Similarity Renormalization Group and Evolution of Many-Body Forces

E.D. Jurgenson

Department of Physics, The Ohio State University

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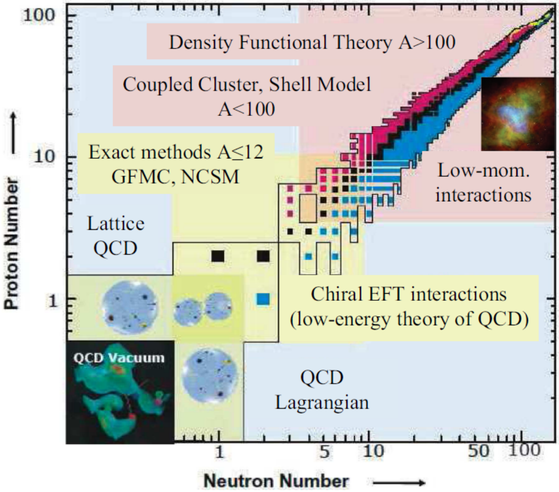
Collaborators: E.R. Anderson, S.K. Bogner, R.J. Furnstahl,

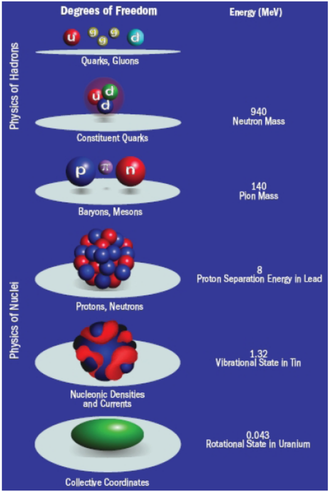
P. Navratil, R.J. Perry, A. Schwenk

Outline

- Overview of Similarity Renormalization Group (SRG) and Decoupling
- Evolving Three-Nucleon Forces (3NFs in 3D!!)
- Insights from a One-Dimensional Model
- Conclusions and Future Work

Degrees of Freedom: From QCD to Nuclei

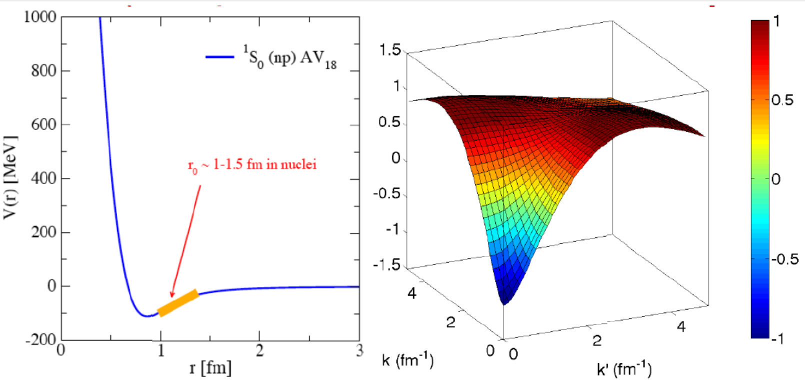




- Renormalization Group $\Longrightarrow$ focus on relevant dof's

- Which picture should I use?

Nuclear Interactions in Momentum Space



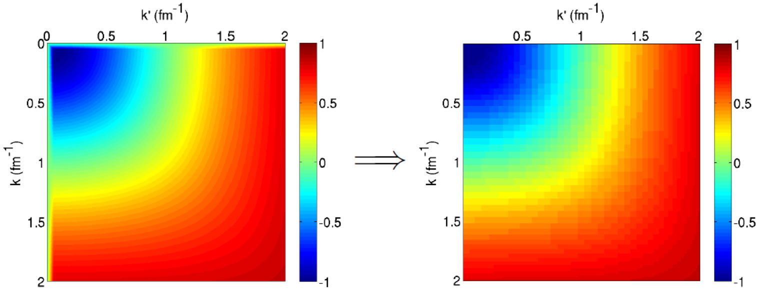
- Fourier transform in partial waves (Bessel transform)

$$V_{L=0}(k, k') = \int d^3r\, j_0(kr) V(r) j_0(k'r) = \langle k | V_{L=0} | k' \rangle$$

- Repulsive core $\Longrightarrow$ big high-k (≥ 2 fm^{-1}) components
- EFTs are softer - but still have high-k components

Computational Aside: Digital Potentials

- Although momentum is continuous in principle, in practice represented as discrete (gaussian quadrature) grid:

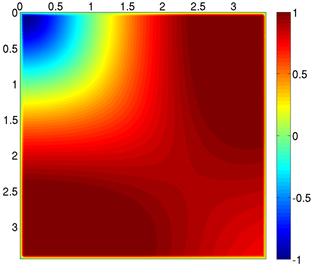


- Calculations become just matrix multiplications! E.g.,

$$\langle k|V|k\rangle + \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{(k^2 - k'^2)/m} + \cdots \Longrightarrow V_{ii} + \sum_{j} V_{ij} V_{ji} \frac{1}{(k_i^2 - k_j^2)/m} + \cdots$$

- 100×100 Resolution is sufficient for many significant figures

Try a Low-Pass Filter



- Start with a potential [AV18 - $^1S_0$]
- Cut at Λ [2.2 fm^{-1}]
- Compute observables [$\delta_0(E)$]
- Compare to uncut

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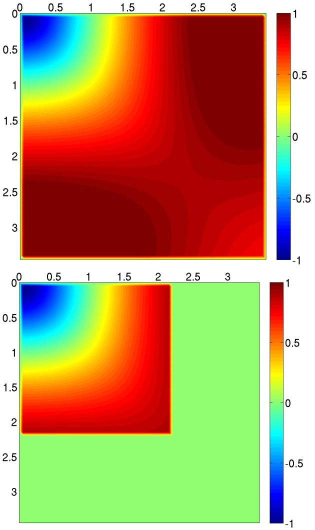

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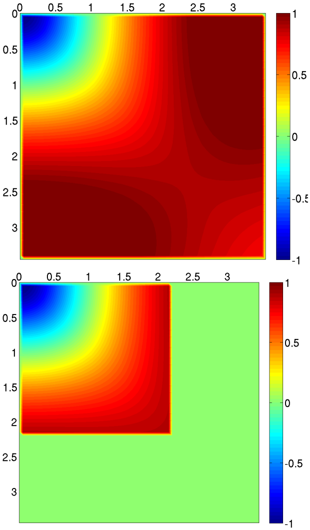

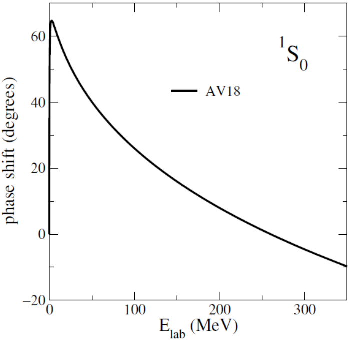

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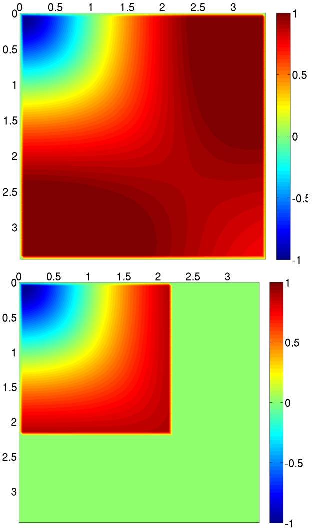

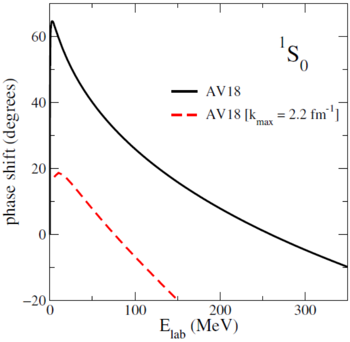

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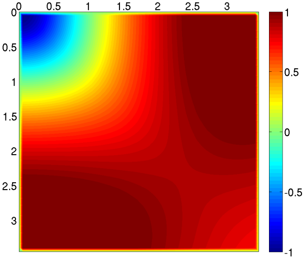
What's wrong with the Low-Pass Filter

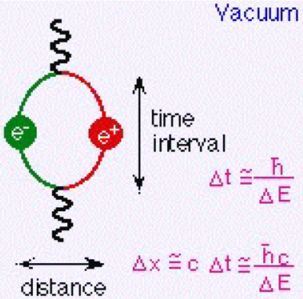
- Basic problem: high and low are coupled!
- Perturbation theory for scattering

$$\langle k|V|k\rangle + \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{(k^2 - k'^2)/m} + \ldots$$

- Can't just change high-momentum elements (intermediate virtual states)
- Absorb high-energy effects into low-energy Hamiltonians ⇒ "Renormalization Group" (Here: "flow equations")
- Unitary transformation:

$$E_n = (\langle\psi_n|U^\dagger)UHU^\dagger(U|\psi_n\rangle)$$





What is the SRG? [arXiv:nucl-th/0611045]

- Transform an initial Free-Space Hamiltonian, $H = T + V_s$

$$H_s = U(s) H U^{\dagger}(s) \equiv T + V_s$$

where s is the flow parameter. Differentiating wrt s:

$$\frac{dH_s}{ds} = [\eta(s), H_s] \quad with \quad \eta(s) = \frac{dU(s)}{ds} U^{\dagger}(s) = -\eta^{\dagger}(s)$$

- $\eta(s)$ is specified by the commutator with generator, G_s:

$$\eta(s) = [G_s, H_s] \ ,$$

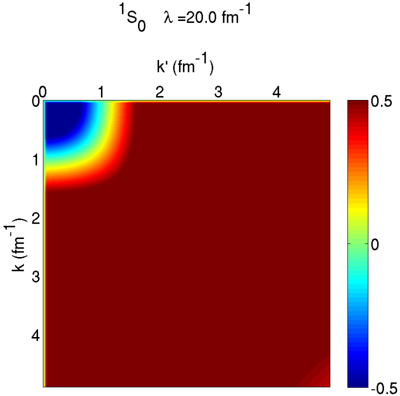
which yields the flow equation,

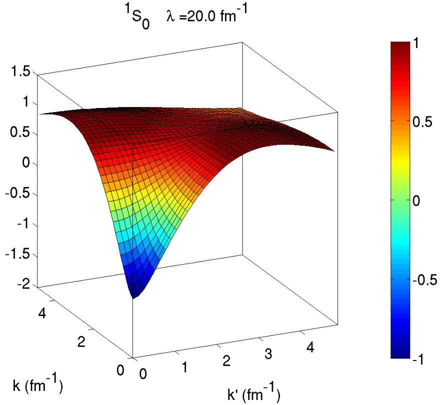
$$\frac{dH_s}{ds} = \frac{dV_s}{ds} = [[G_s, H_s], H_s]$$

- G_s determines flow $\Longrightarrow$ Many choices! (e.g., $G_s = T$)

What is the Similarity Renormalization Group (SRG)?

$$H_s = U(s) H U^\dagger(s) \Longrightarrow \frac{dH_s}{ds} = [[T_{rel}, H_s], H_s] \quad (\lambda = 1/s^{1/4})$$





