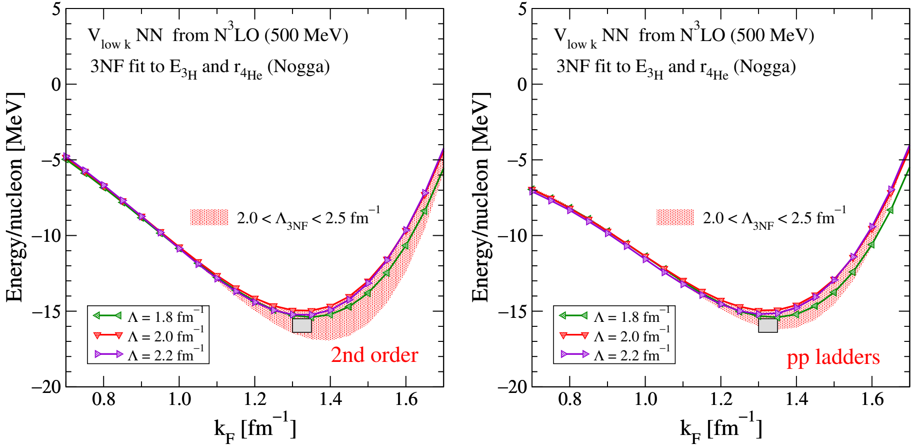
Ab Initio Nuclear DFT Progress Report, Part 2

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

- Use a chiral EFT to a given order (e.g., E/M N^3LO below); soften with RG (evolve to $\Lambda \approx 2\,\mathrm{fm}^{-1}$ 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

Interactions

Chiral EFT

Bonn/Julich (Epelbaum, Nogga)

Idaho/Salamanca (Entem, Machleidt)

↓

Vlowk/SRG

OSU, MSU

TRIUMF (Schwenk)

Ab Initio WF Methods

CC: UT/ORNL (Dean, Hagen, Papenbrock)

FCI: ISU (Maris, Vary)

LLNL (Navratil)

↕

Ab Initio Functional + Nuclear Matter

OSU (Drut, Furnstahl, Platter)

MSU (Bogner, Gebremariam)

(also Saclay, TRIUMF)

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DFT Applications

UT/ORNL (Schunck, Stoitsov)

UW (Bertsch)

Saclay (Duguet, Lesinski, ...)

Participant color key:
- UNEDF
- International collaborator
- Outside UNEDF

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(Epelbaum, Nogga)
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Vlowk/SRG
OSU, MSU
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N3LO 3NF
Explicit Delta's

New 3NF fits

SRG 3NF evolution

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Ab Initio WF Methods
CC: UT/ORNL (Dean, Hagen, Papenbrock)
FCI: ISU (Maris, Vary)
LLNL (Navratil)

Wider range of nuclei
Full 3NF
Ab Initio densities
External potentials

↕

Tests of DME: energies, densities with same H
Vary 3NF, external potential parameters
Cutoff dependence as diagnostic

Ab Initio Functional + Nuclear Matter
OSU (Drut, Furnstahl, Platter)
MSU (Bogner, Gebremariam)
(also Saclay, TRIUMF)

Tests of nuclear matter:
new fits, self−energies, ...
Improved 3NF for DME
Generalized DME
DFT from OPM

↕

Long−range pion contributions
from NN and NNN DME
plus fit residual Skyrme in HFB code

DFT Applications
UT/ORNL (Schunck, Stoitsov)
UW (Bertsch)
Saclay (Duguet, Lesinski, ...)

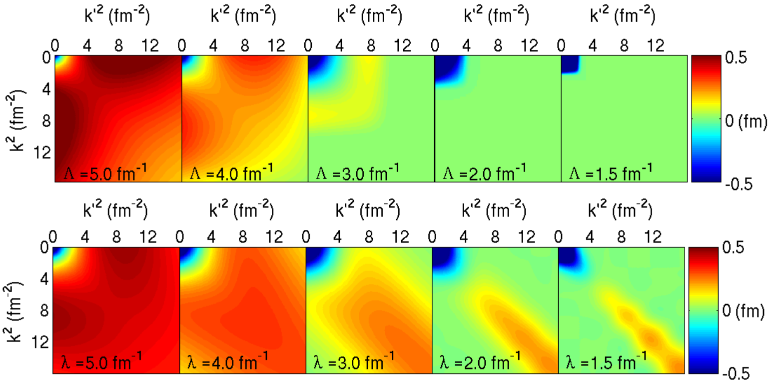
Systematics along
isotope chains
Tests: spin−orbit splittings,
time−odd terms, ...
Non−empirical pairing functional

