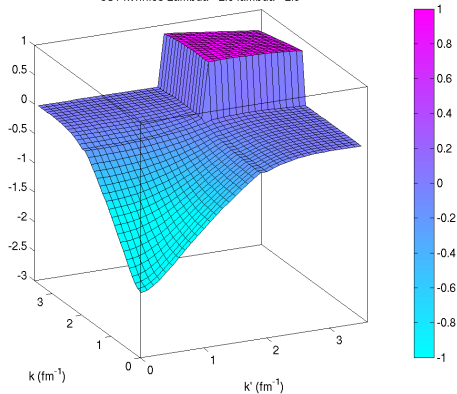
• Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?

• Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$

3S1 kvnn:06 Lambda = 2.0 lambda = 2.5



3S1 kvnn:06 Lambda = 2.0 lambda = 2.5

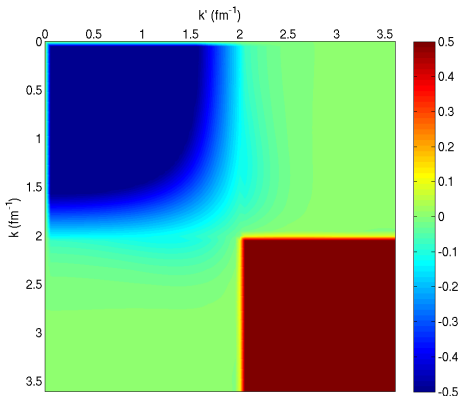


Block Diagonalization Via SRG [arXiv:0801.1098]

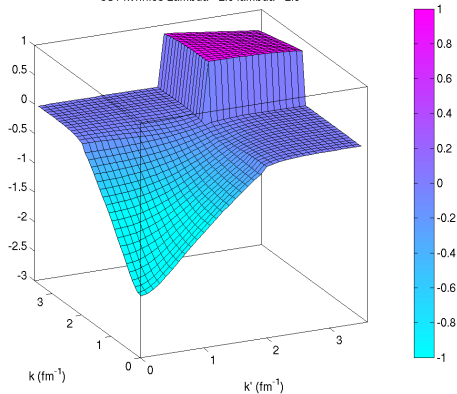
• Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?

• Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$

3S1 kvnn:06 Lambda = 2.0 lambda = 2.0



3S1 kvnn:06 Lambda = 2.0 lambda = 2.0

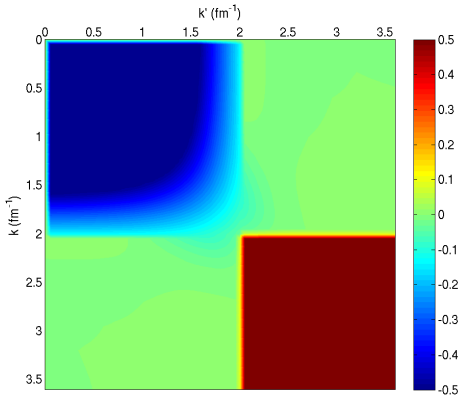


Block Diagonalization Via SRG [arXiv:0801.1098]

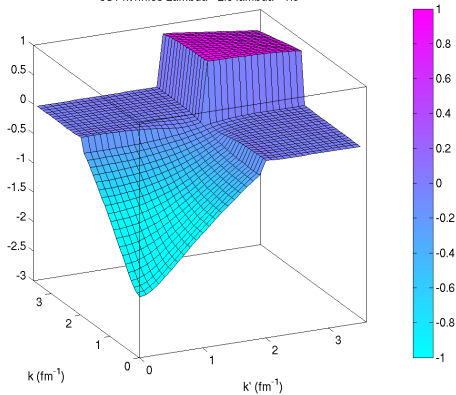
• Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?

• Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$

3S1 kvnn:06 Lambda = 2.0 lambda = 1.5



3S1 kvnn:06 Lambda = 2.0 lambda = 1.5



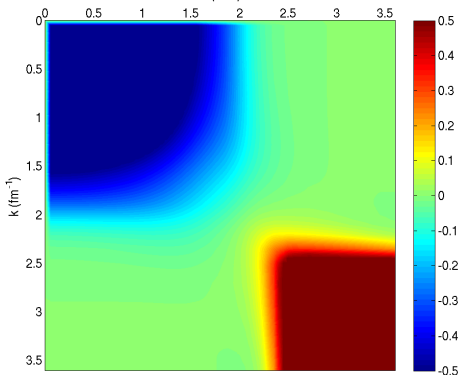
Block Diagonalization Via SRG [arXiv:0801.1098]

- Can we get a $\Lambda = 2 \text{ fm}^{-1}$ $V_{\text{low } k}$ -like potential with SRG?