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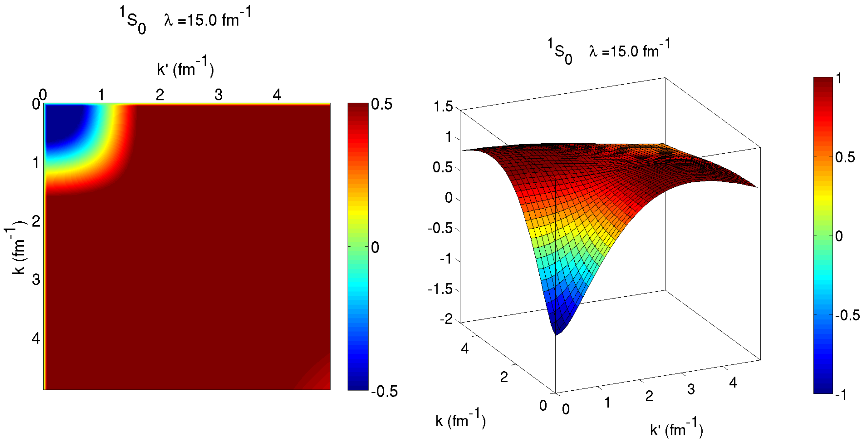

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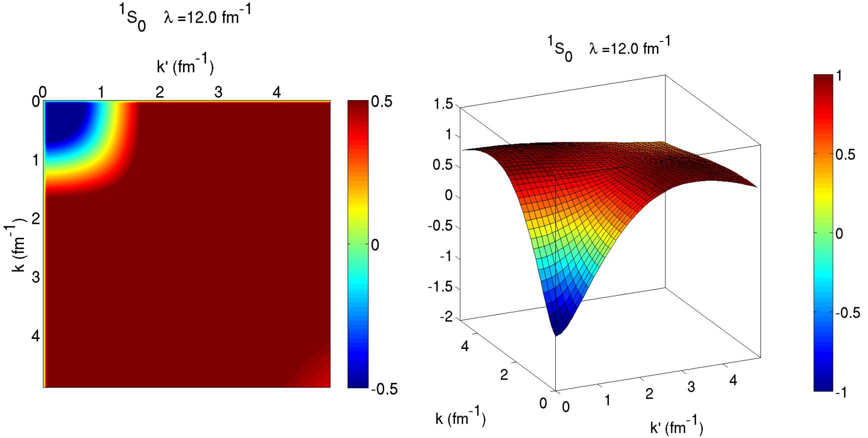

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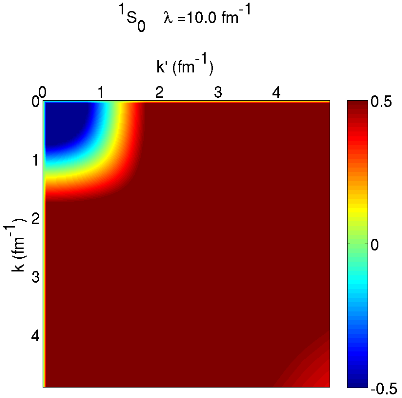

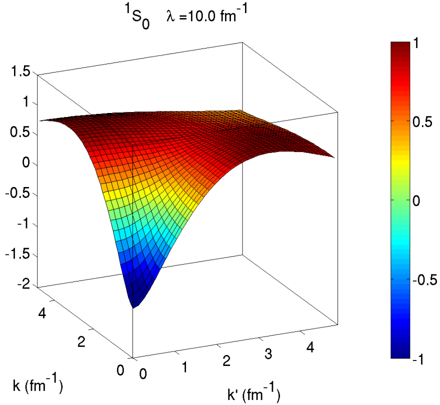

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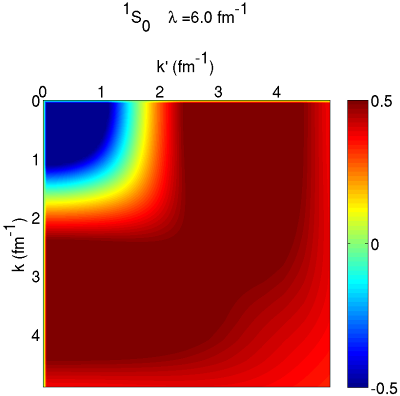

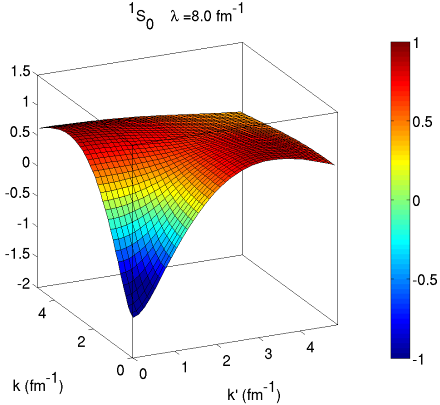

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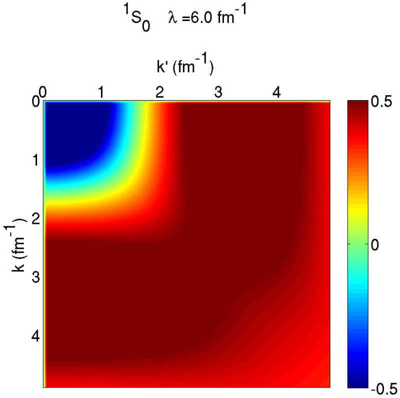

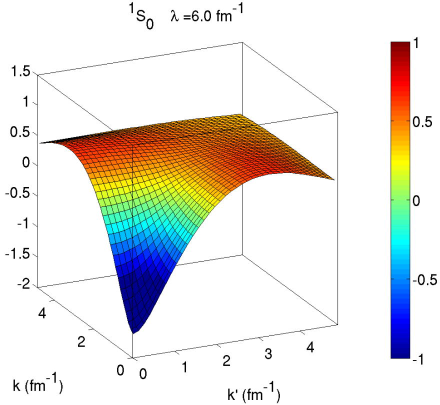

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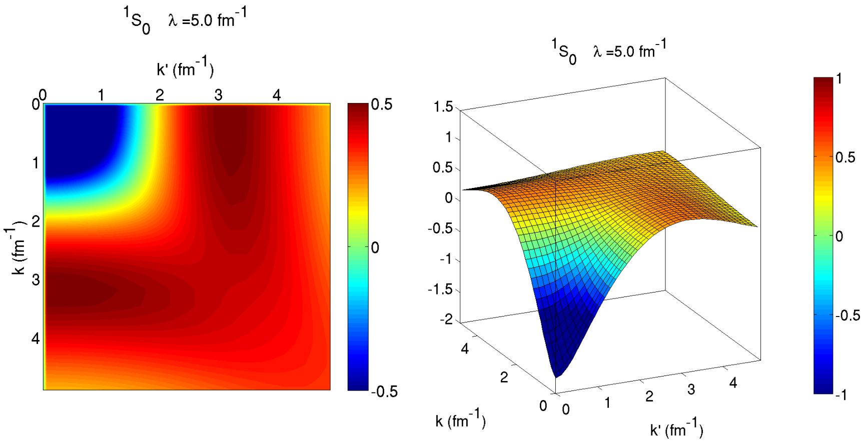

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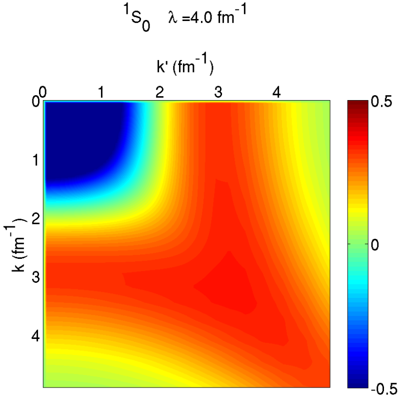

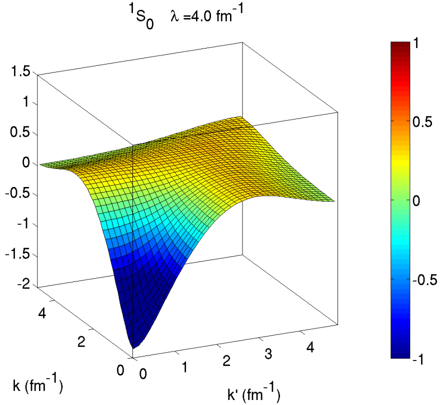

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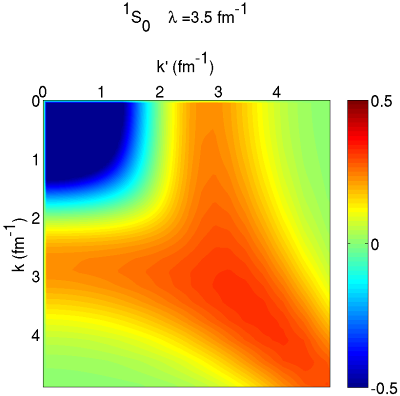

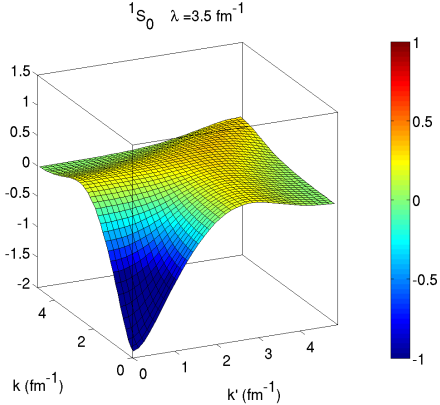

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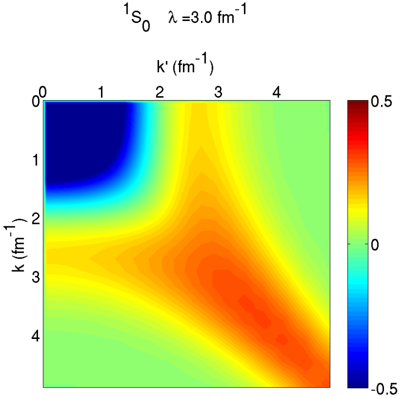

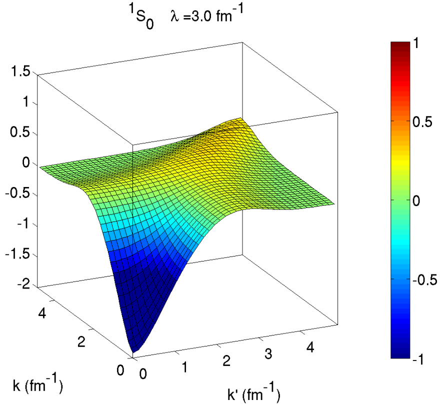

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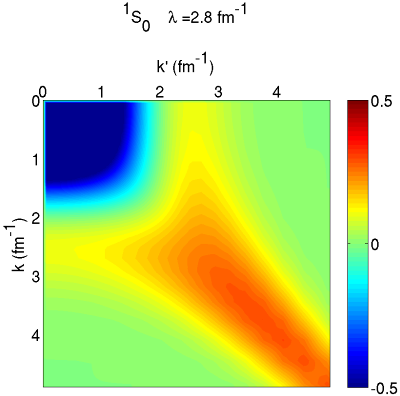

