Atomic Nuclei at Low Resolution

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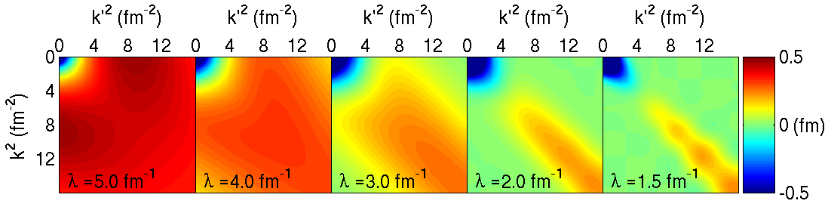
Department of Physics
Ohio State University

July, 2013

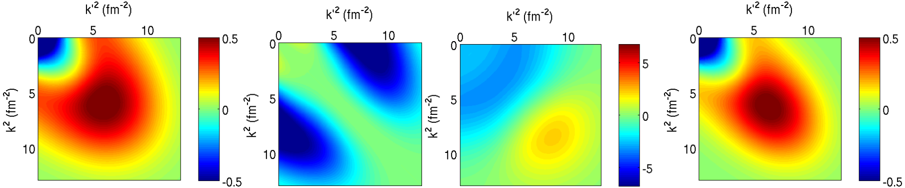


Flow in momentum basis with $\eta(s) = [T, H_s]$

- For $A = 2$, project on rel. momentum states $|k\rangle$, but generic

$$\frac{dV_s}{ds} = [[T_{\rm rel}, V_s], H_s] \qquad \text{with} \quad T_{\rm rel}|k\rangle = \epsilon_k|k\rangle \quad \text{and} \quad \lambda^2 = 1/\sqrt{s}$$

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



$V_{\lambda=3.0}(k,k')$ 1st term 2nd term $V_{\lambda=2.5}(k,k')$

- First term drives $^1S_0$ V_λ toward diagonal:

$$V_\lambda(k,k') = V_{\lambda=\infty}(k,k')\, e^{-[(\epsilon_k - \epsilon_{k'})/\lambda^2]^2} + \cdots$$

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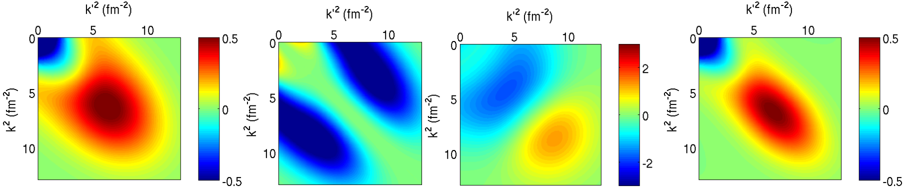

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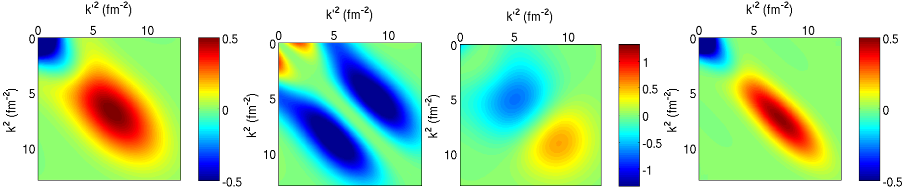

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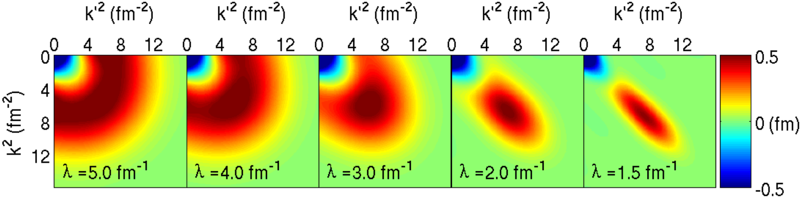
Flow of different N^3LO chiral EFT potentials

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



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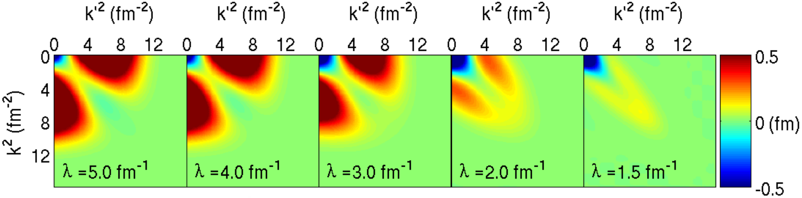

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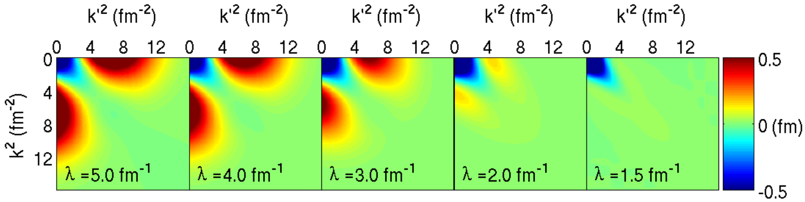

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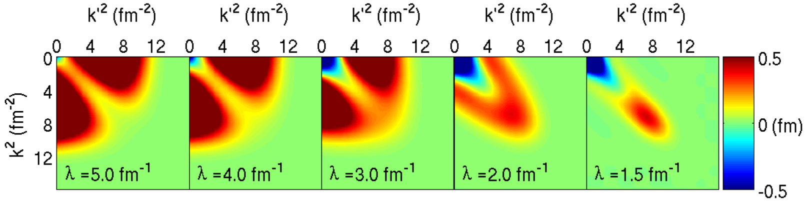

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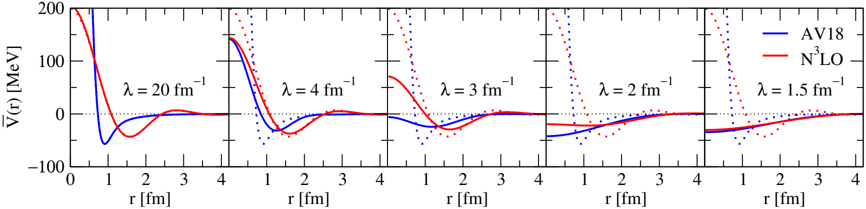
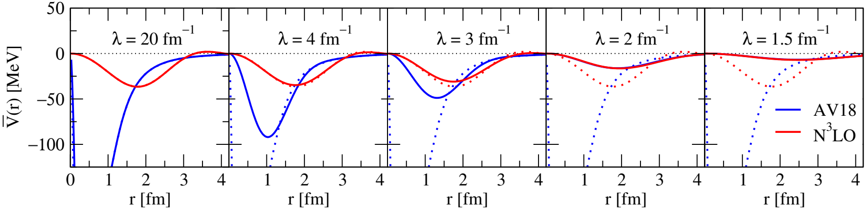
Visualizing the softening of NN interactions

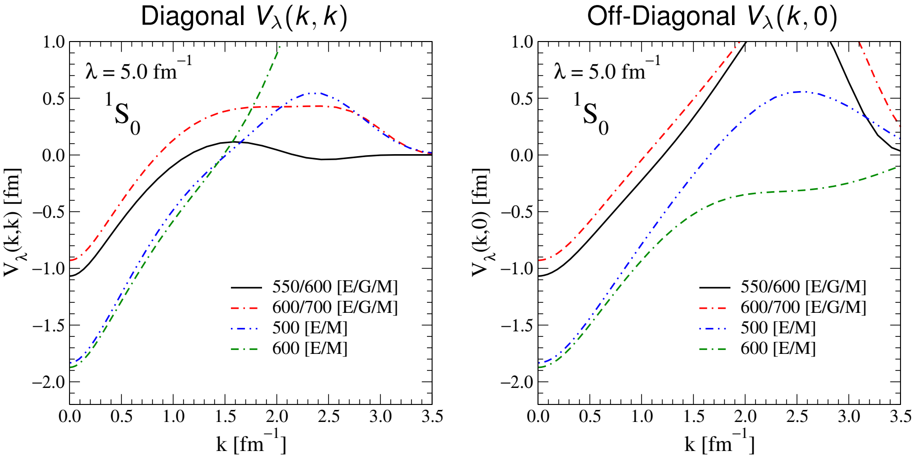
- Project non-local NN potential: $\overline{V}_\lambda(r) = \int d^3r'\, V_\lambda(r, r')$
  - Roughly gives action of potential on long-wavelength nucleons
- Central part (S-wave) [Note: The V_λ's are all phase equivalent!]



- Tensor part (S-D mixing) [graphs from K. Wendt]



Run to lower λ via SRG $\Longrightarrow \approx$Universal V_{NN}



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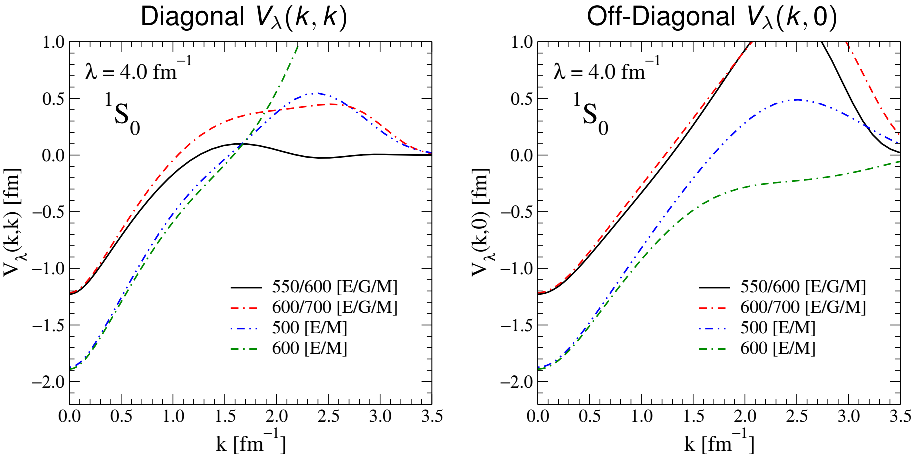

