Applications of Renormalization Group Methods in Nuclear Physics – 2

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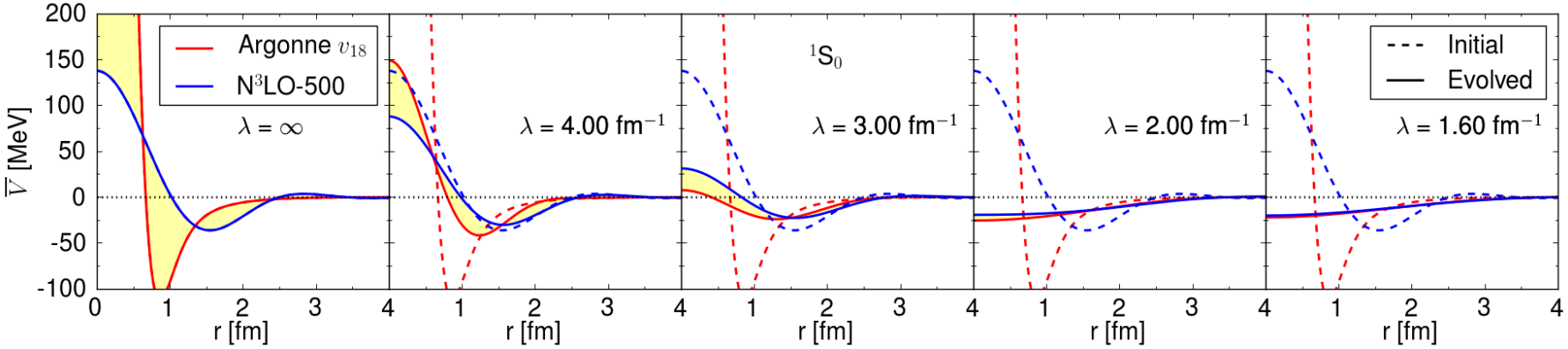
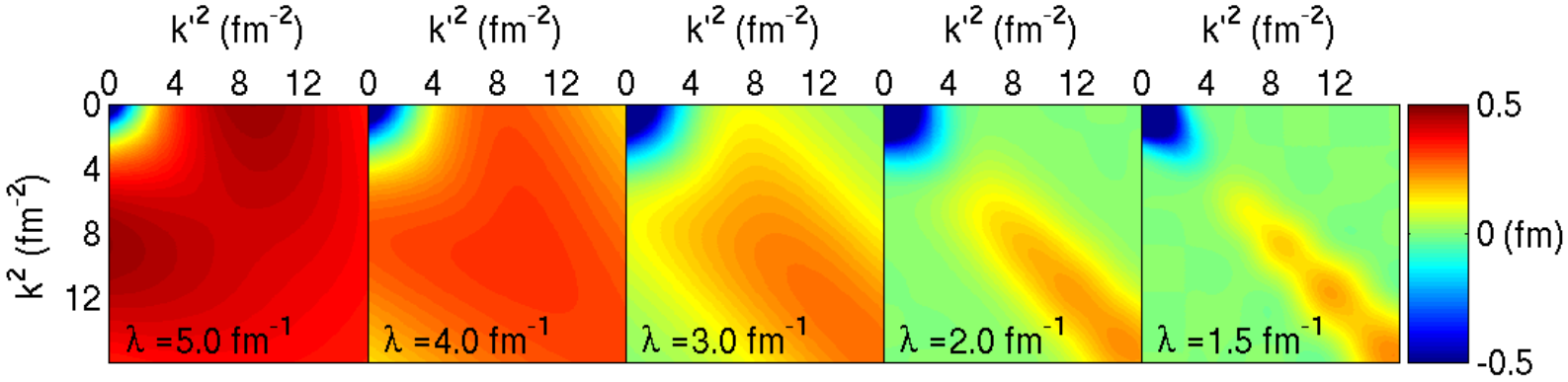
HUGS 2014





Outline: Lecture 2

Lecture 2: SRG in practice

- Recap from lecture 1: decoupling
- Implementing the similarity renormalization group (SRG)
- Block diagonal ("$V_{\mathrm{low},k}$") generator
- Computational aspects
- Quantitative measure of perturbativeness

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Why did our low-pass filter fail?

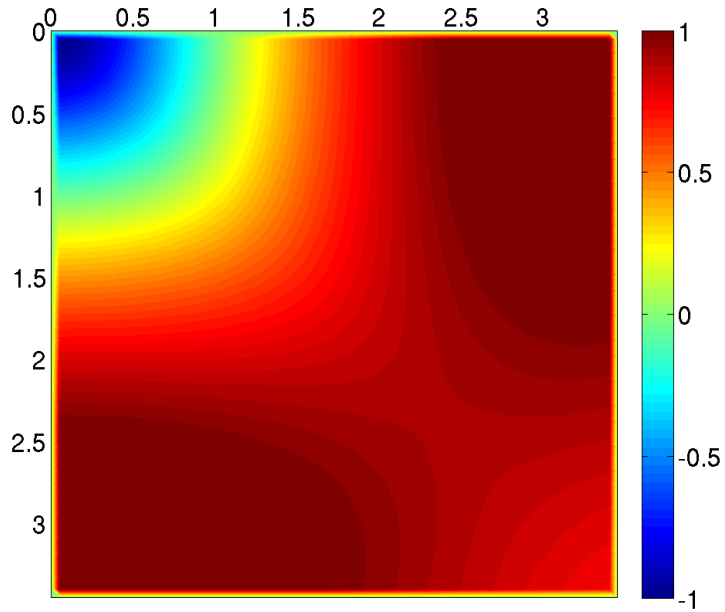
- Basic problem: low k and high k are coupled (mismatched dof's!)
- E.g., perturbation theory for (tangent of) phase shift:

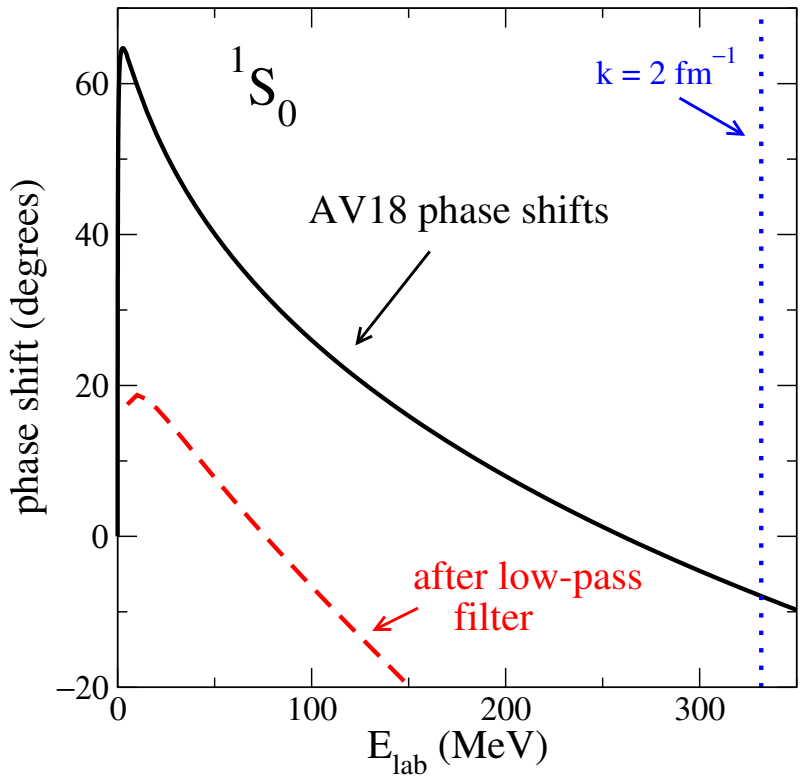
$$\langle k|V|k\rangle + \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{(k^2 - k'^2)/m} + \cdots$$

- Solution: Unitary transformation of the H matrix $\Longrightarrow$ decouple!

$$\begin{aligned} E_n &= \langle \Psi_n|H|\Psi_n\rangle \quad U^\dagger U = 1 \\ &= (\langle \Psi_n|U^\dagger)UHU^\dagger(U|\Psi_n\rangle) \\ &= \langle \widetilde{\Psi}_n|\widetilde{H}|\widetilde{\Psi}_n\rangle \end{aligned}$$

- Here: Decouple using RG





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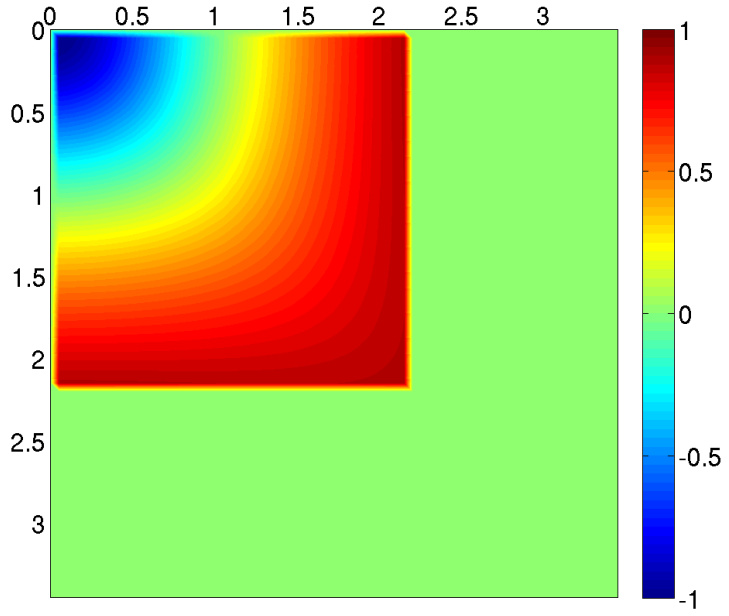

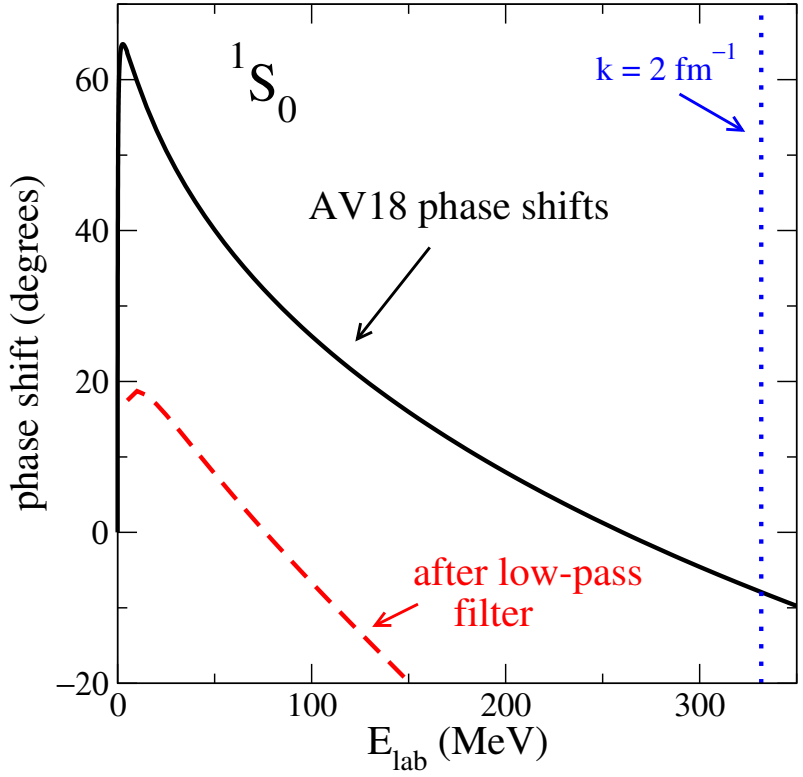

Aside: Unitary transformations of matrices

- Recall that a unitary transformation can be realized as unitary matrices with $U_\alpha^\dagger U_\alpha = I$ (where α is just a label)
  - Often used to simplify nuclear many-body problems, e.g., by making them more perturbative
- If I have a Hamiltonian H with eigenstates $|\psi_n\rangle$ and an operator O, then the new Hamiltonian, operator, and eigenstates are

$$\widetilde{H} = UHU^\dagger \qquad \widetilde{O} = UOU^\dagger \qquad |\widetilde{\psi}_n\rangle = U|\psi_n\rangle$$

  - The energy is unchanged: $\langle\widetilde{\psi}_n|\widetilde{H}|\widetilde{\psi}_n\rangle = \langle\psi_n|H|\psi_n\rangle = E_n$
- Furthermore, matrix elements of O are unchanged:

$$O_{mn} \equiv \langle\psi_m|\widehat{O}|\psi_n\rangle = \left(\langle\psi_m|U^\dagger\right) U\widehat{O}U^\dagger \left(U|\psi_n\rangle\right) = \langle\widetilde{\psi}_m|\widetilde{O}|\widetilde{\psi}_n\rangle \equiv \widetilde{O}_{mn}$$

- If asymptotic (long distance) properties are unchanged, H and $\widetilde{H}$ are equally acceptable physically $\Longrightarrow$ not measurable!
  - Consistency: use O with H and $|\psi_n\rangle$'s but $\widetilde{O}$ with $\widetilde{H}$ and $|\widetilde{\psi}_n\rangle$'s
  - One form may be better for intuition or for calculations
  - Scheme-dependent observables (come back to this later)

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- From “Why the RG is a good thing” [for Francis Low Festschrift]
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- Improving perturbation theory; e.g., in QCD calculations
  - Mismatch of energy scales can generate large logarithms
  - RG: shift between couplings and loop integrals to reduce logs
  - Nuclear: decouple high- and low-momentum modes
- Identifying universality in critical phenomena
  - RG: filter out short-distance degrees of freedom
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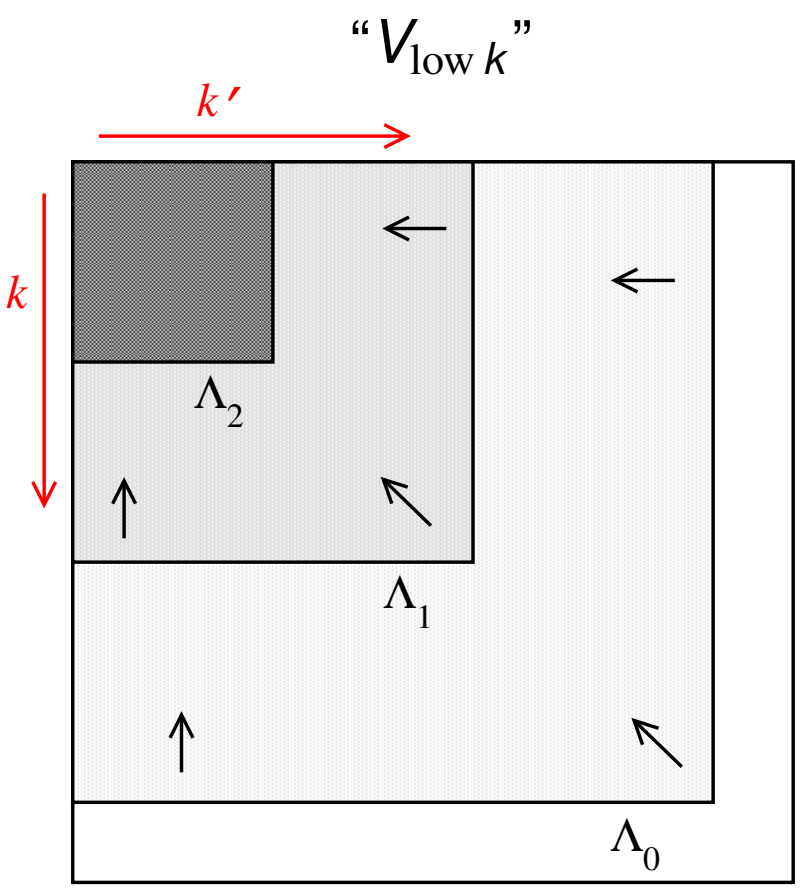
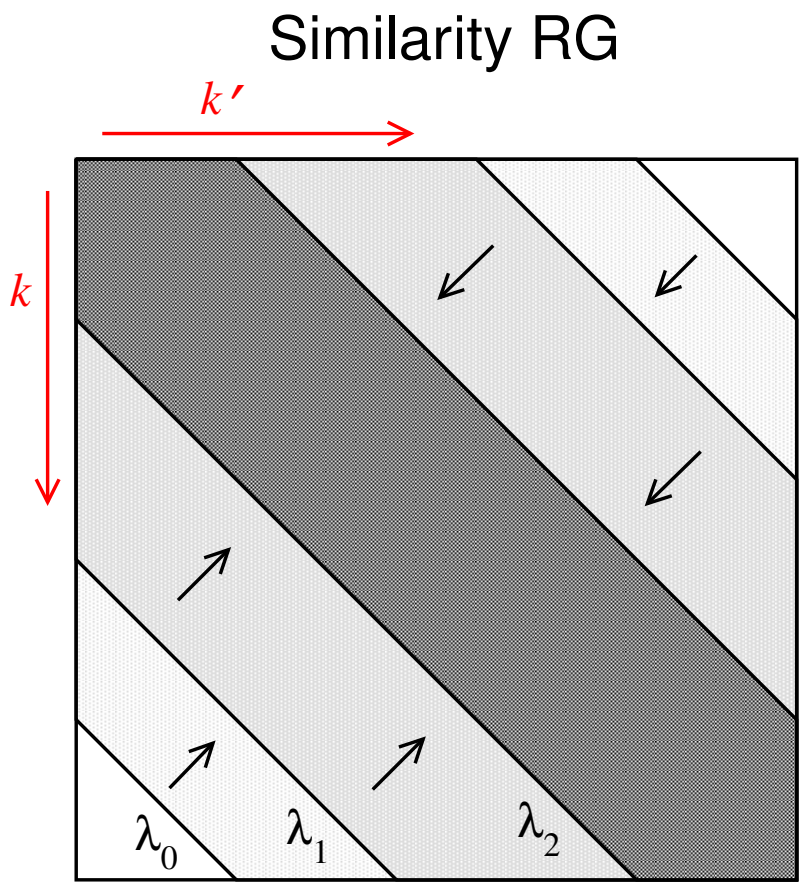
  - Nuclear: evolve toward universal interactions
- Nuclear: simplifying calculations of structure/reactions
  - Make nuclear physics look more like quantum chemistry!
  - RG gains can violate conservation of difficulty!
  - Use RG scale (resolution) dependence as a *probe* or *tool*

Two ways to use RG equations to decouple Hamiltonians





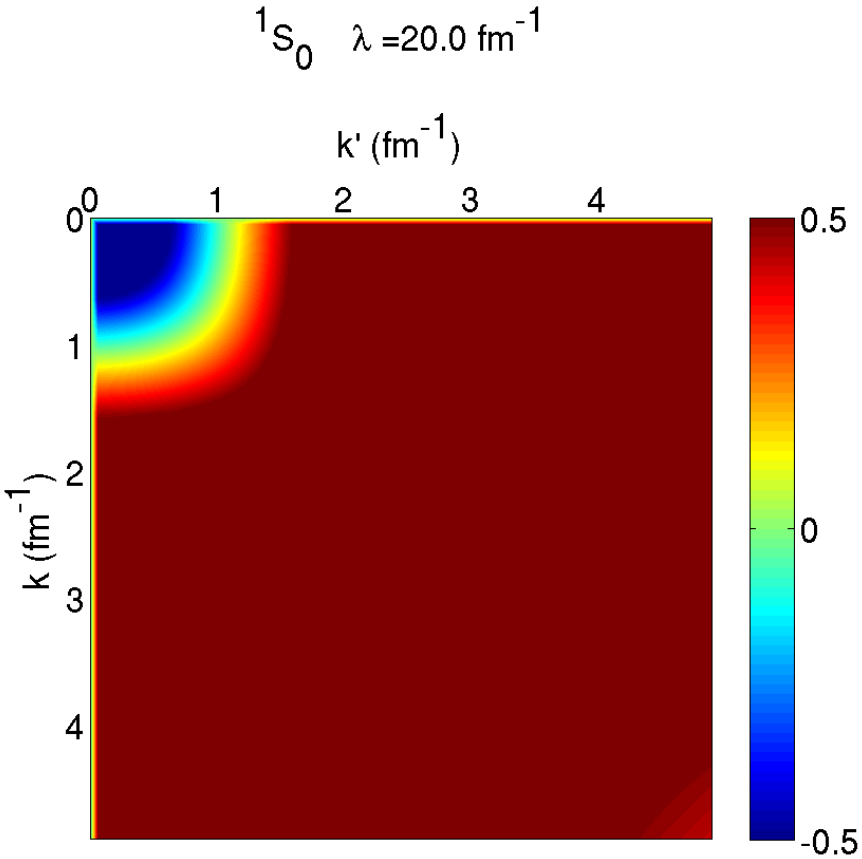
- Lower a cutoff Λ_i in k, k', e.g., demand $dT(k, k'; k^2)/d\Lambda = 0$
- Drive the Hamiltonian toward diagonal with "flow equation" [Wegner; Glazek/Wilson (1990's)]

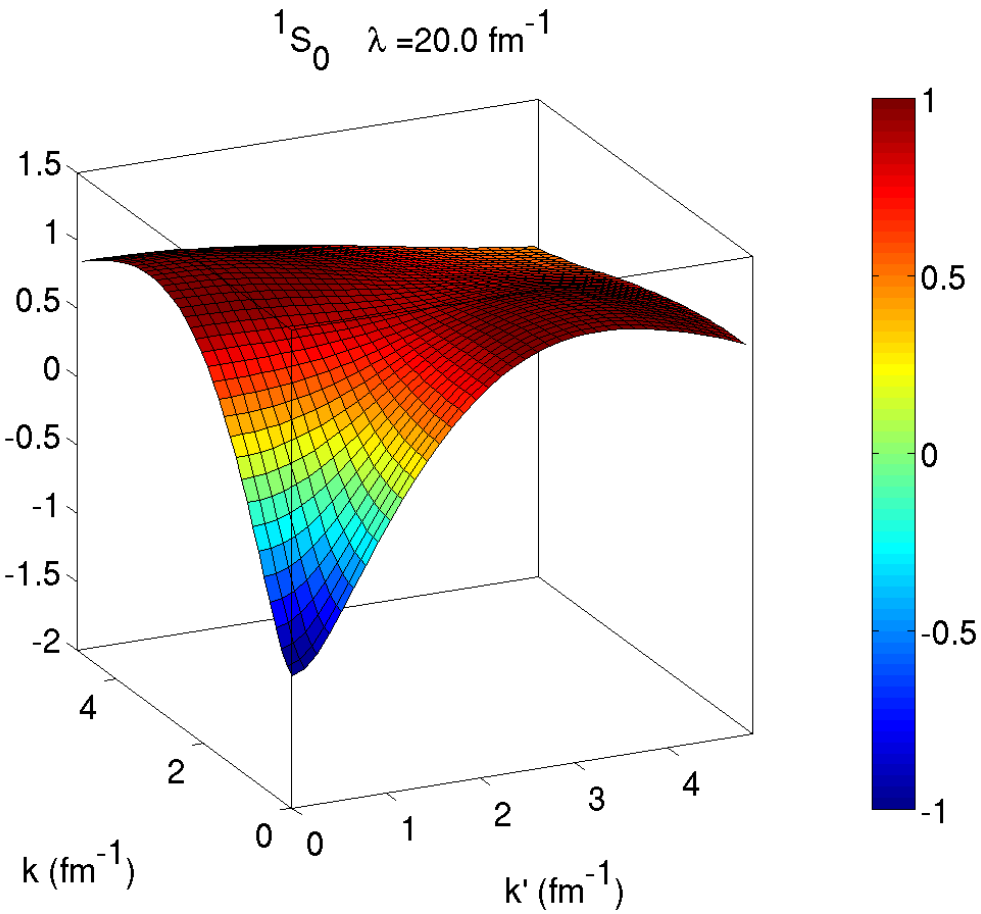
$\Longrightarrow$ Both tend toward universal low-momentum interactions!

Flow equations in action: NN only

- In each partial wave with $\epsilon_k = \hbar^2 k^2/M$ and $\lambda^2 = 1/\sqrt{s}$

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





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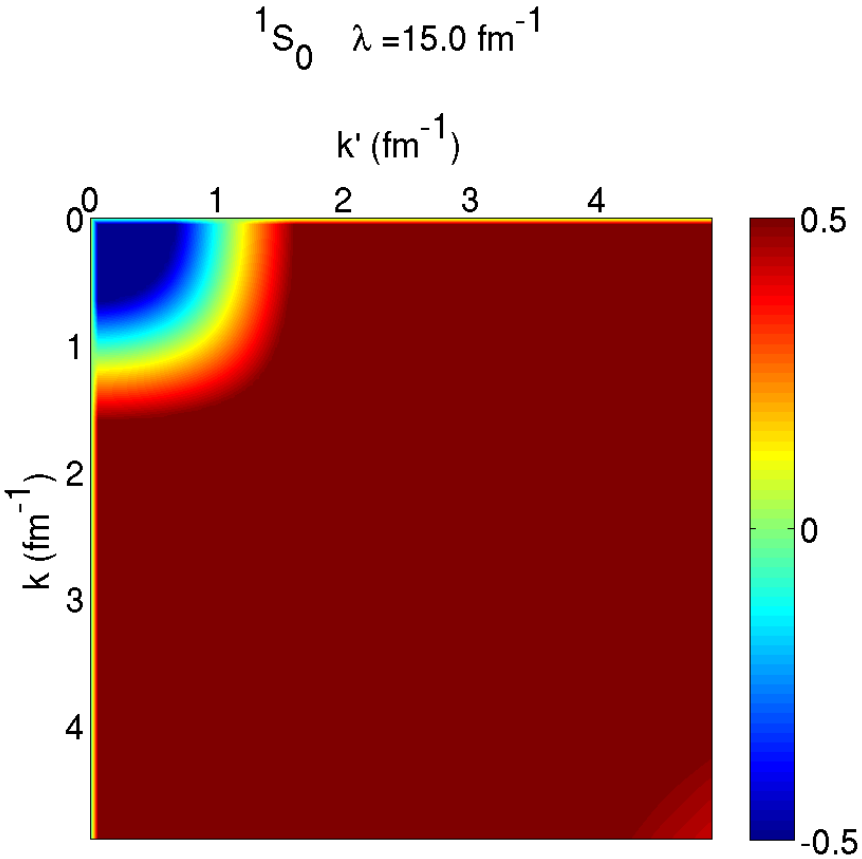

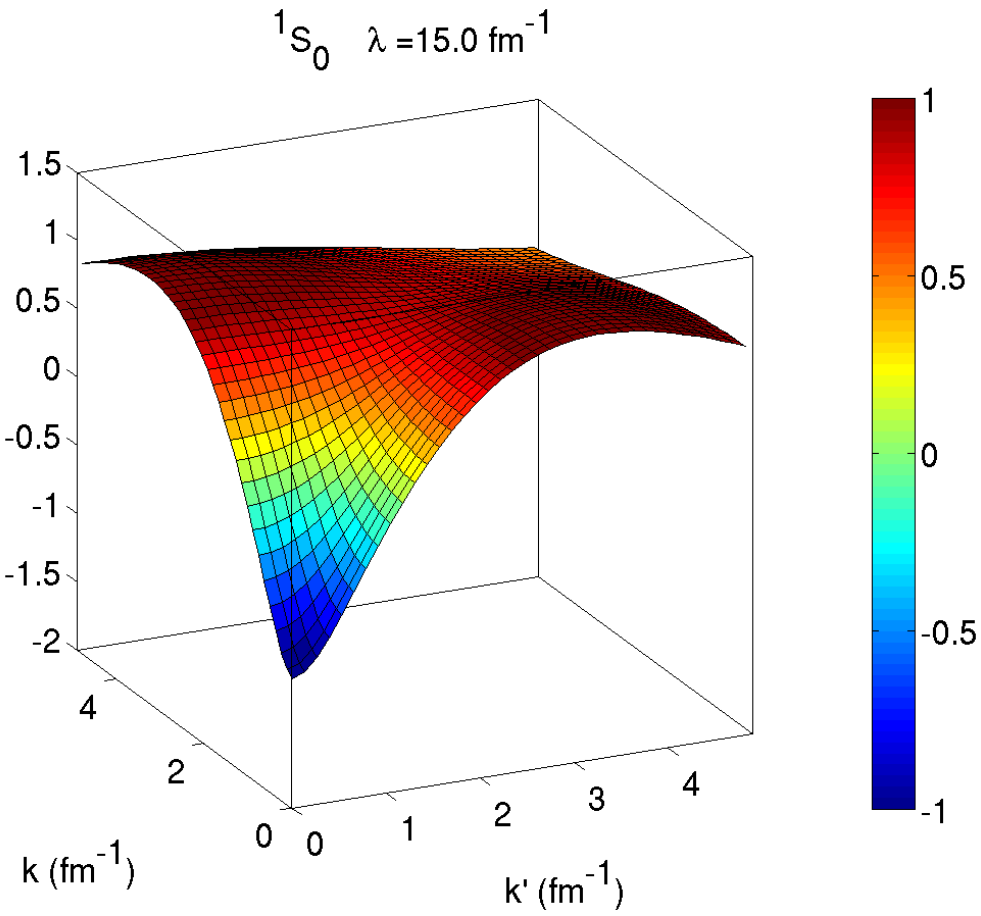

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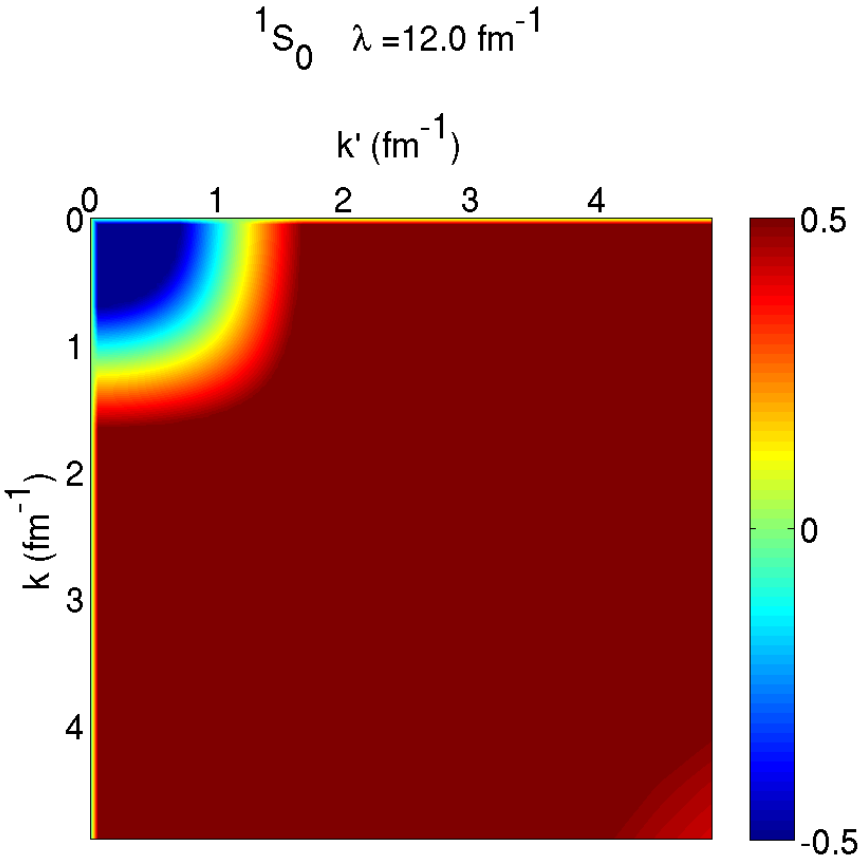

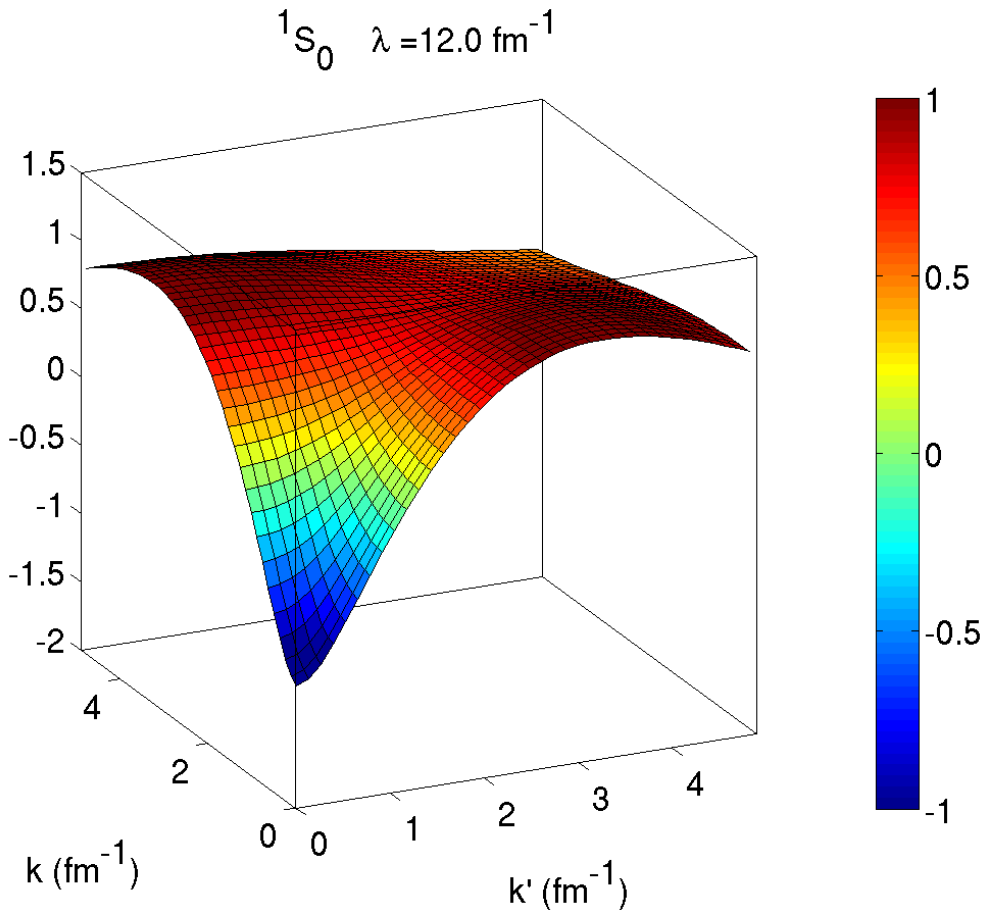

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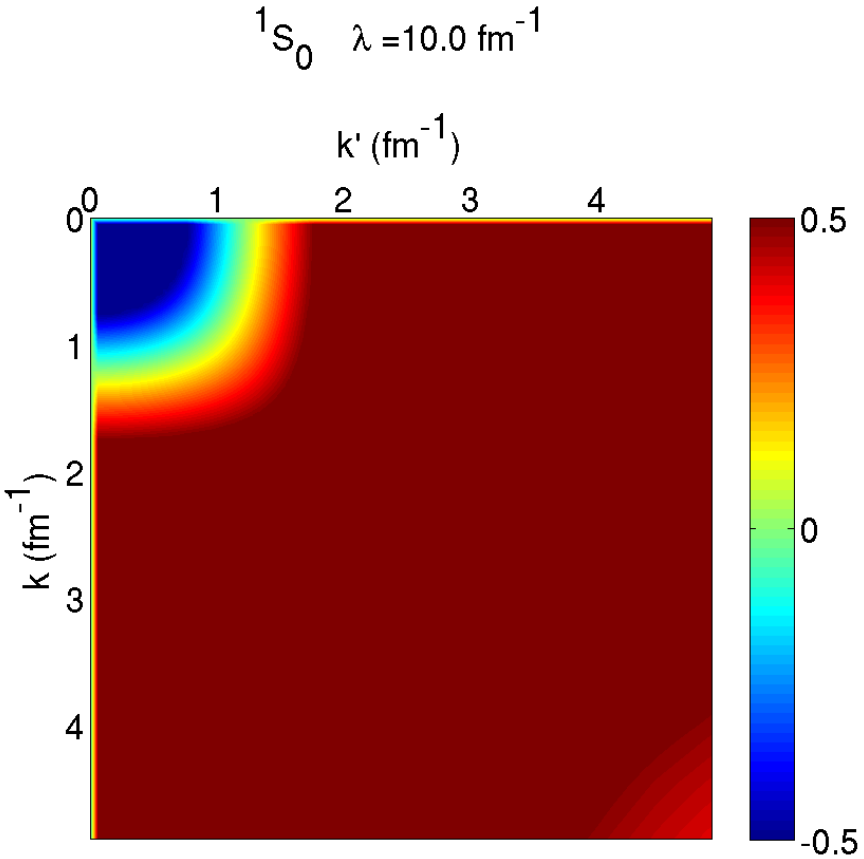