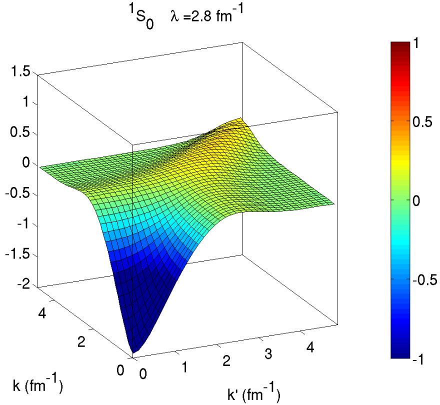

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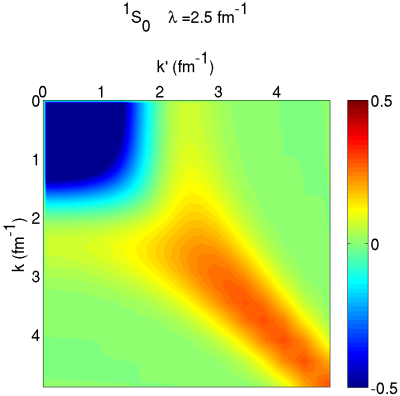

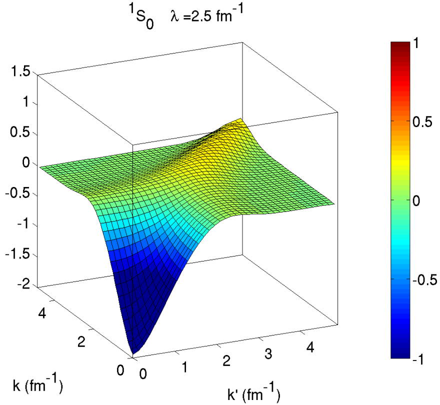

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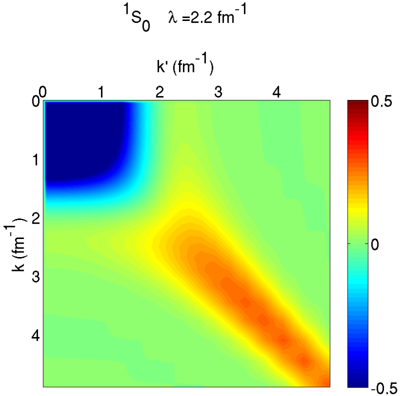

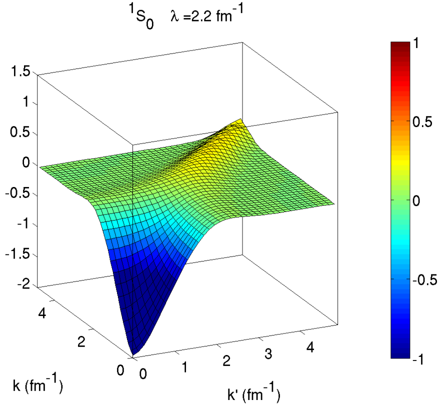

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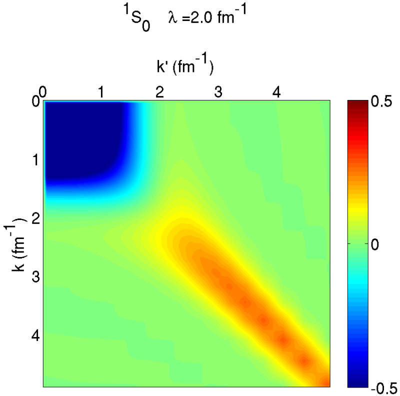
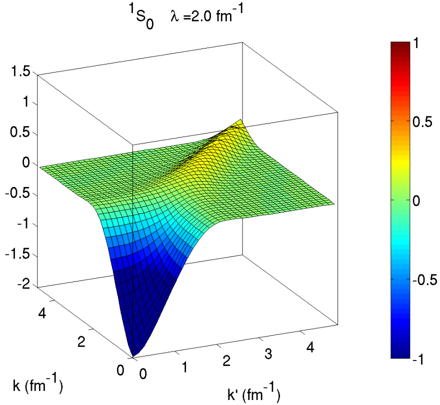
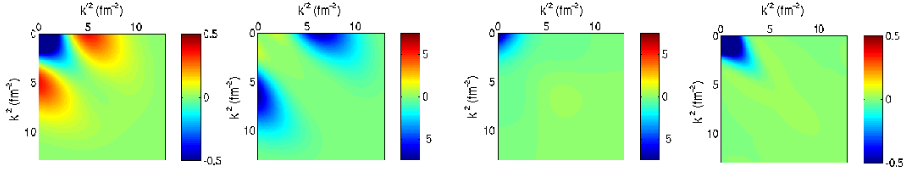




The Mechanics of Decoupling

$$\frac{dV_\lambda}{d\lambda} \propto [[T, V_\lambda], T + V_\lambda] \quad (\epsilon_k \equiv k^2/M)$$

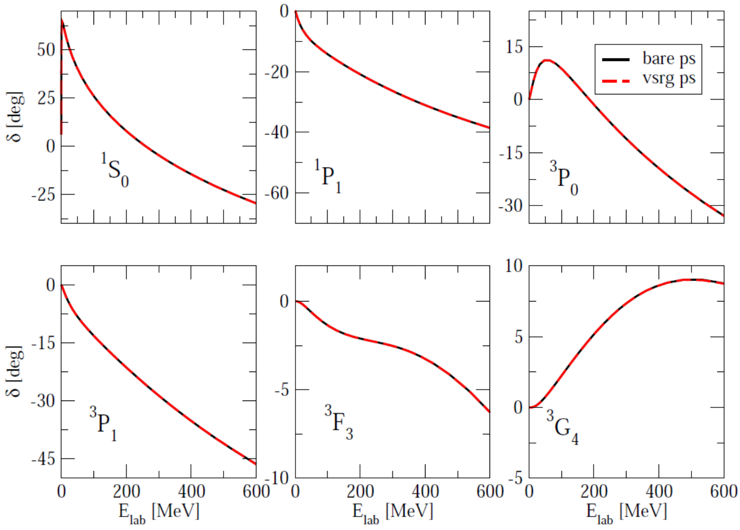
$$\frac{dV_\lambda(k,k')}{d\lambda} = -(\epsilon_k - \epsilon_{k'})^2 V_\lambda(k,k') + \sum_q (\epsilon_k + \epsilon_{k'} - 2\epsilon_q) V_\lambda(k,q) V_\lambda(q,k')$$



$V_{\lambda=2.5}$ $+$ 1st term $+$ 2nd term $\rightarrow$ $V_{\lambda=1.5}$

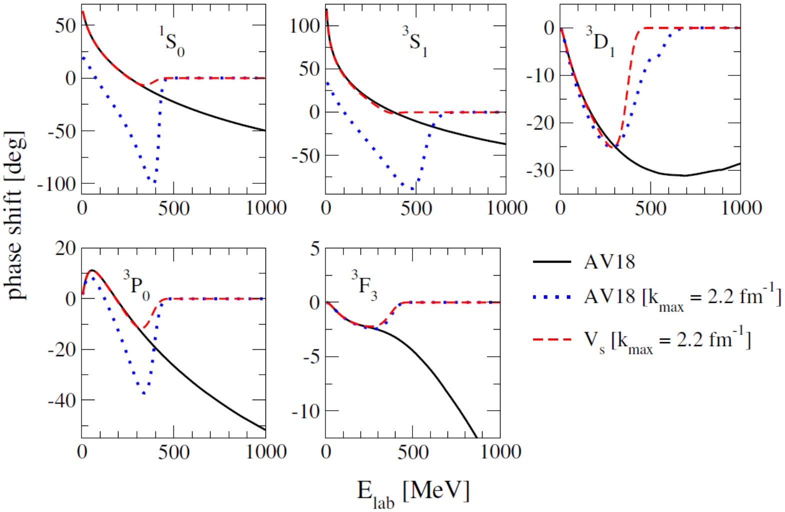
- Off-diagonal elements
  $\Longrightarrow V_\lambda(k,k') \propto V_{NN}(k,k') e^{-[(\epsilon_k - \epsilon_{k'})/\lambda^2]^2}$
- Relevant physics flows to low momentum elements

Unitary Transformations ⟹ Preserve Observables



Now Low-Pass Filters Work!

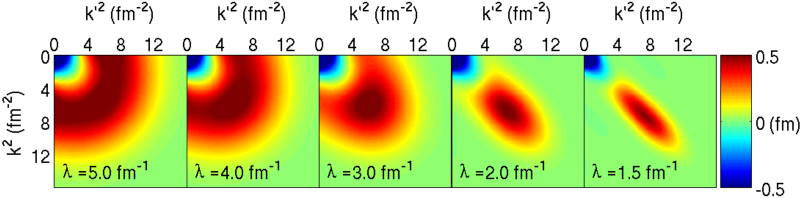
- Phase shifts with $V_s(k, k') = 0$ for $k, k' > k_{max}$



- Tested quantitatively in arXiv: 0711.4252 and 0801.1098

Flow of N^{3}LO Chiral EFT Potentials

- $^1S_0$ from N^{3}LO (500 MeV) of Entem/Machleidt



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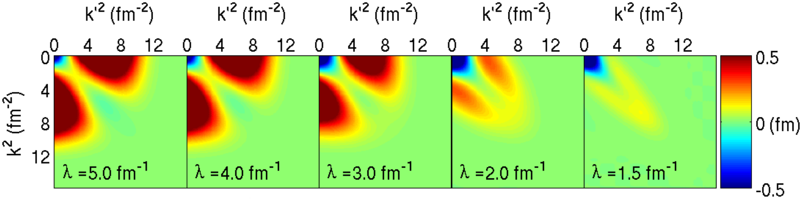

- See http://www.physics.ohio-state.edu/∼ntg/srg/ for more!

