Atomic Nuclei at Low Resolution

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Ohio State University

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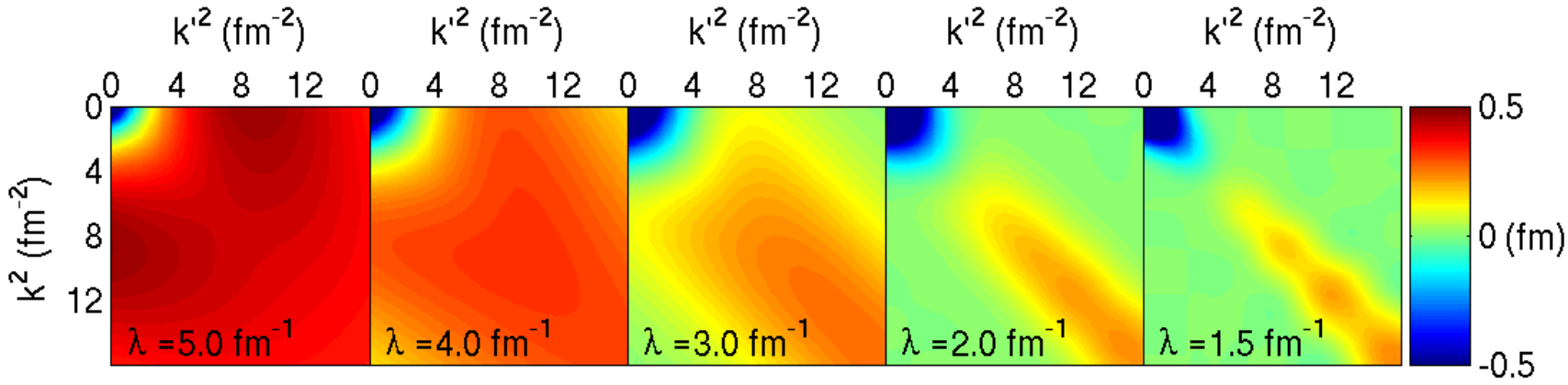

Outline

Overview: Goals of low-energy nuclear physics

Lowering the resolution with RG

Implications of low resolution for nuclear calculations

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Lowering the resolution with RG

Implications of low resolution for nuclear calculations

Questions that drive low-energy nuclear physics

- How do protons and neutrons make stable nuclei and rare isotopes? Where are the limits?
- What are the heaviest nuclei that can exist?
- What is the equation of state of matter made of nucleons?
- What is the origin of simple patterns in complex nuclei?

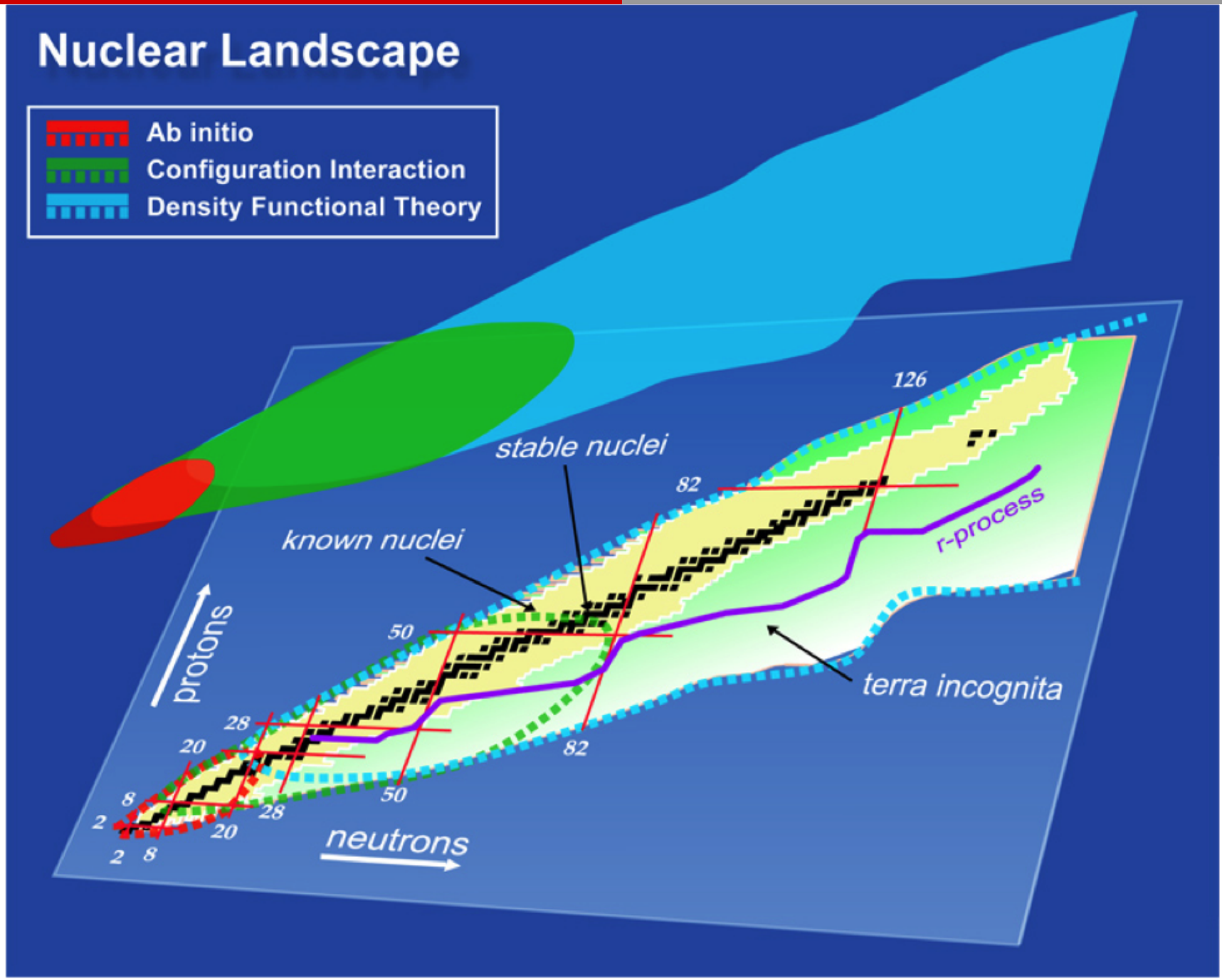
Physics of Nuclei

- When and how did the elements from iron to uranium originate?
- How do stars explode?
- What is the nature of neutron star matter?

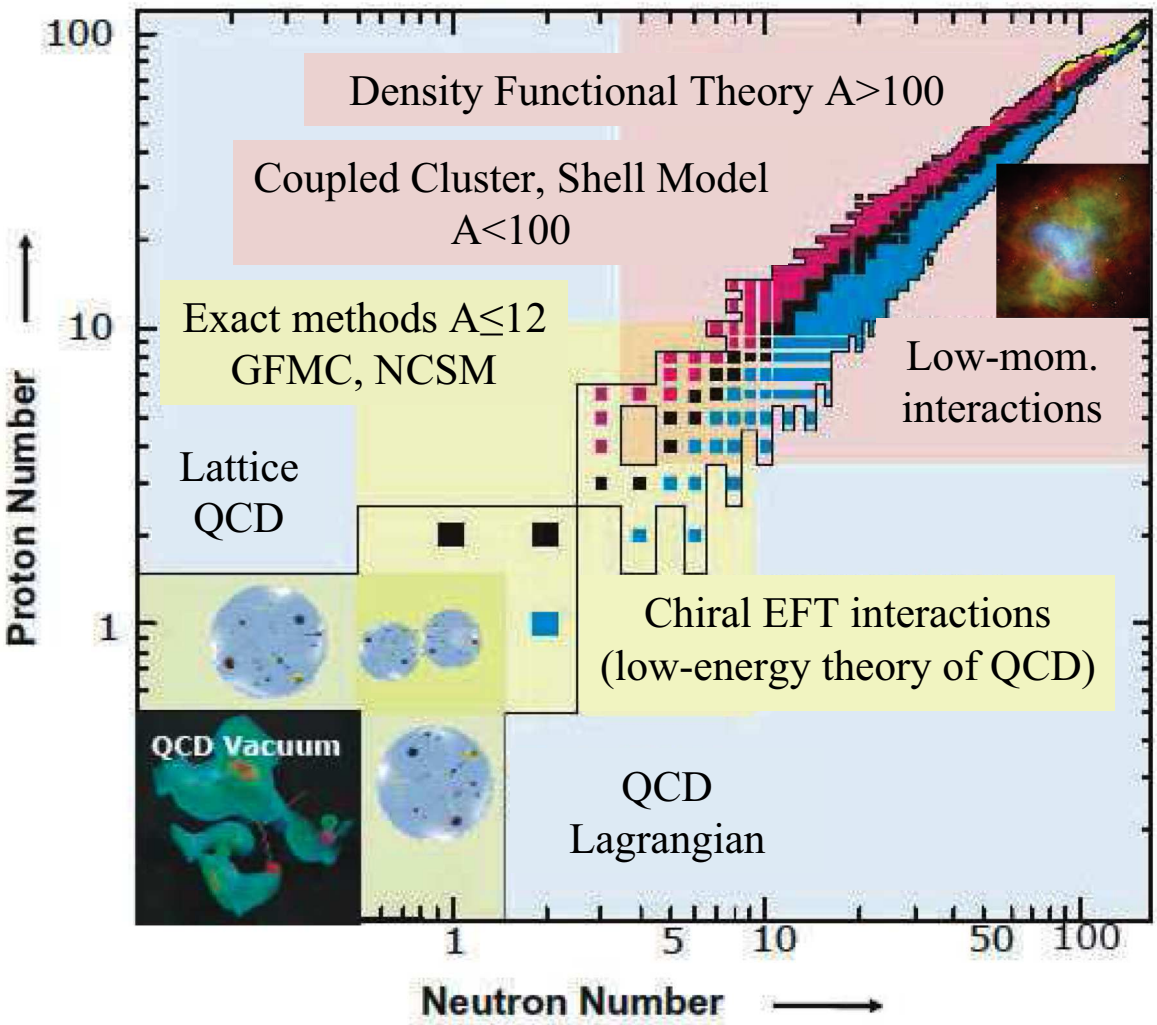
Nuclear Astrophysics

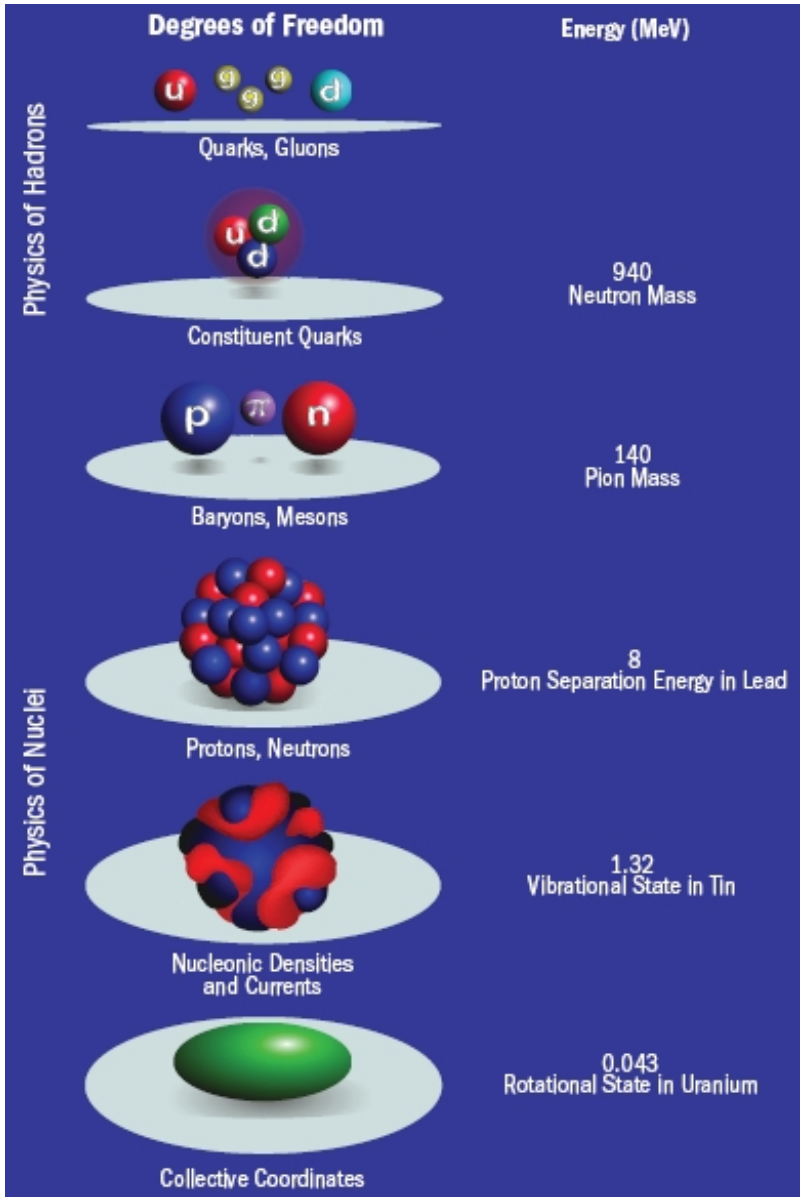
- How can our knowledge of nuclei and our ability to produce them benefit humankind? Life Sciences, Material Sciences, Nuclear Energy, Security

Applications of Nuclei


Nuclear Landscape
Ab initio
Configuration Interaction
Density Functional Theory
stable nuclei
known nuclei
r-process
terra incognita
protons
neutrons
126
82
50
28
20
8
2
2
8
20
28
50
82

The big picture: From QCD to nuclei





Low resolution makes physics easier + efficient

- Weinberg's Third Law of Progress in Theoretical Physics:
  "You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

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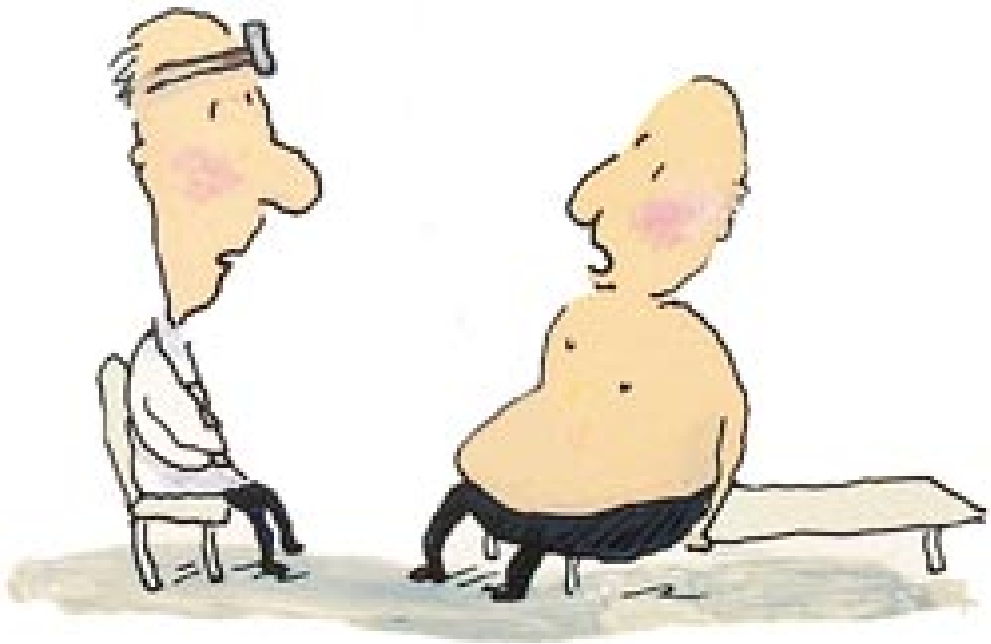

Patient: Doctor, doctor, it hurts when I do this!

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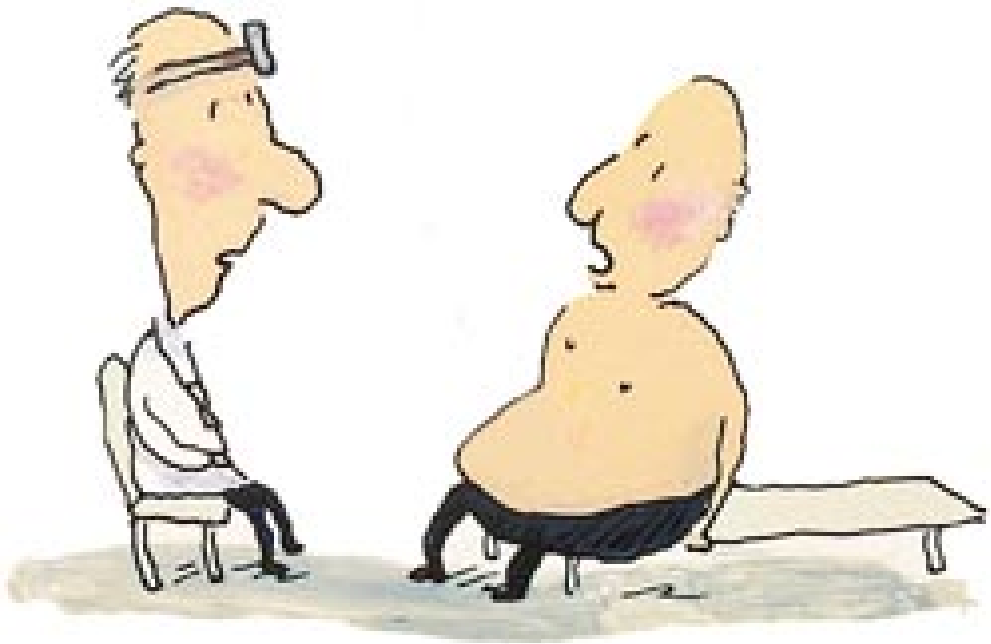
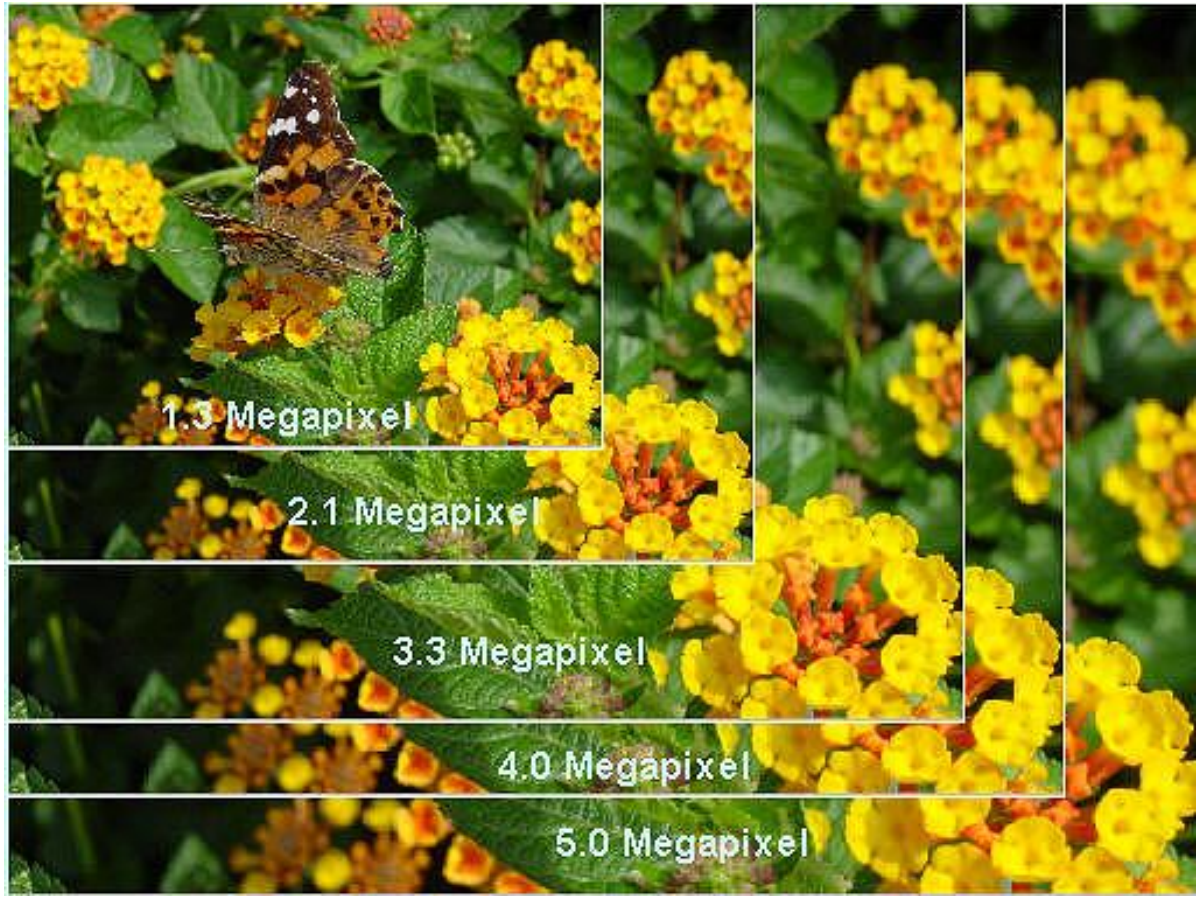


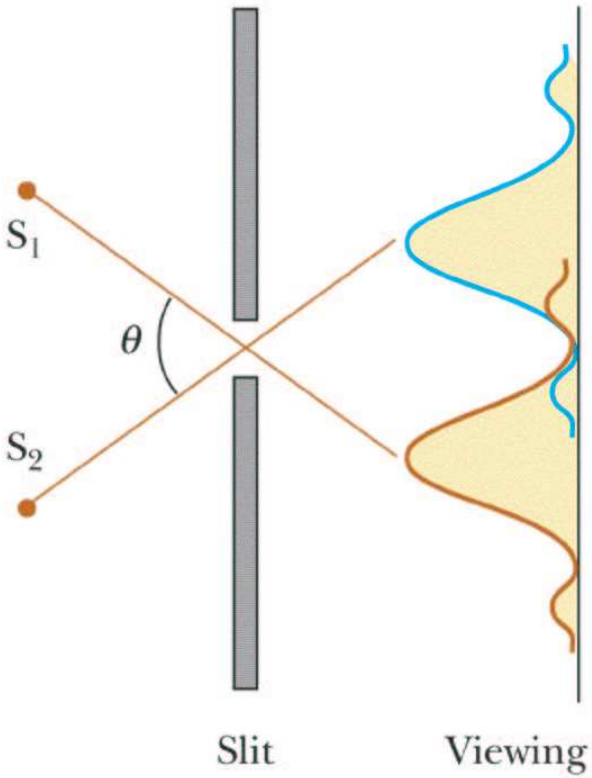
Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don't do that.

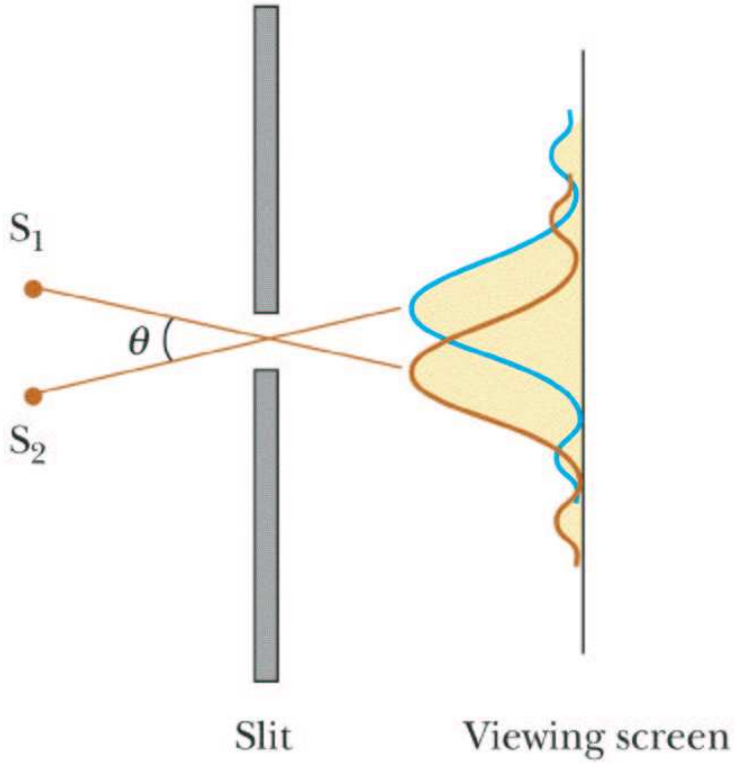
Digital resolution: Higher resolution is better (?)

- Computer screens, printers, digital cameras, TV's ...
- Higher resolution $\Longrightarrow$ more pixels
- Pixel size $\ll$ characteristic scale $\Longrightarrow$ greater detail
- Greater resolution $\Longrightarrow$ more \$\$\$

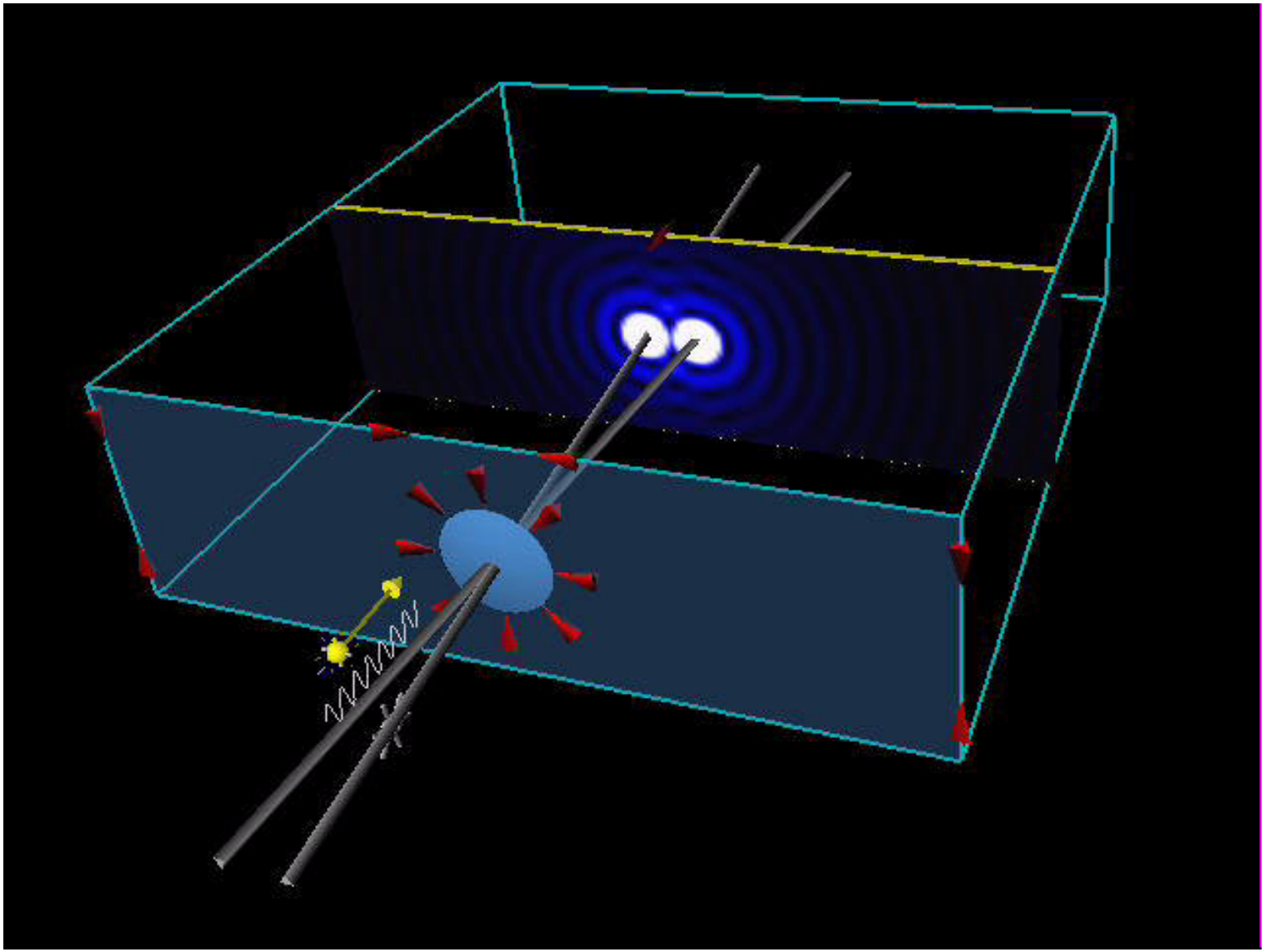


Diffraction and resolution





Wavelength and resolution



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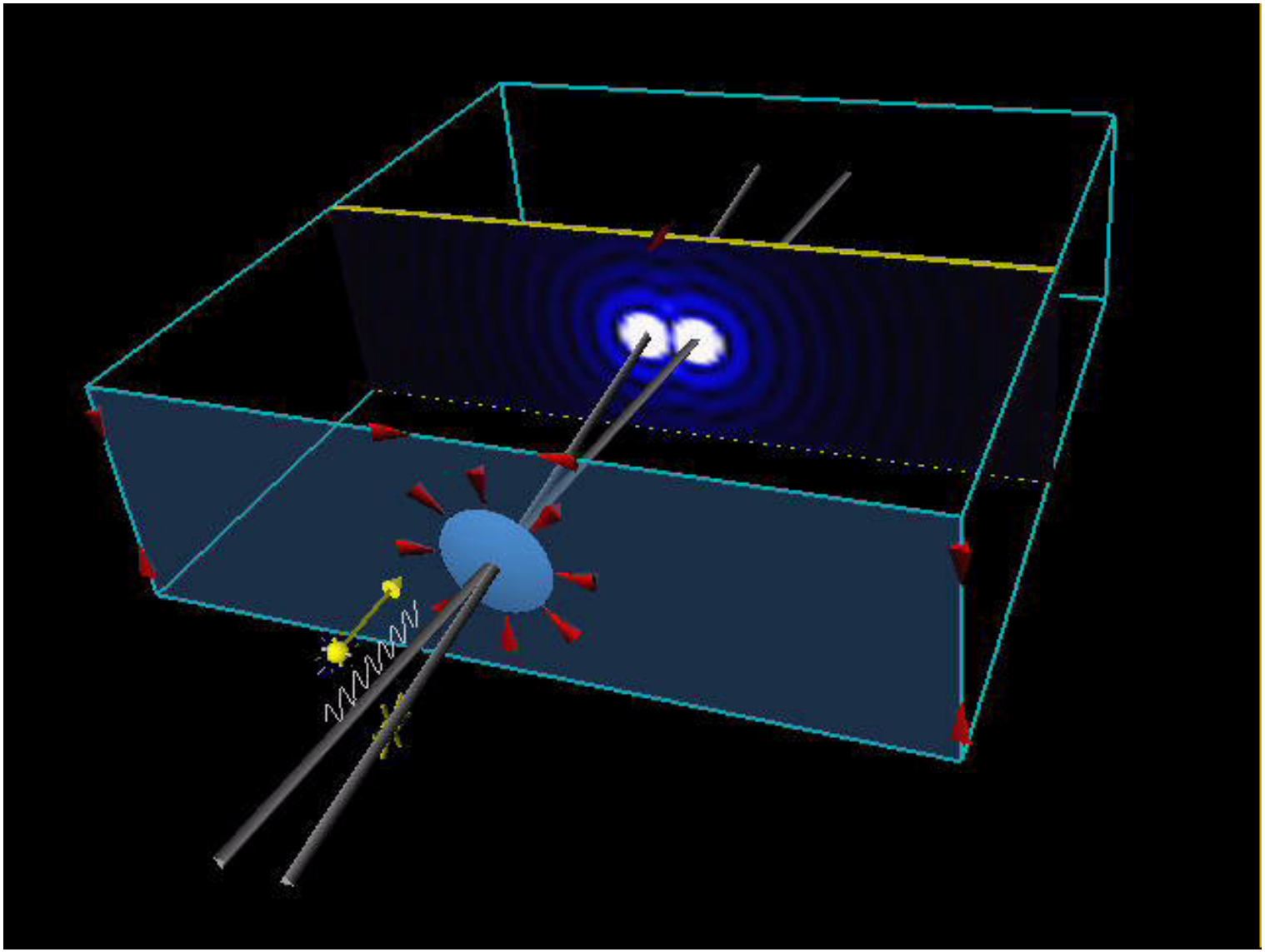

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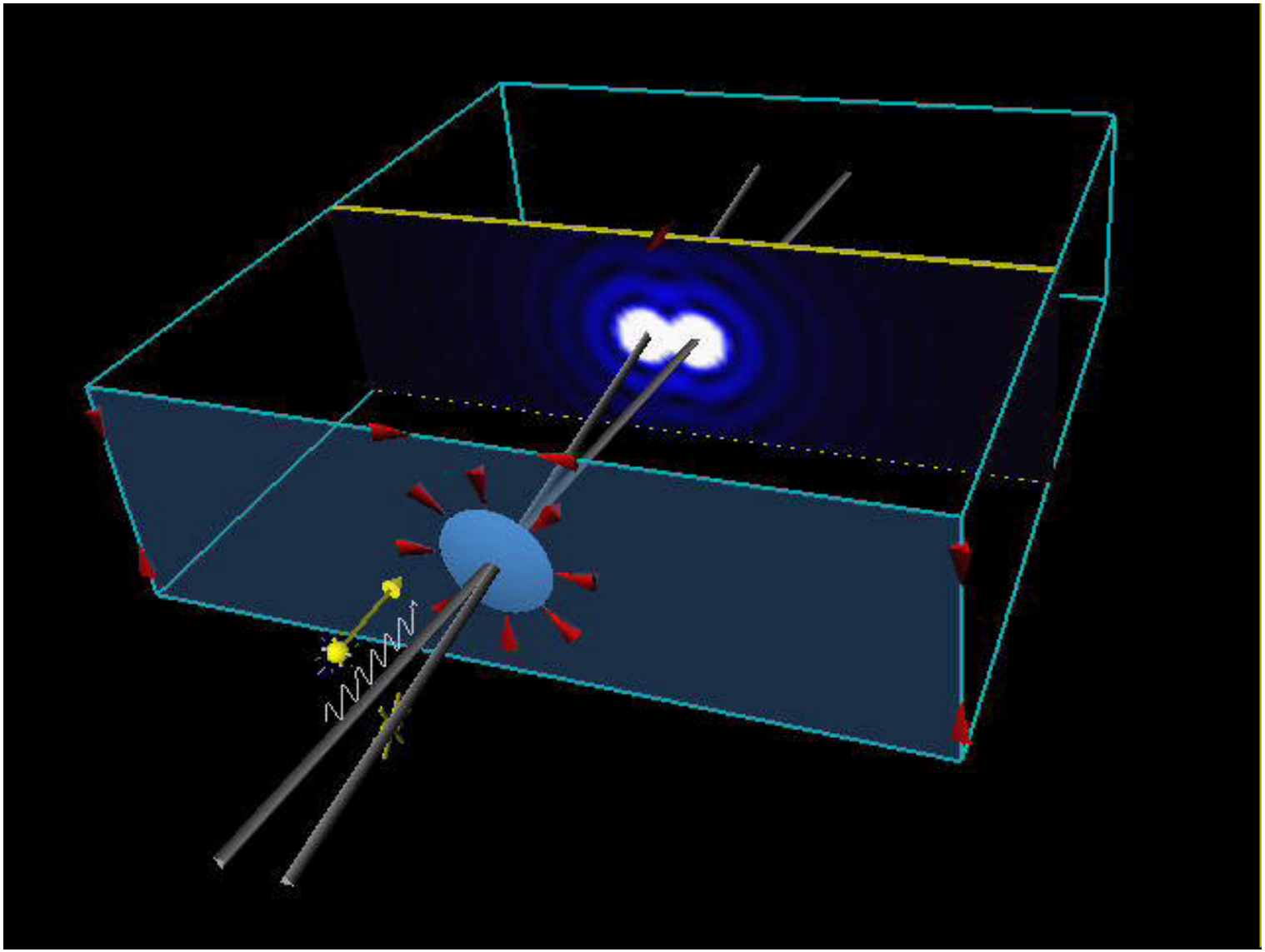

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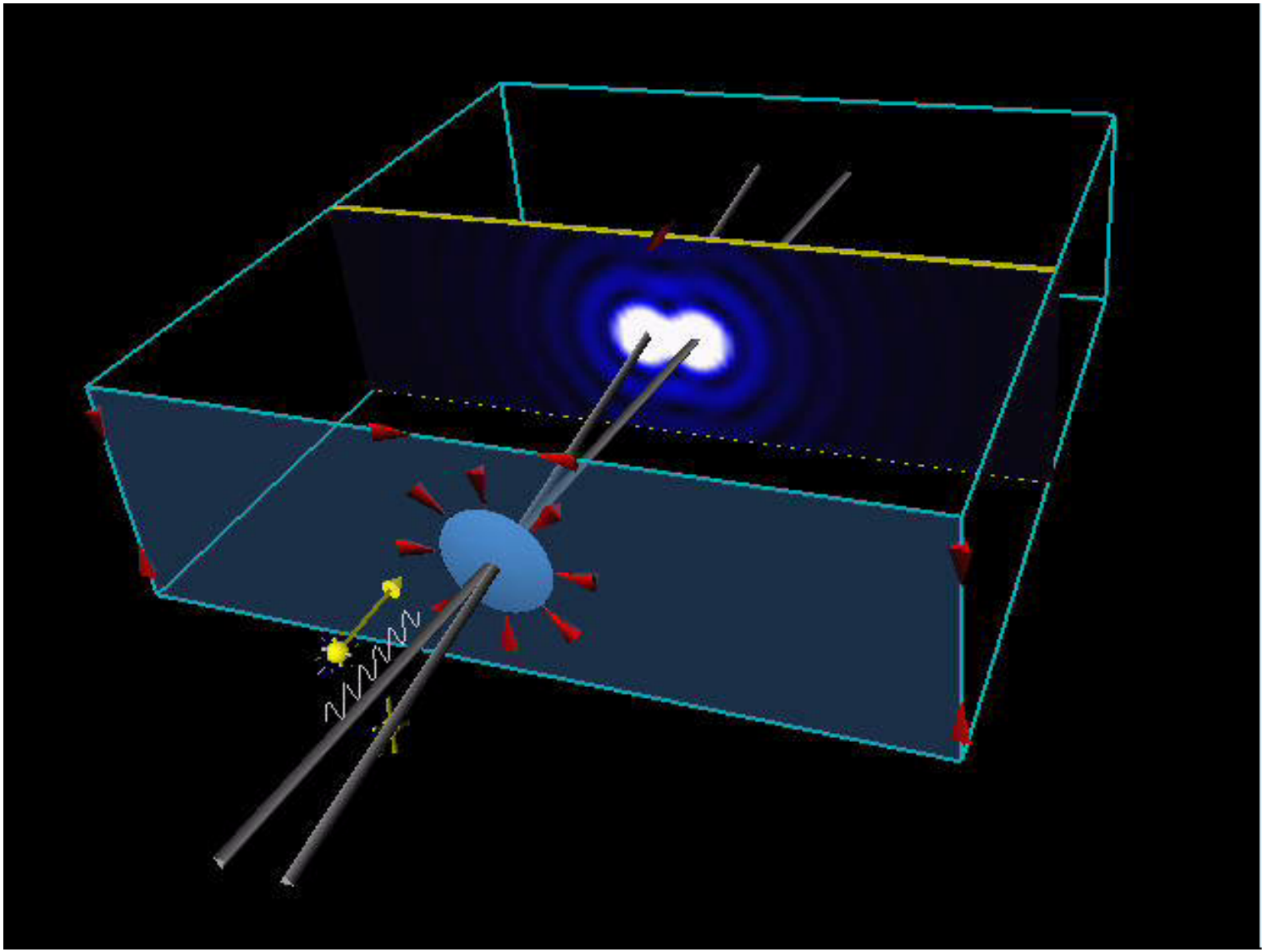

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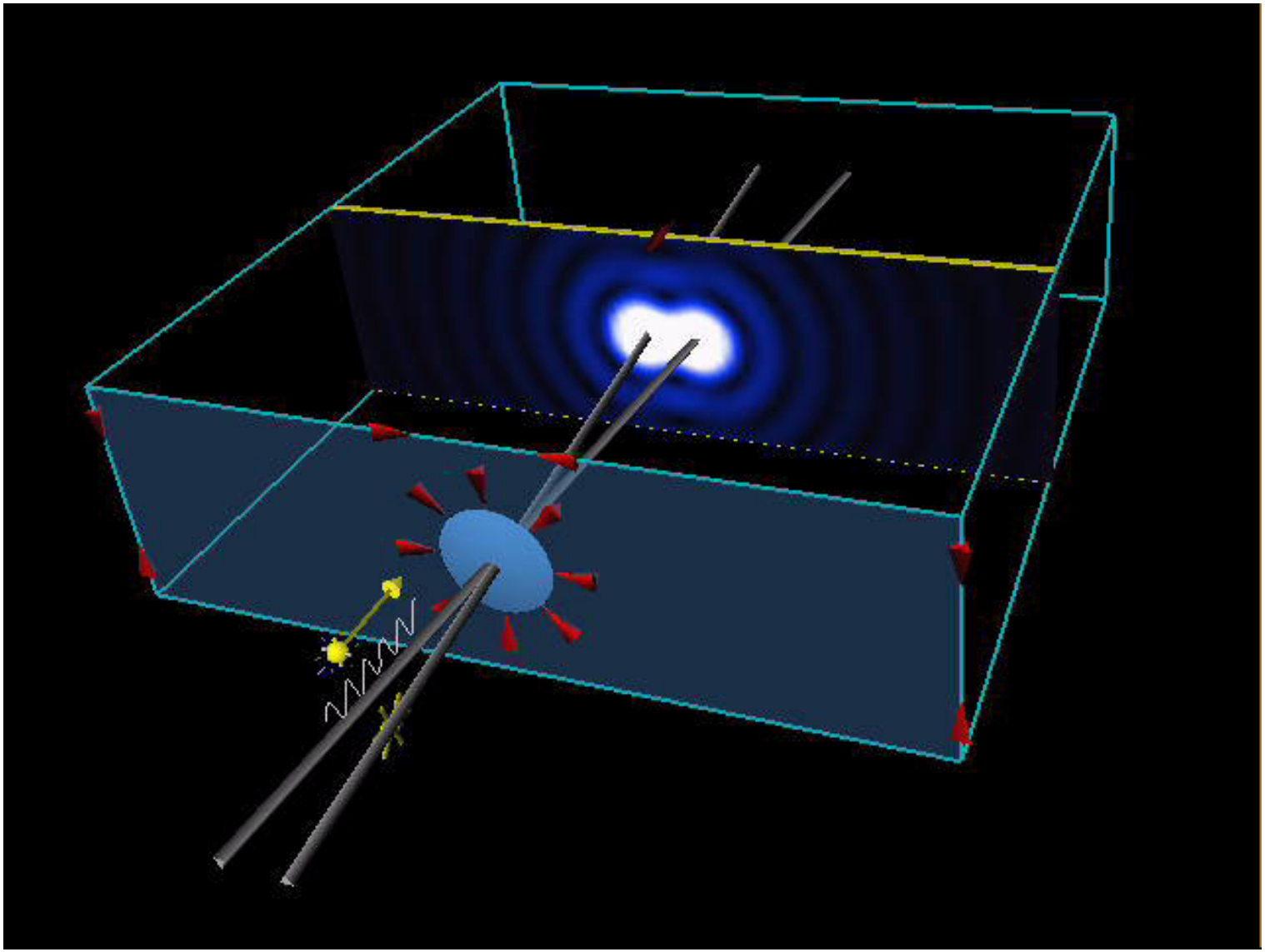

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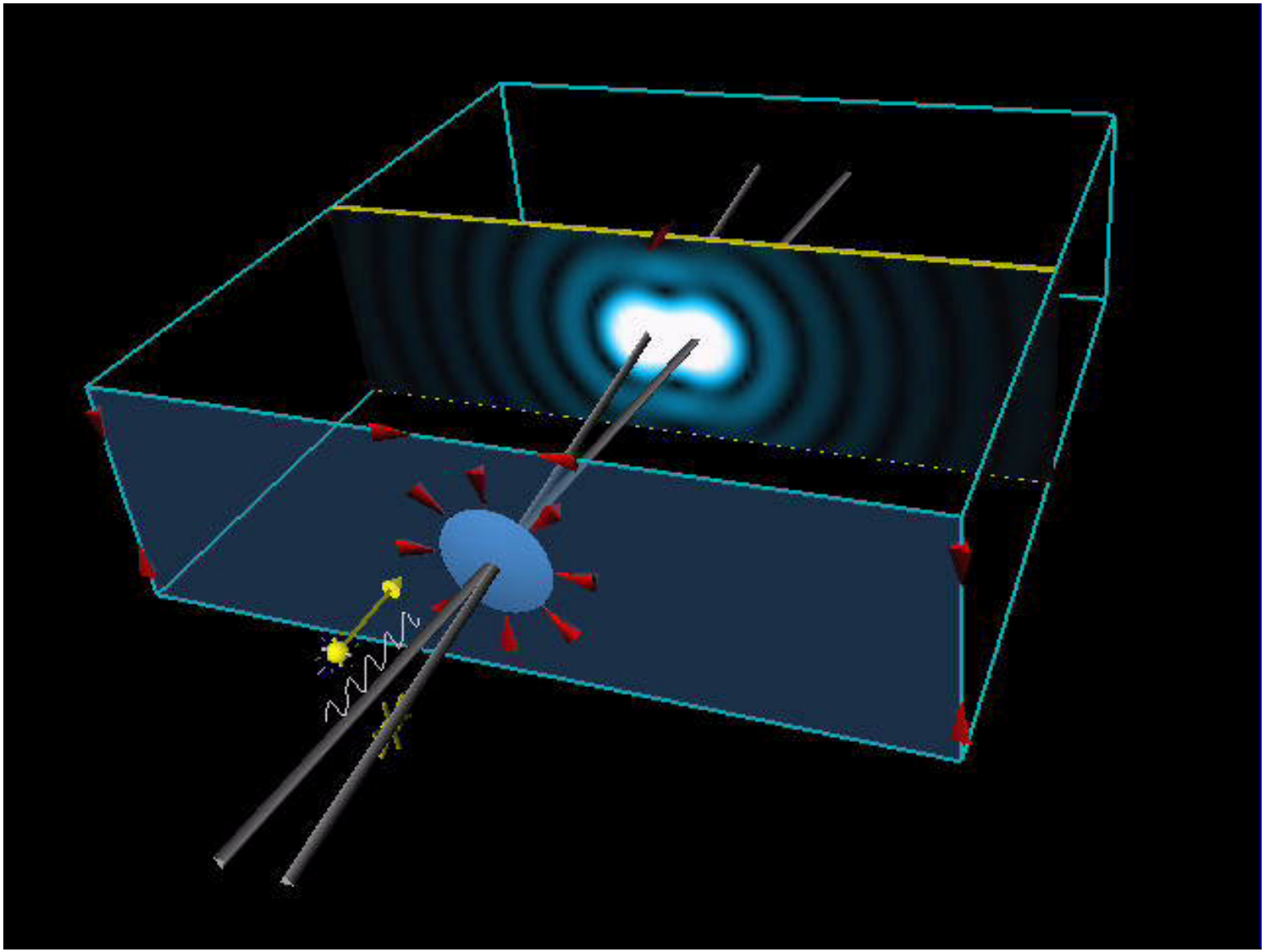