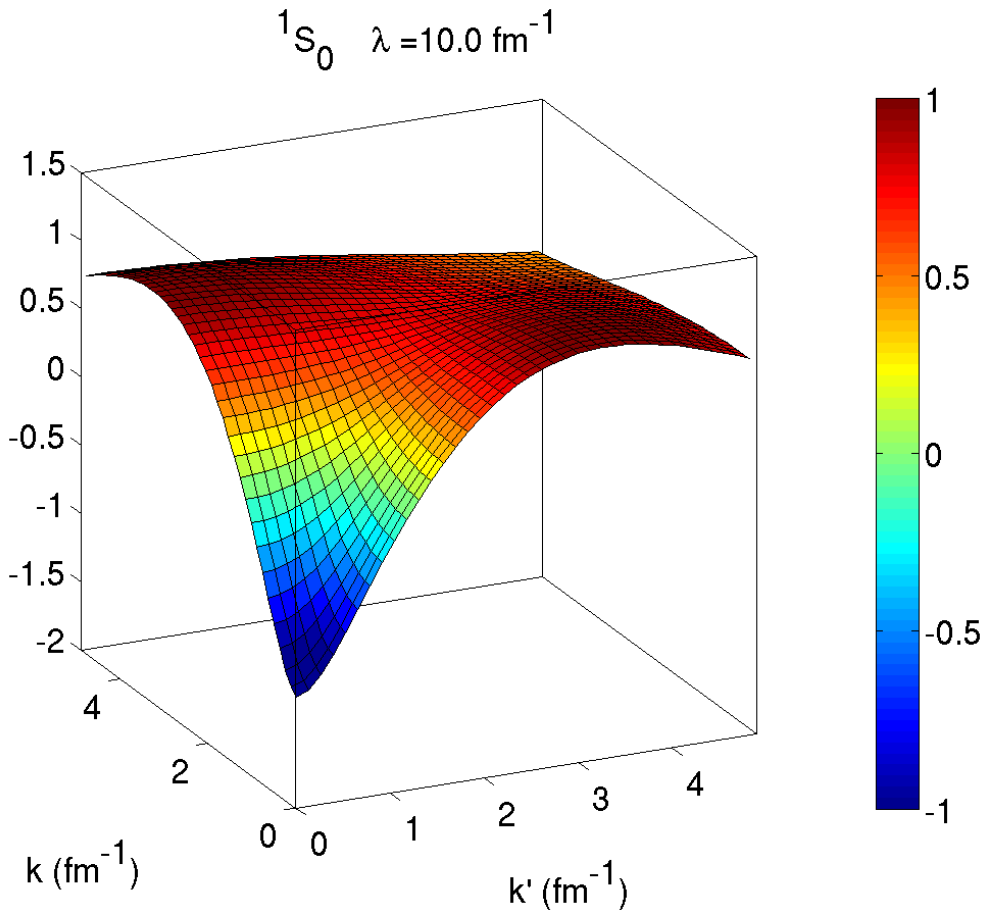

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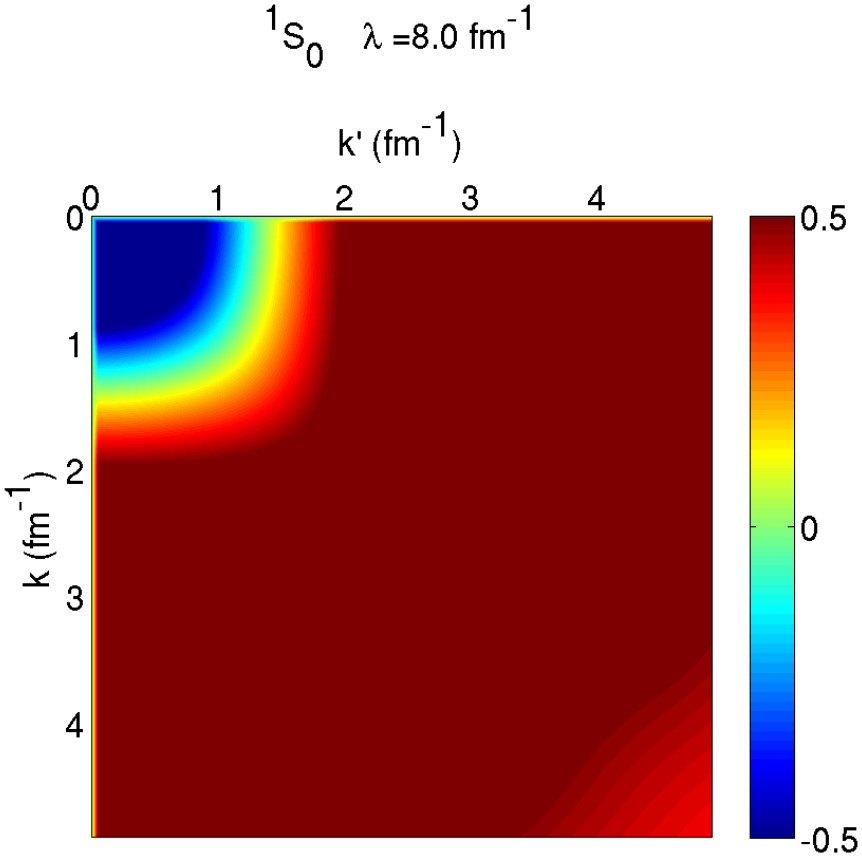

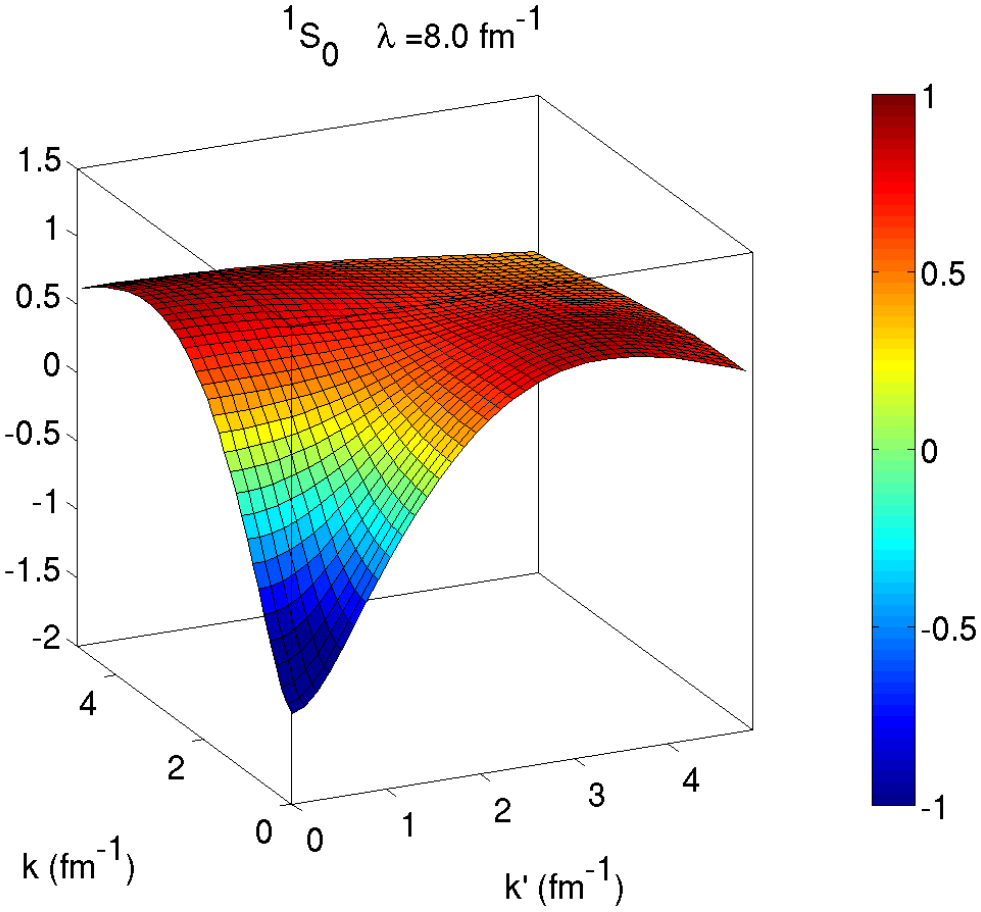

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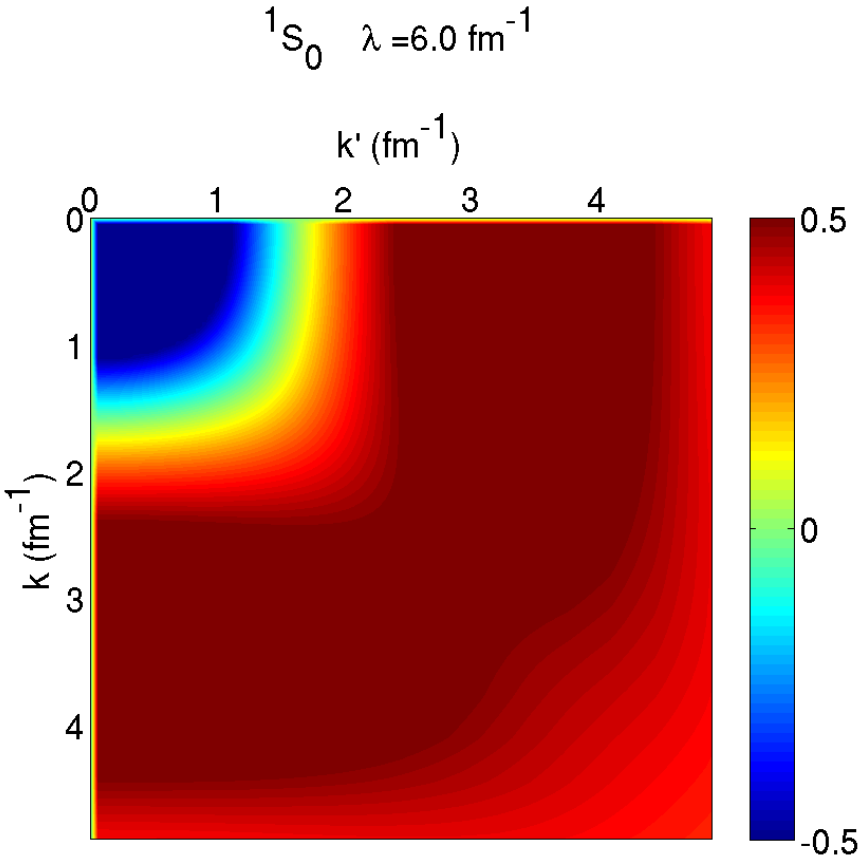

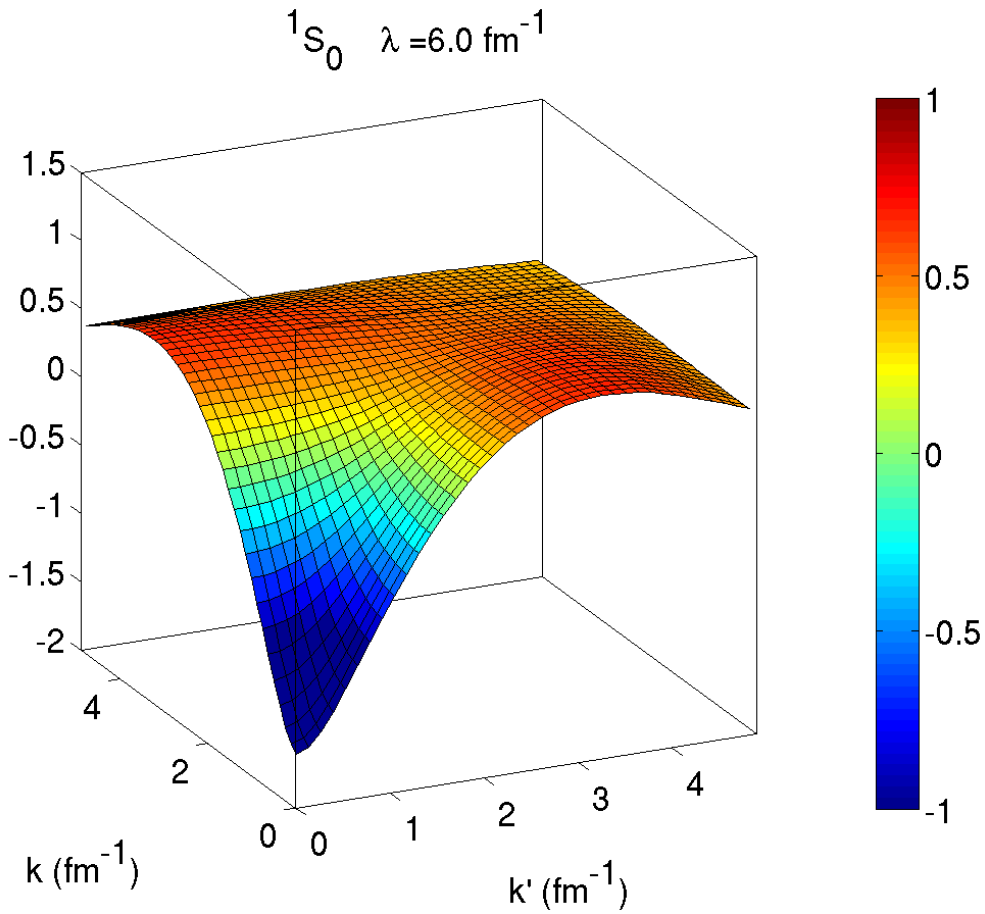

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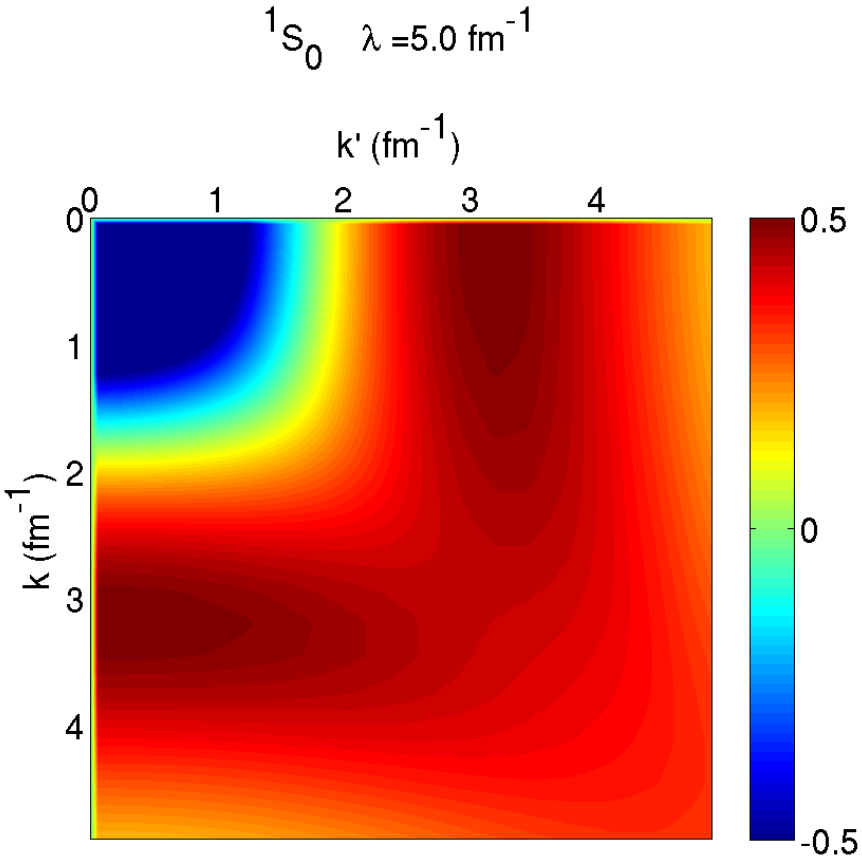

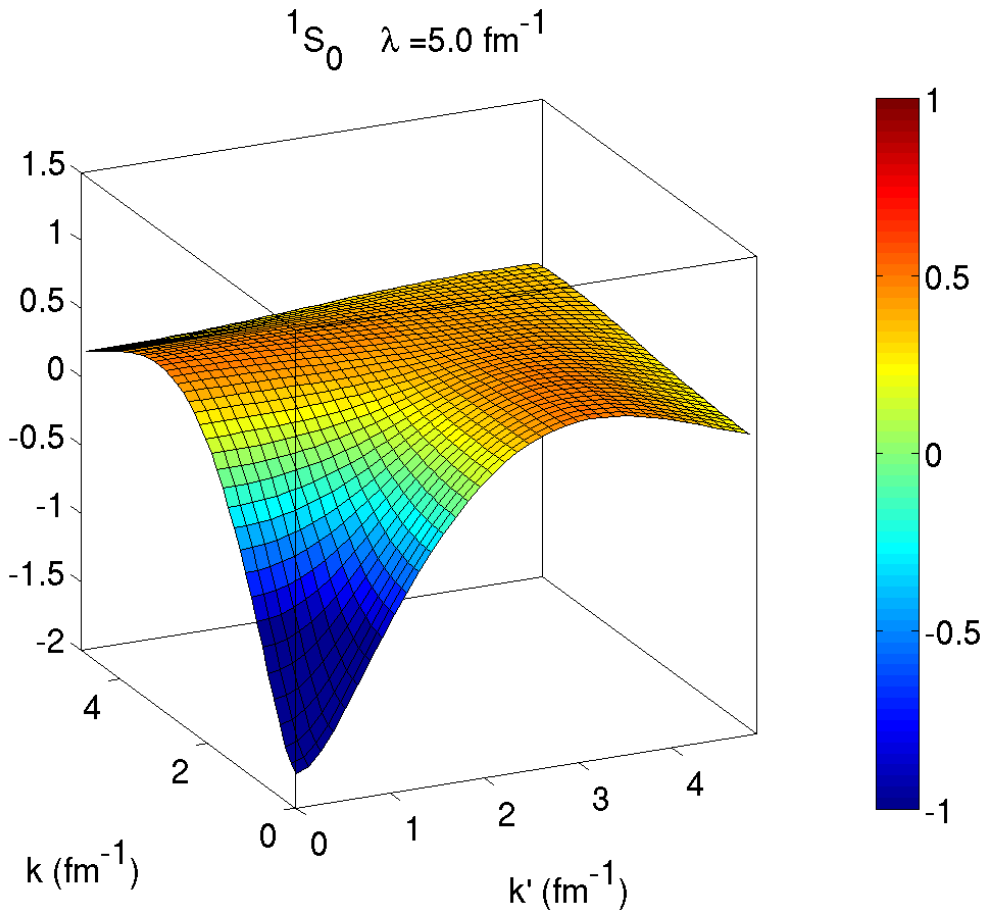

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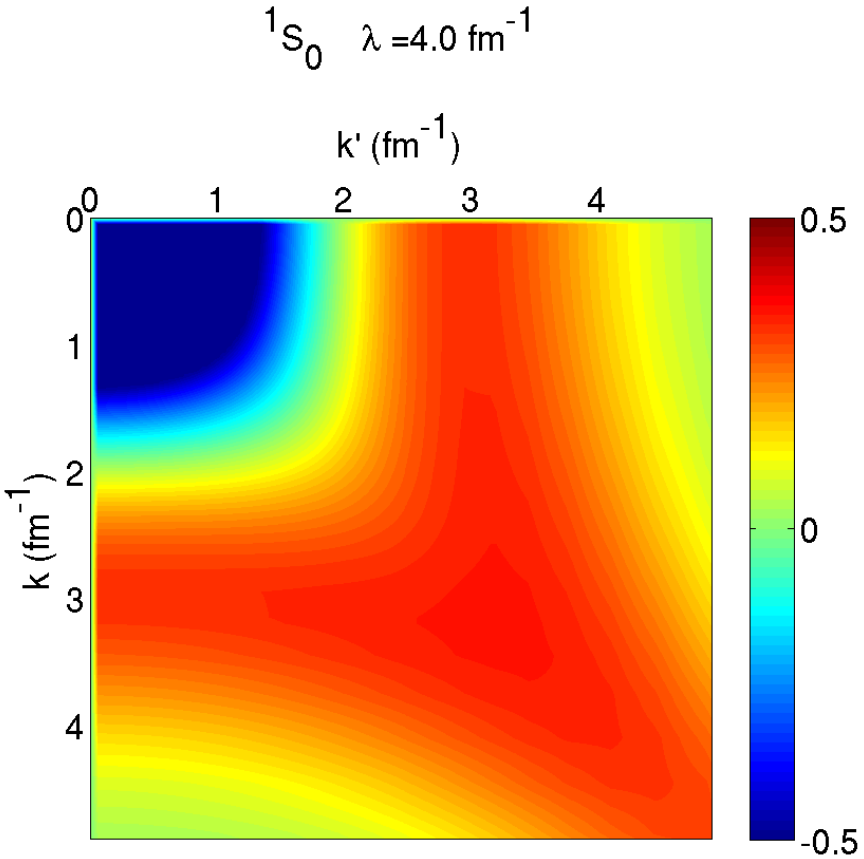

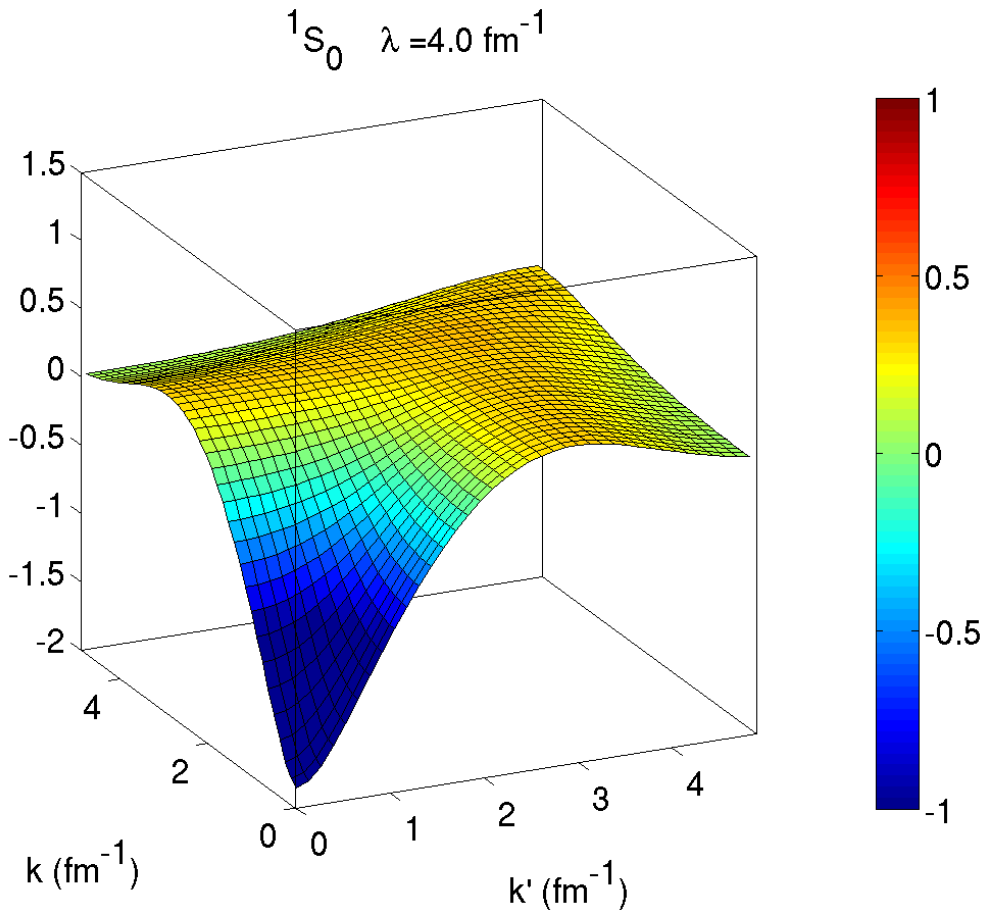

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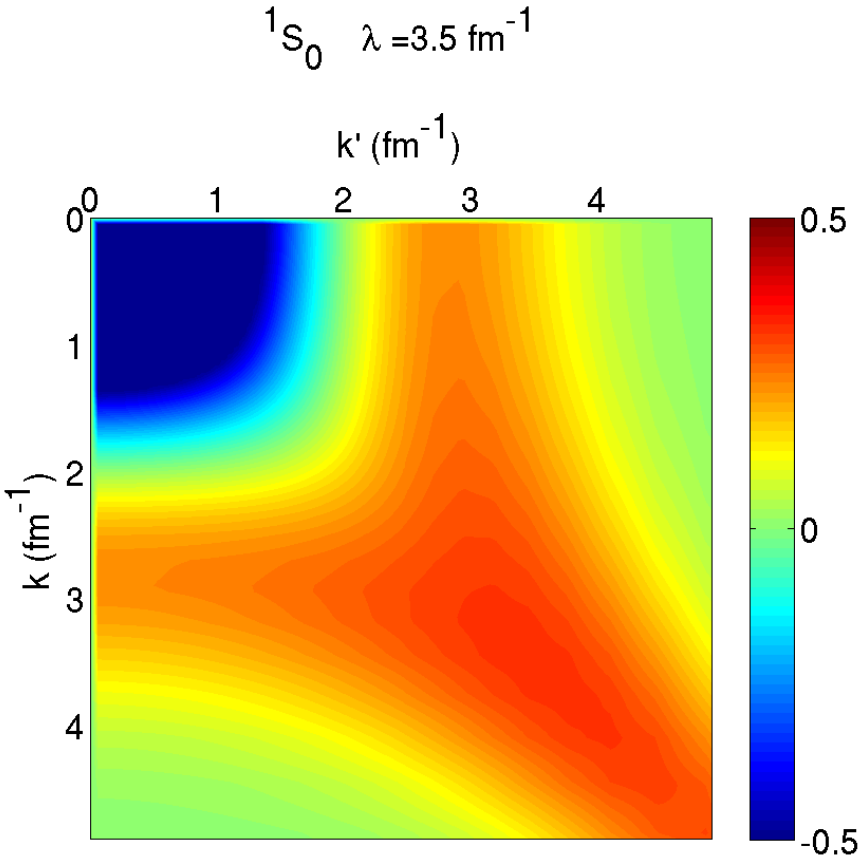

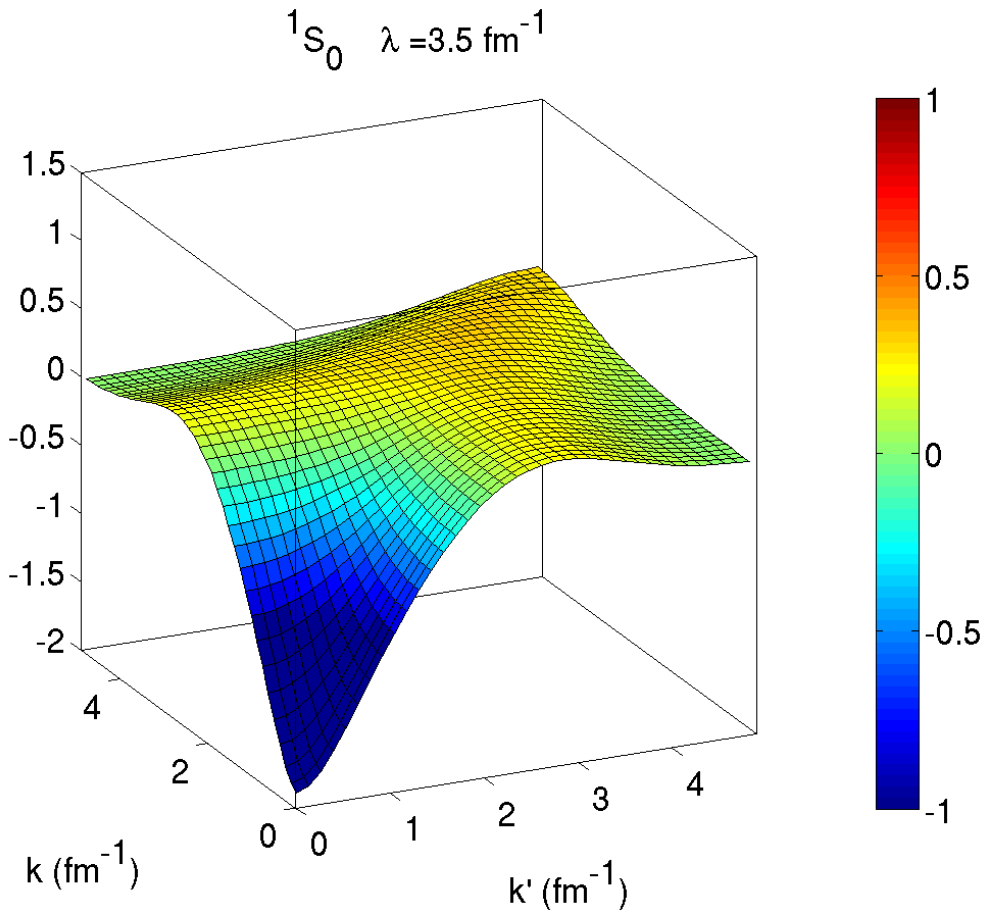

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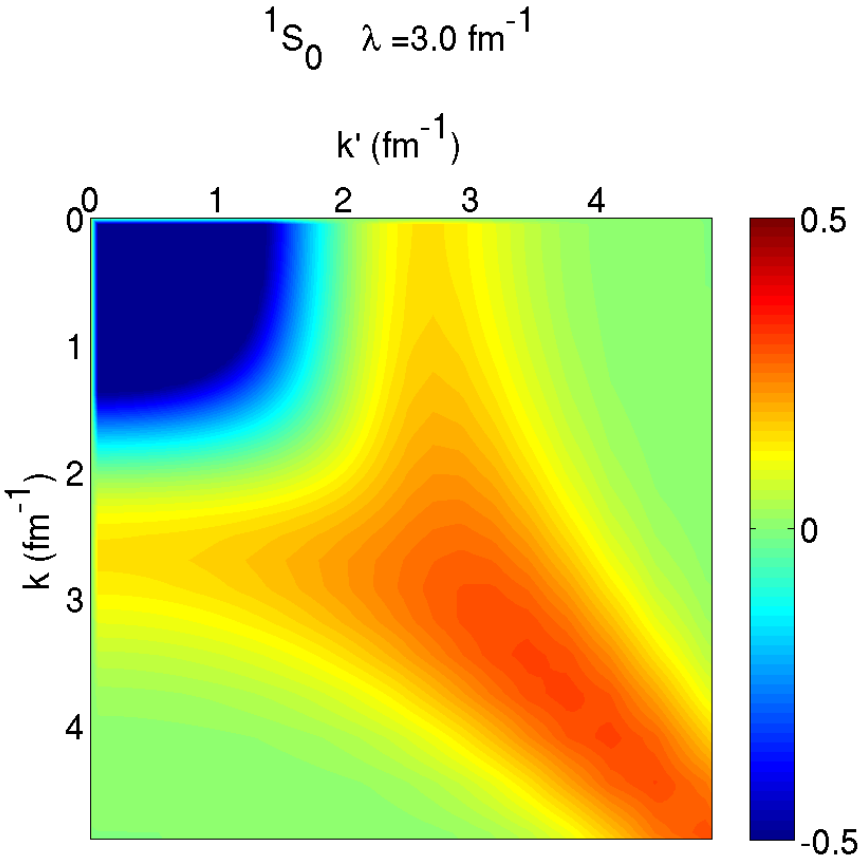

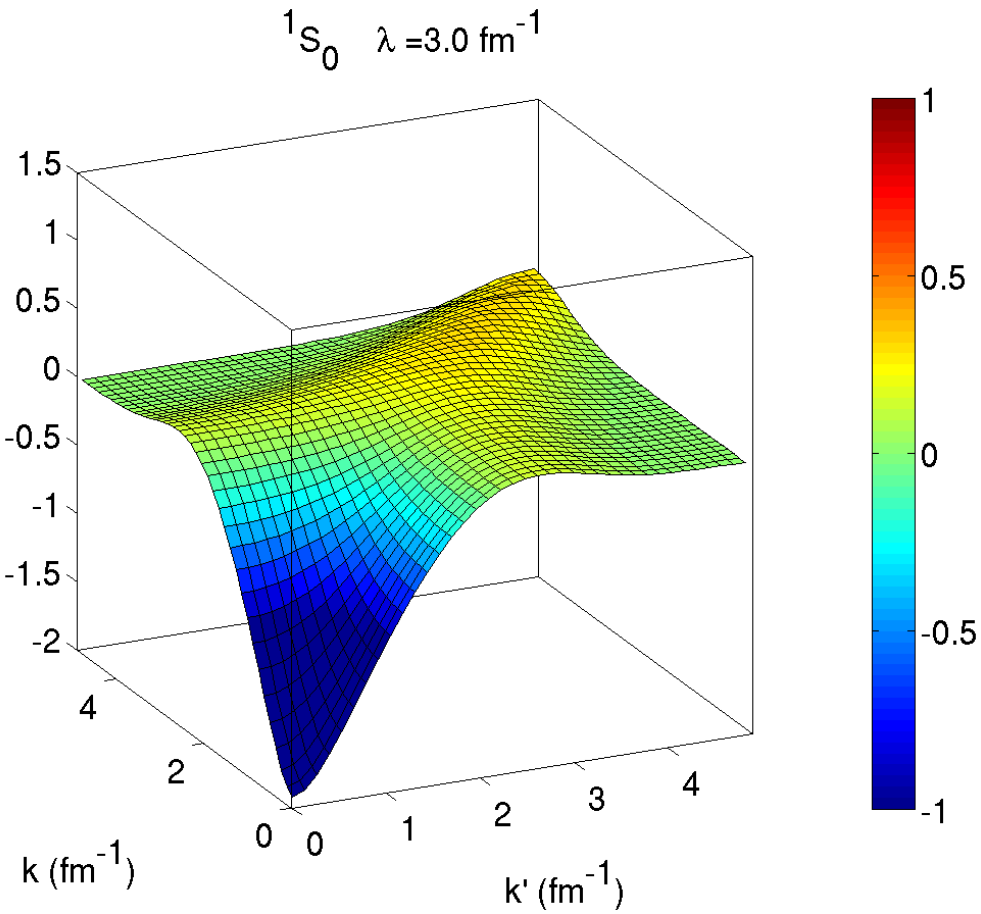

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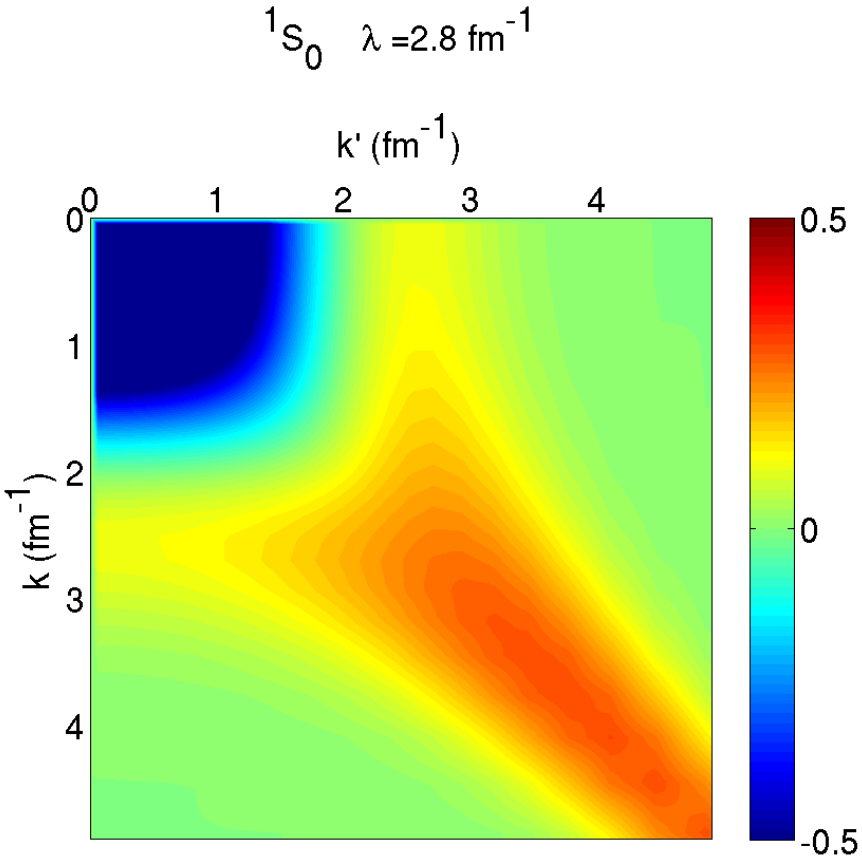