Flow of N^{3}LO Chiral EFT Potentials

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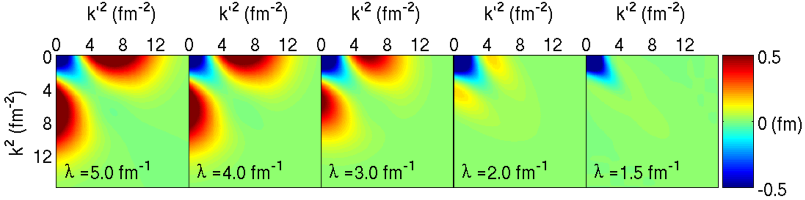

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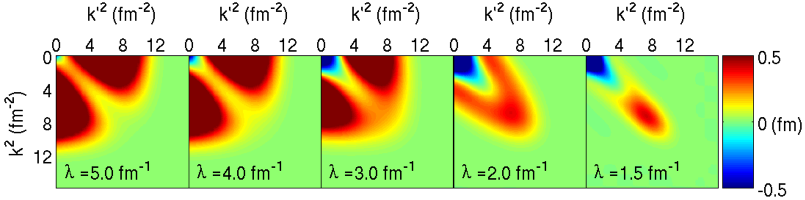

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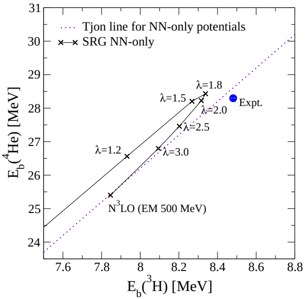
Many-Body Forces

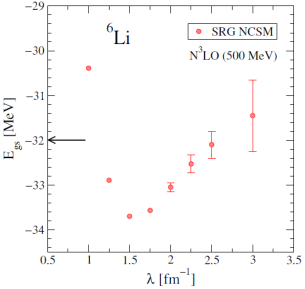
- Why do we need many-body forces?
  - 3NFs arise from eliminating dof's
  - Omitting 3NFs leads to model dependence (Tjon line)
  - 3NF saturates nuclear matter correctly
  - Many-body methods must deal with them (e.g., CI,CC,...)
- SRG will induce many-body forces!

$$\frac{dV}{ds} = [[\sum a^\dagger a, \sum \underbrace{a^\dagger a^\dagger a a}_{2-body}], \sum \underbrace{a^\dagger a^\dagger a a}_{2-body}]$$

$$= \ldots + \sum \underbrace{a^\dagger a^\dagger a^\dagger a a a}_{3-body!} + \ldots$$

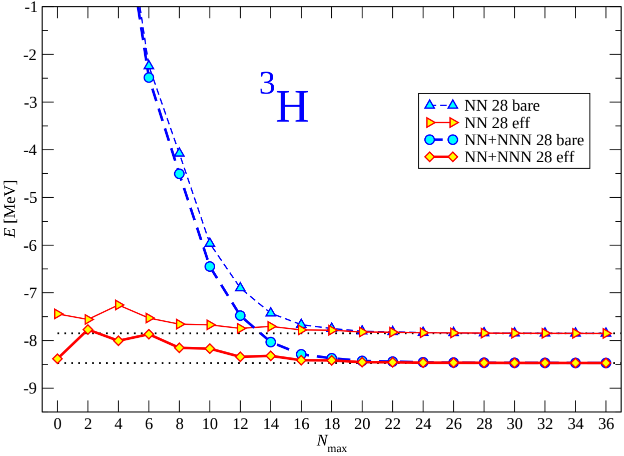
  - Stop evolution if induced 3NF becomes unnatural
  - RG flows with SRG extend consistently to many-body spaces
  - Recent progress: 3NF evolved!!!





Current Realistic NCSM Calculations

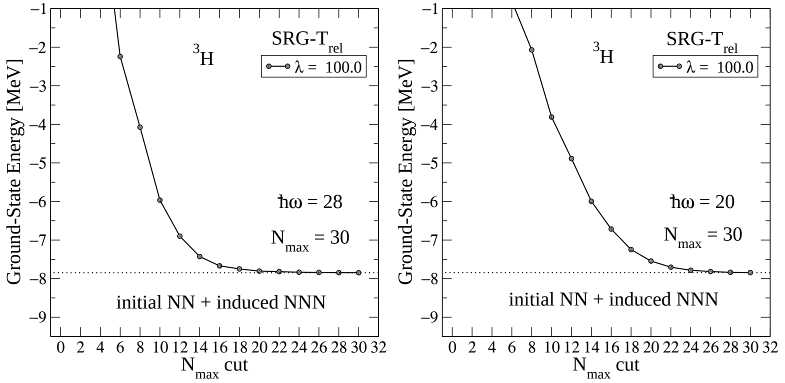
- Triton calculations from P. Navratil (arXiv:0707.4680)



- "eff" ≡ Lee-Suzuki: Generated in large space and cut down with LS
- 3NF is N2LO
- $N_{max} = 40$ converged to within 5keV

- 3NF parameters c_E and c_D are fit to two observables

Evolving NN Forces in NCSM A=3 space



- Unitary evolution of initial NN-only forces!
  - Currently using MATLAB: working toward parallelization
- $\hbar\omega = 28$ is optimal for initial interaction, $\hbar\omega = 20$ for $\lambda = 2$
  - Trade-off in convergence under investigation

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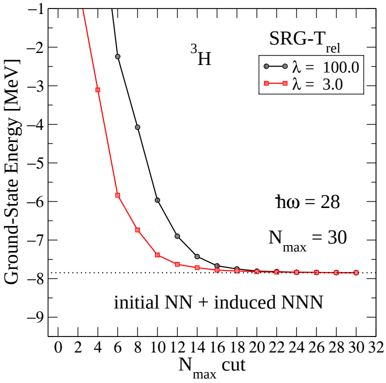

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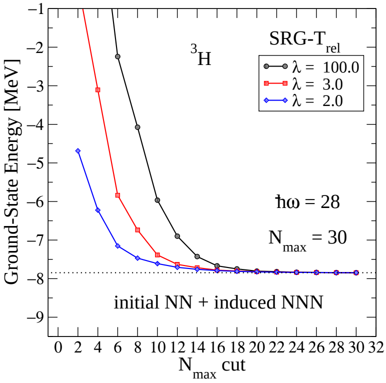
- $\hbar\omega = 28$ is optimal for initial interaction, $\hbar\omega = 20$ for $\lambda = 2$
  - Trade-off in convergence under investigation

Evolving NN Forces in NCSM A=3 space



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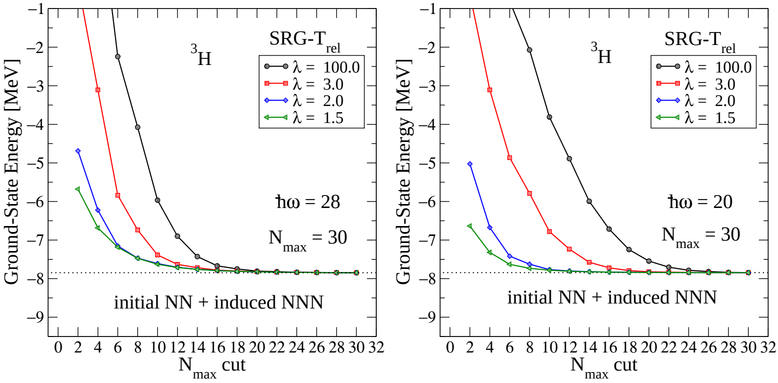

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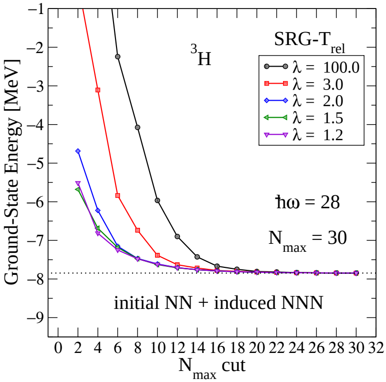

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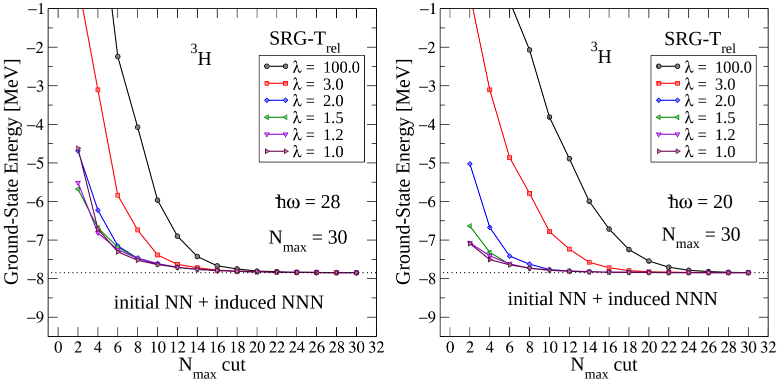

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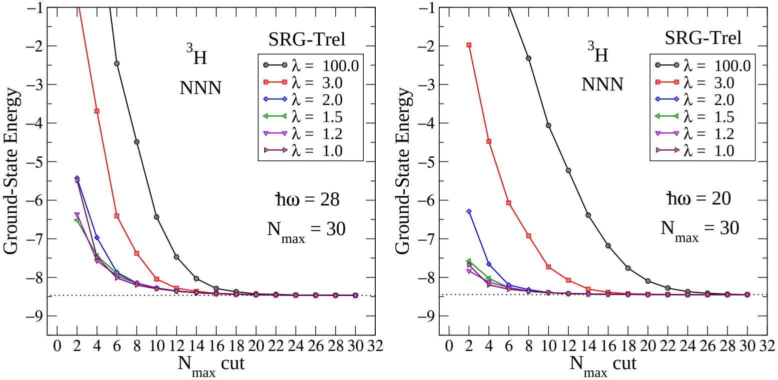
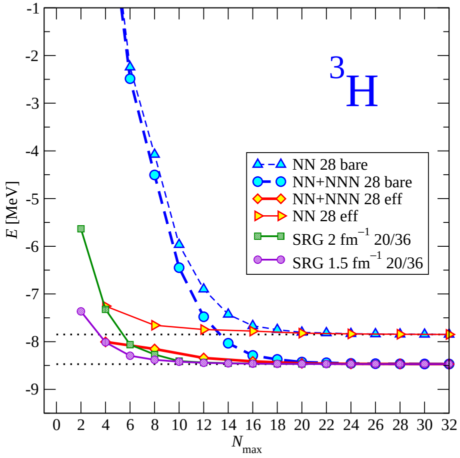
Evolving Three-Body Forces in NCSM!



- Same plots but now including an initial 3NF from N2LO
- Unitary evolution in $A = 3 \implies$ Triton experimental energy preserved

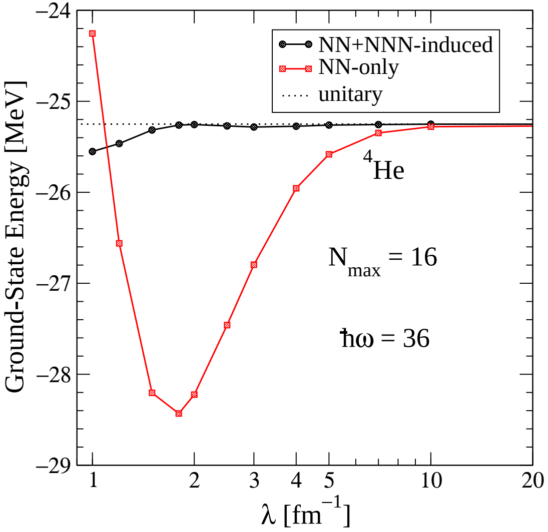
Comparing the SRG to Lee-Suzuki

- SRG converges rapidly and smoothly from above



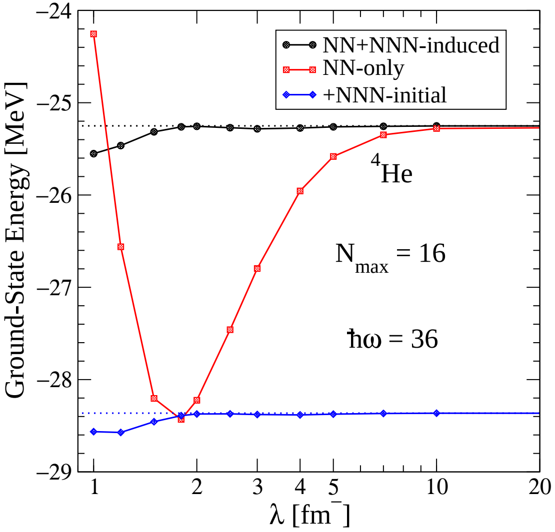
- What about the size of induced 4NFs in ^{4}He?