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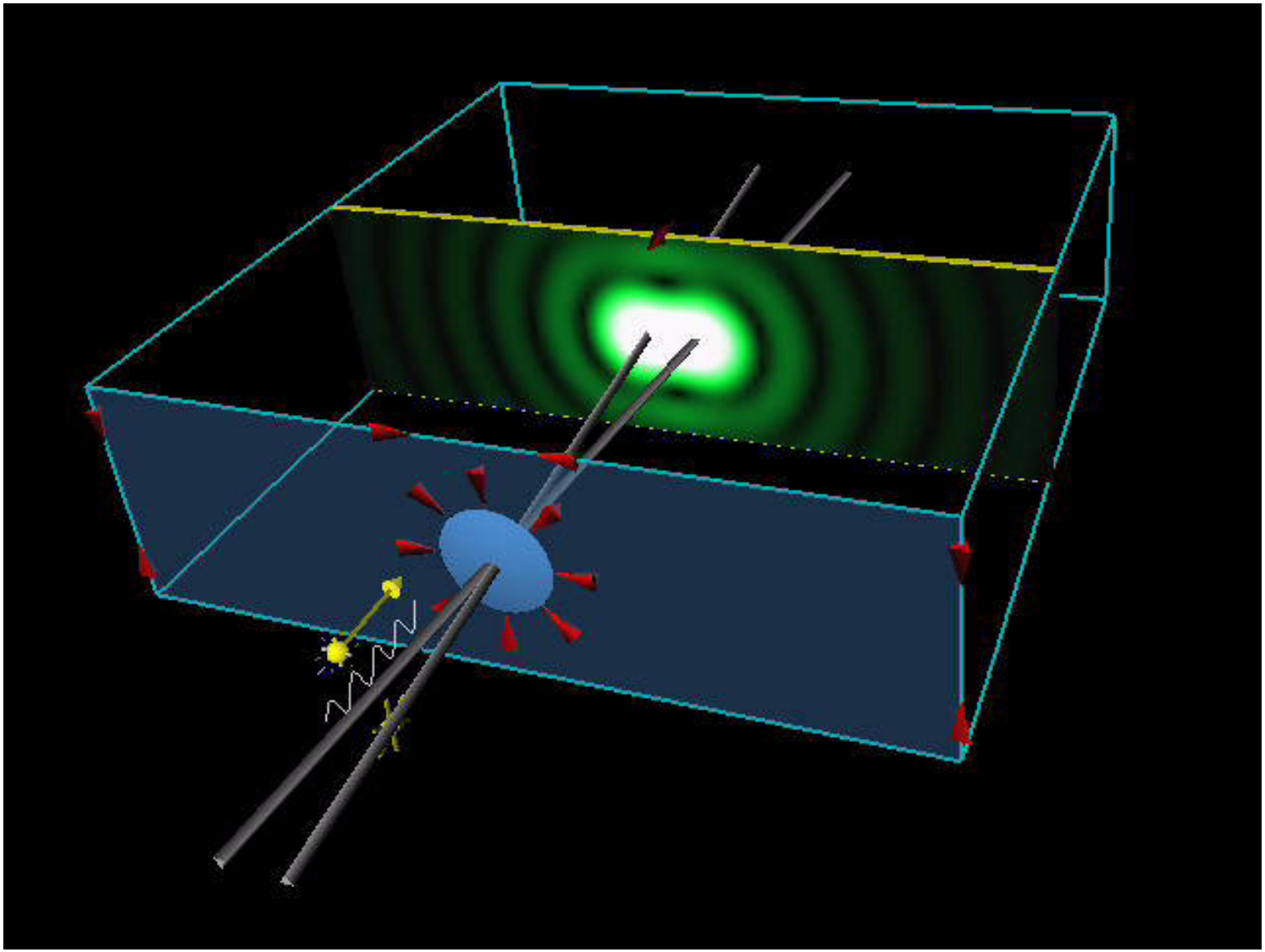

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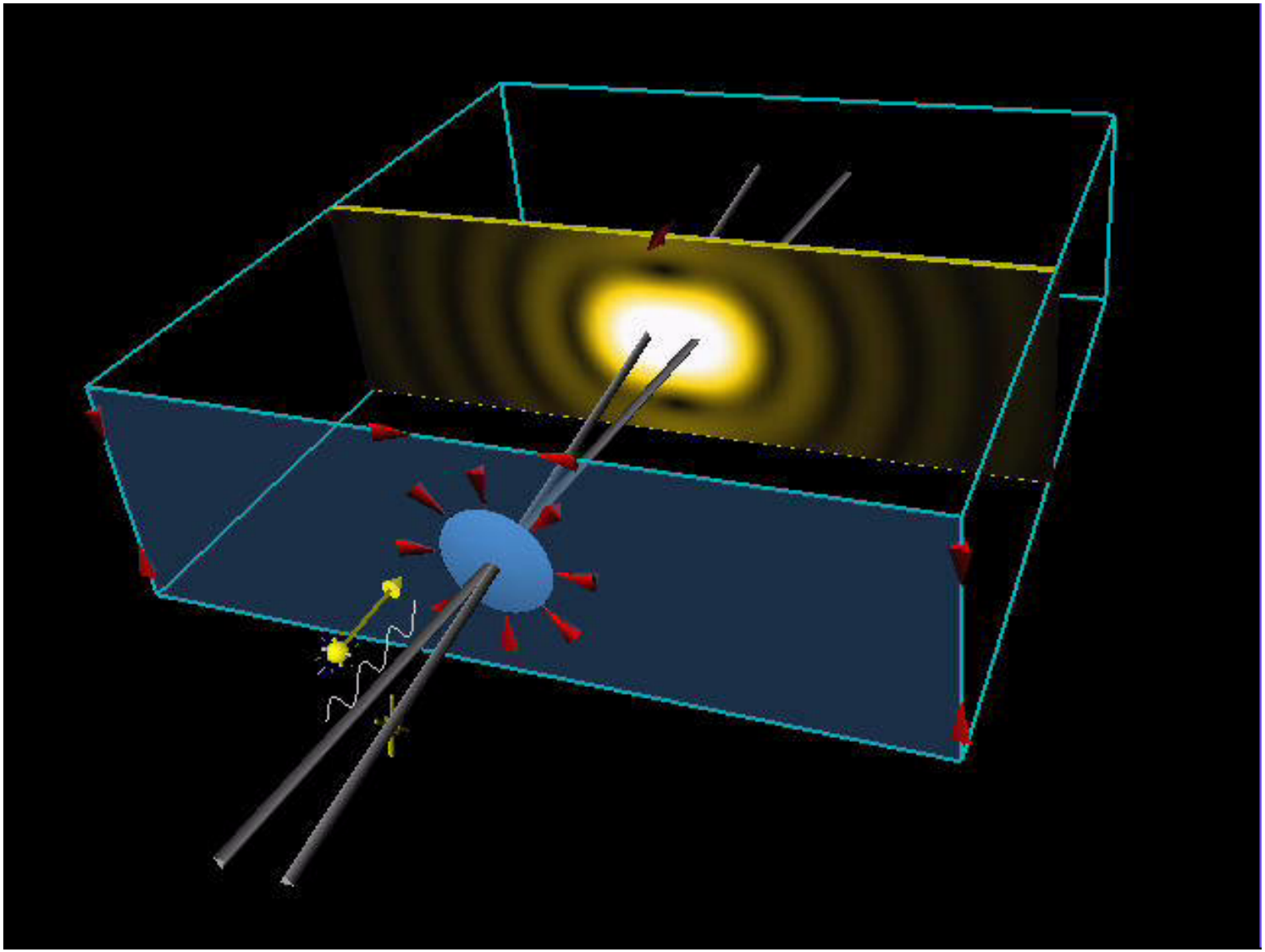

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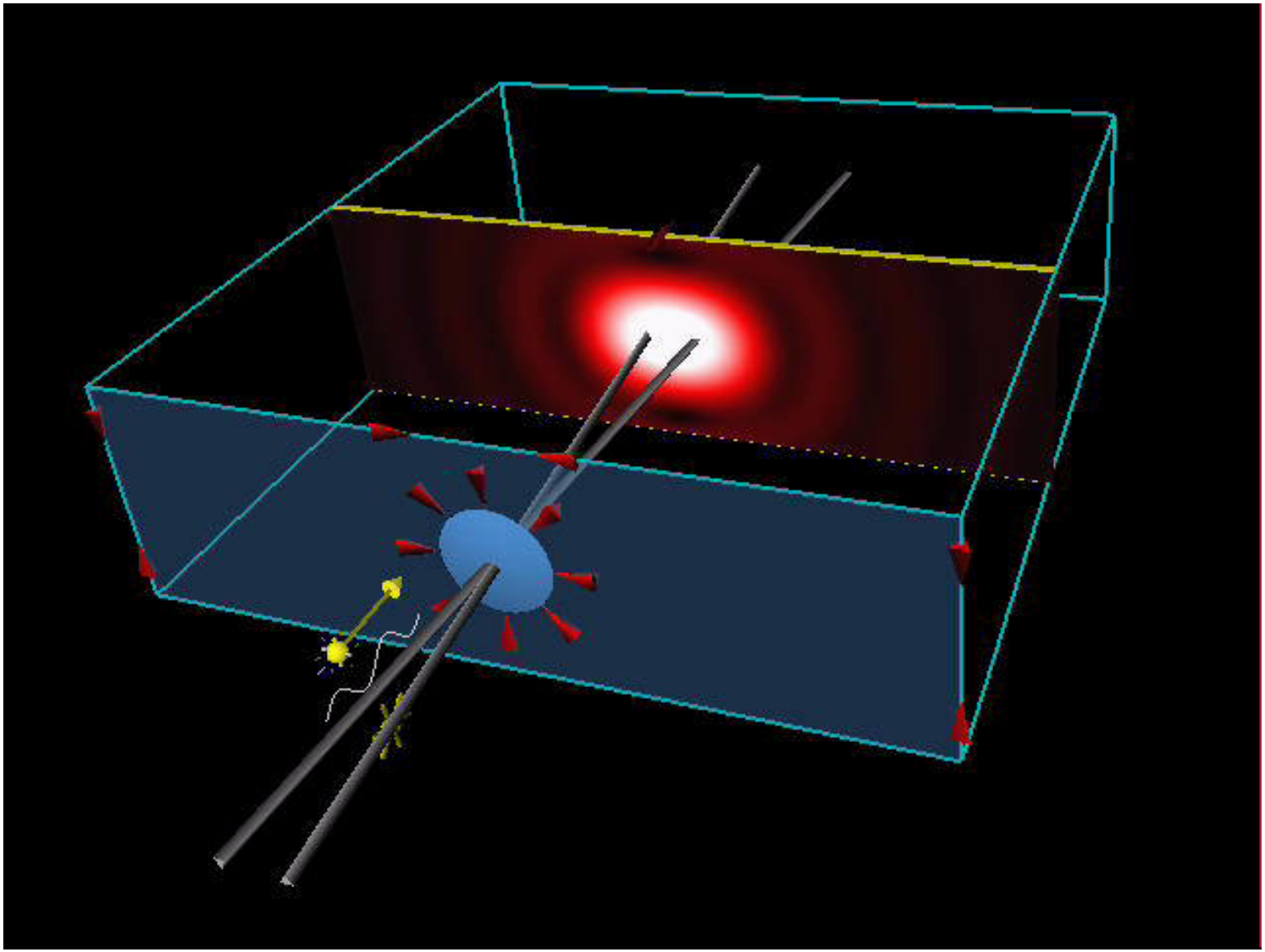
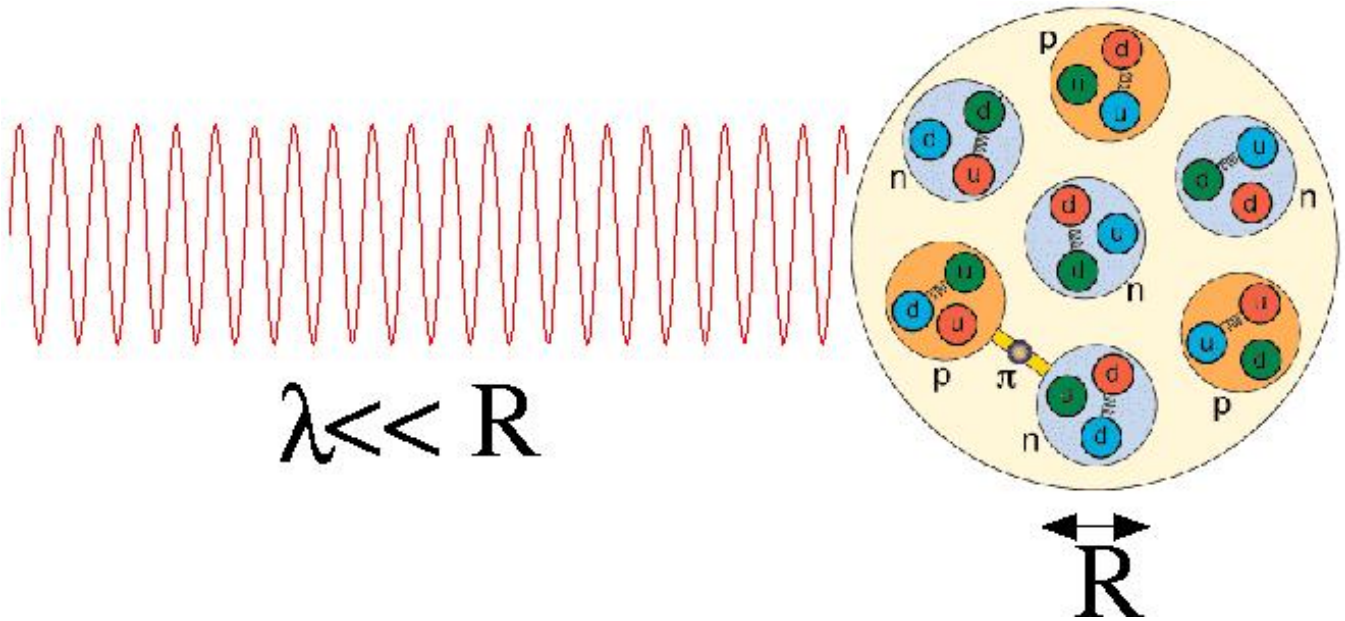


Principle of *any* effective low-energy description



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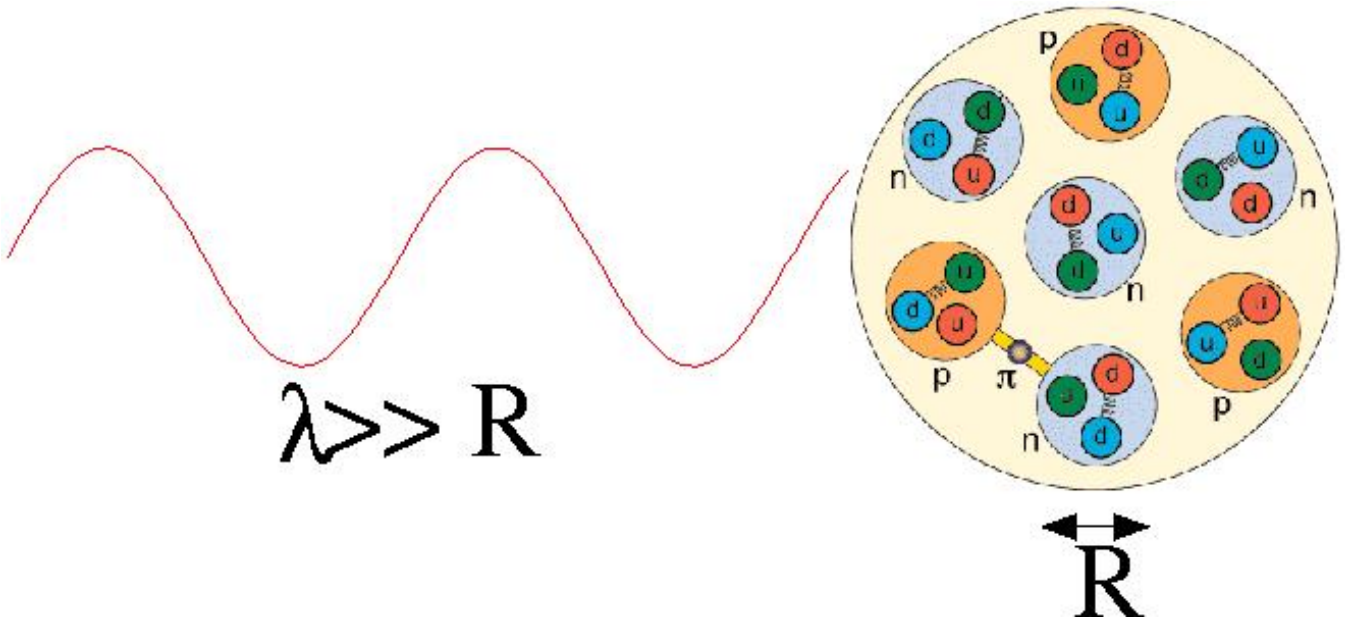

- If system is probed at low energies, fine details not resolved

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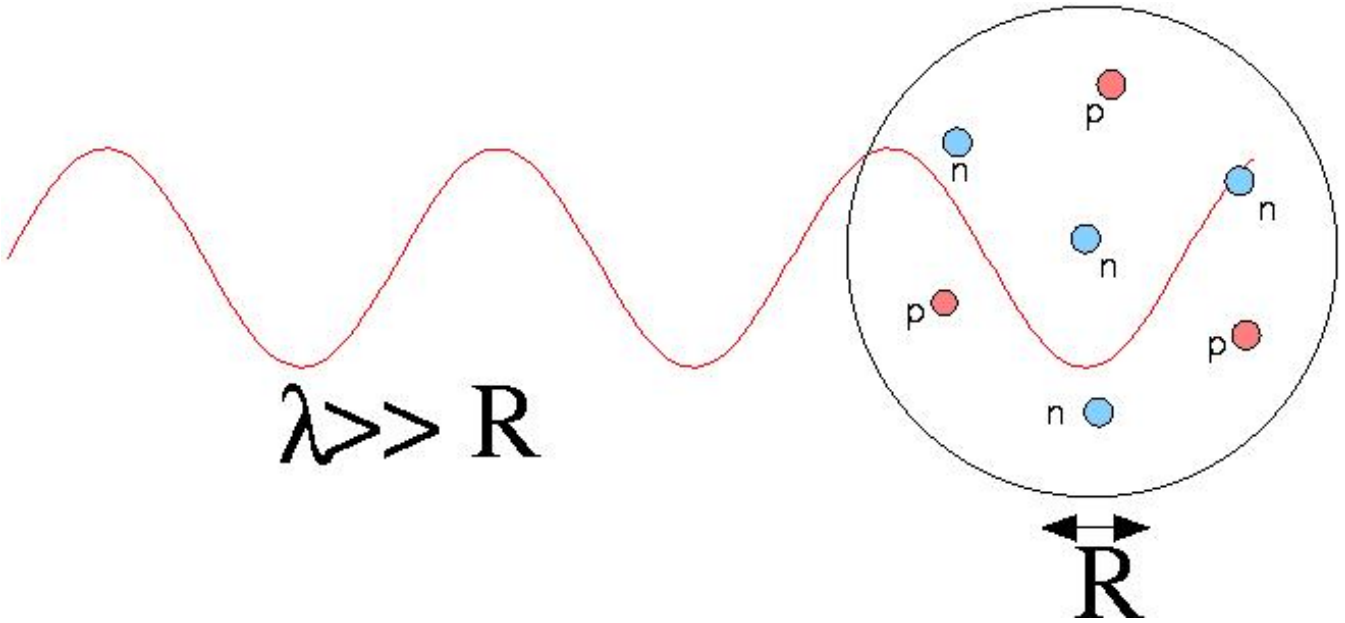

- If system is probed at low energies, fine details not resolved
  - Use low-energy variables for low-energy processes
  - Short-distance structure can be replaced by something simpler without distorting low-energy observables
  - Could be a model or systematic (e.g., effective field theory)
- *Physics interpretation can change with resolution!*

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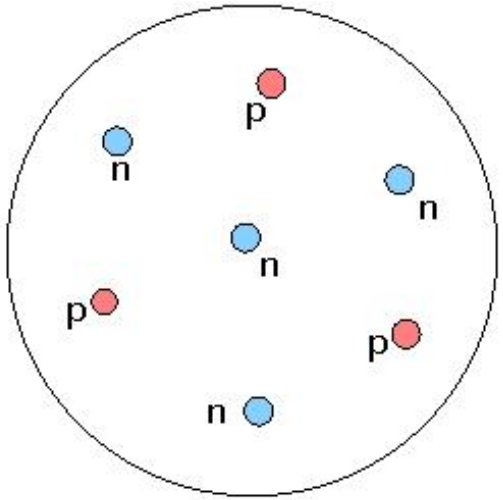

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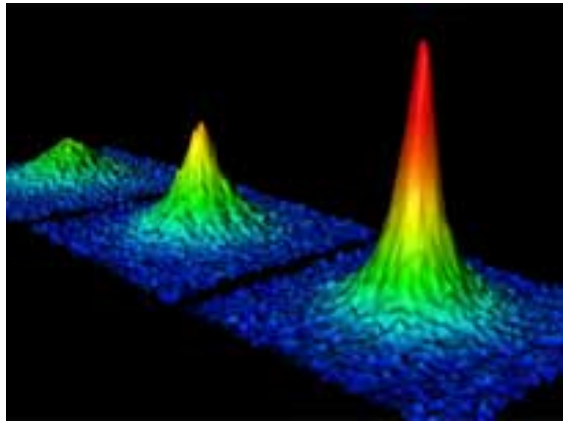
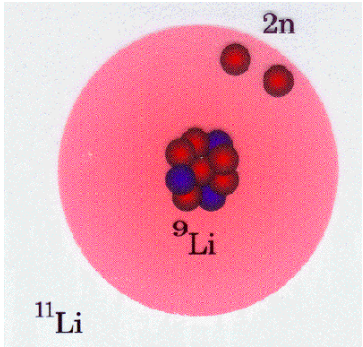
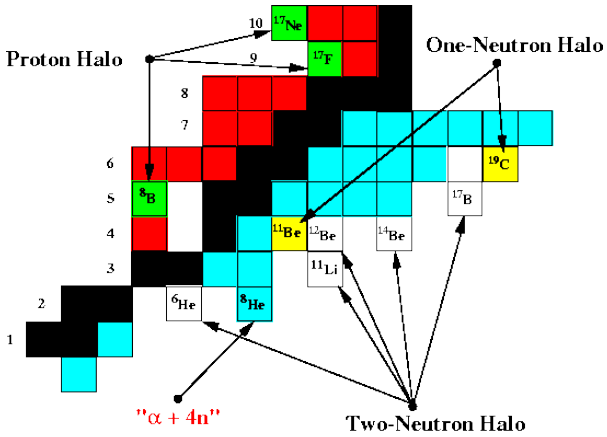
- *Physics interpretation can change with resolution!*
- Low density $\Leftrightarrow$ low interaction energy $\Leftrightarrow$ low resolution (?)

Nuclei at *very* low resolution

- If separation of scales is sufficient, then EFT with pointlike interactions is efficient (e.g., $kR \ll 1$)
- Universal properties (large a_s)
  - connect to cold atom physics
  - low-density neutron matter
  - e.g., Efimov physics
- Pionless EFT
  - e.g., $np \to d\gamma$ with $E_{\rm typ} \approx 0.02$–$0.2\,{\rm MeV}$
- Halo EFT
  - $B_{\rm valence} \ll B_{\rm core}, E_{ex}$
  - $n\alpha$-system (Bedaque et al.) or $\alpha\alpha$-system (Higa et al.) or ...

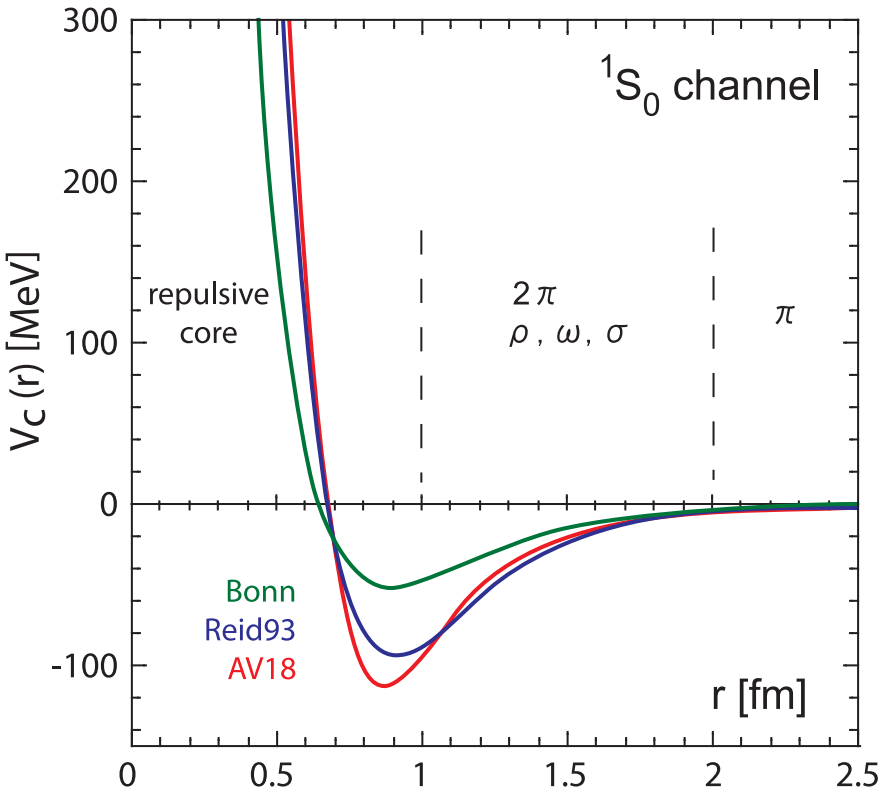


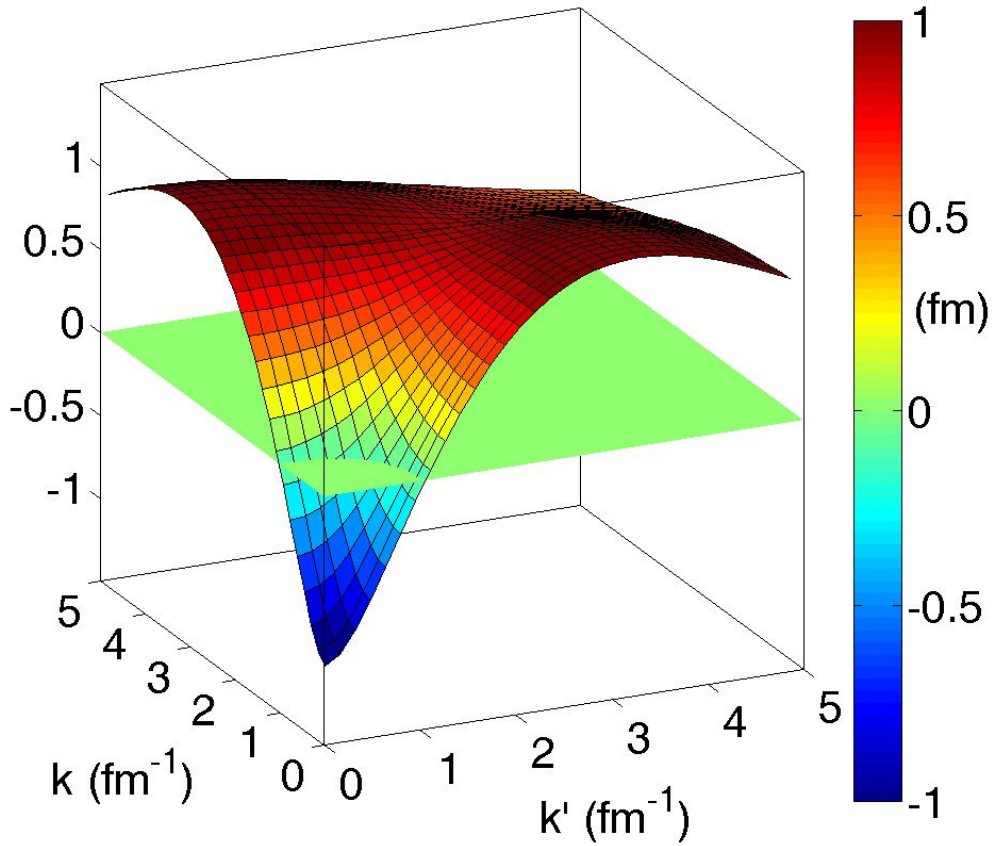




Here: focus on systems where pion exchange is resolved

Why is textbook nuclear physics so hard?





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

- Momentum units ($\hbar = c = 1$): typical relative momentum in large nucleus $\approx 1\,\text{fm}^{-1} \approx 200\,\text{MeV}$ but ...
- Repulsive core $\implies$ large high-k ($\geqslant 2\,\text{fm}^{-1}$) components

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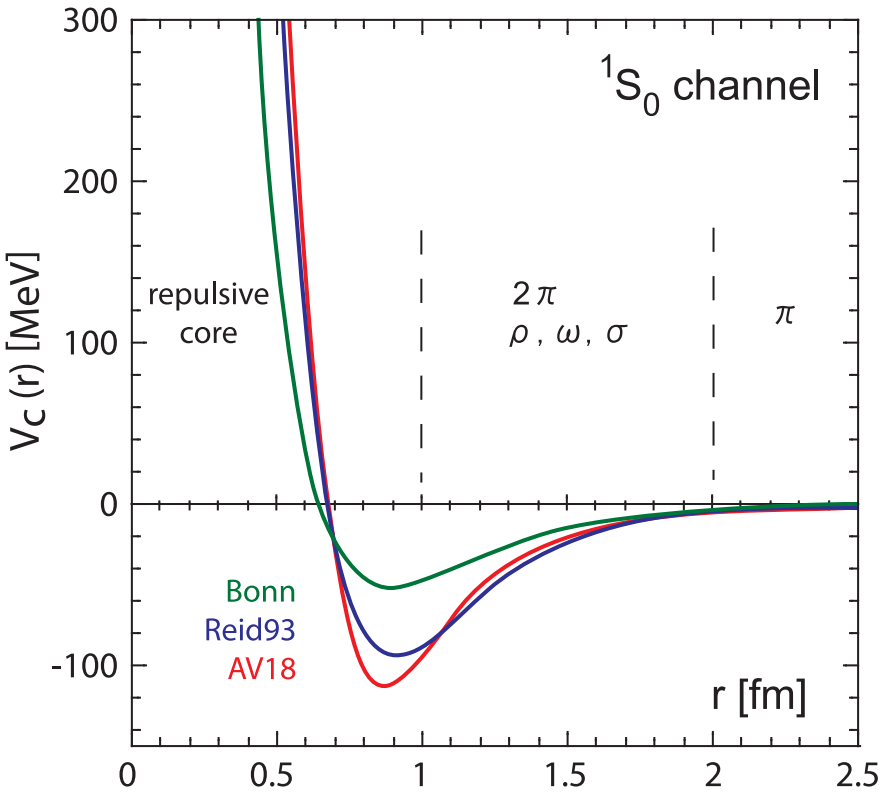

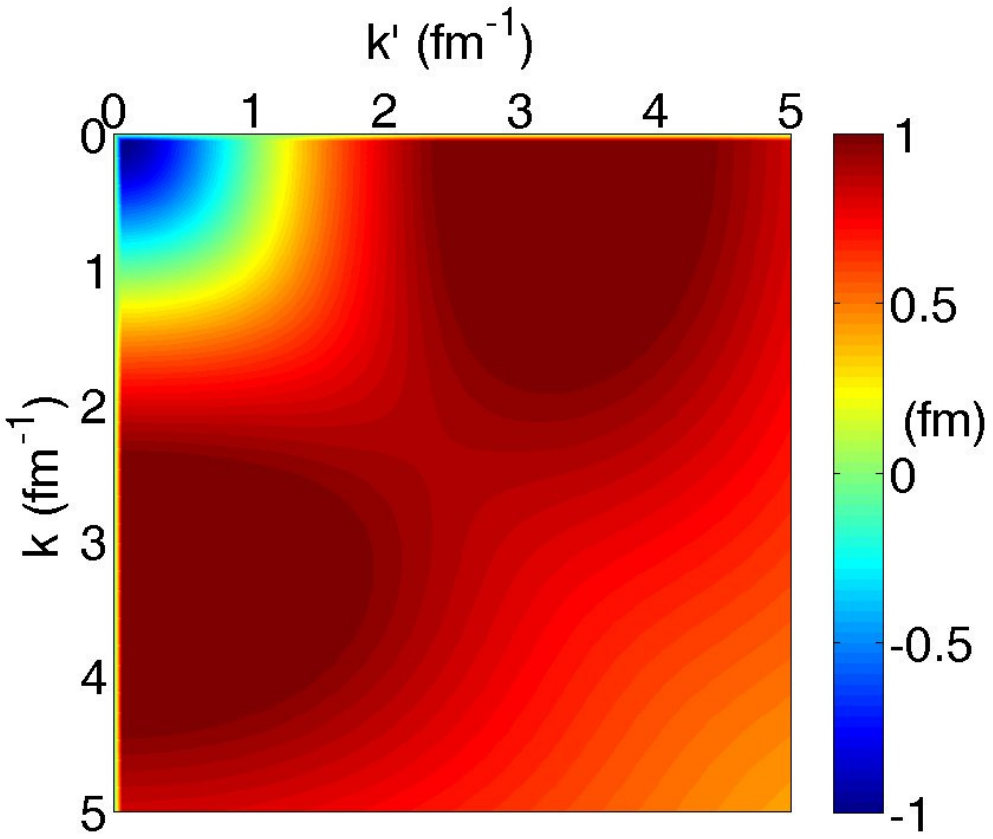

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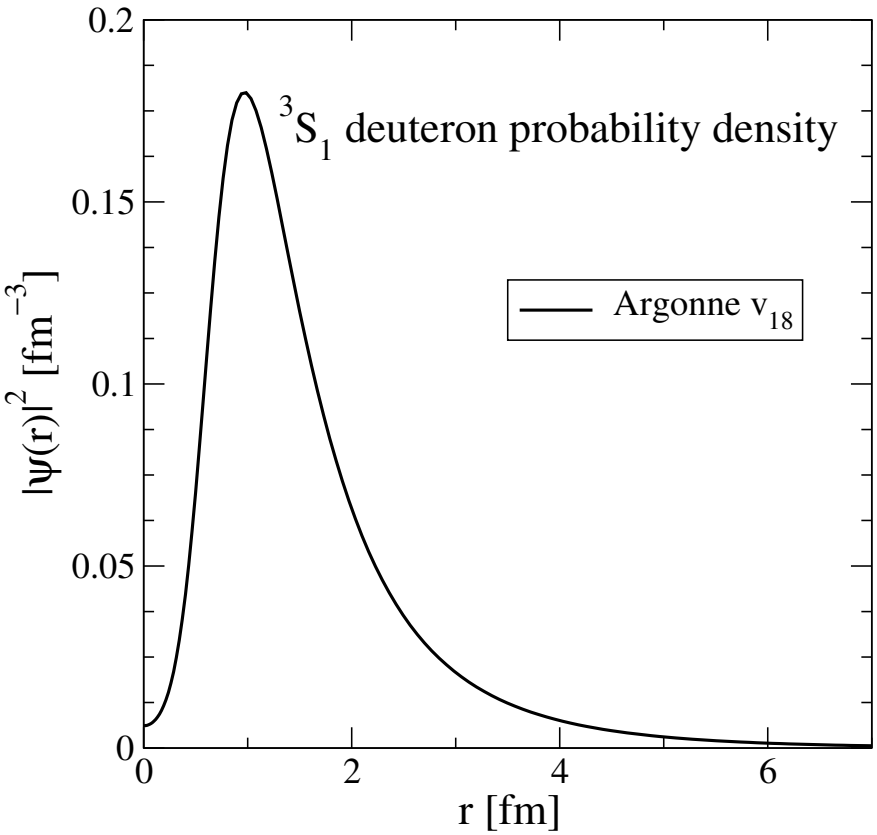
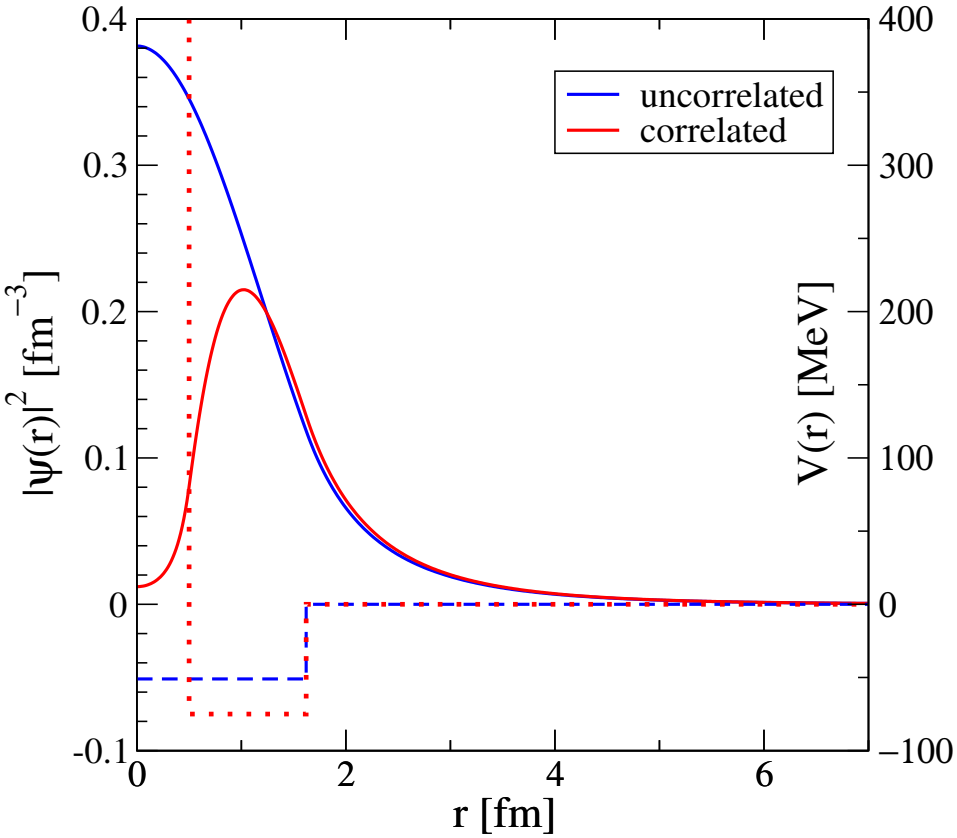
Consequences of a repulsive core

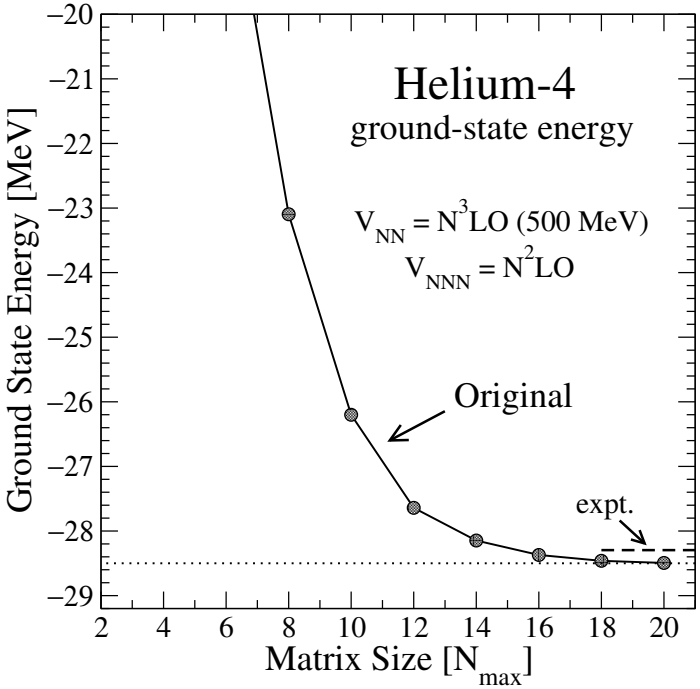


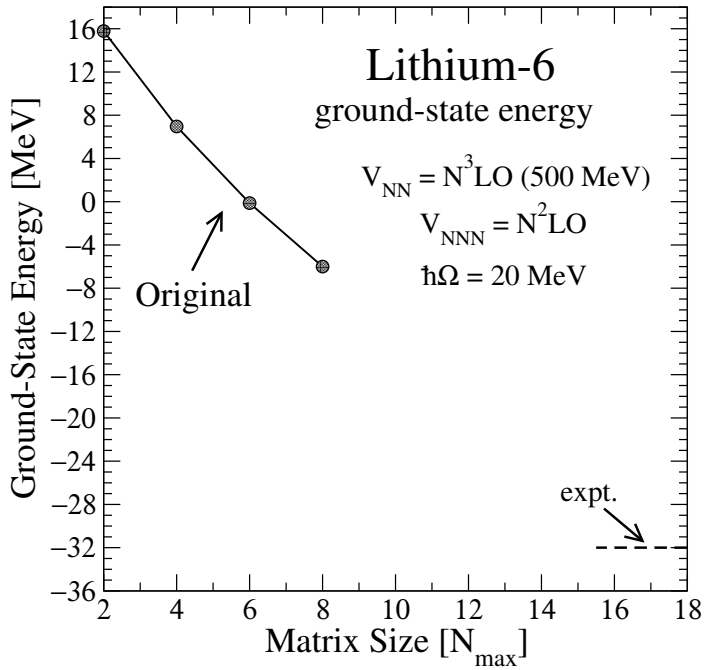


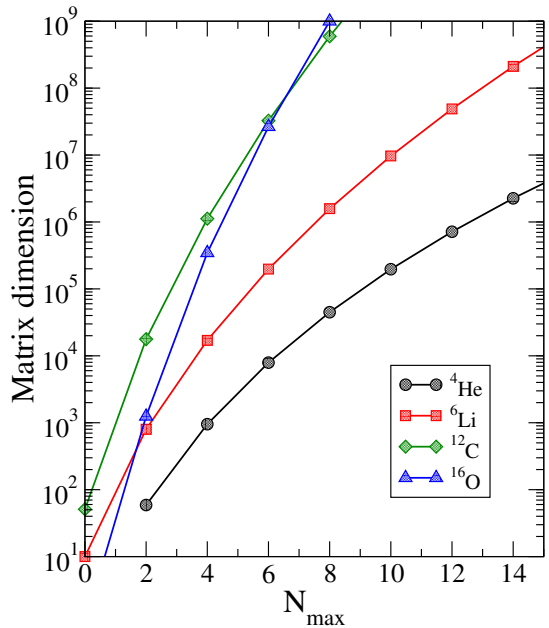
- Probability at short separations suppressed $\Longrightarrow$ “correlations”
- Short-distance structure $\Leftrightarrow$ high-momentum components
- Greatly complicates expansion of many-body wave functions

Many short wavelengths $\Longrightarrow$ Large matrices

- Harmonic oscillator basis with $N_{\max}$ shells for excitations
- Graphs show convergence for *soft* chiral EFT potential (although not at optimal $\hbar\Omega$ for ^{6}Li)

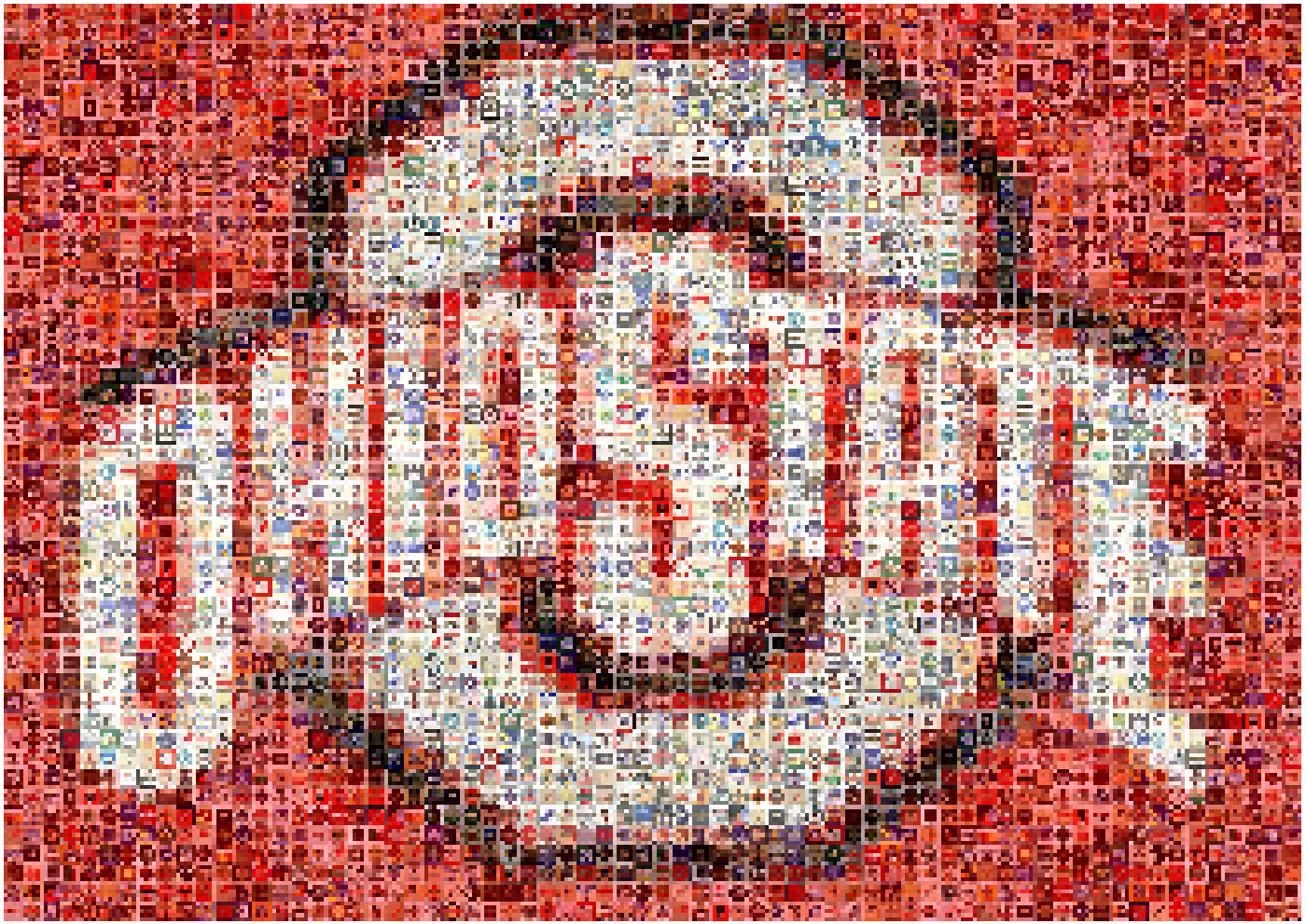






- Factorial growth of basis with $A \Longrightarrow$ limits calculations
- Too much resolution from potential $\Longrightarrow$ mismatch of scales

What if your theory has too much resolution?