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

Bogner, Furnstahl, Perry, Schwenk + OSU students

$V_{\text{low}\,k}$:

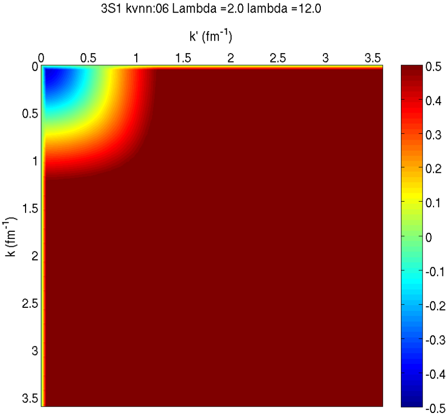
SRG:

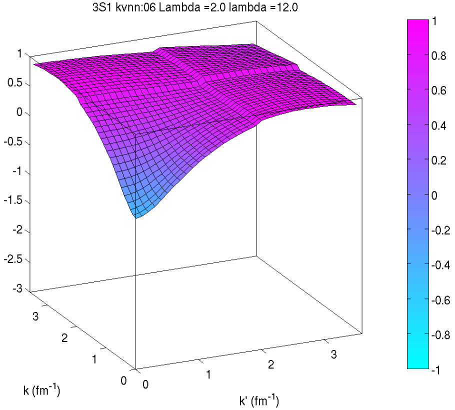


- Website: **http://www.physics.ohio-state.edu/∼srg**
- SRG/$V_{\text{low}\,k}$ NN computer code upgrades; new NNN fits
- Year 2–3 plan: SRG evolution of NNN (1D → 3D). $V_{\text{low}\,k}$?

Block Diagonalization Via SRG [arXiv:0801.1098]

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





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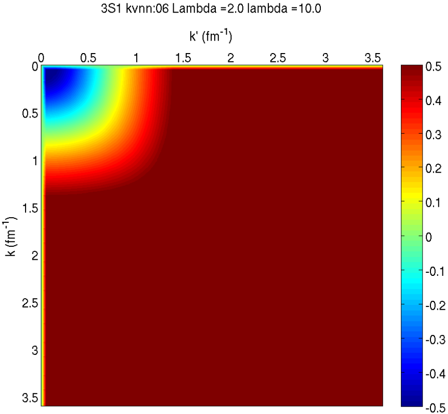

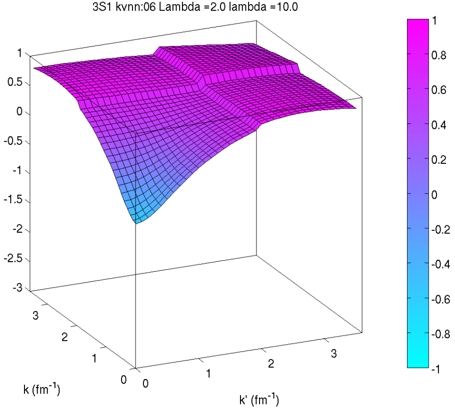

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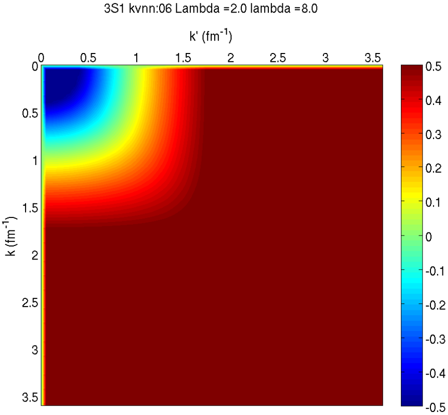

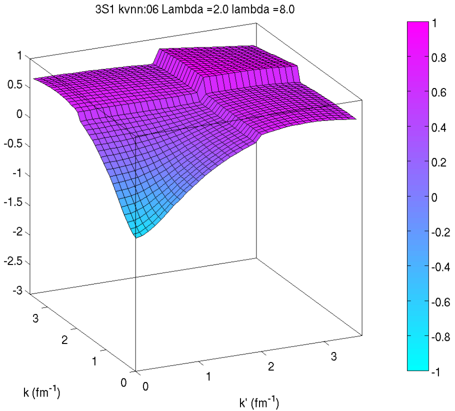

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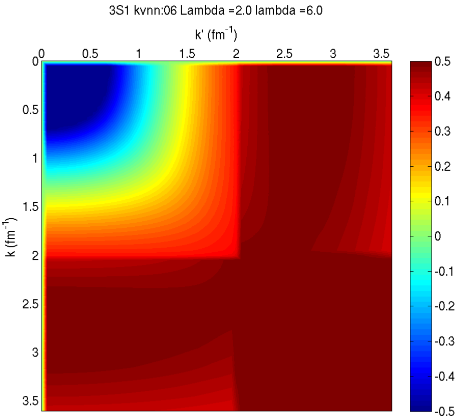