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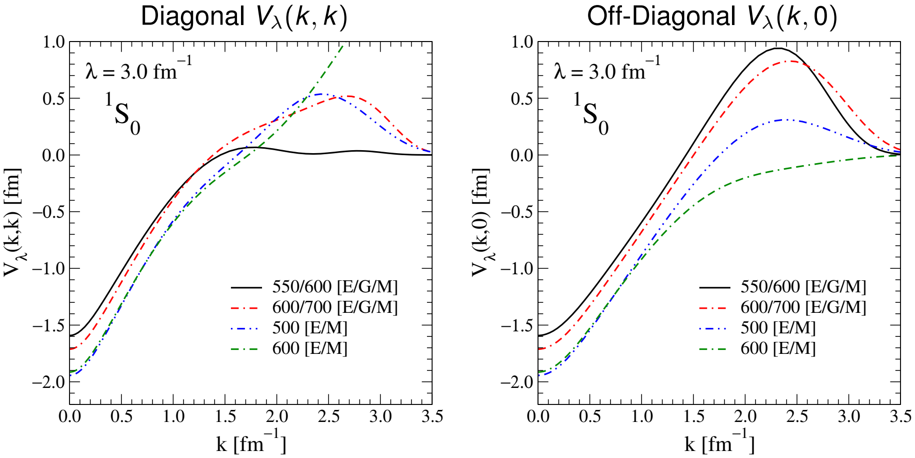

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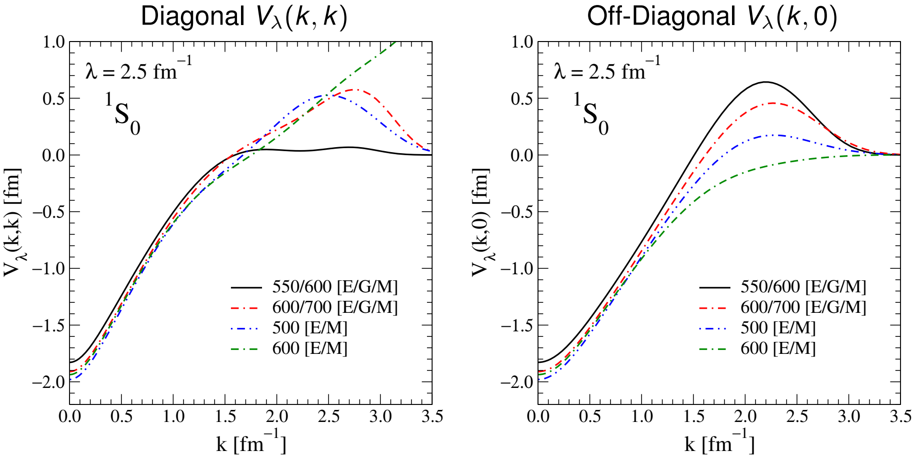

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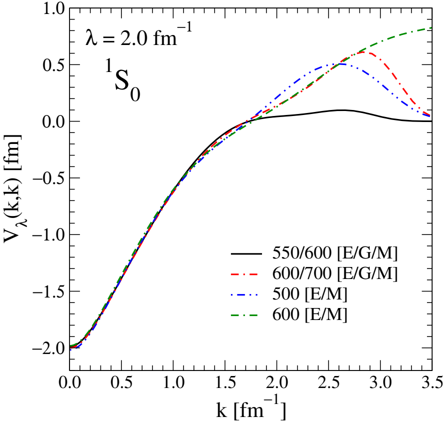
Diagonal $V_\lambda(k,k)$



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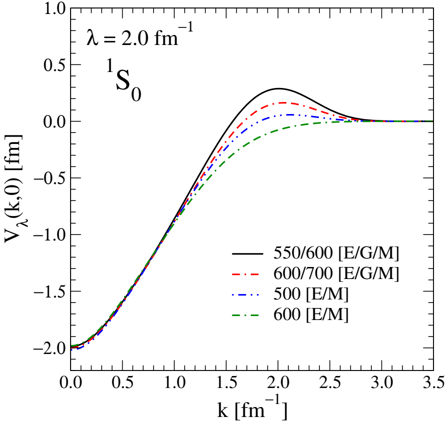

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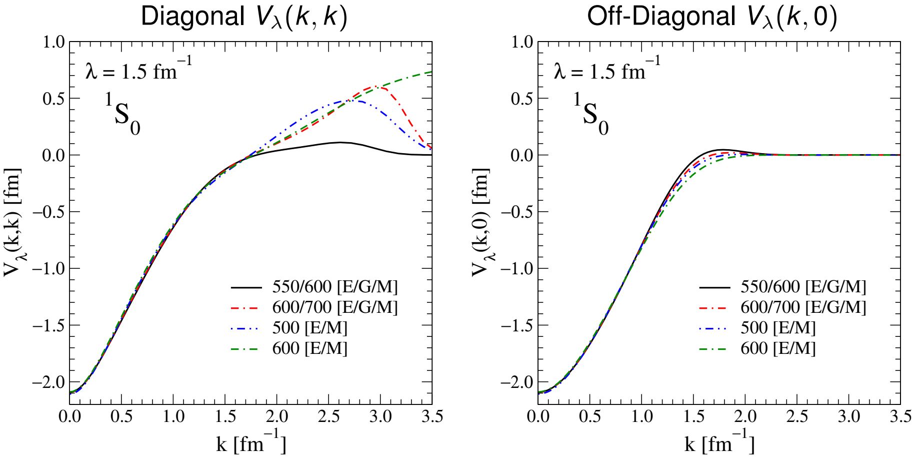

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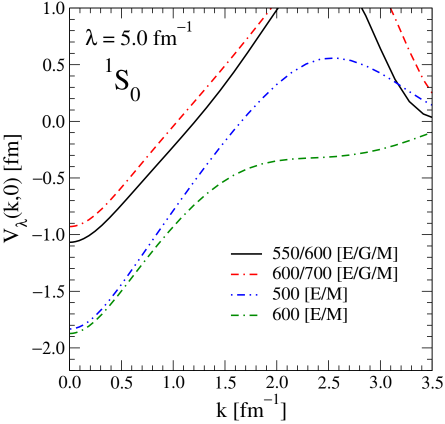

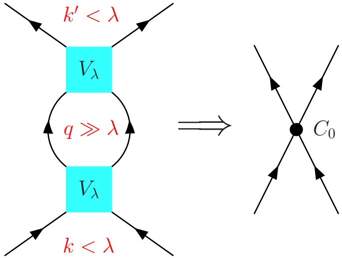

$q \gg \lambda$ (or λ) intermediate states
$\Longrightarrow$ replace with contact term:

$$C_0 \delta^3(\mathbf{x} - \mathbf{x}')$$

[cf. $\mathcal{L}_{\rm eft} = \cdots + \frac{1}{2} C_0 (\psi^\dagger \psi)^2 + \cdots$]

- Similar pattern with phenomenological potentials (e.g., AV18)

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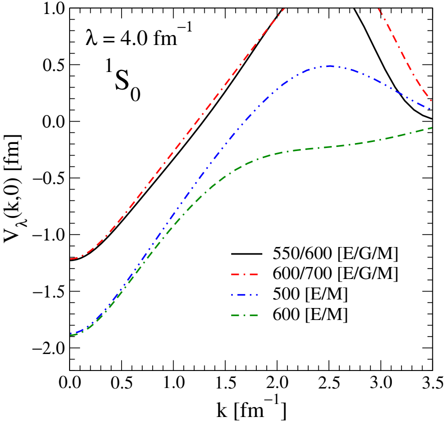

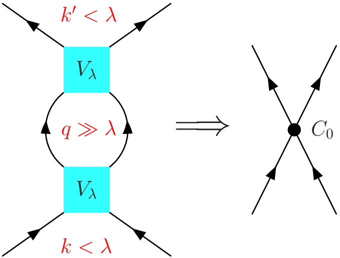

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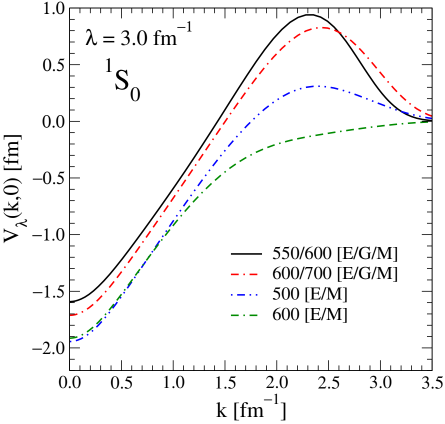

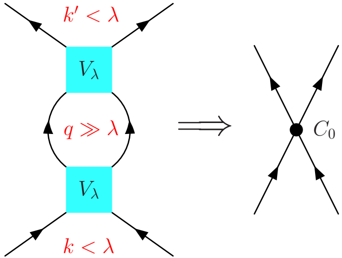

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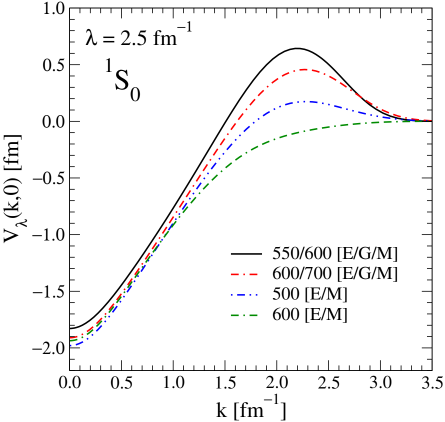

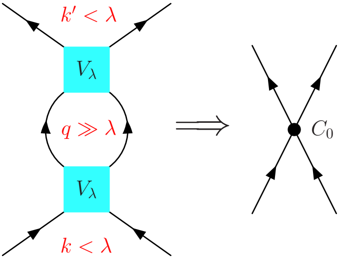

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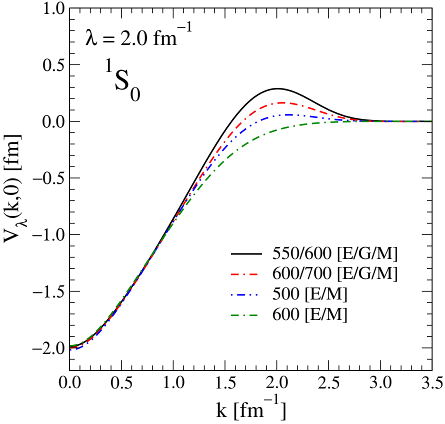

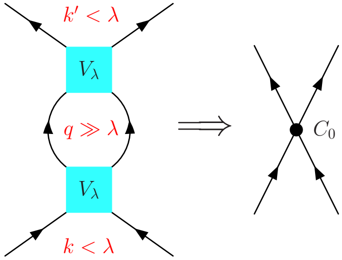

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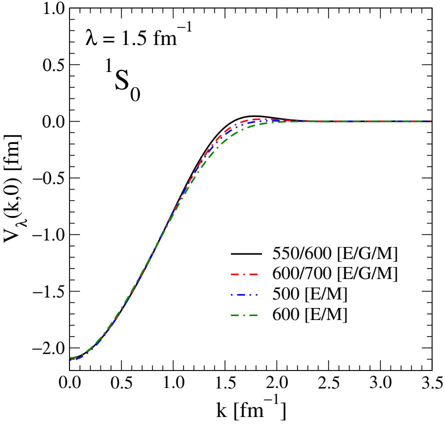