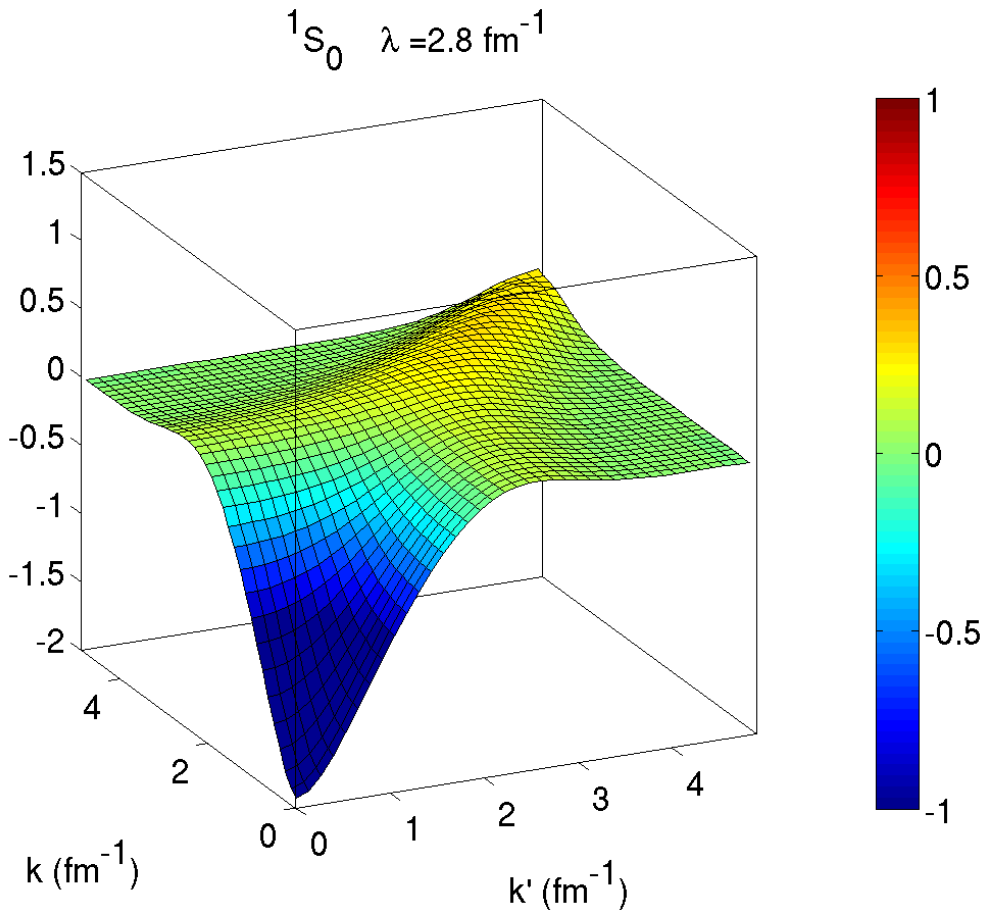

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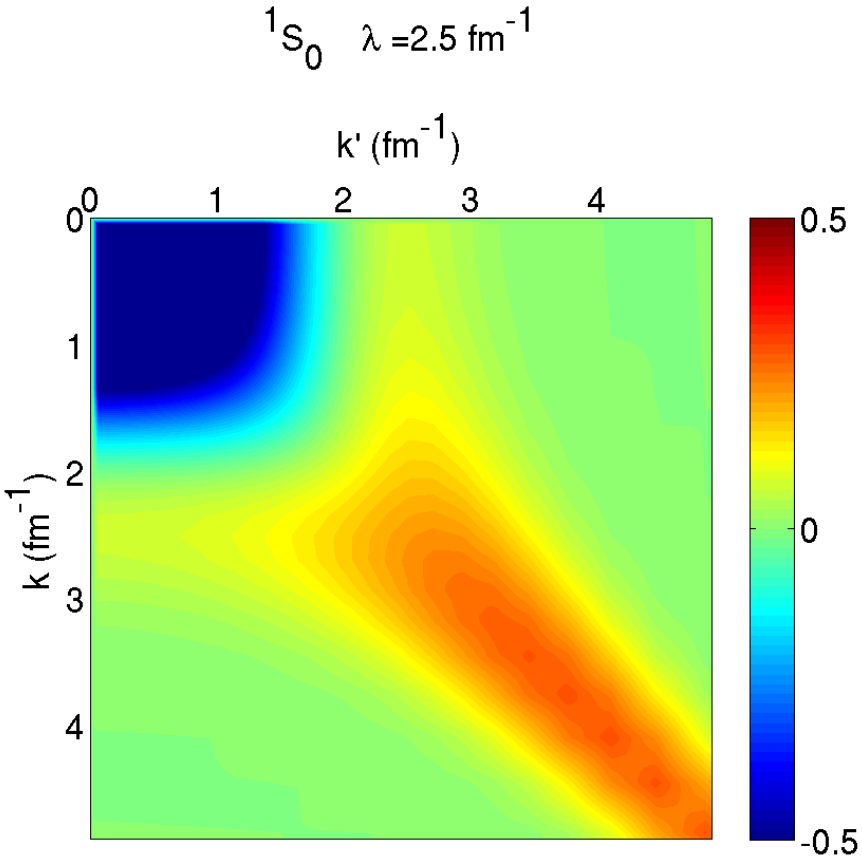

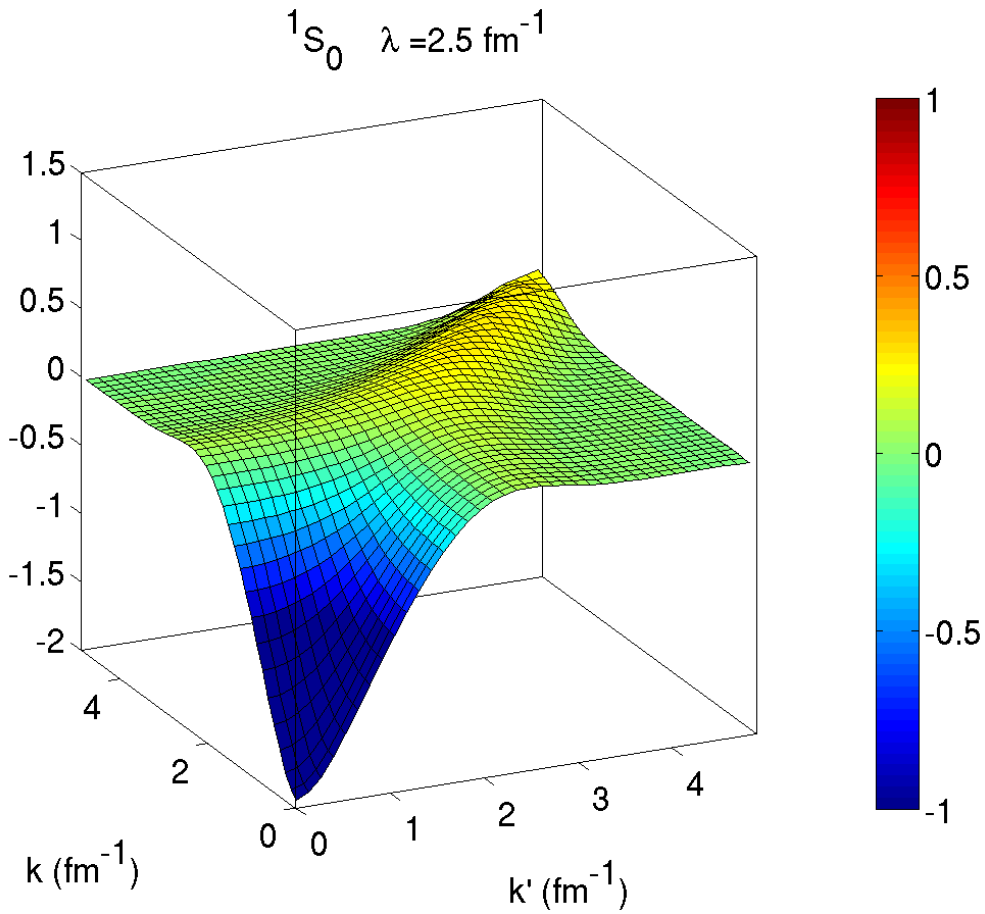

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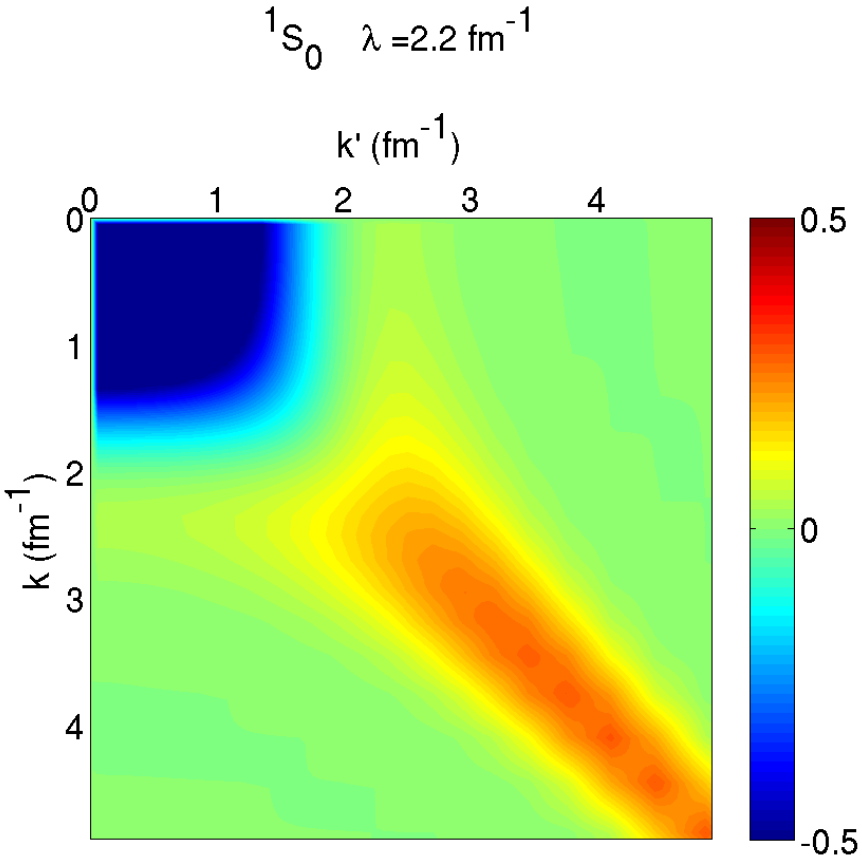

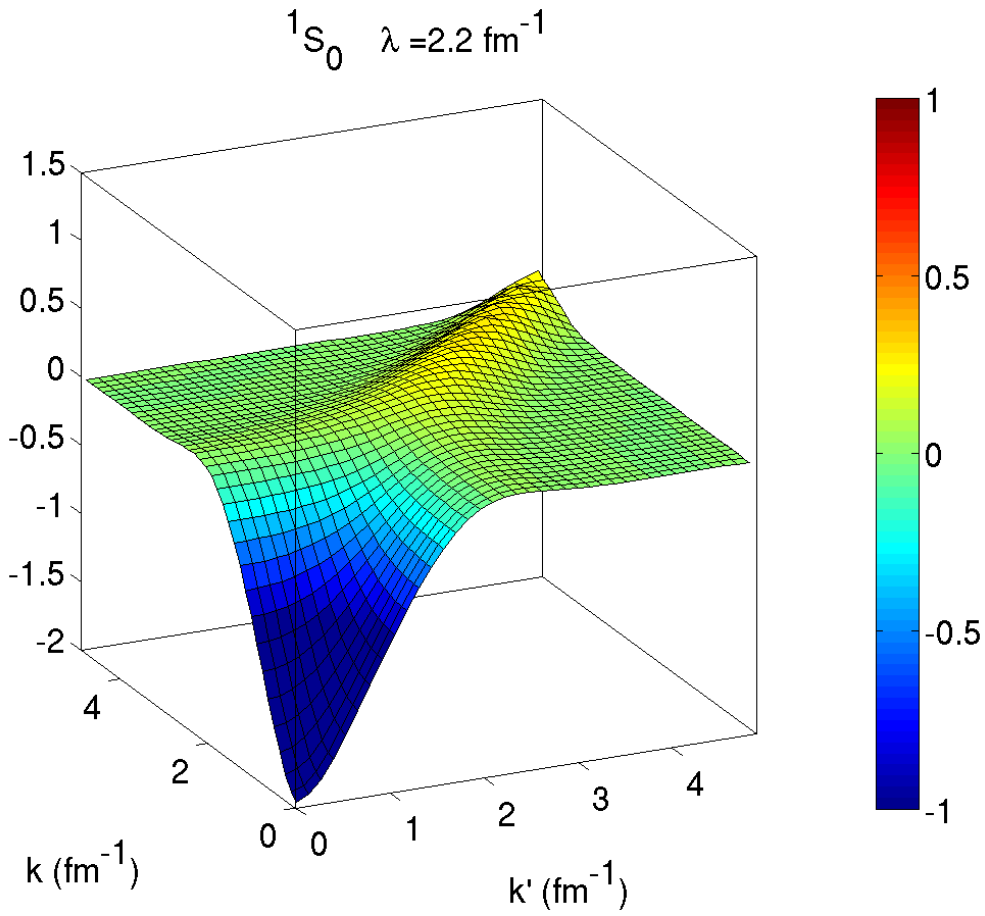

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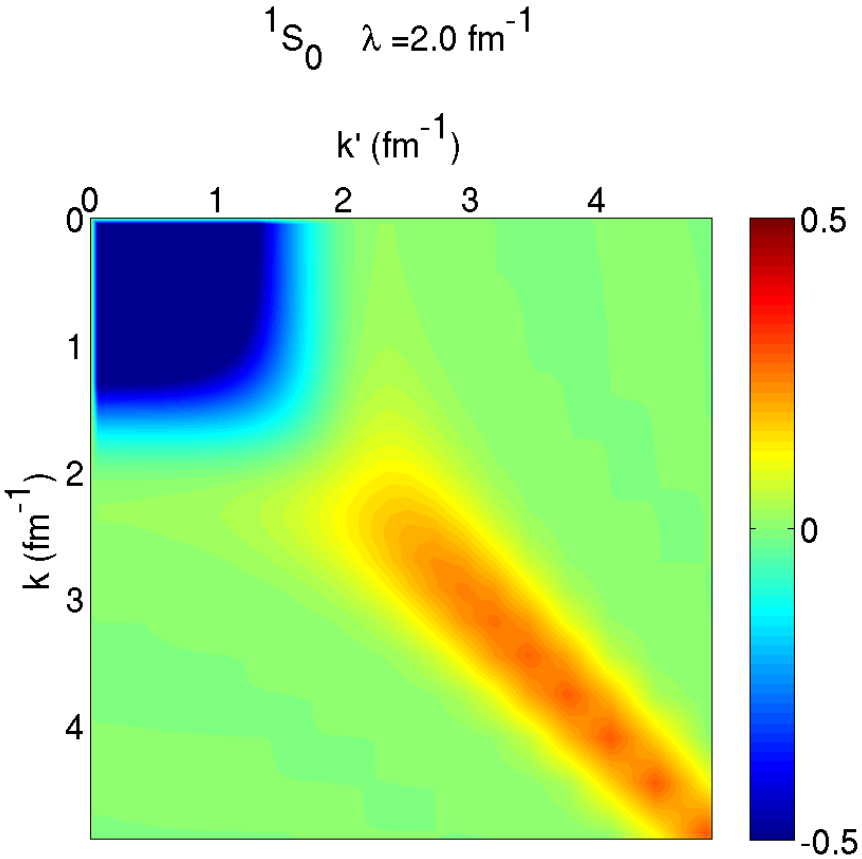
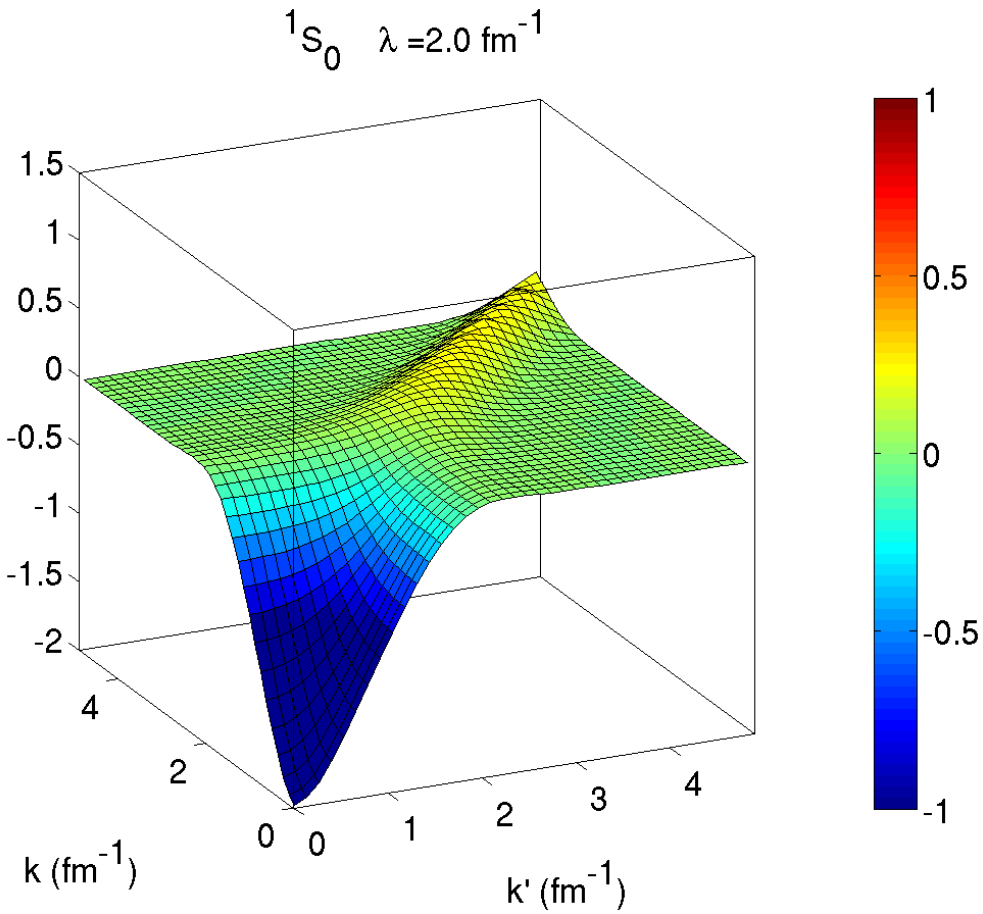
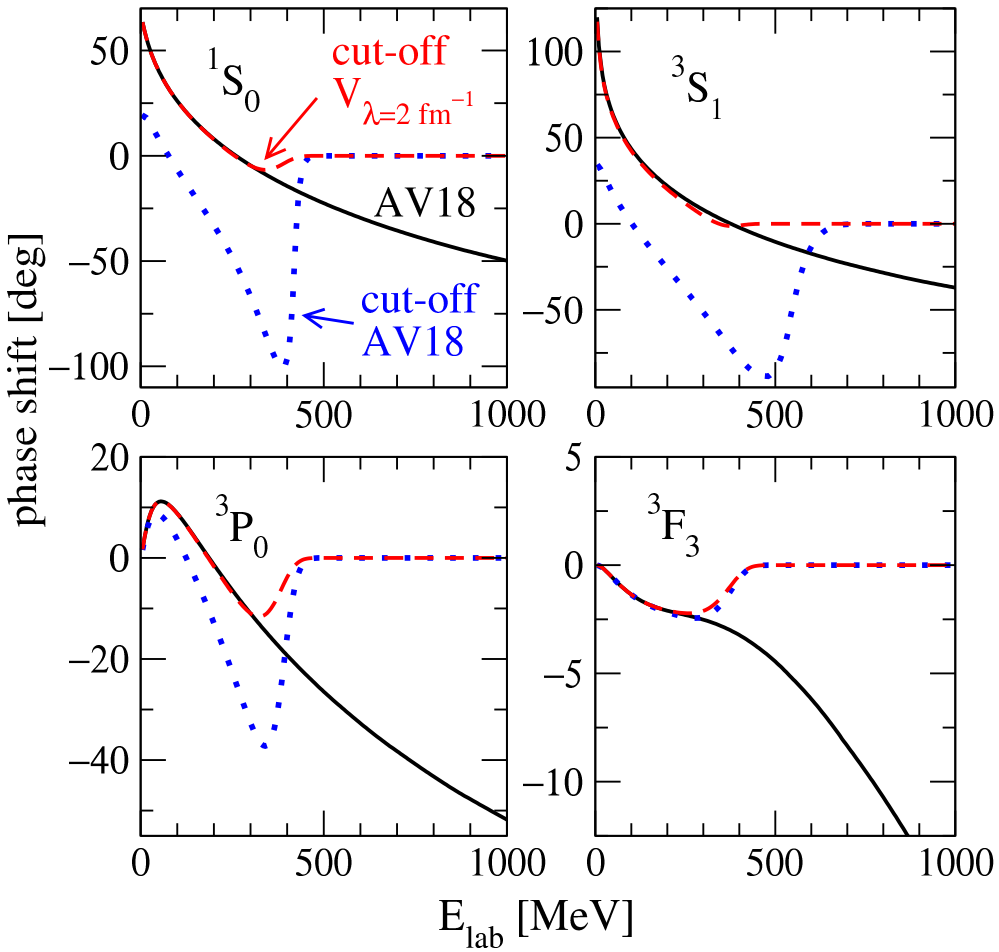




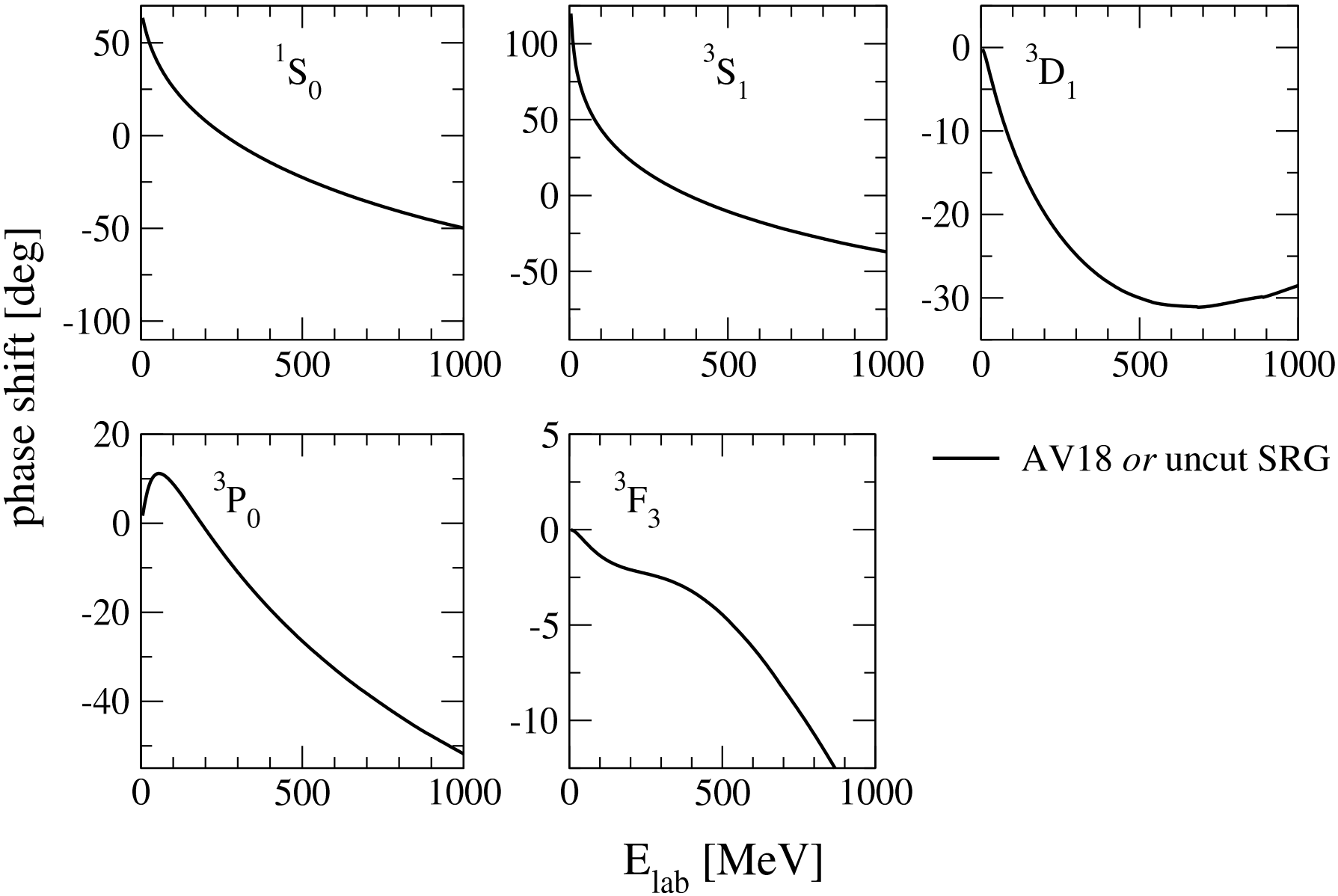
Decoupling and phase shifts: Low-pass filters work!

- Unevolved AV18 phase shifts (black solid line)
- Cutoff AV18 potential at $k = 2.2\,\mathrm{fm}^{-1}$ (dotted blue) $\Longrightarrow$ fails for all but F wave
- Uncut evolved potential agrees perfectly for all energies
- Cutoff evolved potential agrees up to cutoff energy
- F-wave is already soft (π's) $\Longrightarrow$ already decoupled



Low-pass filters work! [Jurgenson et al. (2008)]

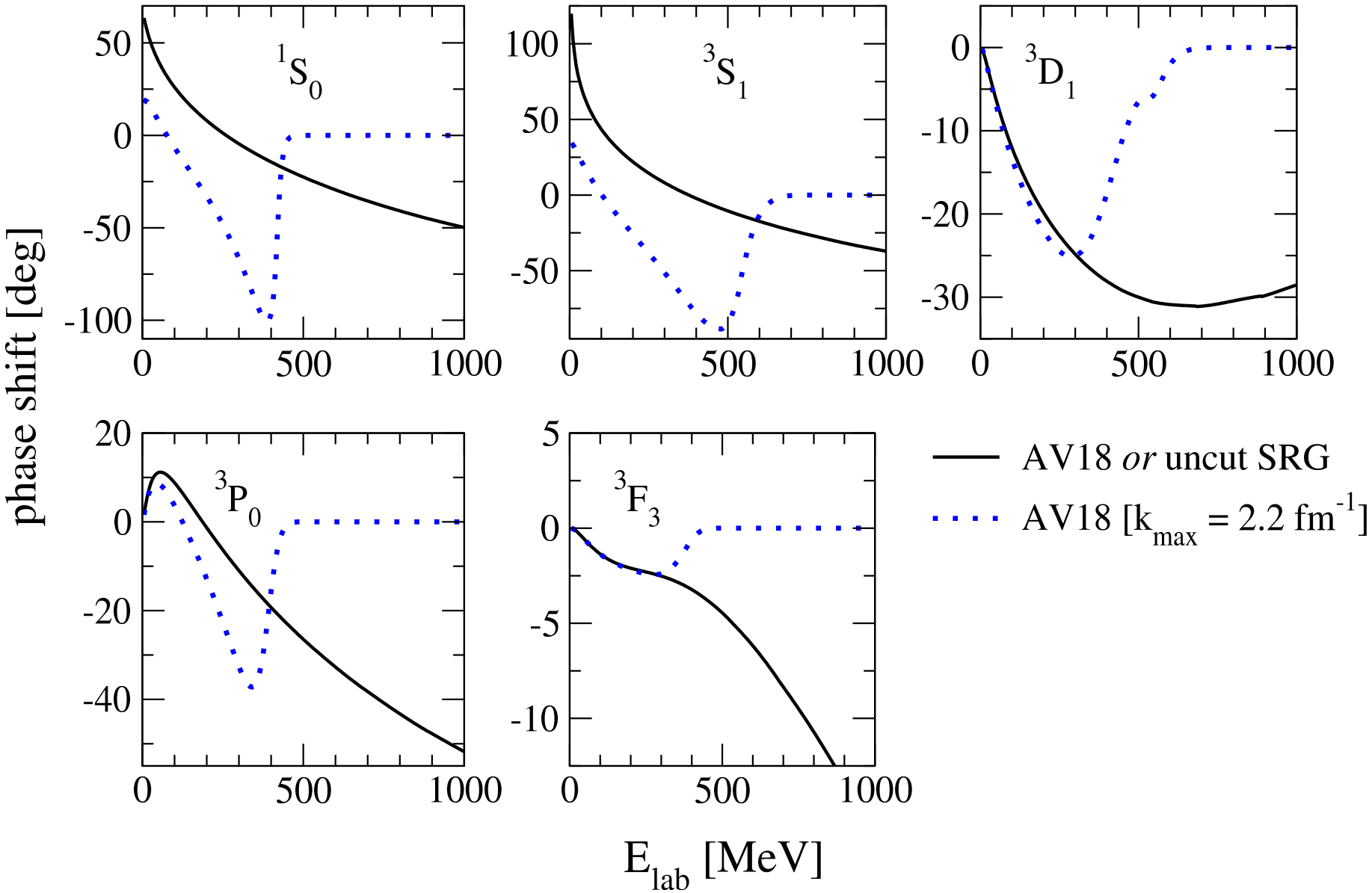
NN phase shifts in different channels: no filter



Uncut evolved potential agrees perfectly for all energies

Low-pass filters work! [Jurgenson et al. (2008)]

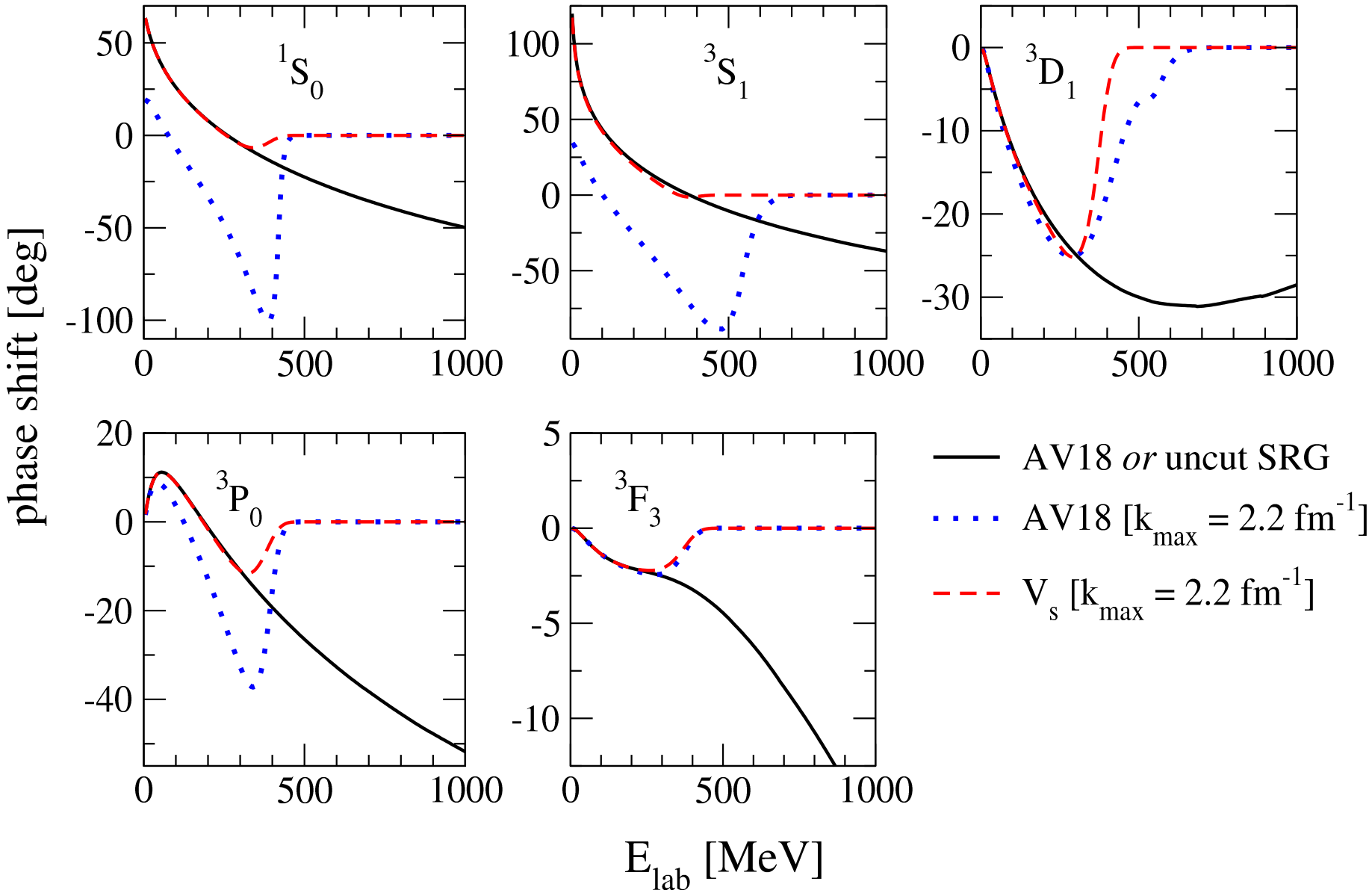
NN phase shifts in different channels: filter full potential



All fail except F-wave (D?) $\Longrightarrow$ already soft (π's) $\Longrightarrow$ already decoupled

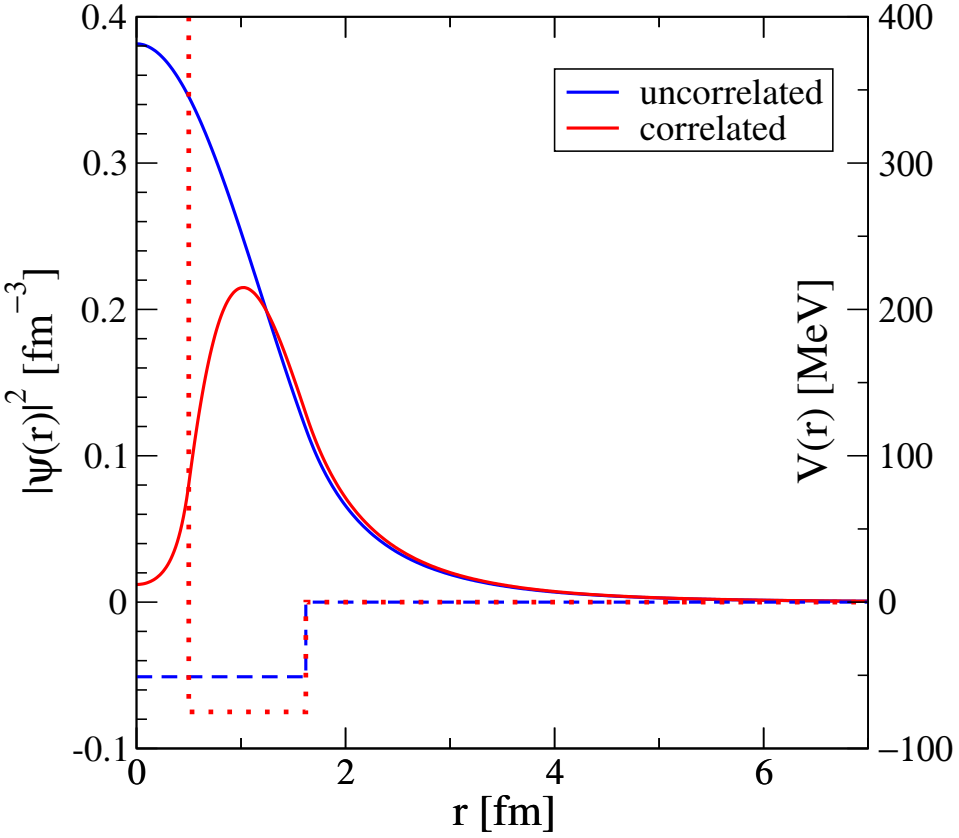
Low-pass filters work! [Jurgenson et al. (2008)]

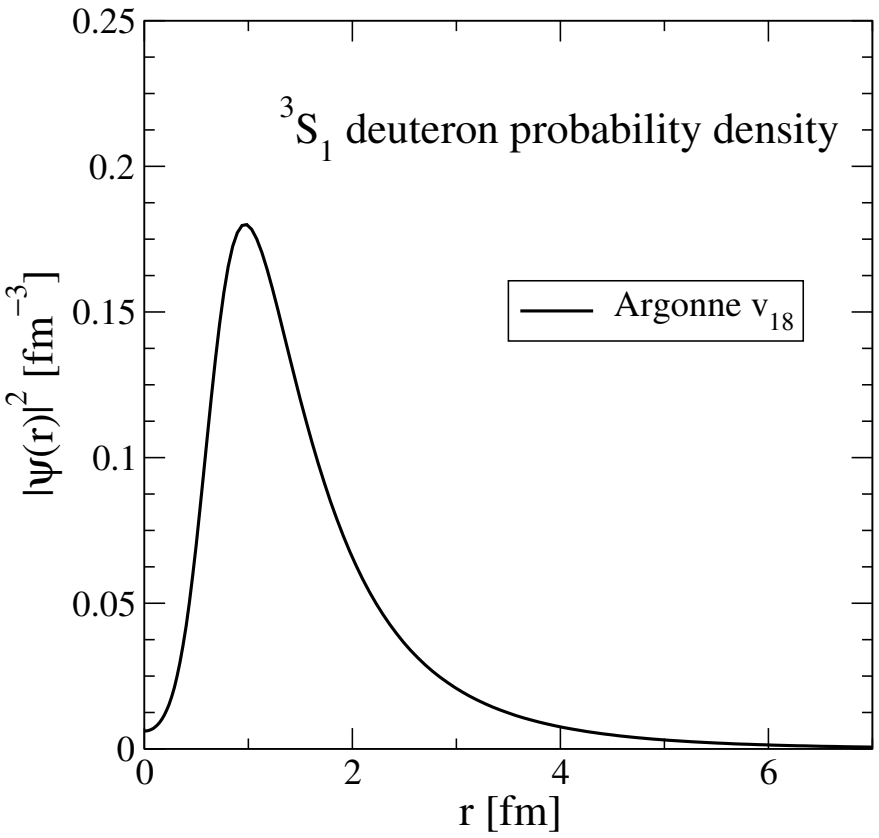
NN phase shifts in different channels: filtered SRG works!