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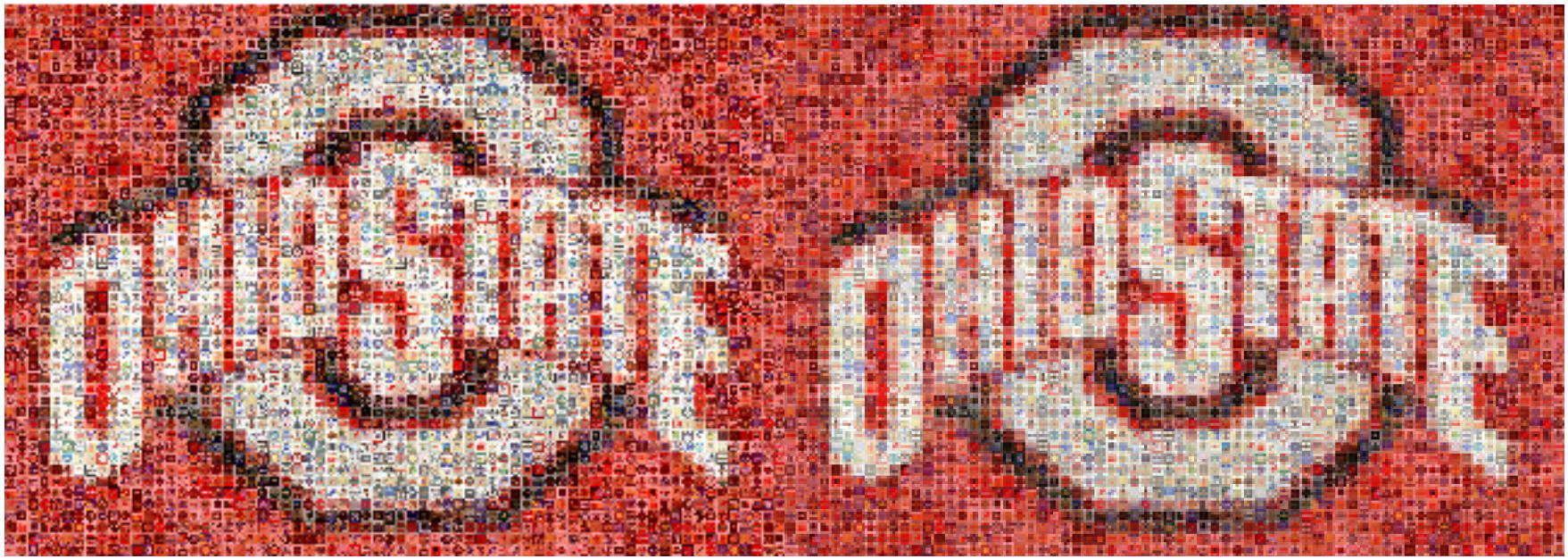
Claim: Nuclear physics with textbook $V(\mathbf{r})$ is like using beer coasters!

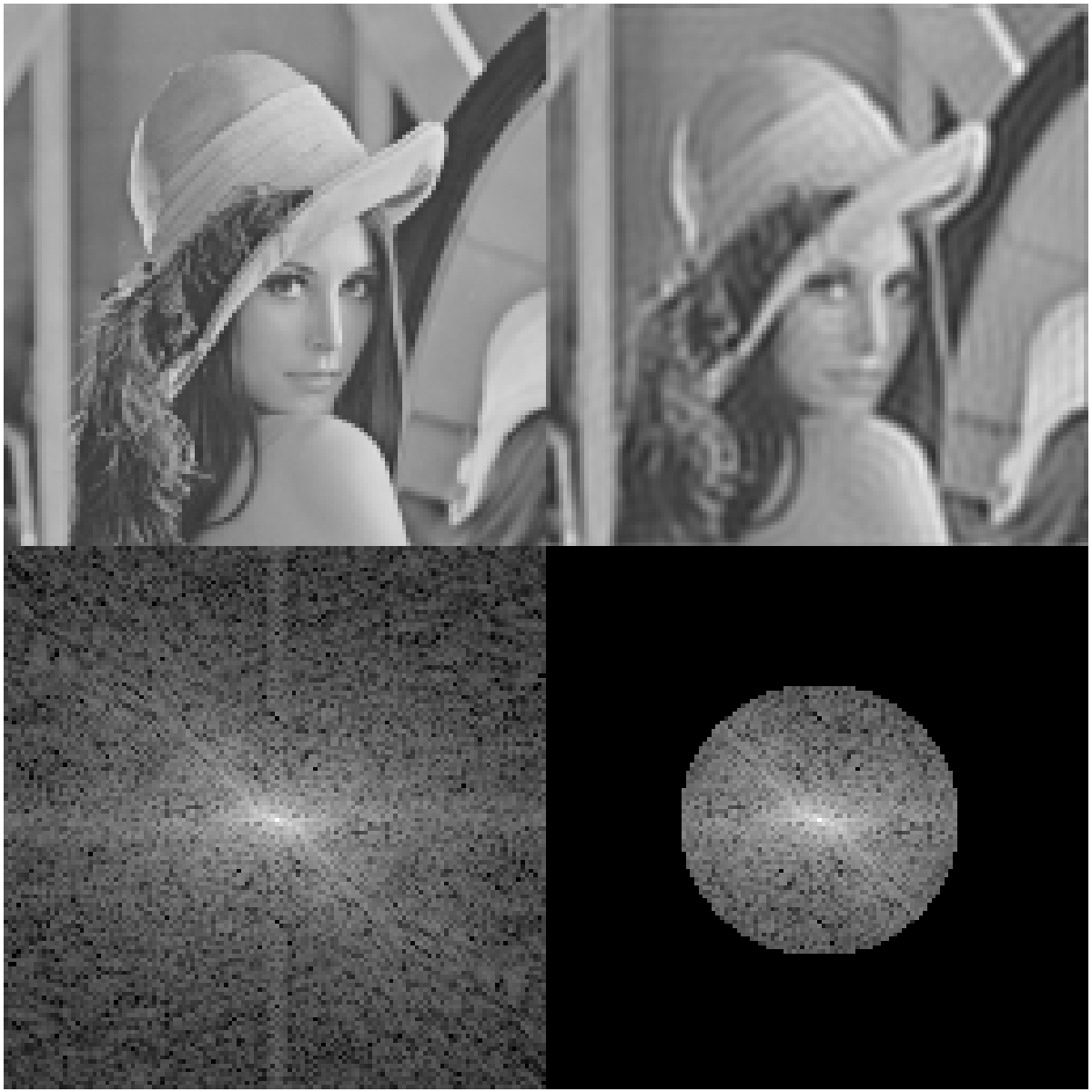
Less painful to use a low-resolution version!

High resolution Low resolution



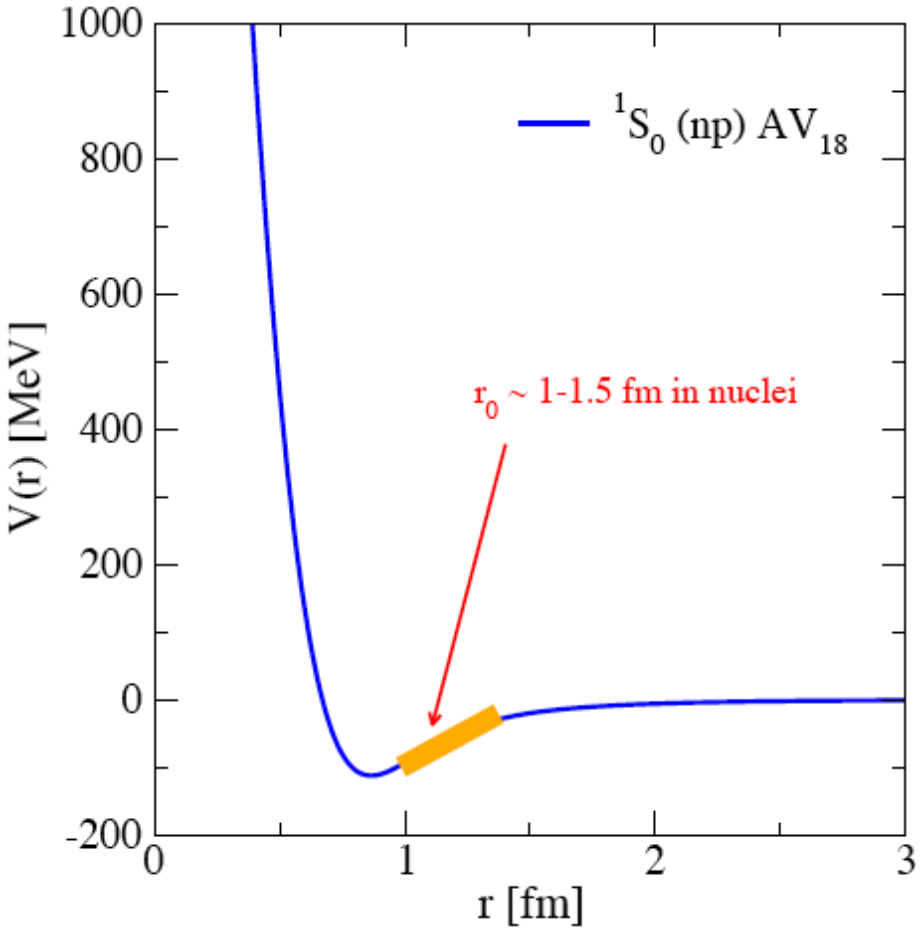
- Can greatly reduce storage without distorting message
- Lower resolution here by “block spinning”
- Alternative: apply a low-pass filter

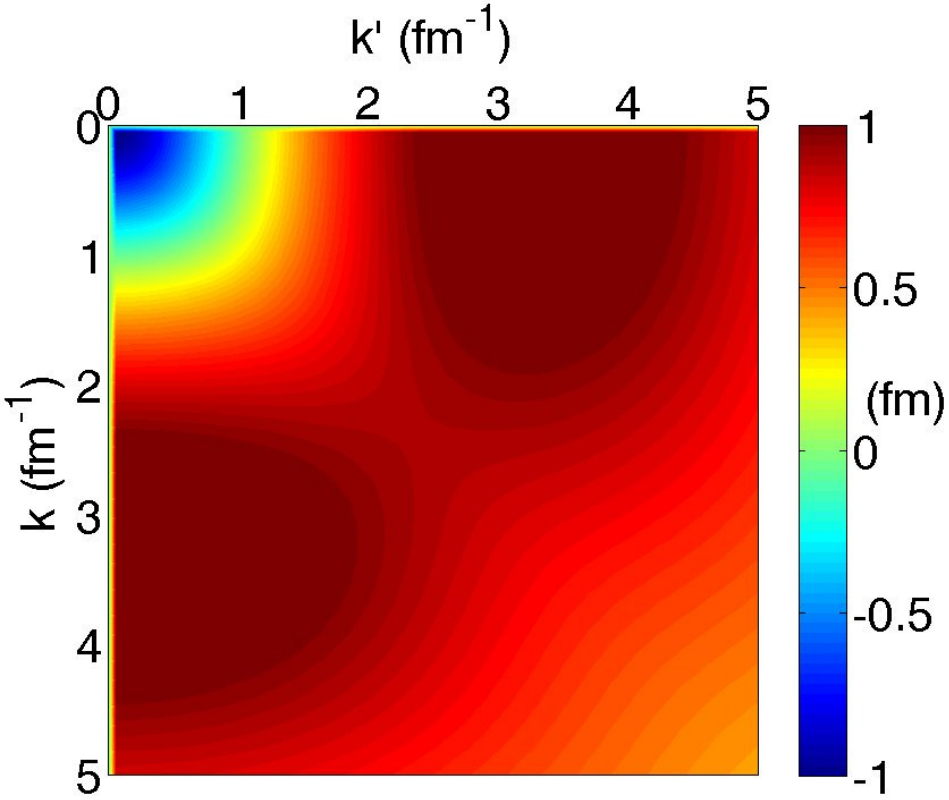
Low-pass filter on an image



- Much less information needed
- Long-wavelength info is preserved

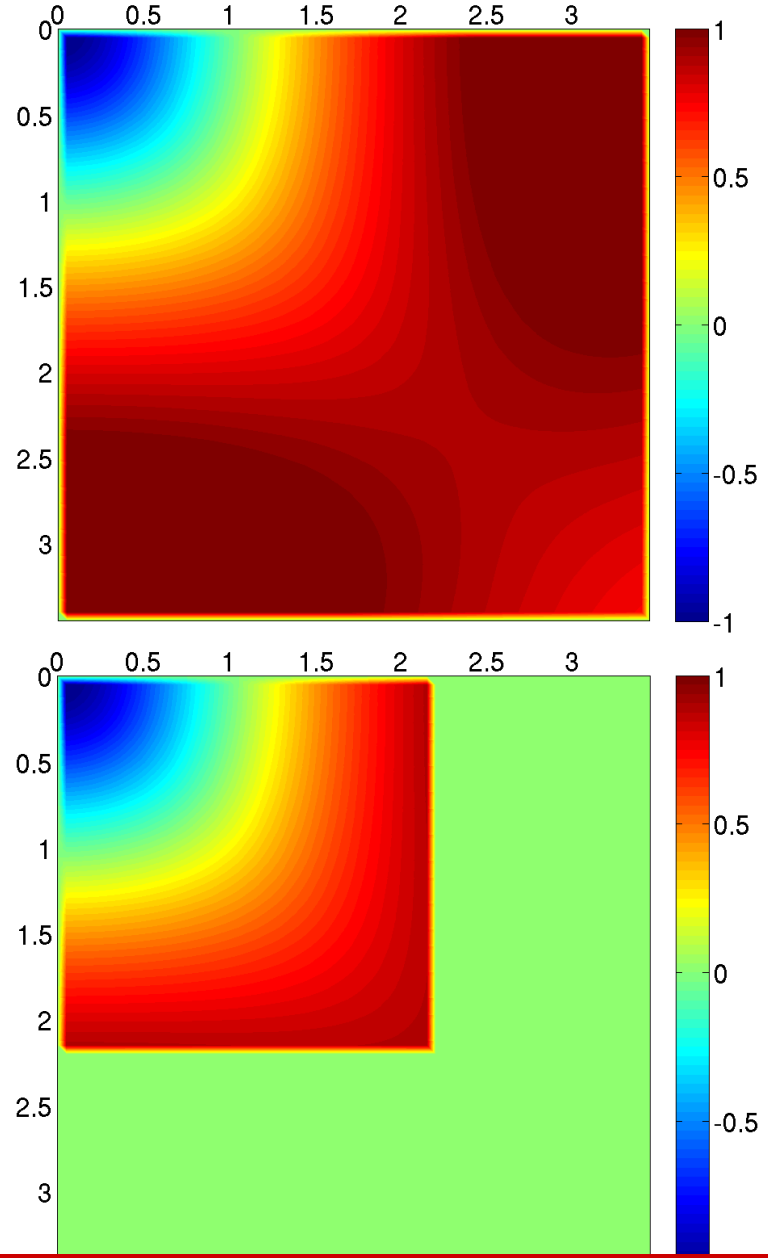
Try a low-pass filter on $V(r)$

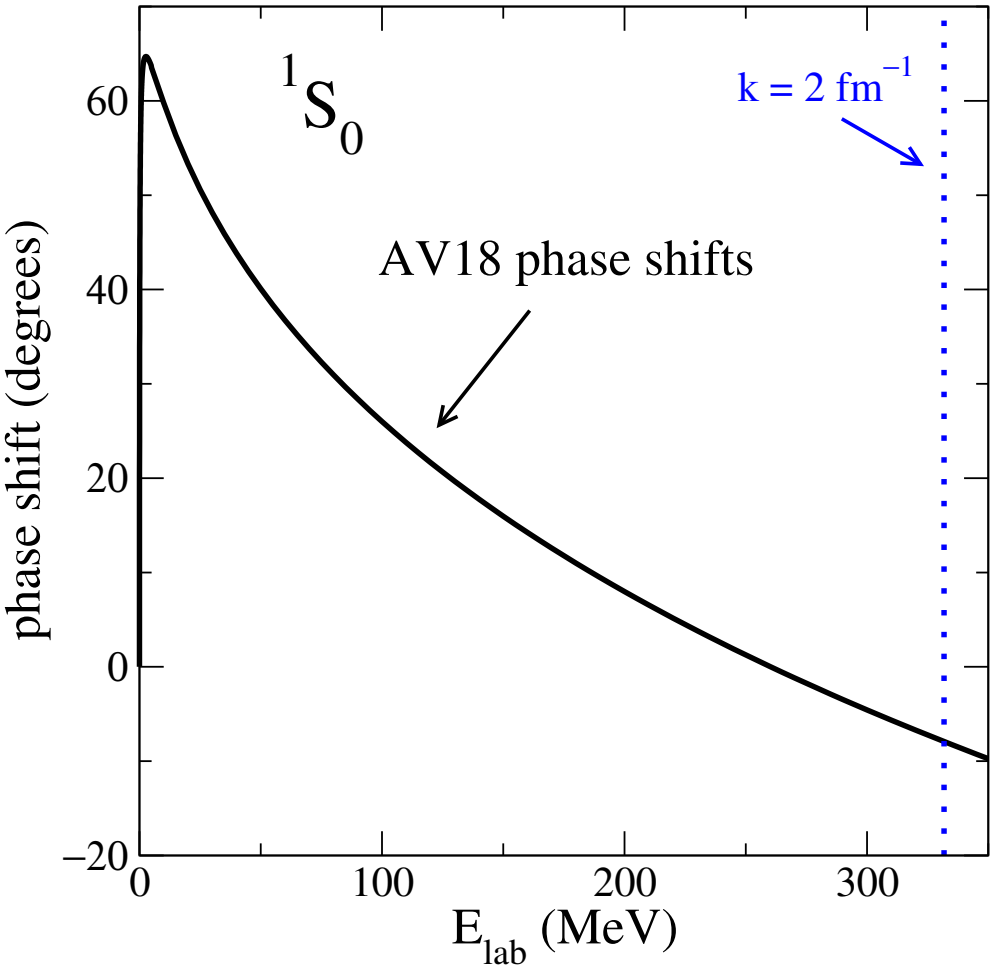




$\Longrightarrow$ Set to zero high momentum ($k \geqslant 2\,\mathrm{fm}^{-1}$) matrix elements and see the effect on low-energy observables

Effect of low-pass filter on observables





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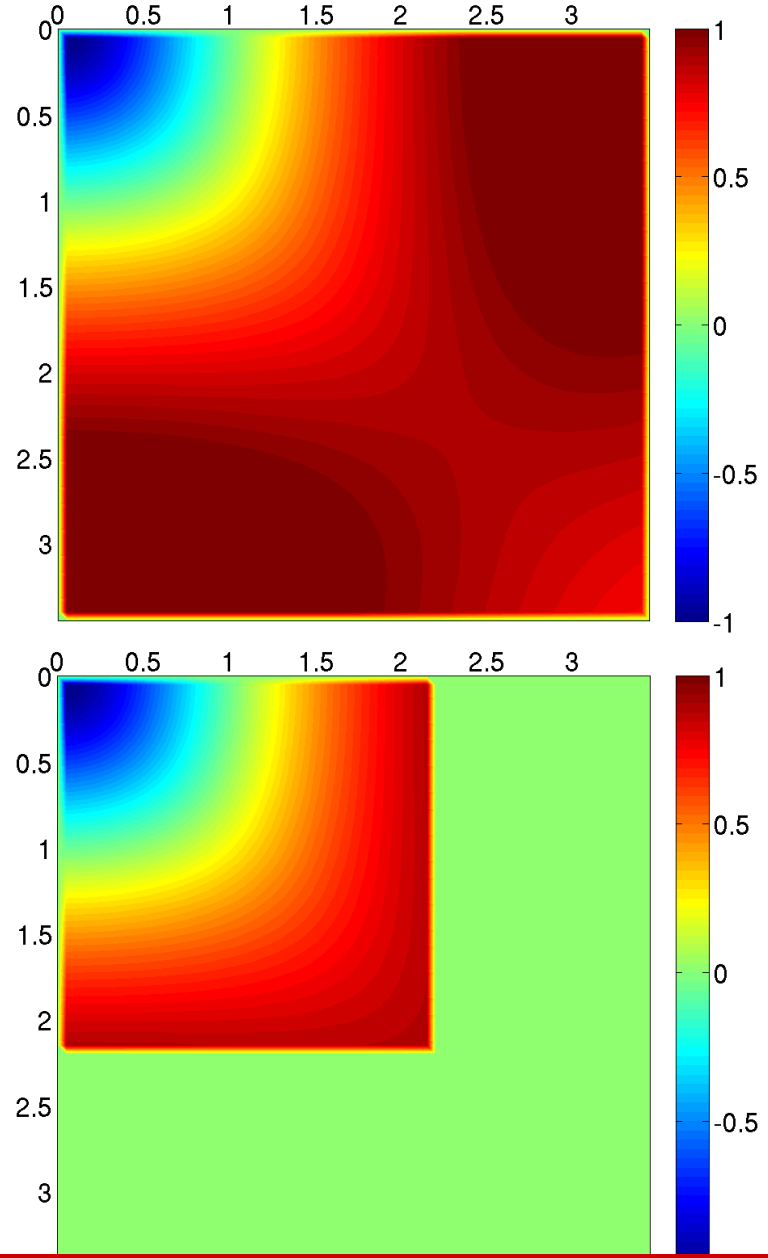
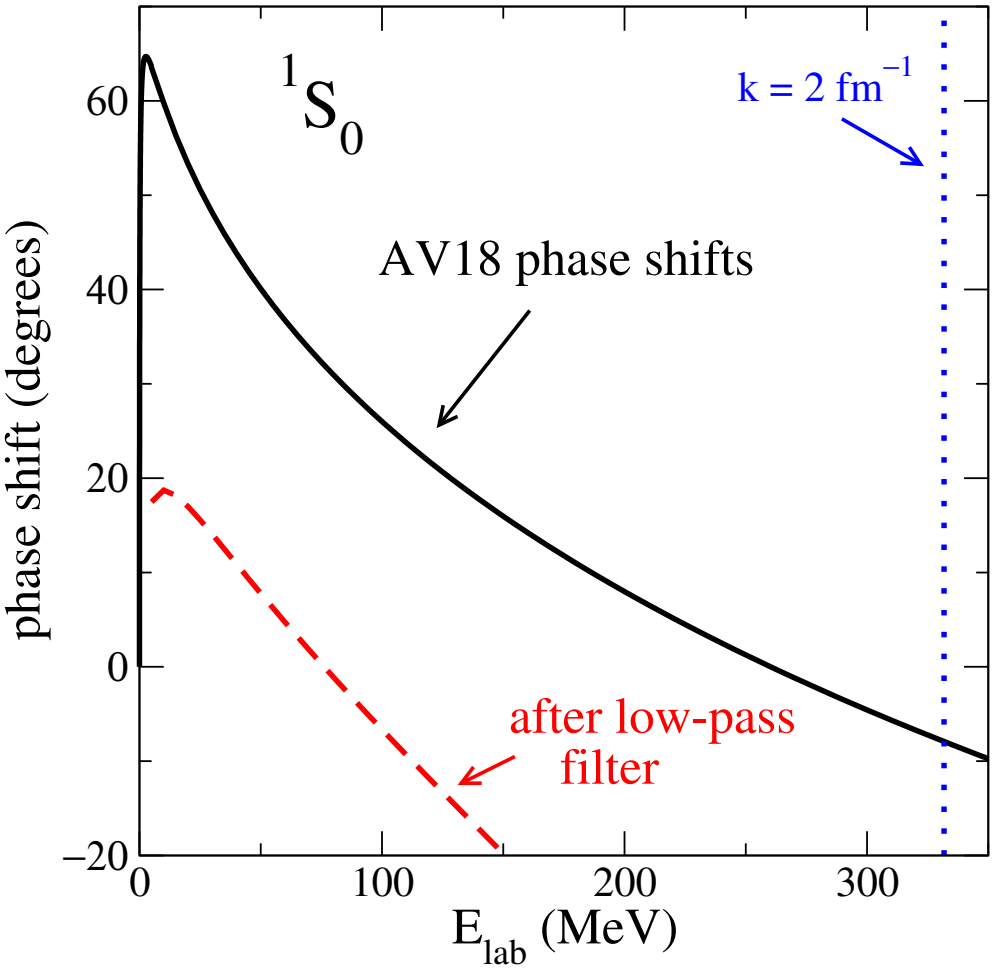




Why did our low-pass filter fail?

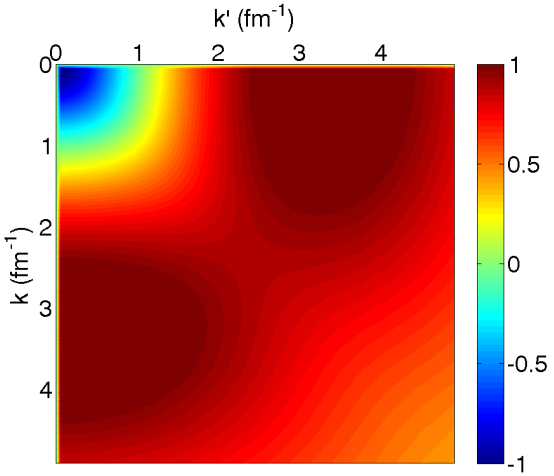
- Basic problem: low k and high k are coupled (mismatched dof's!)
- E.g., perturbation theory for (tangent of) phase shift:

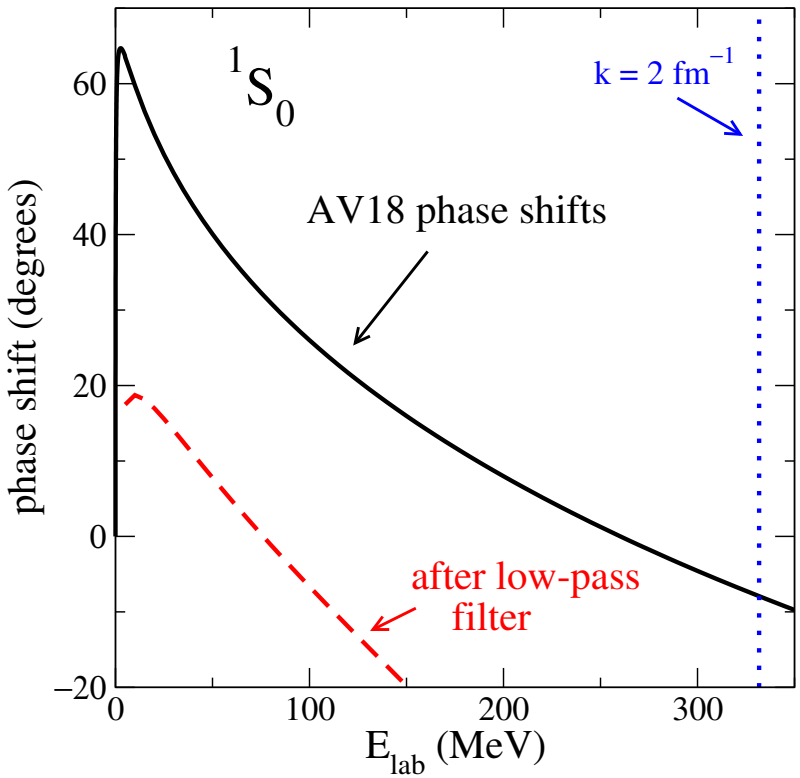
$$\langle k|V|k\rangle + \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{(k^2 - k'^2)/m} + \cdots$$

- 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





S. Weinberg on the Renormalization Group

- From “Why the Renormalization Group is a good thing”

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- Universality in critical phenomena
  - Filter out short-distance degrees of freedom
- Simplifying calculations of nuclear structure/reactions
  - Make nuclear physics look more like quantum chemistry!
  - Like other RG applications, gains can seem like magic
- RG violates the First Law of Progress in Theoretical Physics
  Conservation of Information: "You will get nowhere by churning equations" $\Longrightarrow$ *but with RG you do!*

Outline

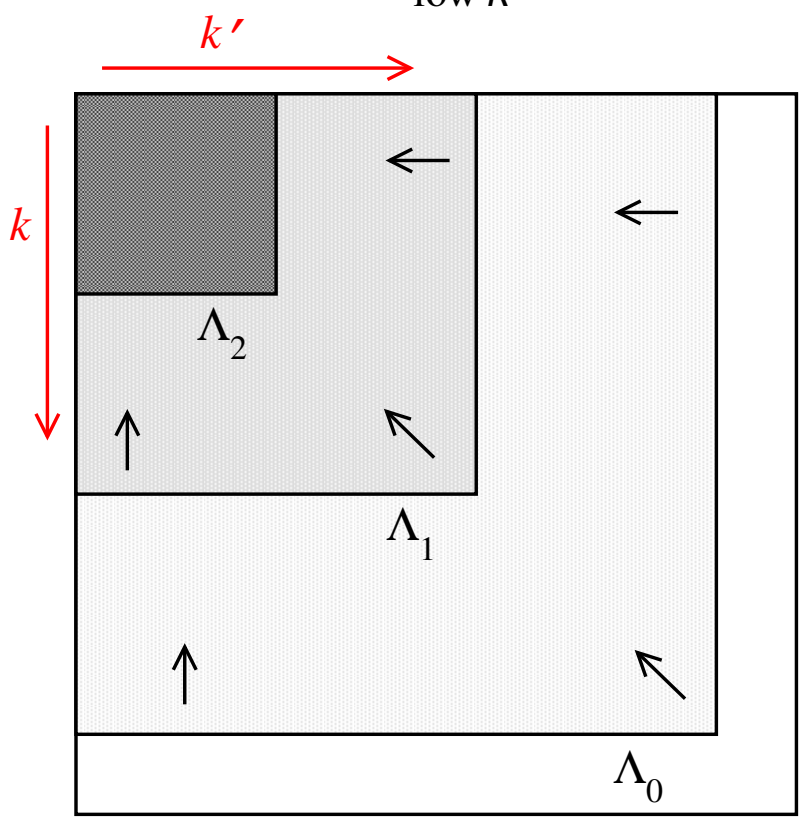
Overview: Goals of low-energy nuclear physics

Lowering the resolution with RG

Implications of low resolution for nuclear calculations

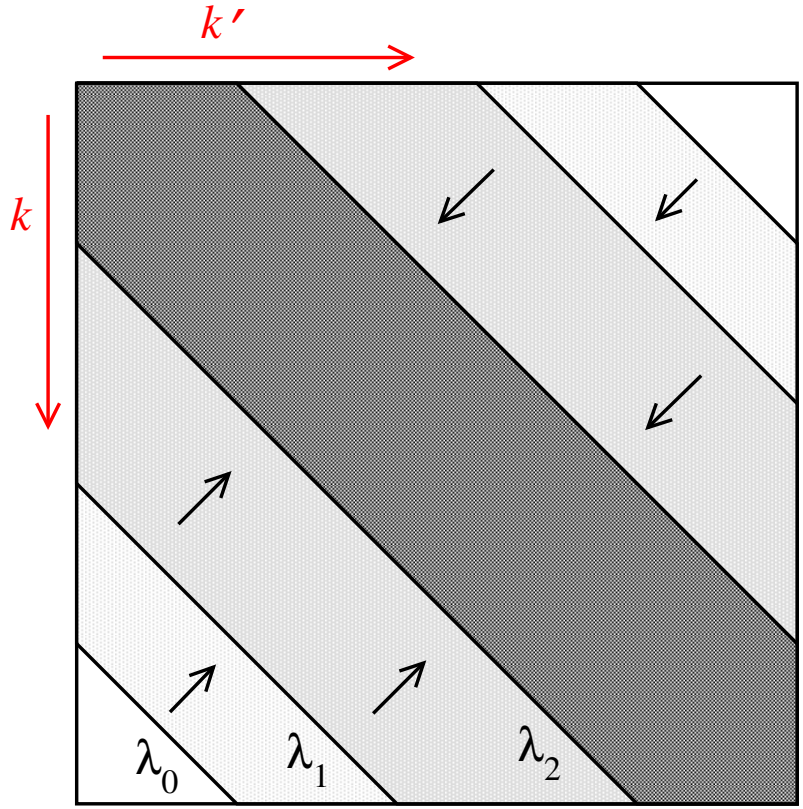
Two ways to decouple with RG equations

"$V_{\text{low } k}$"



- Lower a cutoff Λ_i in k, k', e.g., demand $dT(k, k'; k^2)/d\Lambda = 0$

Similarity RG

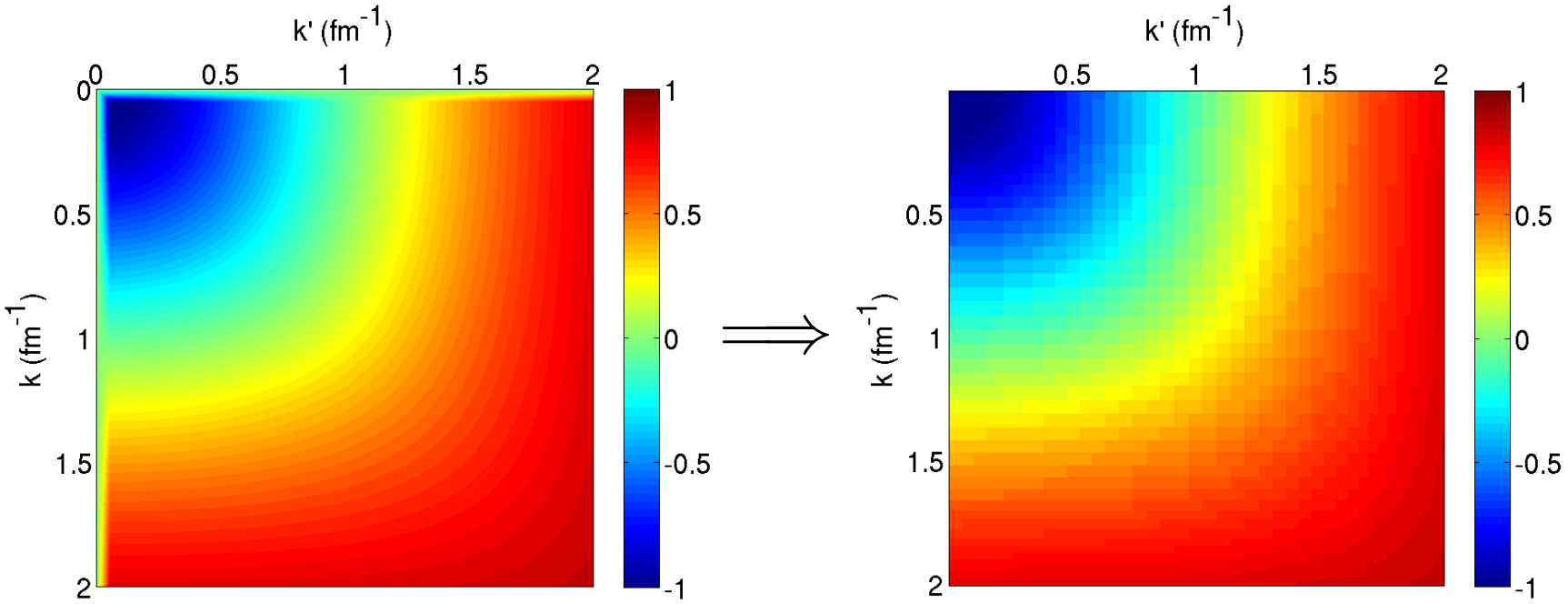


- Drive the Hamiltonian toward diagonal with "flow equation" [Wegner; Glazek/Wilson (1990's)]

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

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.,

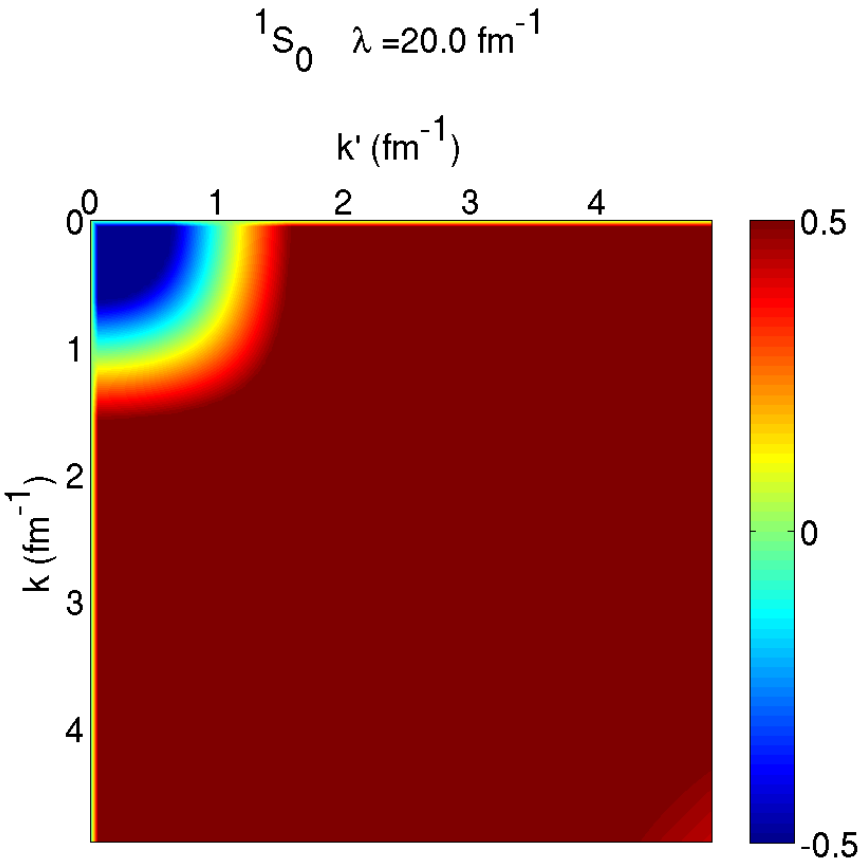
$$\langle k|V|k\rangle + \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{(k^2 - k'^2)/m} + \cdots \Longrightarrow V_{ii} + \sum_j V_{ij} V_{ji} \frac{1}{(k_i^2 - k_j^2)/m} + \cdots$$

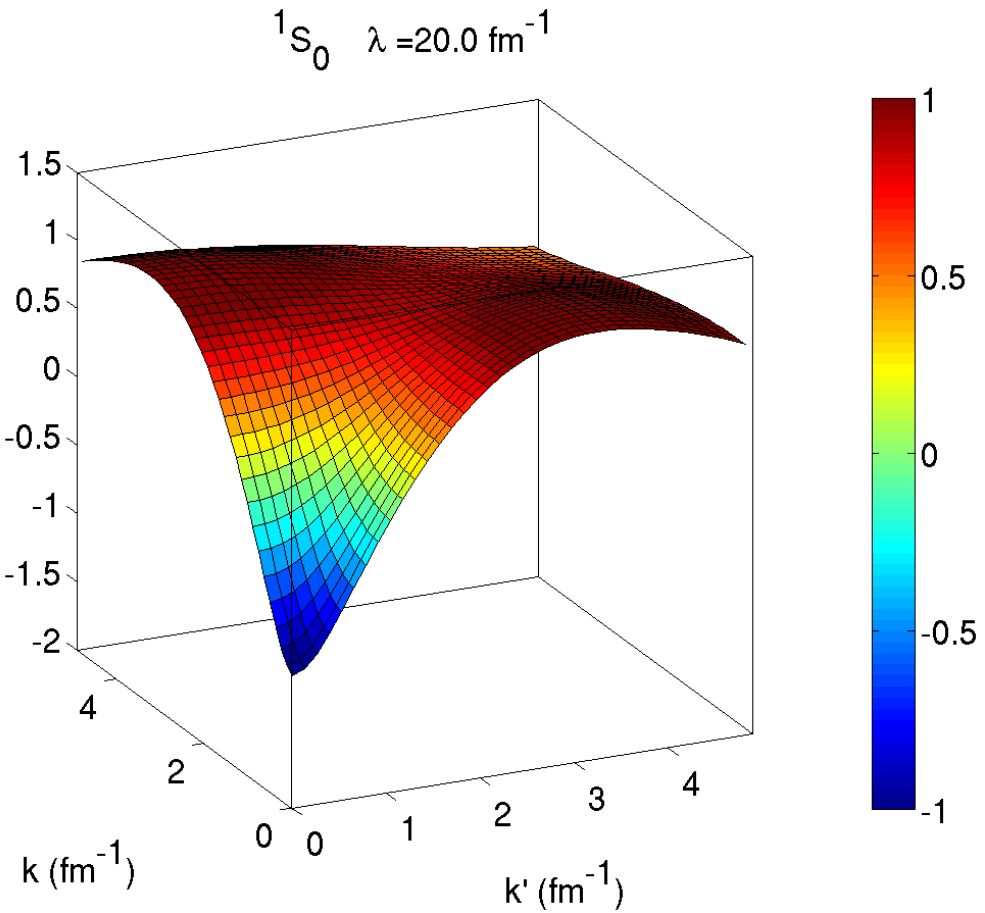
- 100×100 resolution is sufficient for two-body potential

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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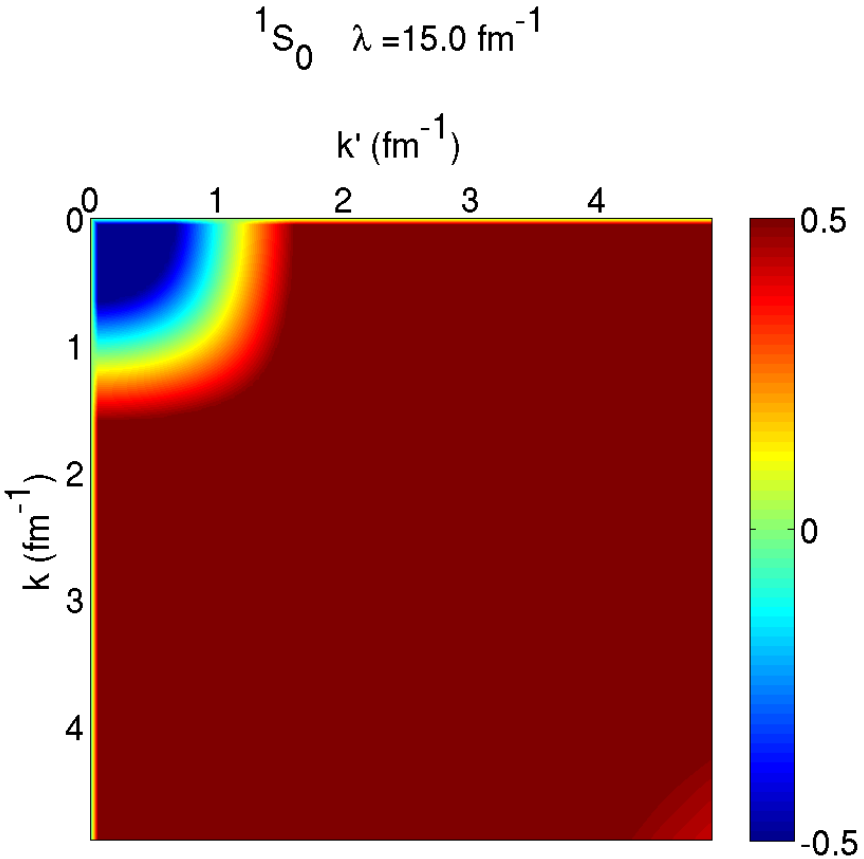