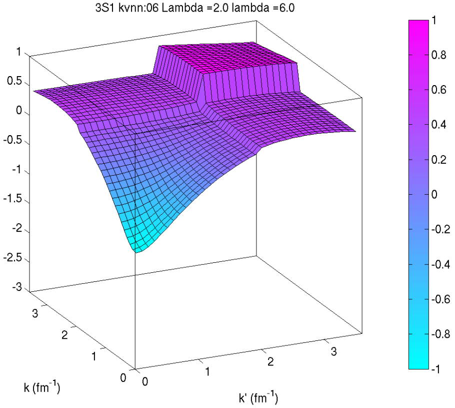

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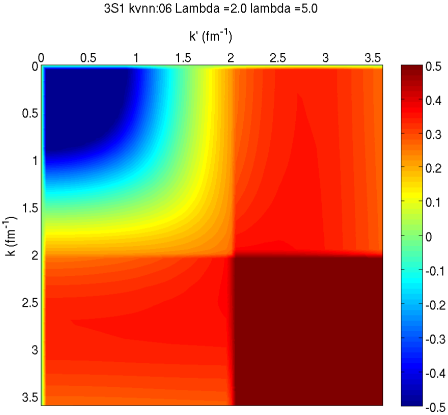

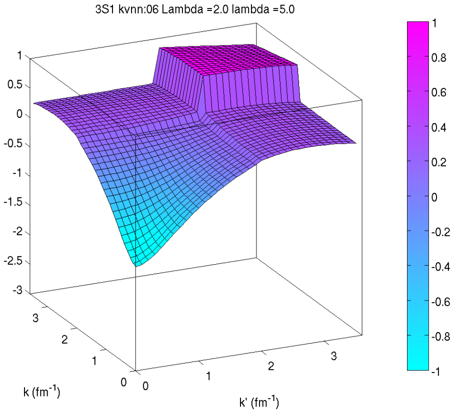

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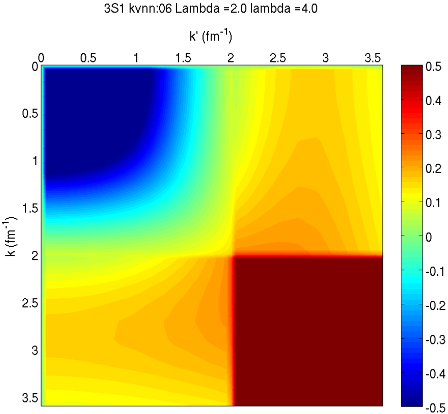

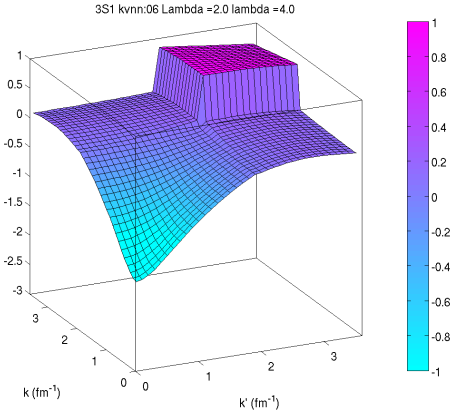

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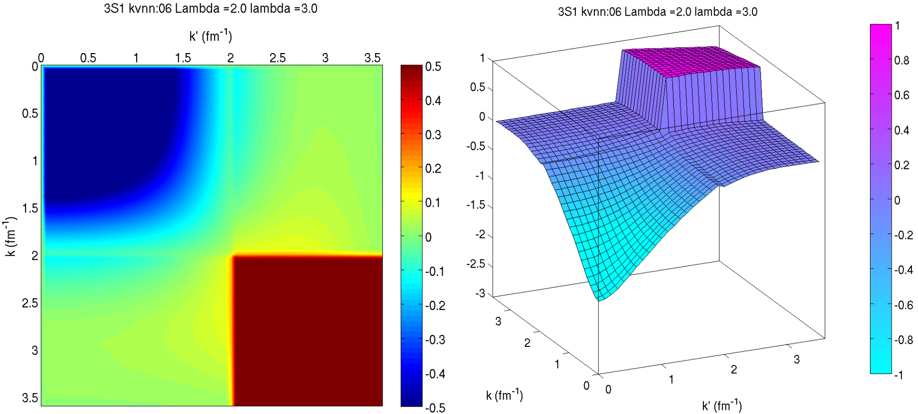