Cutoff evolved potential agrees up to cutoff energy

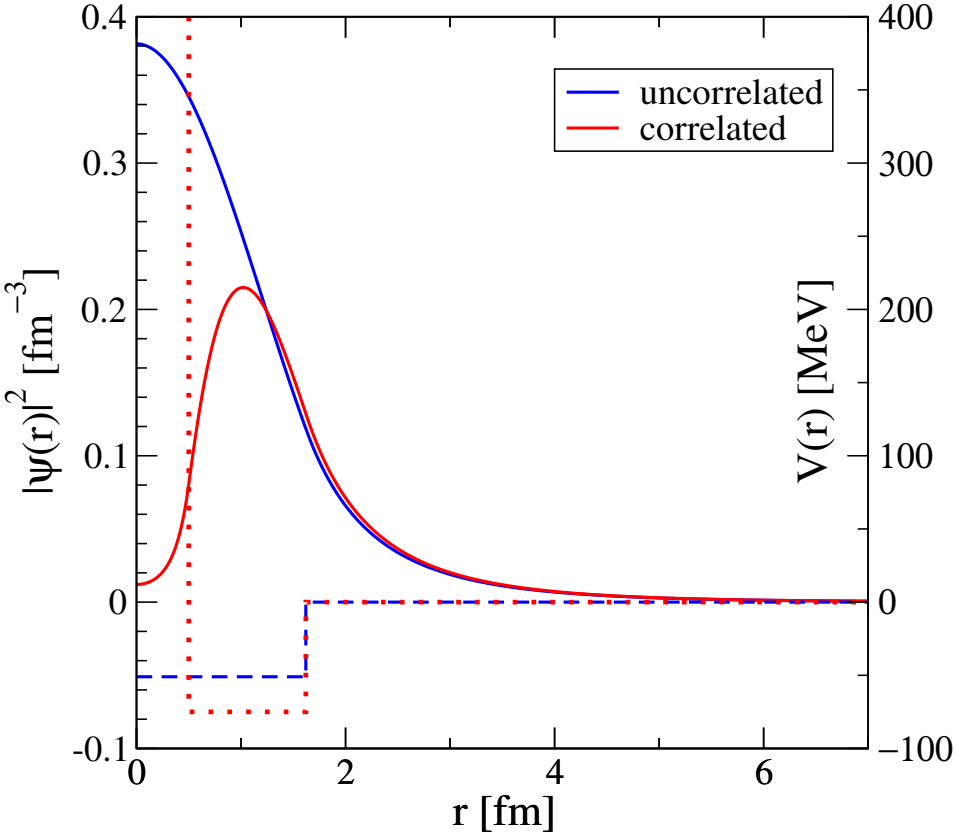
Consequences of a repulsive core revisited

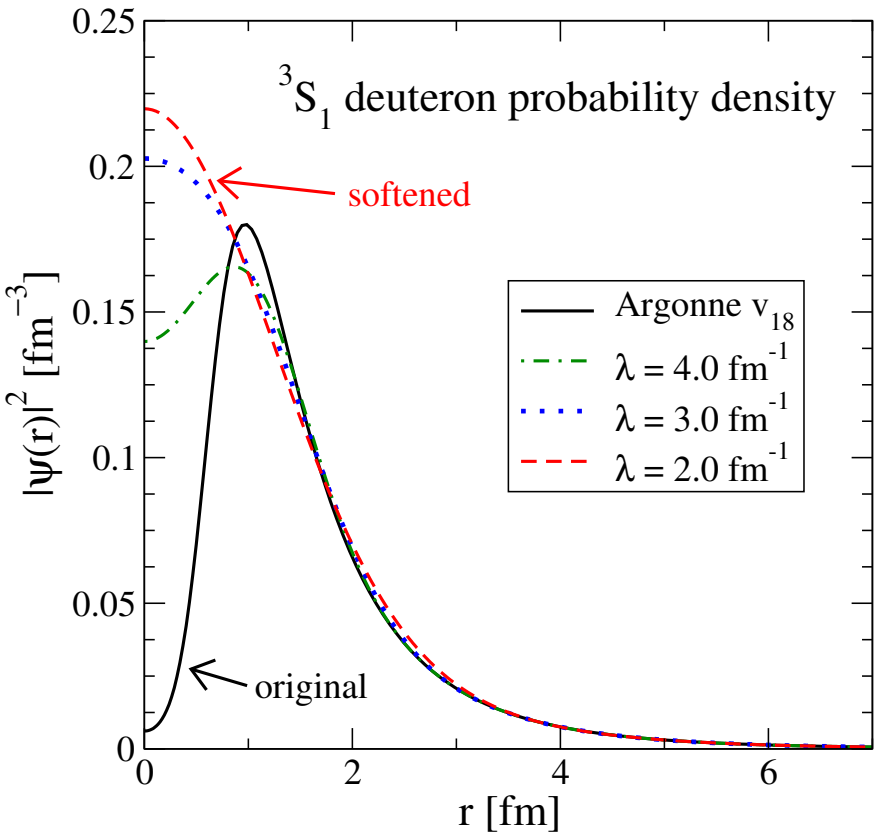




- Probability at short separations suppressed $\Longrightarrow$ "correlations"
- Short-distance structure $\Leftrightarrow$ high-momentum components
- Greatly complicates expansion of many-body wave functions

Consequences of a repulsive core revisited





- Transformed potential $\Longrightarrow$ no short-range correlations in wf!
- Potential is now non-local: $V(\mathbf{r})\psi(\mathbf{r}) \longrightarrow \int d^3\mathbf{r}'\, V(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')$
  - A problem for Green's Function Monte Carlo approach
  - Not a problem for many-body methods using HO matrix elements

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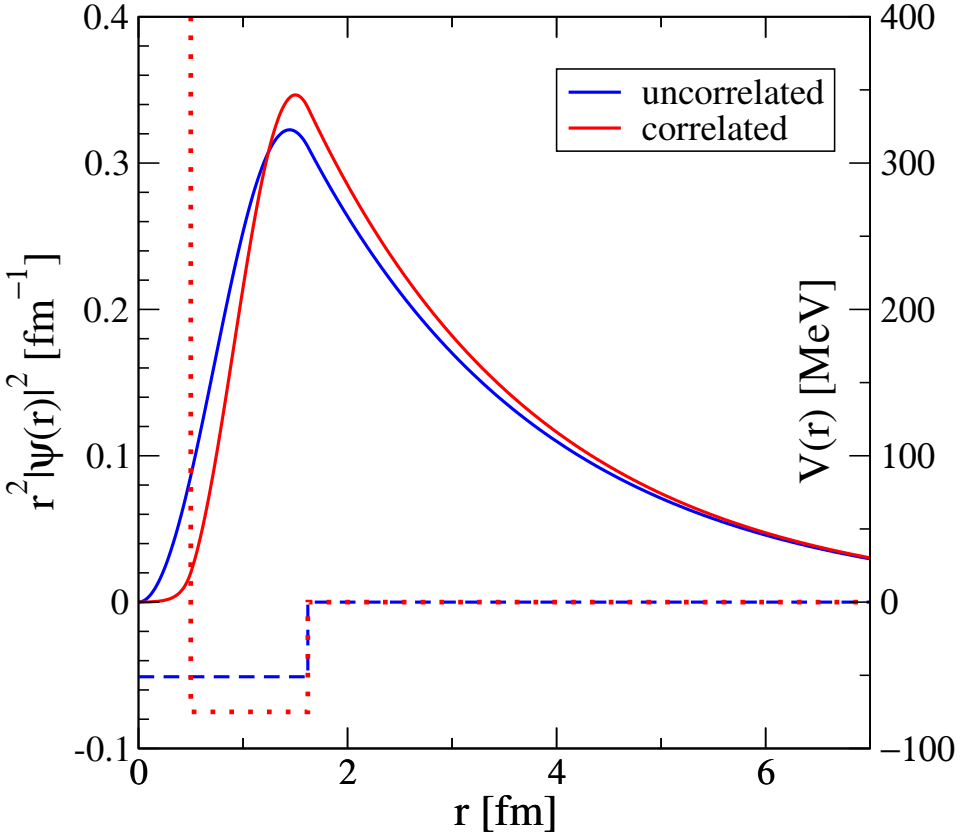

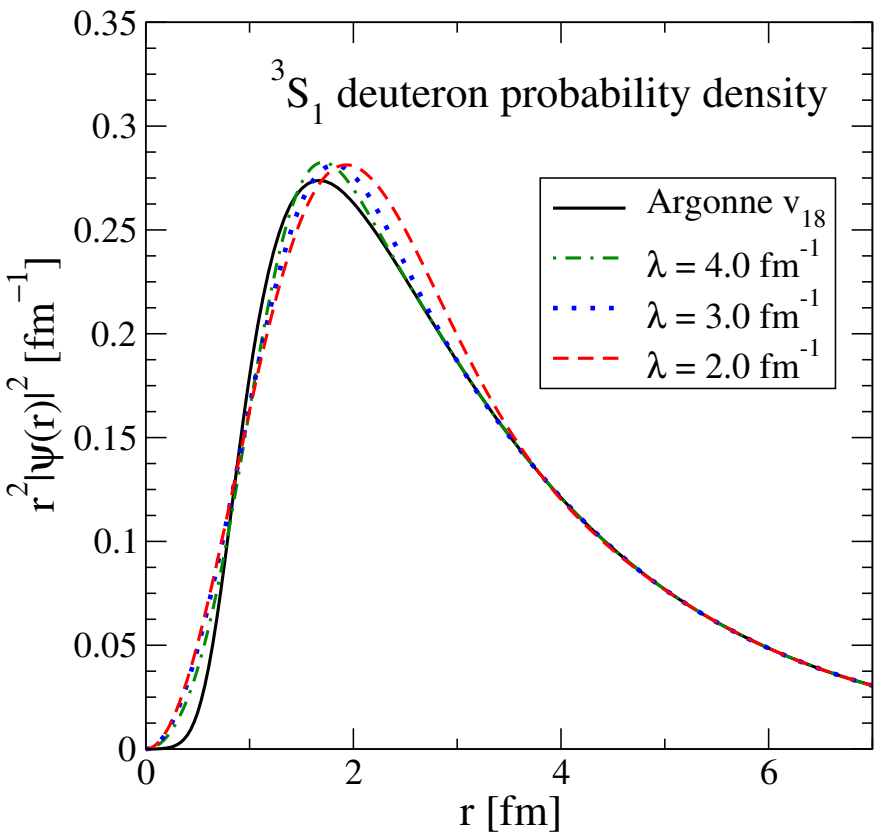

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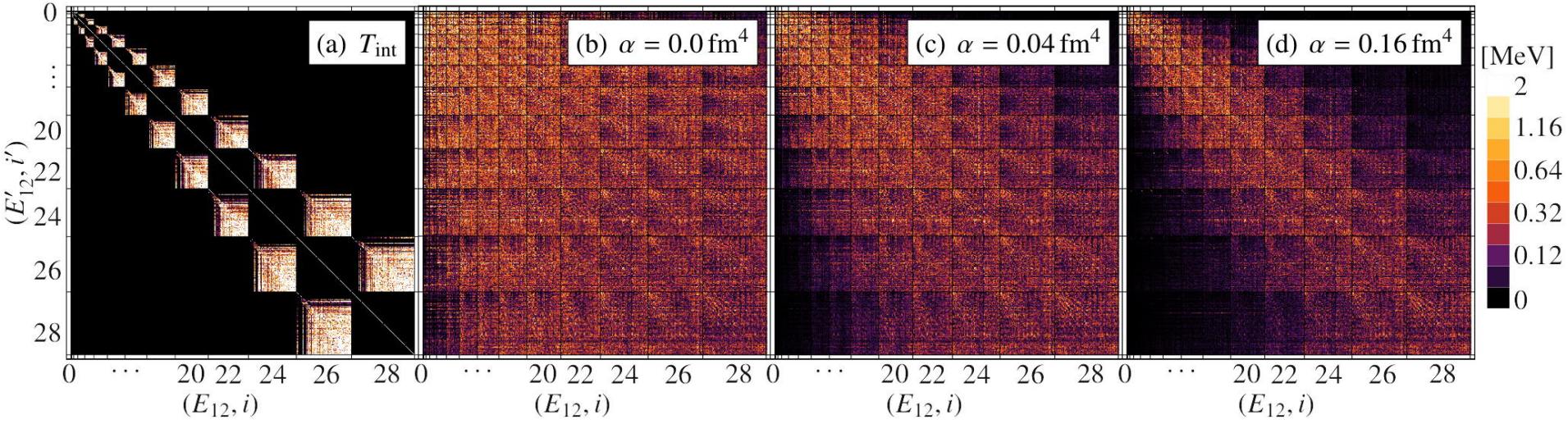
HO matrix elements with SRG flow

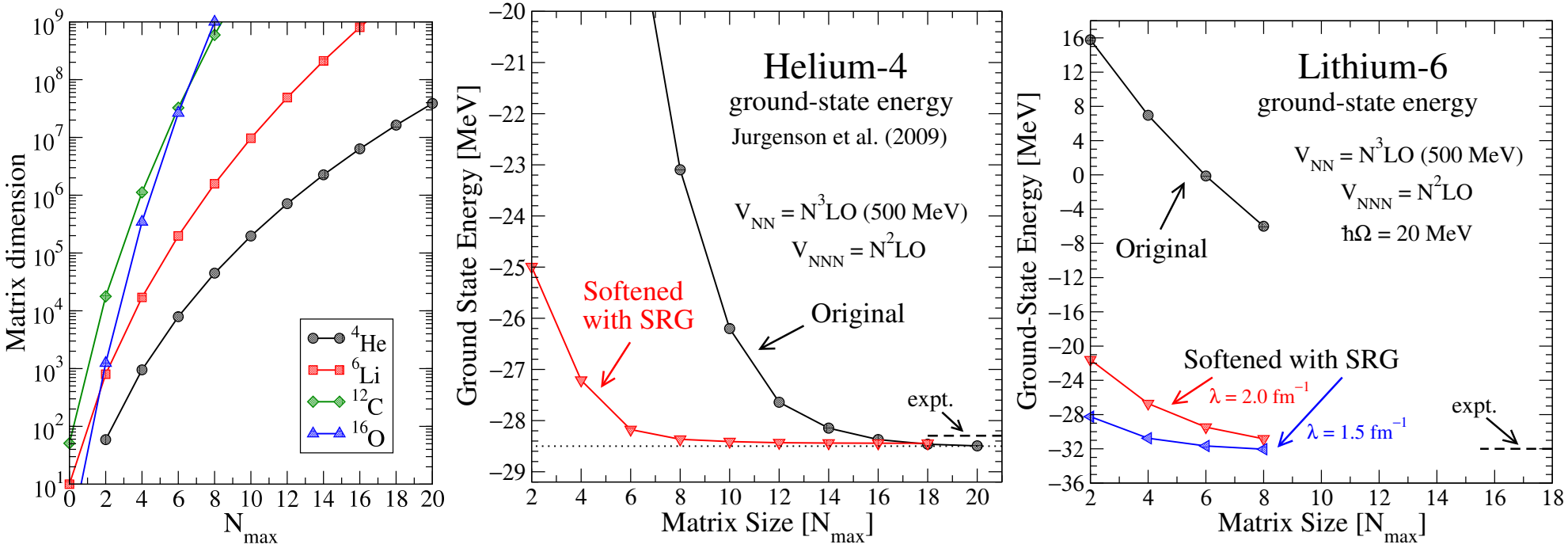
- We've seen that high and low momentum states decouple
- Does this help for harmonic oscilator matrix elements?
- Consider the SRG evolution from R. Roth et al.:



- Yes! We have decoupling of high-energy from low-energy states

Revisit the convergence with matrix size (N_{max})

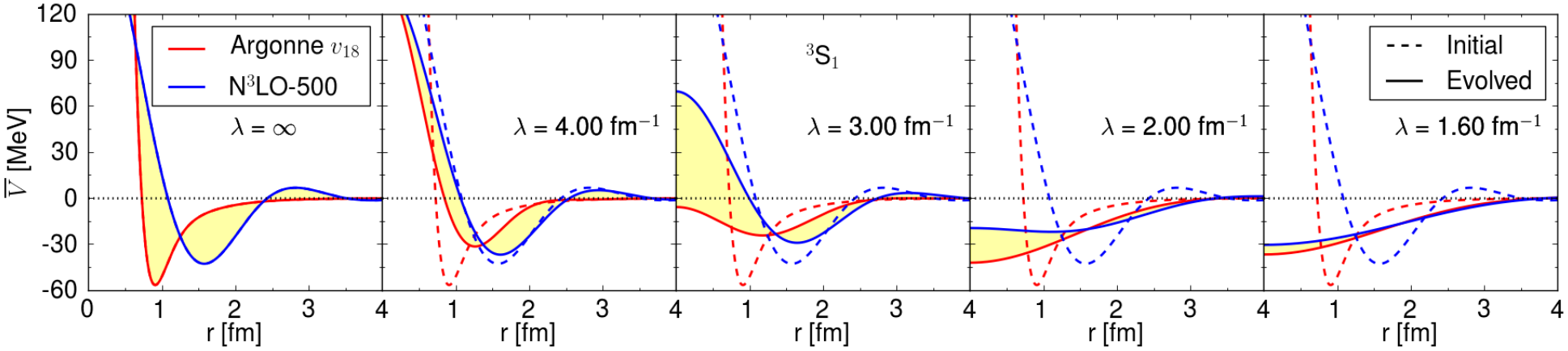
- Harmonic oscillator basis with N_{max} shells for excitations



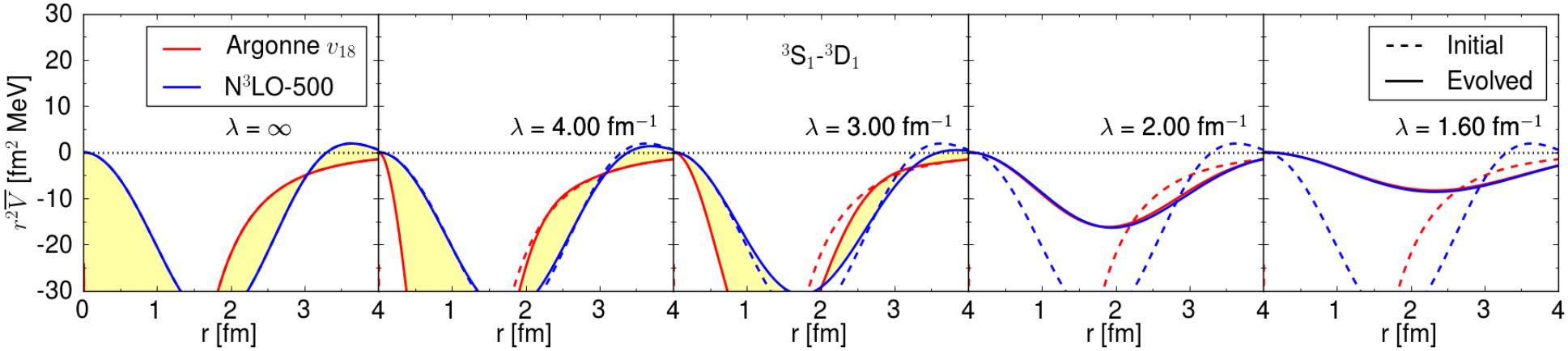
- Graphs show that convergence for *soft* chiral EFT potential is accelerated for evolved SRG potentials
- Rapid growth of basis still a problem; what else can we do?
  - importance sampling of matrix elements
  - e.g., use symmetry: work in a *symplectic* basis

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 et al., PRC (2012)]



$\Longrightarrow$ Flow to universal potentials!

Basics: SRG flow equations [e.g., see arXiv:1203.1779]

- Transform an initial hamiltonian, $H = T + V$, with U_s:

$$H_s = U_s H U_s^\dagger \equiv T + V_s \ ,$$

where s is the *flow parameter*. Differentiating wrt s:

$$\frac{dH_s}{ds} = [\eta_s, H_s] \qquad \text{with} \qquad \eta_s \equiv \frac{dU_s}{ds} U_s^\dagger = -\eta_s^\dagger \ .$$

- η_s is specified by the commutator with Hermitian G_s:

$$\eta_s = [G_s, H_s] \ ,$$

which yields the unitary flow equation (T held fixed),

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

  - Very simple to implement as matrix equation (e.g., MATLAB)
- G_s determines flow $\Longrightarrow$ many choices (T, H_D, H_{BD}, ...)

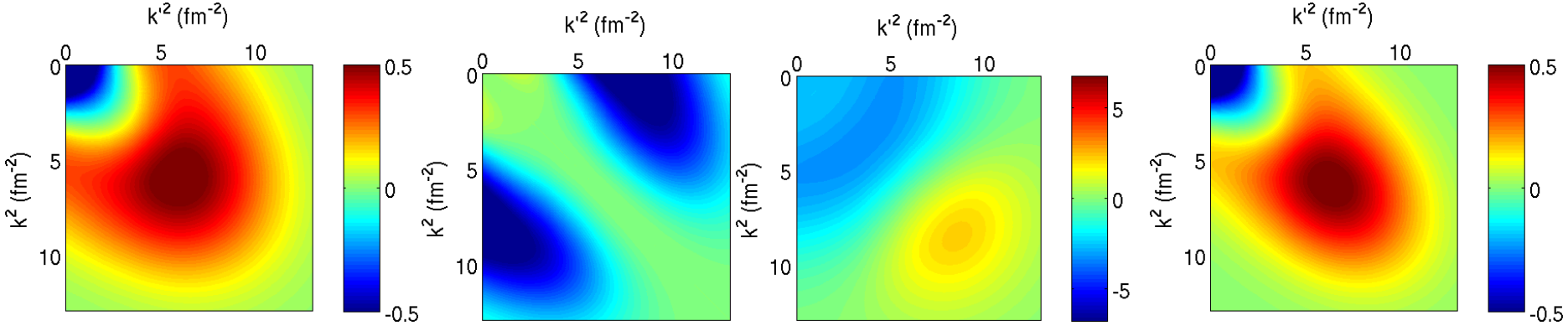
SRG flow of $H = T + V$ in momentum basis

- Takes $H \longrightarrow H_s = U_s H U_s^\dagger$ in small steps labeled by s or λ

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

- For NN, project on relative momentum states $|k\rangle$, but generic

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



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

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

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

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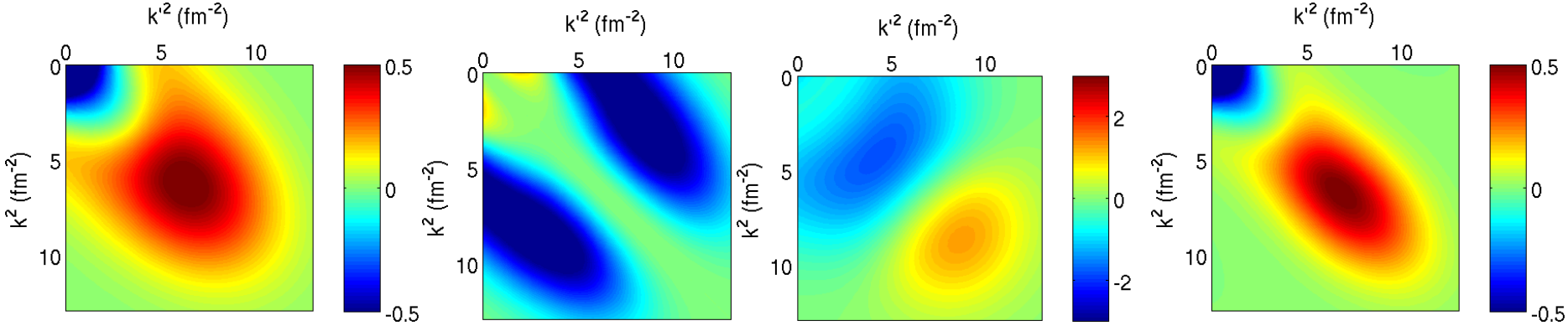

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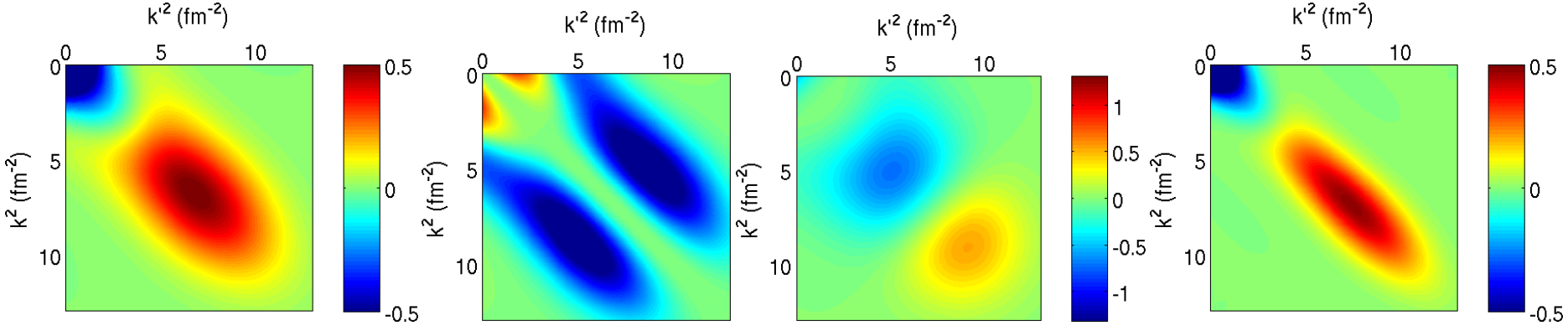

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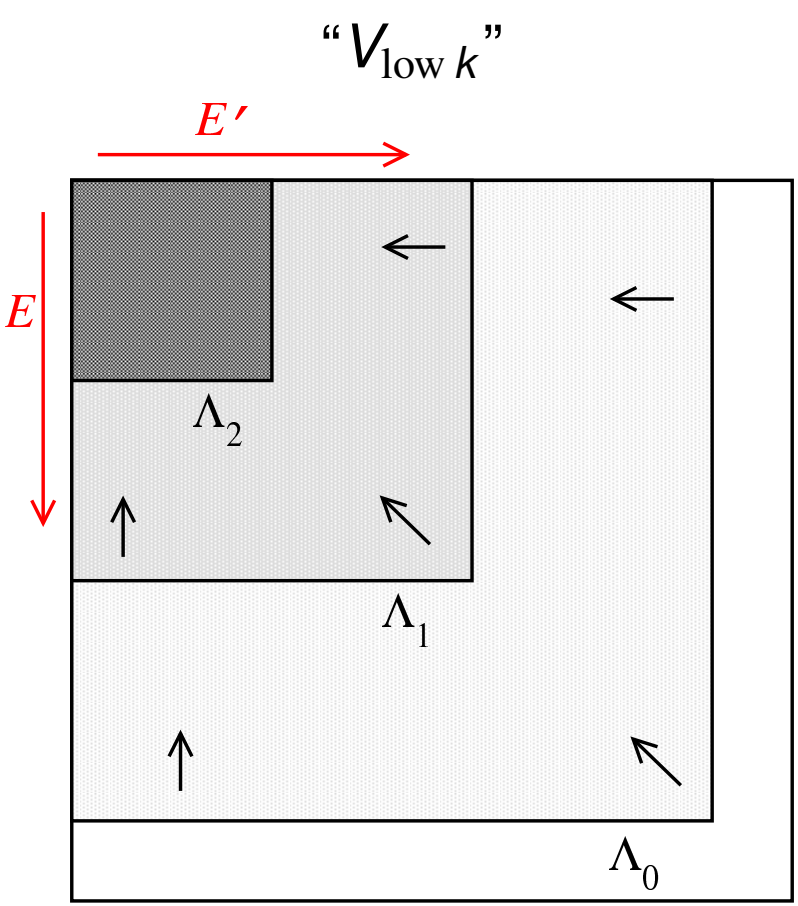
Outline: Lecture 2

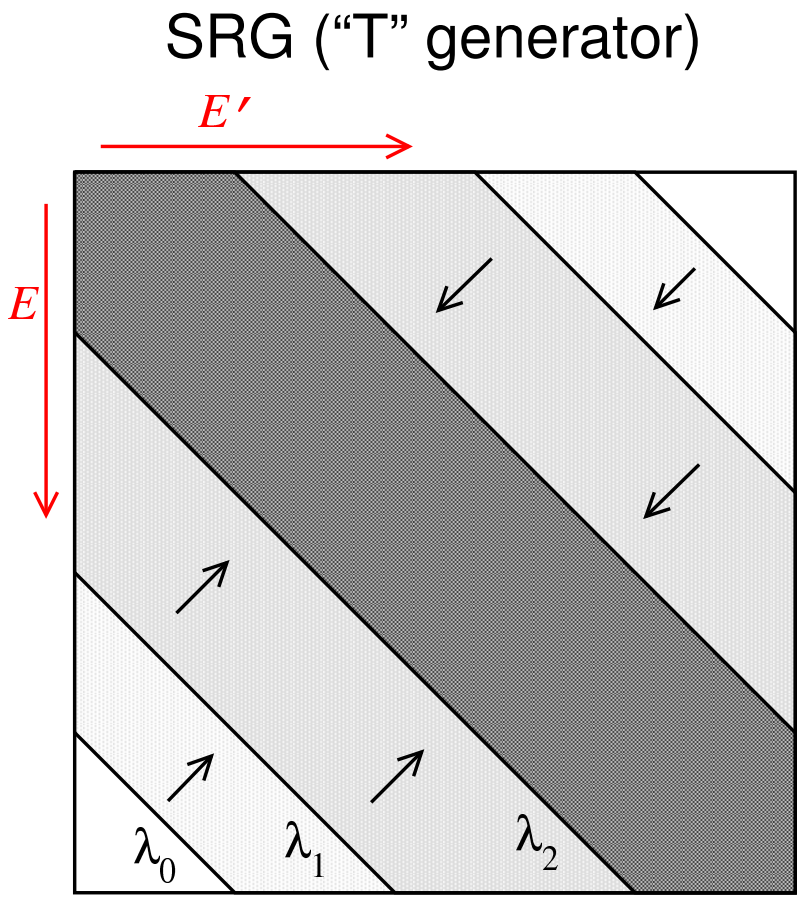
Lecture 2: SRG in practice

- Recap from lecture 1: decoupling
- Implementing the similarity renormalization group (SRG)
- Block diagonal ("$V_{\mathrm{low},k}$") generator
- Computational aspects
- Quantitative measure of perturbativeness

Two ways to use RG equations to decouple Hamiltonians

General form of the flow equation: $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$





General rule: Choose G_s to match the desired final pattern

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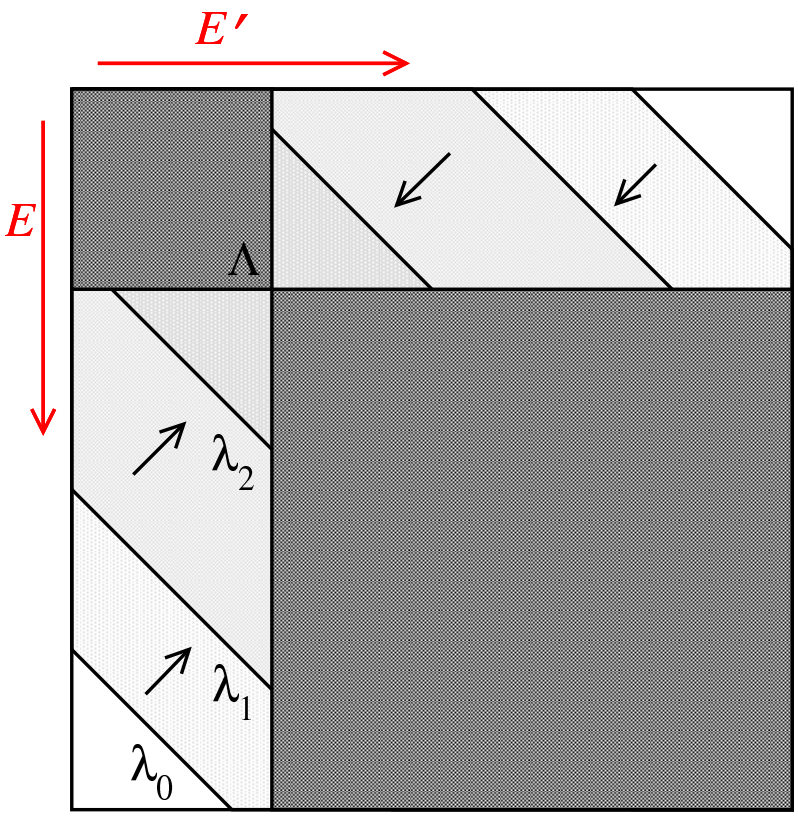
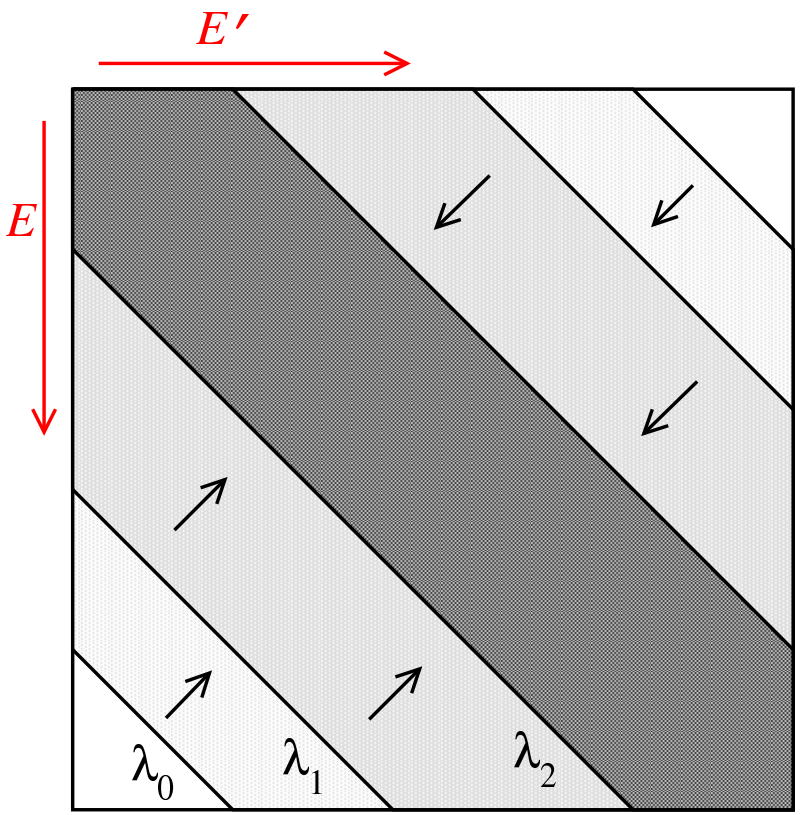
SRG ("BD" generator)



SRG ("T" generator)



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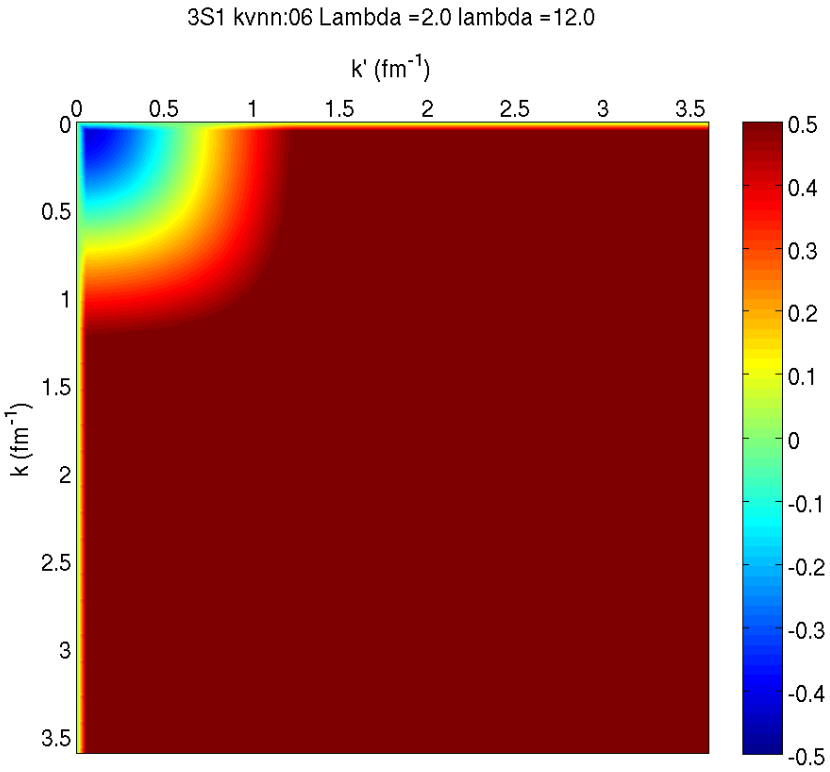
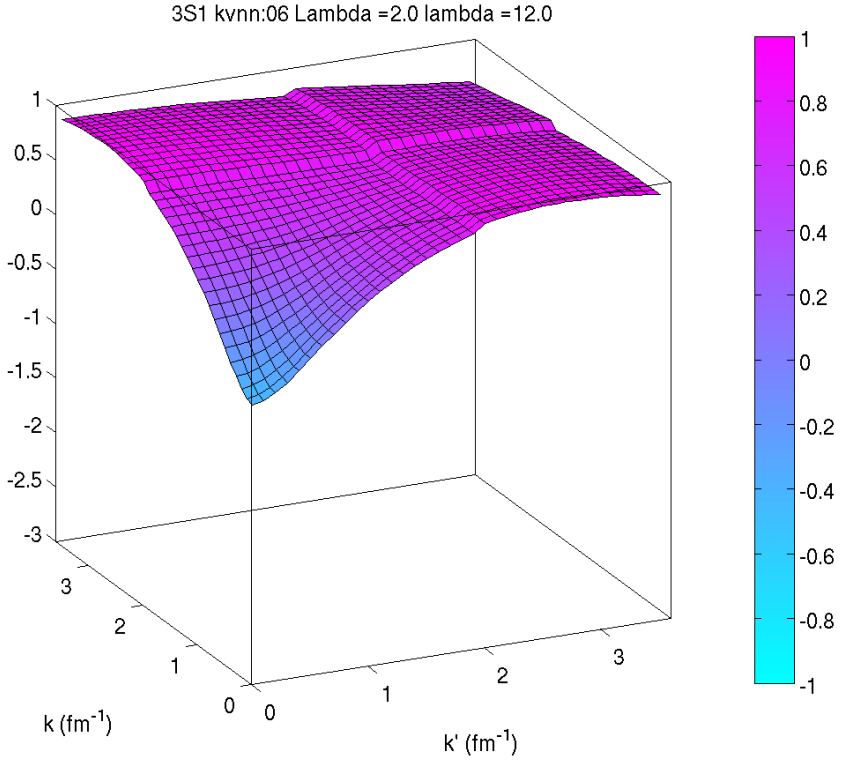
Block diagonalization via SRG $[G_s = H_{BD}]$