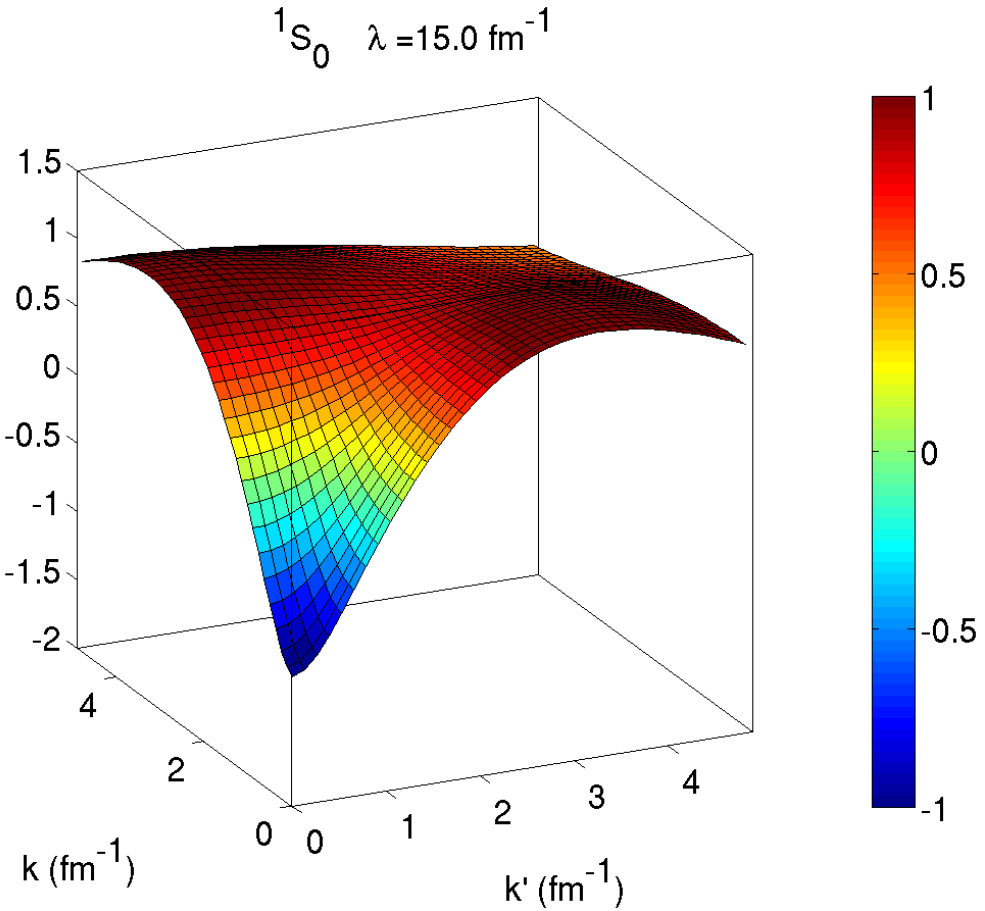

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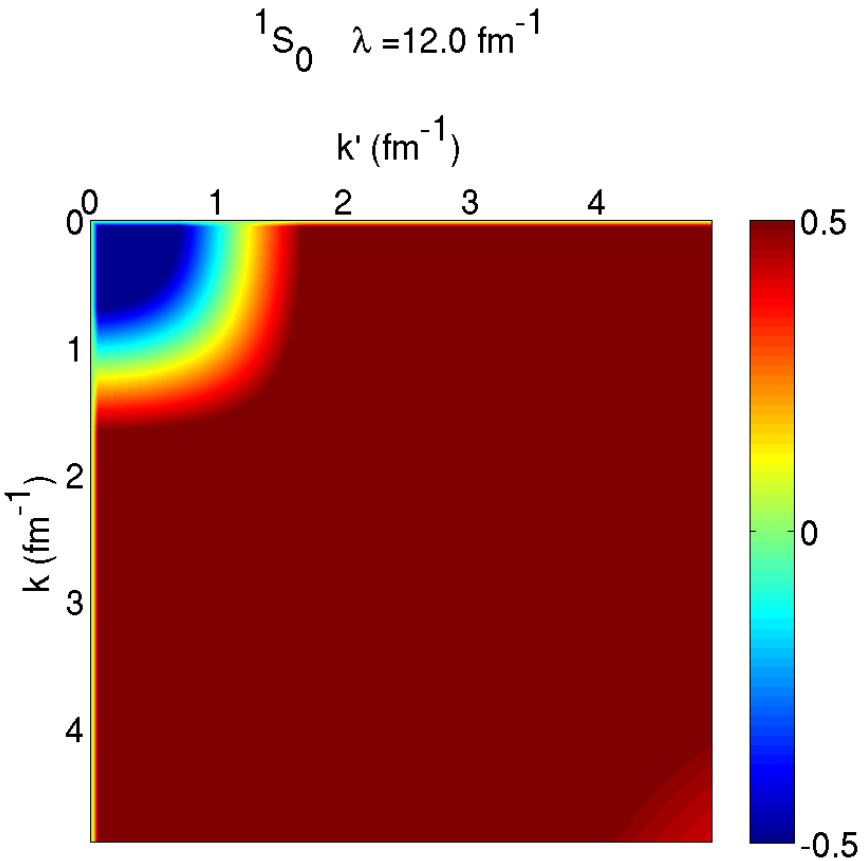

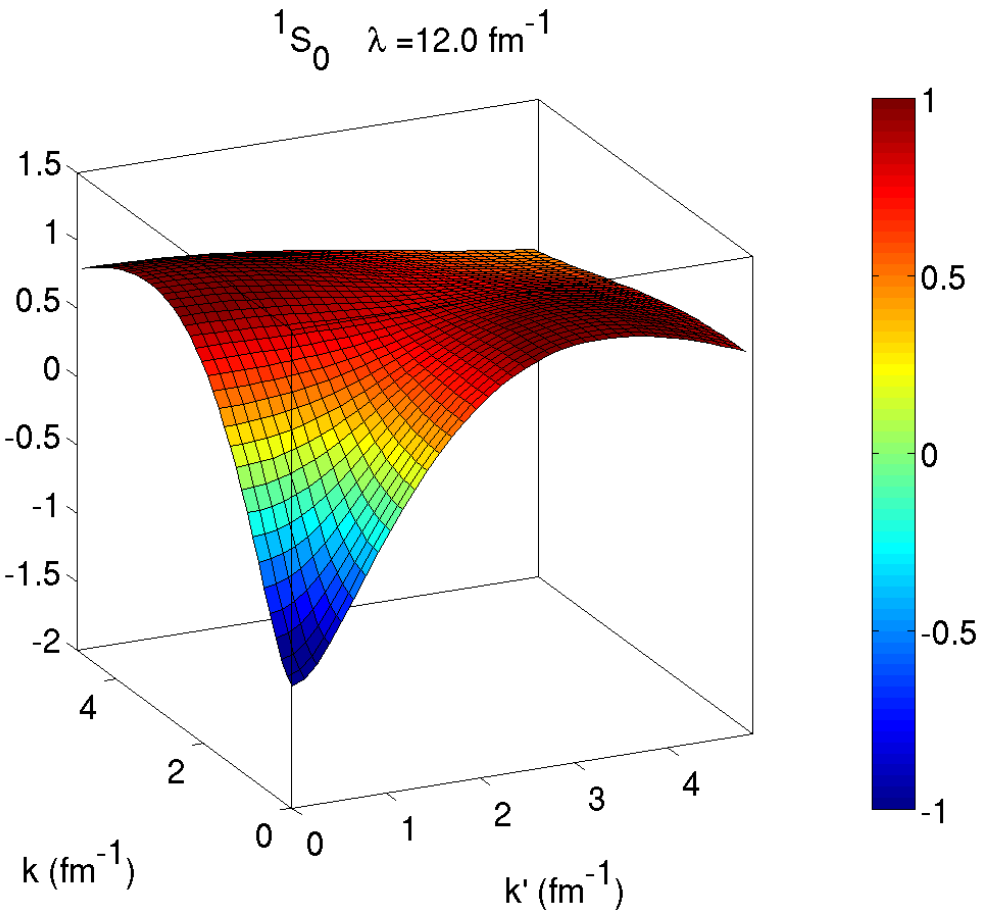

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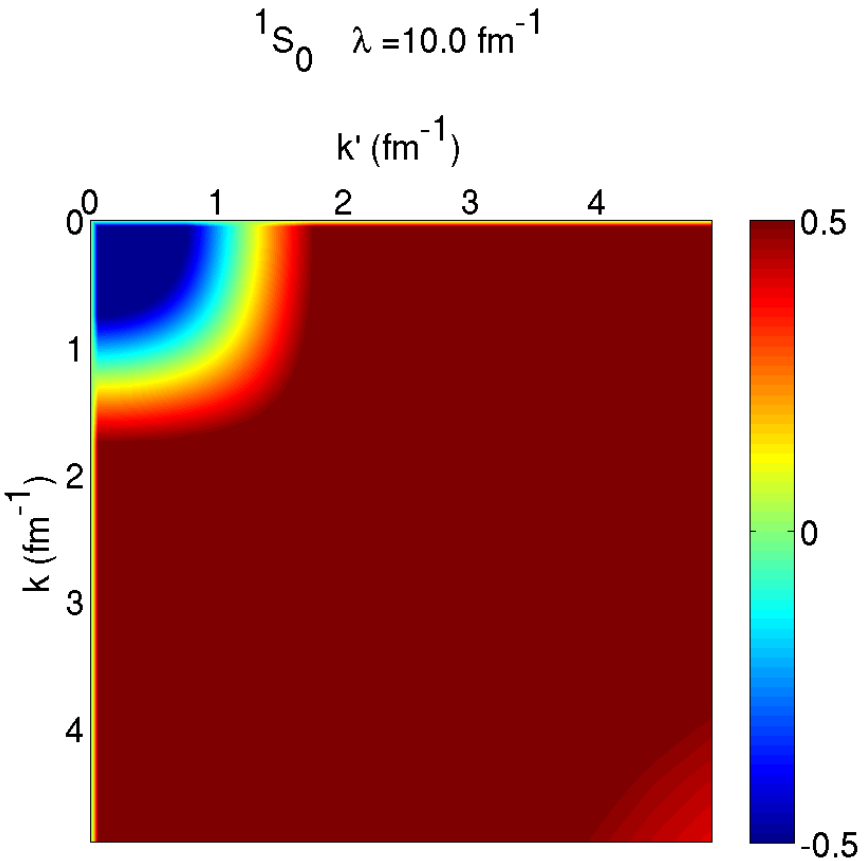

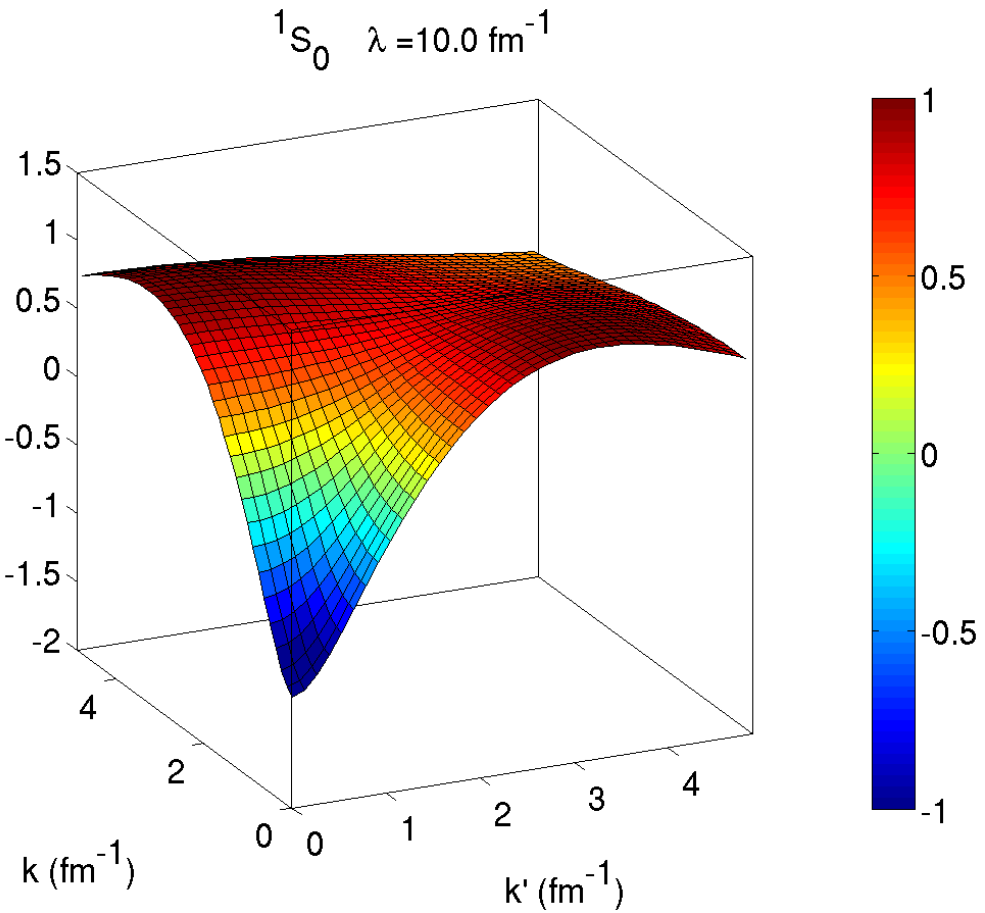

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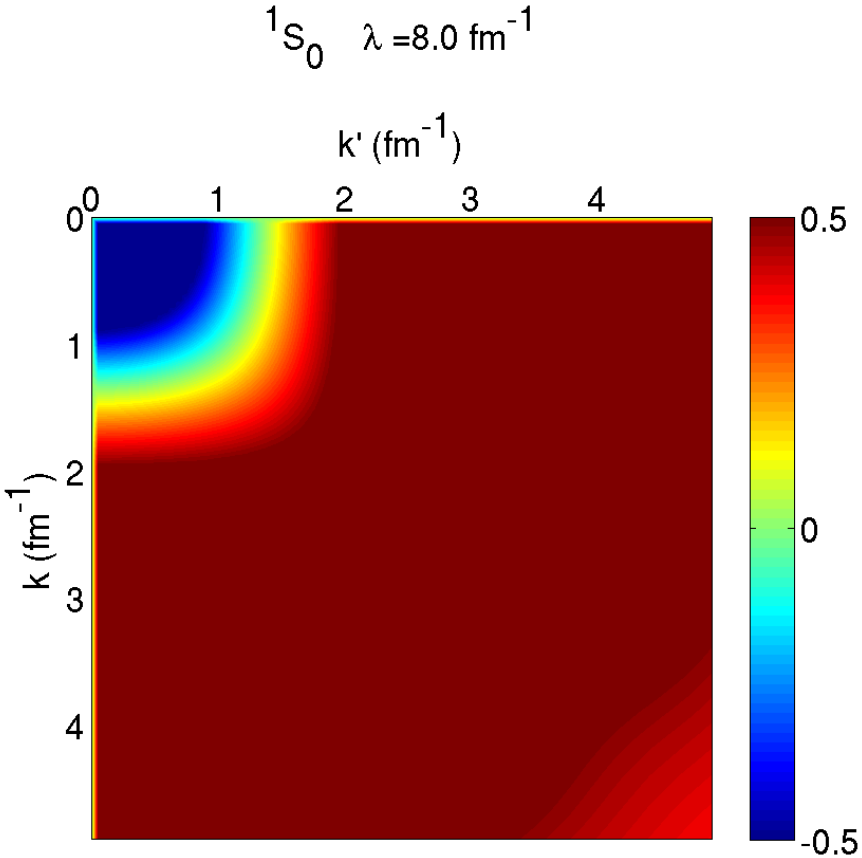

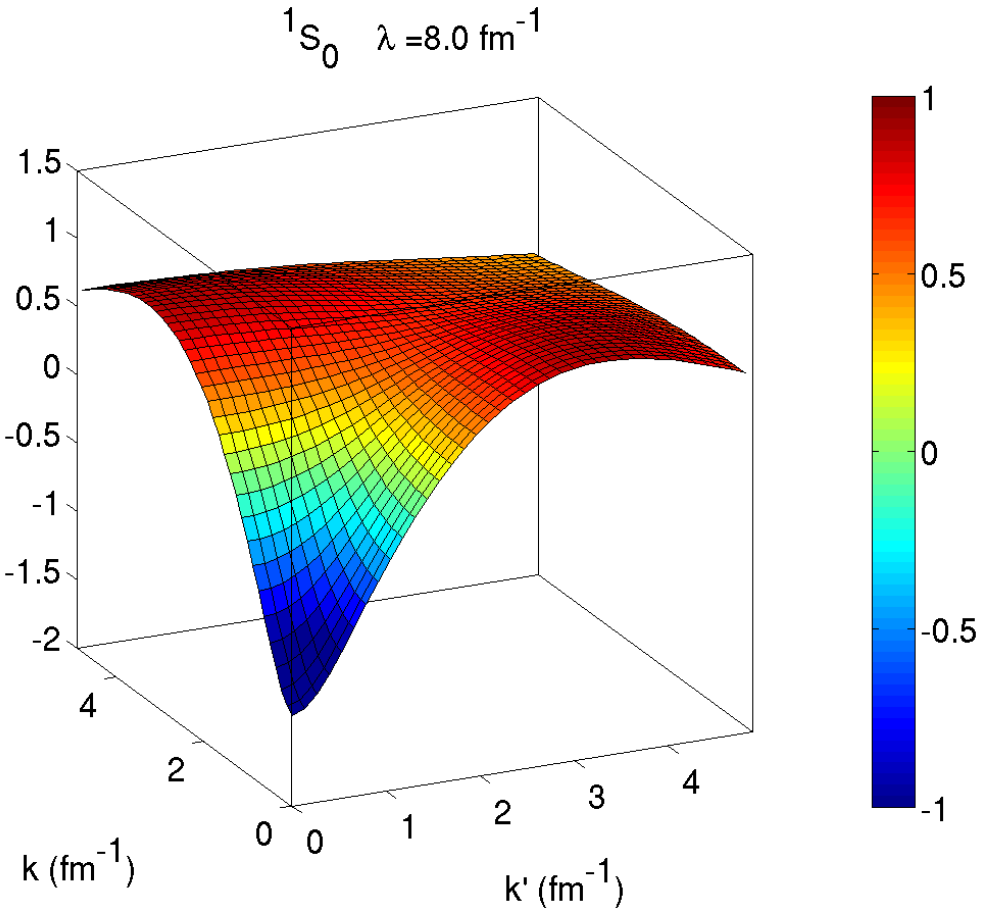

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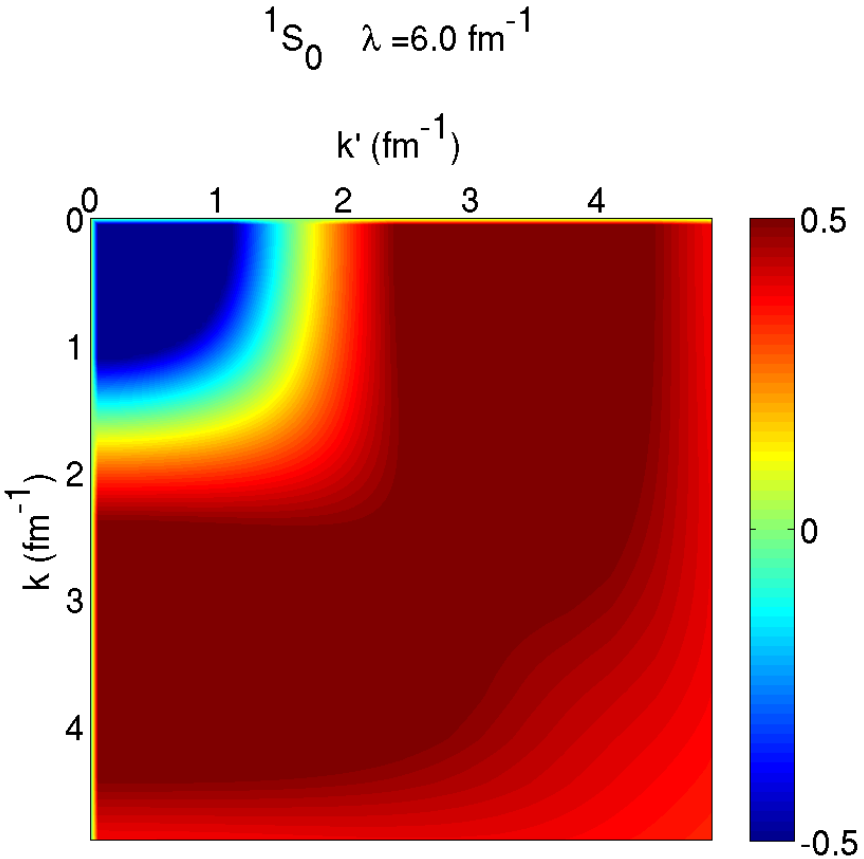

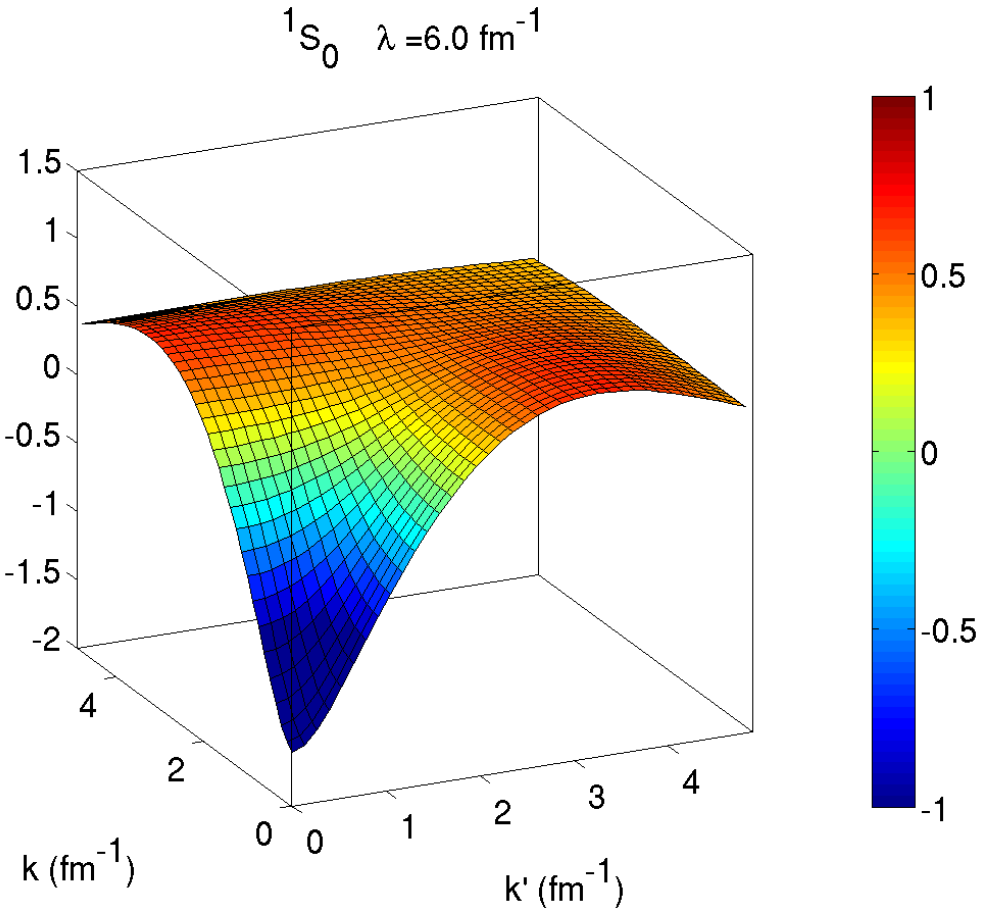

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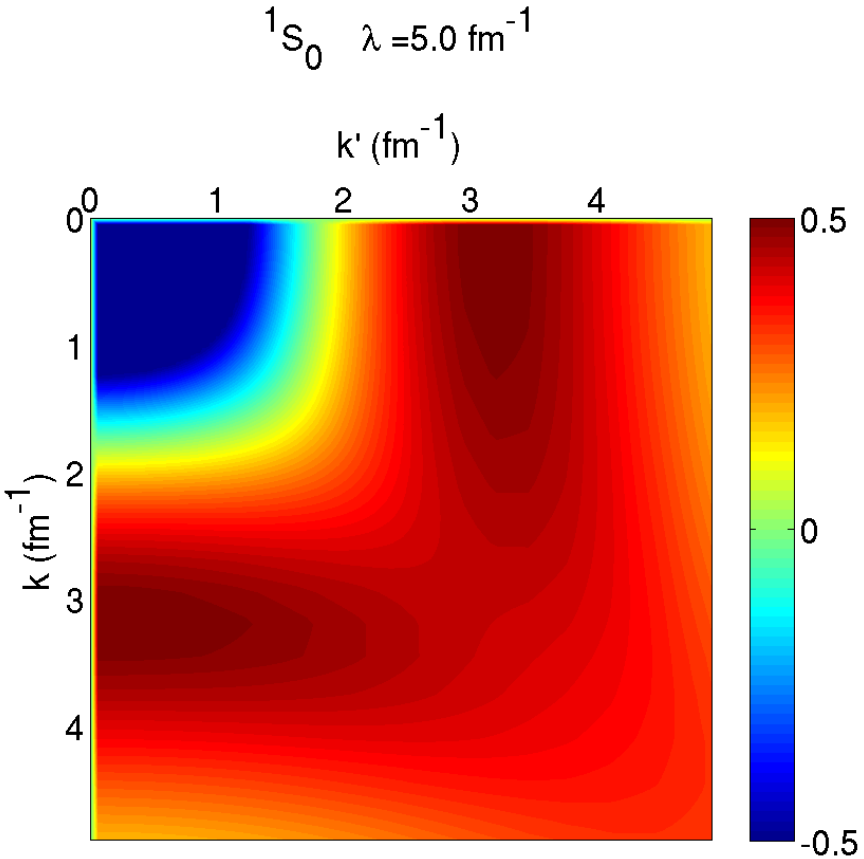

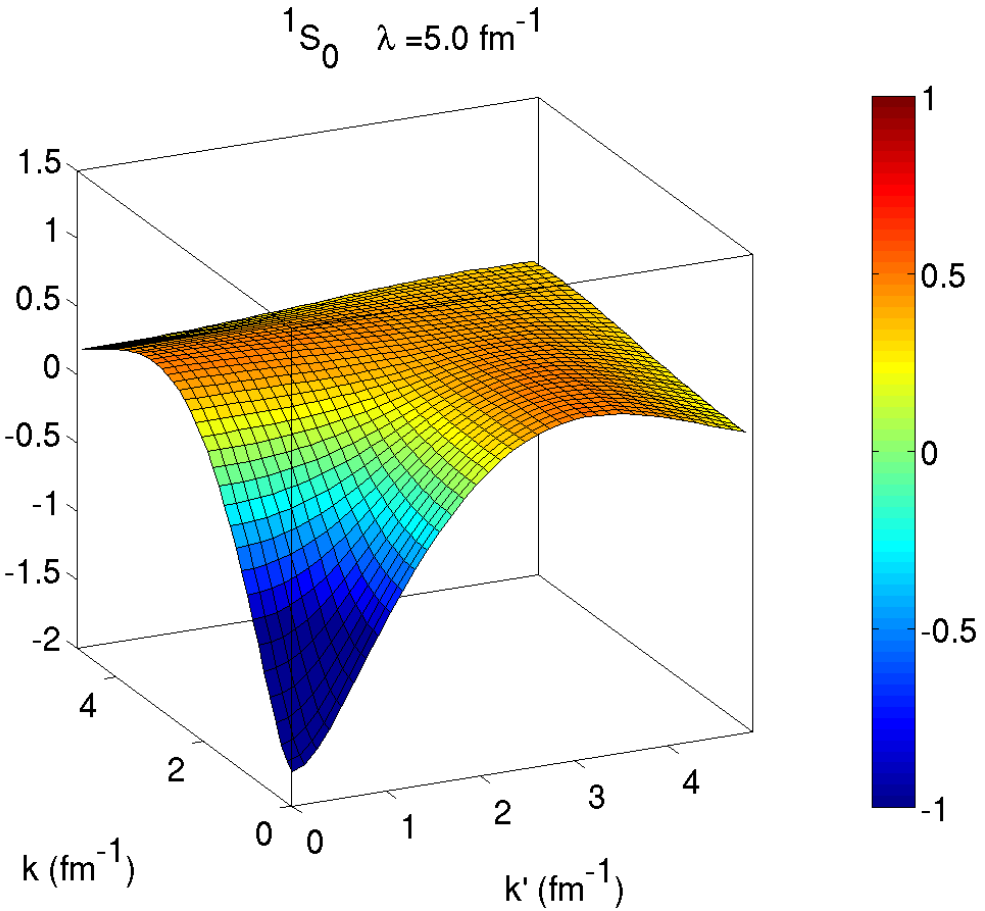

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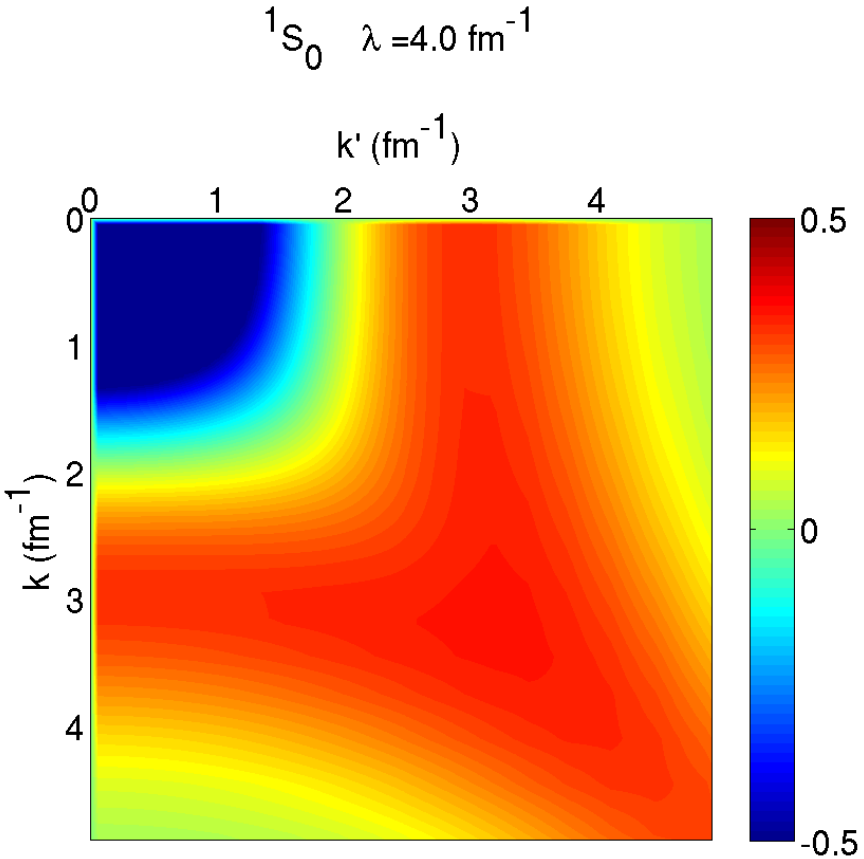

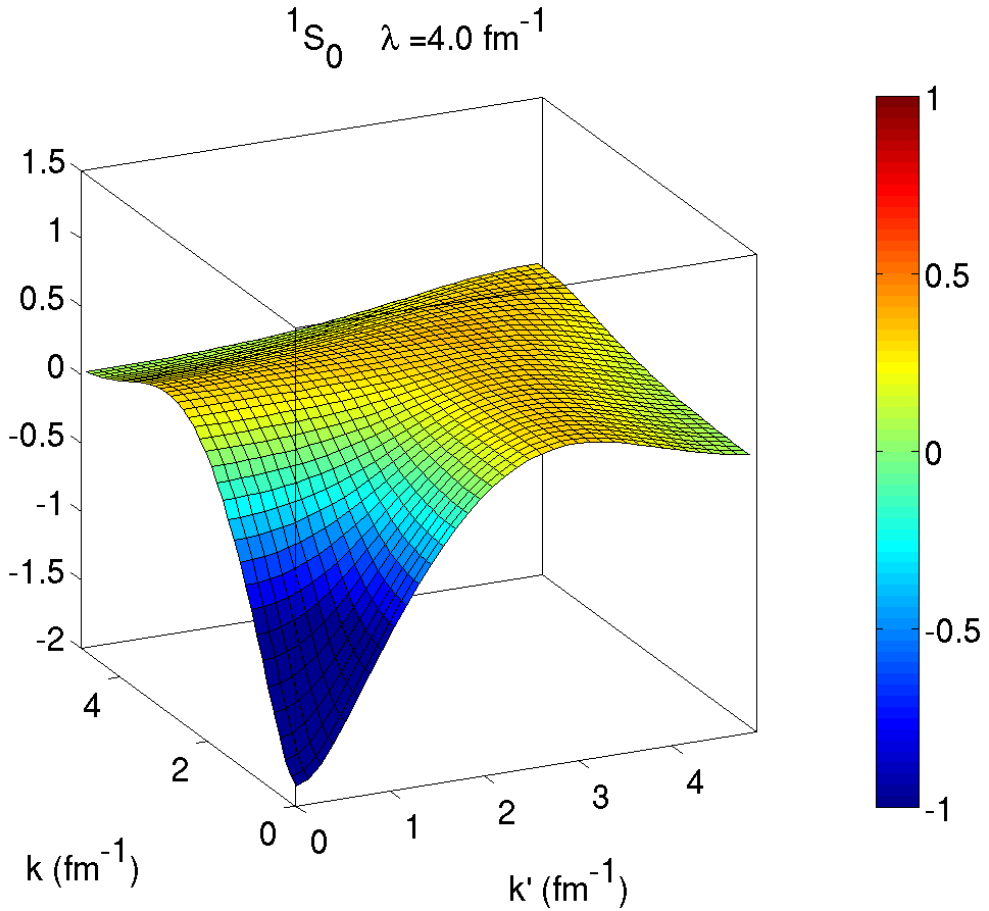

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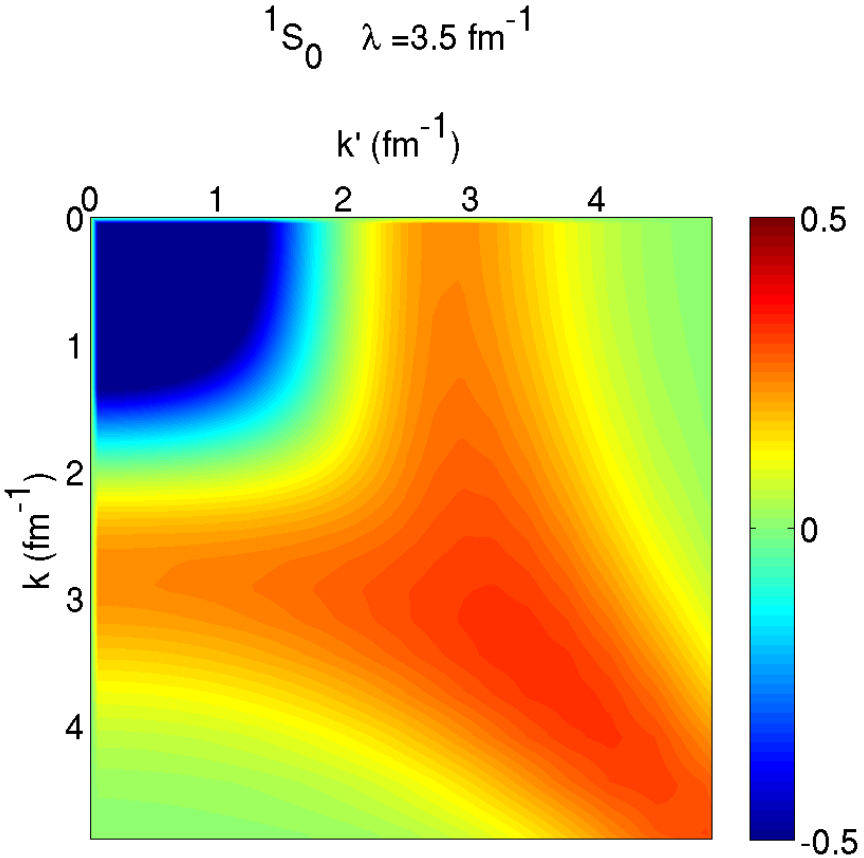

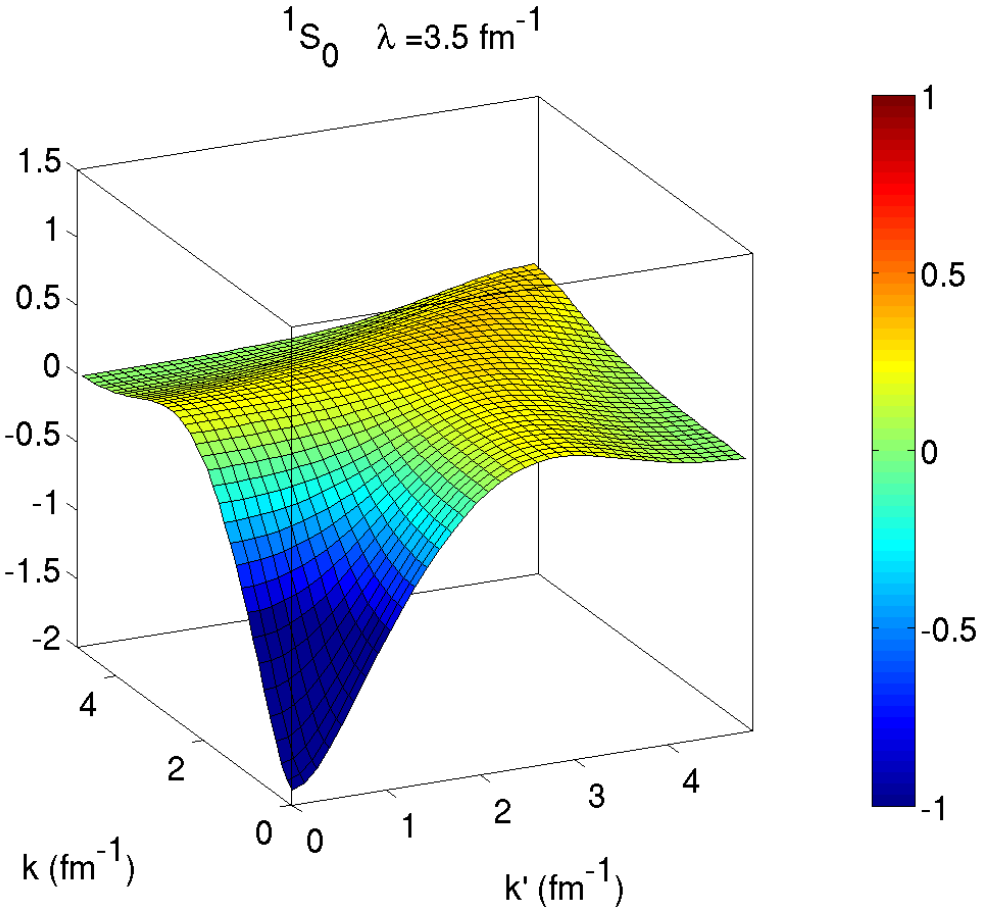

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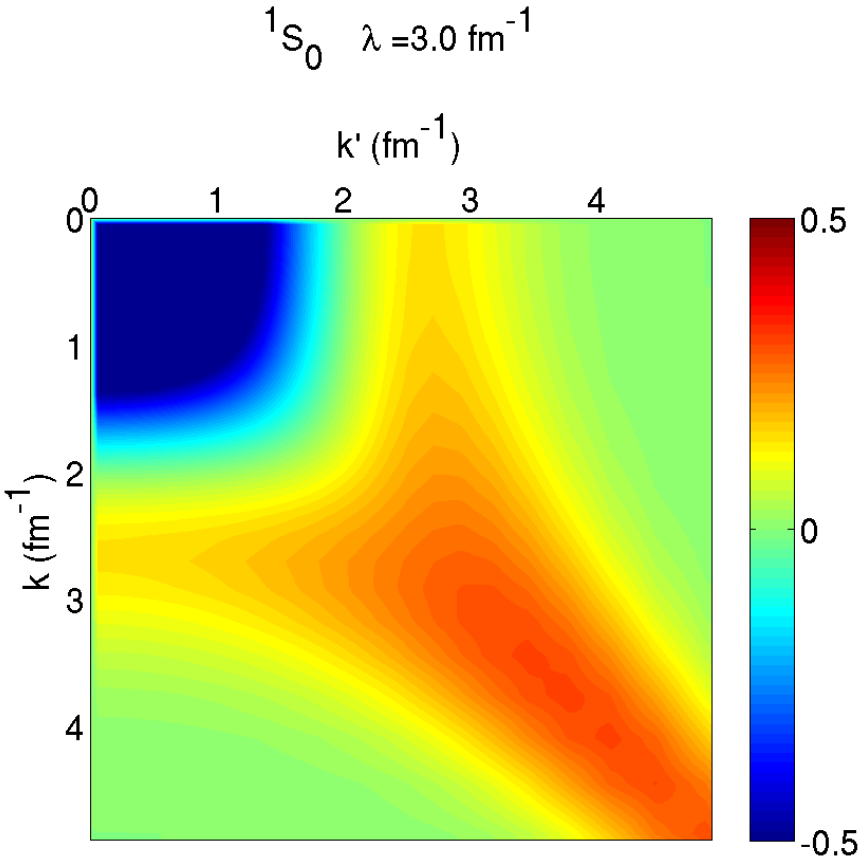

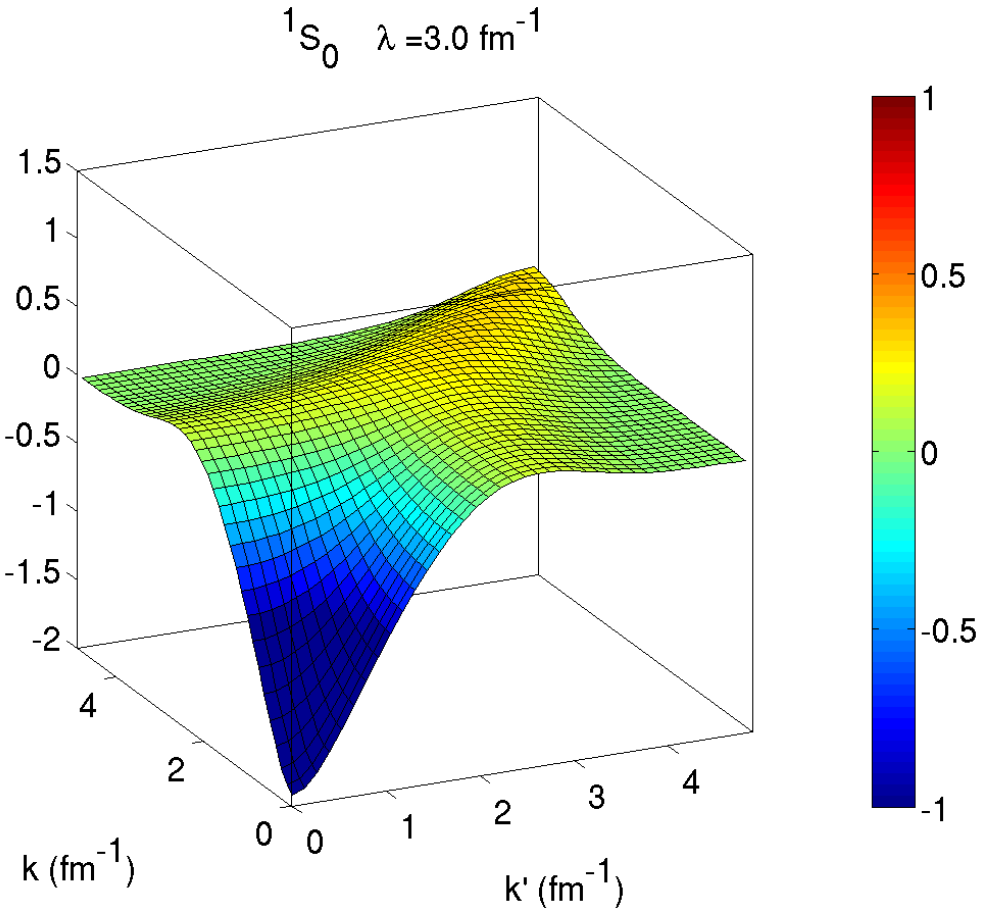

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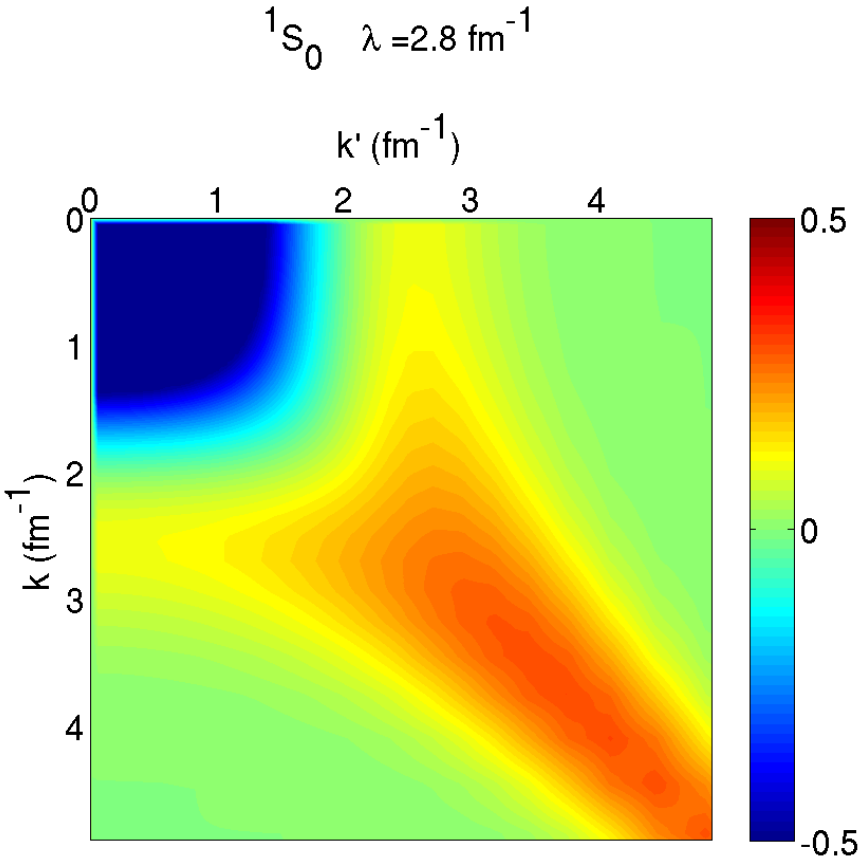