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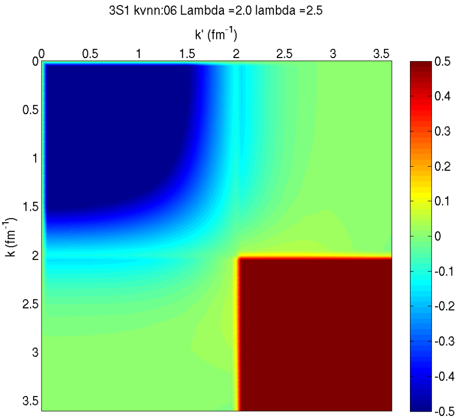

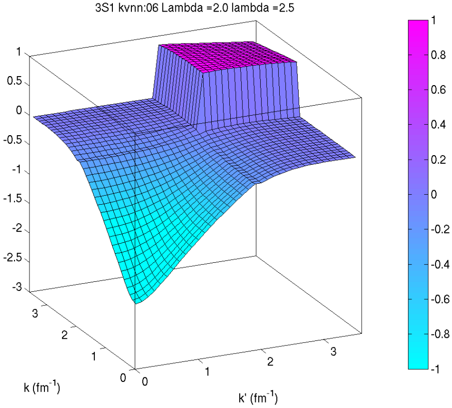

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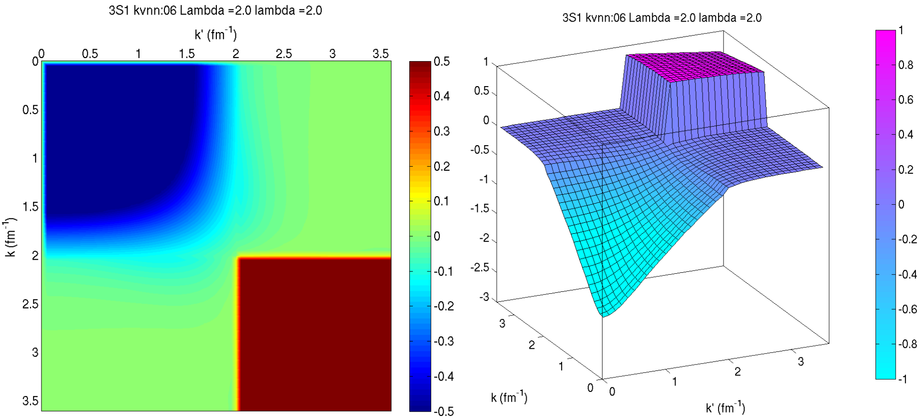

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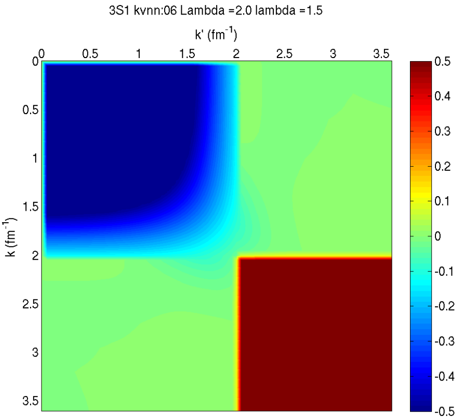