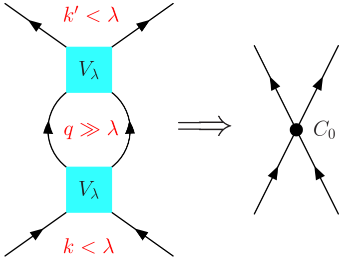

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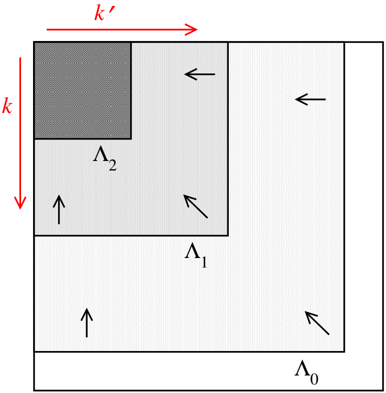
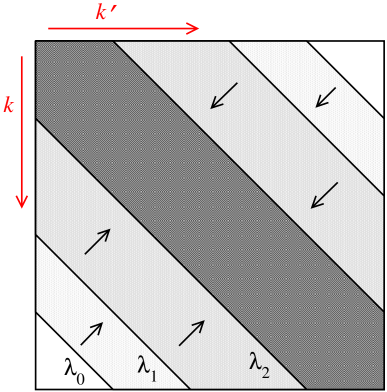
Two ways to decouple with RG equations

“$V_{\text{low}\,k}$”



Similarity RG

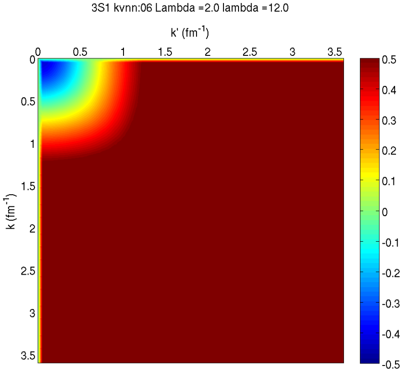


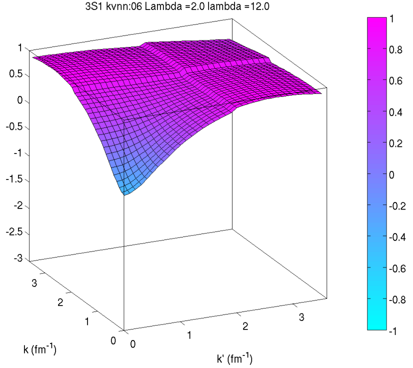
- Lower a cutoff Λ_i in k, k', e.g., demand $dT(k,k';k^2)/d\Lambda = 0$
- Drive the Hamiltonian toward diagonal with “flow equation” [Wegner; Glazek/Wilson (1990’s)]

$\Longrightarrow$ Both tend toward universal low-momentum interactions!

Block diagonalization via SRG $[G_s = H_{BD}]$

- 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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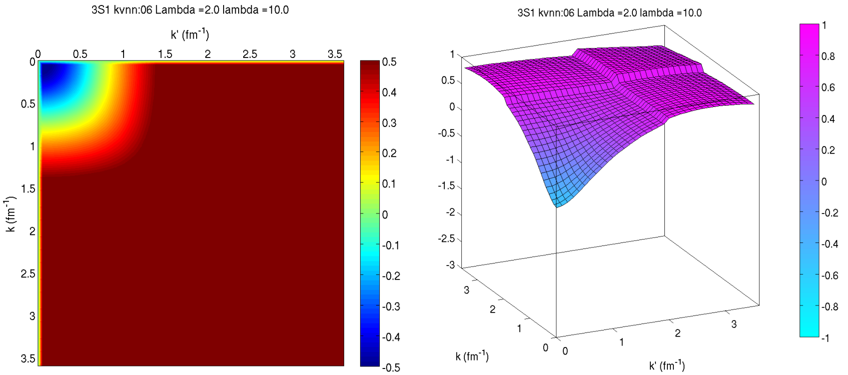

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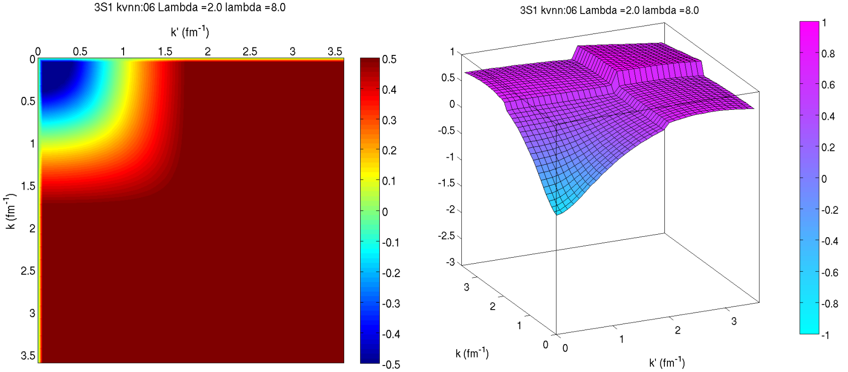

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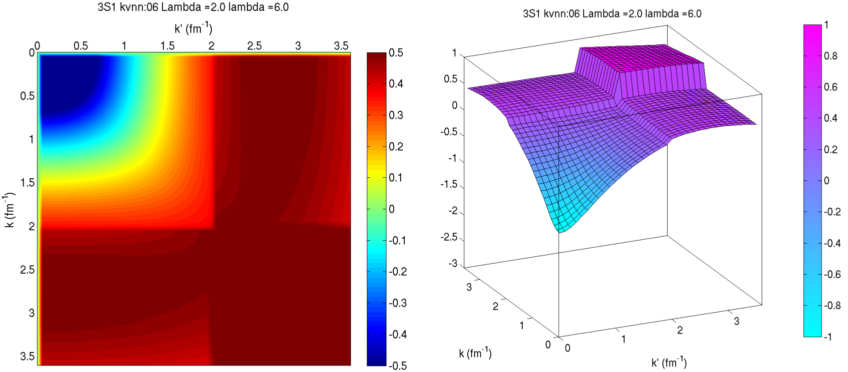

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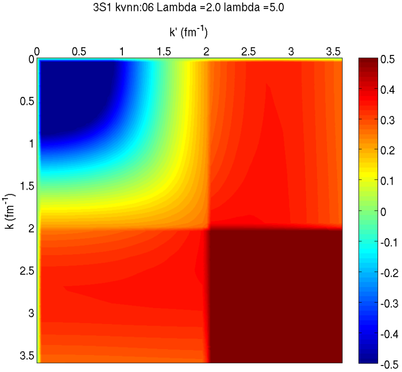

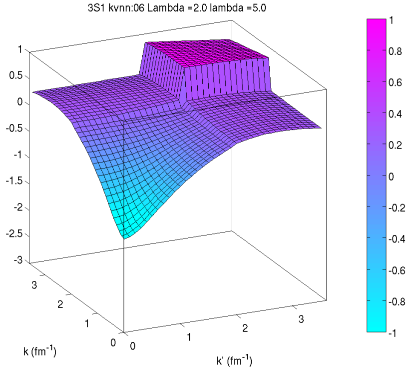

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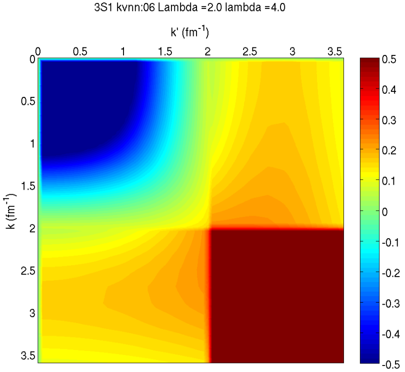

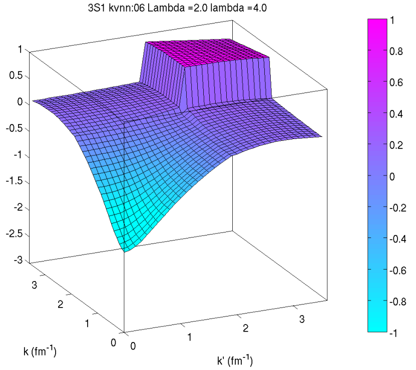

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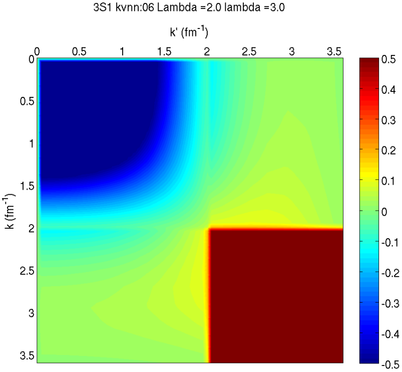

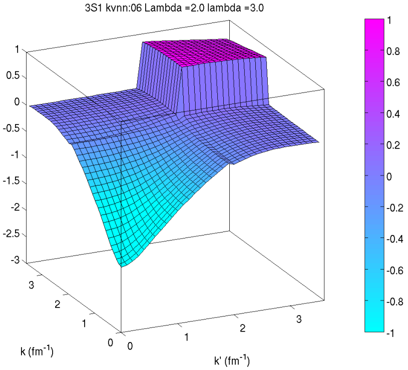

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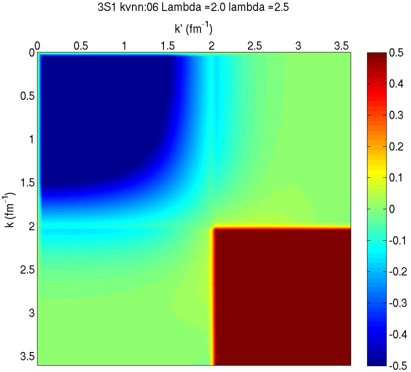

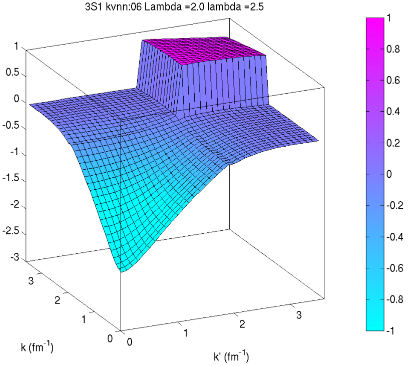

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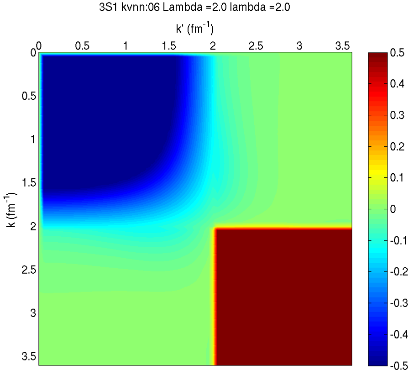