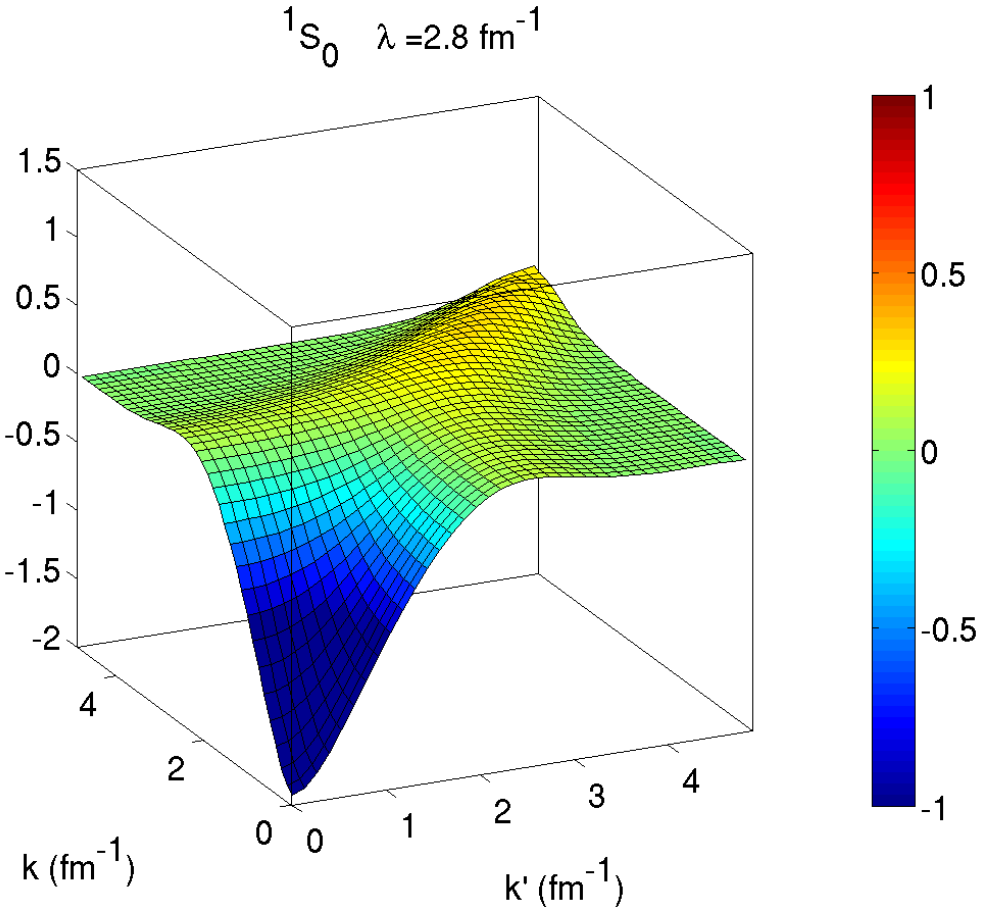

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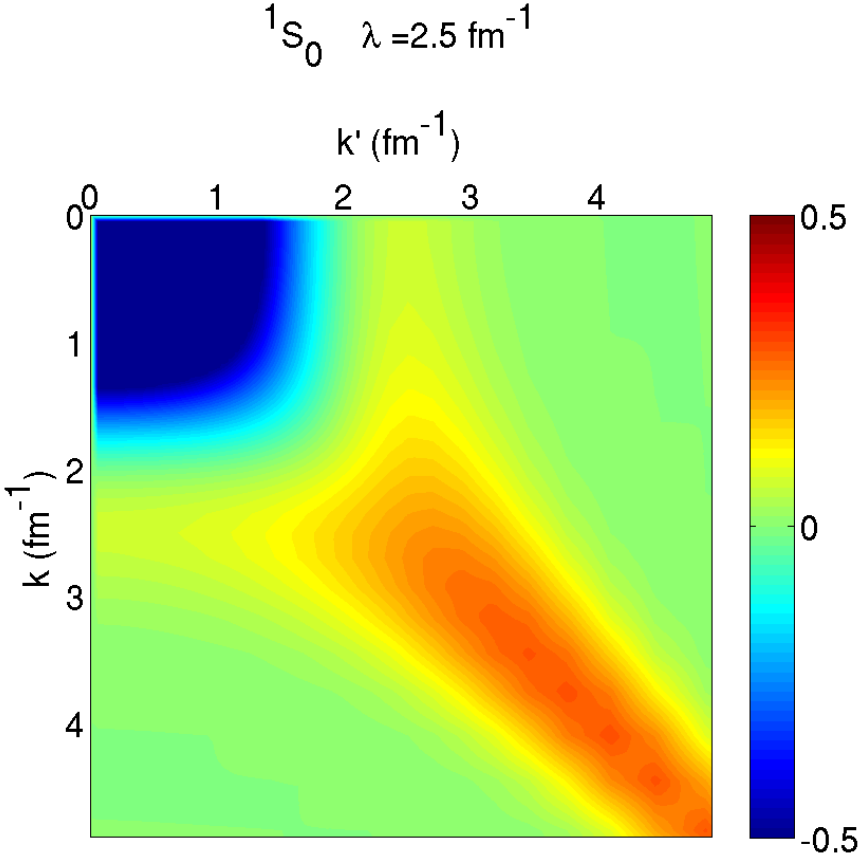

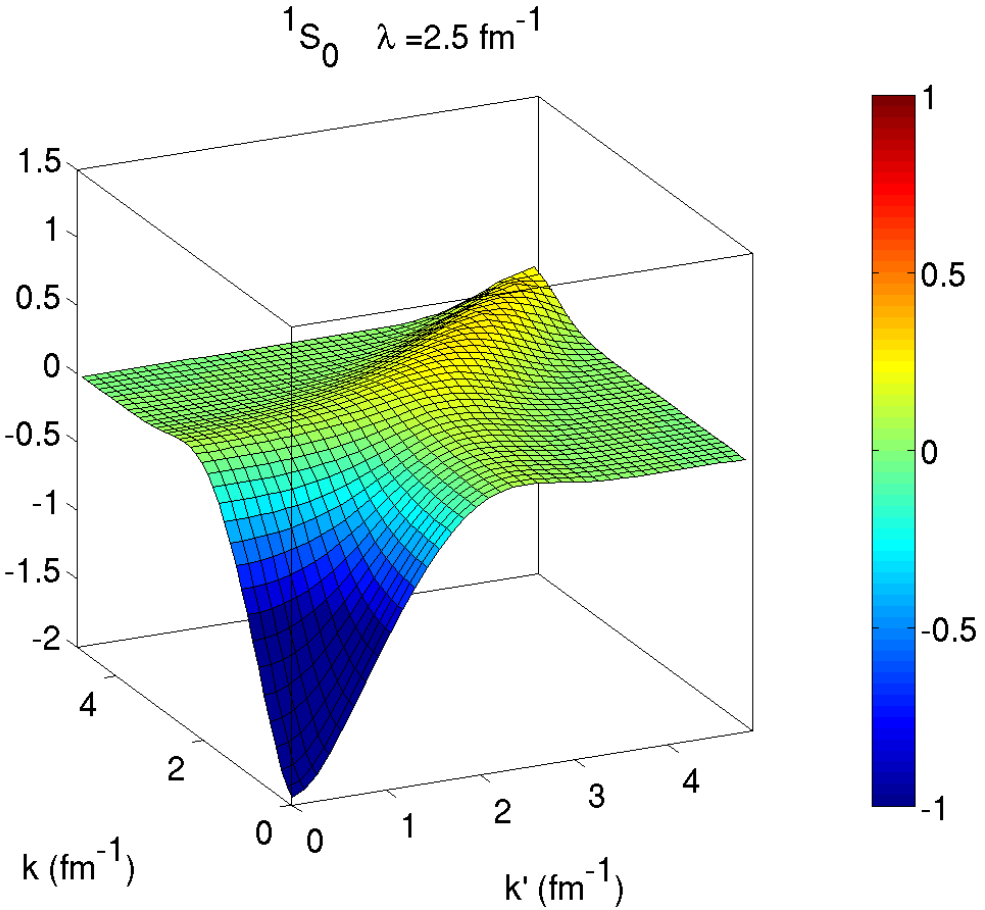

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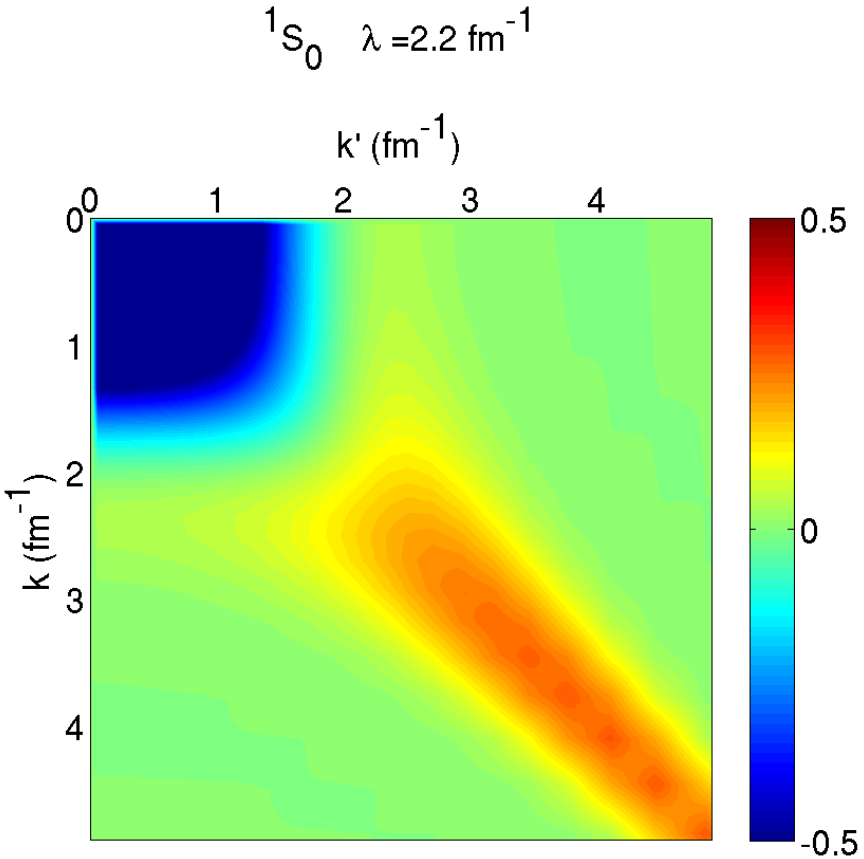

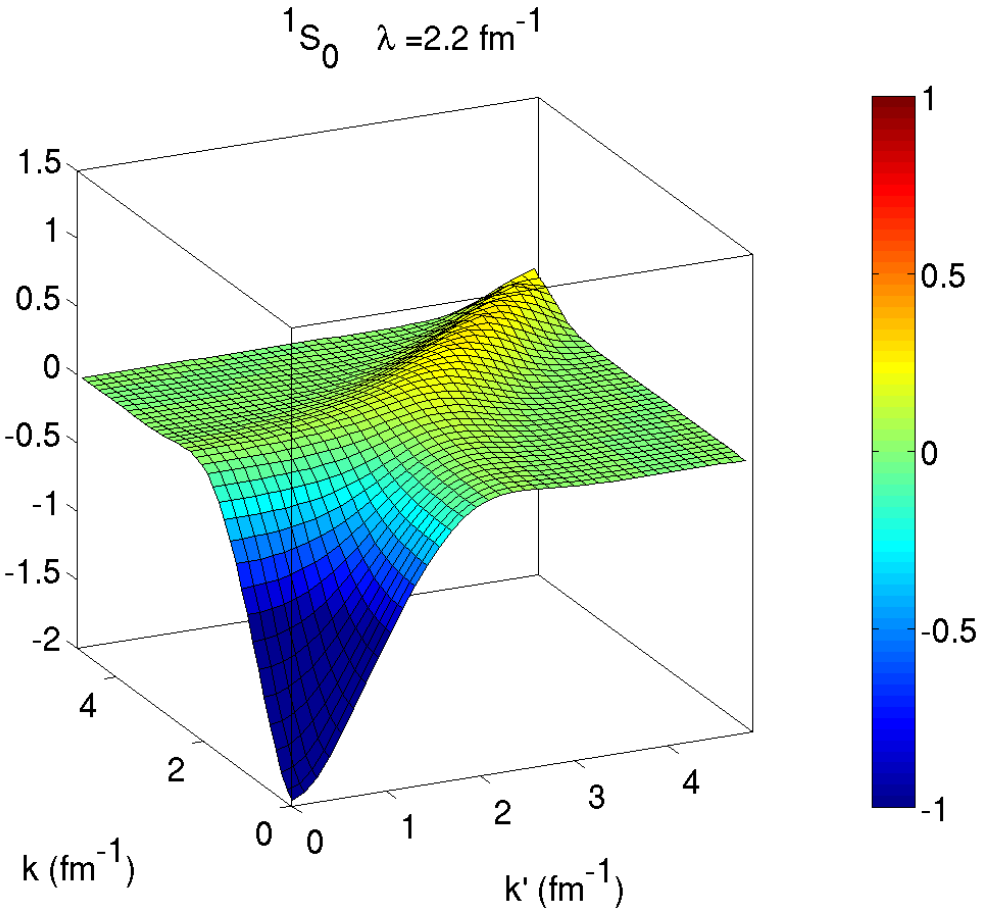

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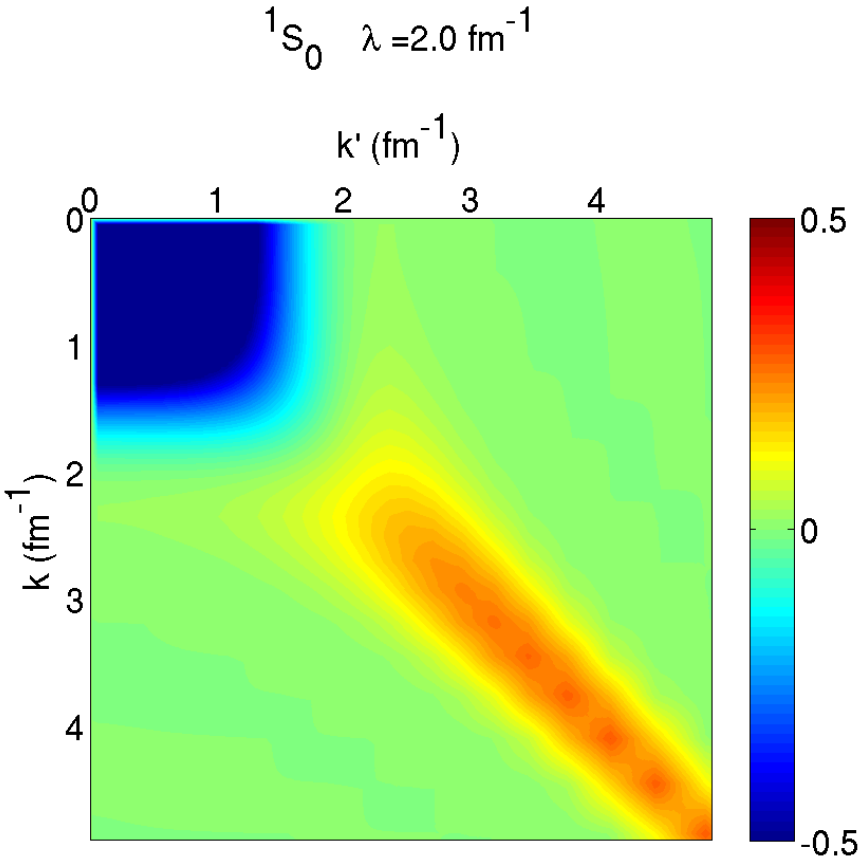
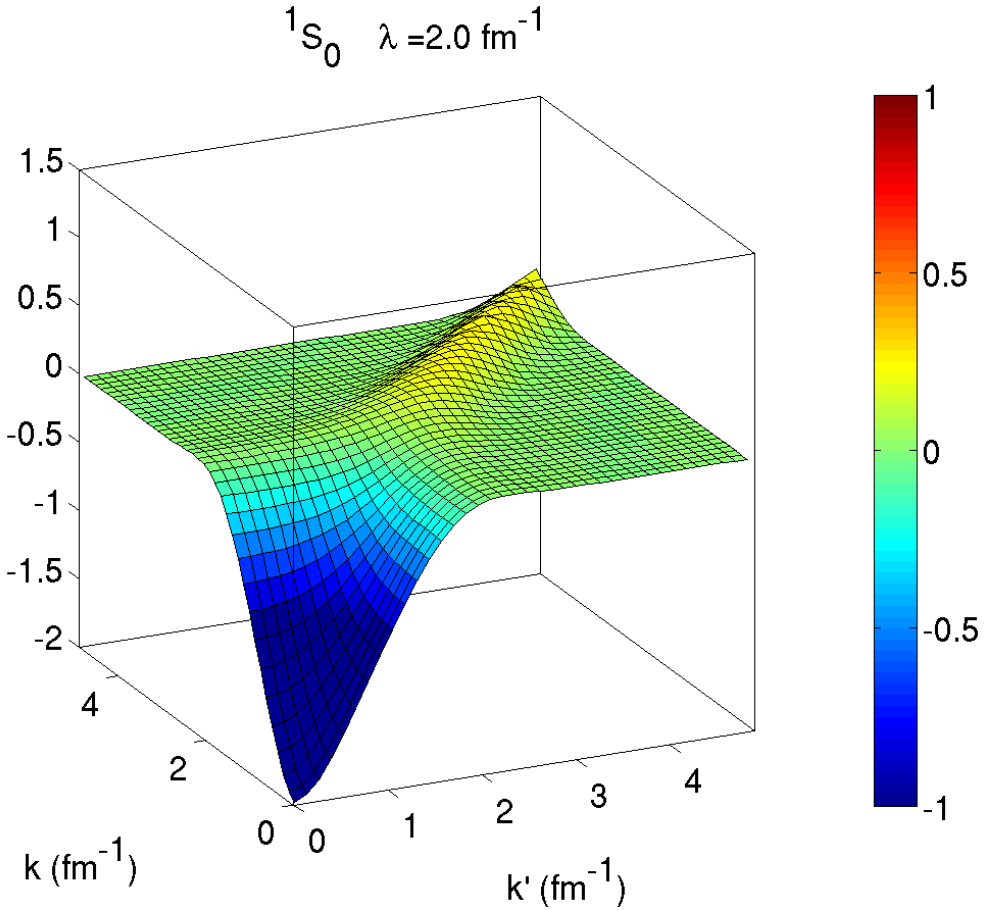
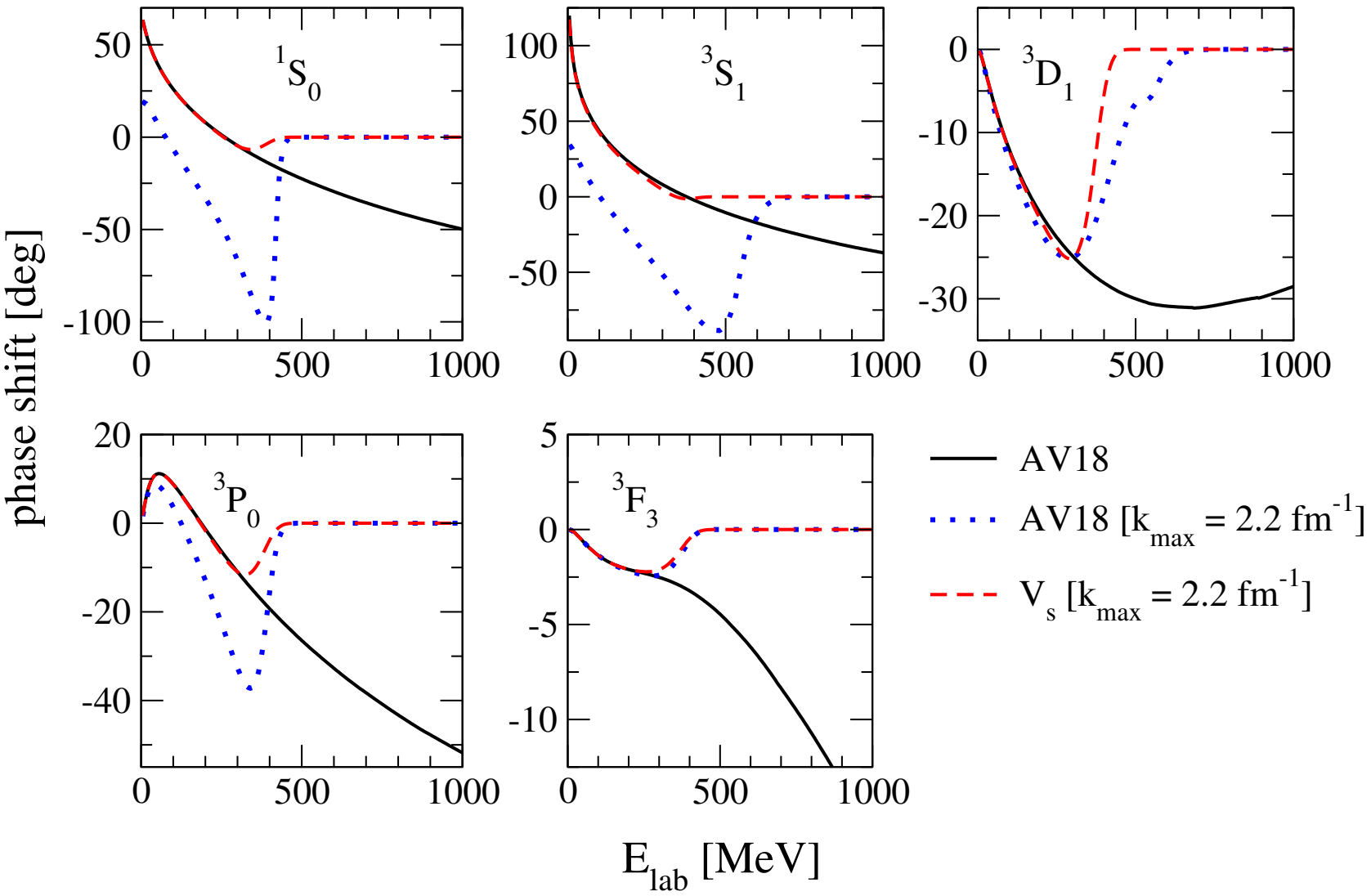


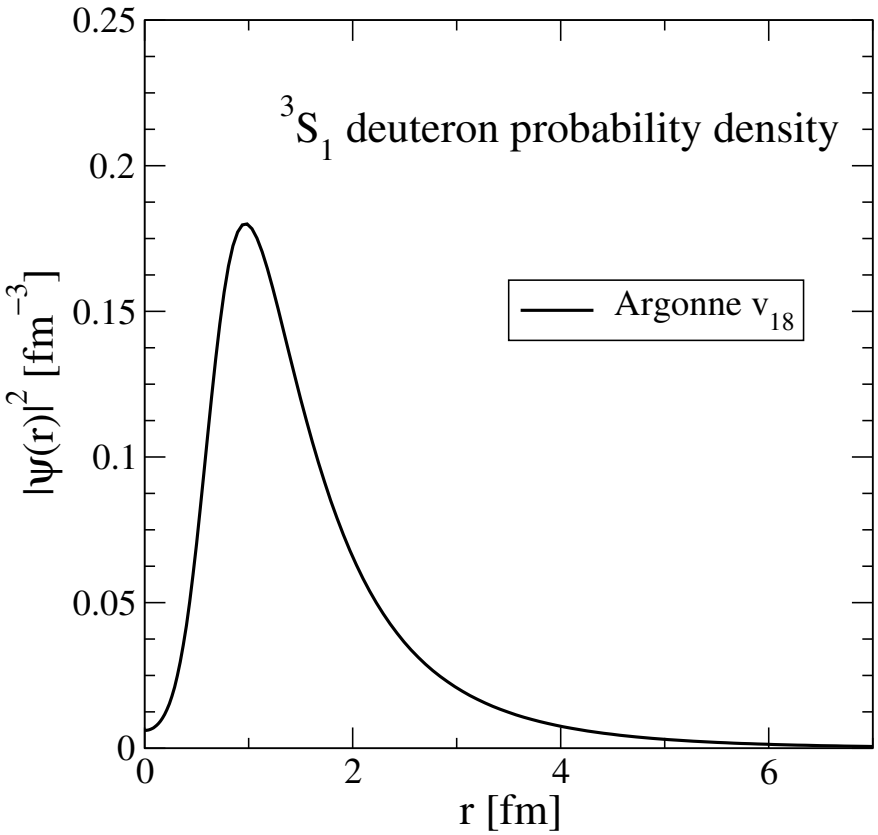


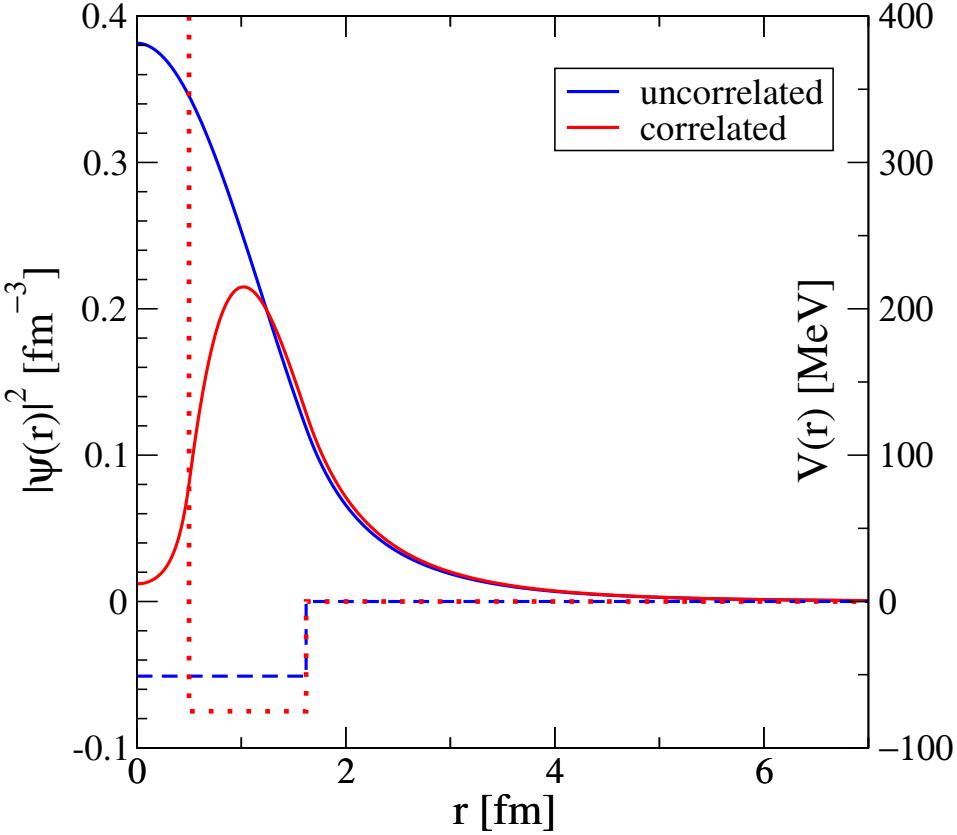
Low-pass filters work! [Jurgenson et al. (2008)]

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



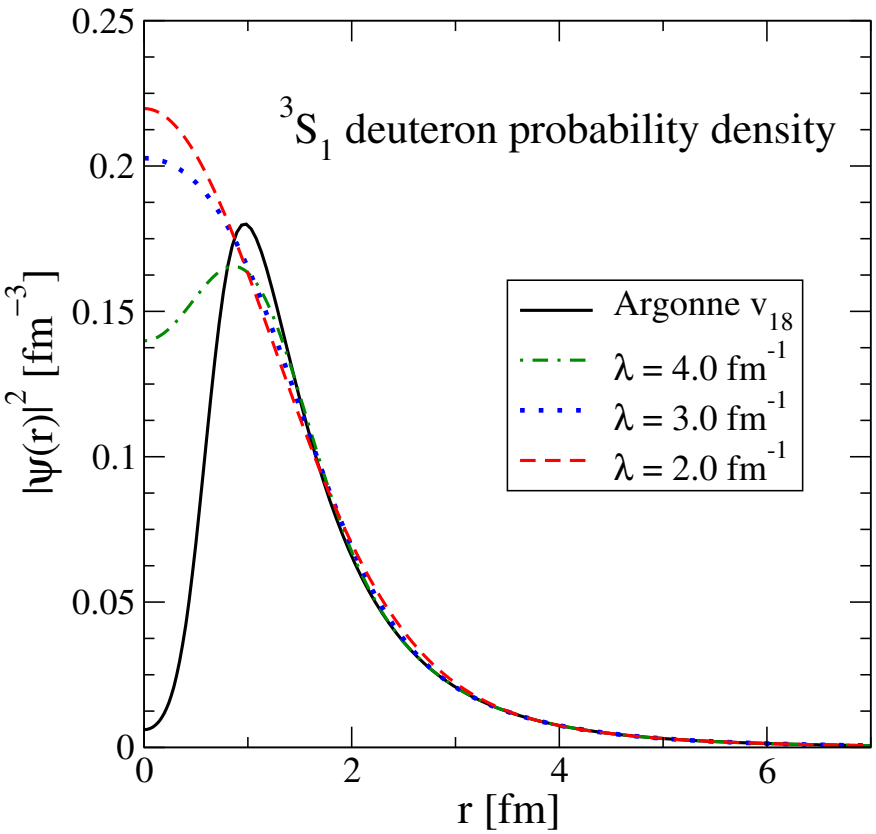
Consequences of a repulsive core revisited

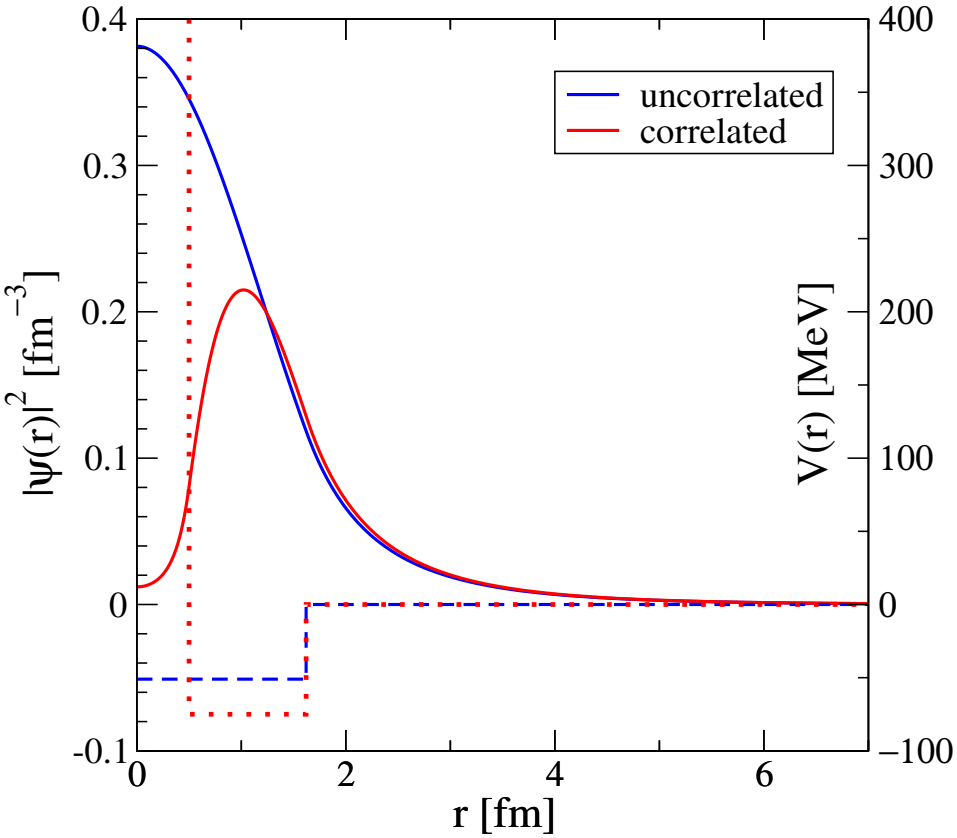




- Probability at short separations suppressed $\Longrightarrow$ “correlations”
- Short-distance structure $\Leftrightarrow$ high-momentum components
- Greatly complicates expansion of many-body wave functions

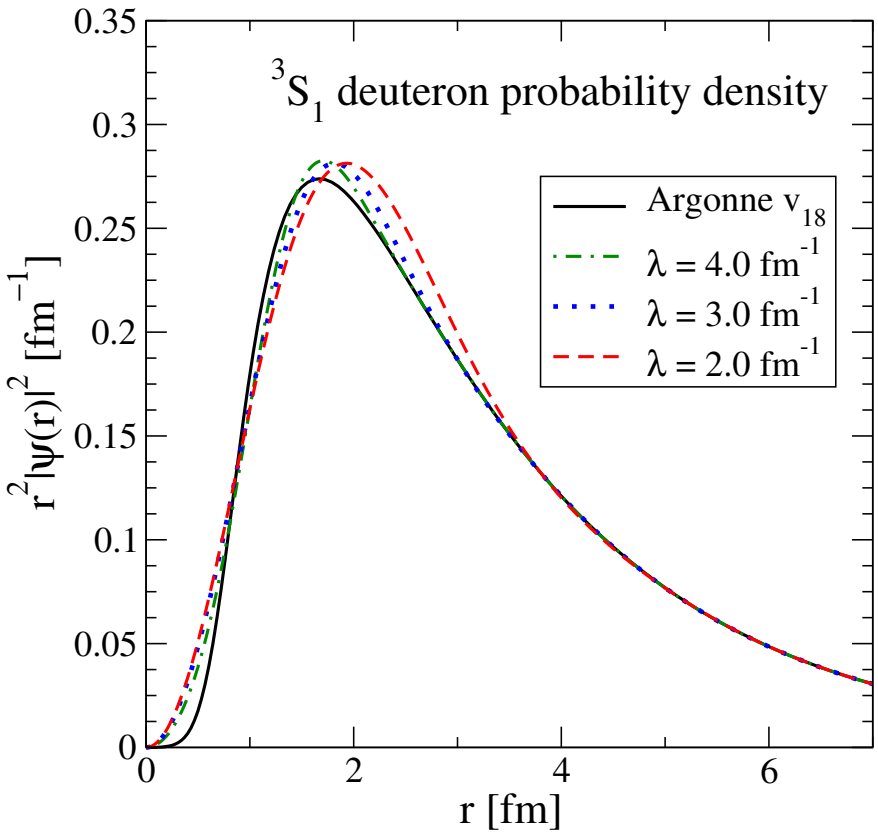
Consequences of a repulsive core revisited

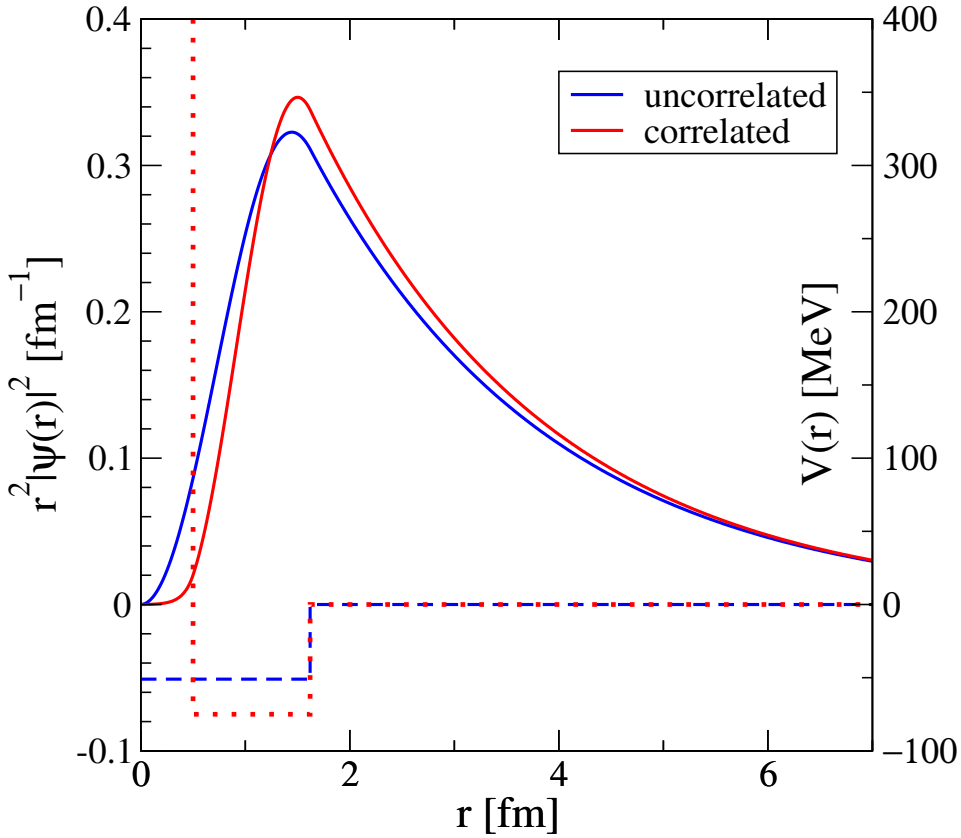




- Transformed potential $\Longrightarrow$ no short-range correlations in wf!
- Potential is now non-local: $V(\mathbf{r})\psi(\mathbf{r}) \longrightarrow \int d^3\mathbf{r}'\, V(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')$
  - A problem for Green's Function Monte Carlo approach
  - Not a problem for many-body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

Consequences of a repulsive core revisited

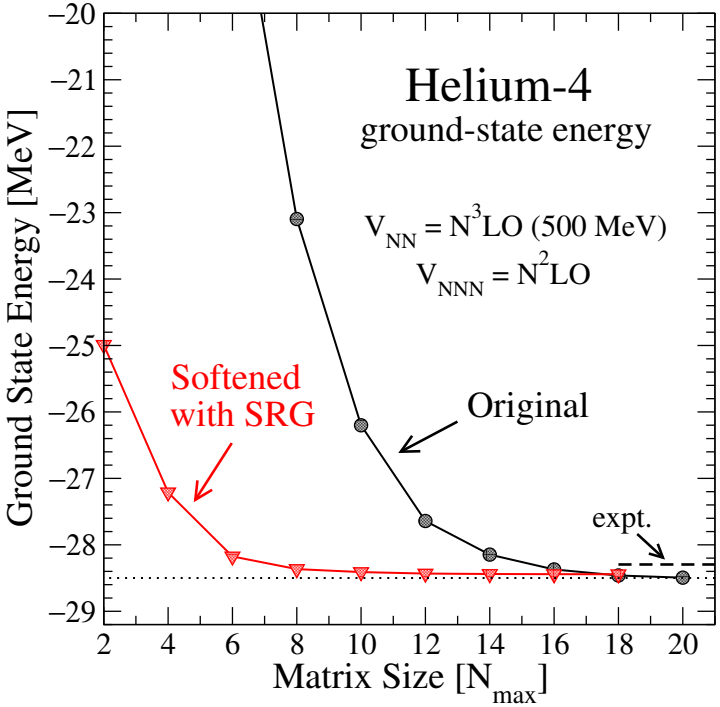


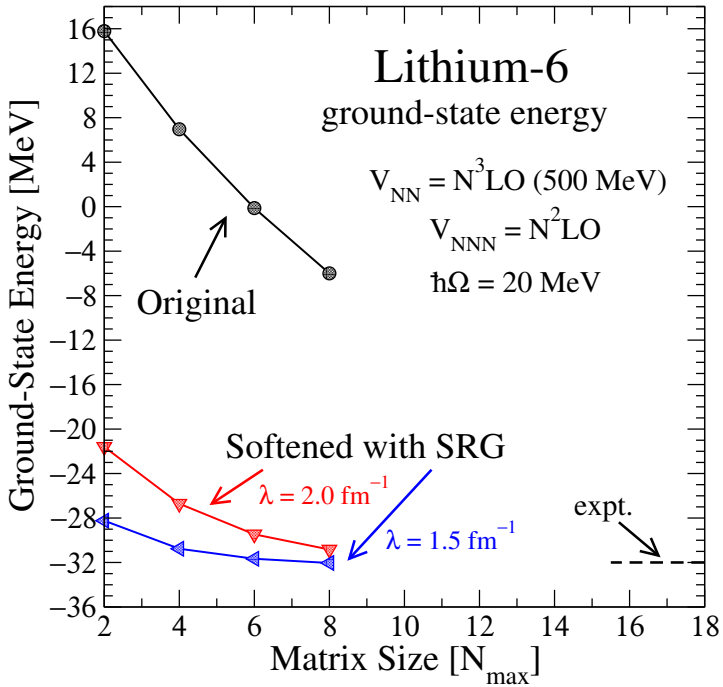


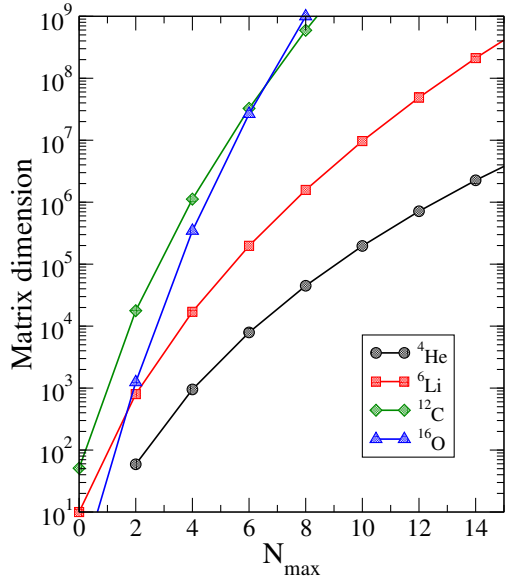
- Transformed potential $\Longrightarrow$ no short-range correlations in wf!
- Potential is now non-local: $V(\mathbf{r})\psi(\mathbf{r}) \longrightarrow \int d^3\mathbf{r}'\, V(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')$
  - A problem for Green's Function Monte Carlo approach
  - Not a problem for many-body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

Many short wavelengths $\Longrightarrow$ Large matrices

- Harmonic oscillator basis with $N_{\max}$ shells for excitations
- Graphs show convergence for *soft* chiral EFT potential and evolved SRG potentials (including NNN)







- Better convergence, but rapid growth of basis still a problem (solution: importance sampling of matrix elements [R. Roth])

Flow equations and the SRG: History

- In the early 1970's, Ken Wilson and Franz Wegner
  $\Longrightarrow$ critical phenomena and renormalization group (RG)
- Twenty years later, Wilson and Wegner innovate again
  - Unitary RG flow to make many-particle Hamiltonians increasingly energy diagonal
  - Glazek and Wilson, "Renormalization of Hamiltonians" (1993)
    $\Longrightarrow$ SRG for QCD on the light front (also Perry, . . .)
  - Wegner, "Flow Equations for Hamiltonians" (1994)
    $\Longrightarrow$ condensed matter problems
- S. Kehrein, "Flow-Equation Approach to Many-Particle Systems"
  - Dissipative quantum systems to correlated electron physics to non-equilibrium problems to . . .
- Particularly well suited for low-energy nuclear physics!
  - Only applied in last few years [arXiv:0912.3688]
  - Technically simpler and more versatile than other methods

Basics: SRG flow equations [arXiv:0912.3688]

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

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

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 "generator" G_s:

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

which yields the flow equation (T held fixed),

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

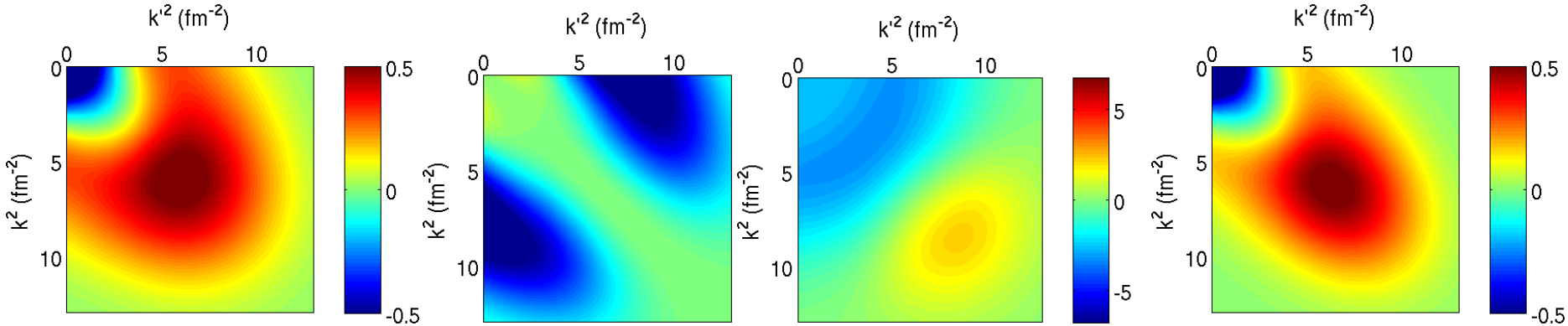
- G_s determines flow $\Longrightarrow$ many choices (T, H_D, H_{BD}, ...)