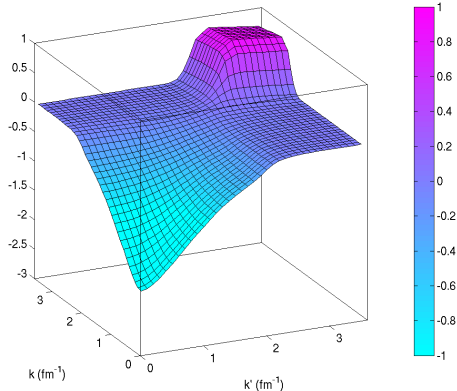
- Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$

3S1 kvnn:06 Lambda =2.0 lambda =2.0

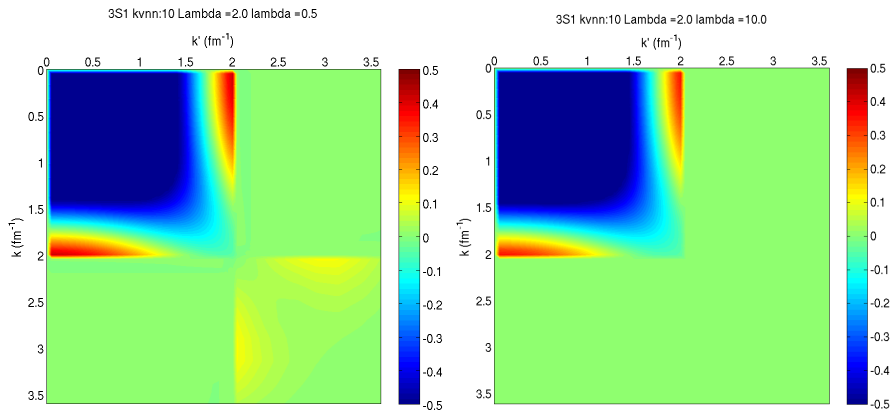
$k' \text{ (fm}^{-1}\text{)}$



3S1 kvnn:06 Lambda =2.0 lambda =2.0

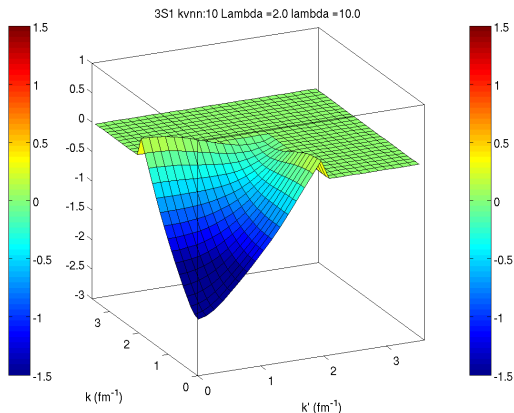
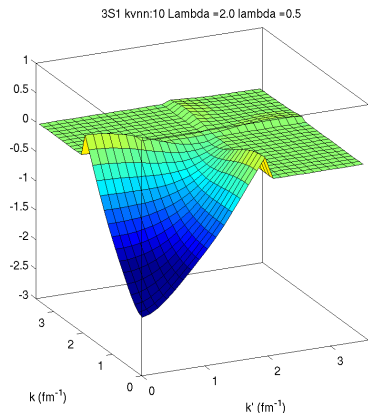


Compare SRG Block Diagonal and $V_{\text{low } k}$



- Decoupling means that they are functionally equivalent
- Can we directly relate Lee-Suzuki $V_{\text{low } k}$ and this SRG?
- Year 2–3: Can we use this SRG to evolve in the 3N system?

Compare SRG Block Diagonal and $V_{\text{low } k}$



- Decoupling means that they are functionally equivalent
- Can we directly relate Lee-Suzuki $V_{\text{low } k}$ and this SRG?
- Year 2–3: Can we use this SRG to evolve in the 3N system?