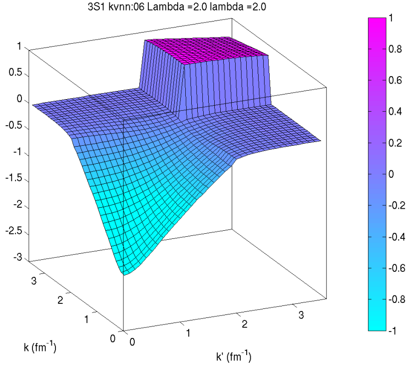

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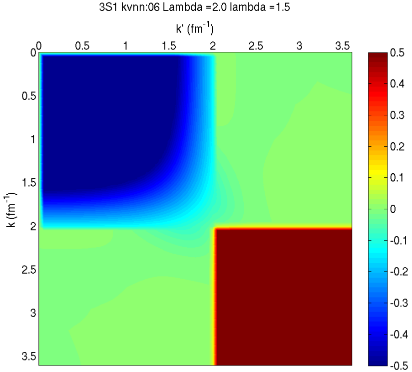

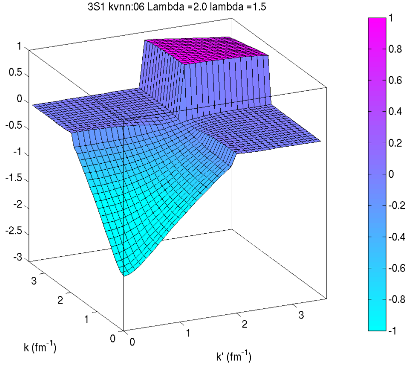

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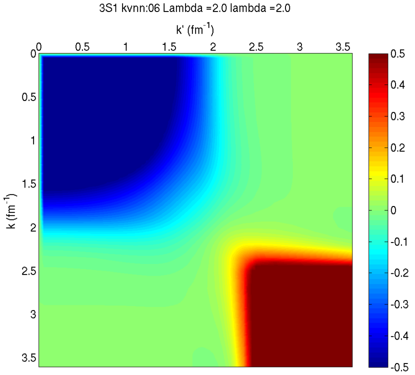

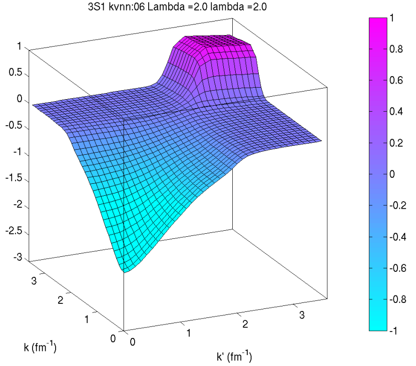

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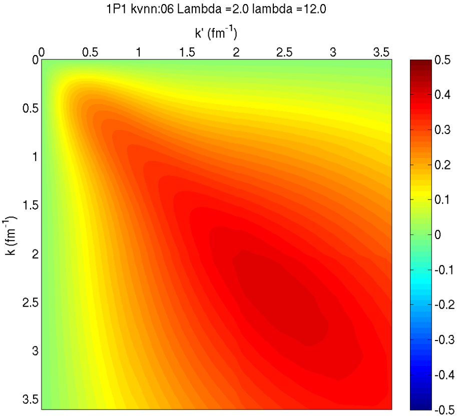
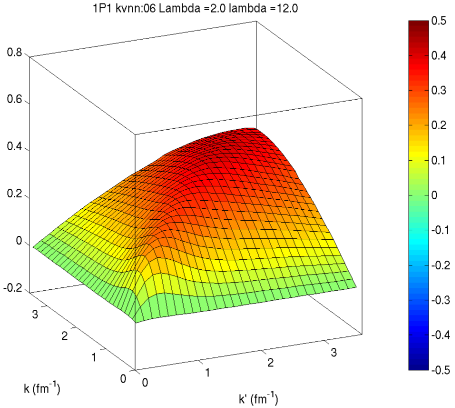
Custom potentials via the SRG

- Can we tailor the potential to other shapes with the SRG?
- Consider $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ in the $^1P_1$ partial wave with a strange choice for G_s





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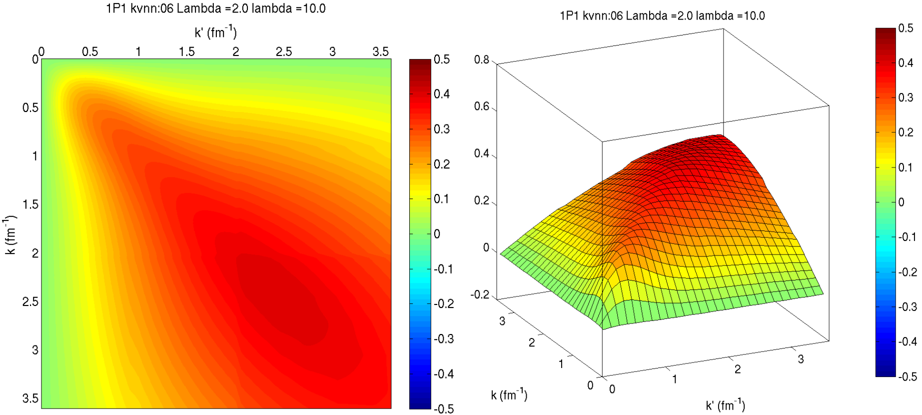

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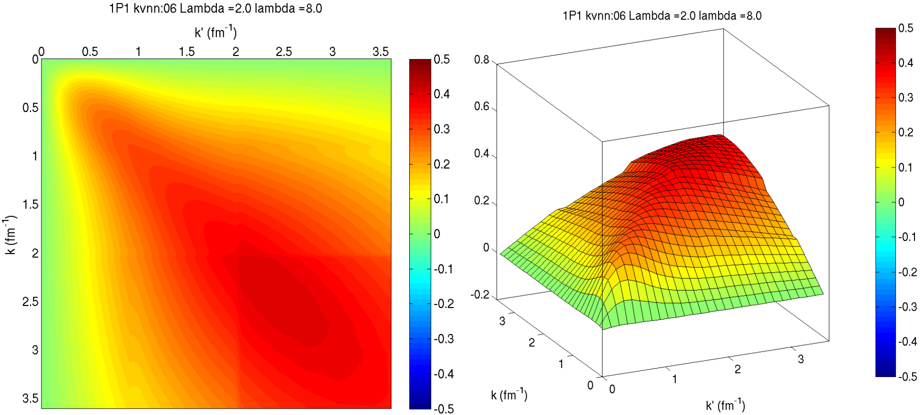

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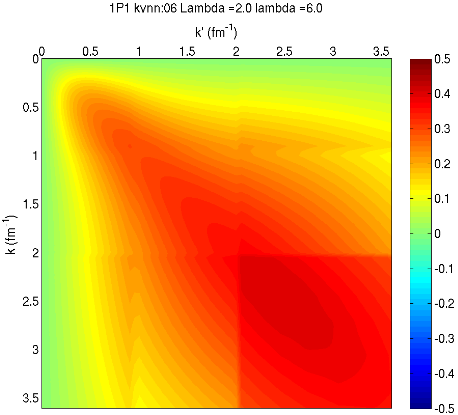

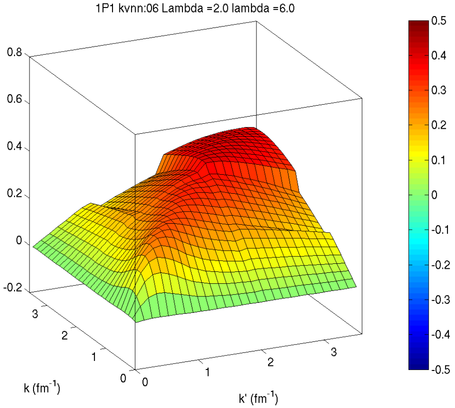

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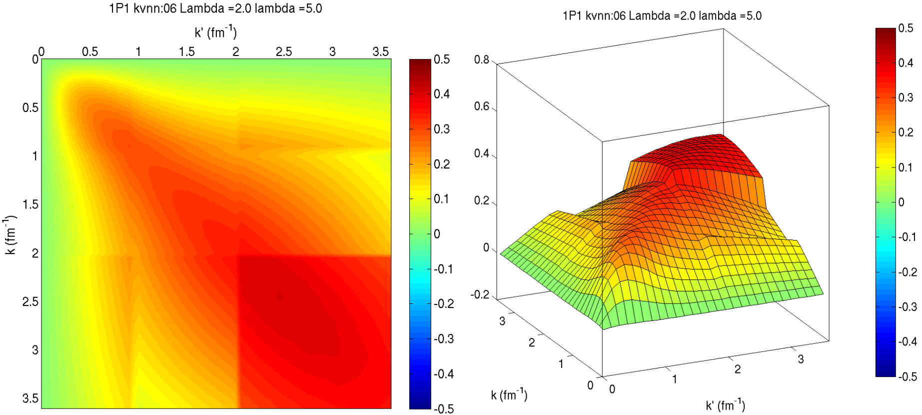

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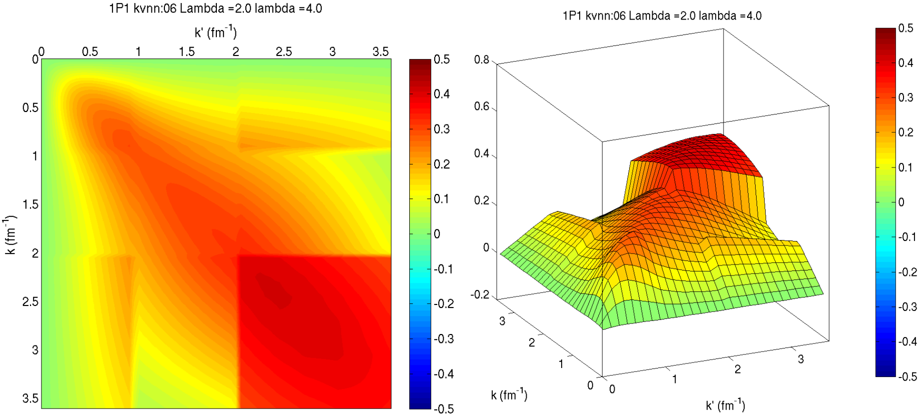