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:

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

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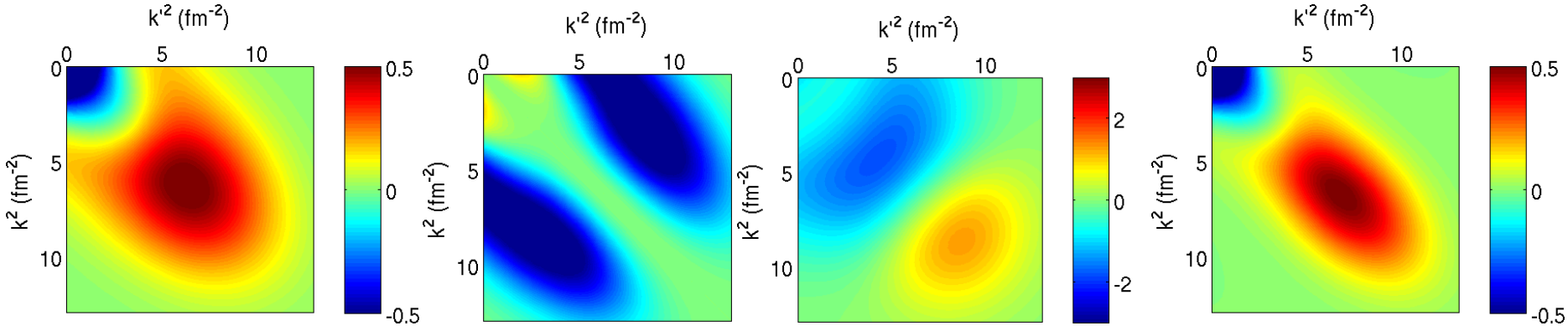

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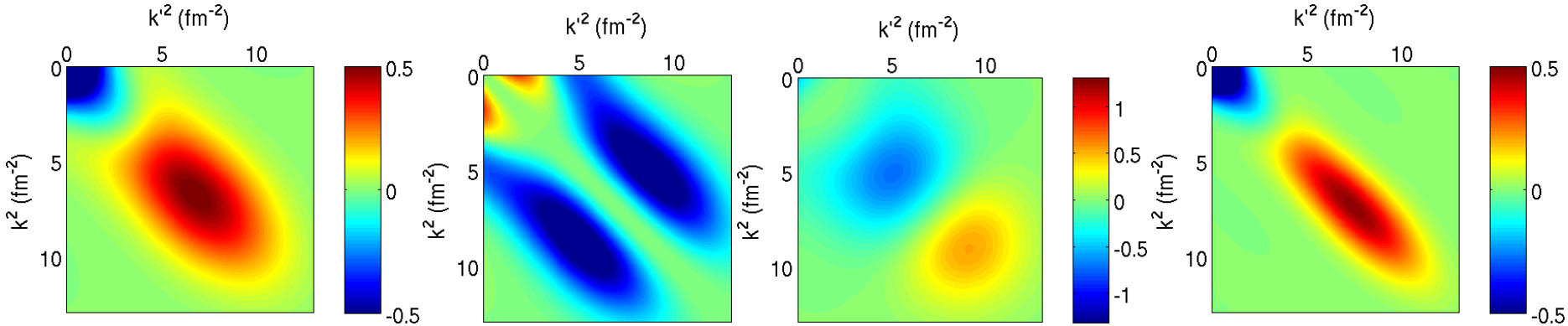

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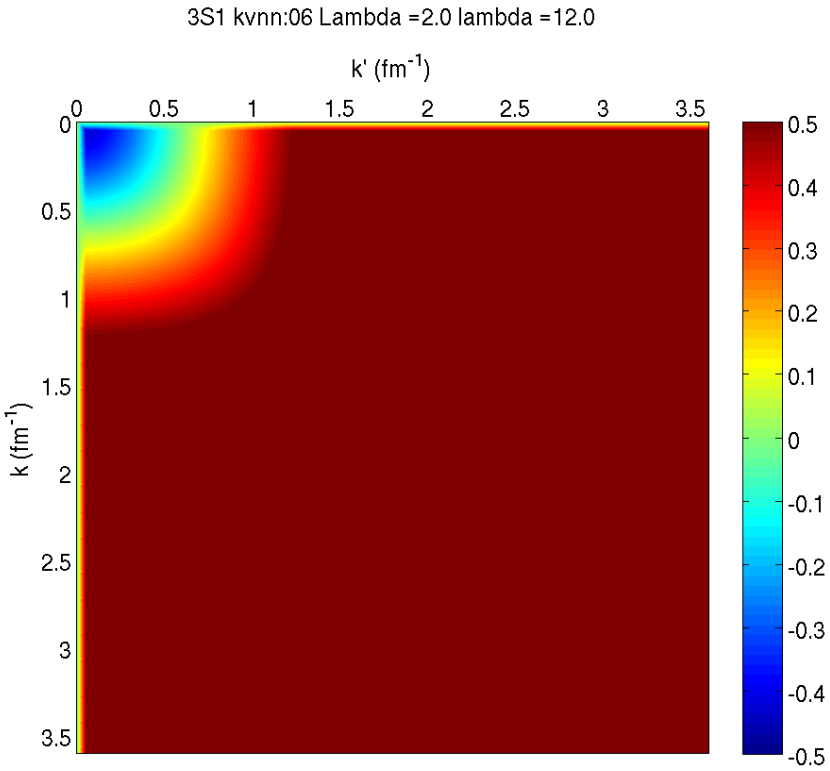
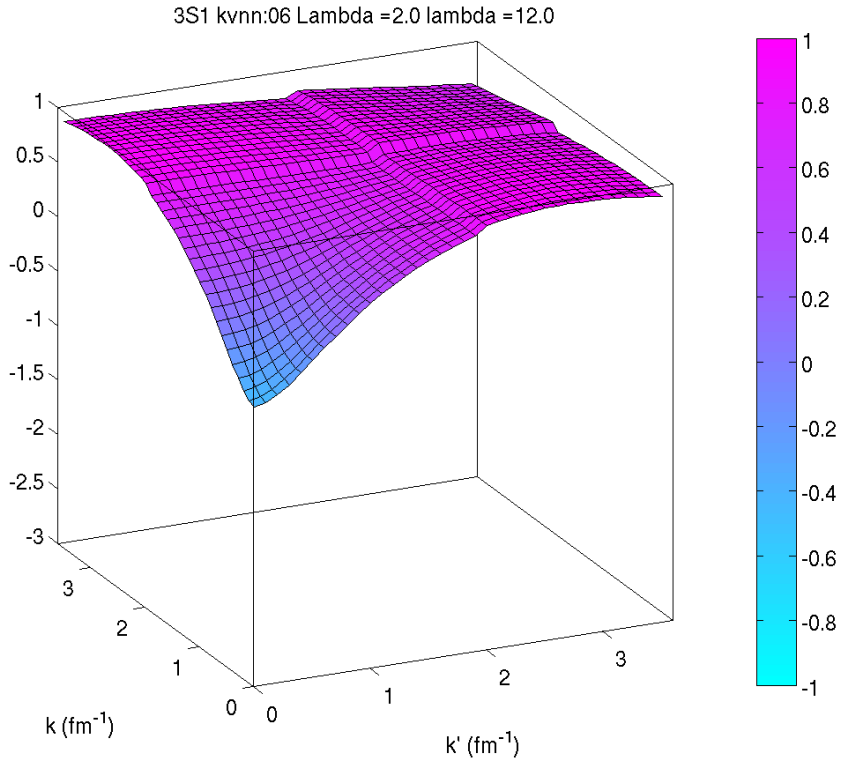
Block diagonalization via SRG $[G_s = H_{BD}]$

- 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 $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$





- What are the best generators for nuclear applications?

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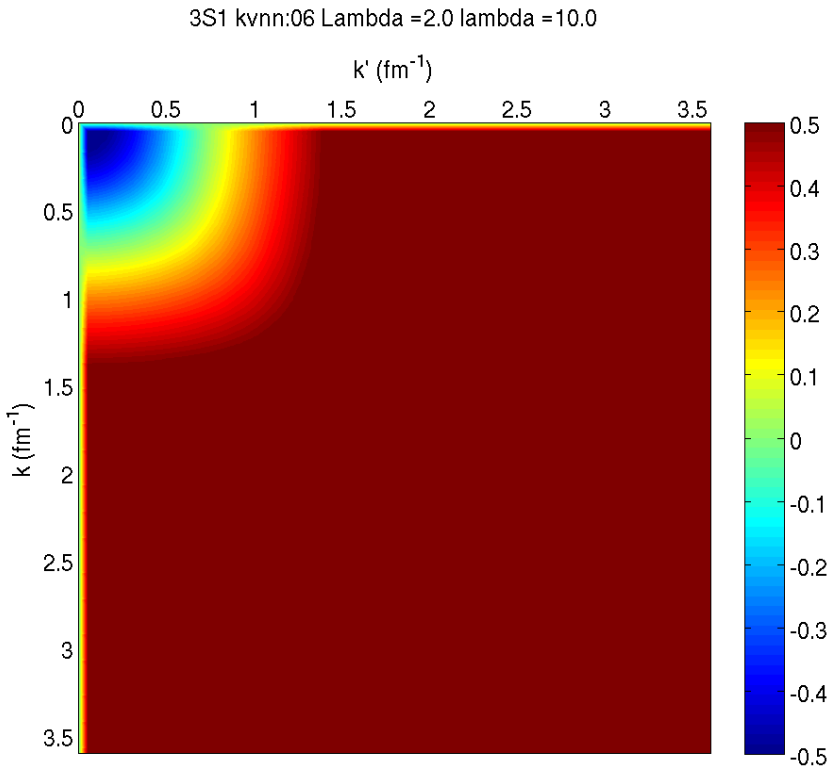

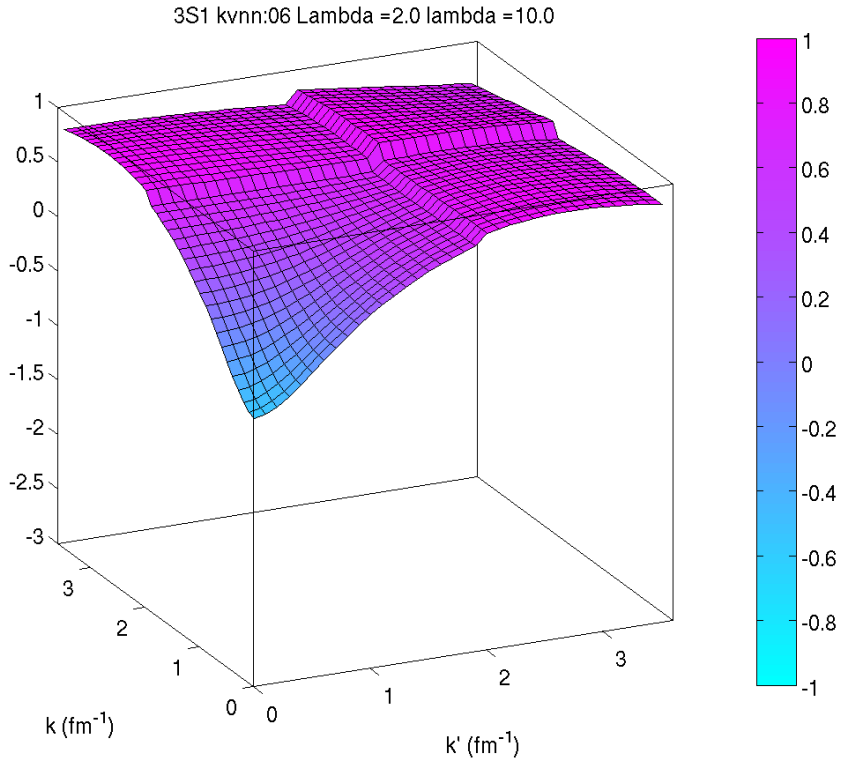

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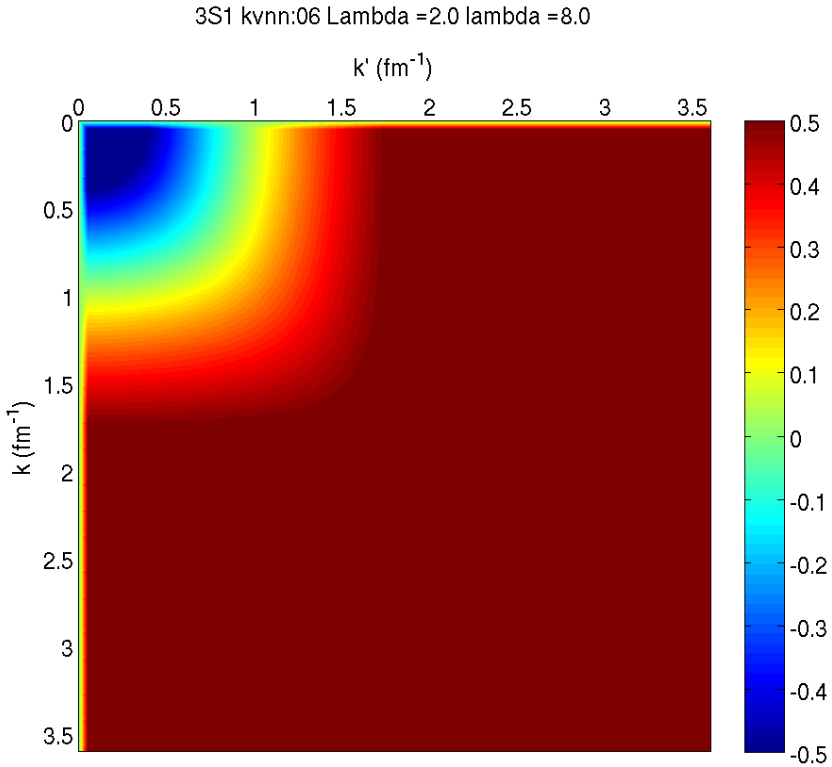

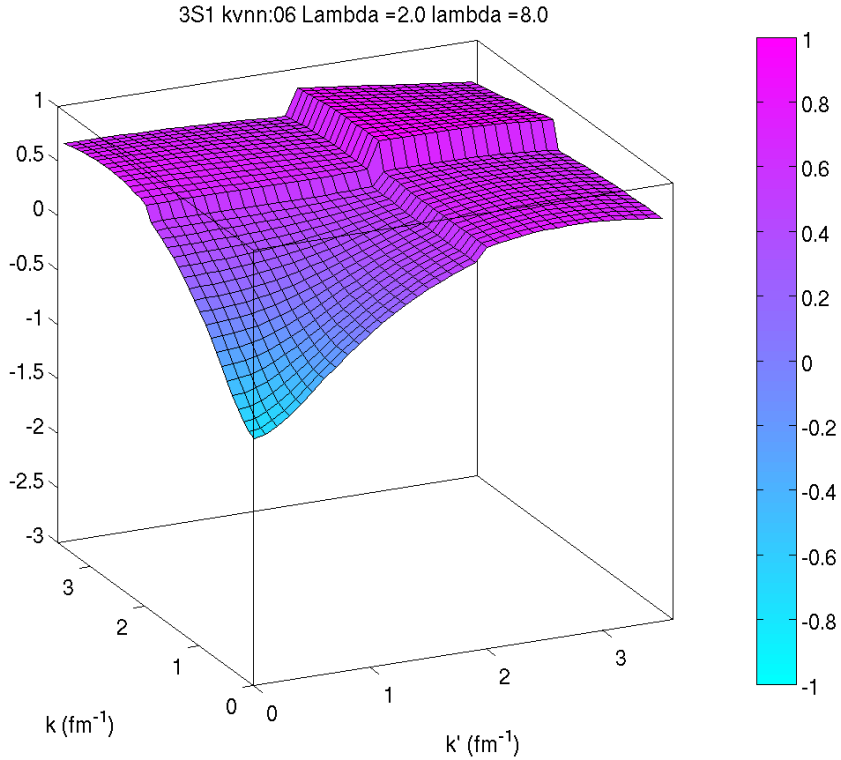

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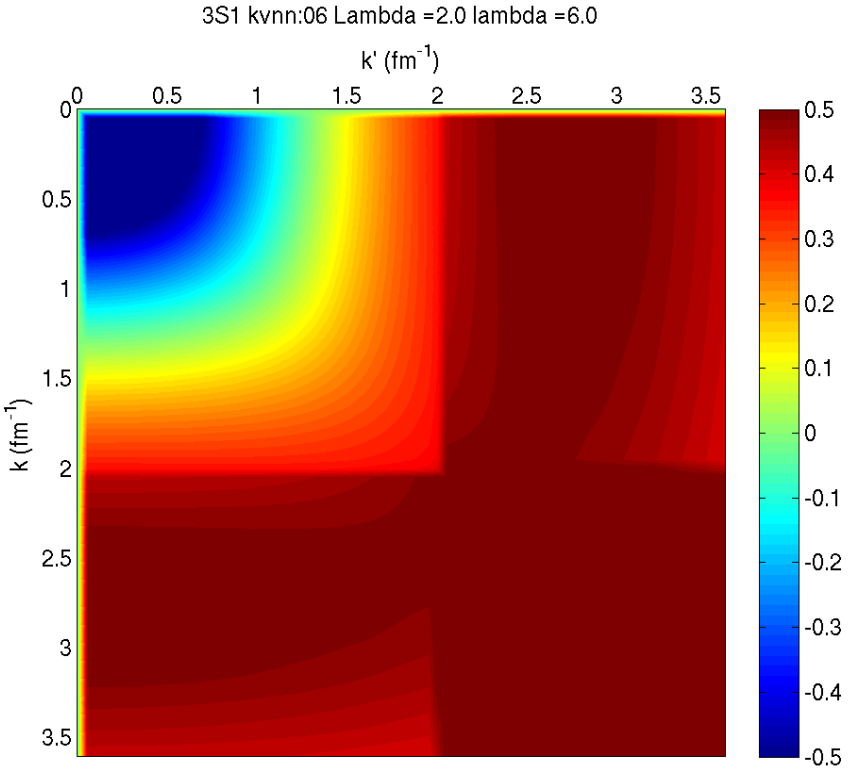

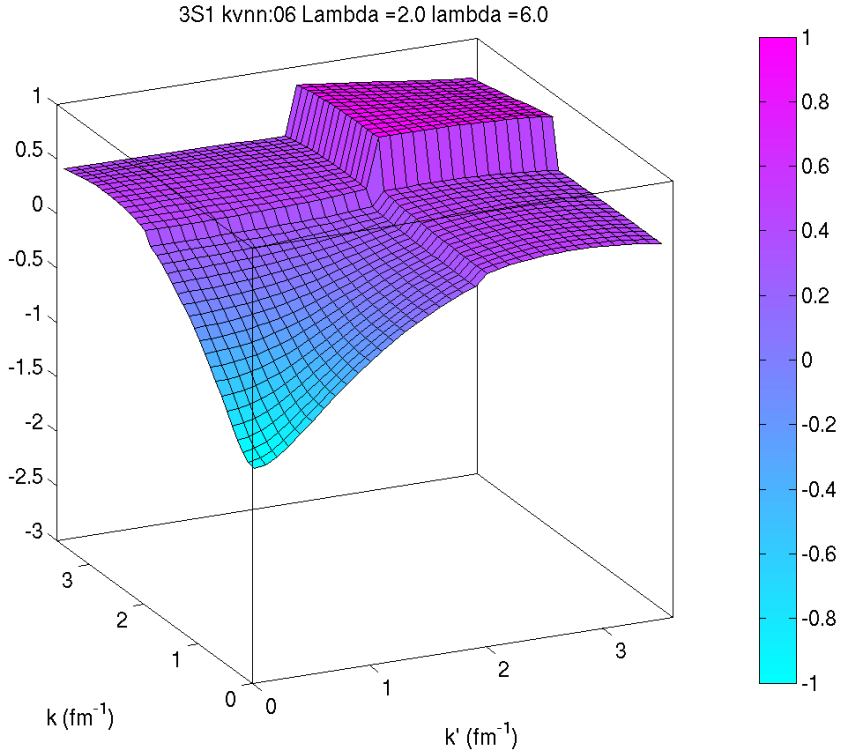

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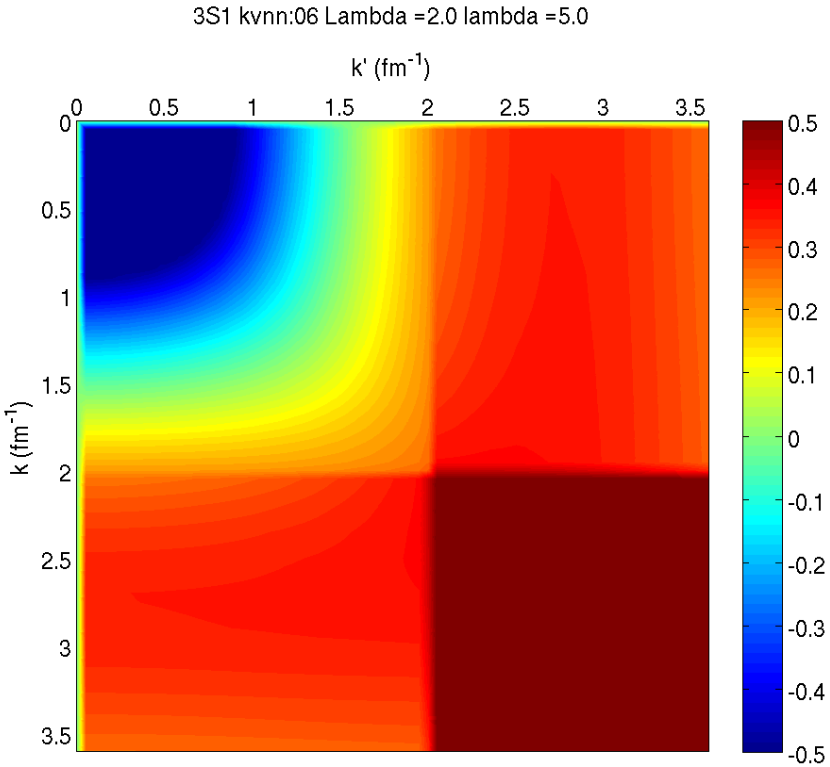

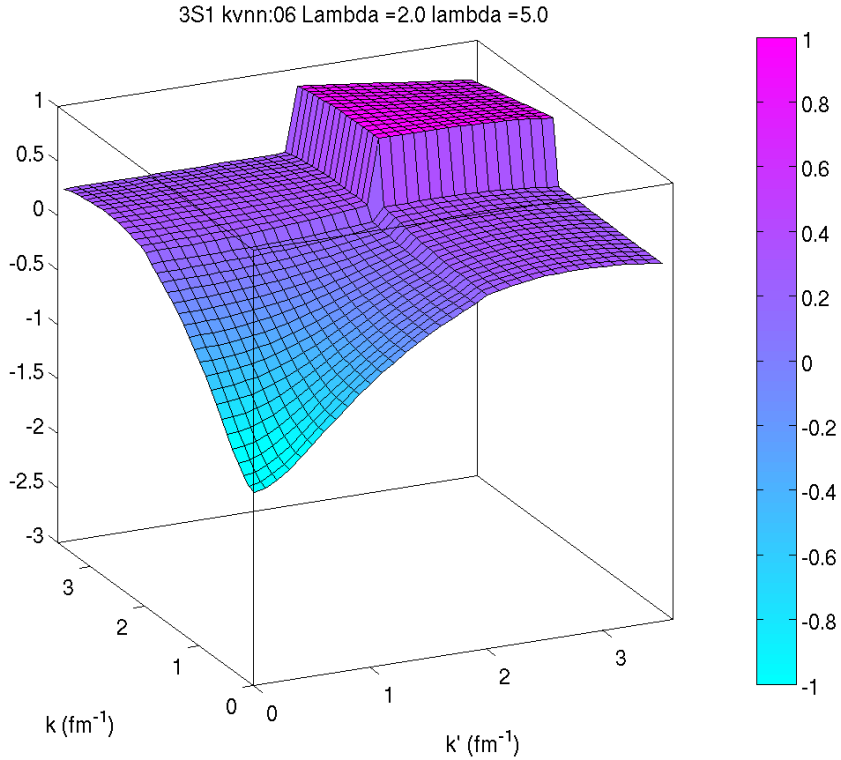

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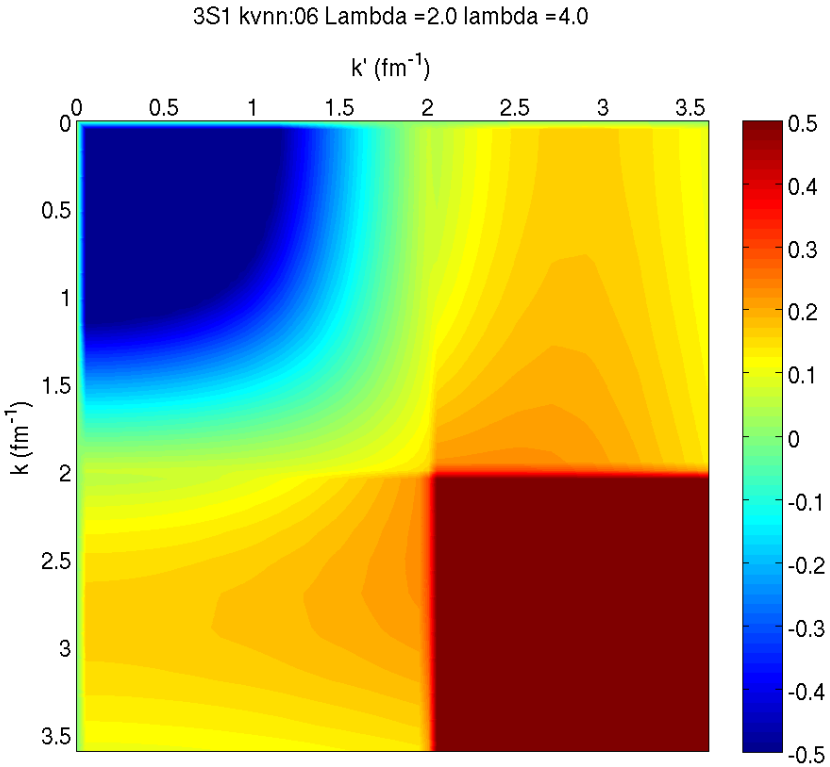

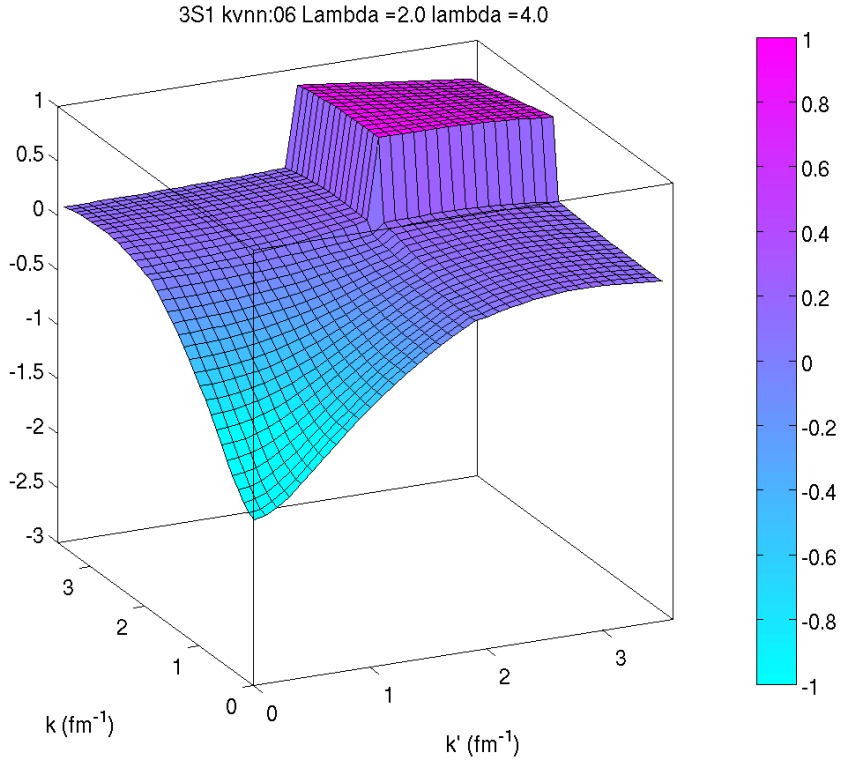

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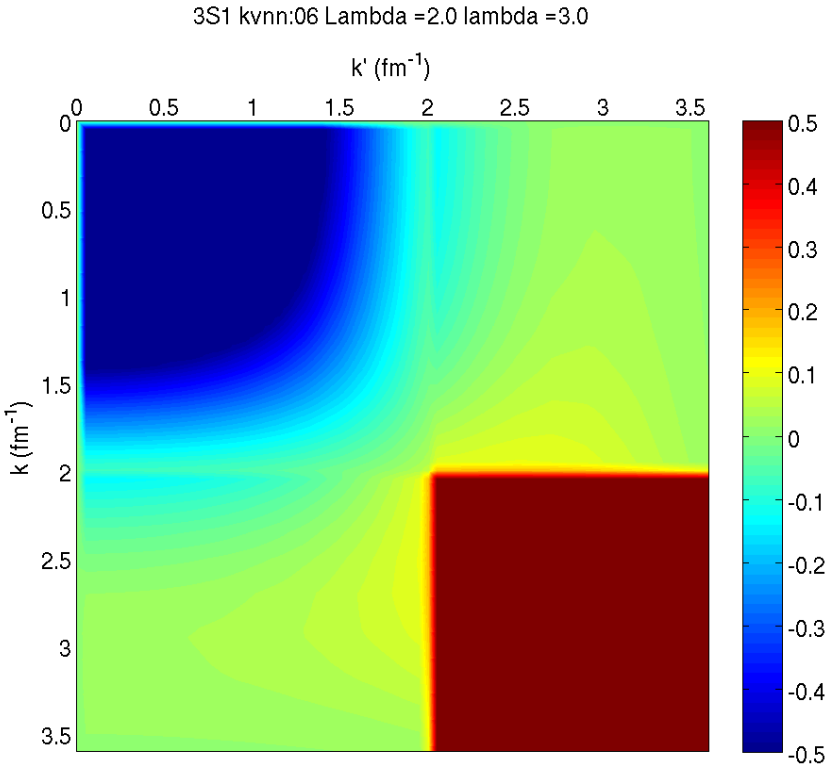

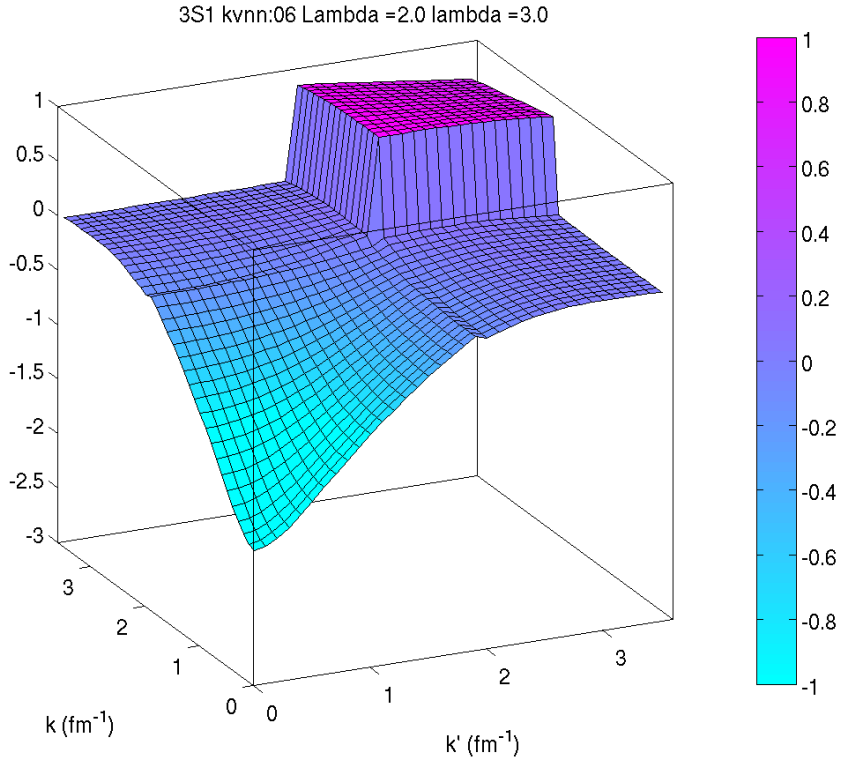

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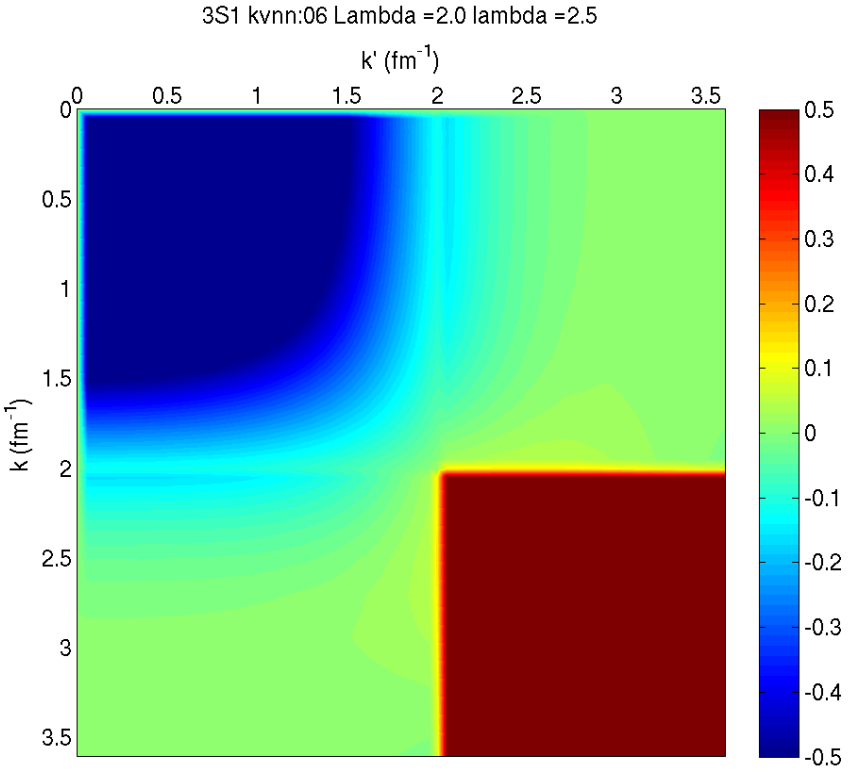

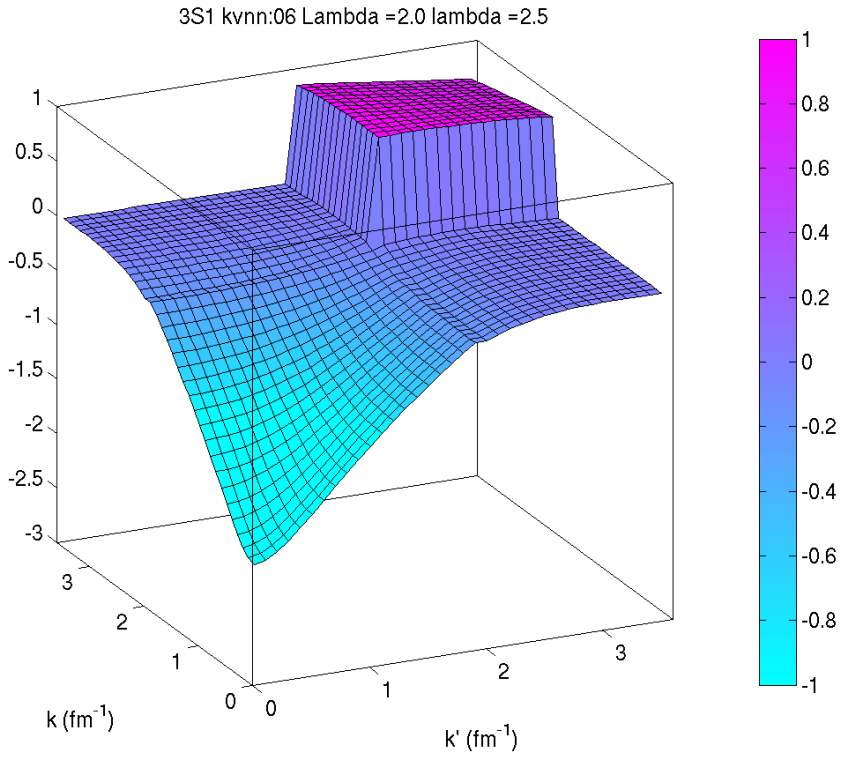

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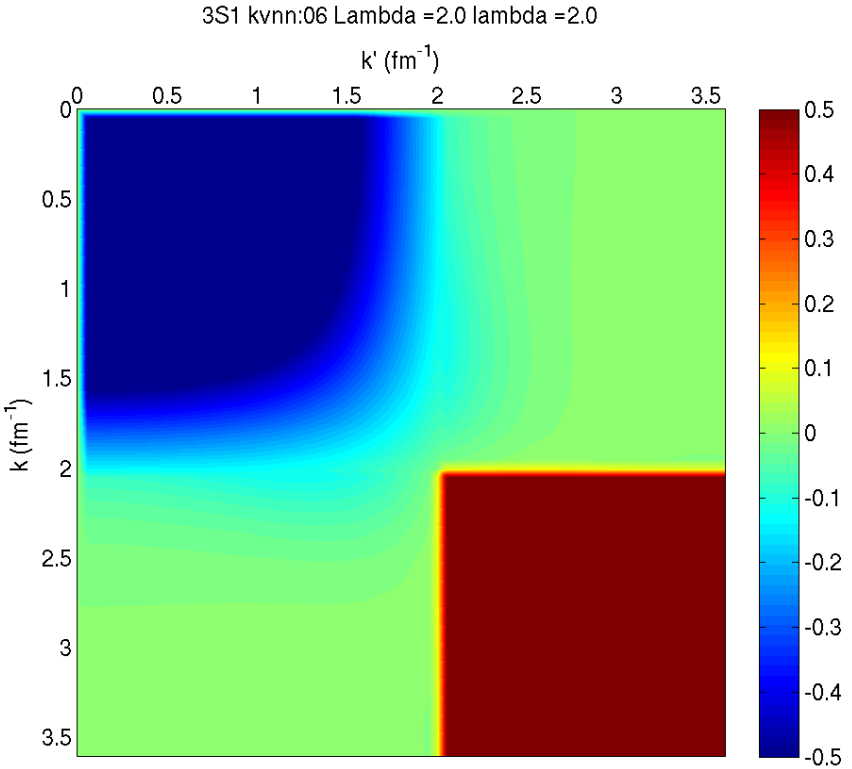

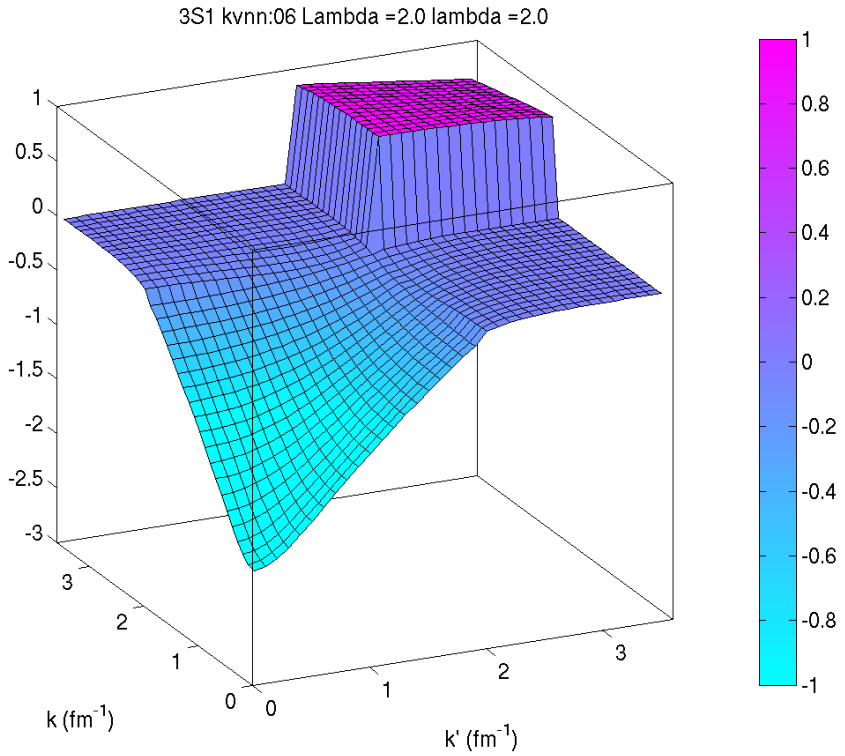

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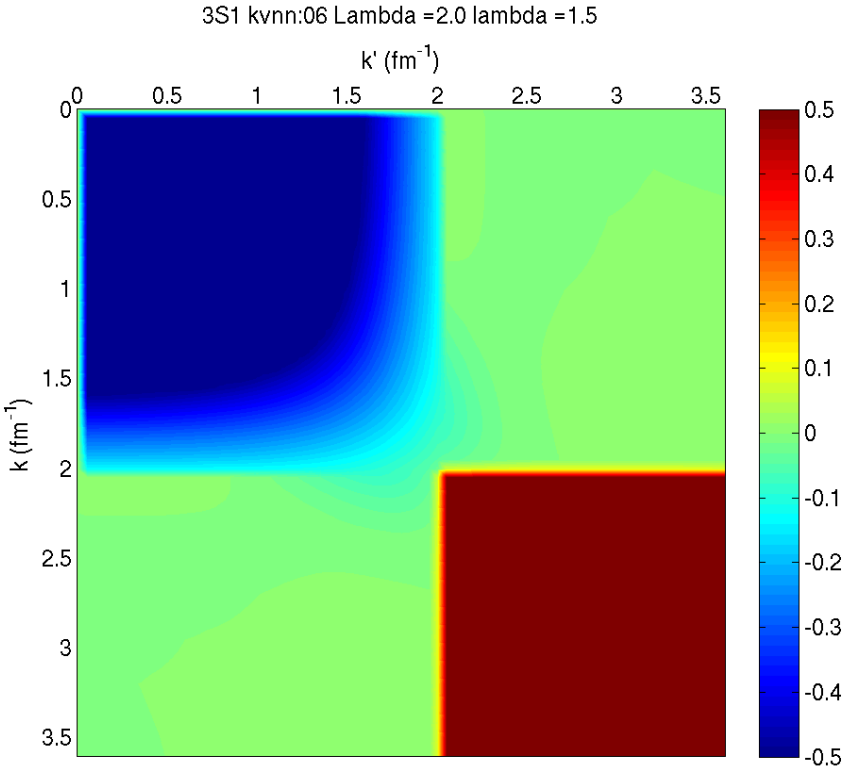

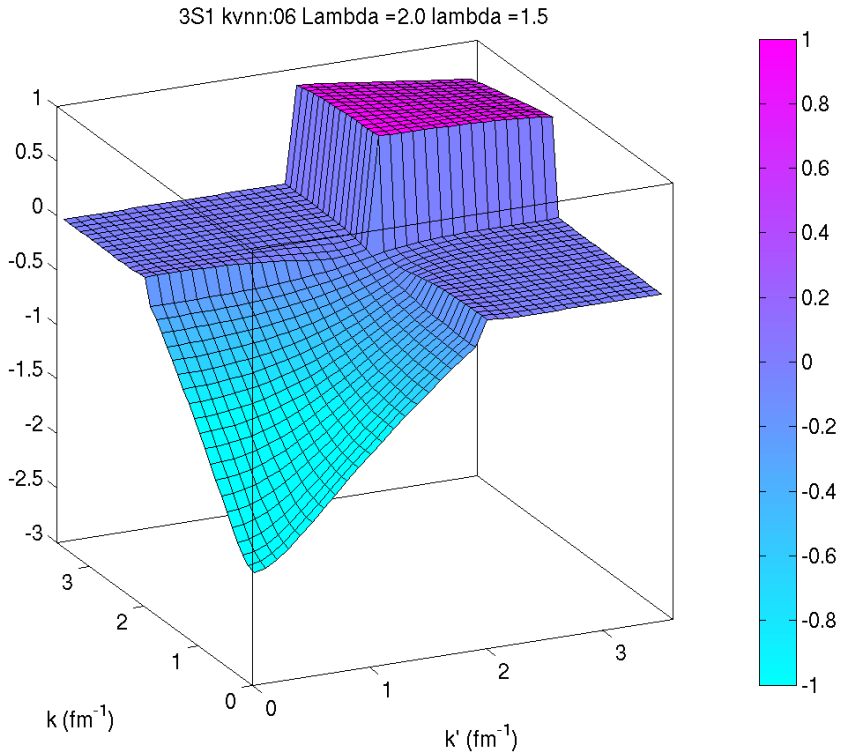

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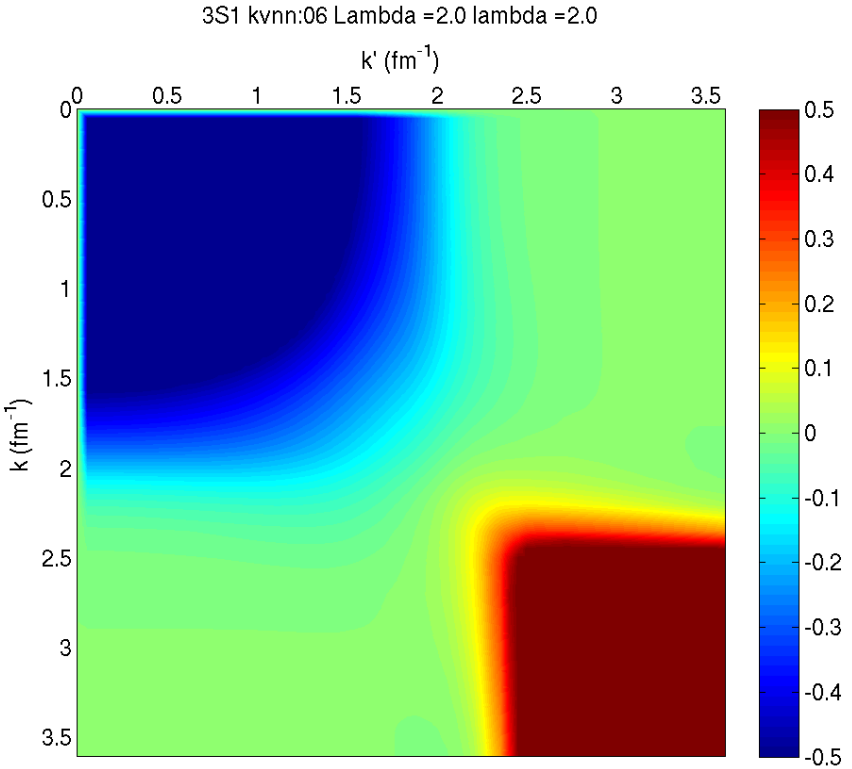