^{4}He results: Brand New!!!



- Low nmax: not fully converged
- Encouraging results even for preliminary procedure
- very small induced 4NF at $\lambda = 2$

^{4}He results: Brand New!!!



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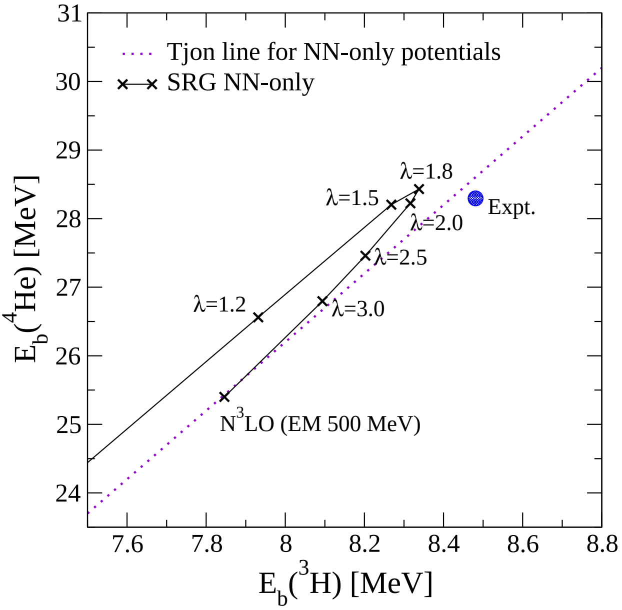
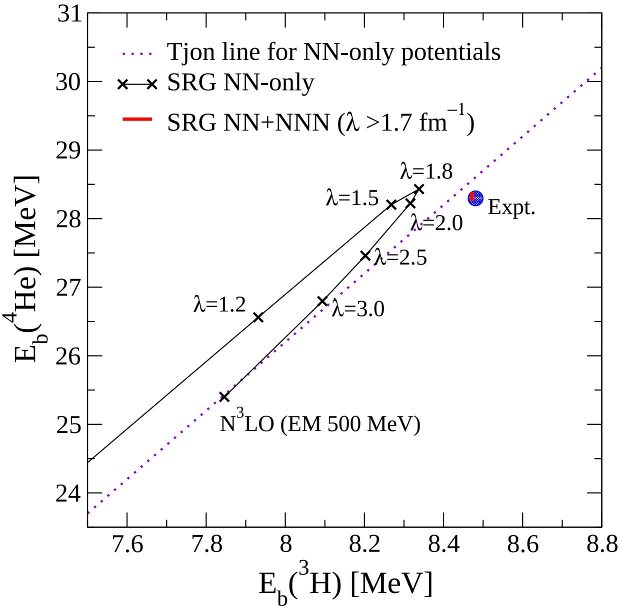
Tjon Line



Tjon line for NN-only potentials
SRG NN-only
λ=1.8
λ=1.5
λ=2.0
λ=2.5
λ=1.2
λ=3.0
Expt.
N³LO (EM 500 MeV)
$E_b(^4He)$ [MeV]
$E_b(^3H)$ [MeV]
31
30
29
28
27
26
25
24
7.6
7.8
8
8.2
8.4
8.6
8.8

Tjon Line



Tjon line for NN-only potentials
SRG NN-only
SRG NN+NNN (λ >1.7 fm^{-1})
λ=1.8
λ=1.5
λ=2.0
λ=2.5
λ=1.2
λ=3.0
Expt.
N^{3}LO (EM 500 MeV)
$E_b(^4He)$ [MeV]
$E_b(^3H)$ [MeV]
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30
29
28
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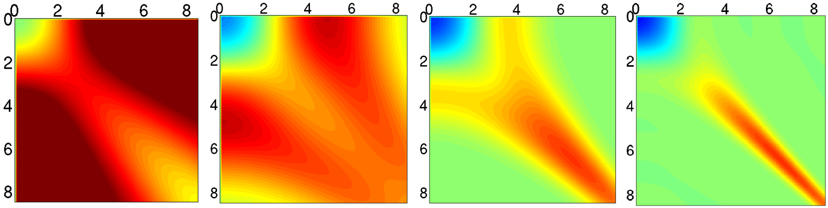
8.8

Insights from the One-Dimensional Model

- 1-D model: $V^{(2)}(x) = \frac{V_1}{\sigma_1\sqrt{\pi}} e^{-x^2/\sigma_1^2} + \frac{V_2}{\sigma_2\sqrt{\pi}} e^{-x^2/\sigma_2^2}$
  [Negele et al.: Phys.Rev.C **39** 1076 (1989)]

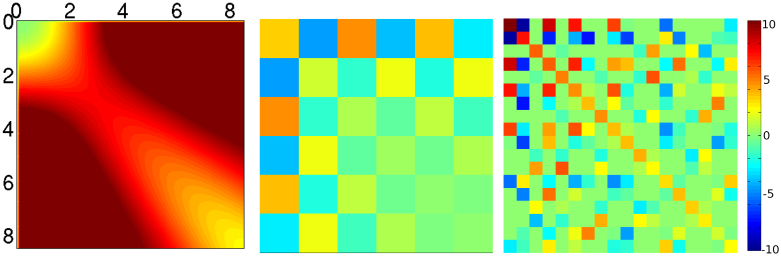


$\lambda = \infty$ $\lambda = 5$ $\lambda = 3$ $\lambda = 2$

- How do we handle many-body forces? $\longrightarrow$ use a discrete basis to avoid "dangerous" delta functions
- EDJ and R. J. Furnstahl - [arXiv:0809.4199]

Embedding: initial potential

- Symmetrized Jacobi Oscillator Basis (here: Bosons)
- EDJ and R. J. Furnstahl - [arXiv:0809.4199]

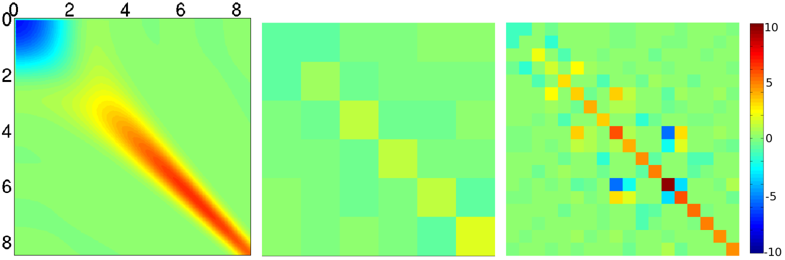


$V(p,p') \longrightarrow V(N_2,N_2') \longrightarrow V(N_3,N_3')$

- diagonalize symmetrizer $\Rightarrow \langle N_A || N_{A-1}; n_{A-1}\rangle$; use recursively
- 3D: Use Navratil et al. technology for NCSM
- embedding is everything, SRG coding is trivial

Embedding: evolved potential - $\lambda = 2$

- Symmetrized Jacobi Oscillator Basis (here: Bosons)
- EDJ and R. J. Furnstahl - [arXiv:0809.4199]



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- embedding is everything, SRG coding is trivial

Some many-body examples

Legend: Embedding, Evolving, BE calculation, Initial 3NF

- A=3 (2N only):

$$V^{(2)}_{osc} \overset{SRG}{\Longrightarrow} V^{(2)}_{\lambda,osc} \overset{embed}{\Longrightarrow} V^{(2)}_{\lambda,3Nosc} \overset{diag}{\Longrightarrow} BE^{(2Nonly)}_3$$

- A=4 (2N only):

$$V^{(2)}_{osc} \overset{SRG}{\Longrightarrow} V^{(2)}_{\lambda,osc} \overset{embed}{\Longrightarrow} V^{(2)}_{\lambda,3Nosc} \overset{embed}{\Longrightarrow} V^{(2)}_{\lambda,4Nosc} \overset{diag}{\Longrightarrow} BE^{(2Nonly)}_4$$

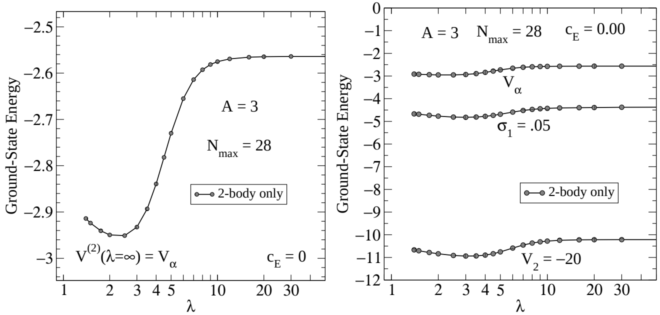
- A=4 (2N+3N only):

$$V^{(2)}_{osc} \overset{embed}{\Longrightarrow} V^{(2)}_{3Nosc} \overset{SRG}{\Longrightarrow} V^{(2+3)}_{\lambda,3Nosc} \overset{embed}{\Longrightarrow} V^{(2+3)}_{\lambda,4Nosc} \overset{diag}{\Longrightarrow} BE^{(2N+3Nonly)}_4$$

$$\overset{3NF}{\Longrightarrow} \quad + V^{(3init)}_{3Nosc} \ldots$$

Induced Many-Body Forces are Small - A=3

$$V^{(2)}(x) = \frac{V_1}{\sigma_1\sqrt{\pi}} e^{-x^2/\sigma_1^2} + \frac{V_2}{\sigma_2\sqrt{\pi}} e^{-x^2/\sigma_2^2}$$



- Basis independent: same evolution in momentum or HO basis
- Black: Same evolution pattern for 2-body only as 3D NN-only