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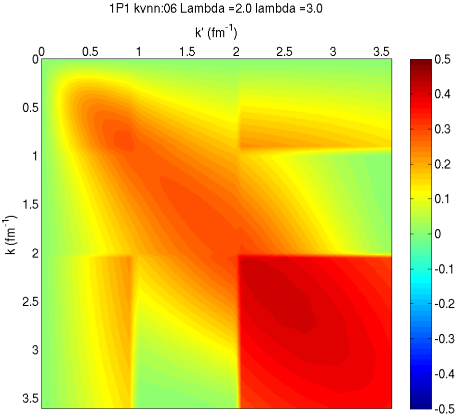

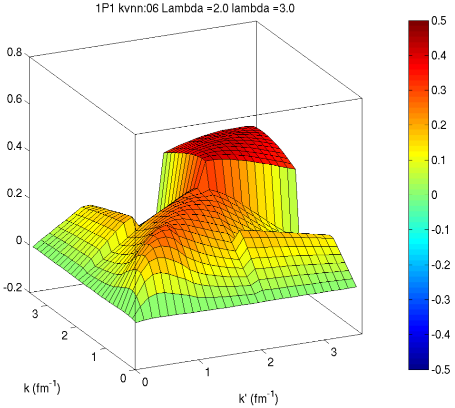

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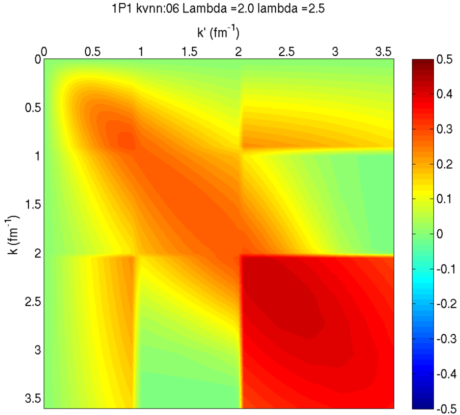

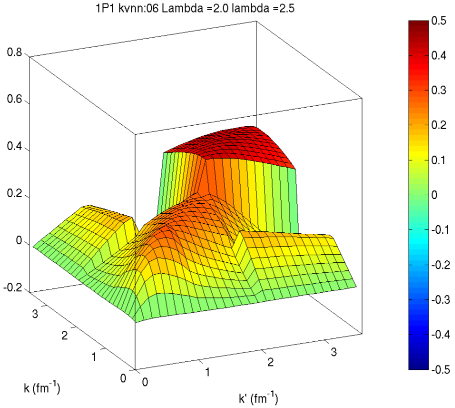

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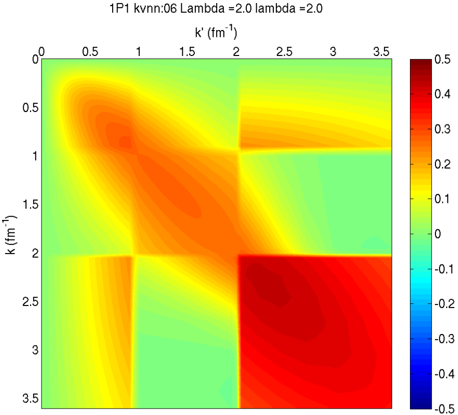

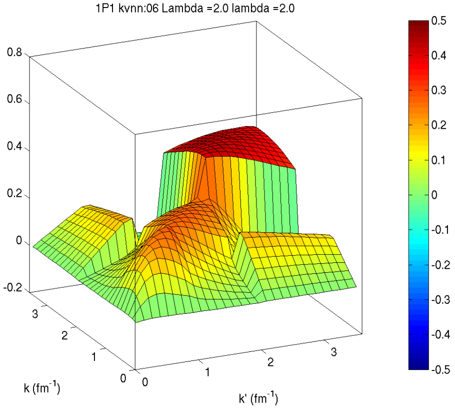

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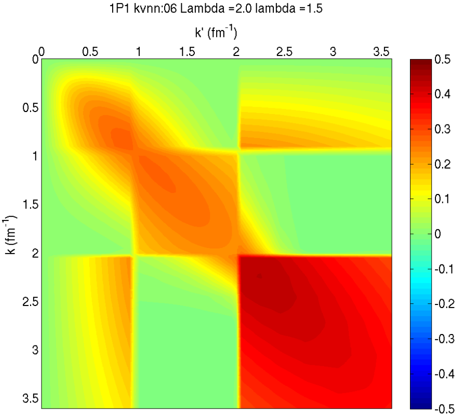

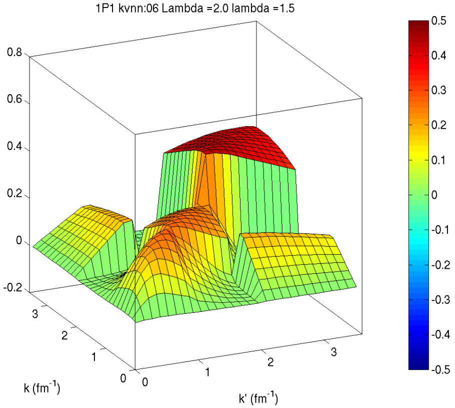

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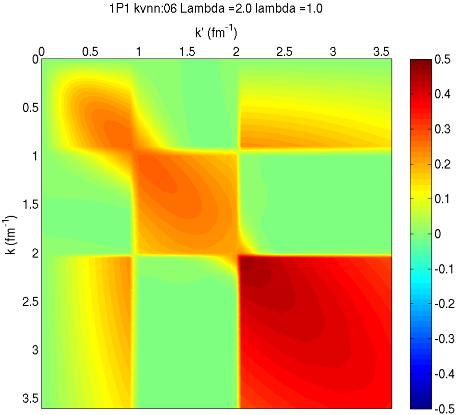
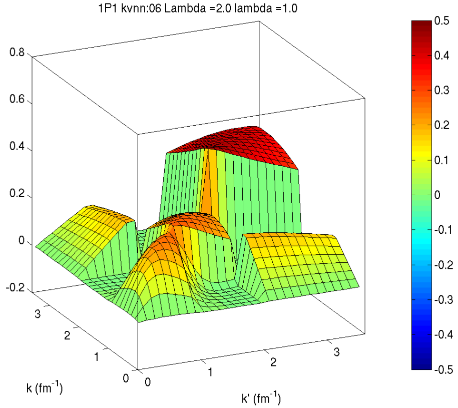
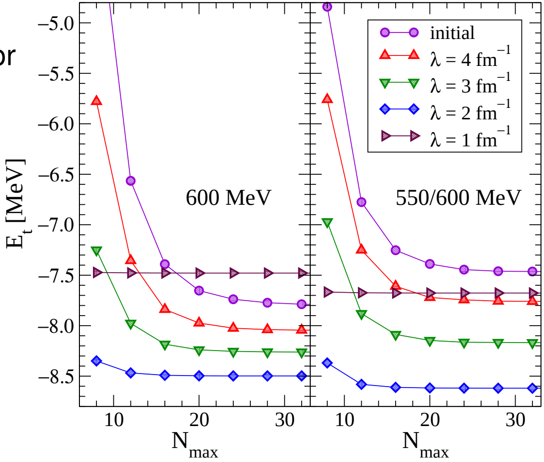




Variational calculations in three-nucleon systems

- Triton ground-state energy vs. size of harmonic oscillator basis ($N_{\max}\hbar\omega$ excitations)
- Rapid convergence as λ decreases
- Note softening already at $\lambda = 3\,\text{fm}^{-1}$ with N^{3}LO EFT $\Lambda = 600\,\text{MeV} = 3\,\text{fm}^{-1}$
- Different binding energies!



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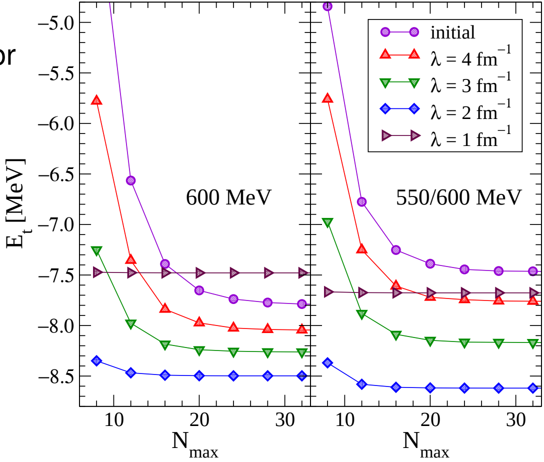
- Nuclear matter doesn't saturate at low λ



Flow equations lead to many-body operators

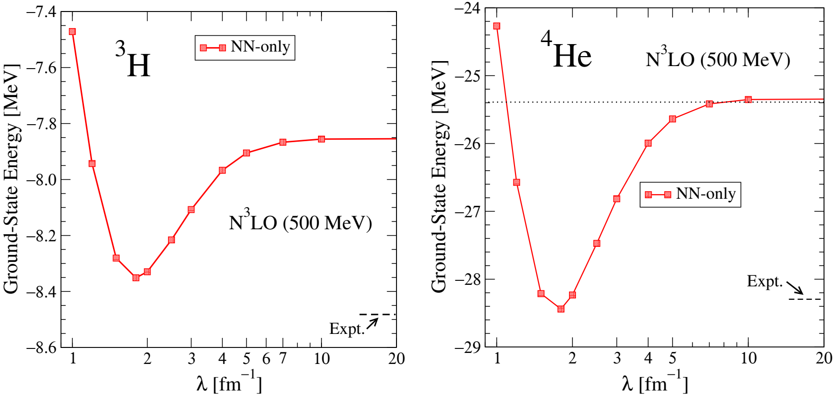
- Consider a's and $a^\dagger$'s wrt s.p. basis and reference state:

$$\frac{dV_s}{ds} = \Big[\Big[\sum \underbrace{a^\dagger a}_{G_s}, \sum \underbrace{a^\dagger a^\dagger a a}_{\text{2-body}}\Big], \sum \underbrace{a^\dagger a^\dagger a a}_{\text{2-body}}\Big] = \cdots + \sum \underbrace{a^\dagger a^\dagger a^\dagger a a a}_{\text{3-body!}} + \cdots$$

  so there will be A-body forces (and operators) generated
- Is this a problem?
  - Ok if "induced" many-body forces are same size as natural ones
- Nuclear 3-body forces already needed in unevolved potential
  - In fact, there are A-body forces (operators) initially
  - Natural hierarchy from chiral EFT
    $\Longrightarrow$ stop flow equations before unnatural or use G_s to suppress
  - Still needed: analytic bounds on A-body growth
- SRG is a tractable method to evolve many-body operators