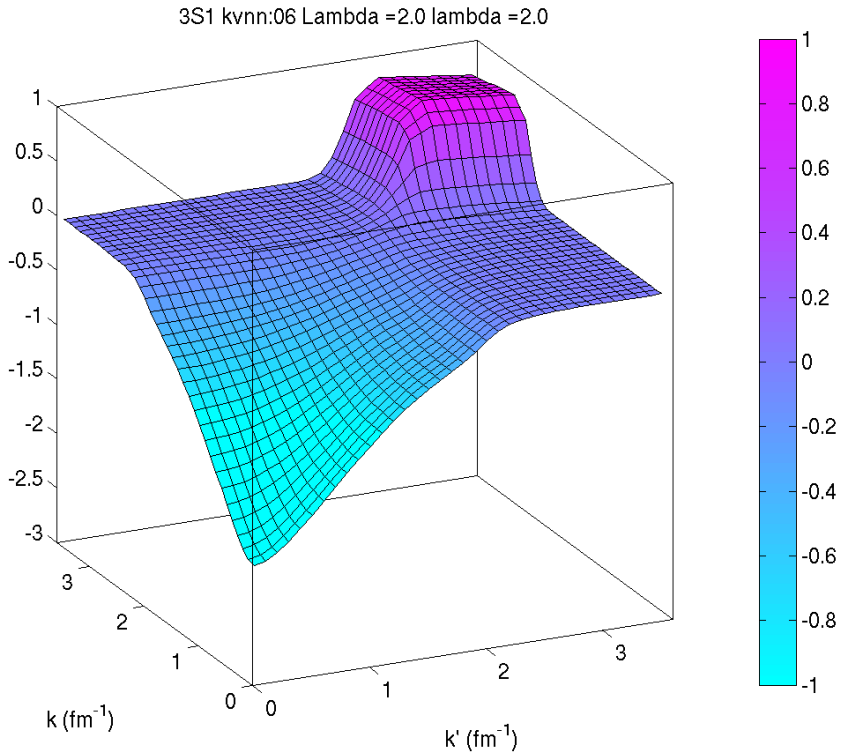

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Flow of different N^{3}LO chiral EFT potentials

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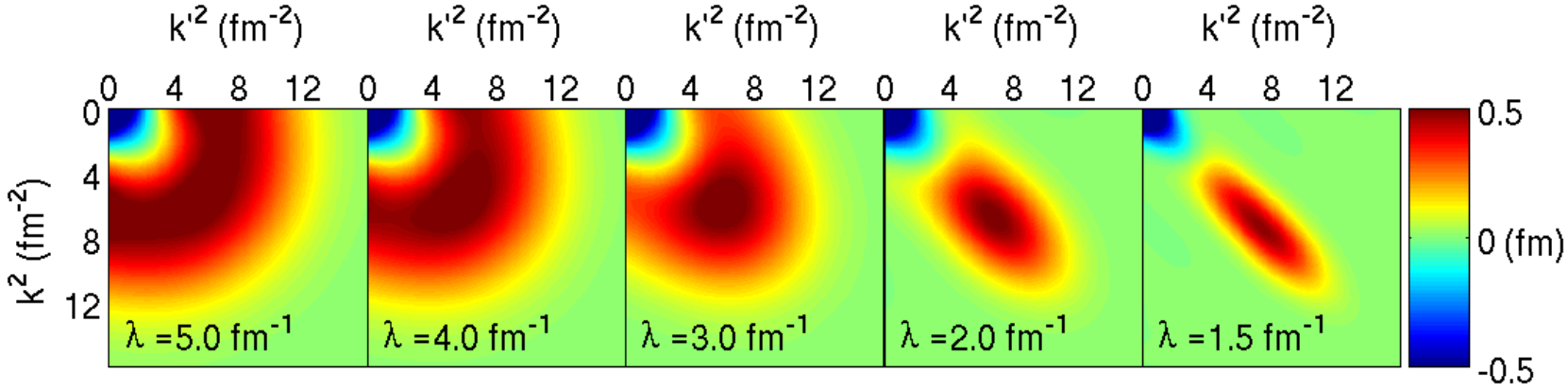

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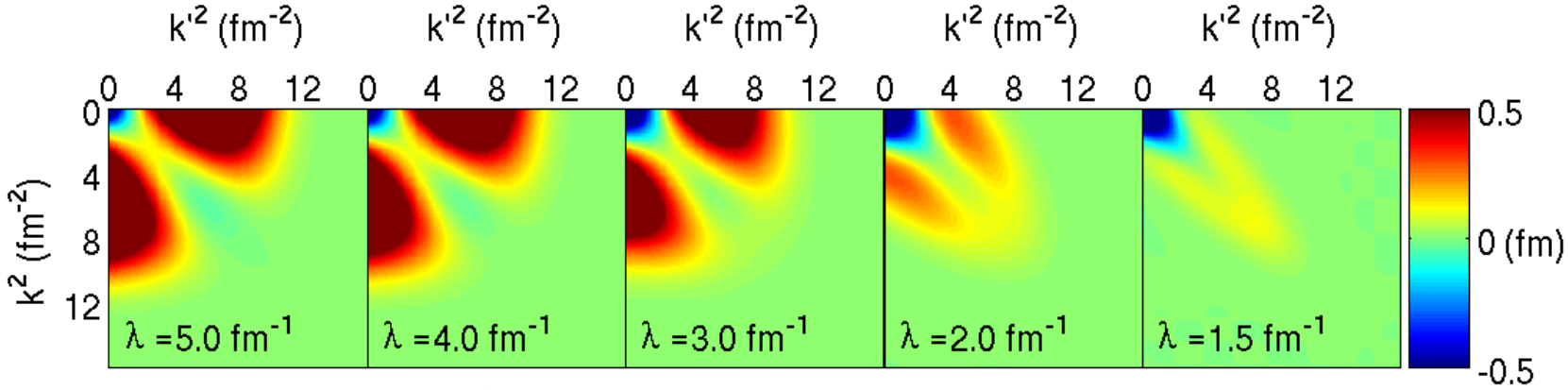

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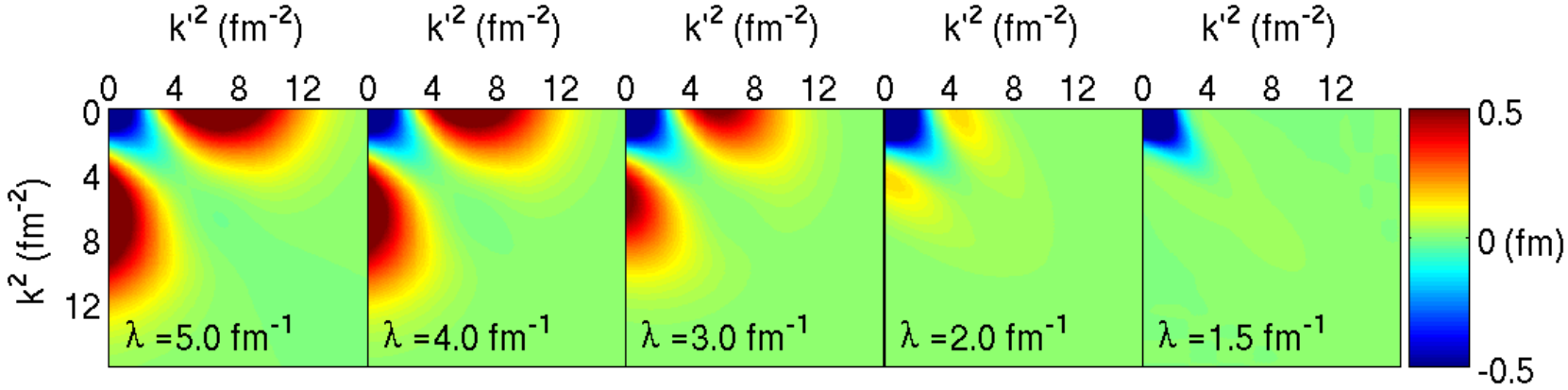

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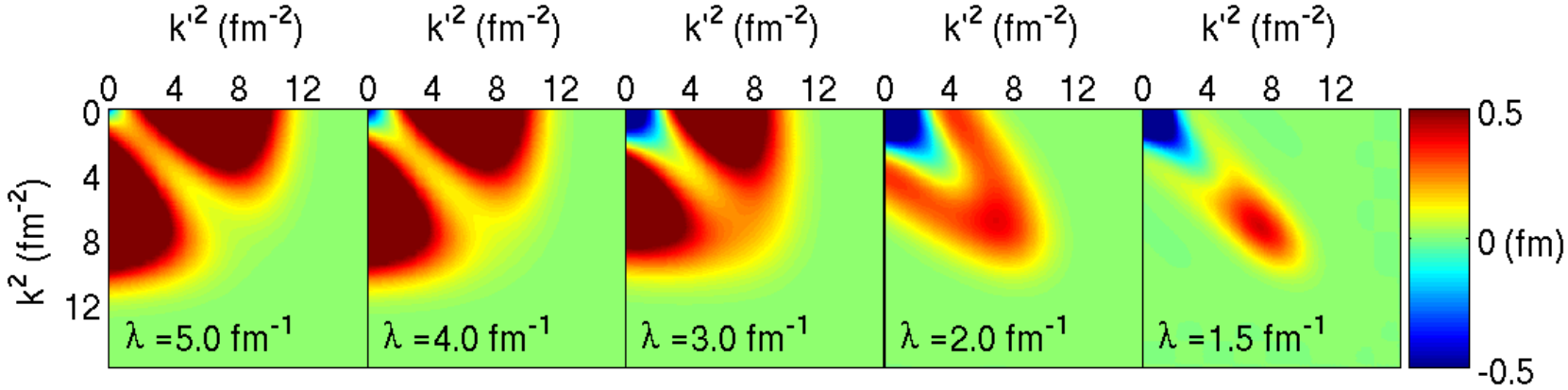

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Run to lower λ via SRG $\Longrightarrow$ $\approx$Universal V_{NN}

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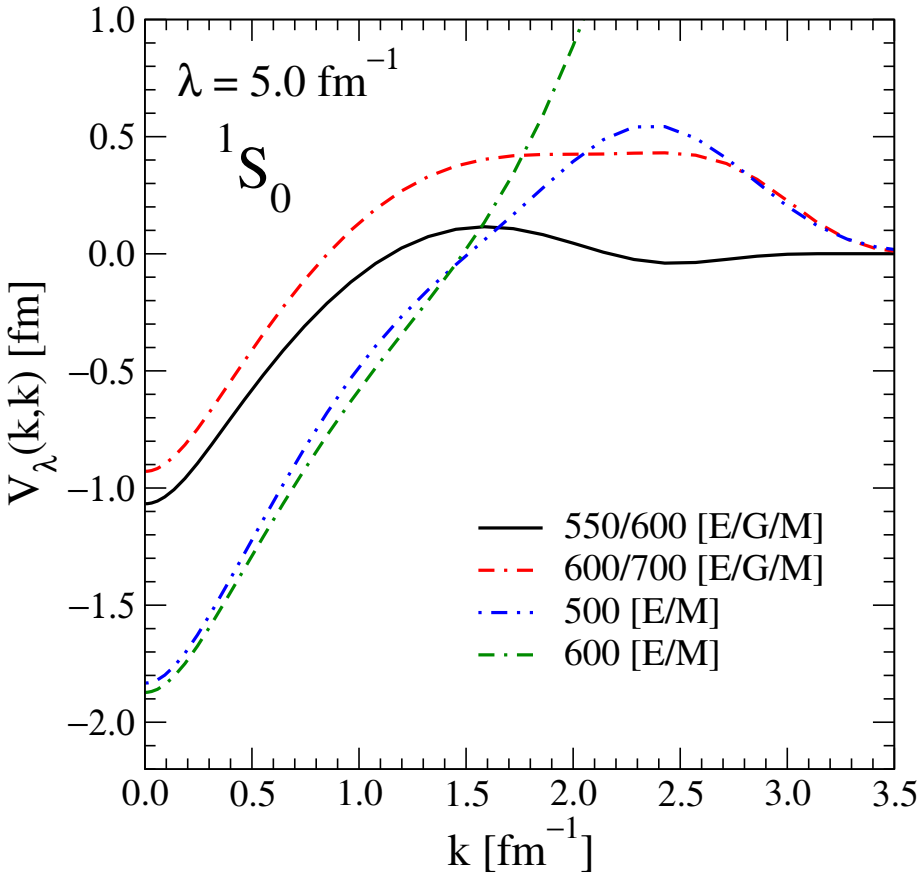
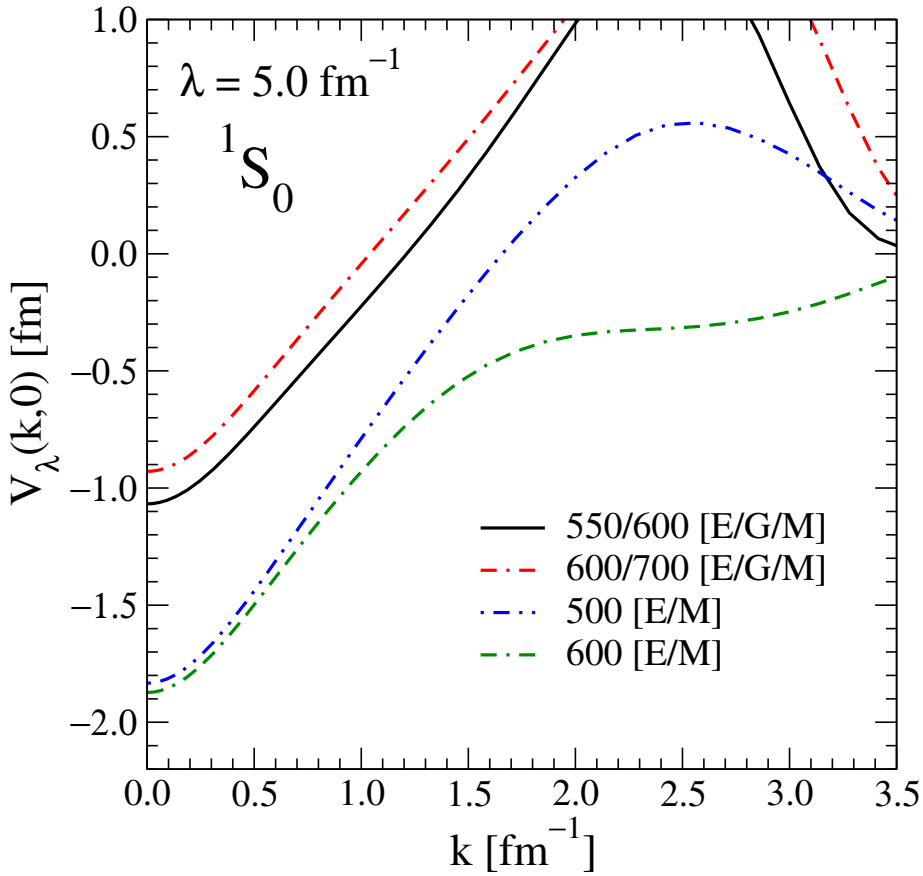


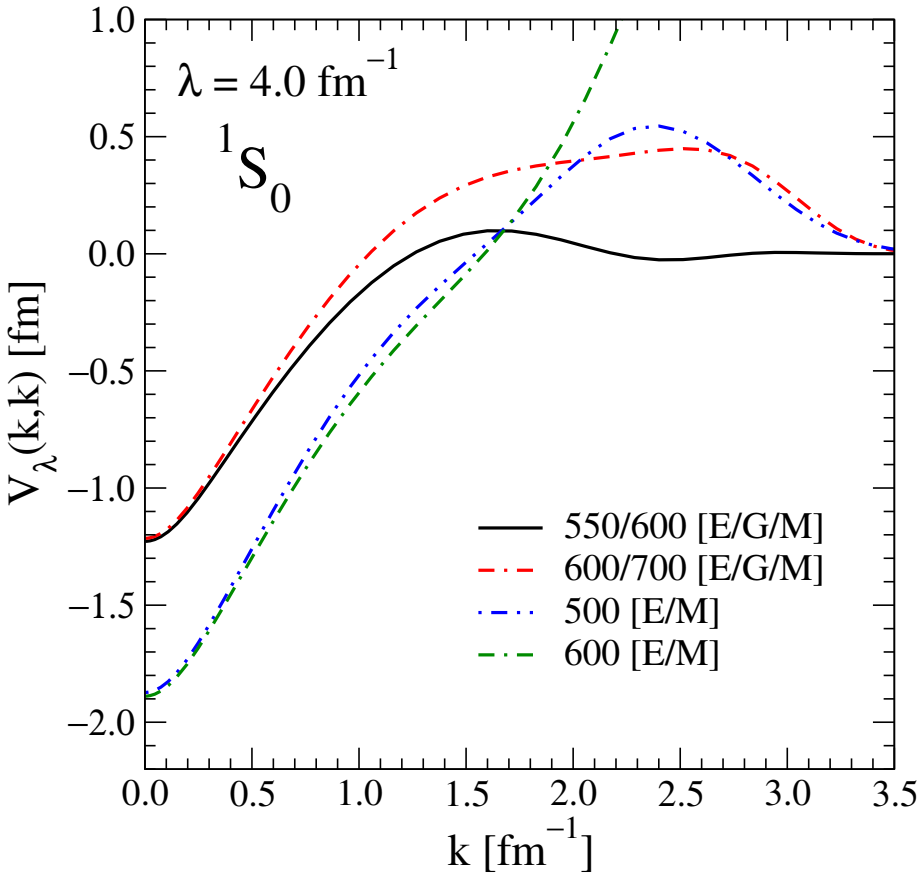
Off-Diagonal $V_\lambda(k,0)$



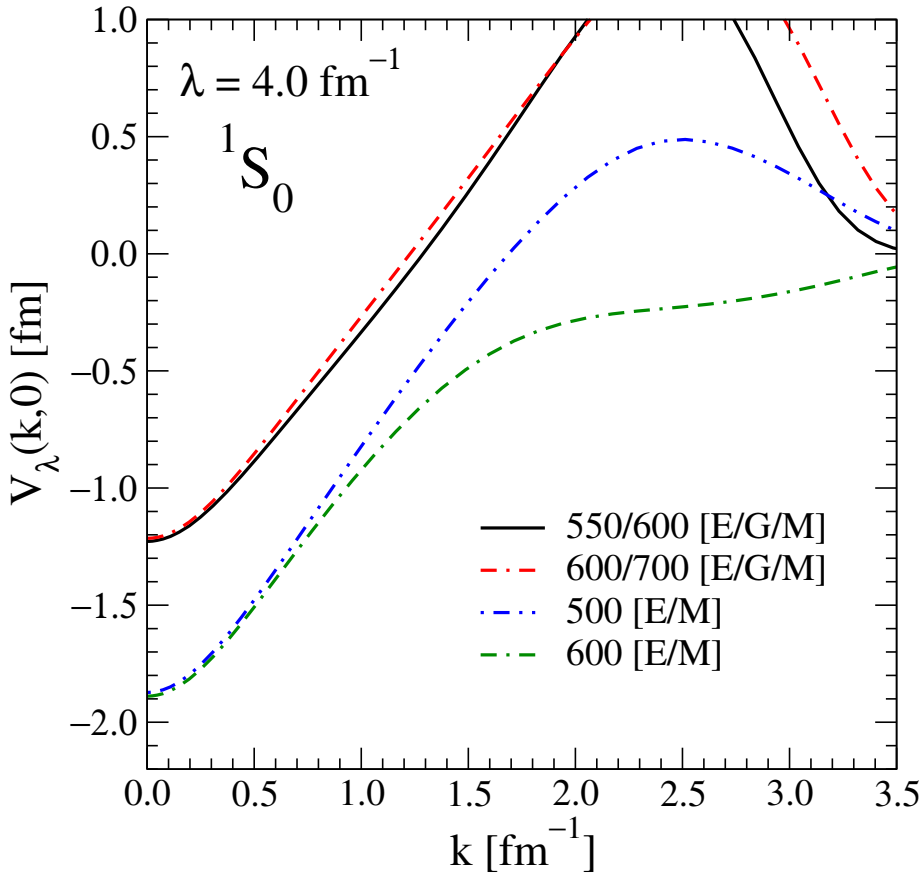
- Cf. inverse scattering in region where S-matrices agree
- Will evolved NNN interactions be universal?

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

Diagonal $V_\lambda(k,k)$



Off-Diagonal $V_\lambda(k,0)$



- Cf. inverse scattering in region where S-matrices agree
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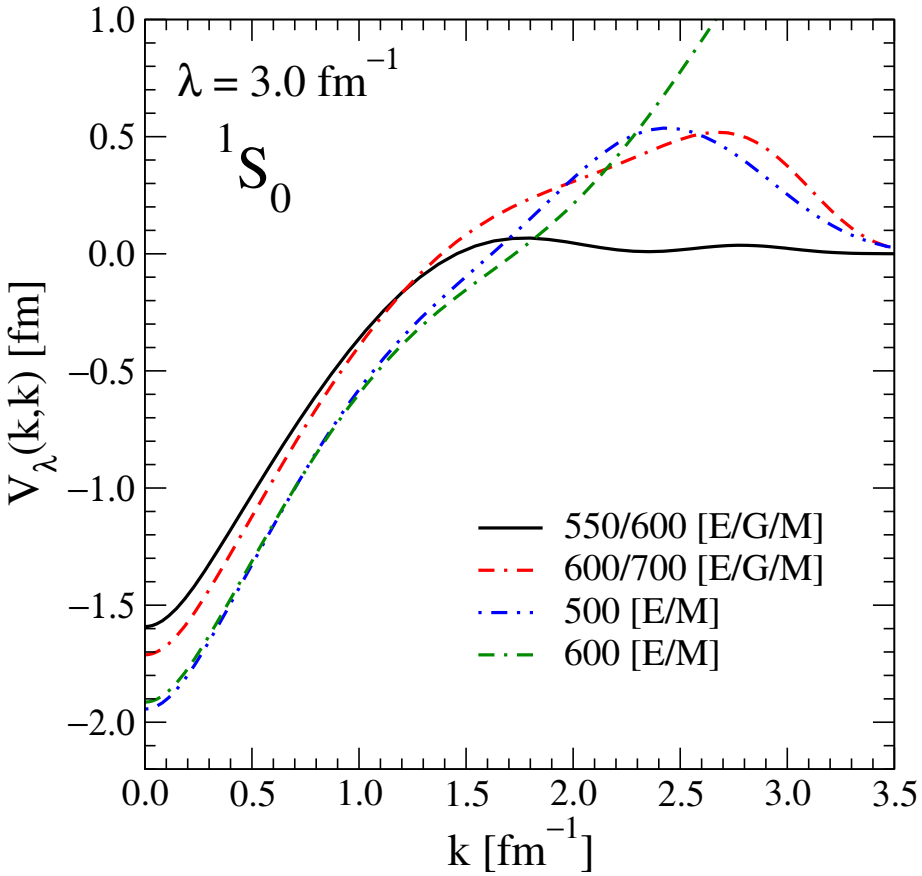

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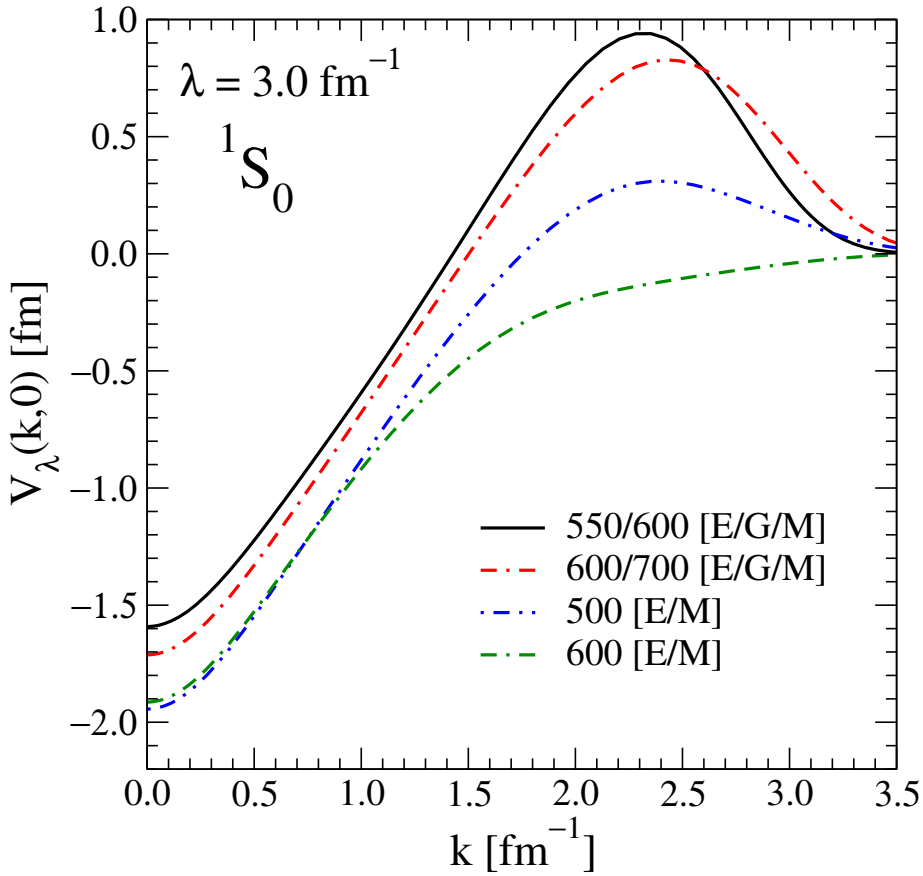

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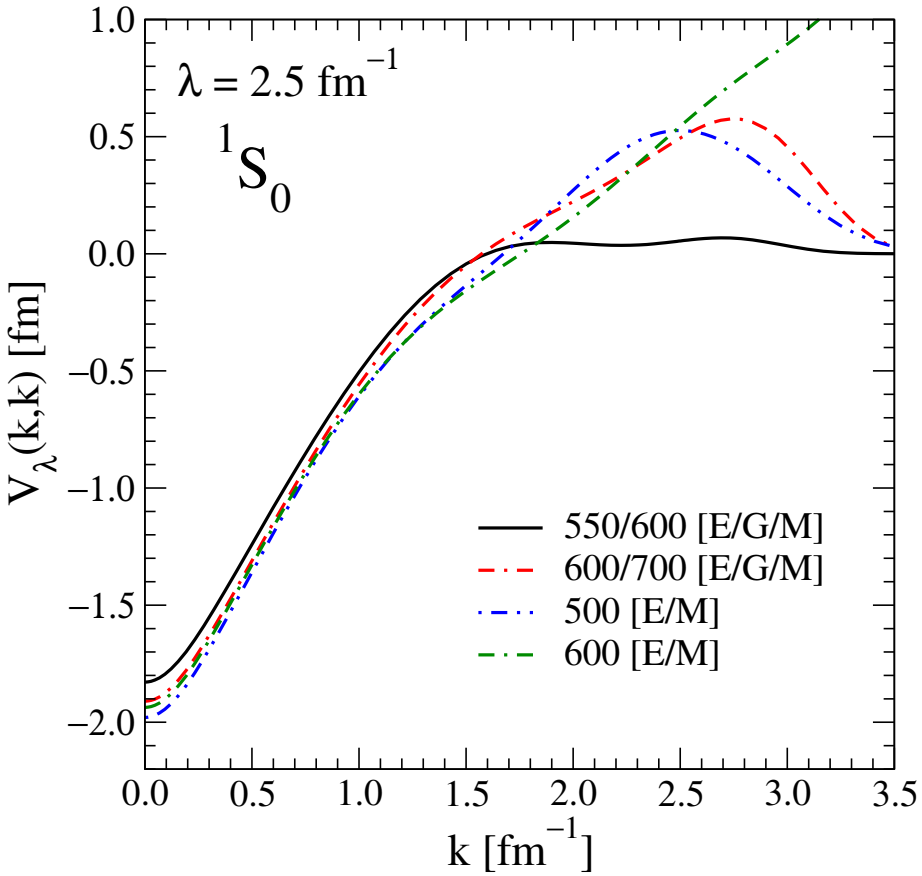

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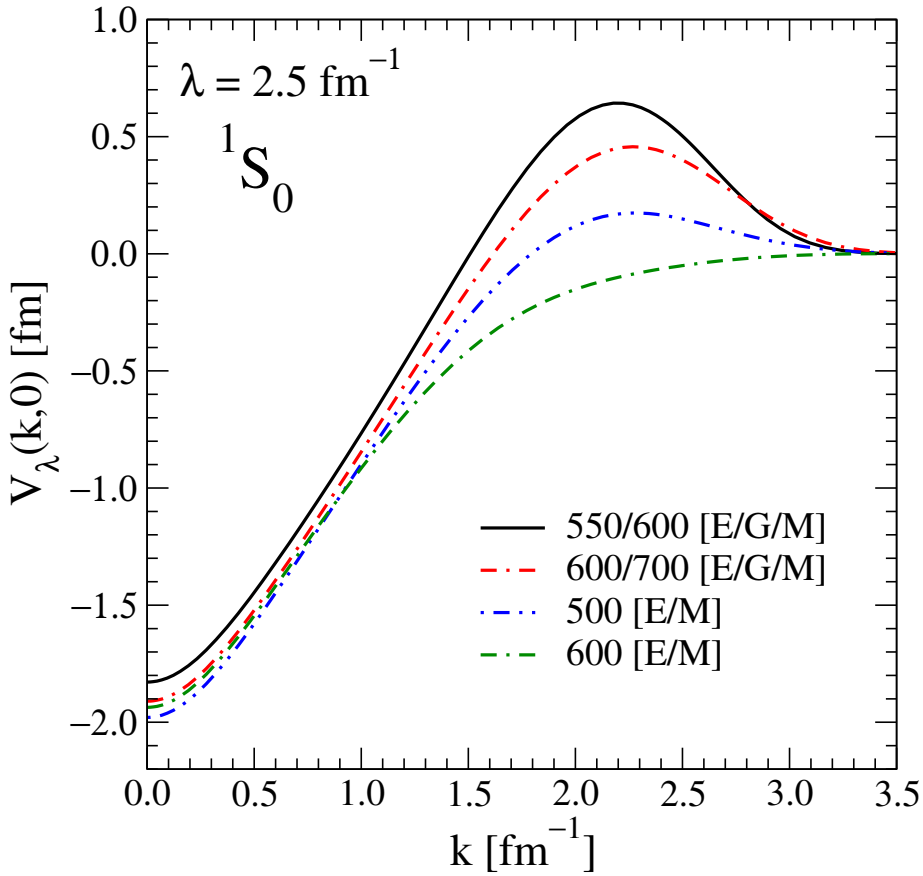

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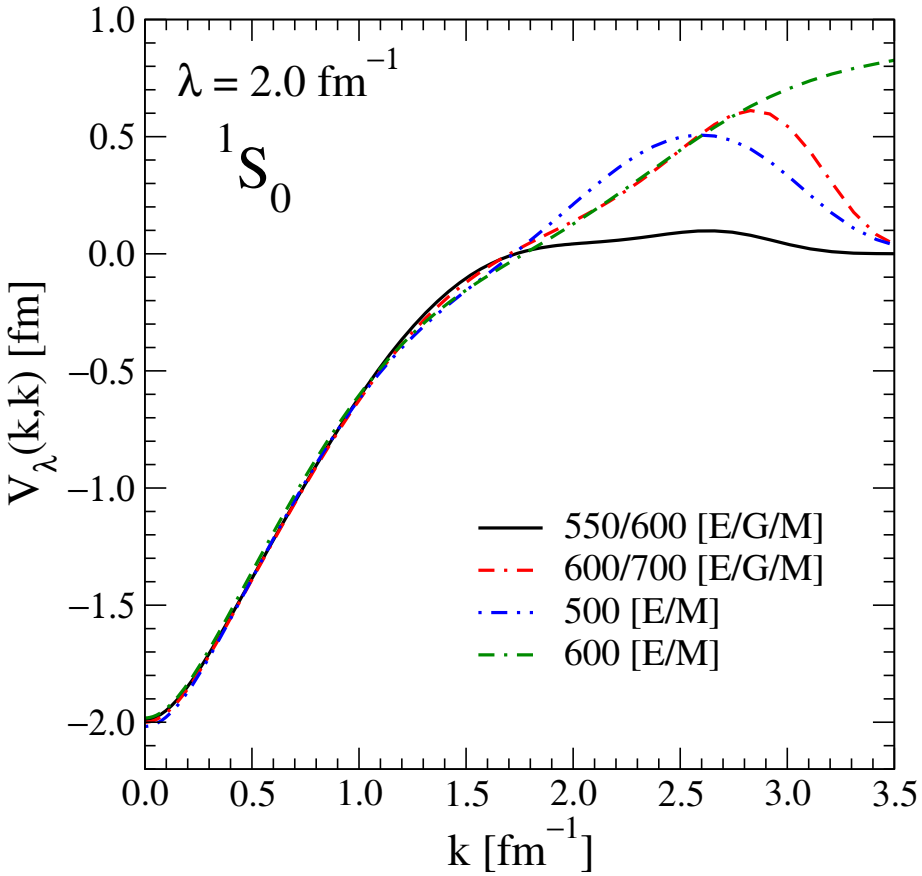

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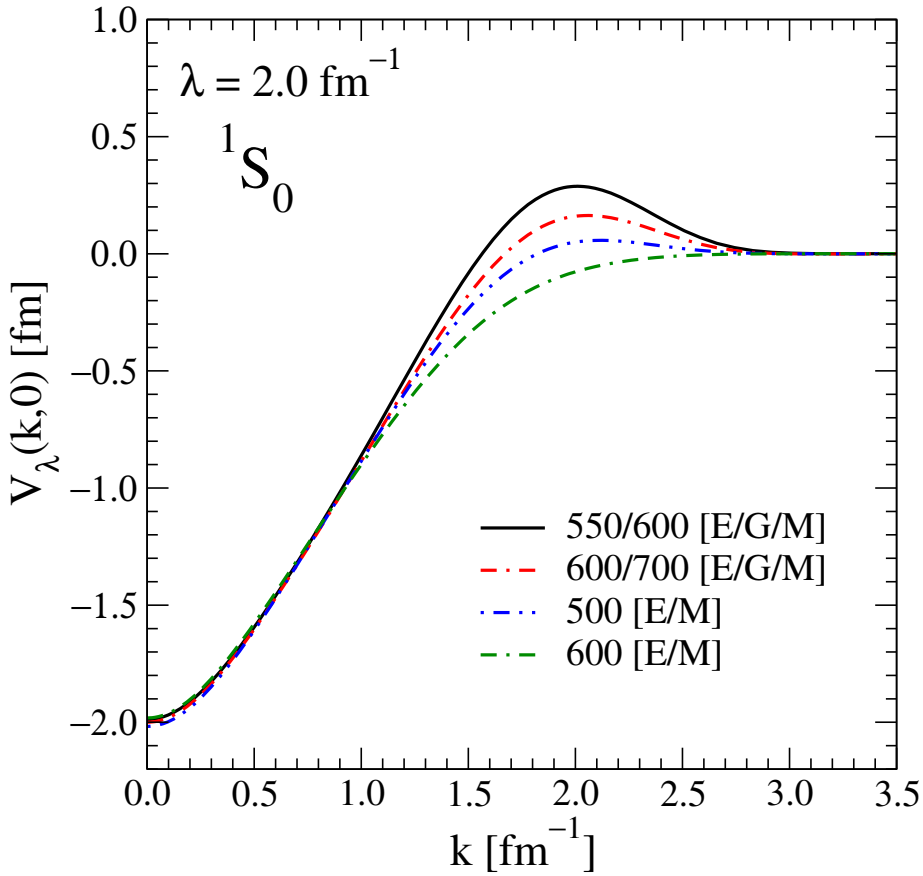

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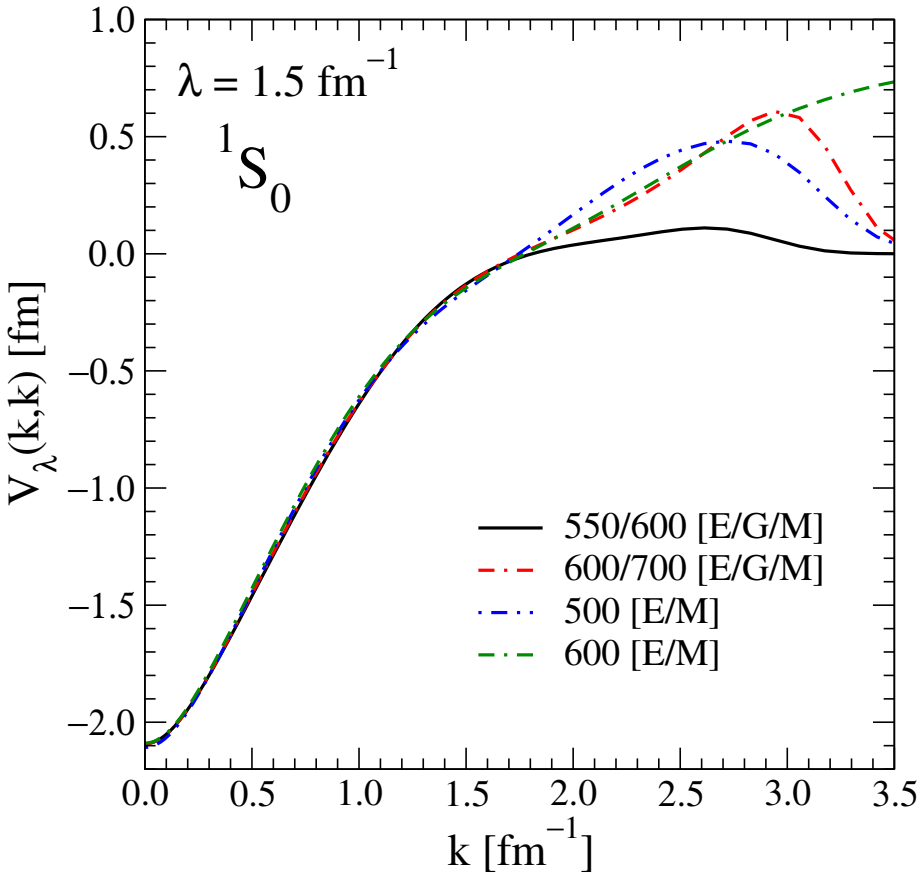

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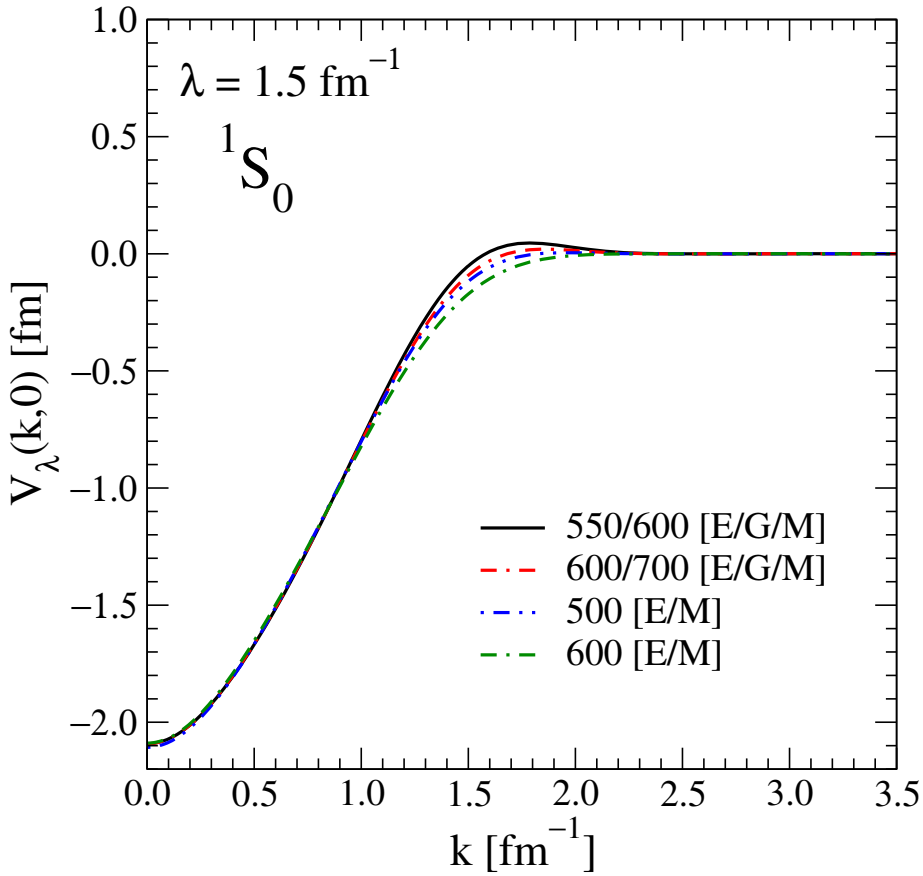

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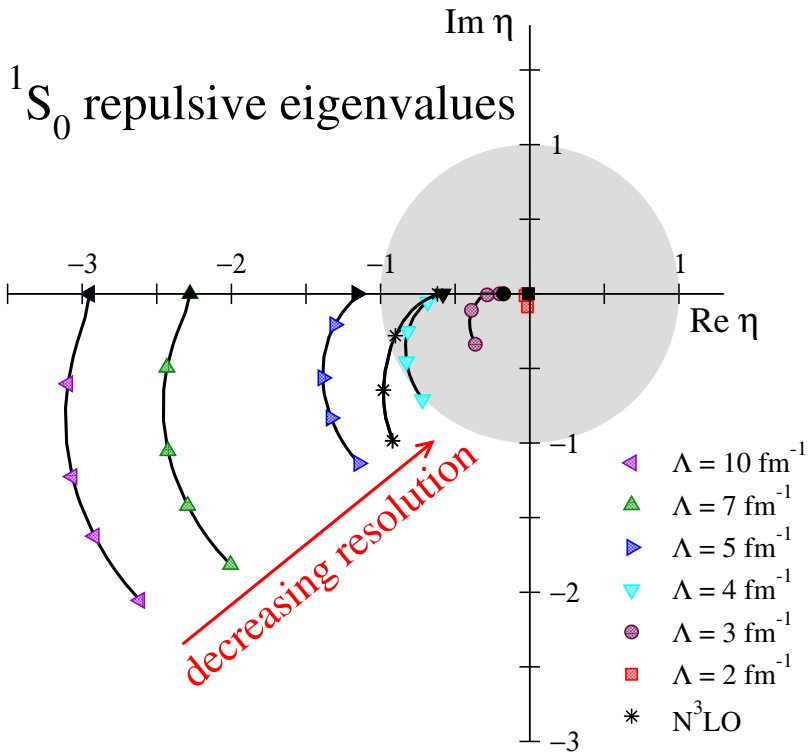
Lowering resolution increases "perturbativeness"

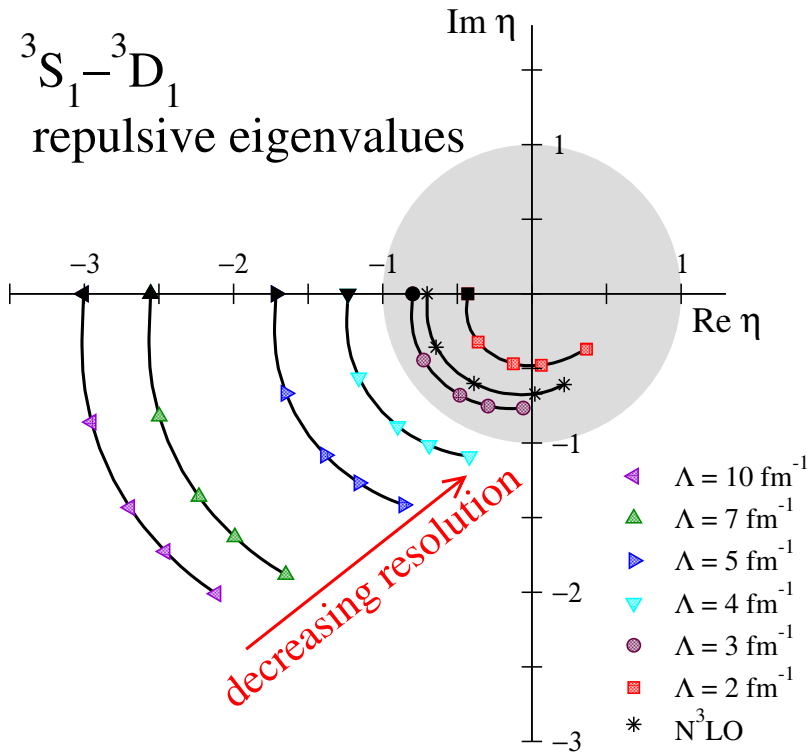
Born Series: $T(E) = V + V\frac{1}{E - H_0}V + V\frac{1}{E - H_0}V\frac{1}{E - H_0}V + \cdots$