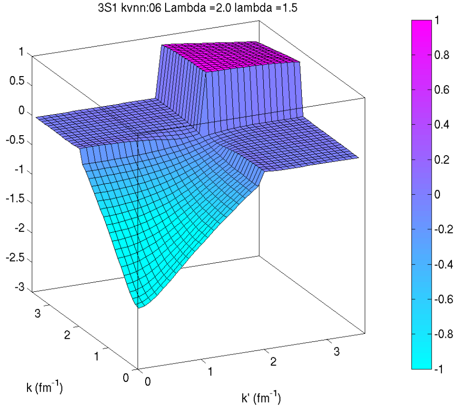

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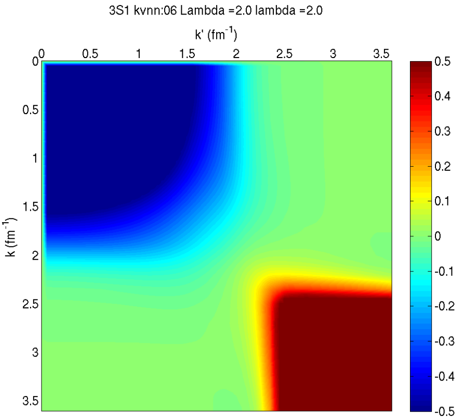
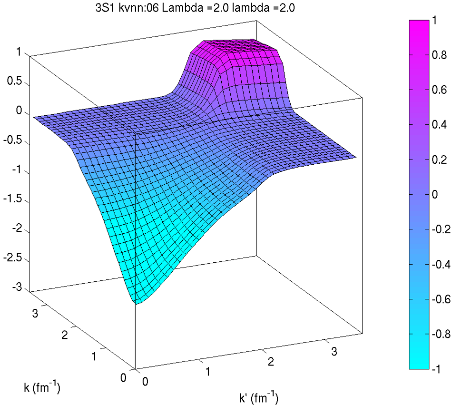
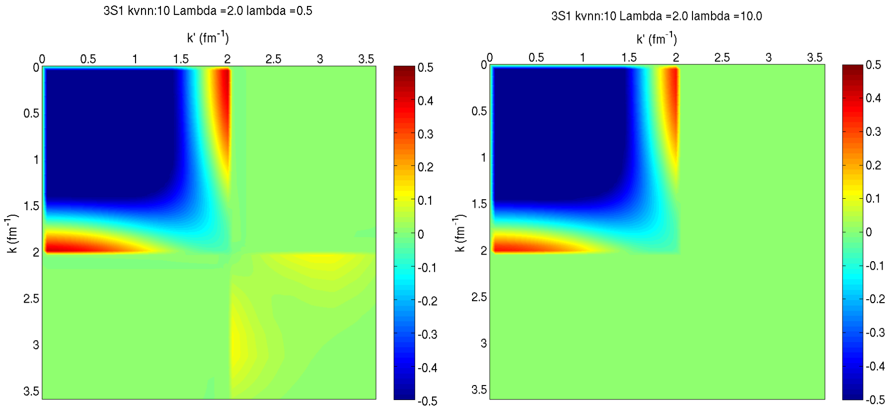




Compare SRG Block Diagonal and $V_{\mathrm{low}\,k}$



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

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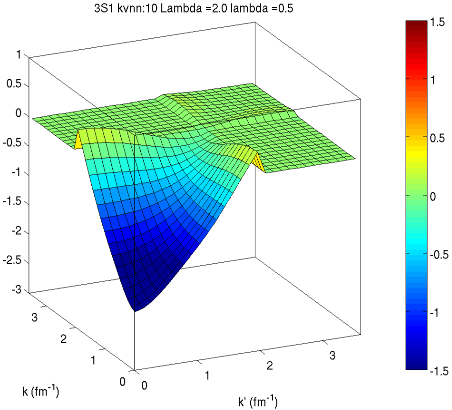

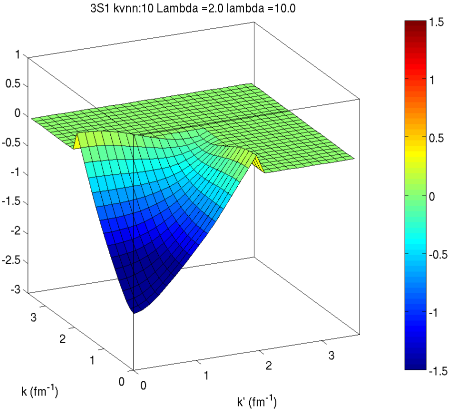

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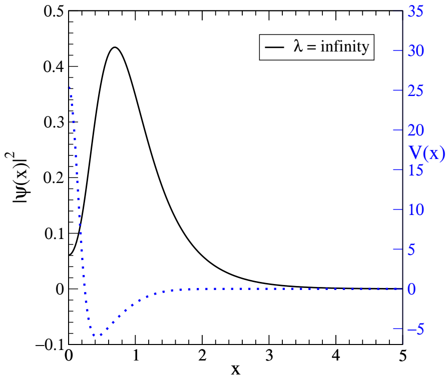
Year 2: 1D Laboratory for SRG Few-Body Physics

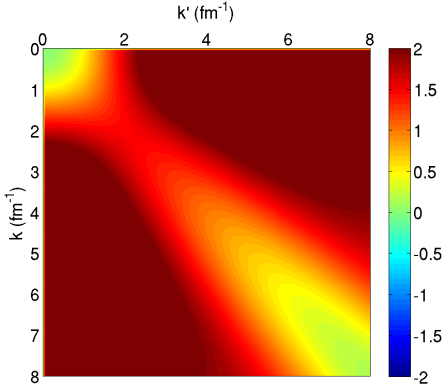
E. Jurgenson et al. [OSU]

- 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 ($A = 3$), ...