- 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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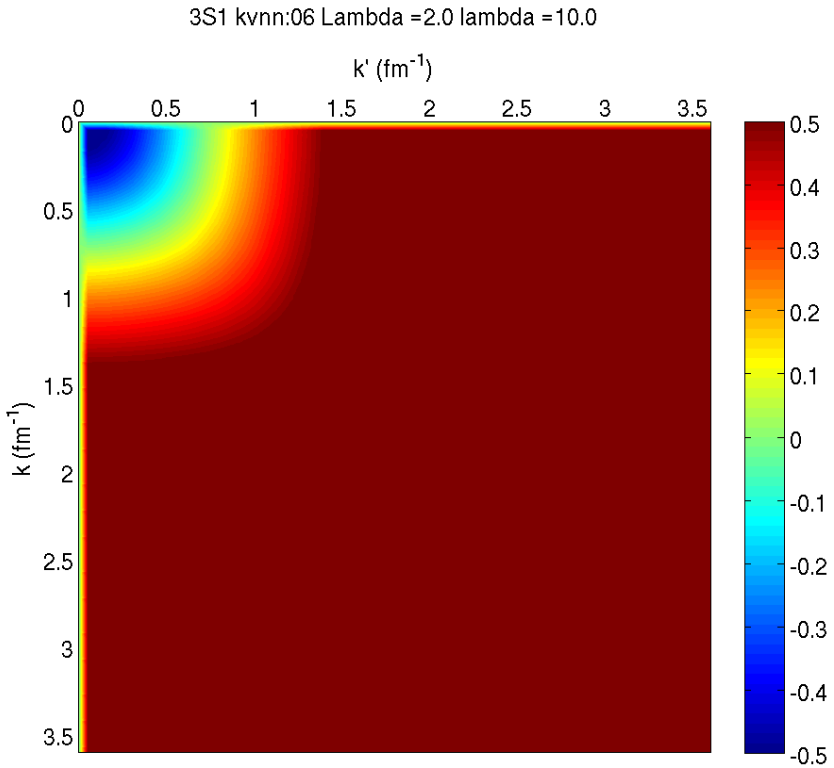

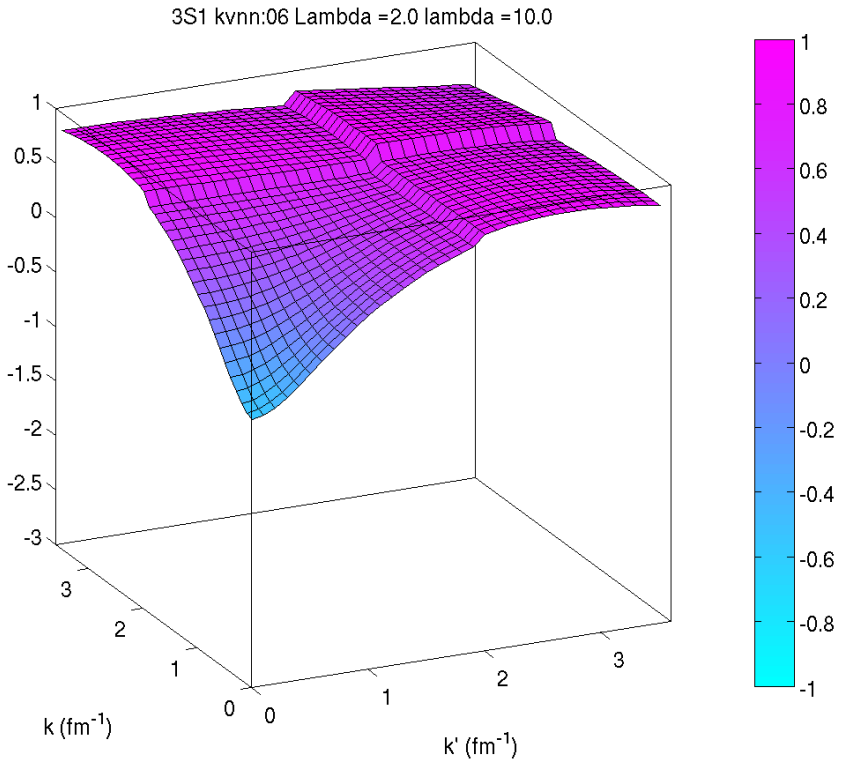

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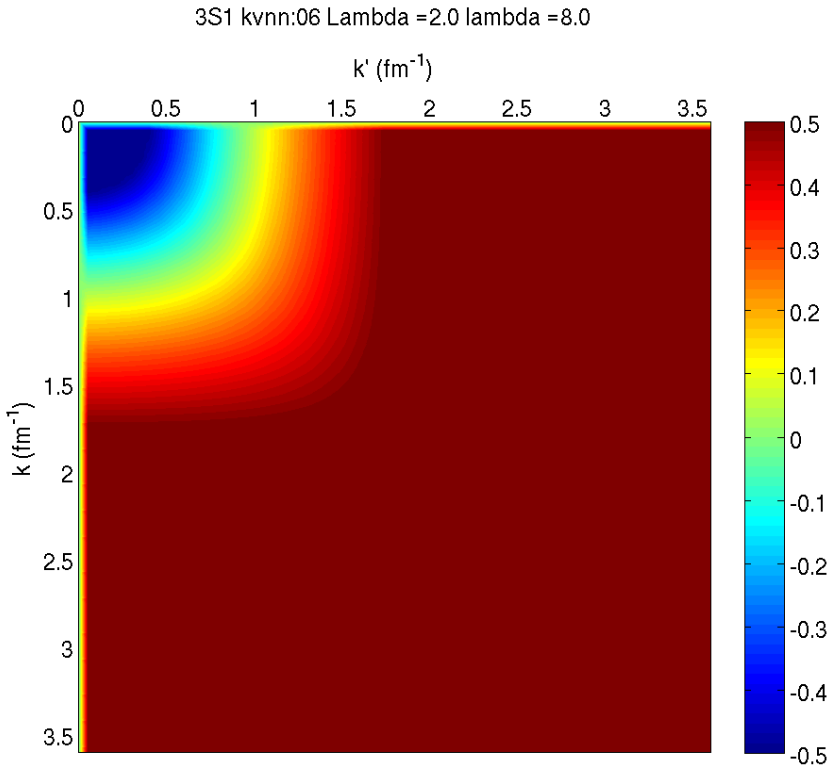

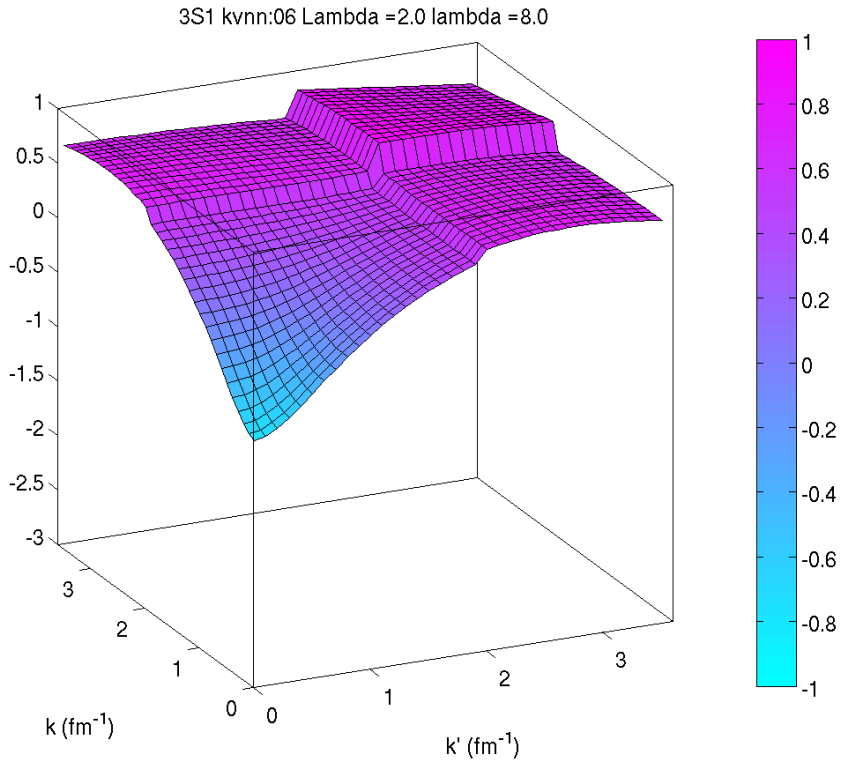

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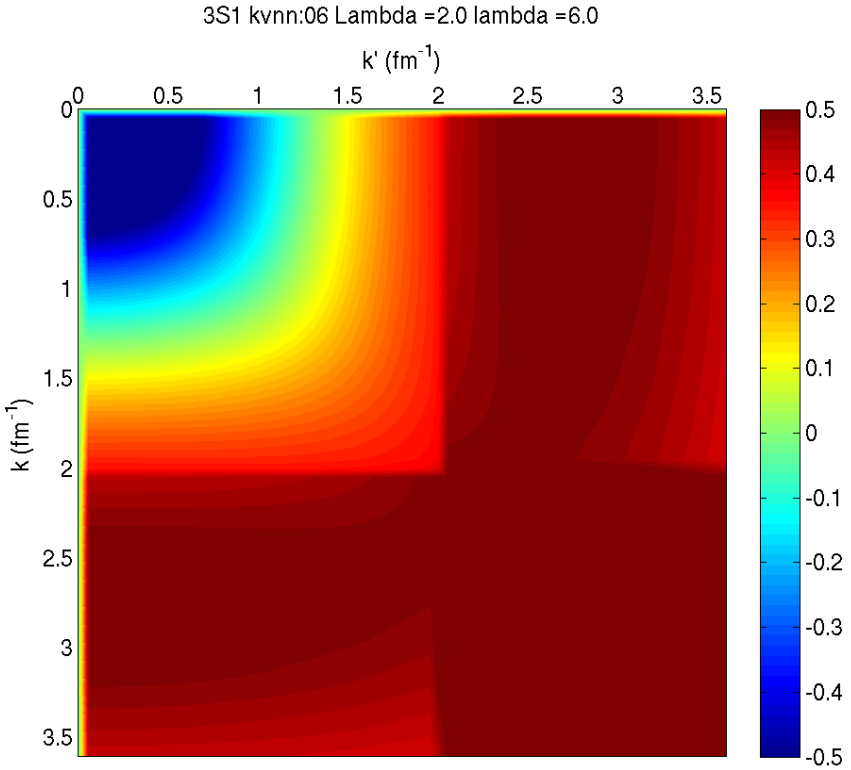

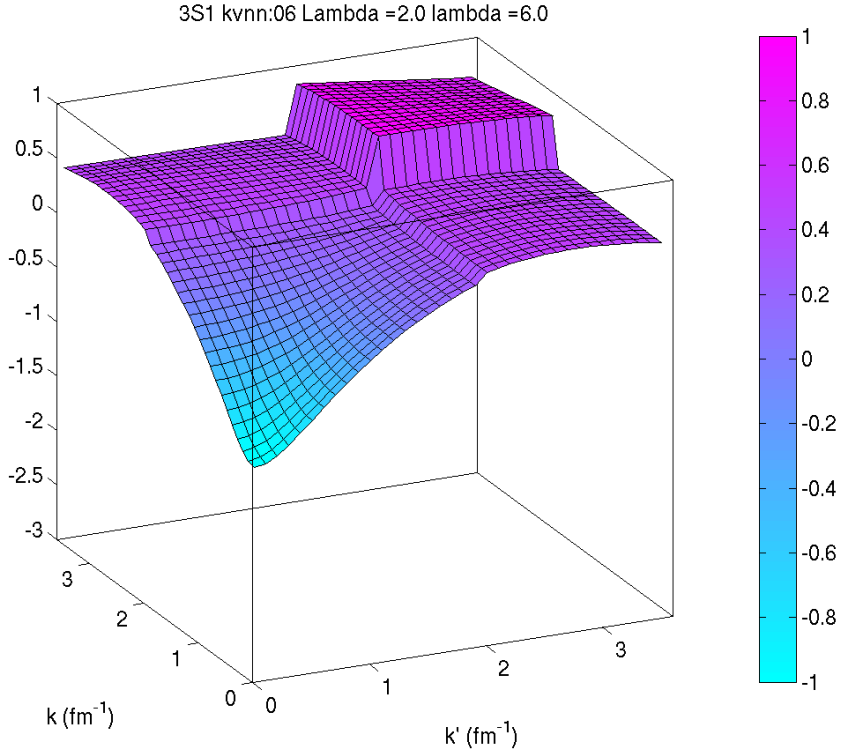

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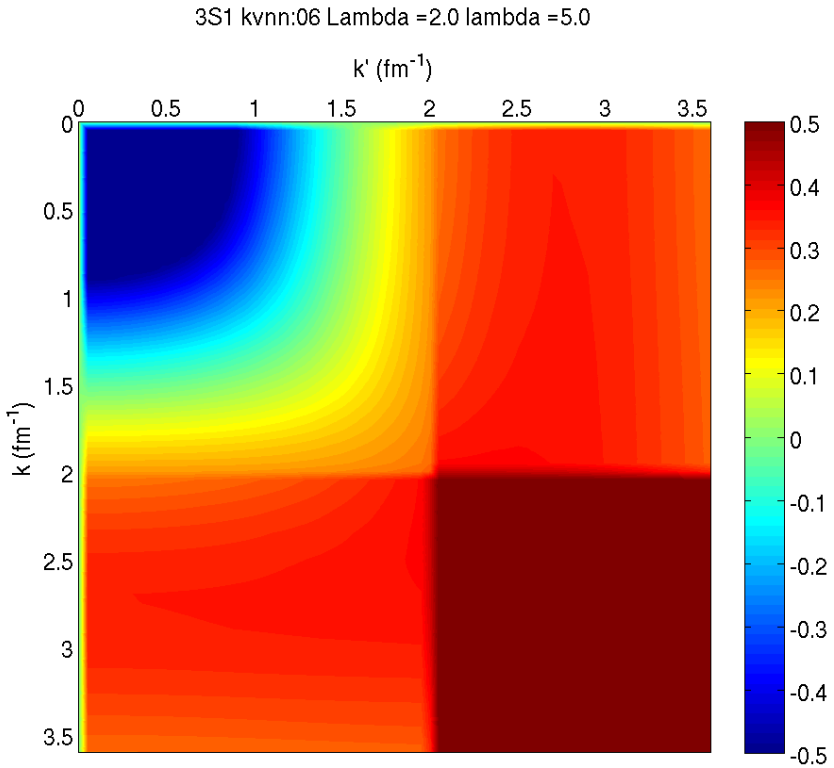

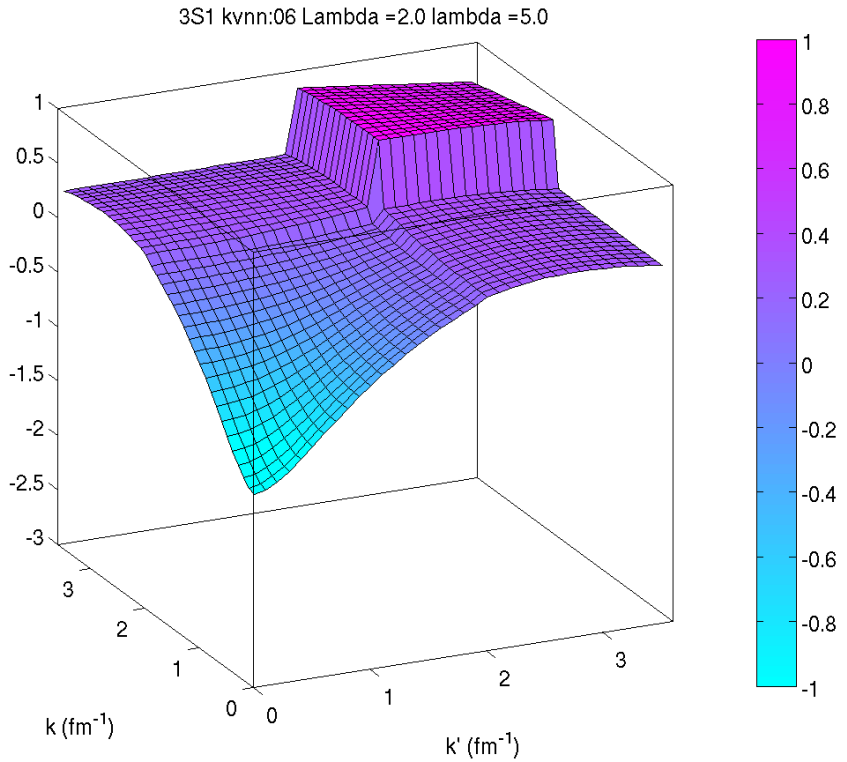

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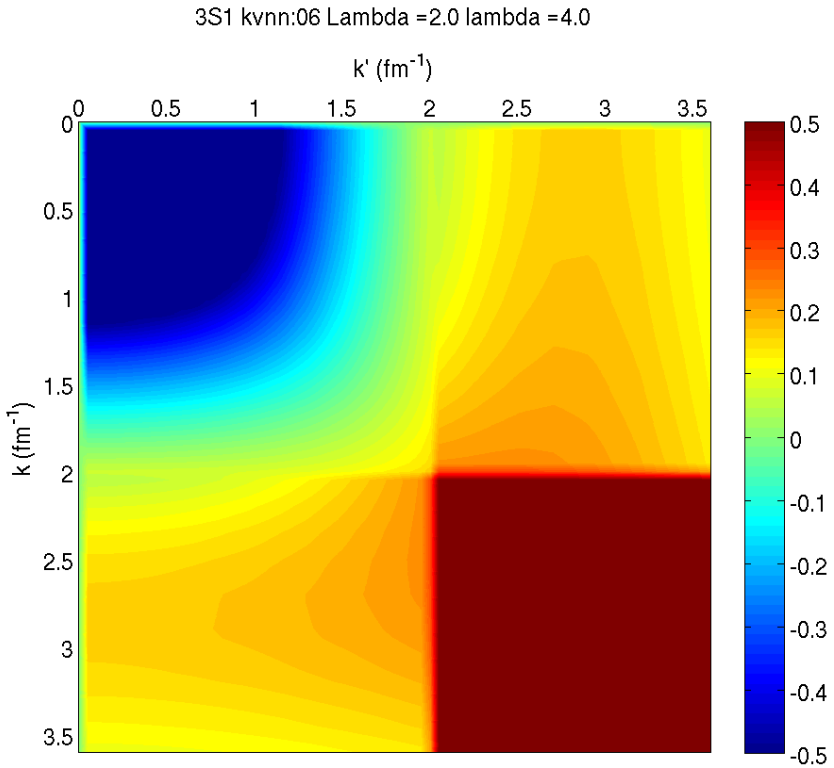

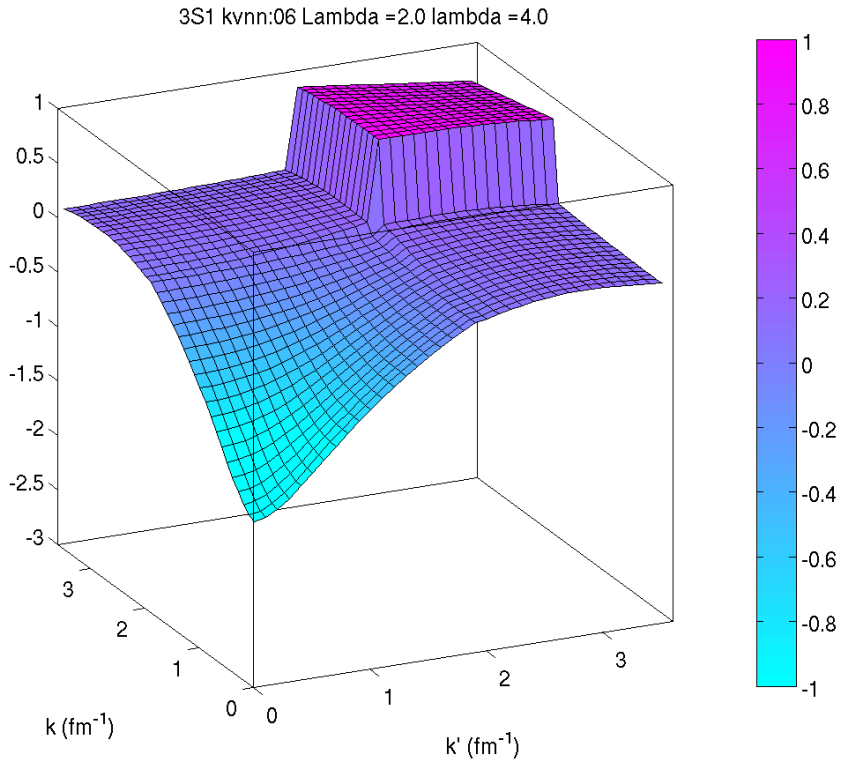

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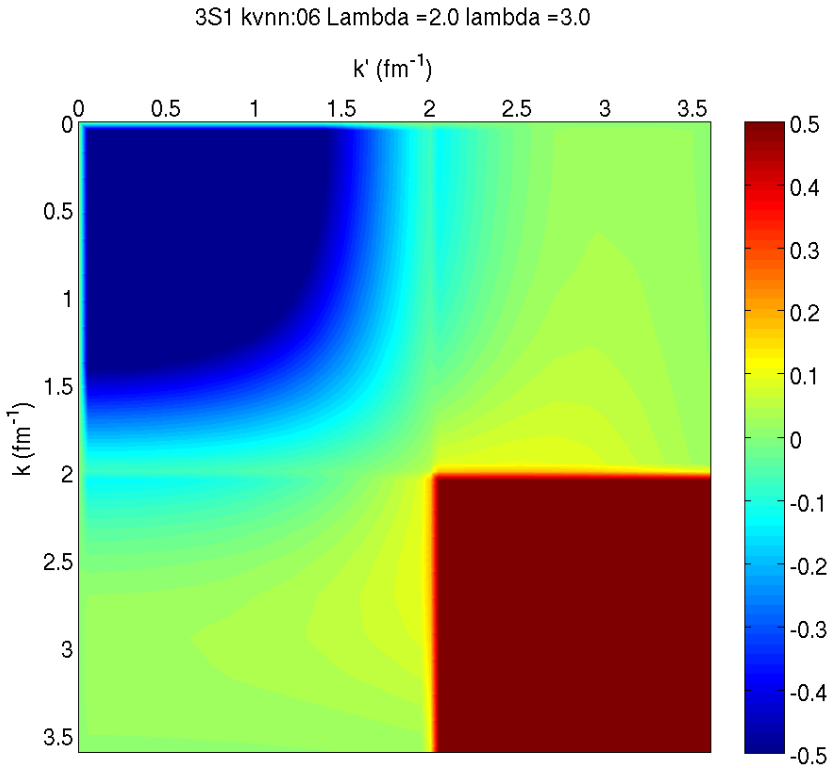

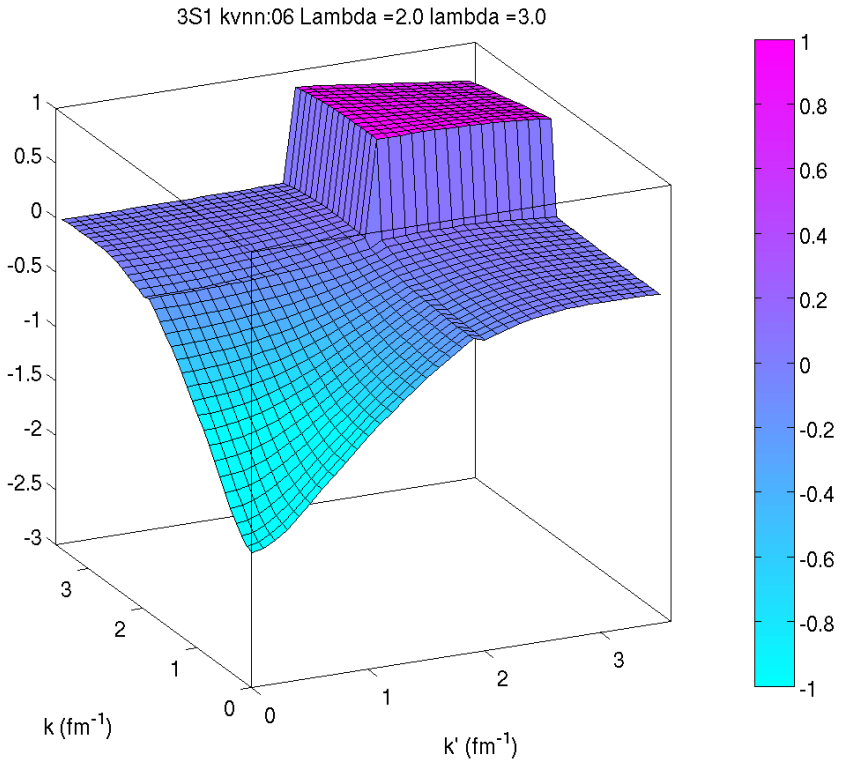

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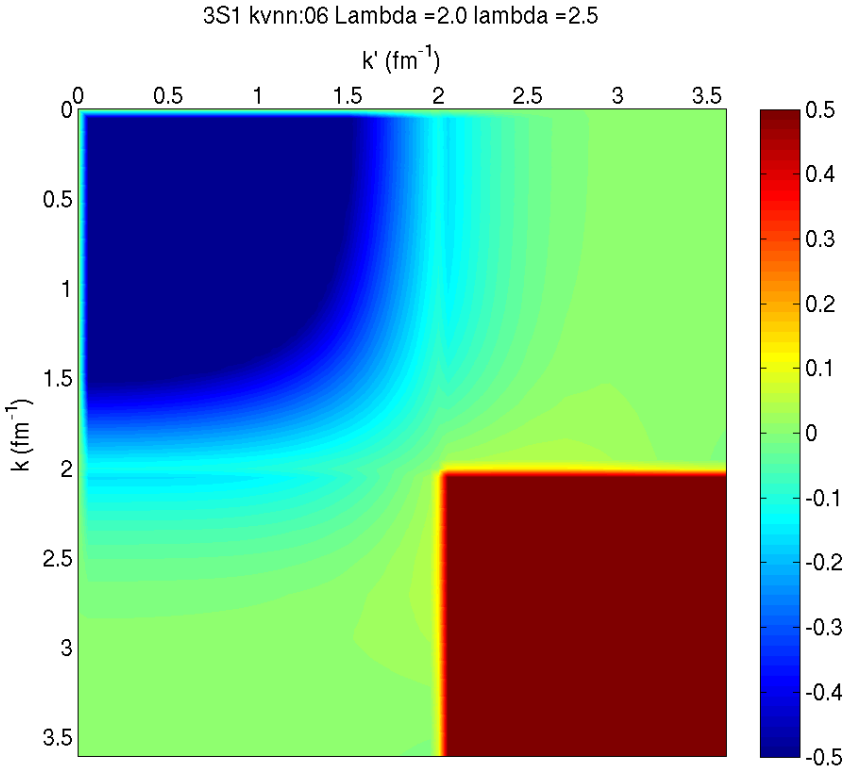

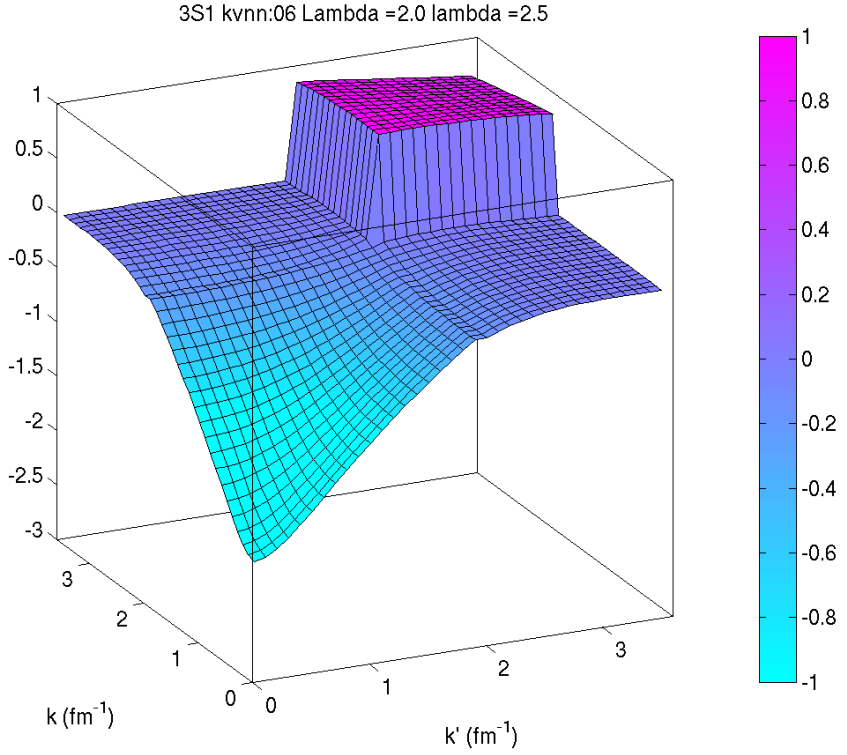

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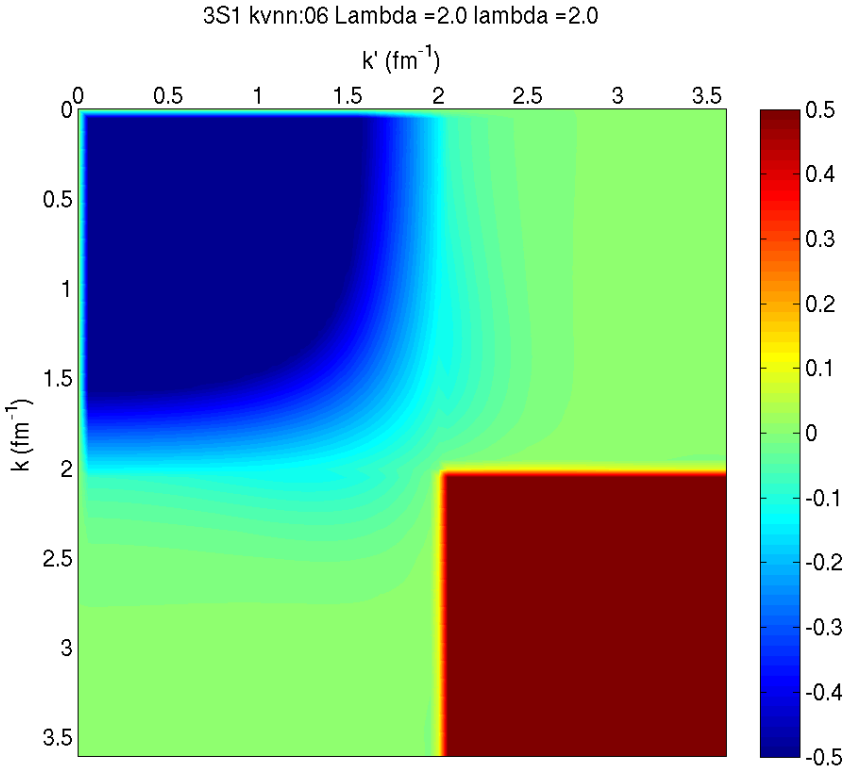

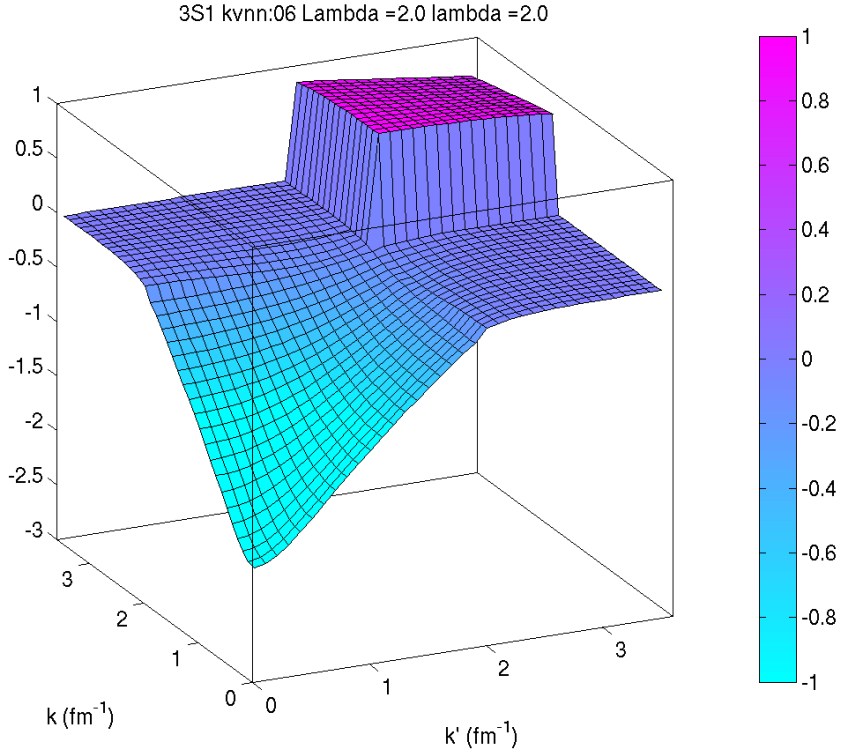

- What are the best generators for nuclear applications?