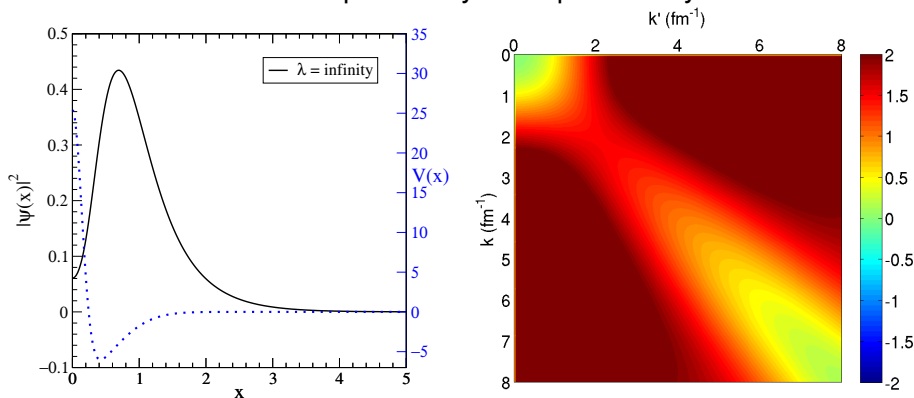
Year 2: 1D Laboratory for SRG Few-Body Physics

E. Jurgenson et al. [OSU]

- Use a simple sum-of-gaussians potential, e.g.,

$$V(x) = 34 e^{-(x/0.2)^2} - 8.5 e^{-(x/0.8)^2}$$

- SRG results in two-particle system qualitatively like NN:



- Bound-state energies: -0.92 ($A = 2$), -2.57 ($A = 3$), ...

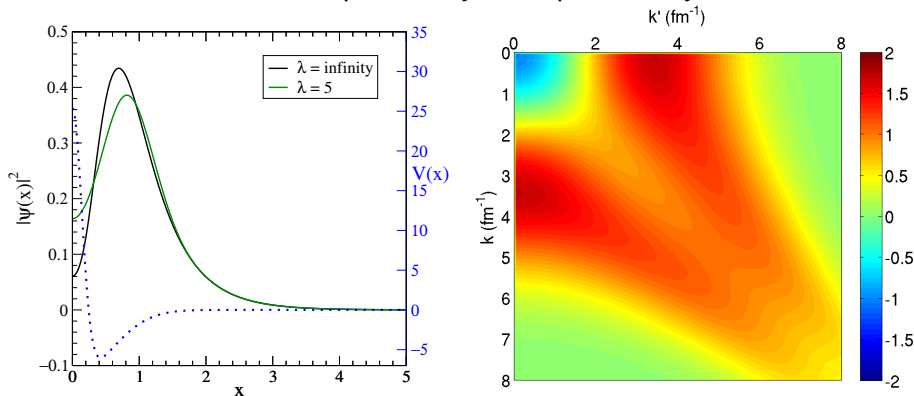
Year 2: 1D Laboratory for SRG Few-Body Physics

E. Jurgenson et al. [OSU]

- Use a simple sum-of-gaussians potential, e.g.,

$$V(x) = 34 e^{-(x/0.2)^2} - 8.5 e^{-(x/0.8)^2}$$

- SRG results in two-particle system qualitatively like NN:



- Bound-state energies: -0.92 ($A = 2$), -2.57 ($A = 3$), ...

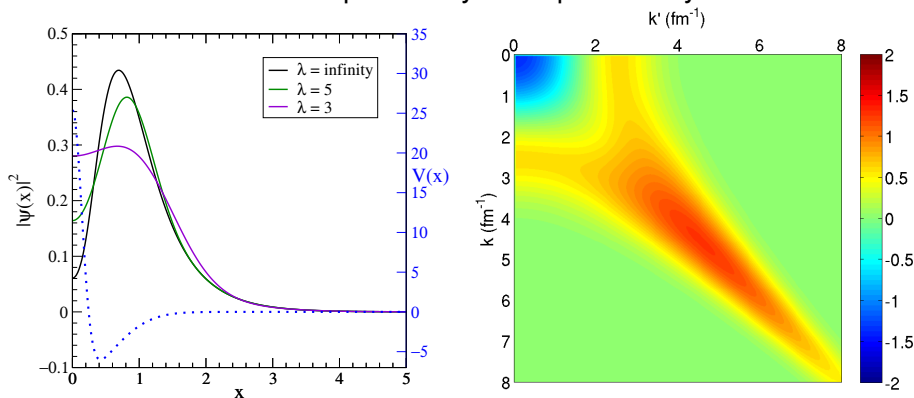
Year 2: 1D Laboratory for SRG Few-Body Physics

E. Jurgenson et al. [OSU]

- Use a simple sum-of-gaussians potential, e.g.,

$$V(x) = 34 e^{-(x/0.2)^2} - 8.5 e^{-(x/0.8)^2}$$

- SRG results in two-particle system qualitatively like NN:



- Bound-state energies: -0.92 ($A = 2$), -2.57 ($A = 3$), ...