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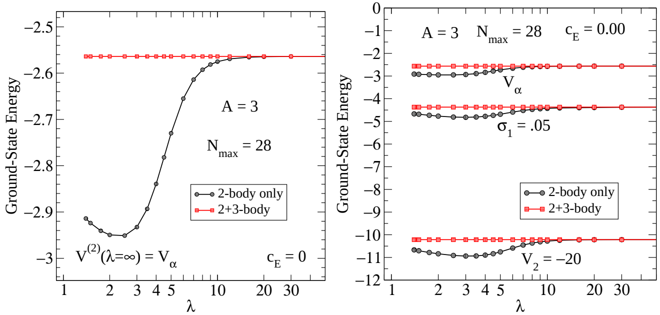
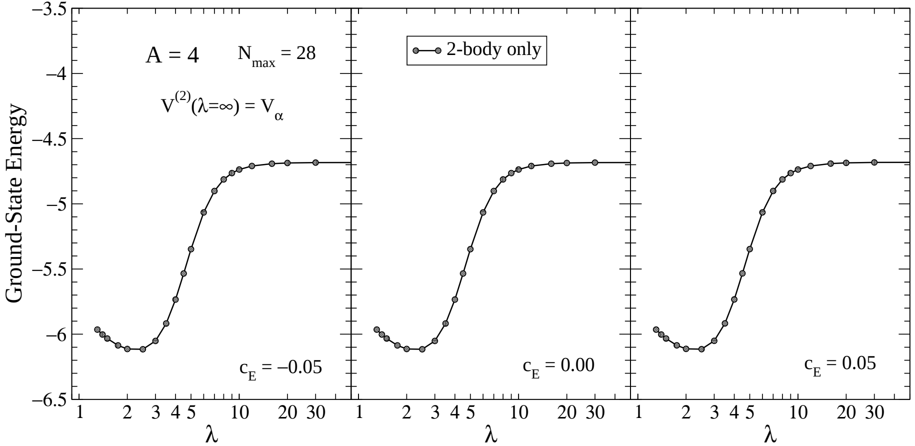


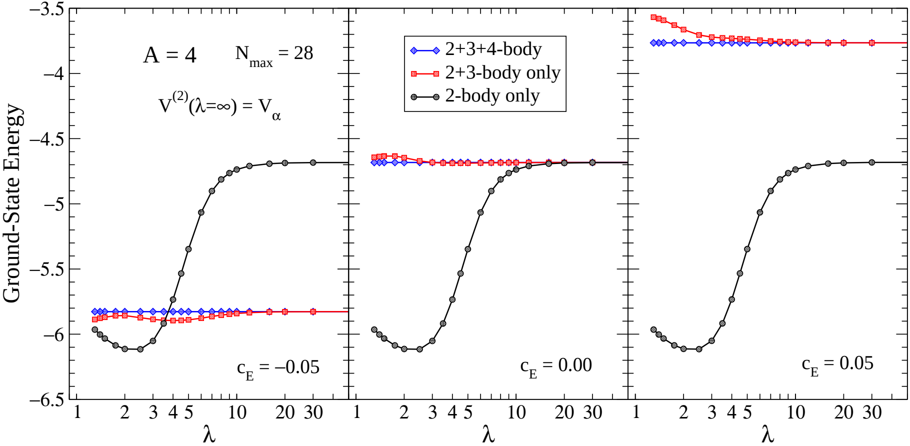
- Basis independent: same evolution in momentum or HO basis
- Black: Same evolution pattern for 2-body only as 3D NN-only
- Red: Three-body forces induced - Unitary!

Induced Many-Body Forces are Small - A=4



$$V^{(3)}(p,q,p',q') = c_E e^{-((p'^2+q'^2)/\Lambda^2)^n} e^{-((p^2+q^2)/\Lambda^2)^n} \quad (\Lambda = 2 \quad n = 4)$$

Induced Many-Body Forces are Small - A=4



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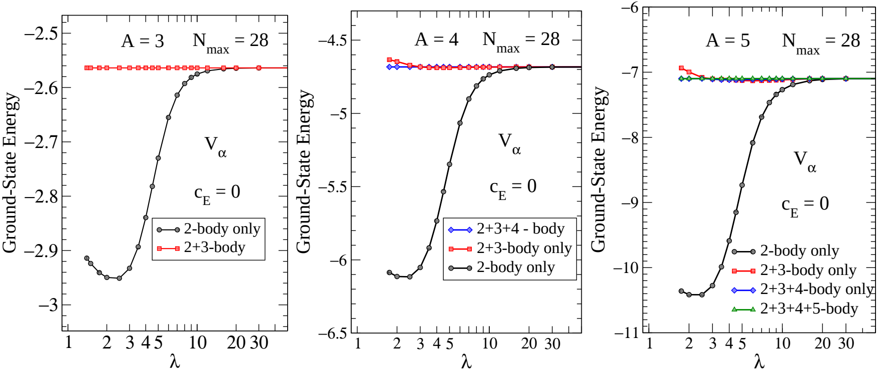
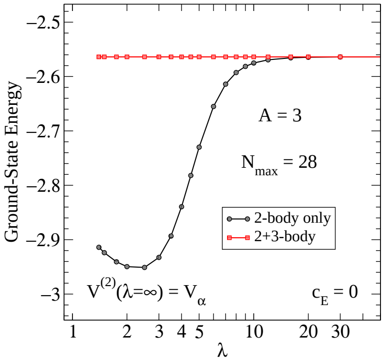
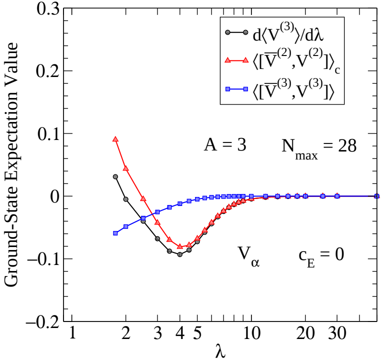
Induced Many-Body Forces are Small - A=5



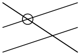
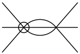
- Five-body force is negligible
- Hierarchy of induced many-body forces

$$\frac{d}{d\lambda}\langle\psi_\lambda^{(3)}|V_\lambda^{(3)}|\psi_\lambda^{(3)}\rangle = \langle\psi_\lambda^{(3)}|[\overline{V}_\lambda^{(2)}, V_\lambda^{(2)}]_c - [\overline{V}_\lambda^{(3)}, V_\lambda^{(3)}]|\psi_\lambda^{(3)}\rangle$$



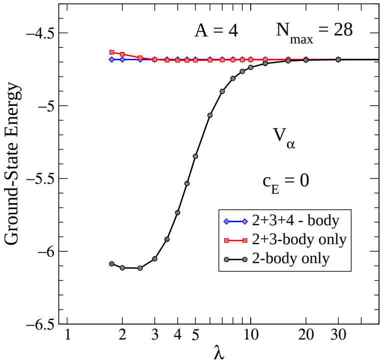


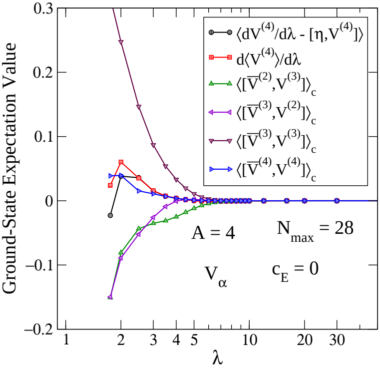
- Majority evolution dominated by $[\overline{V}^{(2)}, V^{(2)}]$, $(\overline{V} \equiv [T, V])$
- Hierarchy of contributions

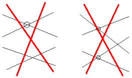
 > 

$V^{(4)}$ analysis

$$\frac{d}{d\lambda}\langle\psi_\lambda^{(4)}|V_\lambda^{(4)}|\psi_\lambda^{(4)}\rangle = \langle\psi_\lambda^{(4)}|[\overline{V}_\lambda^{(2)}, V_\lambda^{(3)}]_c + [\overline{V}_\lambda^{(3)}, V_\lambda^{(2)}]_c + [\overline{V}_\lambda^{(3)}, V_\lambda^{(3)}]_c - [\overline{V}_\lambda^{(4)}, V_\lambda^{(4)}]|\psi_\lambda^{(4)}\rangle$$

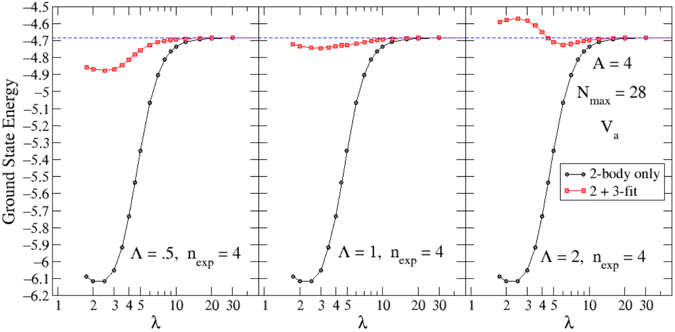




- No $[\overline{V}^{(2)}, V^{(2)}]$: 
- $\therefore$ Induced 4-body is small - Hierarchy persists

Fitting Three-Body Force Evolution

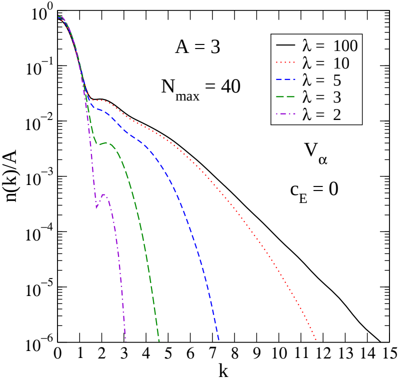
- Evolve in two-particle oscillator space → fit 3-body parameters to missing energy
- One term $V^{(3)} = Ce^{-[(k^2+k'^2)/\Lambda^2]^n}$ reduces λ dependence to the 80-90% level.

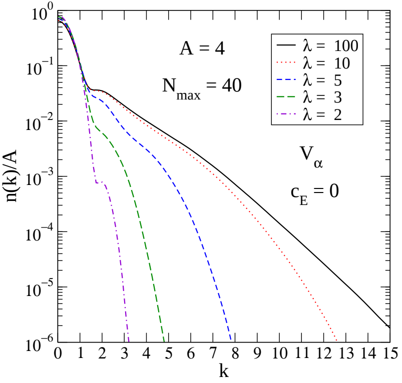


- Future work: add a second, short distance 3NF term with a gradient correction to test systematic reduction

Operator Evolution

- $H_s = U_s^\dagger H_0 U_s \Longrightarrow U_s = \sum_i |\psi_i(0)\rangle\langle\psi_i(s)|$
- Here unevolved operator $(a^\dagger a)$ with evolved wavefuntions

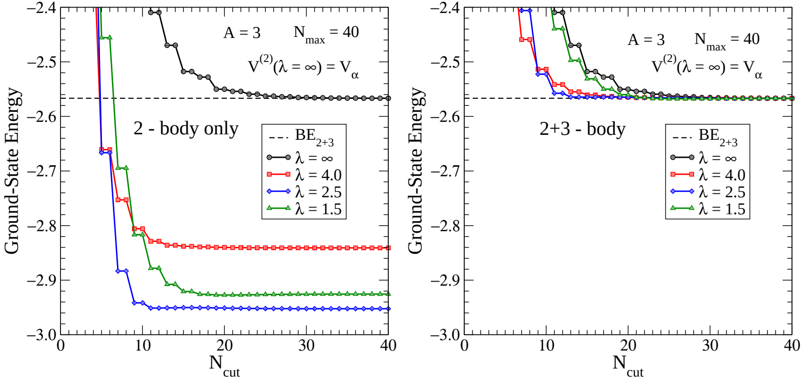




- More of this to come from E. R. Anderson

Decoupling in the Oscillator Basis

$\Rightarrow$ Evolve with T_{rel} and cut off to study decoupling

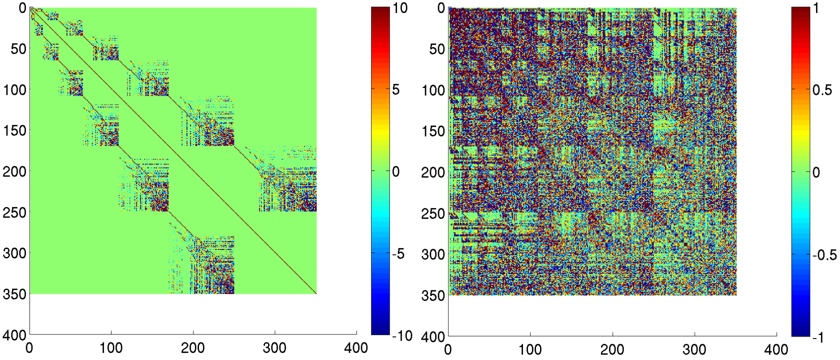


SRG space: 2-body only 3-body

- Decoupling not straightforward with T_{rel} SRG
- Decoupling improves until some λ and then degrades
- What about other SRG generators?