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

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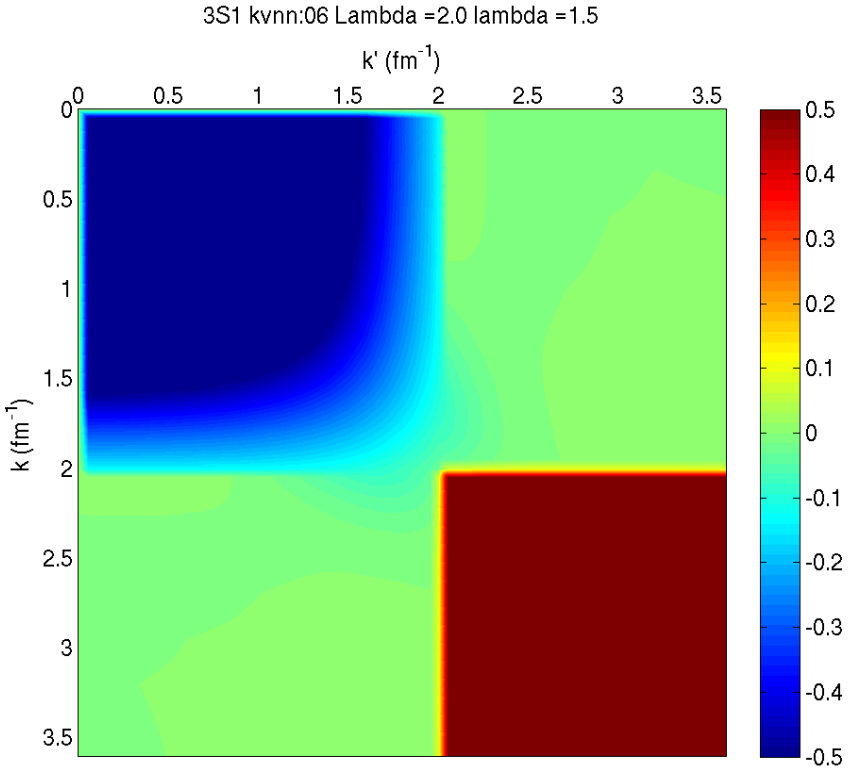

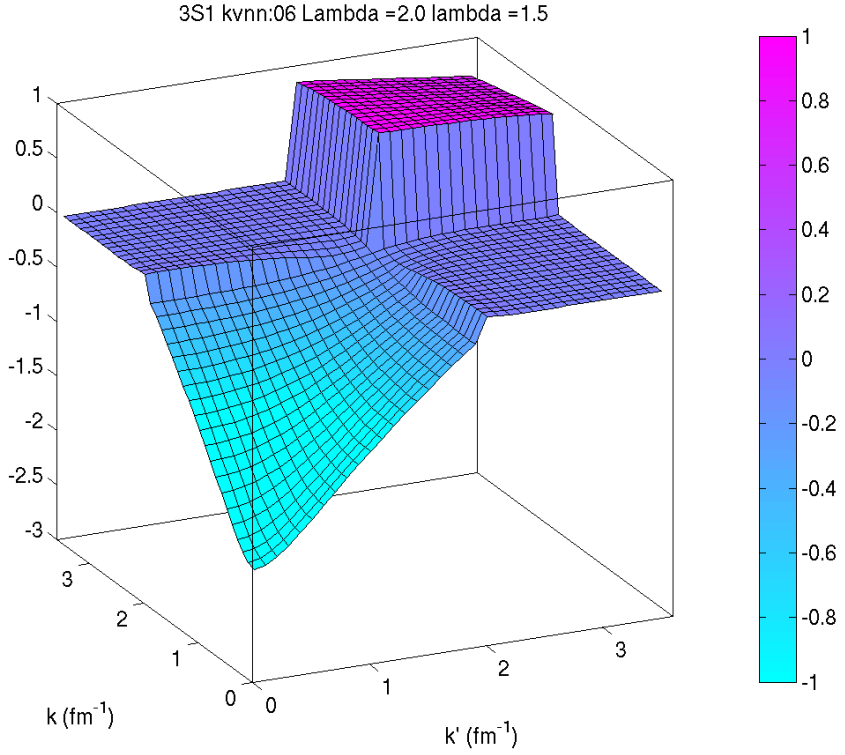

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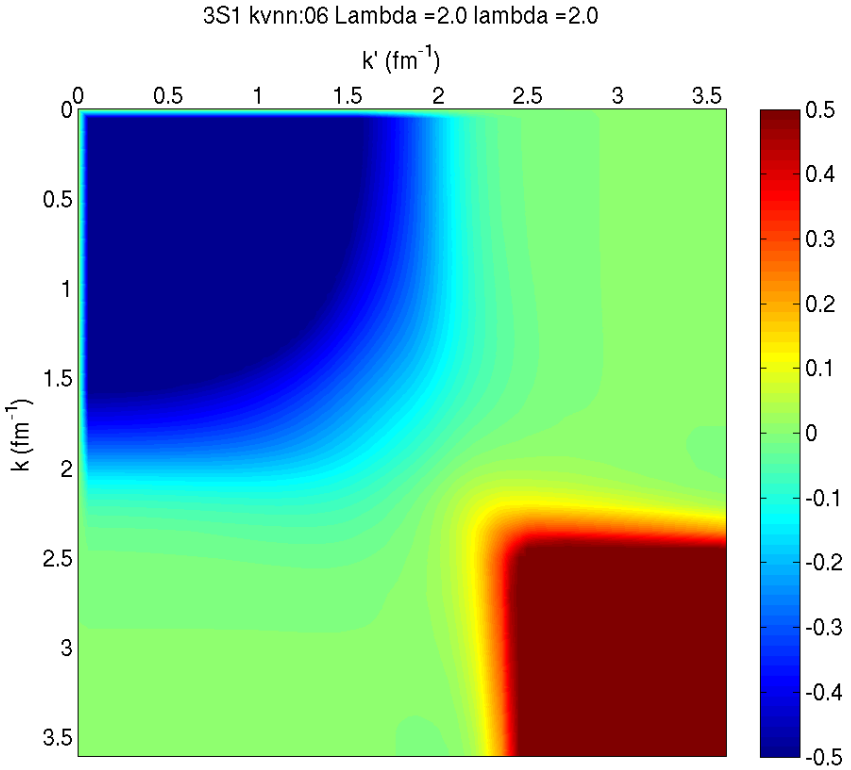

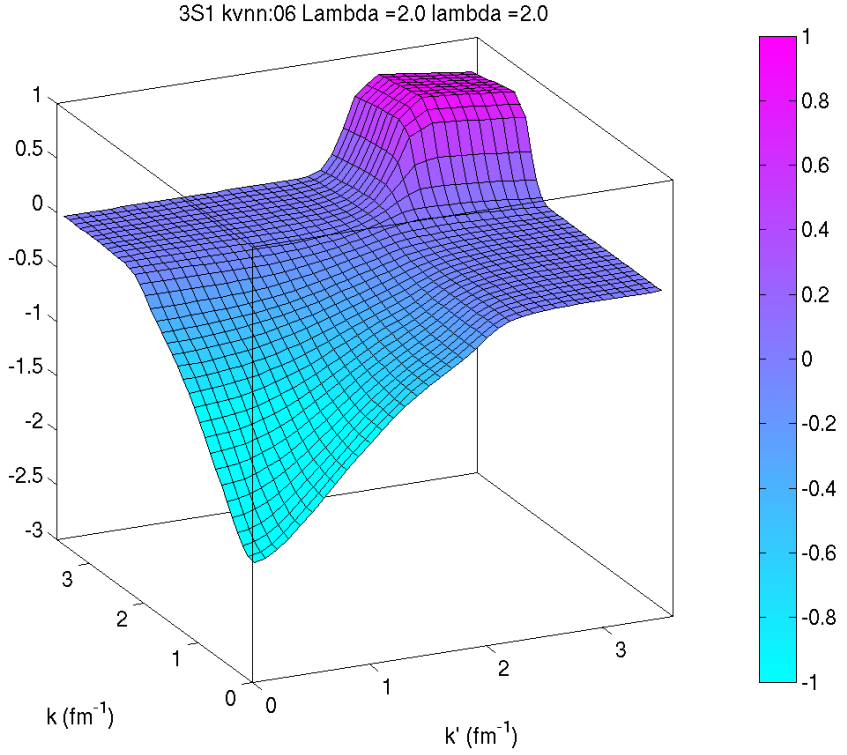

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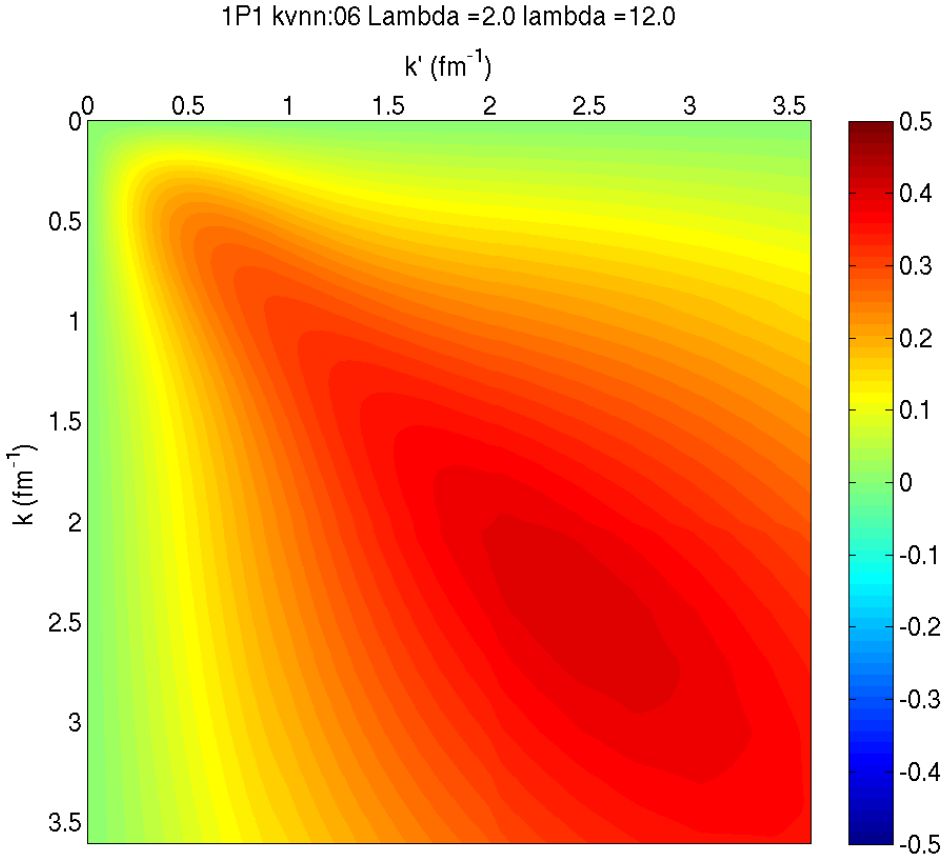

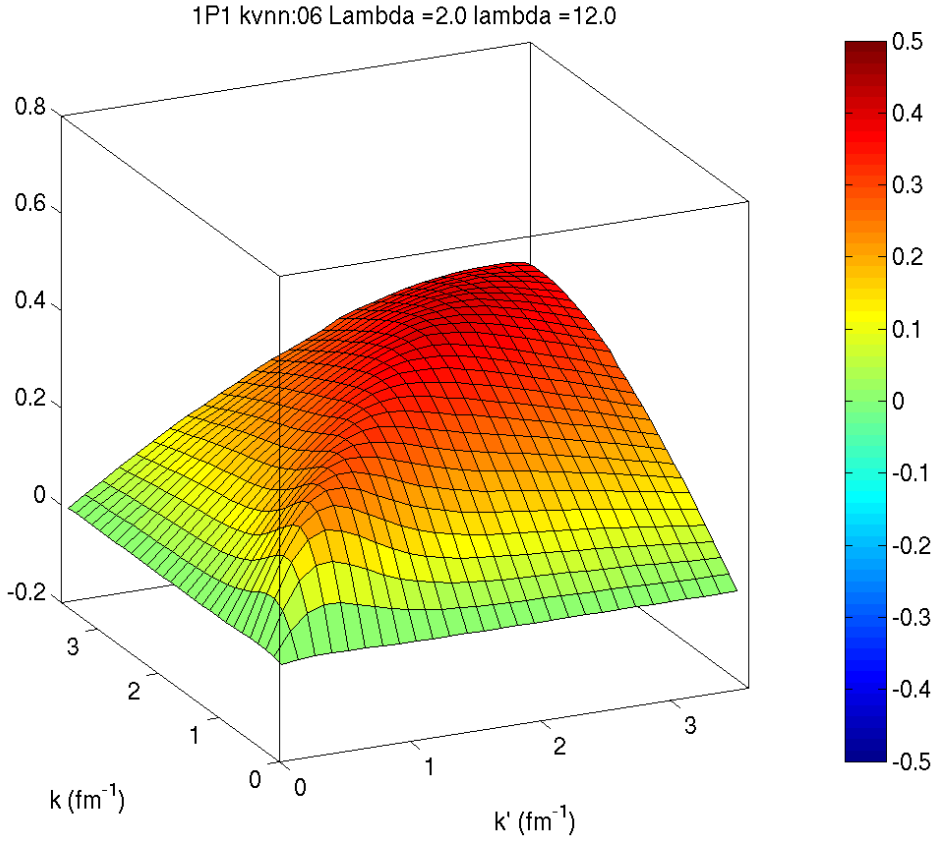

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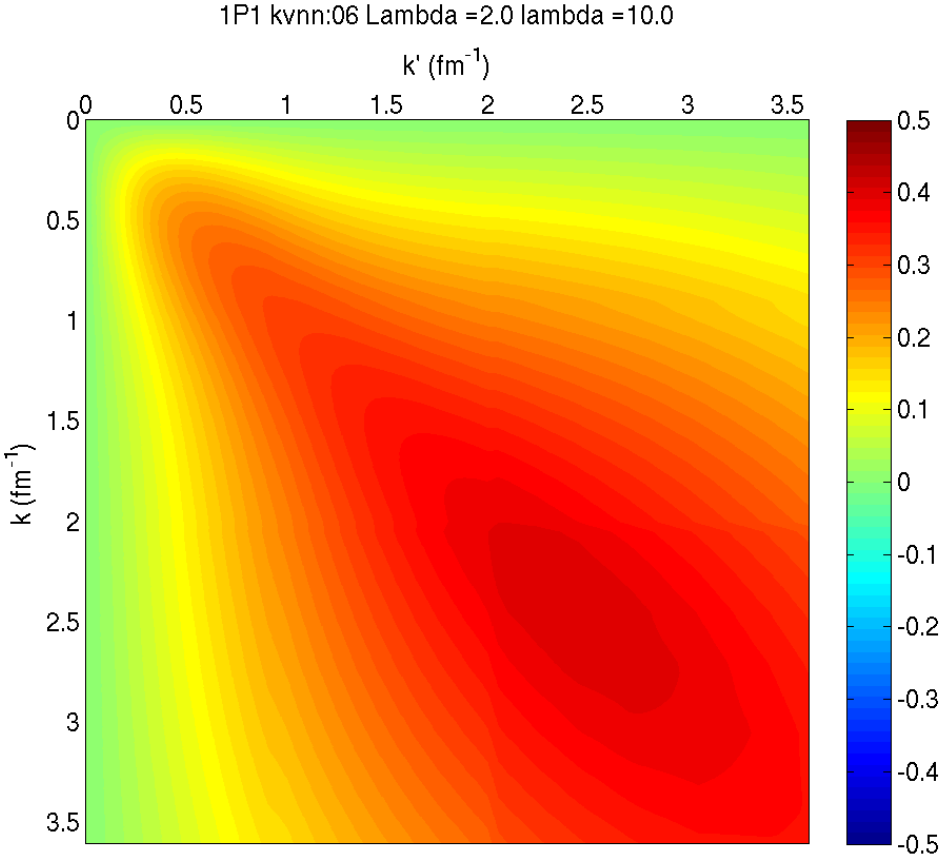

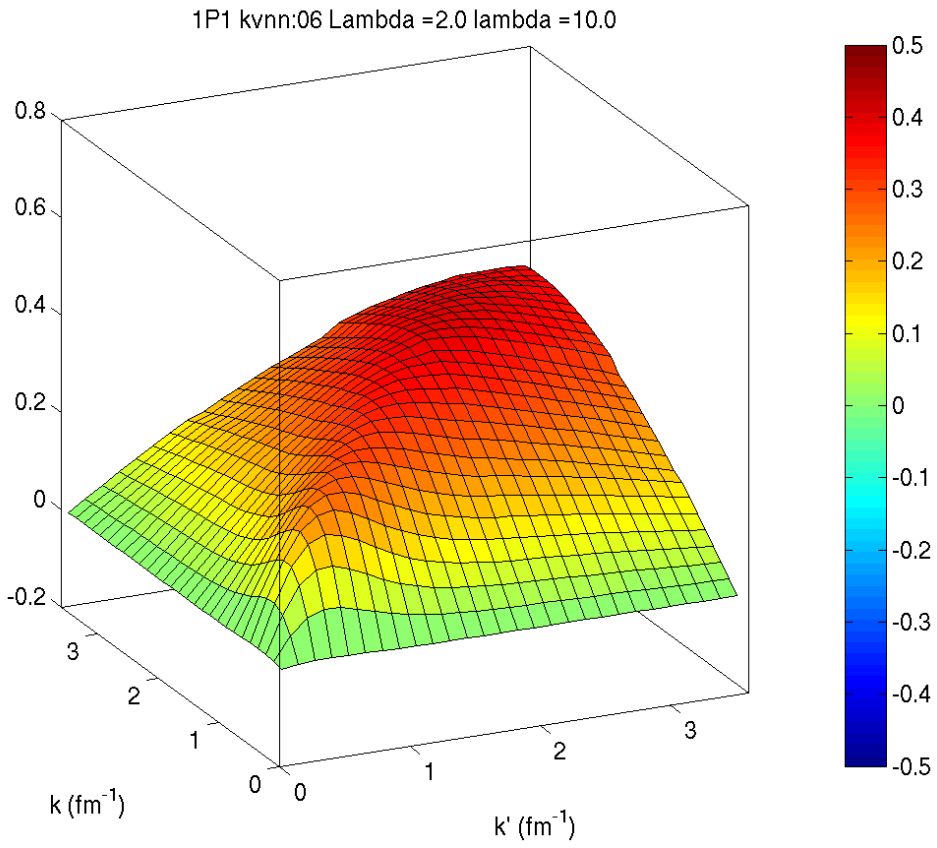

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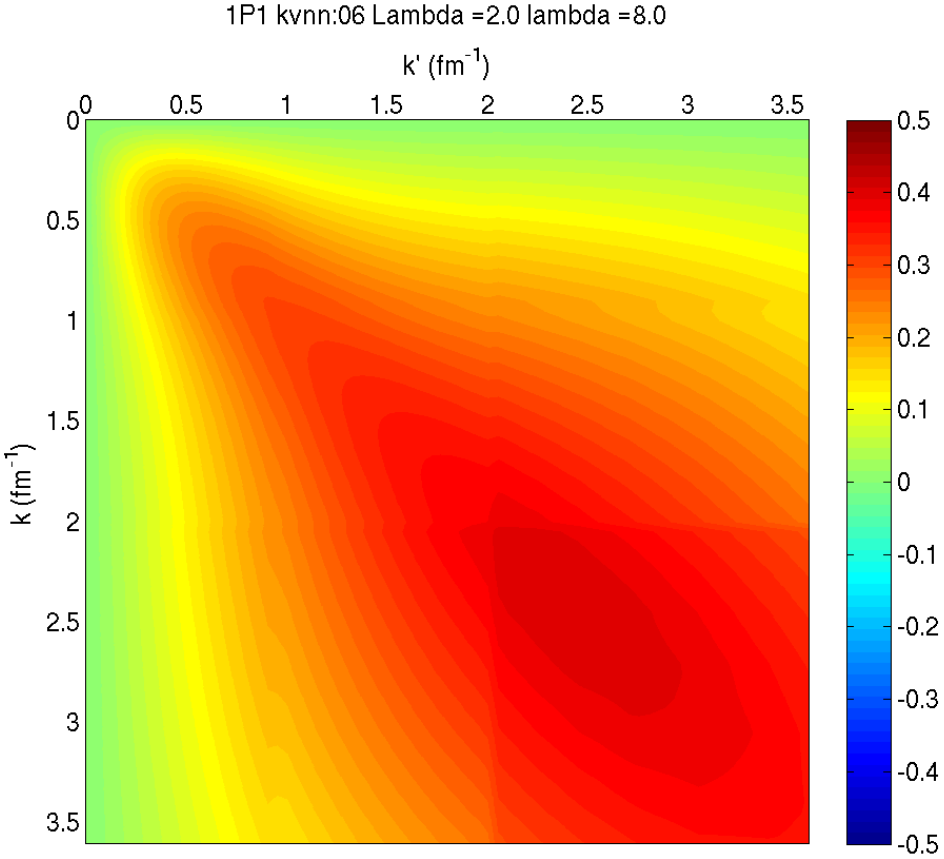

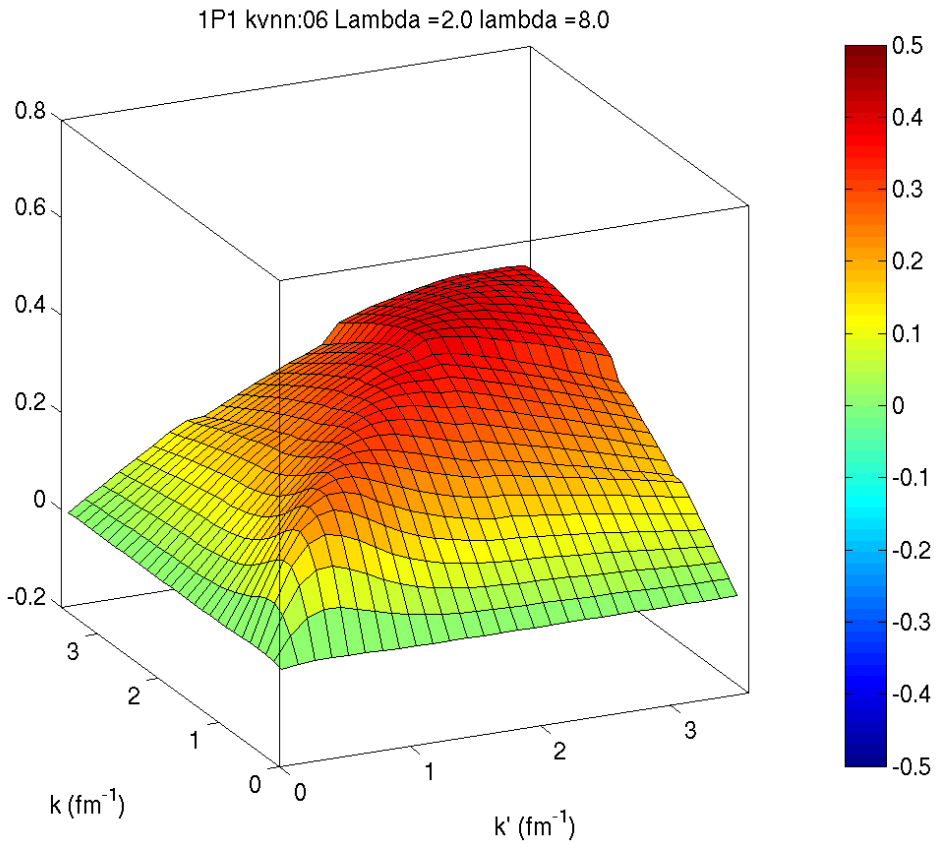

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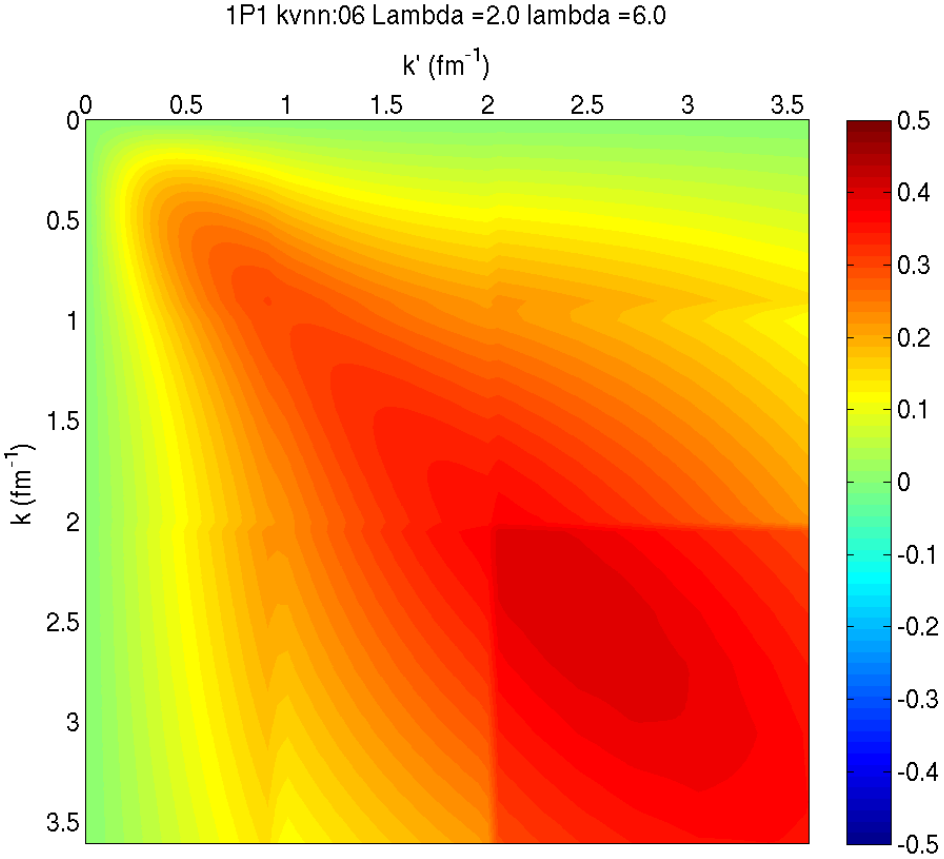

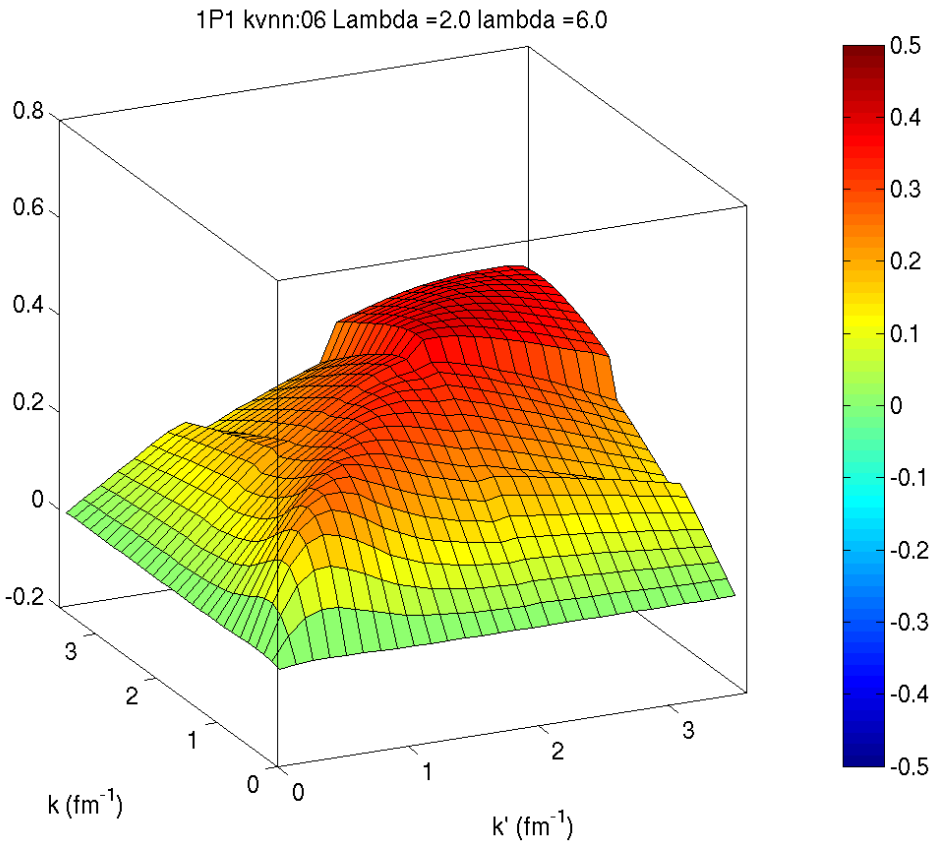

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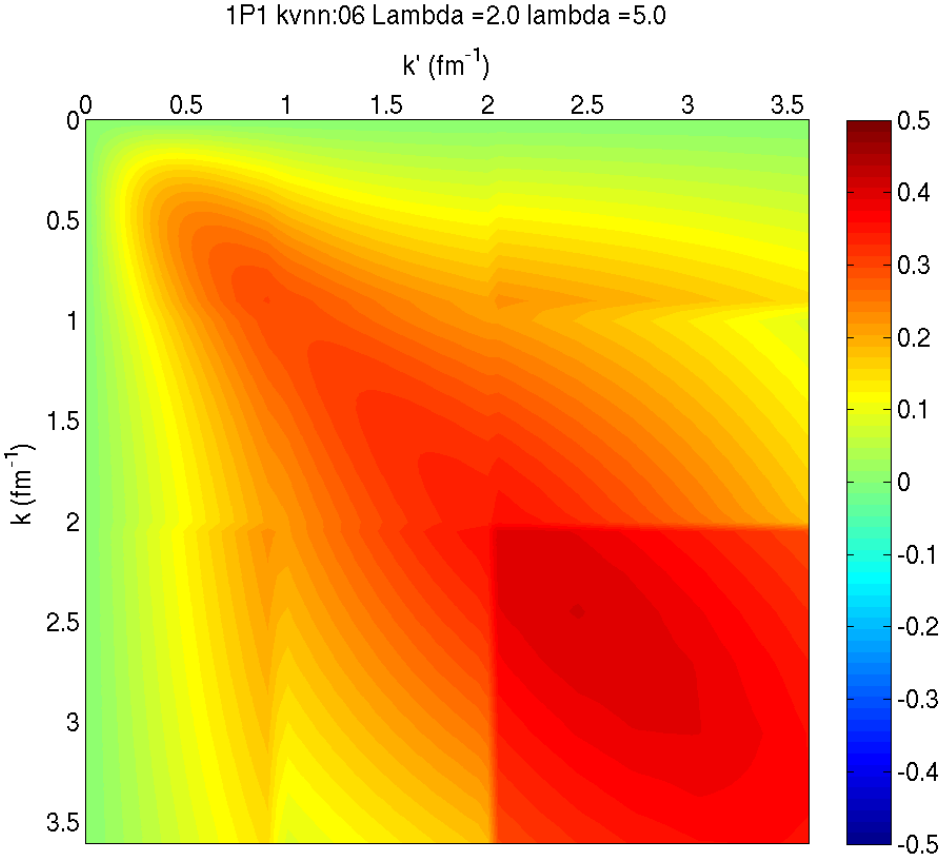

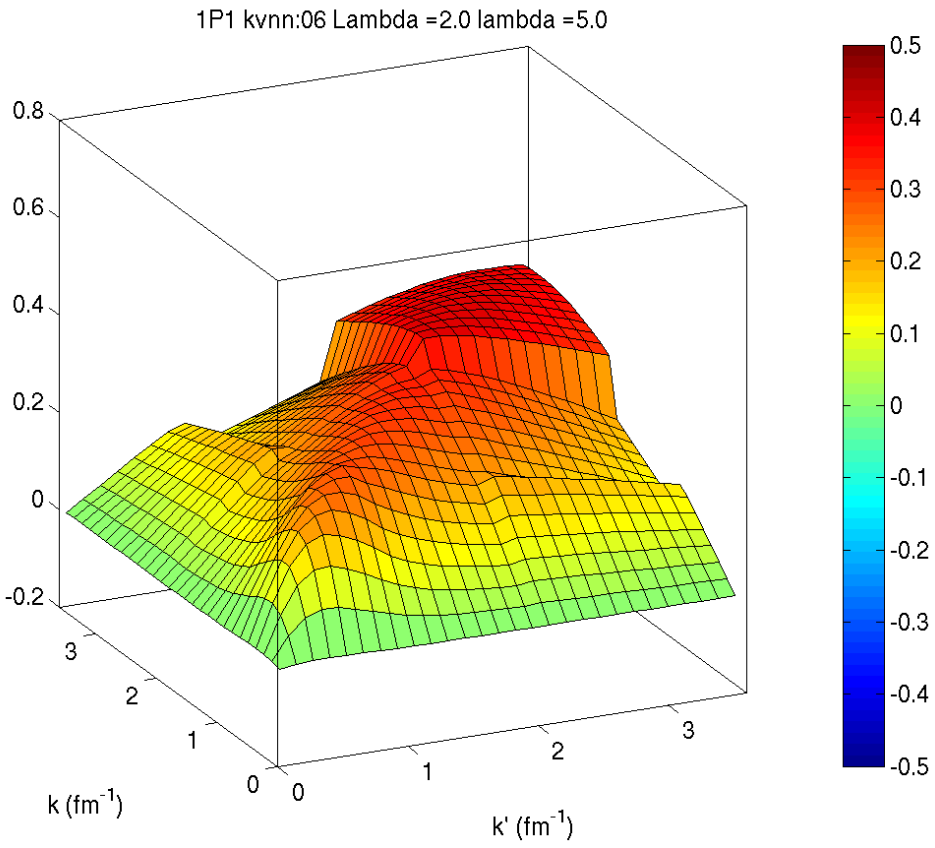

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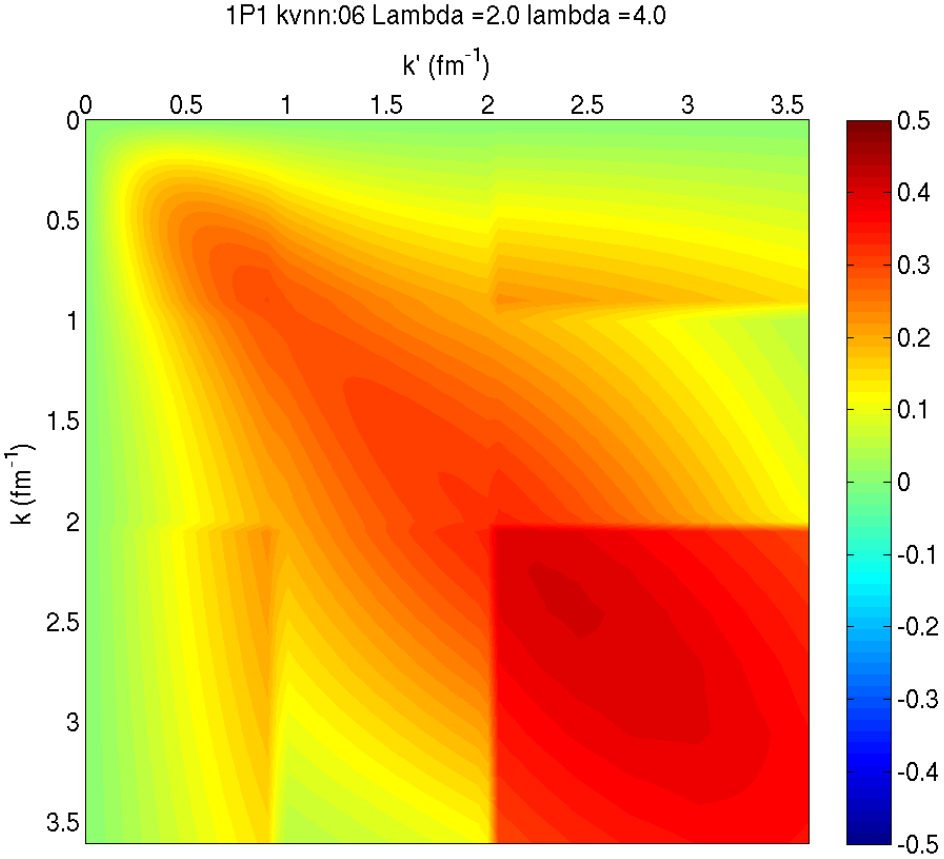

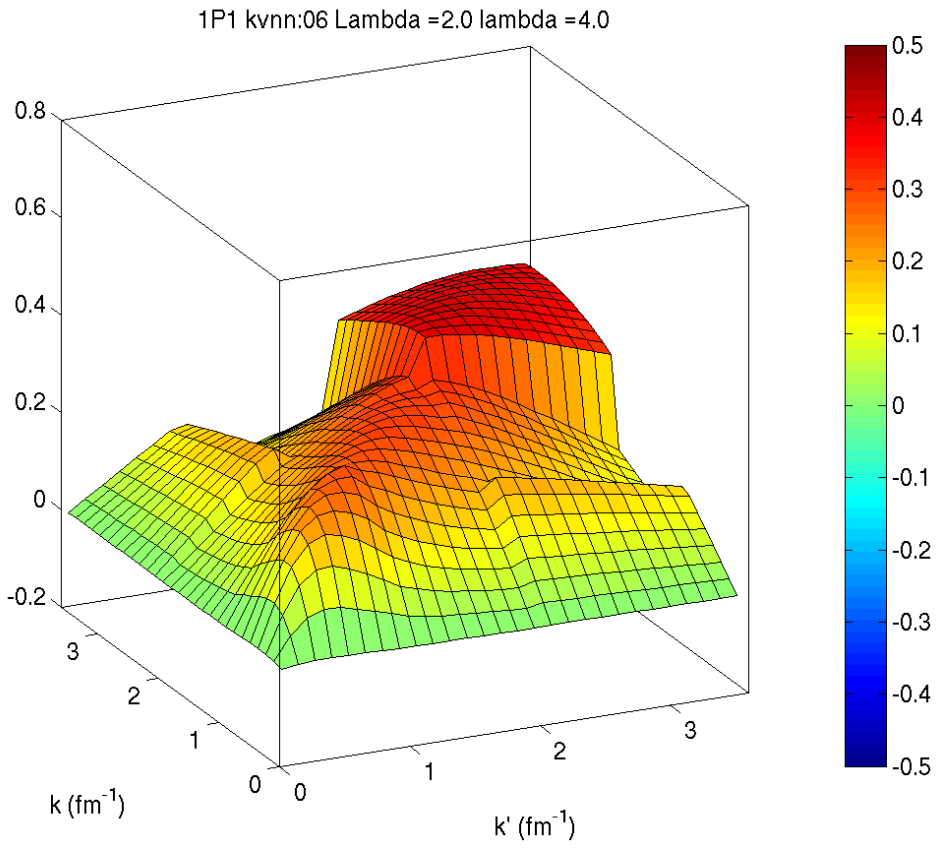

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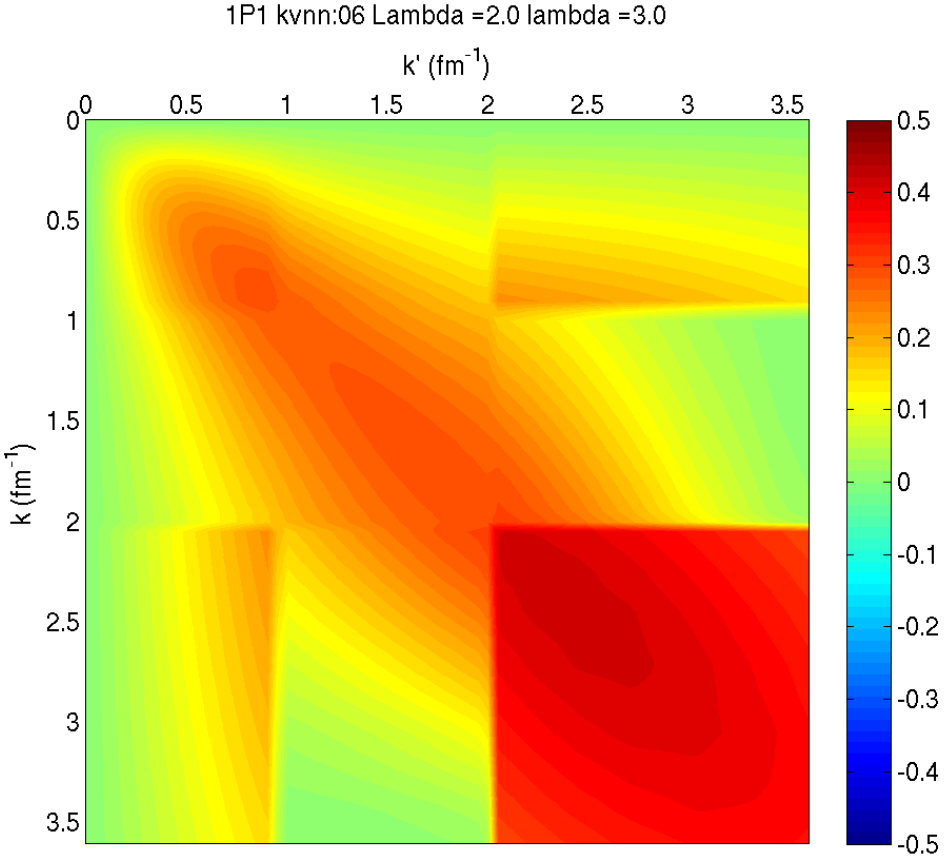