3D SRG evolution with $T_{\rm rel}$ in a Jacobi HO basis

- Can evolve in *any* basis [E. Jurgenson, P. Navrátil, rjf (2009)]
  - Here: use anti-symmetric Jacobi HO basis from NCSM
  - directly obtain SRG matrix elements in HO basis
  - separate 3-body evolution not needed
- Compare 2-body only to full $2+3$-body evolution:



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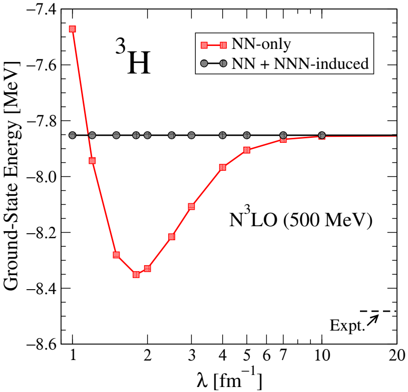

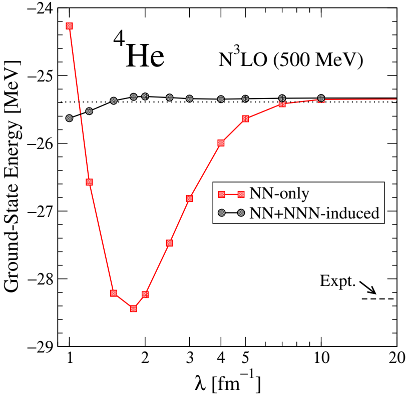

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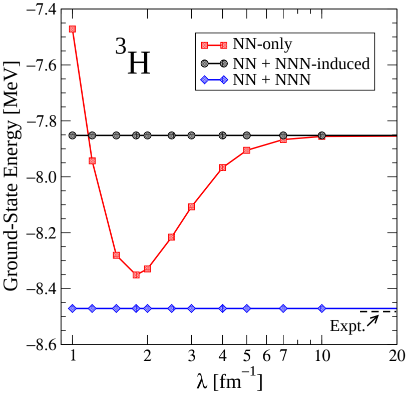
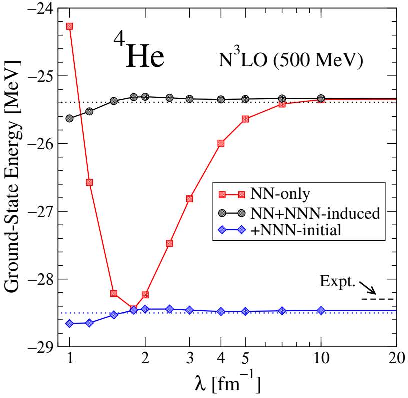
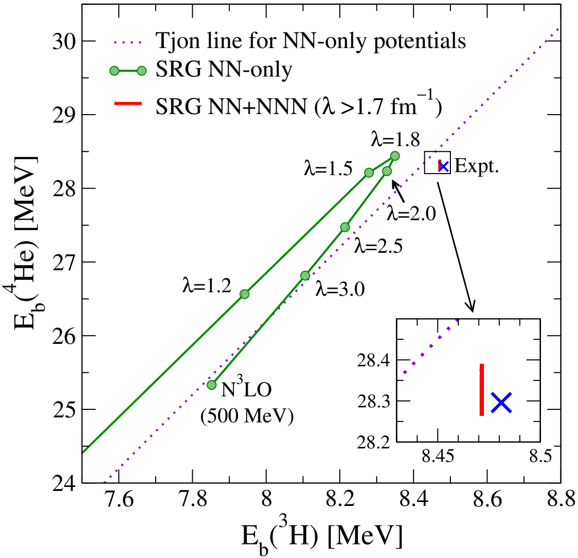


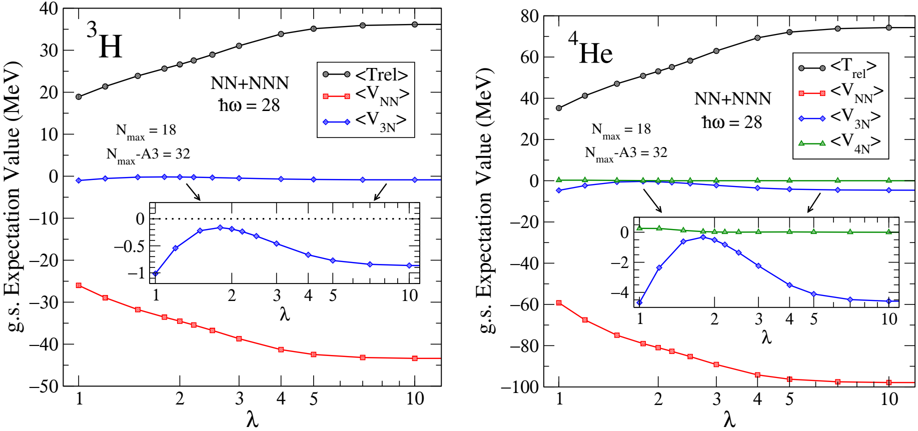


Tjon line revisited



Contributions to the ground-state energy

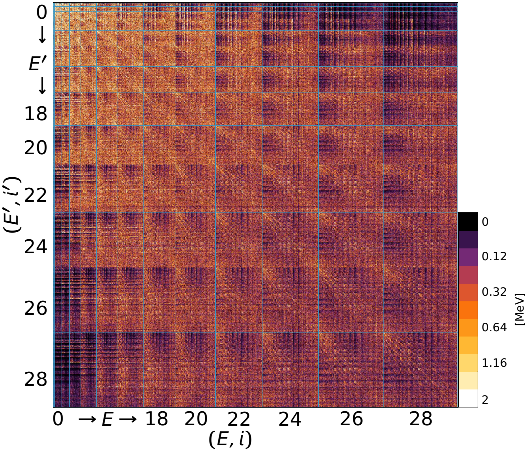
- Look at ground-state matrix elements of KE, NN, 3N, 4N



- Clear hierarchy, but also strong cancellations at NN level
- What about the *A* dependence? Recent results up to ^{48}Ca!

3NF evolution in Jacobi HO basis [Angelo Calci, Trento, 2013]

3B-Jacobi HO matrix elements



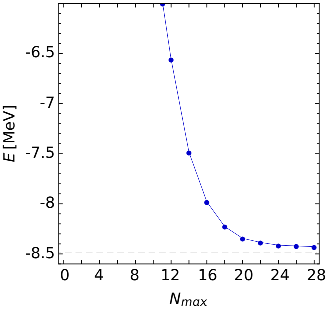
$\alpha = 0.00\,\mathrm{fm}^4$

$\lambda = \infty\,\mathrm{fm}^{-1}$

$\langle E'i'JT | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | EiJT \rangle$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$

NCSM ground state ^{3}H



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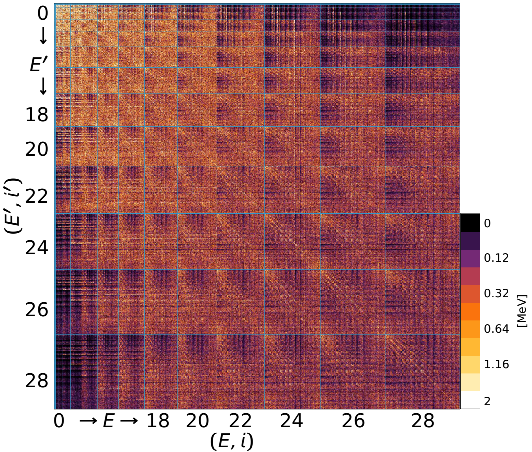

$\alpha = 0.0025\,\mathrm{fm}^4$

$\lambda = 4.47\,\mathrm{fm}^{-1}$

$\langle E' i' JT | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | E i J T \rangle$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$

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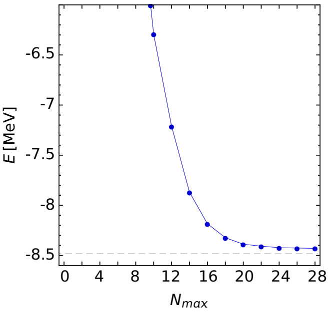

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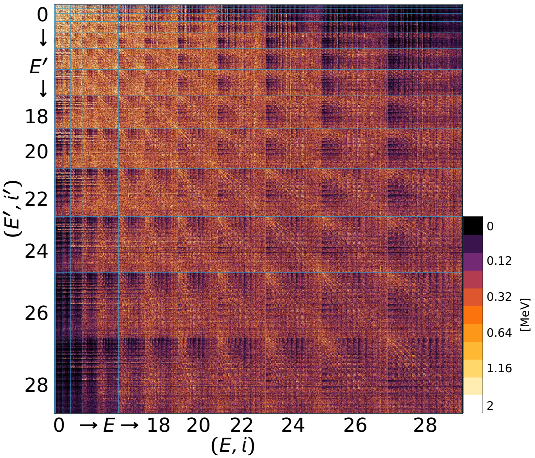

$$\alpha = 0.005\,\text{fm}^4$$

$\lambda = 3.76\,\text{fm}^{-1}$

$$\langle E'i'JT | \widetilde{\text{H}}_\alpha - \text{T}_{\text{int}} | EiJT \rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\text{MeV}$$

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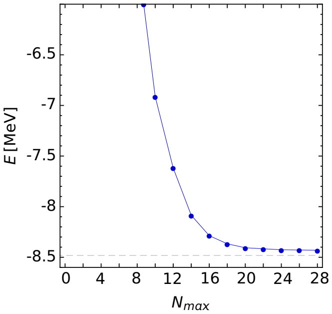

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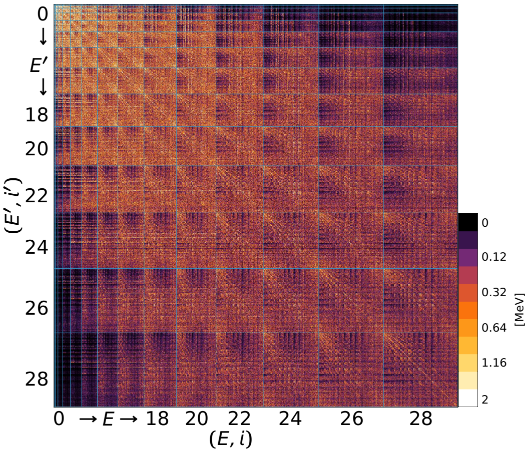

$$\alpha = 0.01\,\mathrm{fm}^4$$

$\lambda = 3.16\,\mathrm{fm}^{-1}$

$$\langle E'i'JT | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | EiJT \rangle$$

$$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$$

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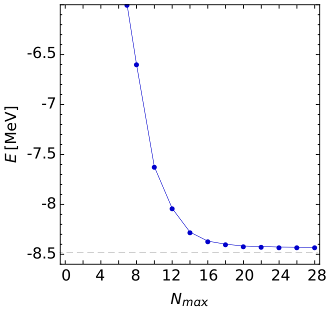