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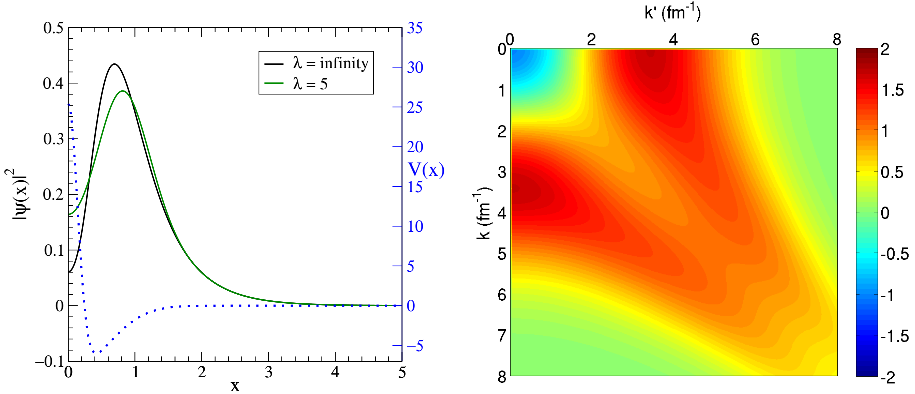

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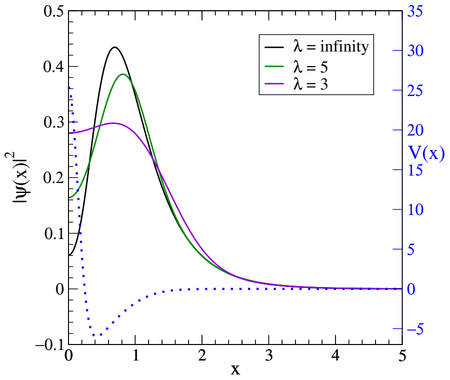

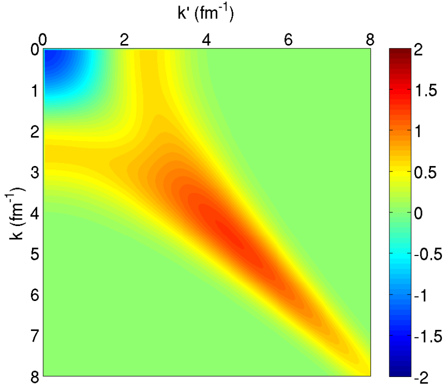

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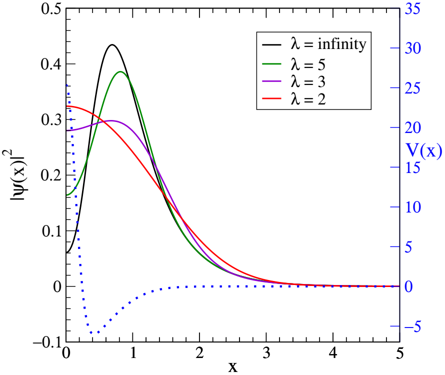

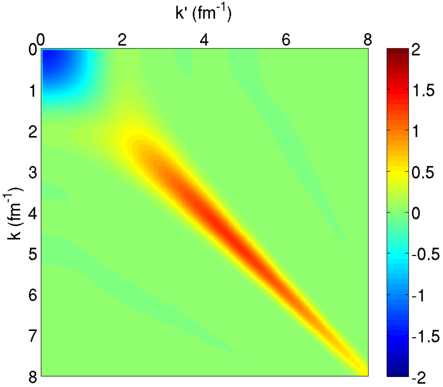

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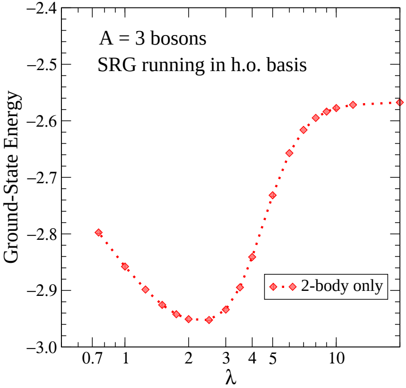
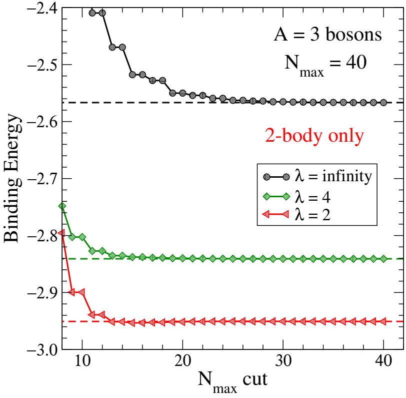
1D SRG Evolution with T_{rel} in a Jacobi HO Basis