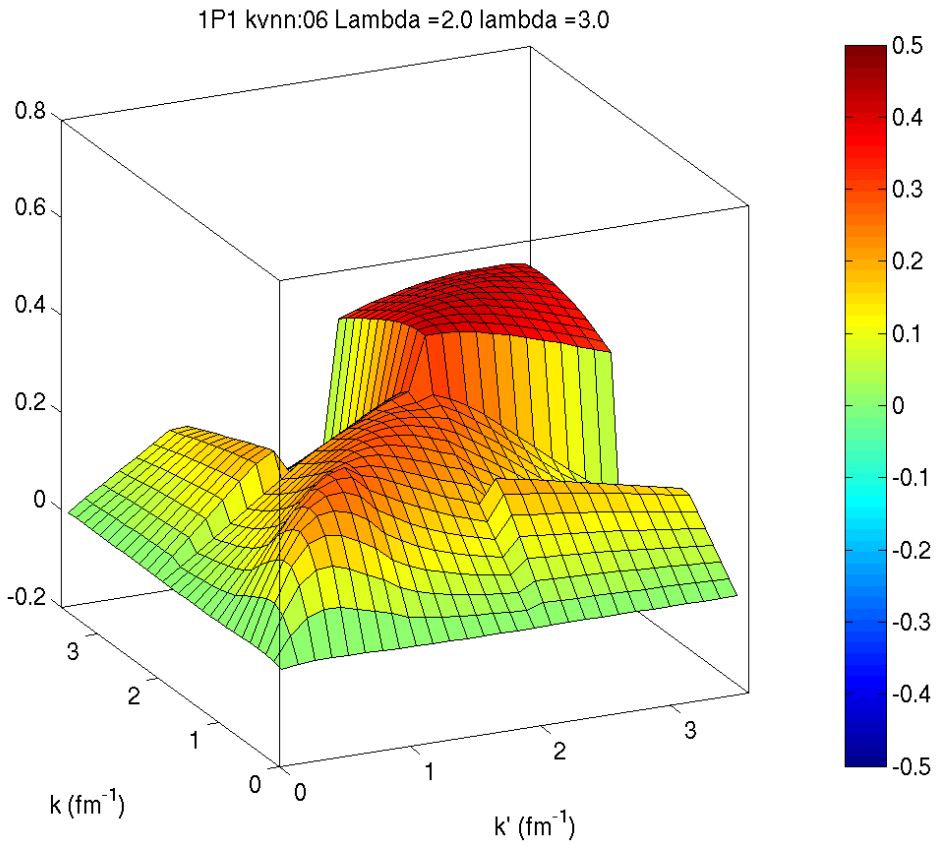

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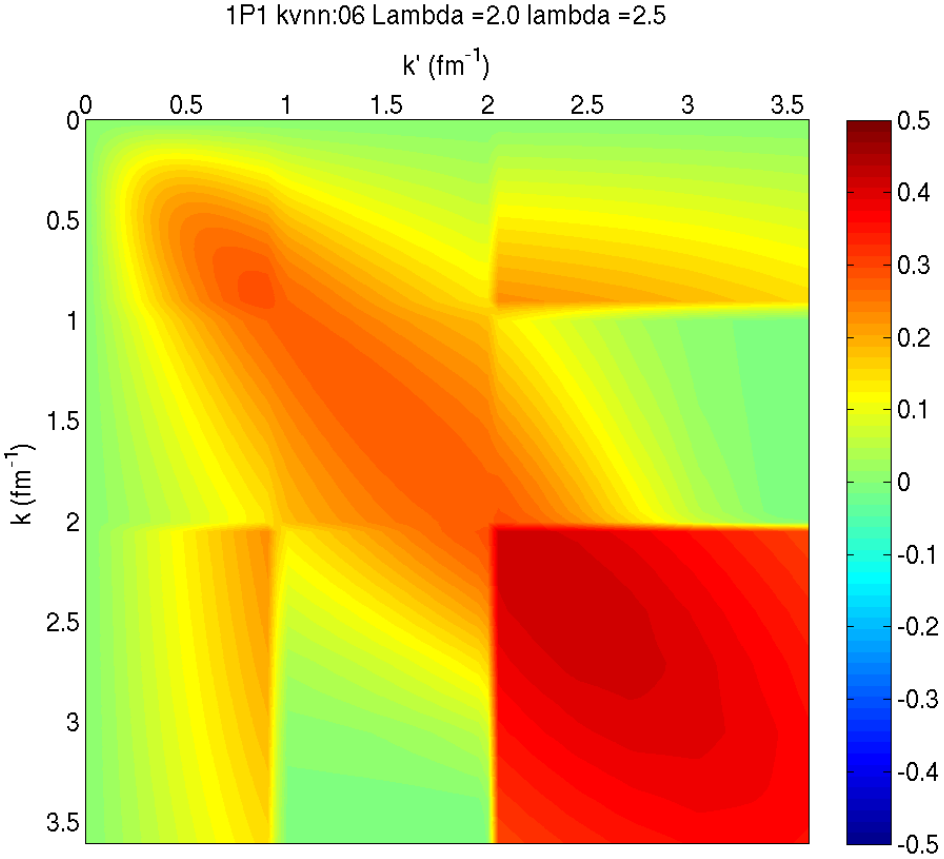

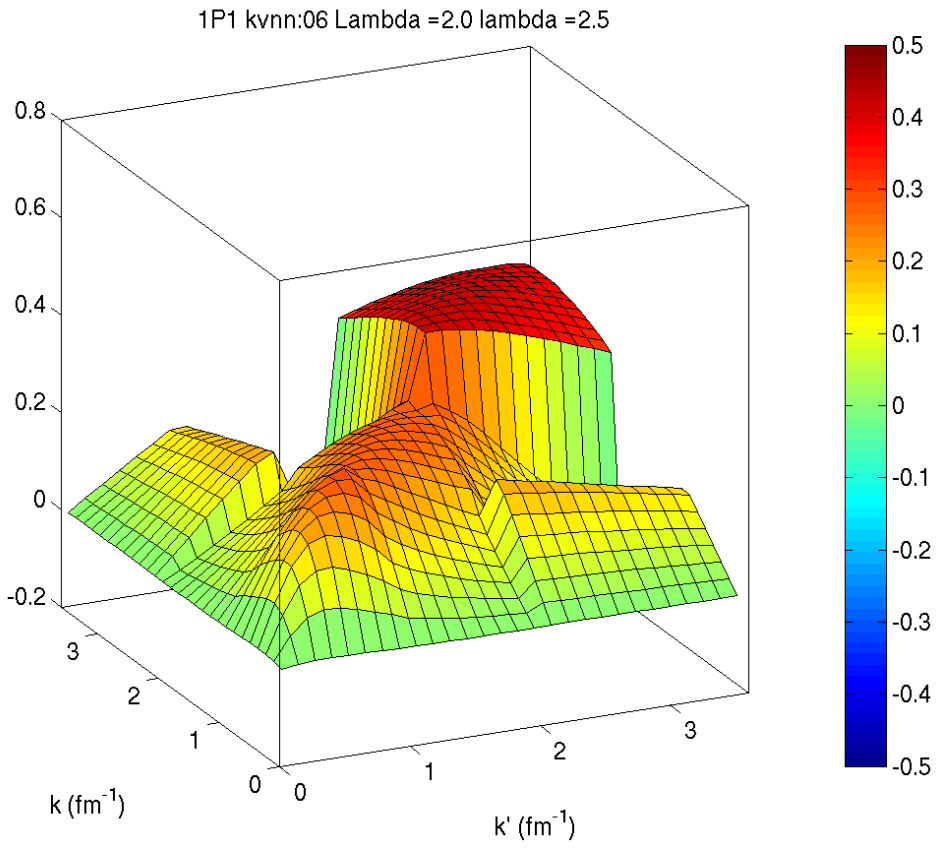

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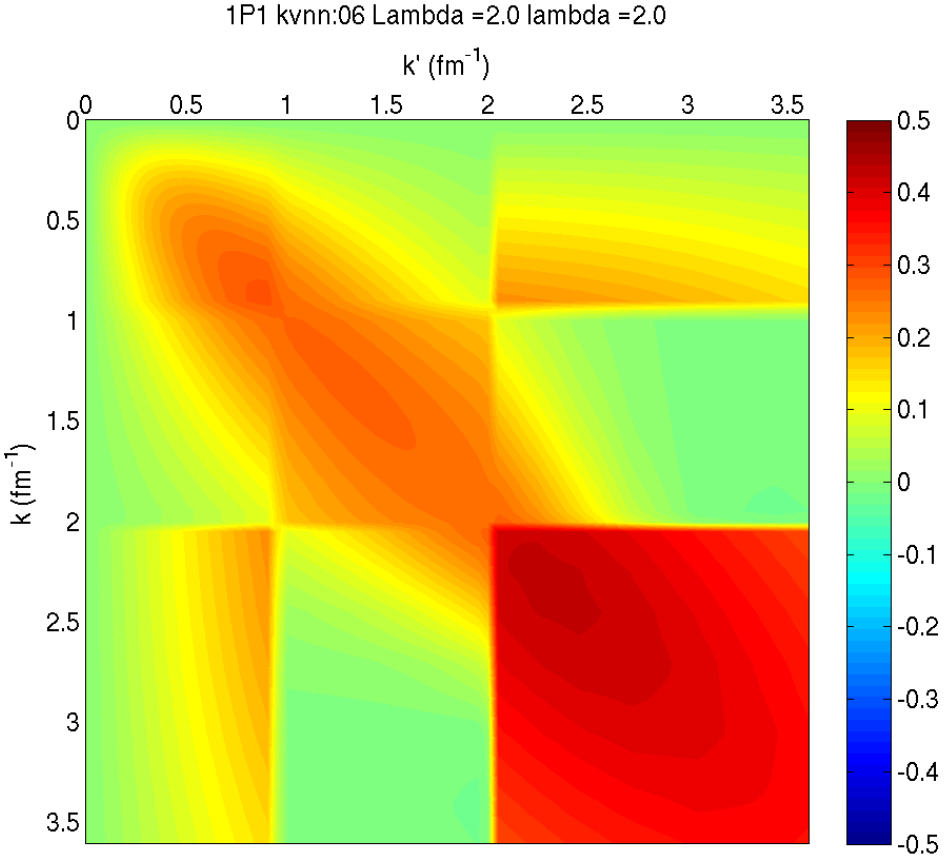

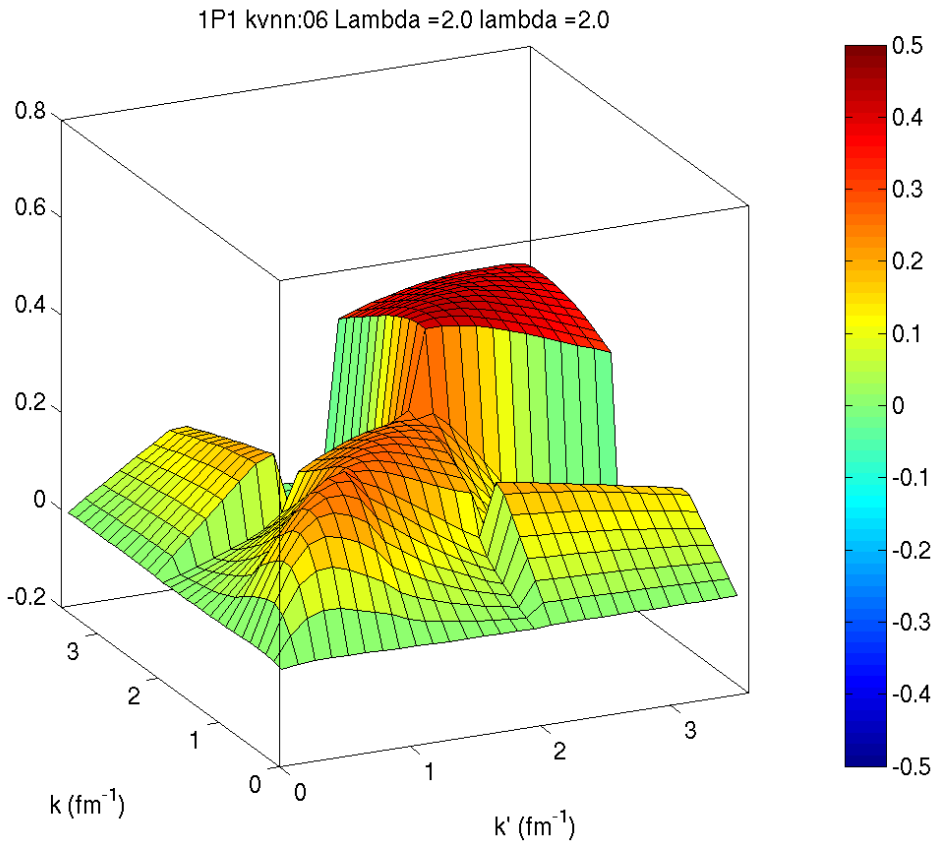

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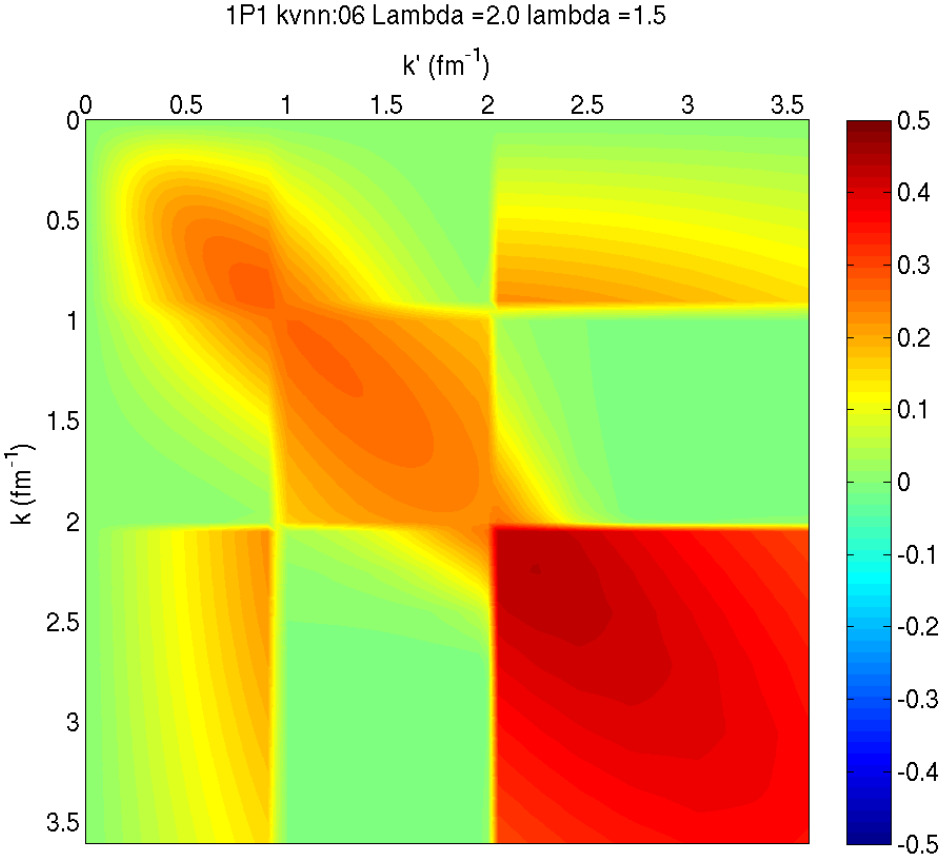

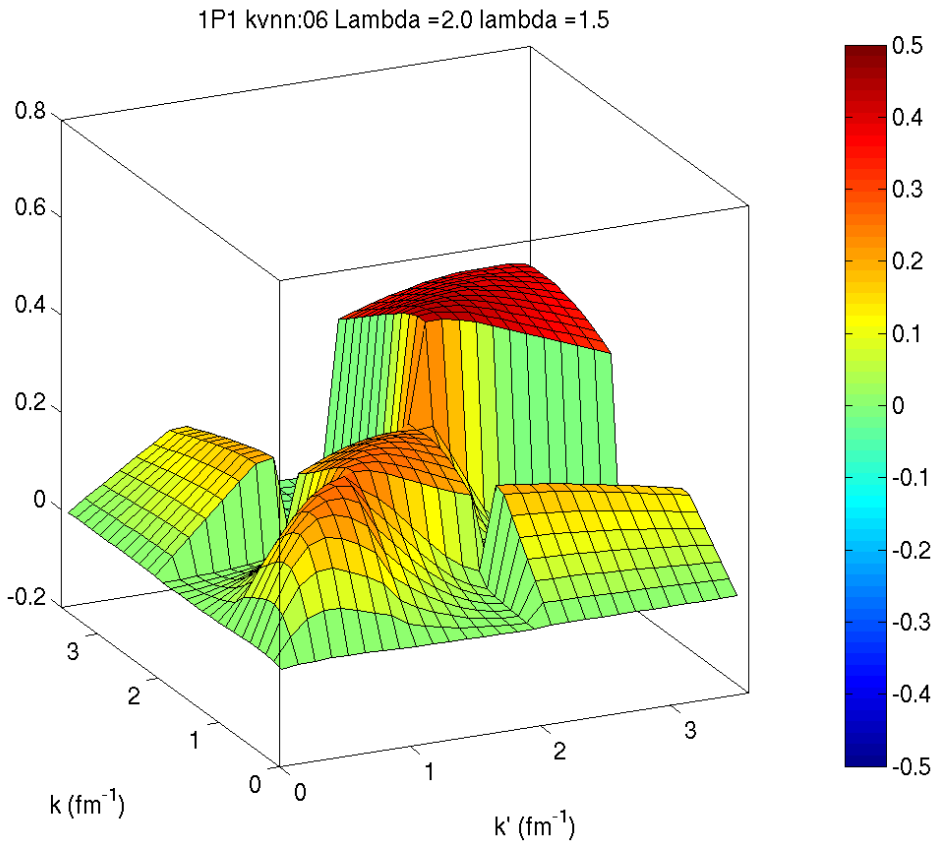

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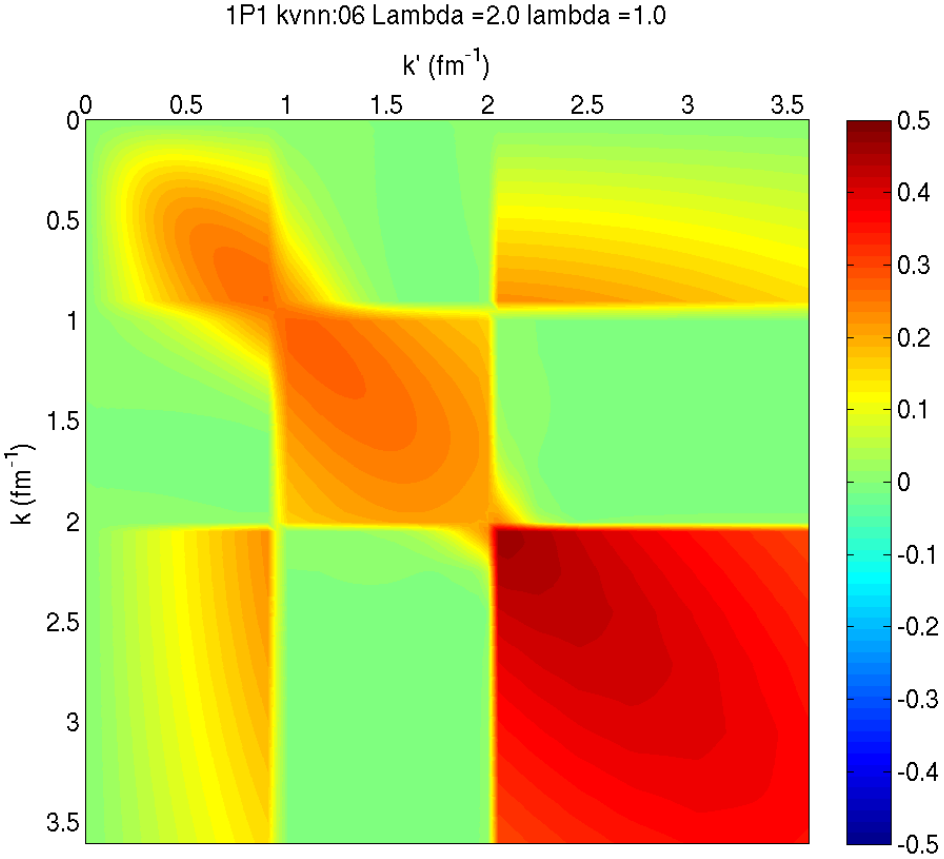
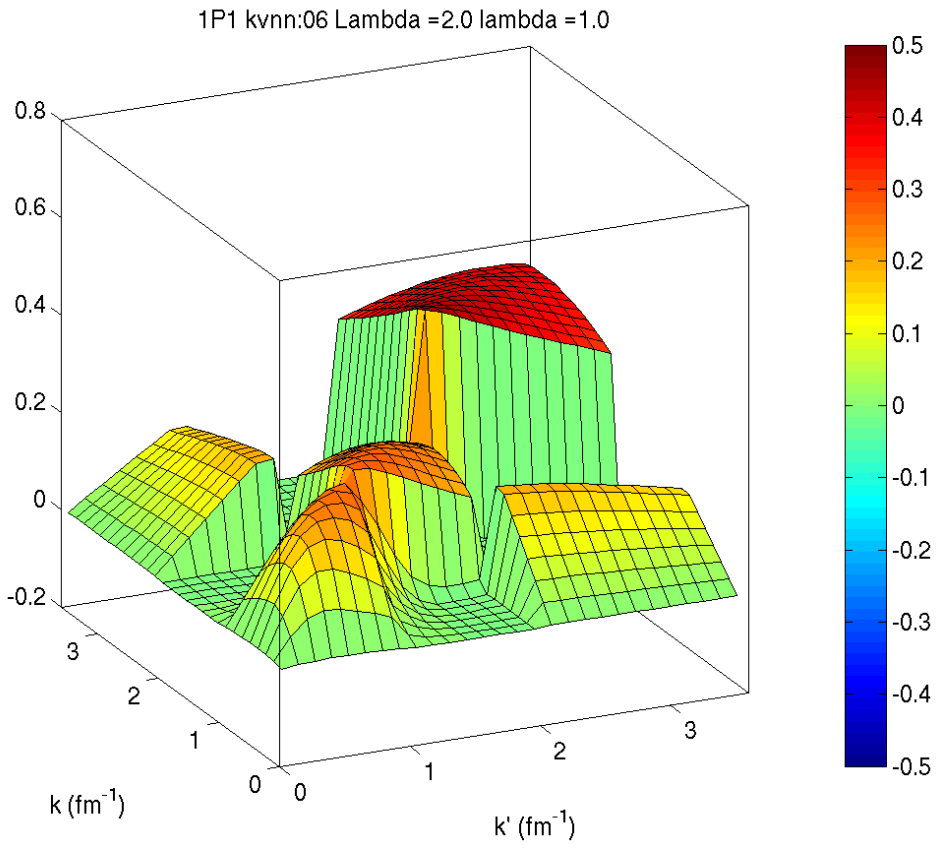


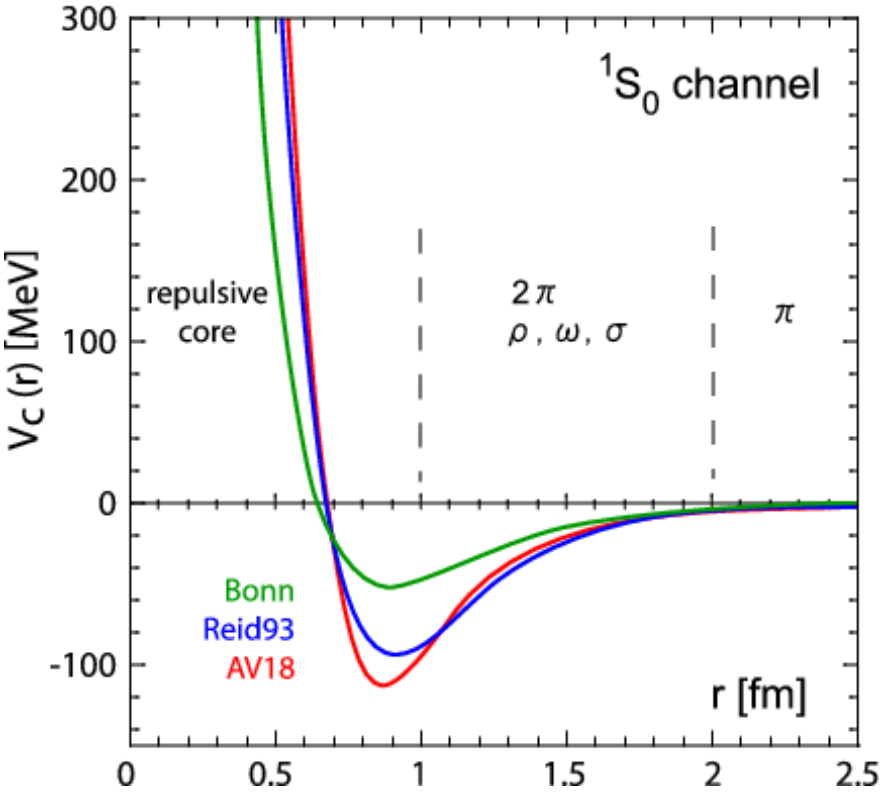


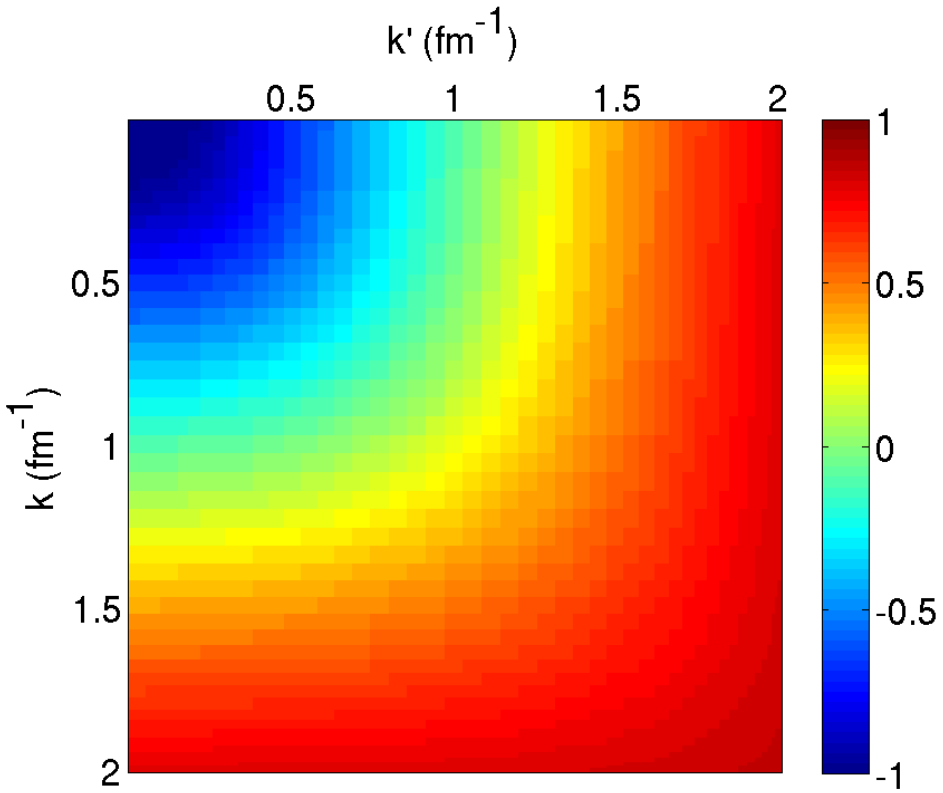
Outline: Lecture 2

Lecture 2: SRG in practice

- Recap from lecture 1: decoupling
- Implementing the similarity renormalization group (SRG)
- Block diagonal ("$V_{\mathrm{low},k}$") generator
- Computational aspects
- Quantitative measure of perturbativeness

S-wave NN potential as momentum-space matrix



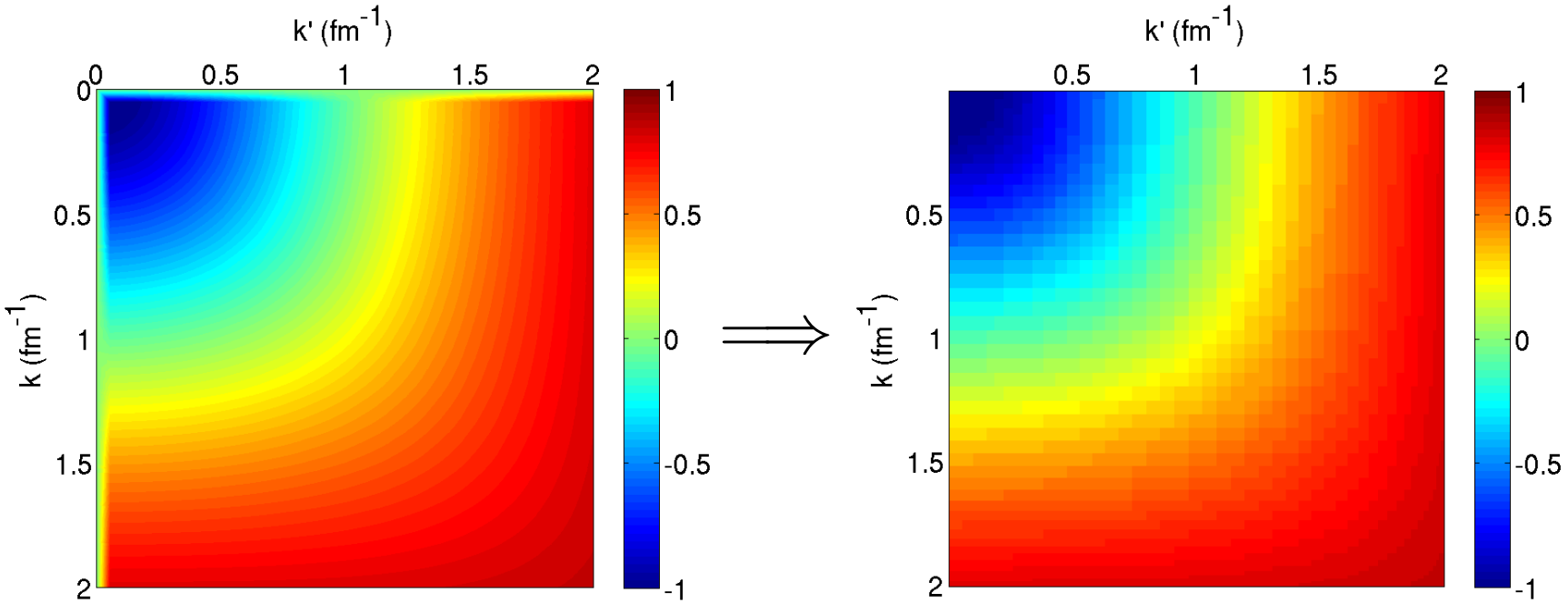


$$\langle k|V_{L=0}|k'\rangle = \int d^3r\, j_0(kr)\, V(r)\, j_0(k'r) \implies V_{kk'} \text{ matrix}$$

- Momentum units ($\hbar = c = 1$): typical relative momentum in large nucleus $\approx 1\,\text{fm}^{-1} \approx 200\,\text{MeV}$
- What would the kinetic energy look like on right?

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
  - For 3NF, harmonic oscillators, discretized partial-wave momentum, and hyperspherical harmonics are available
  - An accurate 3NF evolution in HO basis takes $\sim$ 20 million matrix elements $\Longrightarrow$ that many differential equations

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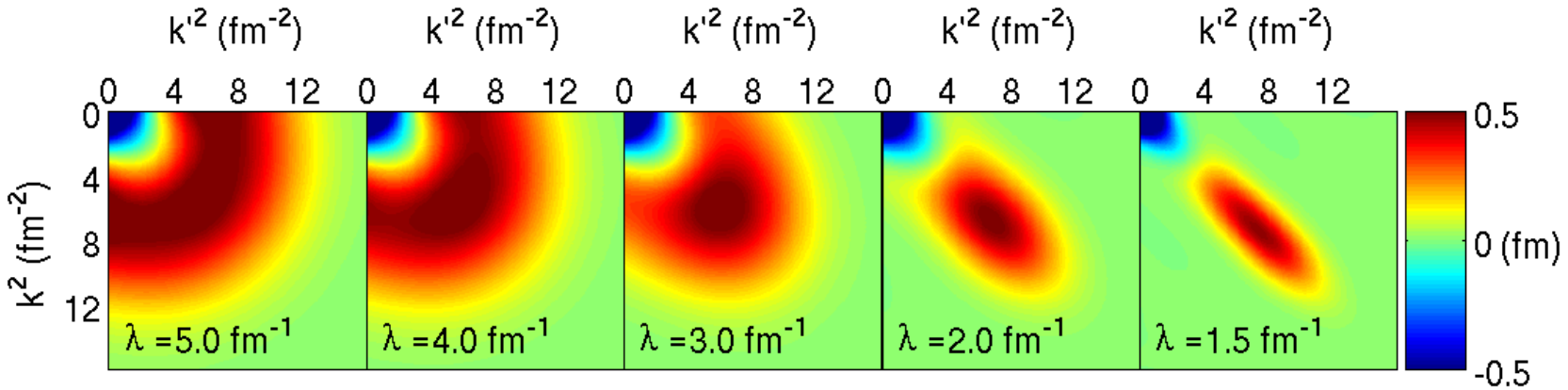
S. Weinberg on the Renormalization Group (RG)

- From "Why the RG is a good thing" [for Francis Low Festschrift]
  "The method in its most general form can I think be understood as a way to arrange in various theories that the degrees of freedom that you're talking about are the relevant degrees of freedom for the problem at hand."
- Improving perturbation theory; e.g., in QCD calculations
  - Mismatch of energy scales can generate large logarithms
  - RG: shift between couplings and loop integrals to reduce logs
  - Nuclear: decouple high- and low-momentum modes
- Identifying universality in critical phenomena
  - RG: filter out short-distance degrees of freedom
  - Nuclear: evolve toward universal interactions
- Nuclear: simplifying calculations of structure/reactions
  - Make nuclear physics look more like quantum chemistry!
  - RG gains can violate conservation of difficulty!
  - Use RG scale (resolution) dependence as a *probe* or *tool*

Flow of different N^{3}LO chiral EFT potentials

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



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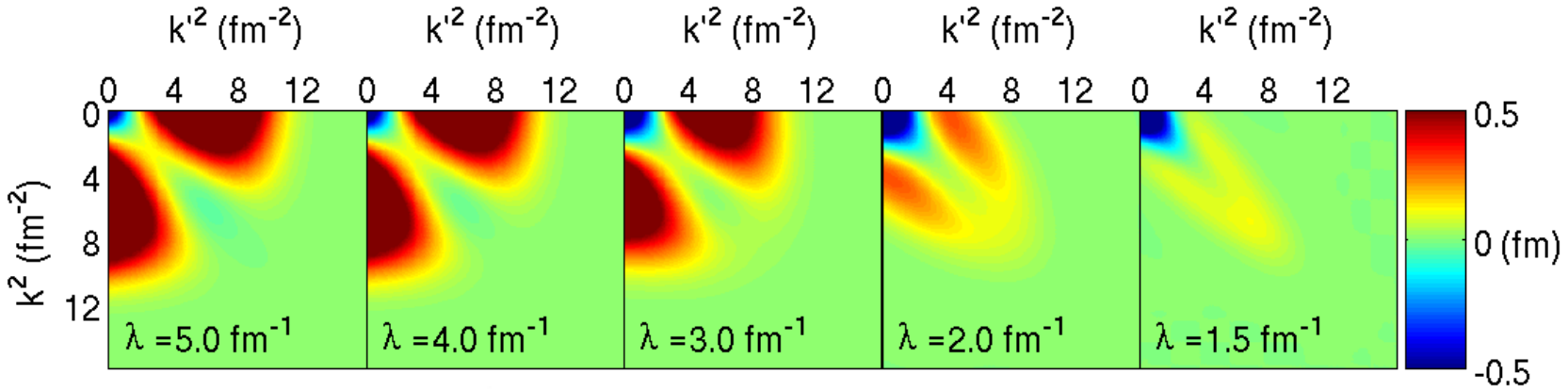

- Decoupling $\Longrightarrow$ perturbation theory is more effective

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

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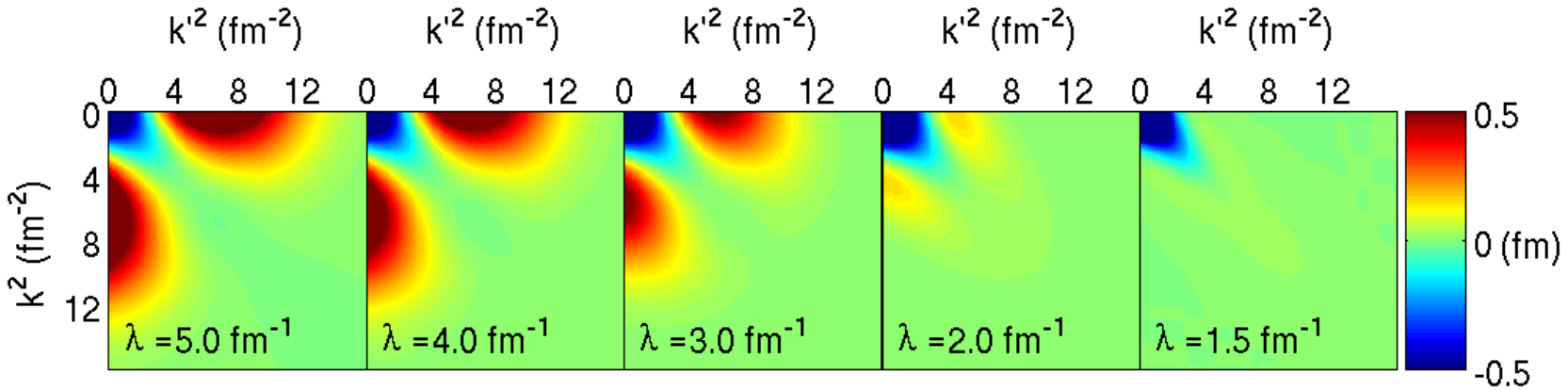