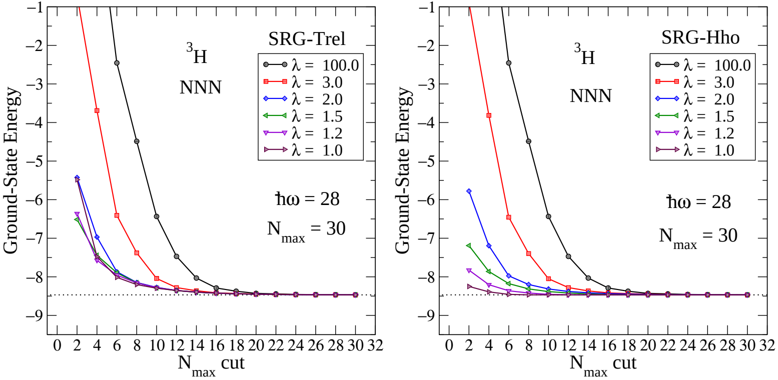
Using other SRG Generators

- Matrices in NCSM basis for $T_{\rm rel}$ and V



- In this basis T_{rel} will not drive to diagonal
- Harmonic Oscillator Hamiltonian ($H_{\rm ho} = T_{\rm rel} + V_{\rm ho}$) is diagonal in this basis

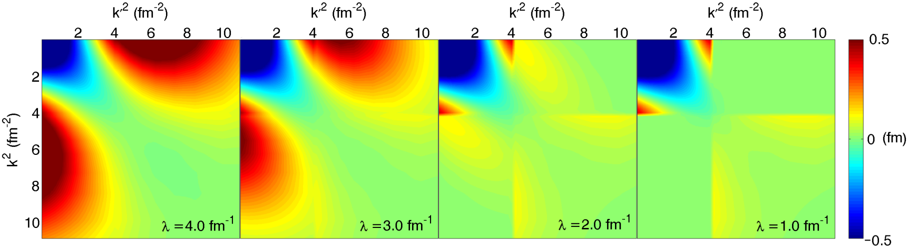
Using $G = H_{ho}$ improves convergence dramatically



- Compare T_{rel} on the left with H_{ho} on the right
- Work in progress: Spurious bound states contaminate evolution with H_{ho} $\rightarrow$ need further investigation

Block-Diagonal SRG: [arXiv:0801.1098]

- [Anderson, Bogner, Furnstahl, EDJ, Perry, Schwenk - arXiv:0801.1098]
- $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$
- $H_\infty = \begin{pmatrix} PH_\infty P & 0 \\ 0 & QH_\infty Q \end{pmatrix} \Longrightarrow G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$



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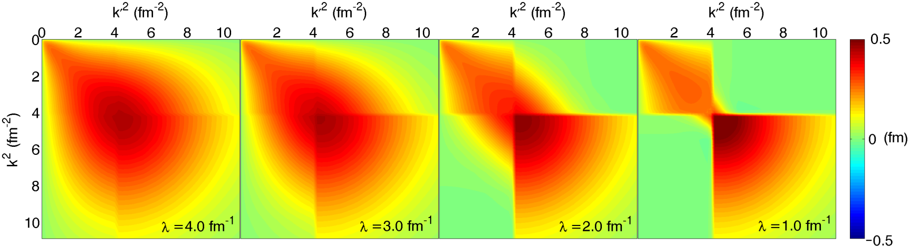


Recap

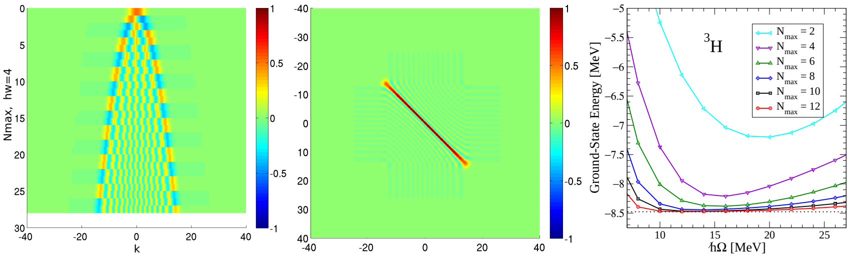
- SRG Decouples high- and low-energy DOF
- SRG is very flexible - can use different generators to evolve potentials
- One-D model gives proof-of-principle of many-body hierarchy
  - provides toolbox to gain intuition quickly - everything is directly applicable to 3D NCSM
- Results for 3NF evolution in the NCSM basis are very encouraging!

Future Work

- Some items to investigate
  - Operator evolution
  - SRG generators (H_{ho}, H_{BD}, H_D)
  - Basis issues
  - Fitting procedures
- All of these can be started in 3D now
- Door is opening quickly to other areas (CI,CC,...)

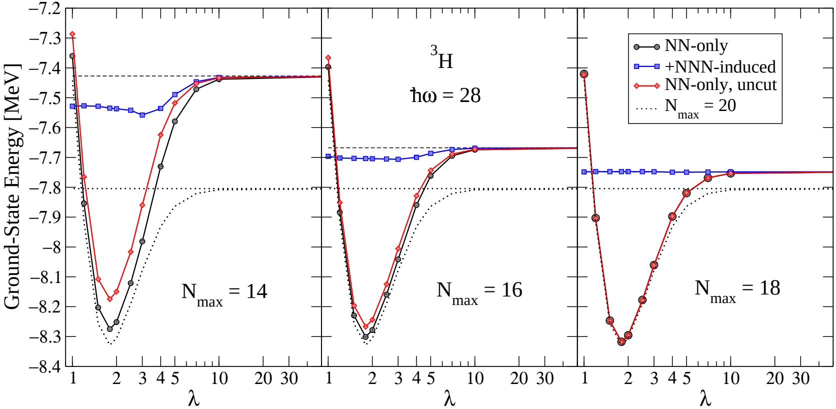
Extra Slides

Harmonic Oscillator Basis Overview



- HO wavefunction examples $\psi_n(k)$ with $\hbar\omega = 4$
- resulting truncated delta function
  $\widetilde{\delta}(k - k') = \sum_{n=0}^{N_{max}} |\psi_n(k)\rangle\langle\psi_n(k')|$
- tradeoff between small $\hbar\omega$ resolution and large $\hbar\omega$ scope
- bigger $N_{max} \rightarrow$ flatter in $\hbar\omega$
- optimal $\hbar\omega$ will shift with SRG evolution

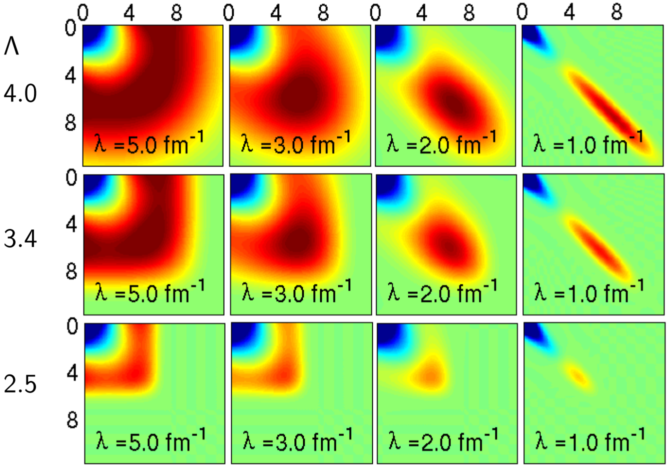
^{3}H results: Brand New!!!



- Good NN convergence even at $N_{max}=20$
- Try this another way (cut in A=2)

Testing Decoupling Quantitatively

- [EDJ, Bogner, Furnstahl, Perry - arXiv:0711.4252]



Tool for Study

1 - run SRG to λ

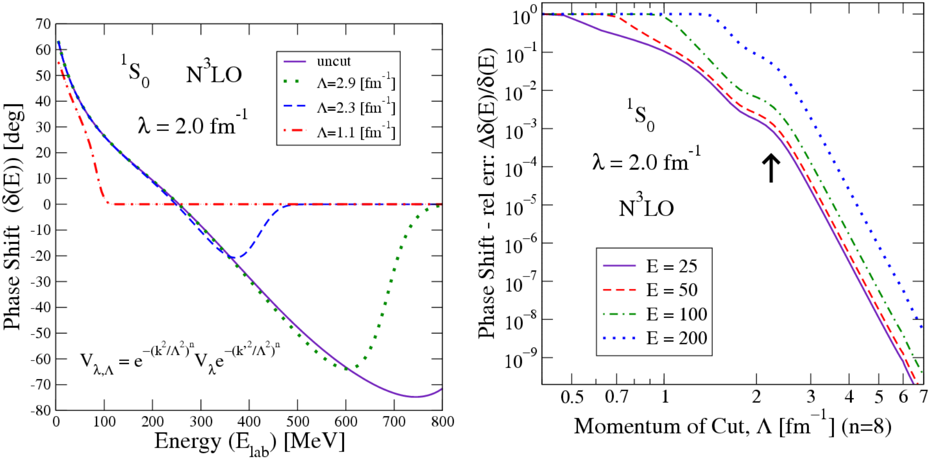
2 - set tail to zero

- $V_{s,\Lambda} = e^{-(\frac{k^2}{\Lambda^2})^n} V_s e^{-(\frac{k'^2}{\Lambda^2})^n}$
- n $=$ 4,8,12,...