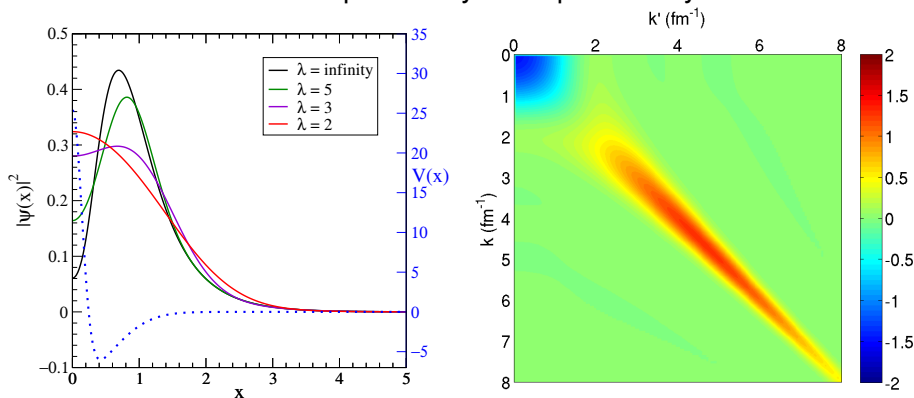
Year 2: 1D Laboratory for SRG Few-Body Physics

E. Jurgenson et al. [OSU]

- Use a simple sum-of-gaussians potential, e.g.,

$$V(x) = 34 e^{-(x/0.2)^2} - 8.5 e^{-(x/0.8)^2}$$

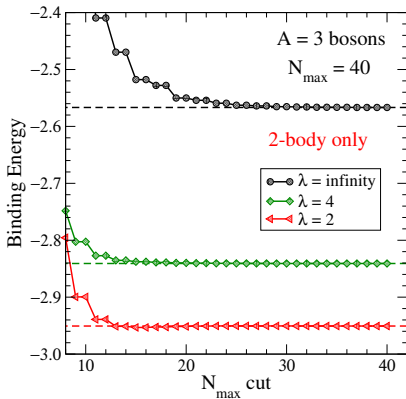
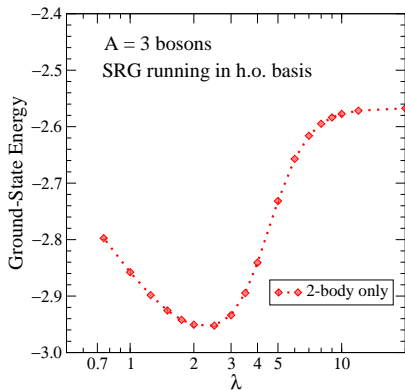
- SRG results in two-particle system qualitatively like NN:



- Bound-state energies: -0.92 ($A = 2$), -2.57 ($A = 3$), ...

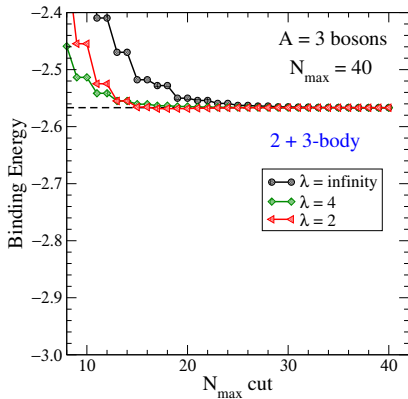
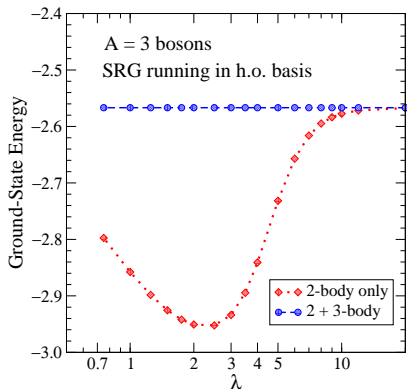
1D SRG Evolution with T_{rel} in a Jacobi HO Basis