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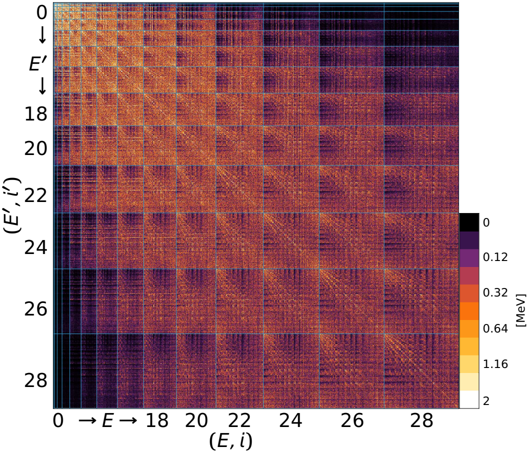


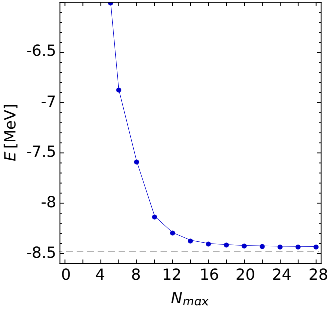
$$\alpha = 0.02\,\mathrm{fm}^4$$

$\lambda = 2.66\,\mathrm{fm}^{-1}$

$$\langle E'i'JT | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | EiJT \rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$$

NCSM ground state ^{3}H



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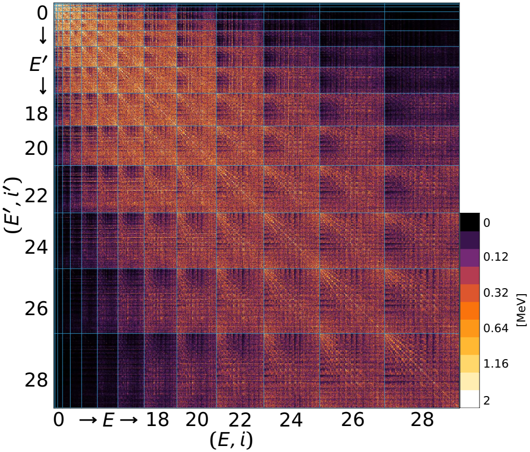

$\alpha = 0.04\,\mathrm{fm}^4$

$\lambda = 2.24\,\mathrm{fm}^{-1}$

$\langle E' i' J T | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | E i J T \rangle$

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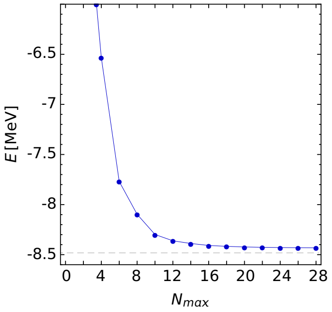

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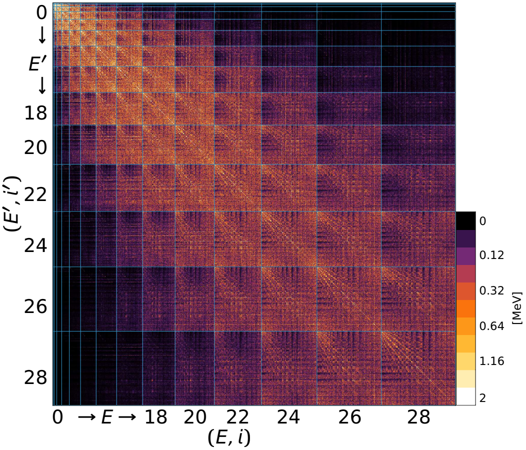

$$\alpha = 0.08\,\mathrm{fm}^4$$

$\lambda = 1.88\,\mathrm{fm}^{-1}$

$$\langle E' i' JT | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | E i JT \rangle$$

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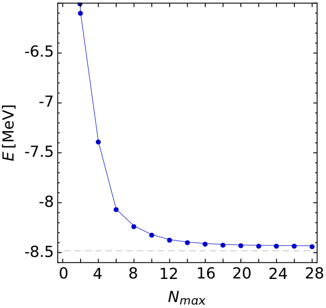

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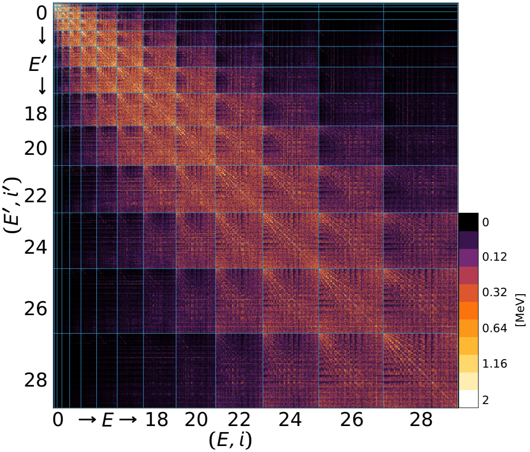


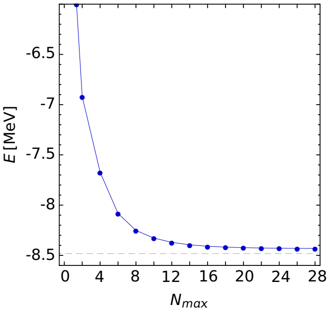
$$\alpha = 0.16\,\mathrm{fm}^4$$

$\lambda = 1.58\,\mathrm{fm}^{-1}$

$$\langle E' i' J T | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | E i J T \rangle$$

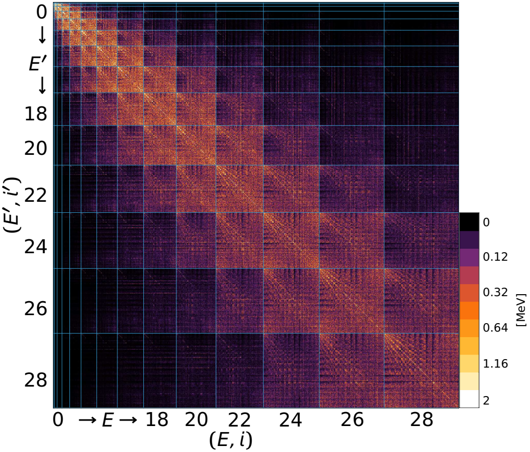
$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$$

NCSM ground state ^{3}H



3NF evolution in Jacobi HO basis [Angelo Calci, Trento, 2013]

3B-Jacobi HO matrix elements



$$\alpha = 0.32\,\text{fm}^4$$

$\lambda = 1.33\,\text{fm}^{-1}$

$$\langle E'i'JT | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\text{int}} | EiJT \rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\text{MeV}$$

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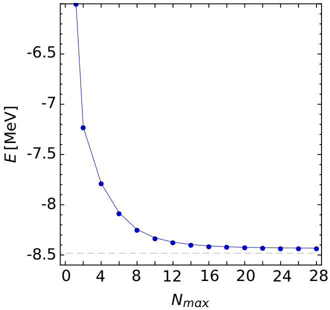

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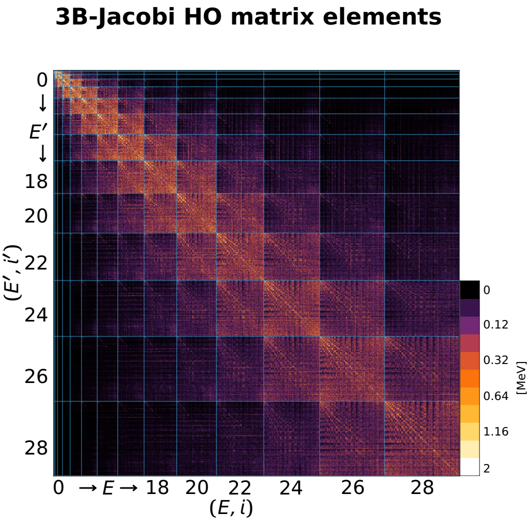
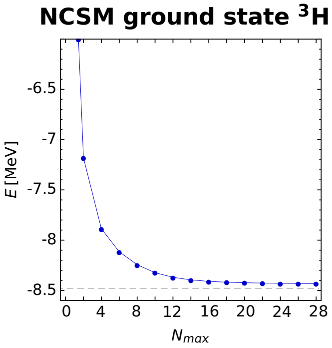


$\alpha = 0.64\,\mathrm{fm}^4$

$\lambda = 1.12\,\mathrm{fm}^{-1}$

$\langle E' i' J T | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | E i J T \rangle$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$



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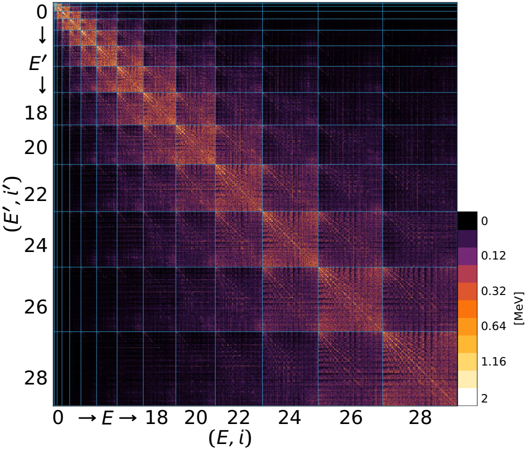


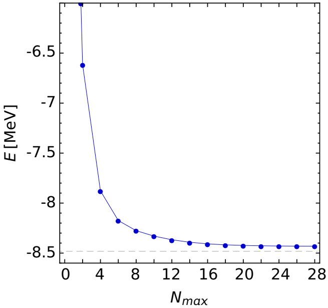
$$\alpha = 1.28\,\mathrm{fm}^4$$

$\lambda = 0.94\,\mathrm{fm}^{-1}$

$$\langle E'i'JT | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} | EiJT \rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$$