3 - relative errors

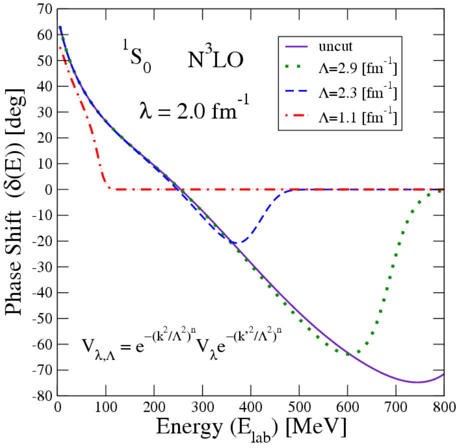
- $^1S_0$ Partial Wave, N^3LO (500 MeV) E/M

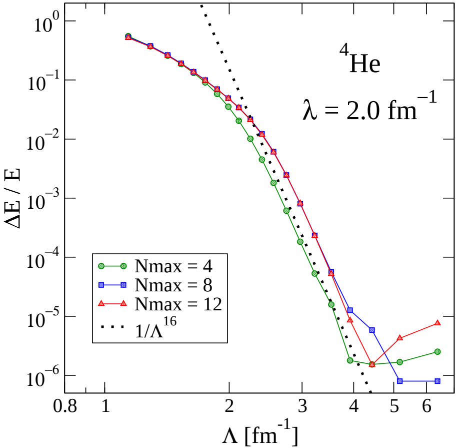
Decoupling above λ



- Decoupling clean and universal for all observables!

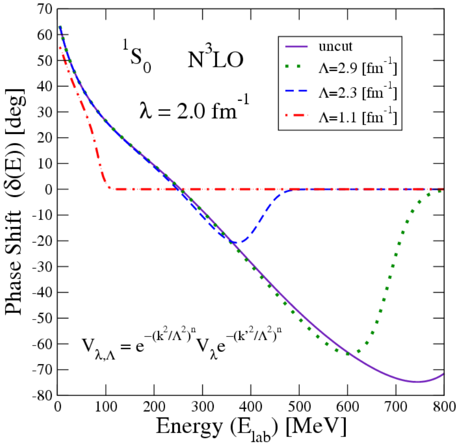
Decoupling above λ

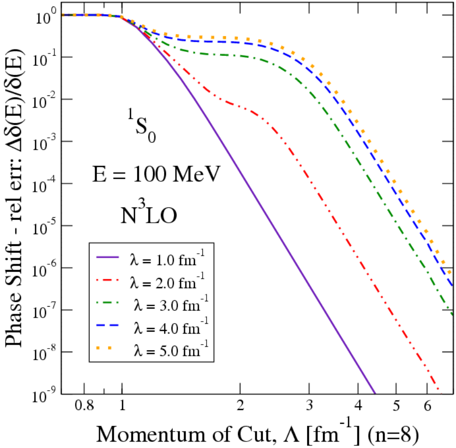




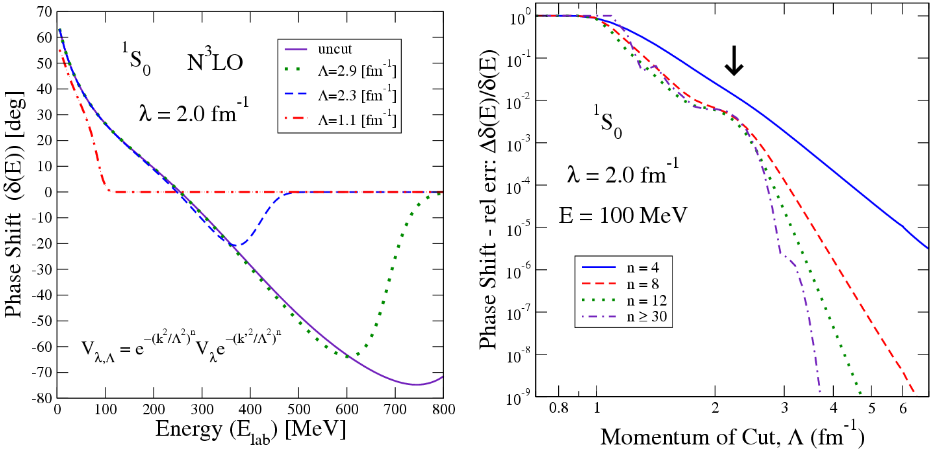
- Decoupling clean and universal for all observables!

Phase Shifts:Decoupled above λ - vary λ





- Relevant physics flows to low momentum → Decoupling!

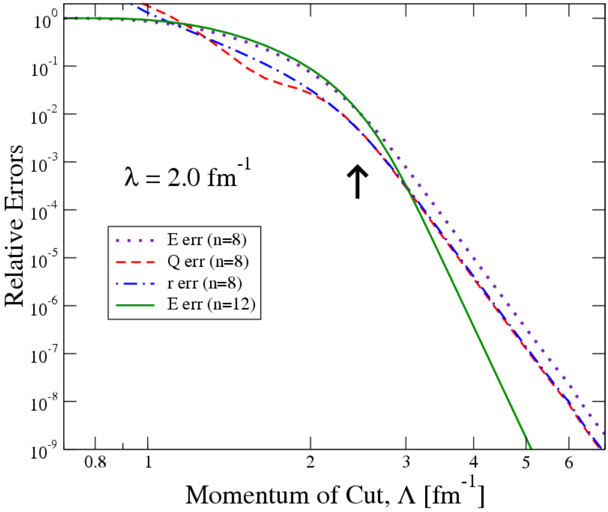


- Relevant physics flows to low momentum → Decoupling!

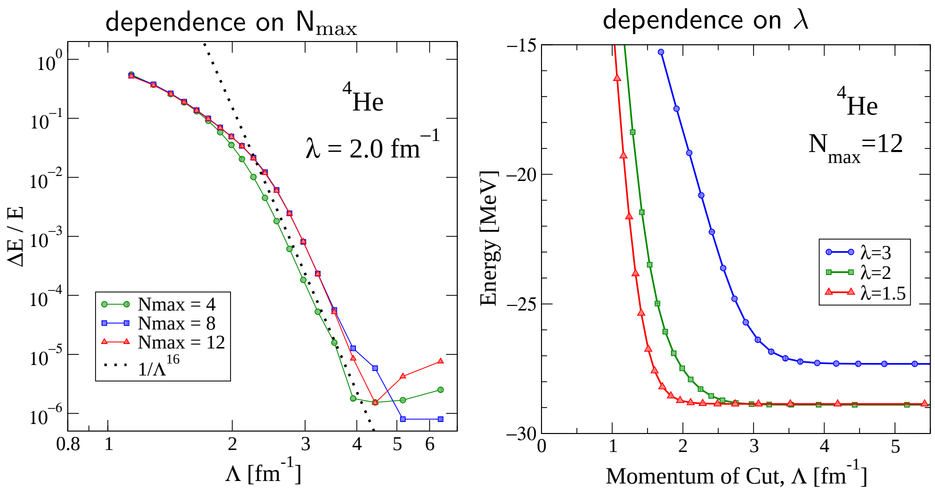
Deuteron Observables

Deuteron Observables

- Binding Energy
- Quadrupole Moment
- RMS radius

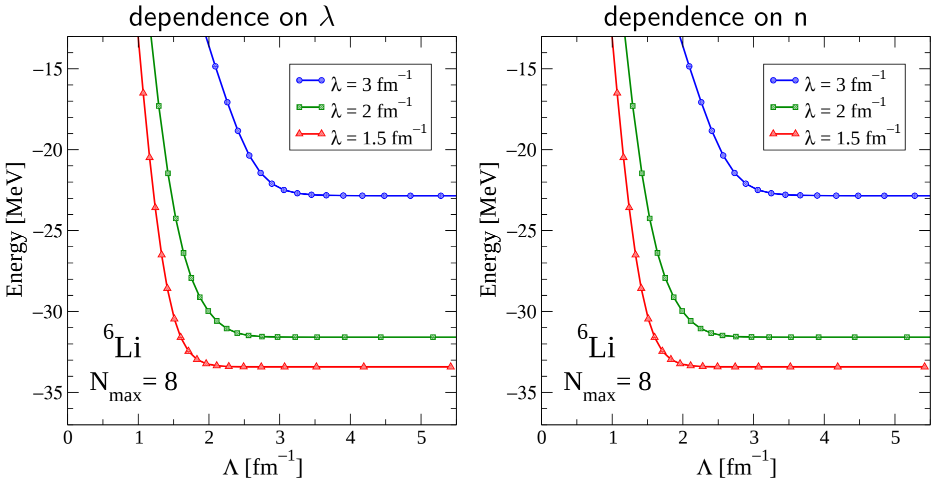


^{4}He Energy using No Core Shell Model



- SRG improves convergence with basis size in NCSM
- NN-only $\Longrightarrow$ different ^{4}He Binding Energies

^{6}Li Energy using No Core Shell Model



- SRG improves convergence with basis size in NCSM
- NN-only $\Longrightarrow$ different ^{6}Li Binding Energies

Block Diagonalization

- See edj et al.: arXiv:0801.1098

$$\mathrm{Goal} \longrightarrow \mathrm{H}_\infty = \begin{pmatrix} PH_\infty P & 0 \\ 0 & QH_\infty Q \end{pmatrix}$$

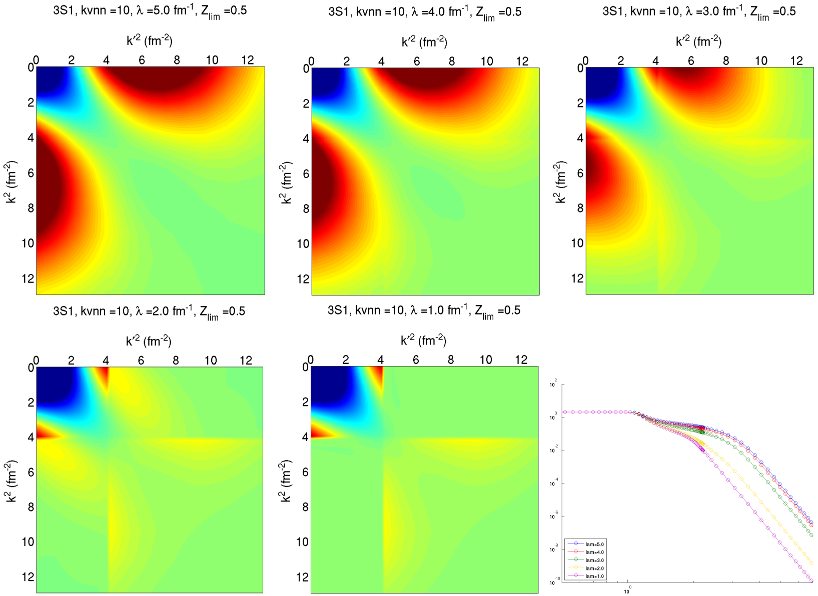
$$\mathrm{SRG} \longrightarrow \frac{\mathrm{dH_s}}{\mathrm{ds}} = [\eta_\mathrm{s}, \mathrm{H_s}] = [[\mathrm{G_s}, \mathrm{H_s}], \mathrm{H_s}]$$

$$\mathrm{sharp} \longrightarrow \mathrm{G_s} = \begin{pmatrix} PH_s P & 0 \\ 0 & QH_s Q \end{pmatrix}$$

$$\mathrm{smooth} \longrightarrow \mathrm{G_s} = \mathrm{fH_sf} + (1-\mathrm{f})\mathrm{H_s}(1-\mathrm{f})$$

$$f(k) = e^{-(k^2/\Lambda_{BD}^2)^n}$$

Block-Diagonal SRG - Sharp



Block-Diagonal SRG - Smooth (n=4)