- Rather than evolving in momentum space
 - use recursive symmetrization formalism developed for NCSM
 - directly obtain SRG matrix elements in HO basis
 - separate 3-body evolution not needed
- Compare $A = 3$ 2-body only to full 2 + 3-body evolution:



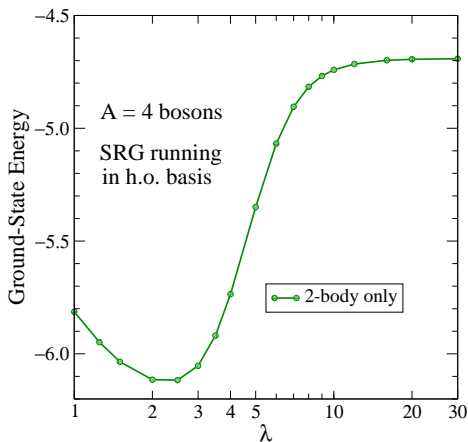
1D SRG Evolution with T_{rel} in a Jacobi HO Basis

- Rather than evolving in momentum space
 - use recursive symmetrization formalism developed for NCSM
 - directly obtain SRG matrix elements in HO basis
 - separate 3-body evolution not needed
- Compare $A = 3$ 2-body only to full 2 + 3-body evolution:



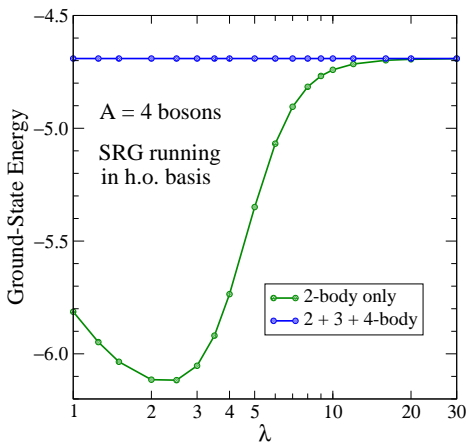
1D SRG Evolution with T_{rel} in a Jacobi HO Basis

- $A \geq 4$ follows by embedding $A - 1$ in A (Navratil et al.)
- Compare $A = 4$ 2-body only to full 2 + 3 + 4-body evolution



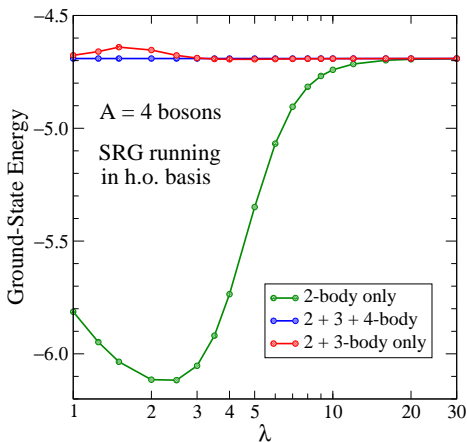
1D SRG Evolution with T_{rel} in a Jacobi HO Basis

- $A \geq 4$ follows by embedding $A - 1$ in A (Navratil et al.)
- Compare $A = 4$ **2-body only** to full **2 + 3 + 4-body** evolution



1D SRG Evolution with T_{rel} in a Jacobi HO Basis

- $A \geq 4$ follows by embedding $A - 1$ in A (Navratil et al.)
- Compare $A = 4$ **2-body only** to full **2 + 3 + 4-body** evolution
- Now extract 3NF from $A = 3$ and look at **2 + 3-body only**



- Year 2–3: other generators/schemes, scaling analysis, **3D**

Articles and Preprints Citing SCIDAC Support

- Posted and Published since Pack Forest 2007
 - “Convergence in the no-core shell model with low-momentum two-nucleon interactions,” S.K. Bogner, R.J. Furnstahl, P. Maris, R.J. Perry, A. Schwenk, and J.P. Vary, Nucl. Phys. A **801**, 21 (2008).
 - “Block Diagonalization using SRG Flow Equations,” Anderson, Bogner, Furnstahl, Jurgenson, Perry, Schwenk, Phys. Rev. C **77**, 037001 (2008) [arXiv:0801.1098].
 - “Exact Relations for a Strongly-interacting Fermi Gas from the Operator Product Expansion,” E. Braaten and L. Platter, Phys. Rev. Lett. **100**, 205301 (2008).
 - “Effective Field Theory and Finite Density Systems,” Furnstahl, Rupak, Schafer, Ann. Rev. Nucl. Part. Phys. [arXiv:0806.1365].
- Posted or Soon-to-be Posted (preprints available)
 - “Density Matrix Expansion for Low-Momentum Interactions,” S.K. Bogner, R.J. Furnstahl, and L. Platter
 - “Decoupling in the Similarity Renormalization Group for Nucleon-Nucleon Forces,” Jurgenson, Bogner, Furnstahl, Perry, Phys. Rev. C, [arXiv:0711.4252].
 - “Similarity Renormalization Group Evolution of Many-Body Forces in

Plans for Rest of Year 2 and Year 3 and ...