- 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:





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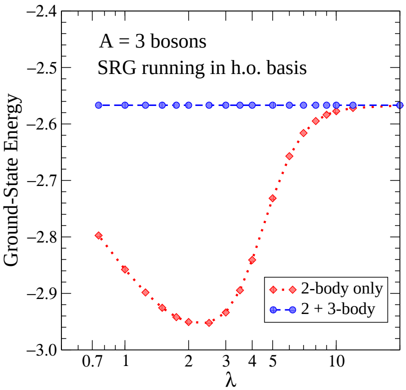
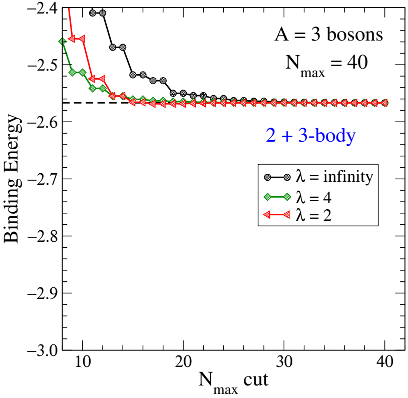
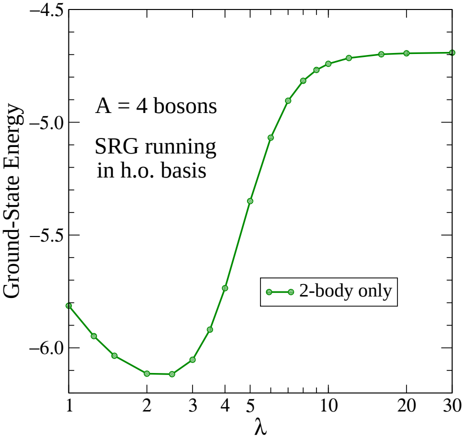




1D SRG Evolution with $T_{\rm rel}$ in a Jacobi HO Basis

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



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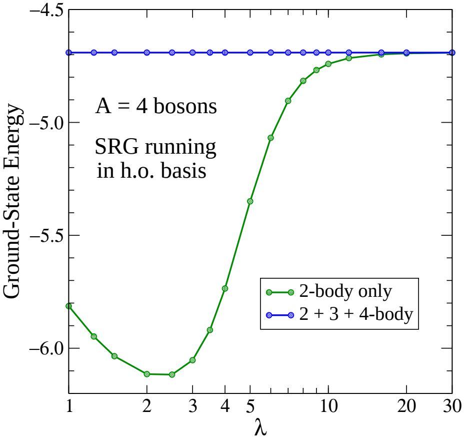

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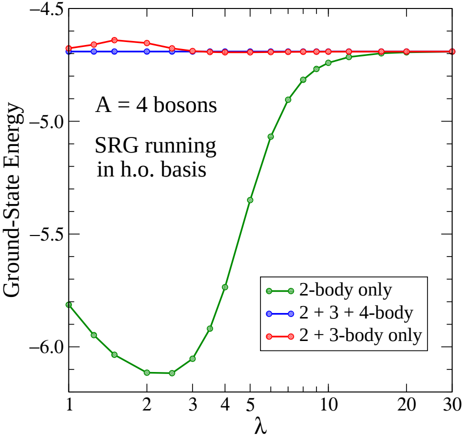
- $A \geq 4$ follows by embedding $A - 1$ in A (Navratil et al.)
- Compare $A = 4$ 2-body only to full $2 + 3 + 4$-body evolution
- Now extract 3NF from $A = 3$ and look at 2 + 3-body only