NCSM ground state ^{3}H



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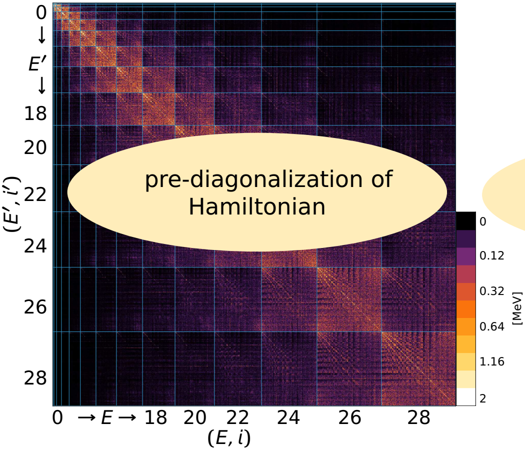


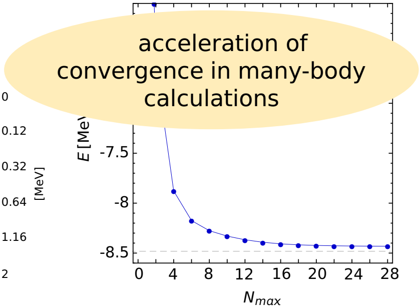
$\alpha = 1.28\,\mathrm{fm}^4$

$\lambda = 0.94\,\mathrm{fm}^{-1}$

$\langle E' i' J T | \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\rm int} | E i J T \rangle$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$

NCSM ground state ^{3}H



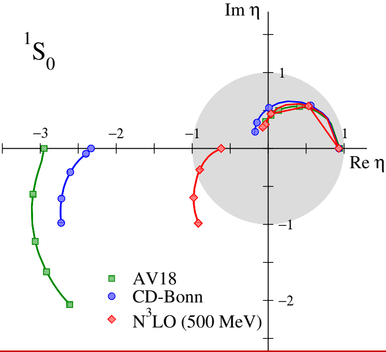
Weinberg eigenvalue analysis of convergence

Born Series: $$T(E) = V + V\frac{1}{E-H_0}V + V\frac{1}{E-H_0}V\frac{1}{E-H_0}V + \cdots$$

- For fixed E, find (complex) eigenvalues $\eta_\nu(E)$ [Weinberg]

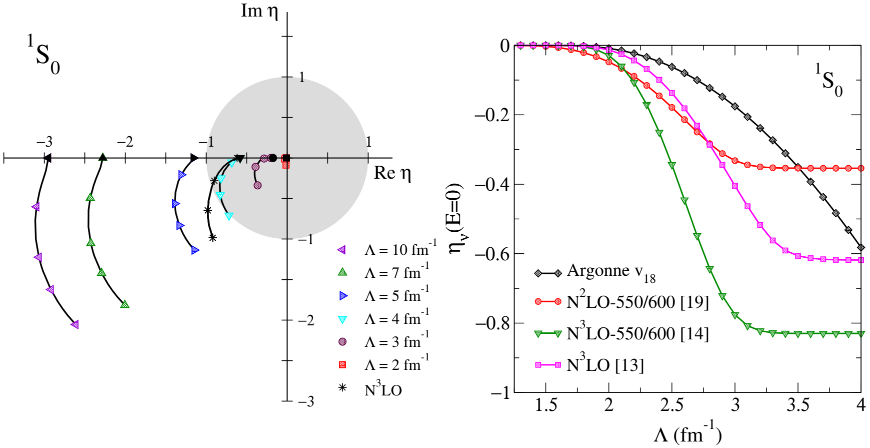
$$\frac{1}{E-H_0}V|\Gamma_\nu\rangle = \eta_\nu|\Gamma_\nu\rangle \quad \Longrightarrow \quad T(E)|\Gamma_\nu\rangle = V|\Gamma_\nu\rangle(1+\eta_\nu+\eta_\nu^2+\cdots)$$

$\Longrightarrow$ T diverges if *any* $|\eta_\nu(E)| \geq 1$ [nucl-th/0602060]



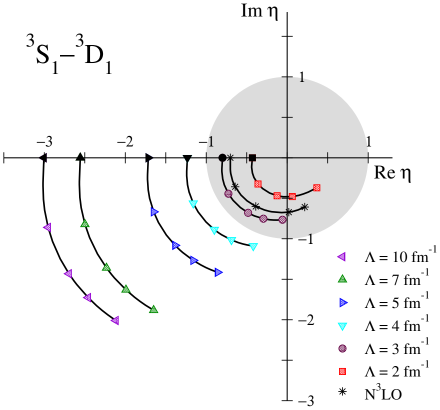
Lowering the cutoff increases "perturbativeness"

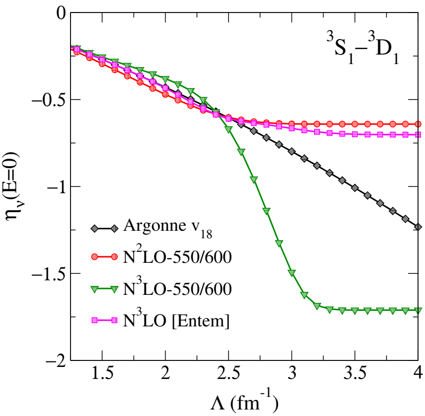
- Weinberg eigenvalue analysis (repulsive) [nucl-th/0602060]



Lowering the cutoff increases "perturbativeness"

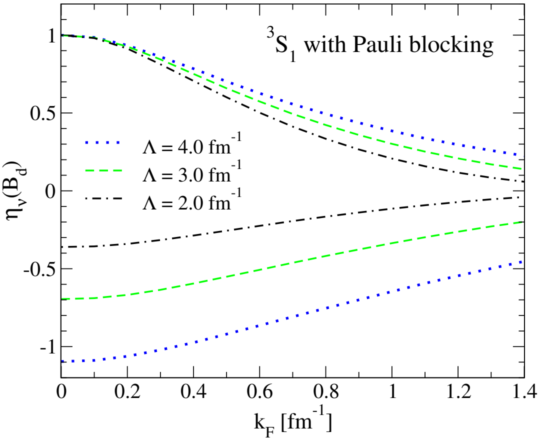
- Weinberg eigenvalue analysis (repulsive) [nucl-th/0602060]





Lowering the cutoff increases "perturbativeness"

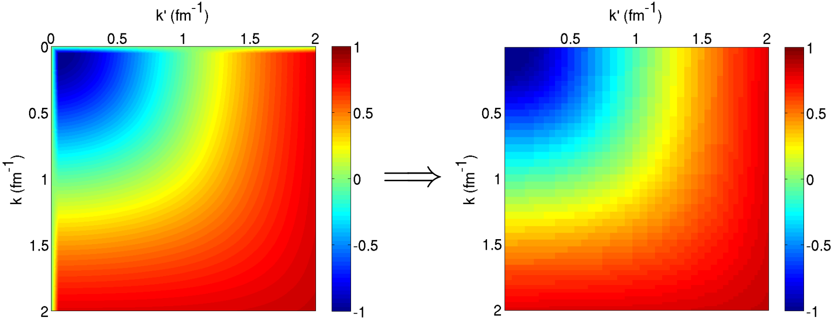
- Weinberg eigenvalue analysis (η_ν at -2.22 MeV vs. density)



- Pauli blocking in nuclear matter increases it even more!
  - at Fermi surface, pairing revealed by $|\eta_\nu| > 1$

Comments on computational aspects

- 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 two-body potential

Discretization of integrals $\Longrightarrow$ matrices!

- Momentum-space flow equations have integrals like:

$$I(p,q) \equiv \int dk\, k^2\, V(p,k)V(k,q)$$

- Introduce gaussian nodes and weights $\{k_n, w_n\}$ $(n = 1, N)$

$$\Longrightarrow \quad \int dk\, f(k) \approx \sum_n w_n\, f(k_n)$$

- Then $I(p,q) \to I_{ij}$, where $p = k_i$ and $q = k_j$, and

$$I_{ij} = \sum_n k_n^2 w_n\, V_{in} V_{nj} \to \sum_n \widetilde{V}_{in} \widetilde{V}_{nj} \quad \text{where} \quad \widetilde{V}_{ij} = \sqrt{w_i} k_i\, V_{ij}\, k_j \sqrt{w_j}$$

- Lets us solve SRG equations, integral equation for phase shift, Schrödinger equation in momentum representation, ...
- In practice, N=100 gauss points more than enough for accurate nucleon-nucleon partial waves

MATLAB Code for SRG is a direct translation!

- The flow equation $\frac{d}{ds}V_s = [[T, H_s], H_s]$ is solved by discretizing, so it is just matrix multiplication.
- If the matrix V_s is converted to a vector by “reshaping”, it can be fed to a differential equation solver, with the right side:

```
% V_s is a vector of the current potential; convert to square matrix
V_s_matrix = reshape(V_s, tot_pts, tot_pts);
H_s_matrix = T_matrix + V_s_matrix;  % form the Hamiltontian

% Matrix for the right side of the SRG differential equation
if (strcmp(evolution,'T'))
  rhs_matrix = my_commutator( my_commutator(T_matrix, H_s_matrix), ...
                              H_s_matrix );

elseif (strcmp(evolution,'Wegner'))
  rhs_matrix = my_commutator( my_commutator(diag(diag(H_s_matrix)), ...
                                     H_s_matrix), H_s_matrix );
```

[etc.]

```
% convert the right side matrix to a vector to be returned
dVds = reshape(rhs_matrix, tot_pts*tot_pts, 1);
```

Pseudocode for SRG evolution

1. Set up basis (e.g., momentum grid with gaussian quadrature or HO wave functions with $N_{\rm max}$)
2. Calculate (or input) the initial Hamiltonian and G_s matrix elements (including any weight factors)
3. Reshape the right side $[[G_s, H_s], H_s]$ to a vector and pass it to a coupled differential equation solver
4. Integrate V_s to desired s (or $\lambda = s^{-1/4}$)
5. Diagonalize H_s with standard symmetric eigensolver $\Longrightarrow$ energies and eigenvectors
6. Form $U = \sum_i |\psi_s^{(i)}\rangle\langle\psi_{s=0}^{(i)}|$ from the eigenvectors
7. Output or plot or calculate observables

Many versions of SRG codes are in use

- Mathematica, MATLAB, Python, C++, Fortran-90
  - Instructive computational project for undergraduates!
- Once there are discretized matrices, the solver is the same with any size basis in any number of dimensions!
- Still the same solution code for a many-particle basis
- Any basis can be used
  - So far discretized momentum and harmonic oscillators
  - An accurate 3NF evolution in HO basis takes $\sim$ 20 million matrix elements $\Longrightarrow$ that many differential equations
  - Other possibilities: hyperspherical harmonics, correlated gaussians, . . .