Plans are nothing; planning is everything. — Dwight D. Eisenhower

- NNN fits and tests
 - NNN project to interface $V_{\text{low } k}$ chiral EFT NNN with FCI
 - Test new fits with CC and FCI in larger nuclei (e.g., λ/Λ dependence)
 - Use FCI in light nuclei for fits of $N^2\text{LO}$ 3NF coefficients C_D , C_E (and c_i 's) for many SRG and smooth $V_{\text{low } k}$ cutoffs
- Evolving NNN with SRG
 - Continue exploring one-dimensional models
 - Understand many-body power counting and use to estimate higher-body interactions; evolve operators
 - Full three-dimensional NNN evolution (!)
 - Harmonic oscillator matrix elements for input to NCSM, CC
- Upgrade SRG input as it develops ($N^3\text{LO}$ NNN, Δ 's, ...)
 - Run different chiral EFT's at $N^n\text{LO}$ and different cutoffs

Plans for Rest of Year 2 and Year 3 and ...

Plans are nothing; planning is everything. — Dwight D. Eisenhower

- Nuclear matter studies
 - Complete and publish the G-matrix and BBG study
 - ⇒ test power counting with numerical examples
 - Study cutoff dependence for SRG/smooth $V_{low k}$ with fit NNN
 - Explore nuclear matter fine tuning ⇒ create data sets
 - Nonperturbativeness in the particle-hole channel
 - Pairing, e.g., in 3S_1
- Nuclear matter calculational extensions
 - Full 2nd order calculation with fit NNN
 - Asymmetric nuclear matter (just needs to be coded)
 - Explore coupled cluster calculations for nuclear matter
 - MBPT via symbolic manipulation (as in quantum chemistry)
- Export nuclear matter code with control over spin-isospin channels/partial waves for Skyrme EDF benchmarking

Plans for Rest of Year 2 and Year 3 and ...

Plans are nothing; planning is everything. — Dwight D. Eisenhower

- Isovector and Spin-Unsaturated (s.o., tensor, ..) terms
 - Λ -independent finite range contributions (nontrivial ρ -dependencies)
 - All 2N contributions through N³LO
 - All 3N contributions through N²LO
- Other DME Developments
 - Phase space averaging
 - Merge non-empirical pairing and DME
 - Alternatives for local k_F
 - DME beyond HF level — dispersive effects using short-time/factorization methods
-

Plans for Rest of Year 2 and Year 3 and ...

Plans are nothing; planning is everything. — Dwight D. Eisenhower

- Validating (or invalidating) DME
 - Compare energies, ρ 's to CC, FCI with same Hamiltonian
 - Vary contact 3NF strength
 - Full 3NF-fitted $V_{\text{low } k}$ /SRG
 - Compare in external potentials with FCI, CC
 - $V_{\text{low } k}$ /SRG with contact (full) 3NF
 - neutron drops
- Beyond DME
 - 1D (3D) development of orbital based nuclear DFT
-

EFT and the (Nuclear) Many-Body Problem

- See “Effective Field Theory and Finite Density Systems” [rjf, G. Rupak, T. Schäfer, arXiv:0801.0729]
- Most applications to date use EFT only for interaction then apply conventional few- and many-body methods
 - important to maintain EFT perspective
 - RG methods are not alternatives but supplements
- New approaches (partial list)
 - EFT for shell model [I. Stetcu et al.]
 - Lattice approaches [D. Lee et al.]
 - “Exact Relations for a Strongly-interacting Fermi Gas from the Operator Product Expansion” [E. Braaten and L. Platter, arXiv:0803.1125]
- Nuclear DFT could use more direct EFT!
- INT Program in spring 2009: “Effective Field Theories and the Many-Body Problem” [C. Johnson, rjf, E. Ormand, Bira]