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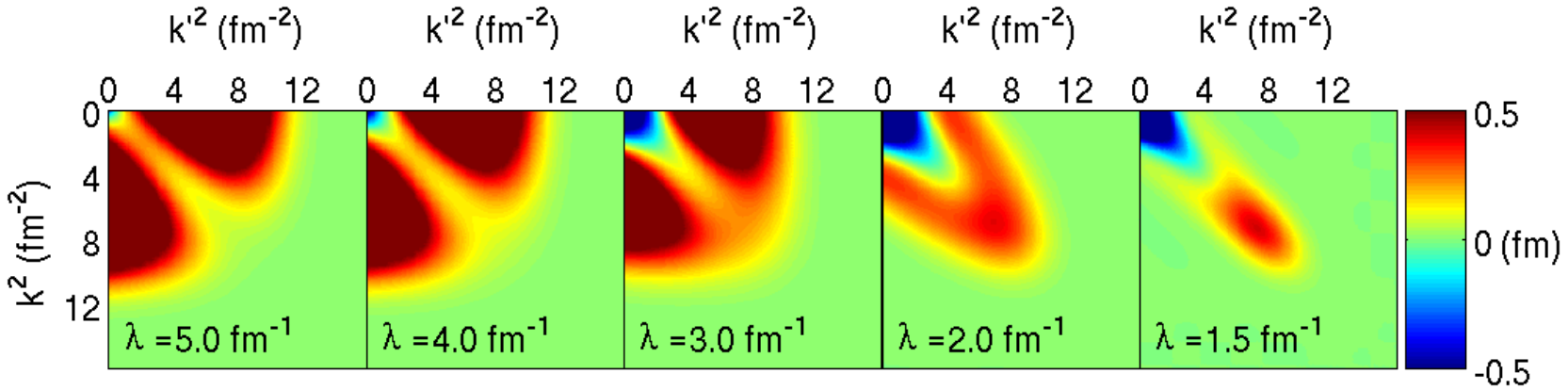

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Convergence of the Born series for scattering

- Consider whether the Born series converges for given z

$$T(z) = V + V\frac{1}{z - H_0}V + V\frac{1}{z - H_0}V\frac{1}{z - H_0}V + \cdots$$

- If bound state $|b\rangle$, series must diverge at $z = E_b$, where

$$(H_0 + V)|b\rangle = E_b|b\rangle \quad \Longrightarrow \quad V|b\rangle = (E_b - H_0)|b\rangle$$

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- For fixed E, generalize to find eigenvalue η_ν [Weinberg]

$$\frac{1}{E_b - H_0}V|b\rangle = |b\rangle \qquad \Longrightarrow \qquad \frac{1}{E - H_0}V|\Gamma_\nu\rangle = \eta_\nu|\Gamma_\nu\rangle$$

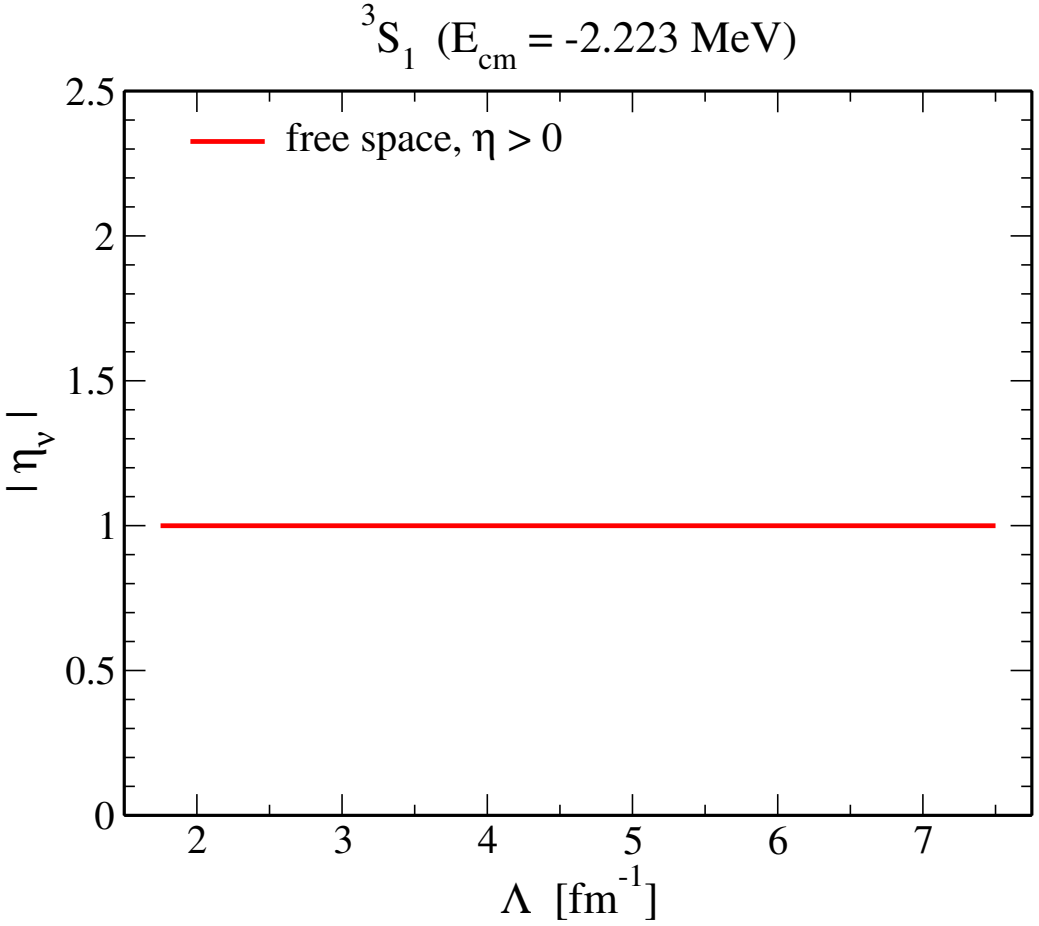
- From T applied to eigenstate, divergence for $|\eta_\nu(E)| \geq 1$:

$$T(E)|\Gamma_\nu\rangle = V|\Gamma_\nu\rangle(1 + \eta_\nu + \eta_\nu^2 + \cdots)$$

$\Longrightarrow$ $T(E)$ diverges if bound state at E for V/η_ν with $|\eta_\nu| \geq 1$

Weinberg eigenvalues as function of cutoff Λ/λ

- Consider $\eta_\nu(E = -2.22\,\text{MeV})$
- Deuteron $\Longrightarrow$ attractive eigenvalue $\eta_\nu = 1$
  - $\Lambda \downarrow \Longrightarrow$ unchanged



Weinberg eigenvalues as function of cutoff Λ/λ

- Consider $\eta_\nu(E = -2.22\,\text{MeV})$
- Deuteron $\Longrightarrow$ attractive eigenvalue $\eta_\nu = 1$
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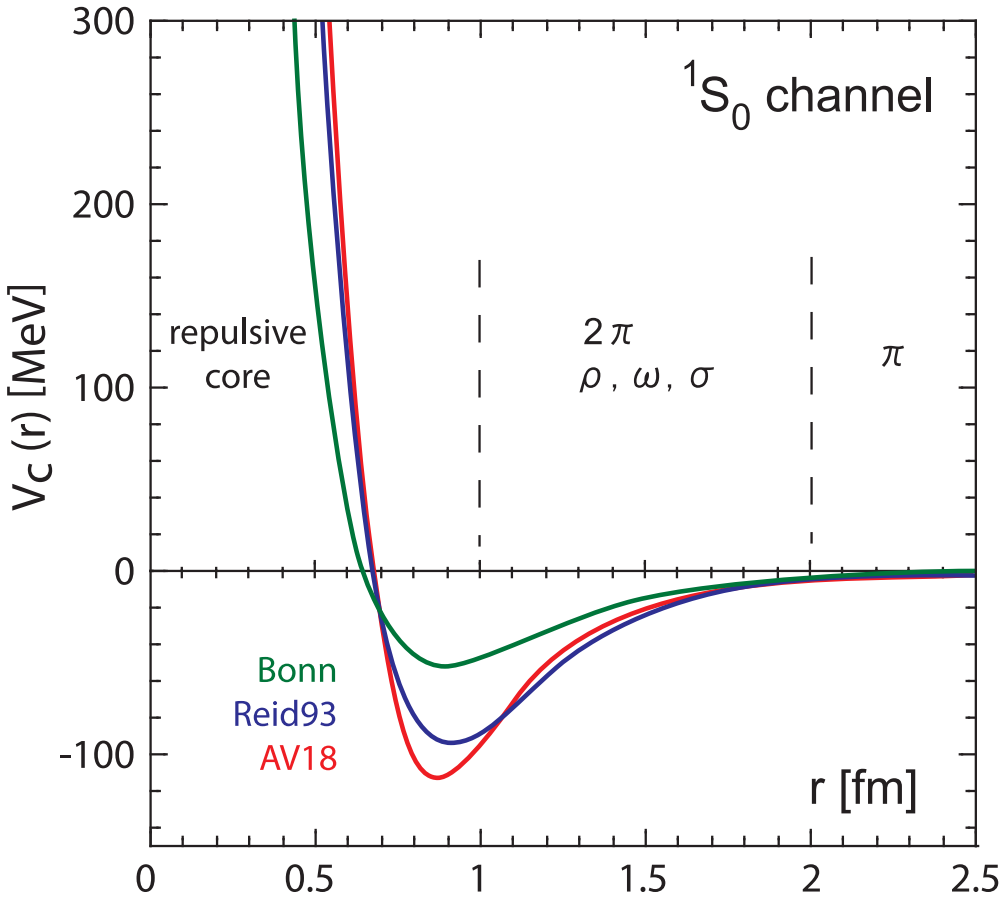
- But η_ν can be negative, so $V/\eta_\nu \Longrightarrow$ flip potential



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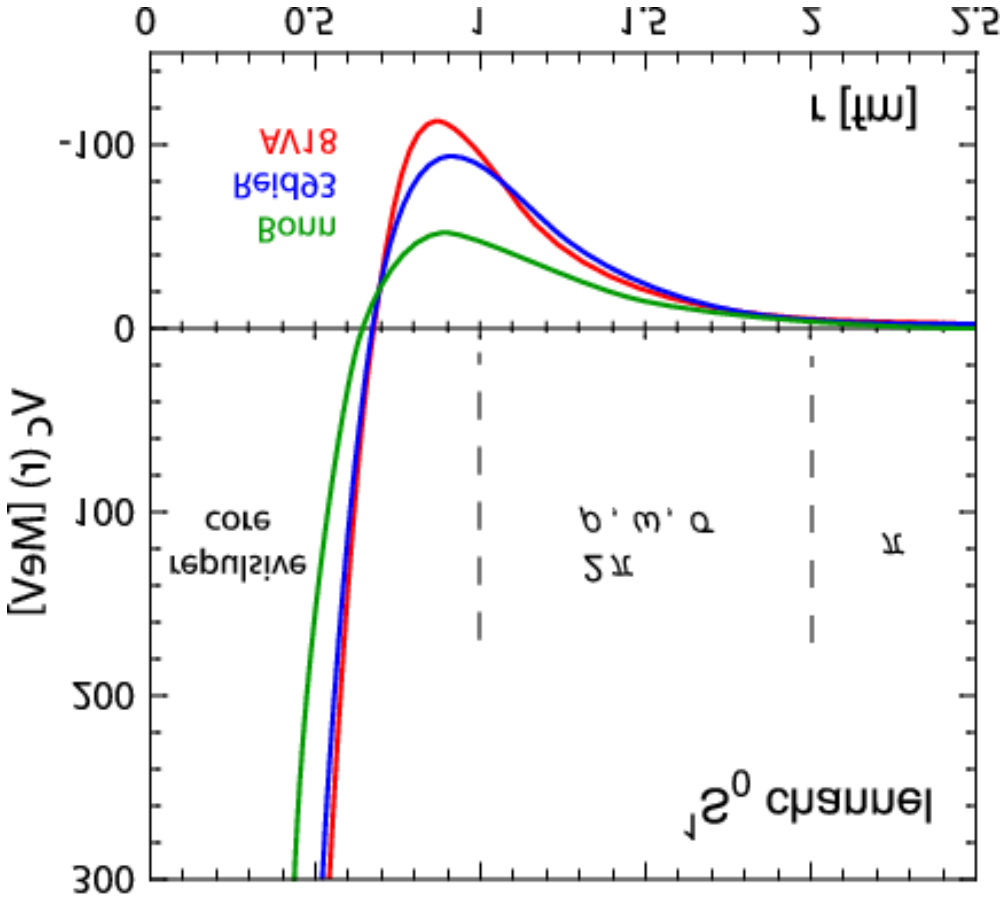

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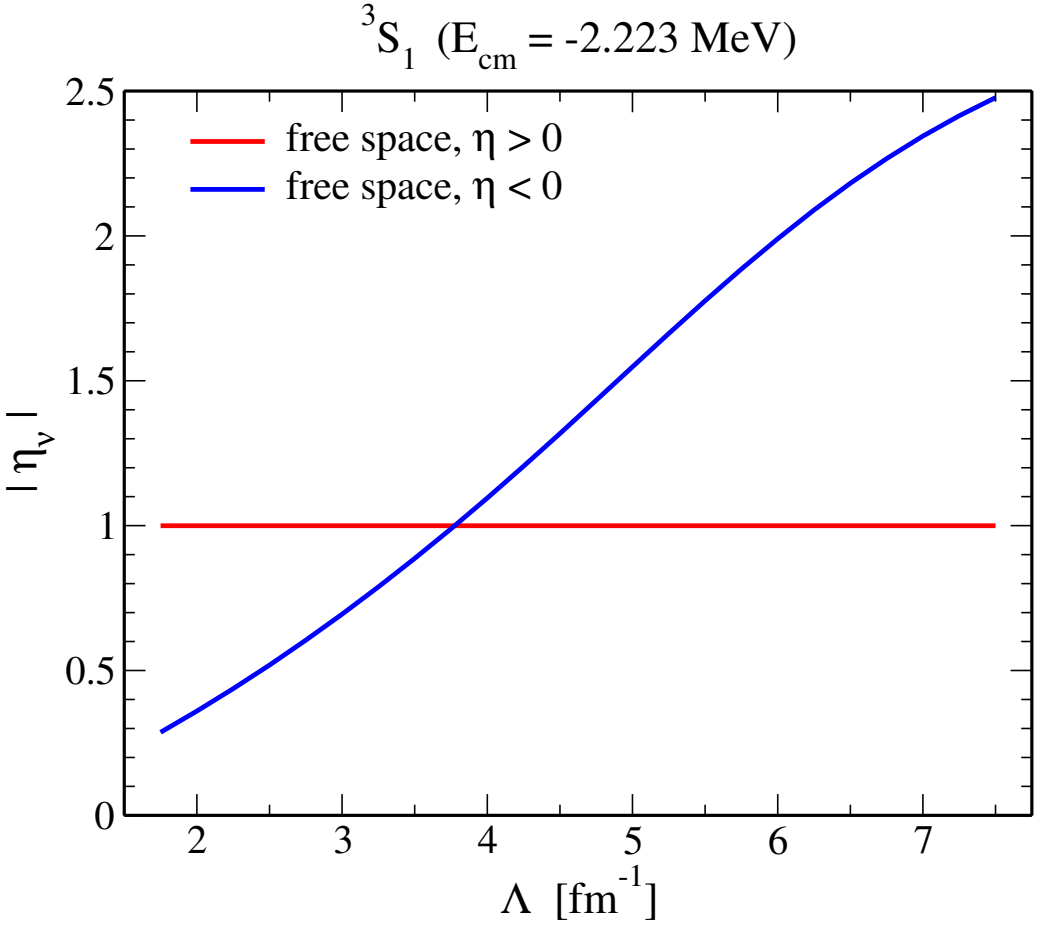

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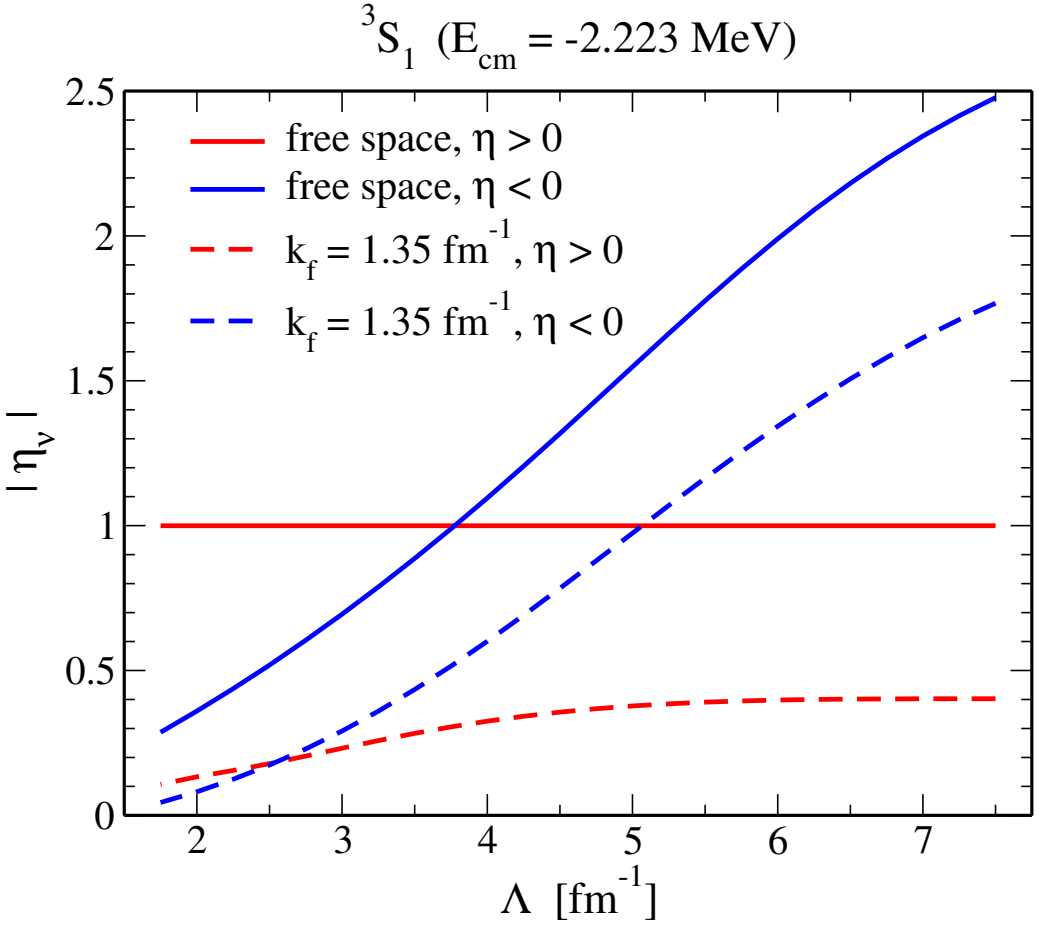
- Deuteron $\Longrightarrow$ attractive eigenvalue $\eta_\nu = 1$
  - $\Lambda \downarrow \Longrightarrow$ unchanged
- But η_ν can be negative, so $V/\eta_\nu \Longrightarrow$ flip potential
- Hard core $\Longrightarrow$ repulsive eigenvalue η_ν
  - $\Lambda \downarrow \Longrightarrow$ reduced
- In medium: both reduced
  - $\eta_\nu \ll 1$ for $\Lambda \approx 2\,\text{fm}^{-1}$

$\Longrightarrow$ perturbative (at least for particle-particle channel)



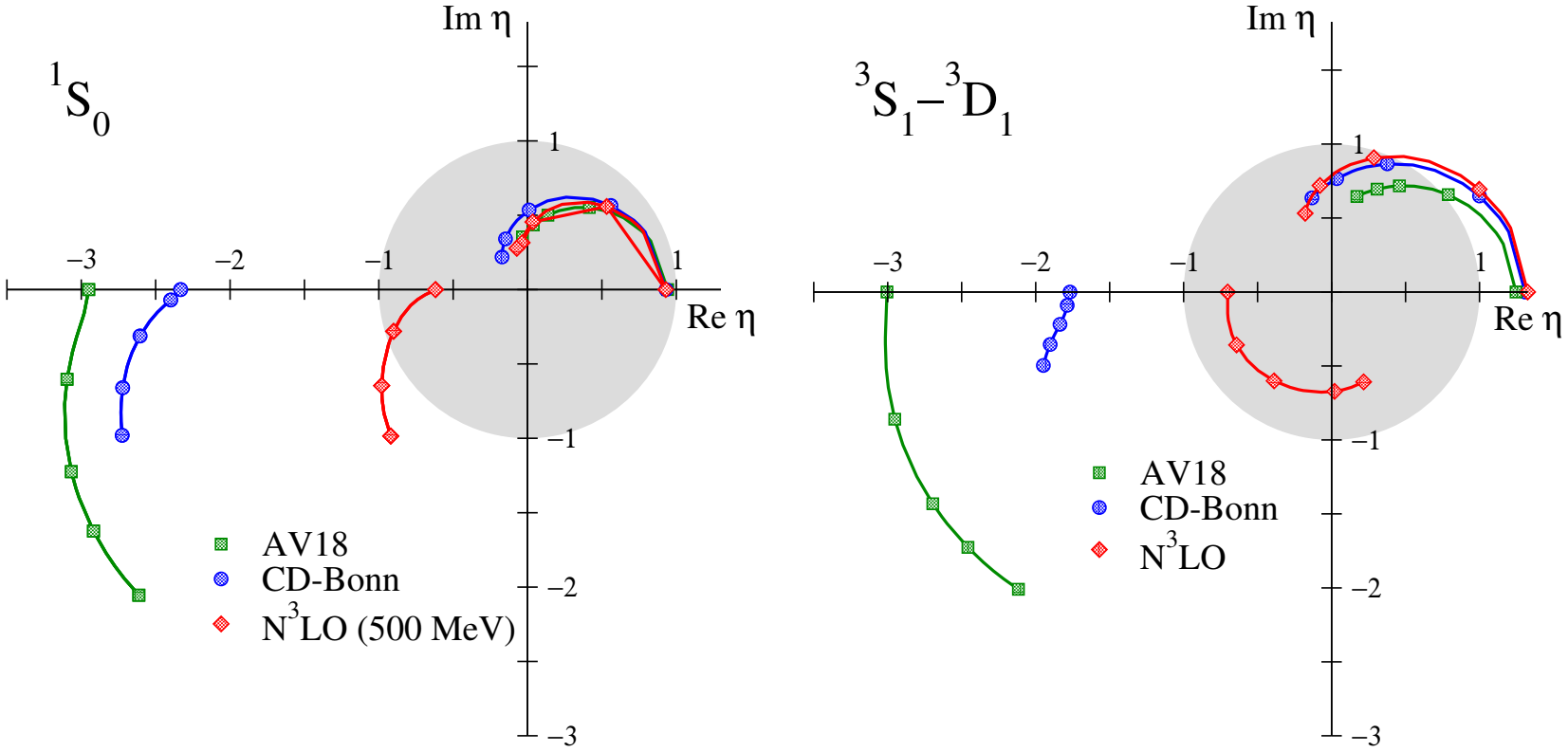
Weinberg eigenvalue analysis of convergence

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]

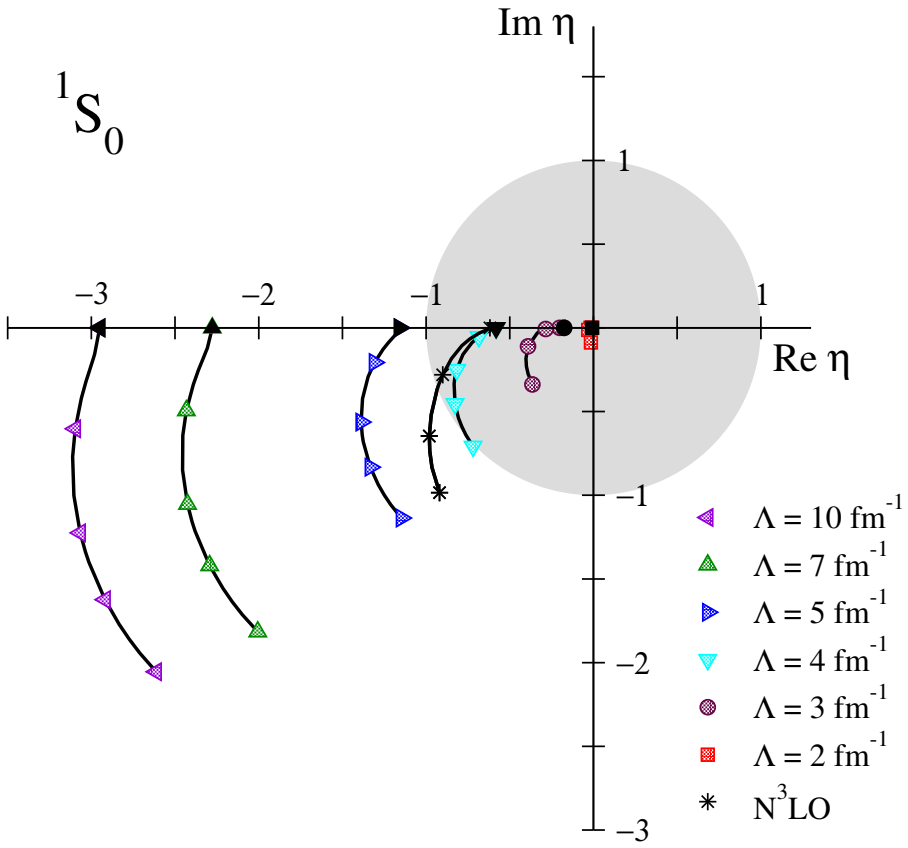
$$\frac{1}{E-H_0}V|\Gamma_\nu\rangle = \eta_\nu|\Gamma_\nu\rangle \quad \Longrightarrow \quad T(E)|\Gamma_\nu\rangle = V|\Gamma_\nu\rangle(1+\eta_\nu+\eta_\nu^2+\cdots)$$

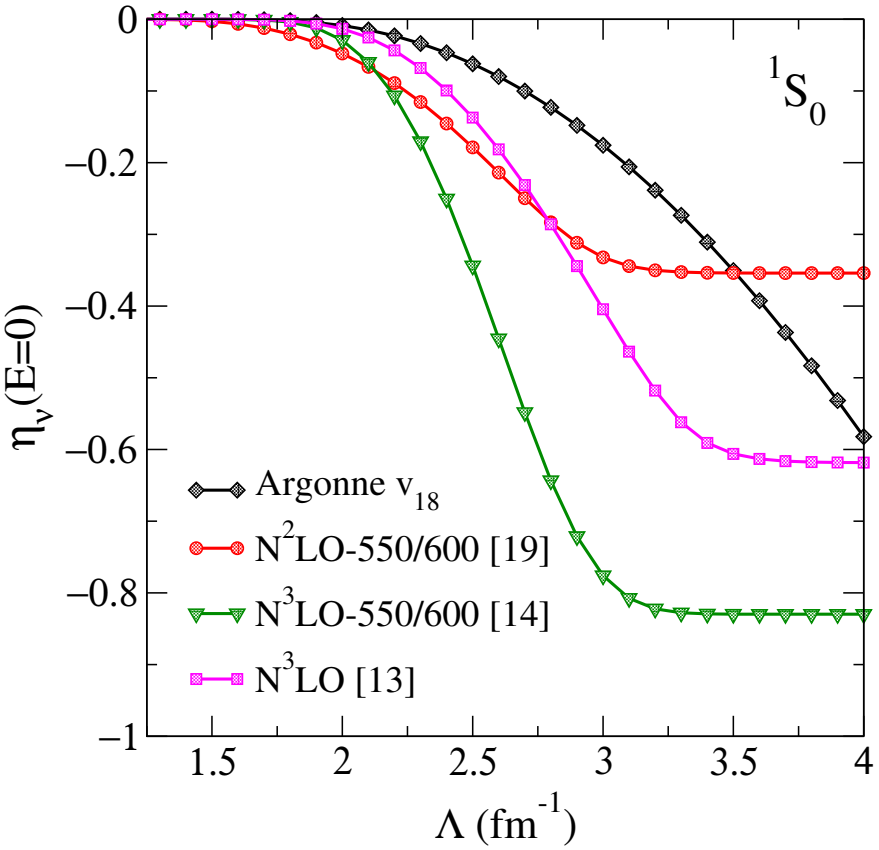
$\Longrightarrow$ T diverges if *any* $|\eta_\nu(E)| \geq 1$ [nucl-th/0602060]



Lowering the cutoff increases “perturbativeness”

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





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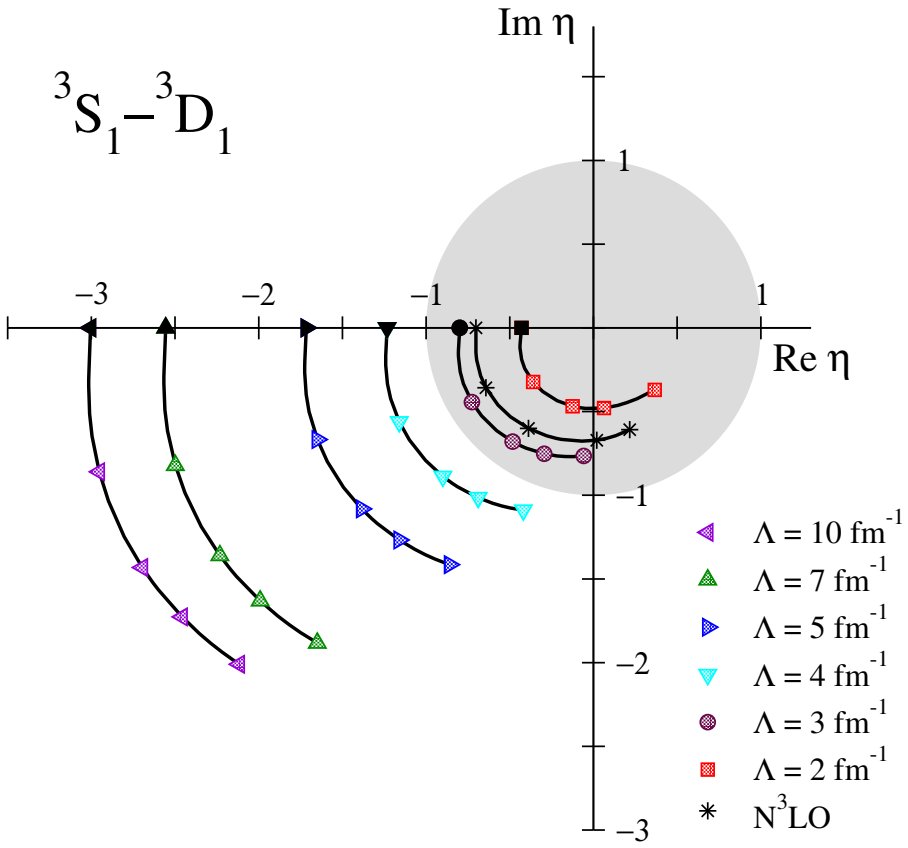
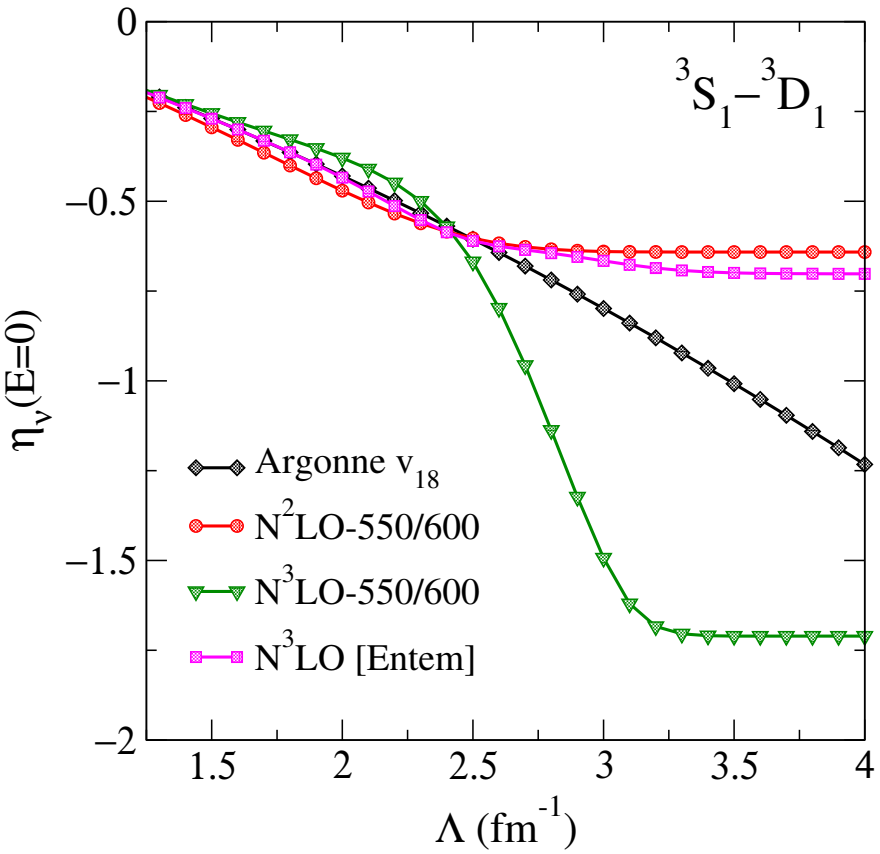
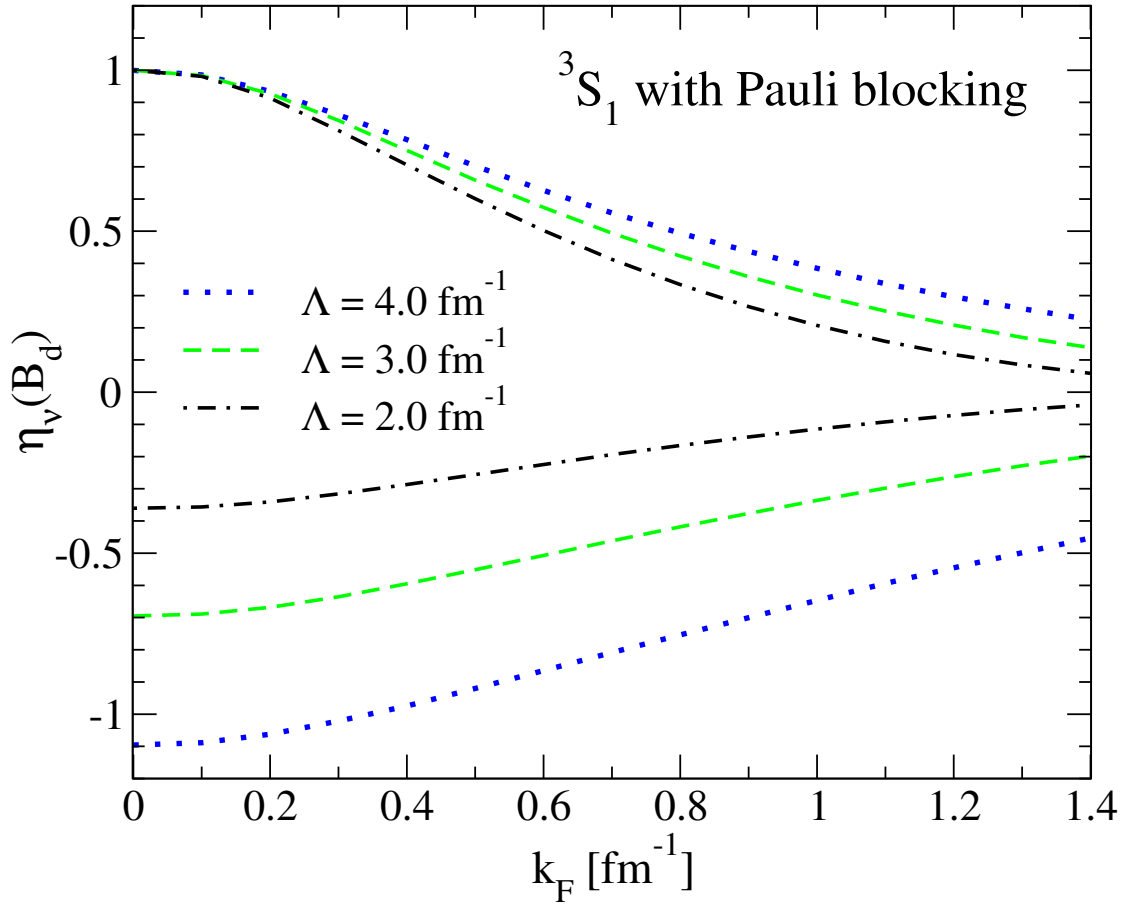




Lowering the cutoff increases "perturbativeness"

- 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 $|\eta_\nu| > 1$