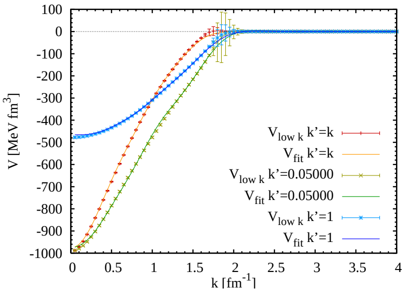


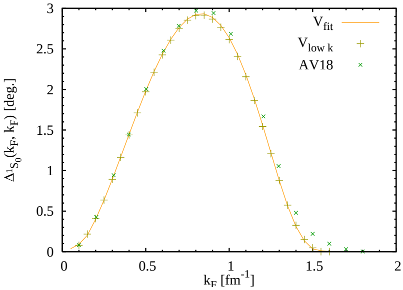
- Year 2–3: other generators/schemes, scaling analysis, 3D

Non-Empirical Pairing Functional for Nuclei

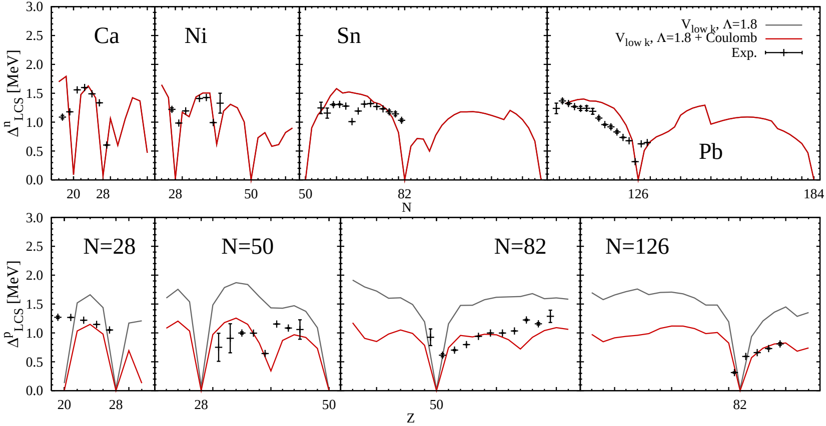
T. Duguet (Saclay); T. Lesinski, K. Bennaceur, J. Meyer (Lyon)

- New spherical code BSLHFB
  - spherical Bessel function basis
  - finite-range / non-local pairing interactions in EDF
  - operator representation: sum of separable terms (rank 2 for $V_{\text{low}\,k}$)
- Pairing at lowest order in NN (nuclear + Coulomb)
  - use $V_{\text{low}\,k}$ at $\Lambda \approx 2\,\text{fm}^{-1}$ as NN pairing interaction
  - Use SLY5 Skyrme for ph EDF with fixed $m_0^*/m = 0.7$
- Studied $m^*(k, k_F)$ for cutoffs Λ (K. Hebeler, T.D., A. Schwenk)
  - consistent ph/pp scales needed
  - $V_{\text{low}\,k}$ ok with $m^*_{\text{Skyrme}}(k_F)$





Pairing Gaps from $V_{\mathrm{low}\,k}$ + Coulomb Near Data!



- Current limitations
  - Three-body force missing
  - No density/spin/isospin fluctuations (Milan: +40%!?)
  - Phenom. ph functional and momentum-independent m_0^*
- Upgrade plans
  - Other observables (Lesinski), deformed nuclei (Rotival)
  - Incorporate NNN (Lesinski)
  - Check fluctuations
  - Construct ph part (BG, VR)

Articles and Preprints Citing SCIDAC Support

- Published and Posted (or soon) 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].
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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 $V_{\mathrm{low}\,k}$ 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^2LO 3NF coefficients C_D, C_E (and c_i's) for many SRG and smooth $V_{\mathrm{low}\,k}$ 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
- Develop in-medium SRG
- Upgrade SRG input as it develops (N^3LO NNN, Δ's, . . .)

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

- Nuclear matter studies
  - Complete and publish the G-matrix and BBG study
    $\Longrightarrow$ test power counting with numerical examples
  - Study cutoff dependence for SRG/smooth $V_{\mathrm{low}\,k}$ with fit NNN
  - Explore nuclear matter fine tuning $\Longrightarrow$ 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
- Export nuclear matter code with control over spin-isopin channels/partial waves for Skyrme EDF benchmarking

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

- Isovector and Spin-Unsaturated (s.o., tensor, ..) terms
  - Λ-independent finite range contributions
    - All 2N contributions through N^2LO (N^3LO)
    - All 3N contributions through N^2LO
  - Incorporate in HFB DME codes; refit generalized Skyrme
- Extensions of DME
  - Phase space averaging; alternatives for local k_F
  - Merge non-empirical pairing and DME
  - DME beyond HF level — dispersive effects using short-time/factorization methods
- 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]