- 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* $|\eta_\nu(E)| \geq 1$ [Bogner et al. (2006)]





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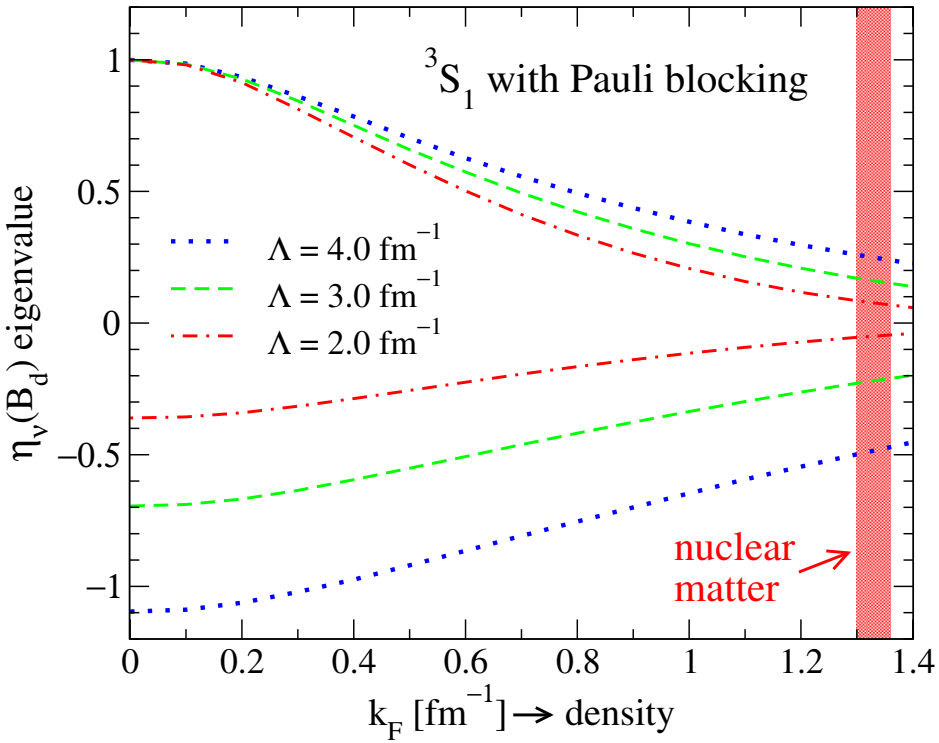
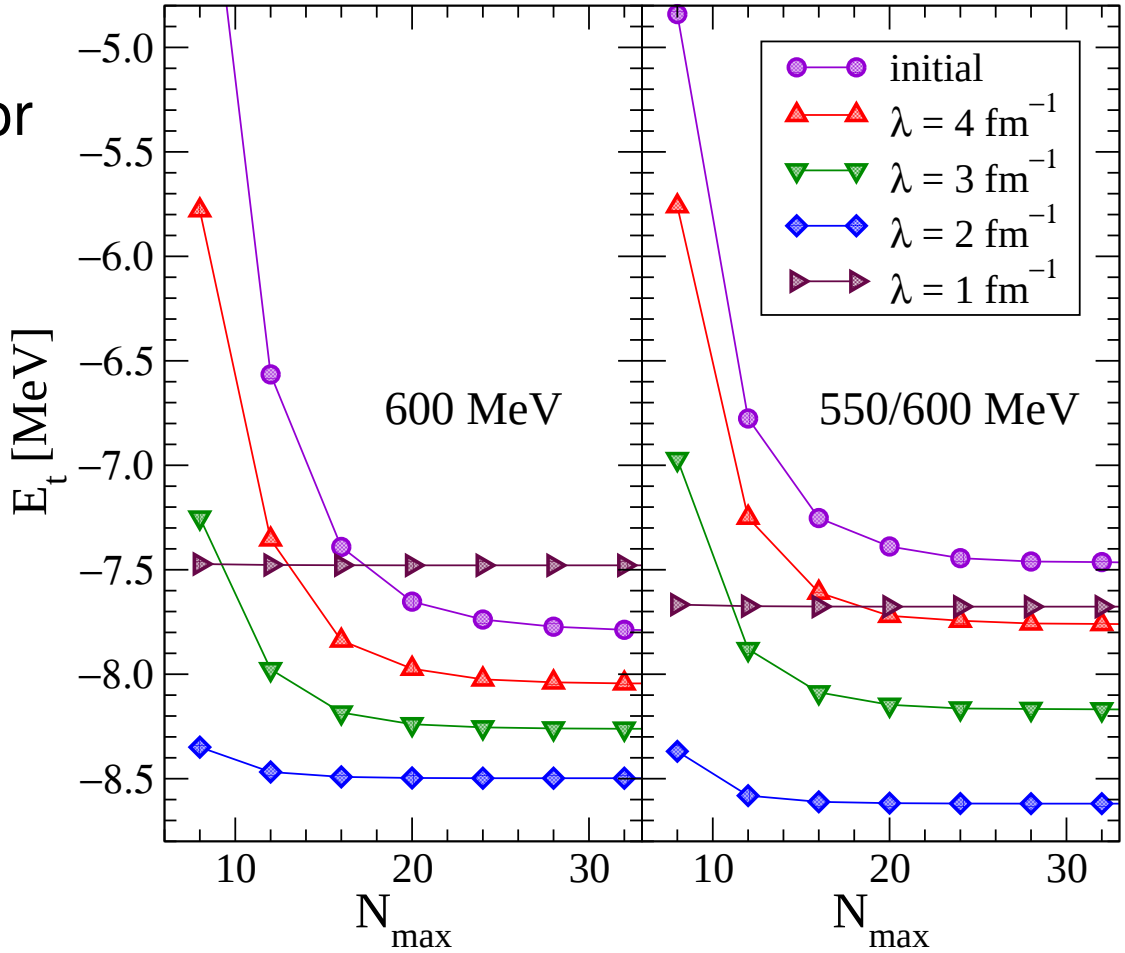


Variational calculations in three-nucleon systems

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



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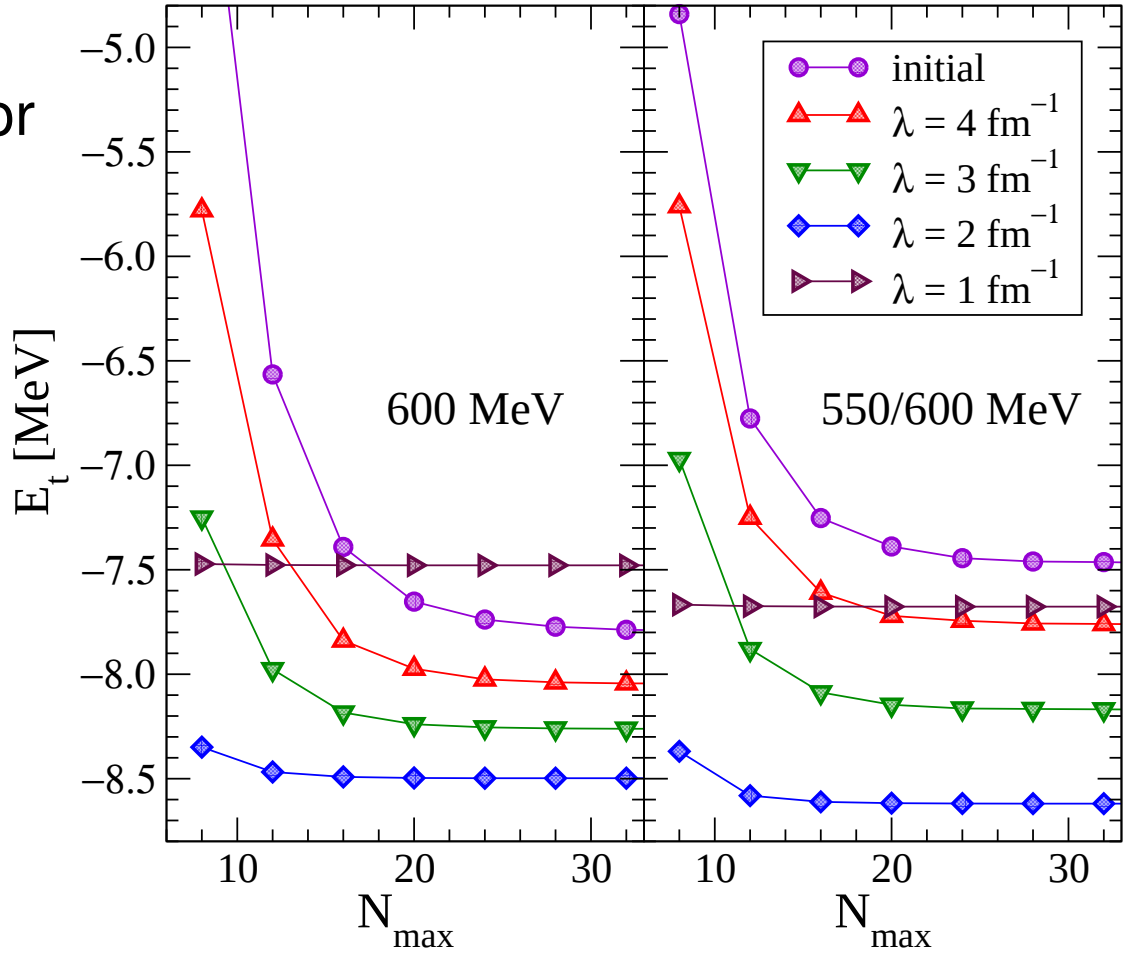
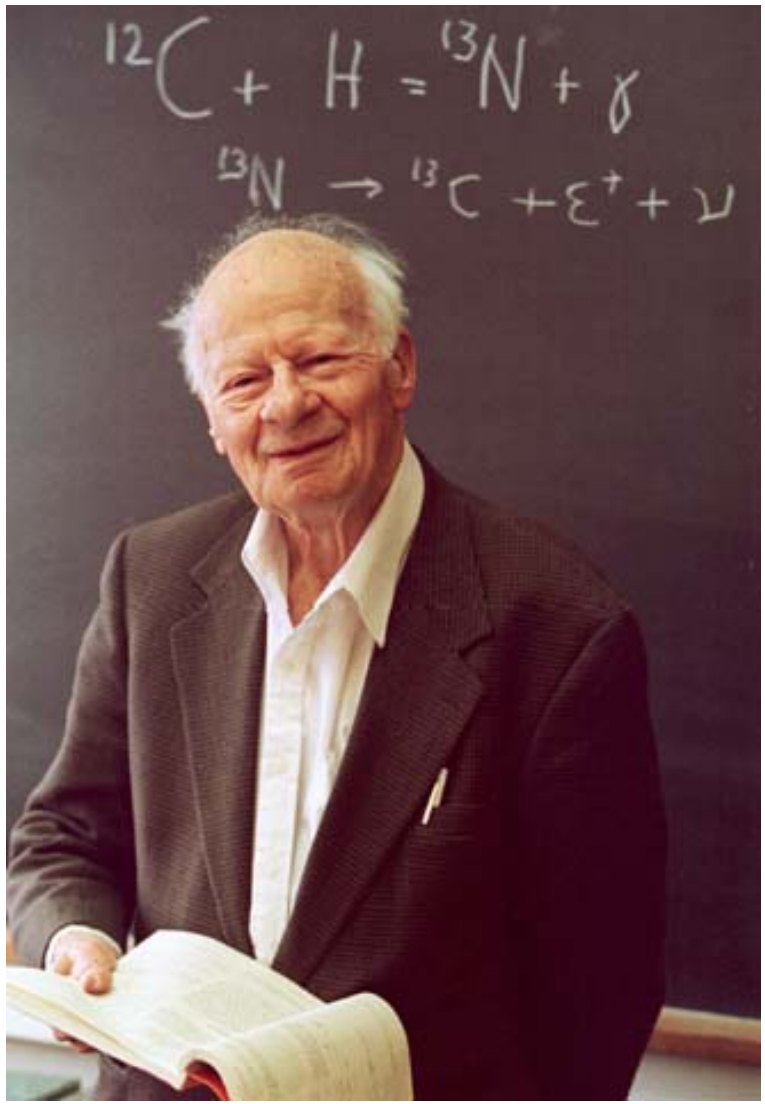
- Different binding energies!
- Nuclear matter doesn't saturate at low λ



Deja vu all over again?

- There were active attempts to transform away hard cores and soften the tensor interaction in the late sixties and early seventies.
- But the requiem for soft potentials was given by Bethe (1971):
  "Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."
- Next 35+ years struggling to solve accurately with "hard" potential



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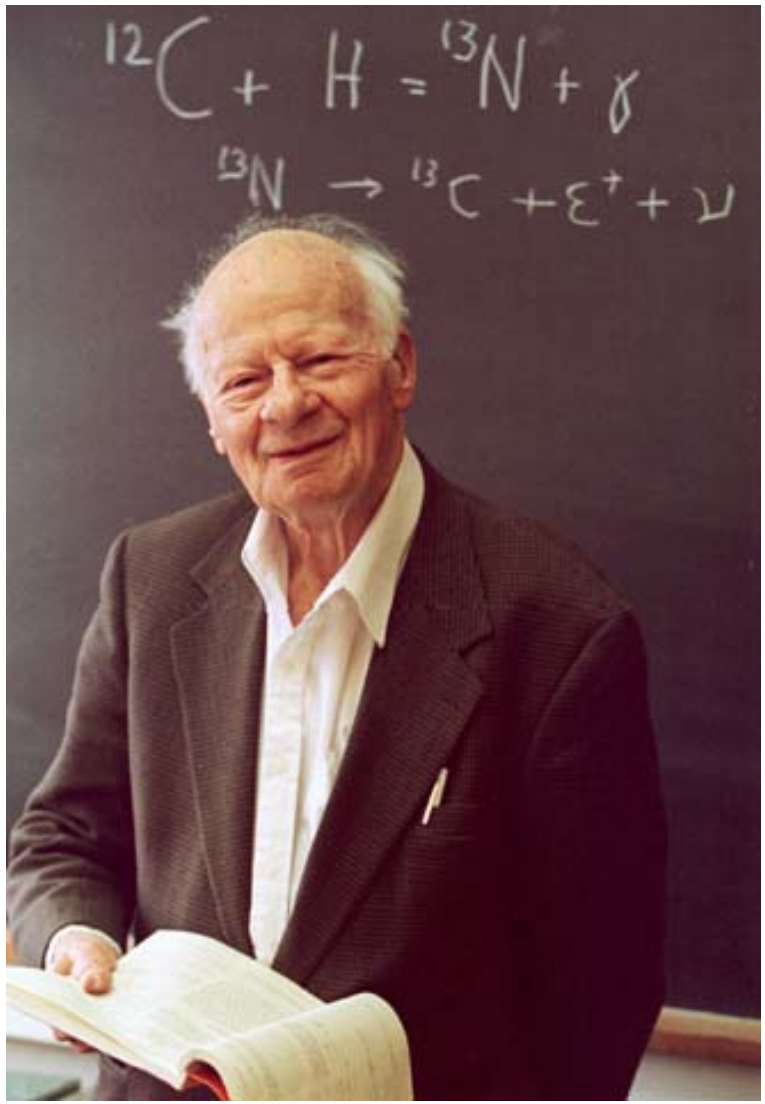
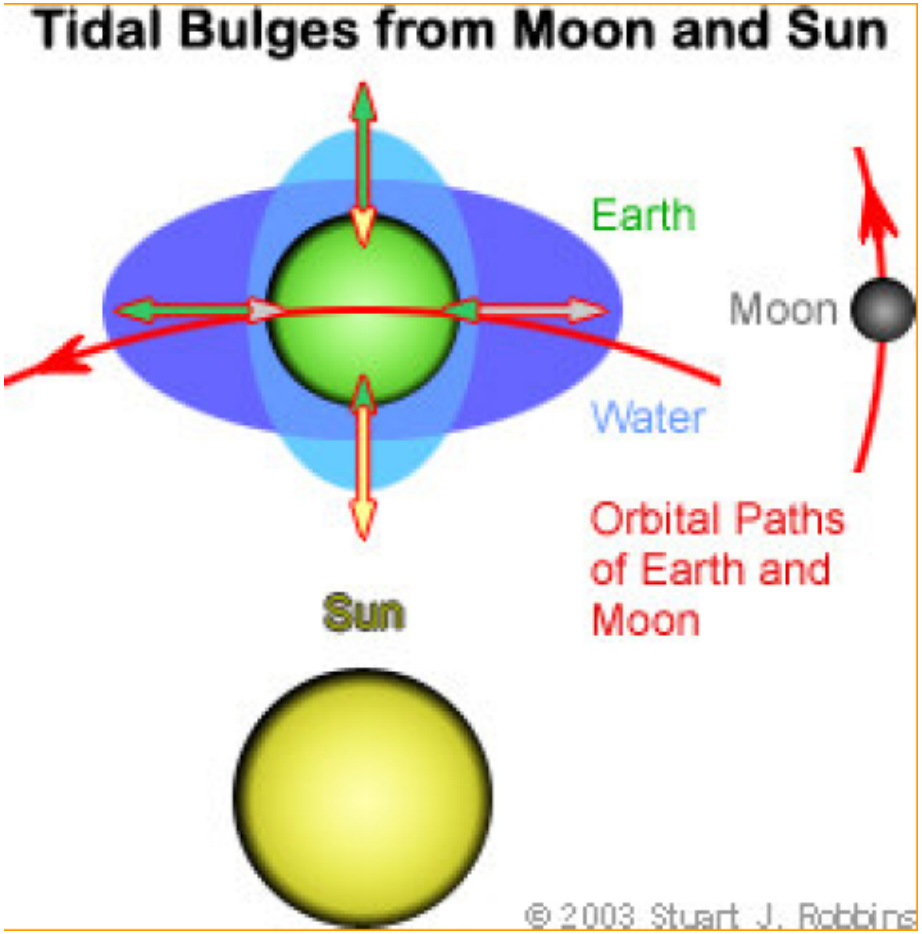
- But the story is not complete: three-nucleon forces (3NF)!



Tidal analog to nuclear 3-body forces

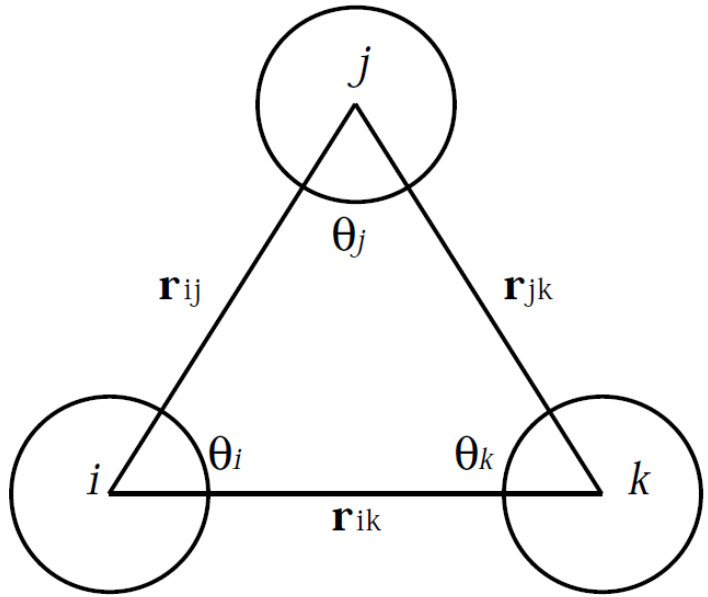
- Three-body forces between protons and neutrons are not negligible
- Analogous to tidal forces: the gravitational force on the Earth is not just the pairwise sum of Earth-Moon and Earth-Sun forces



Atomic 3-body forces: Axilrod-Teller term (1943)

- Three-body potential for atoms/molecules from triple-dipole mutual polarization (3rd-order perturbation correction)

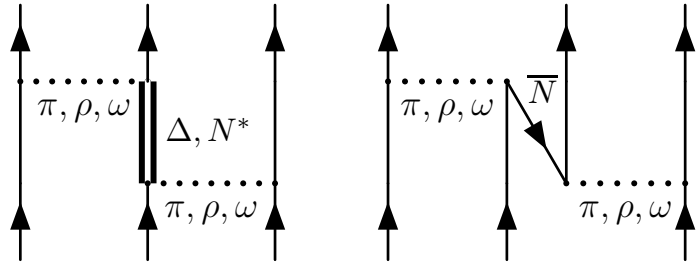
$$V(i,j,k) = \frac{\nu(1 + 3\cos\theta_i \cos\theta_j \cos\theta_k)}{(r_{ij} r_{ik} r_{jk})^3}$$

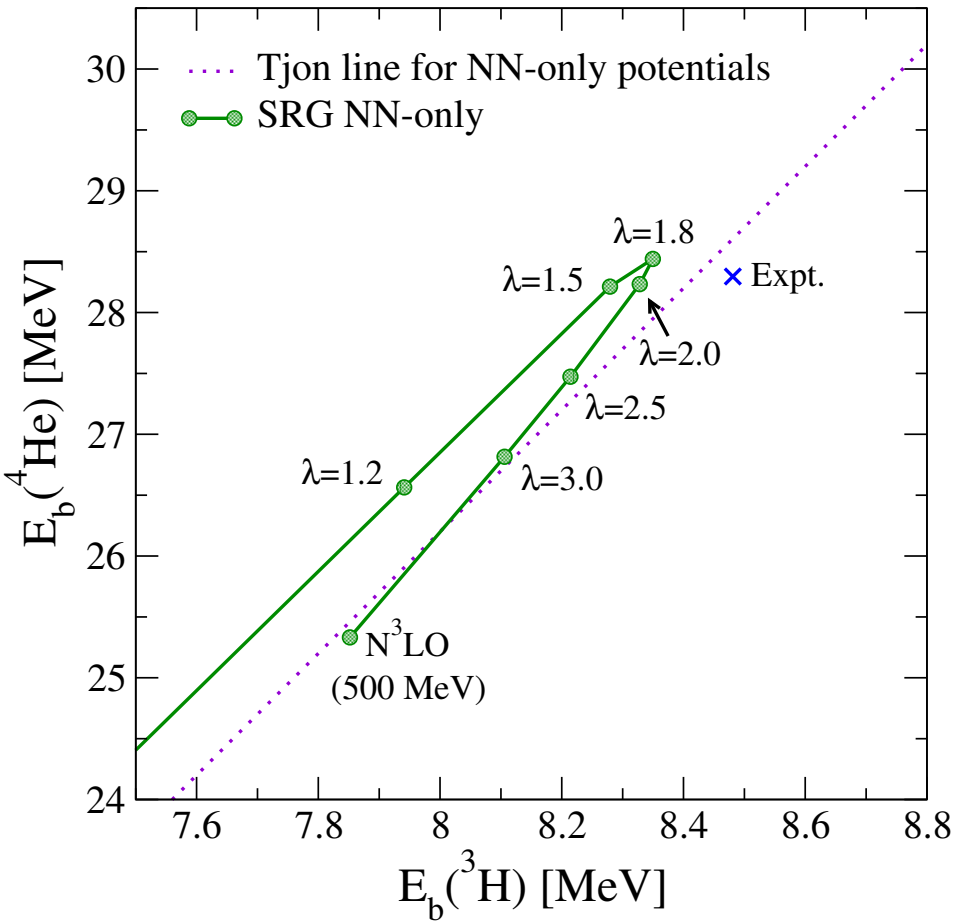


- Usually negligible in metals and semiconductors
- Can be important for ground-state energy of solids bound by van der Waals potentials
- Bell and Zuker (1976): 10% of energy in solid xenon

Observations on three-body forces

- Three-body forces arise from eliminating/decoupling dof's
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
  - observables depend on Λ/λ
  - cutoff dependence as tool





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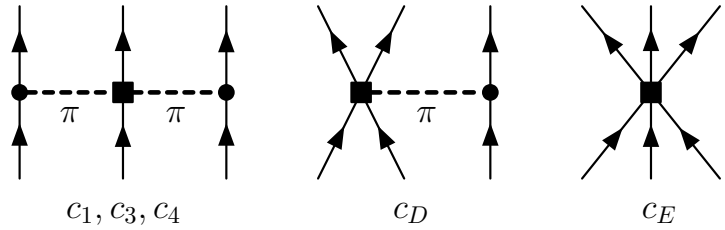
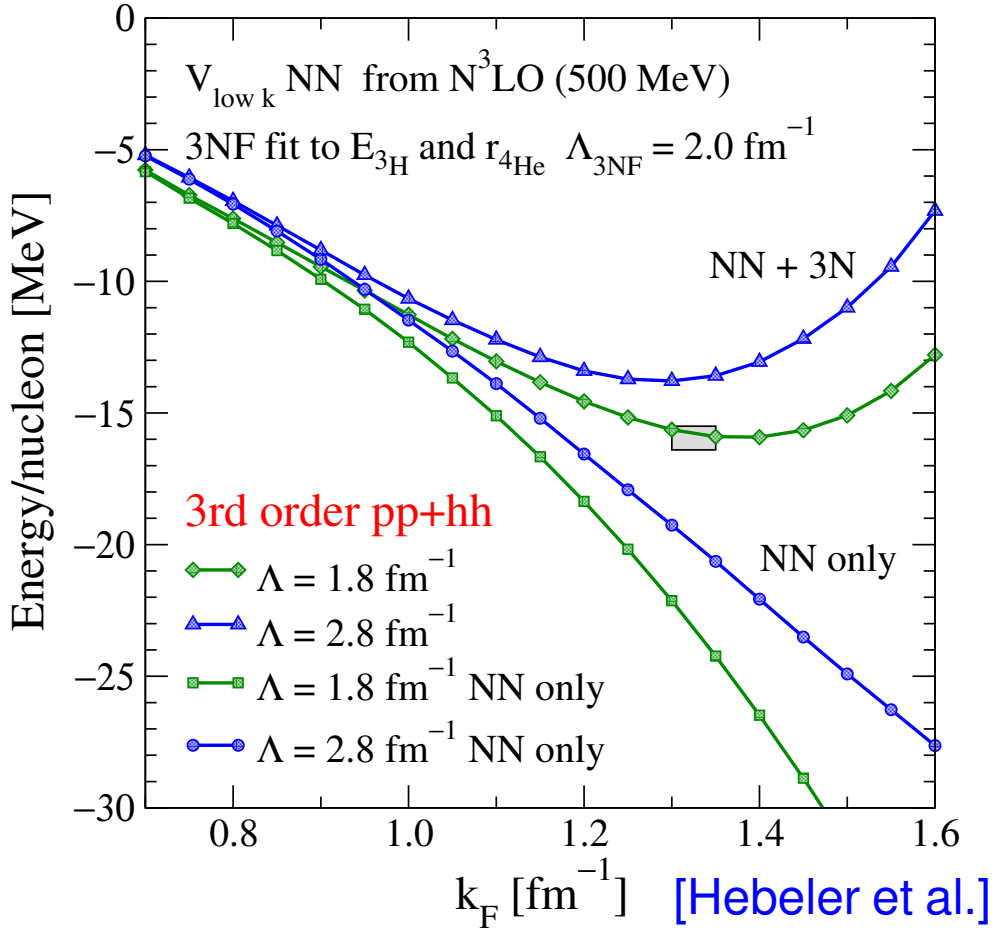
- Omitting 3-body forces leads to model dependence
  - observables depend on Λ/λ
  - cutoff dependence as tool
- NNN at different Λ/λ must be fit or evolved to χEFT
  - NNN contribution is important at low resolution (e.g., nuclear matter)





[Hebeler et al.]

Flow equations lead to many-body operators

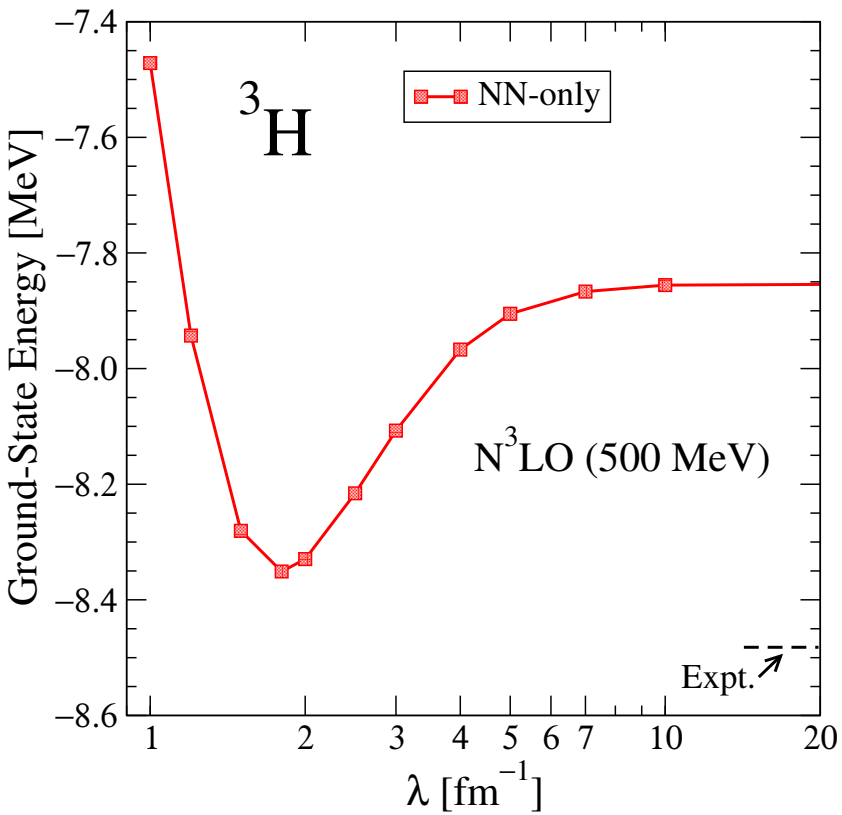
- Consider a's and $a^\dagger$'s wrt s.p. basis and reference state:

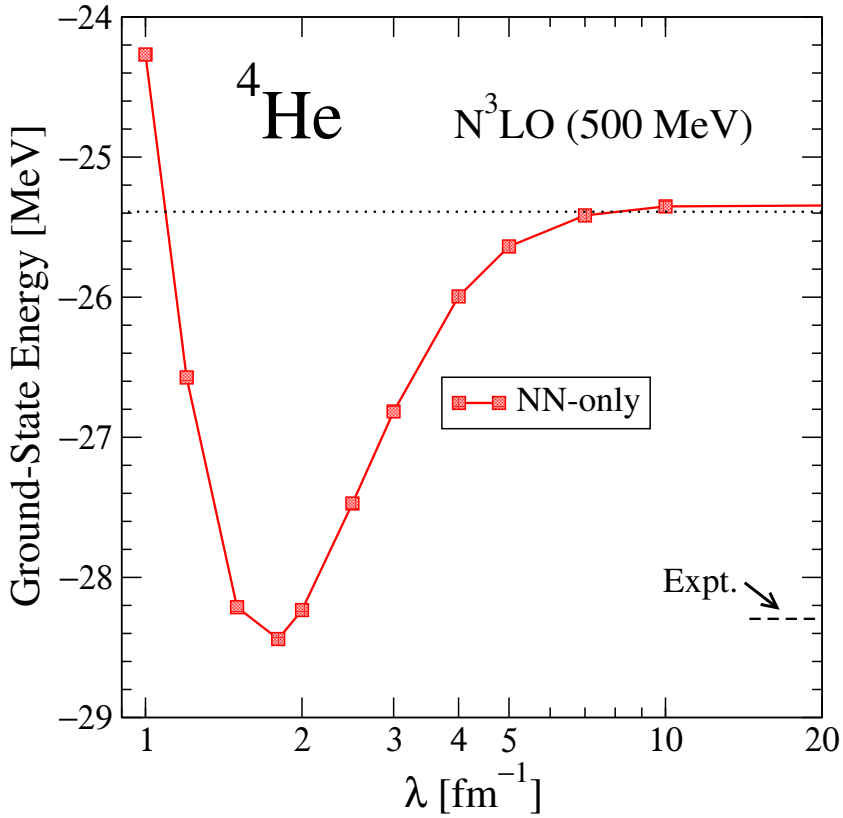
$$\frac{dV_s}{ds} = \Big[\Big[\sum \underbrace{a^\dagger a}_{G_s}, \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}\Big], \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}\Big] = \cdots + \sum \underbrace{a^\dagger a^\dagger a^\dagger aaa}_{\text{3-body!}} + \cdots$$

  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
- Alternative: choose a non-vacuum reference state
  $\Longrightarrow$ in-medium SRG (e.g., HF reference state)

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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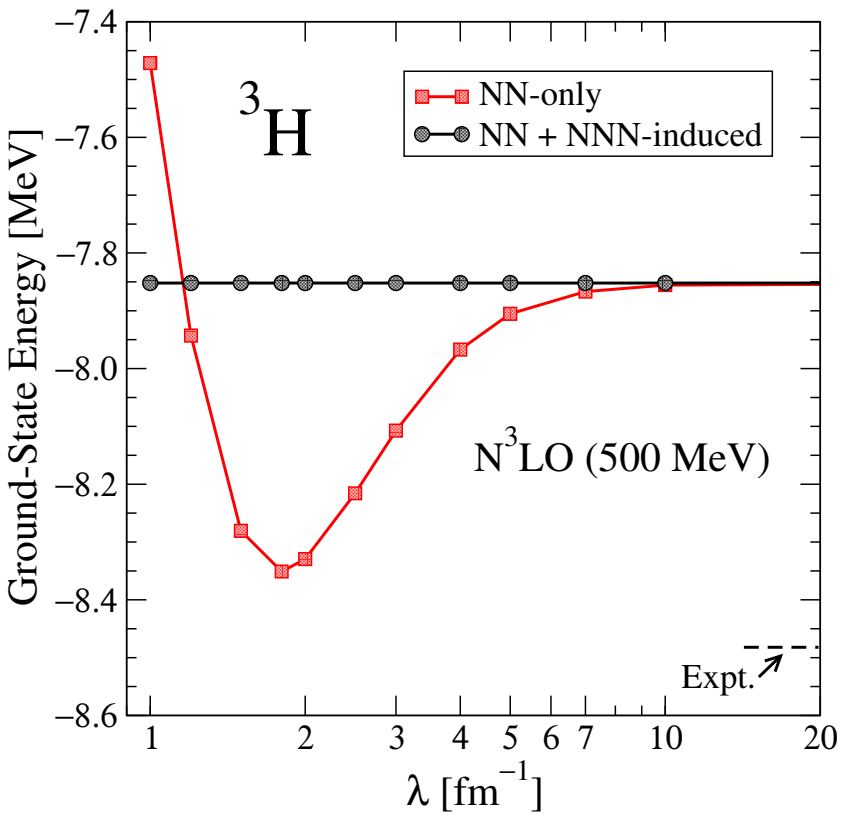

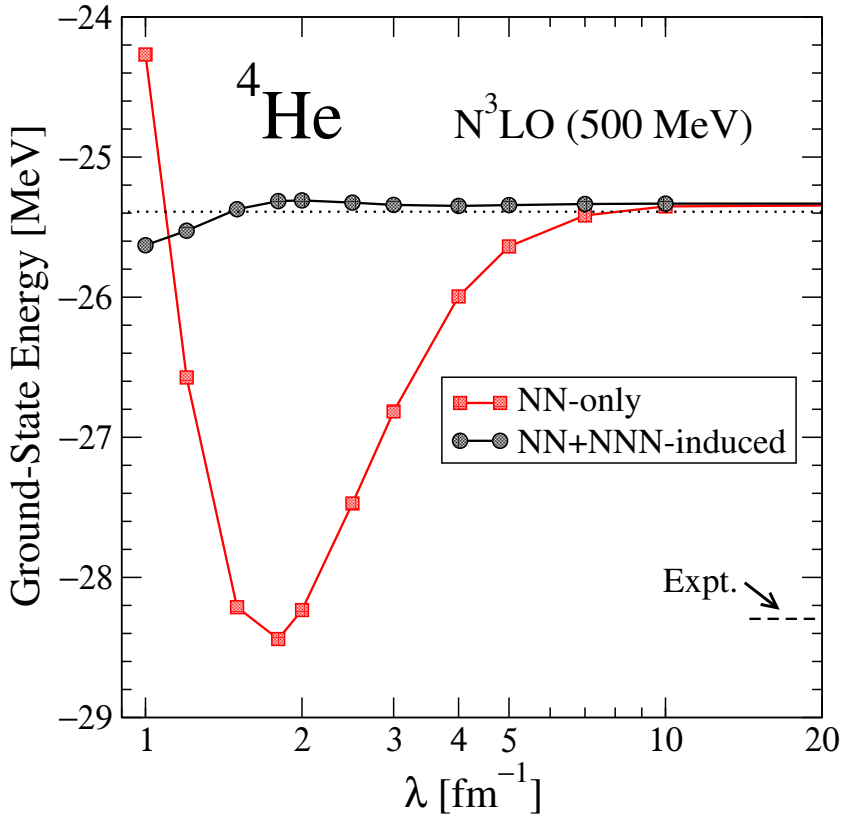

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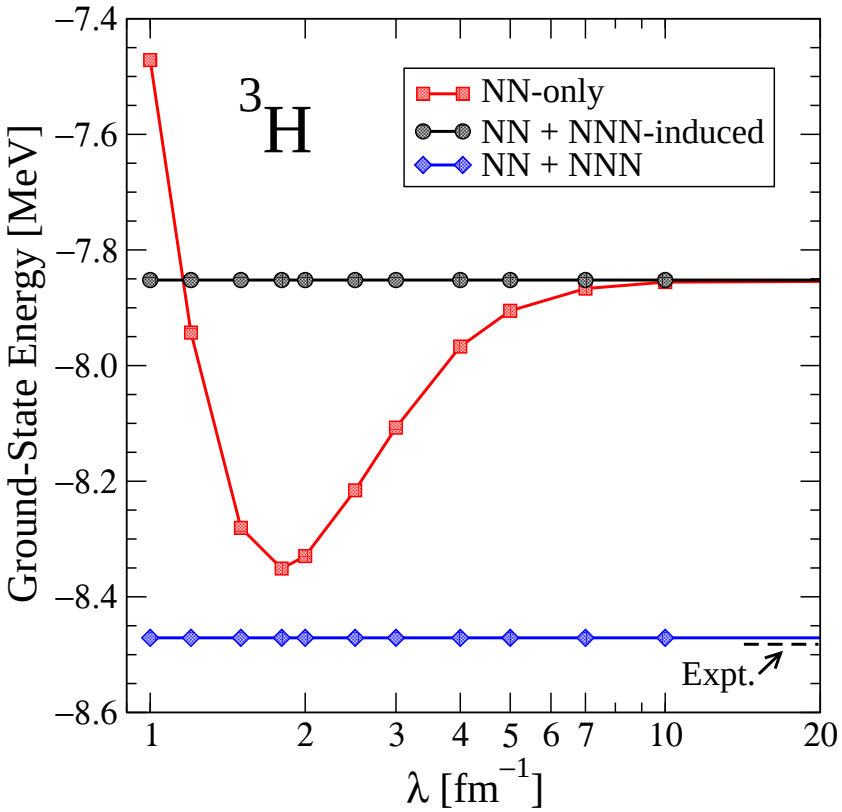
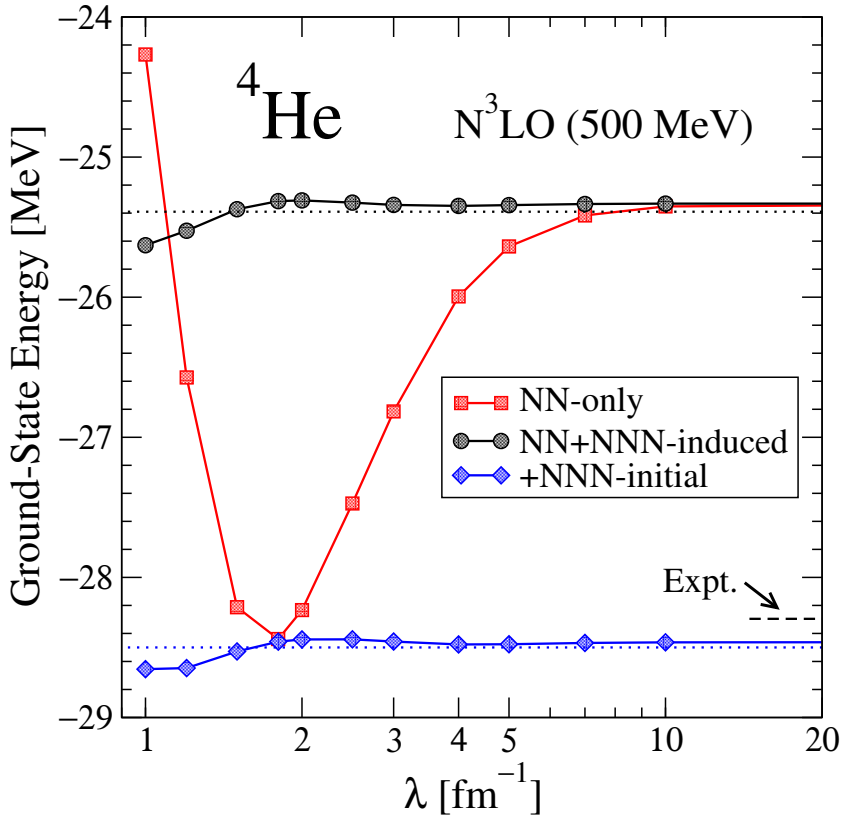
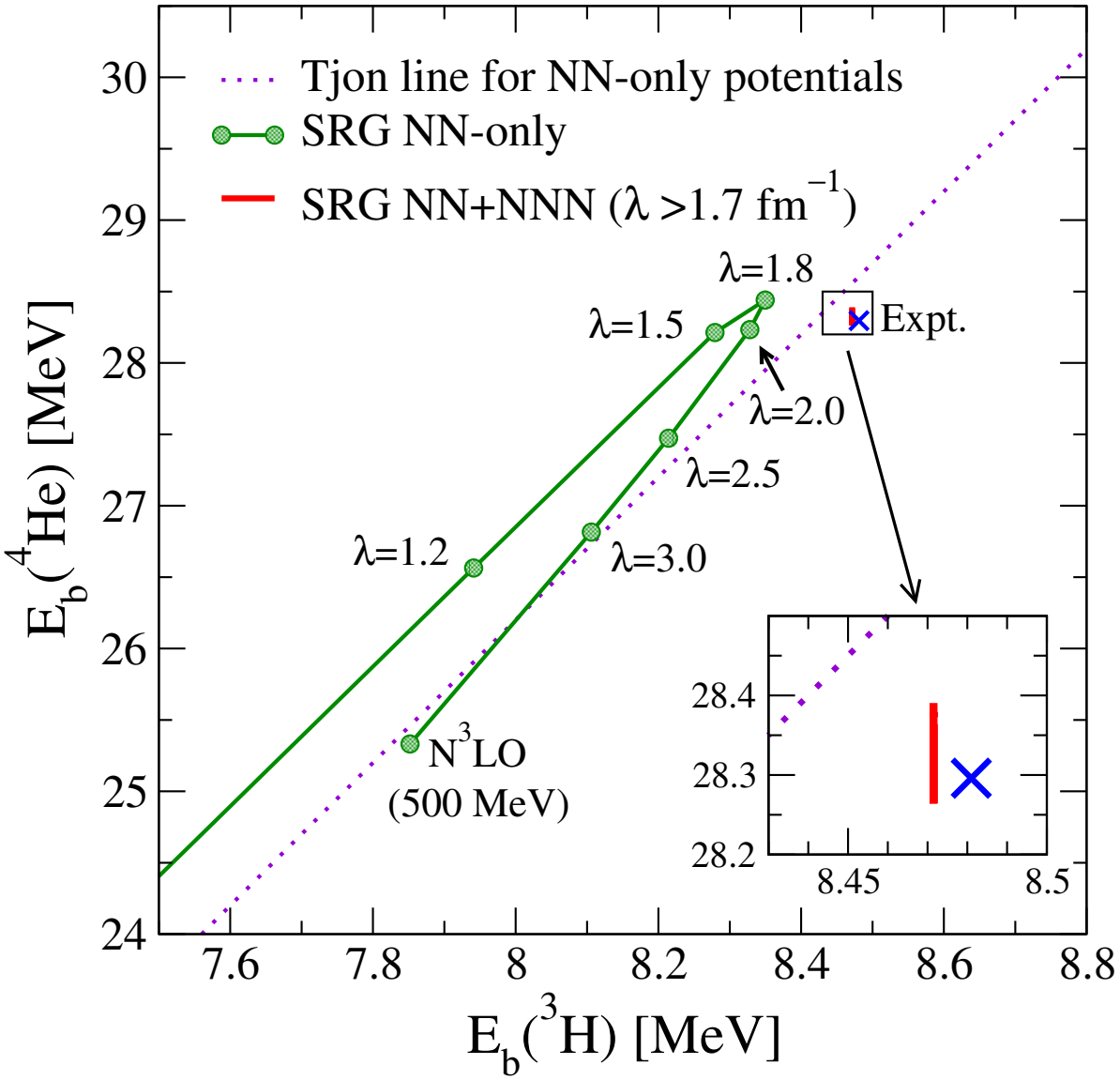


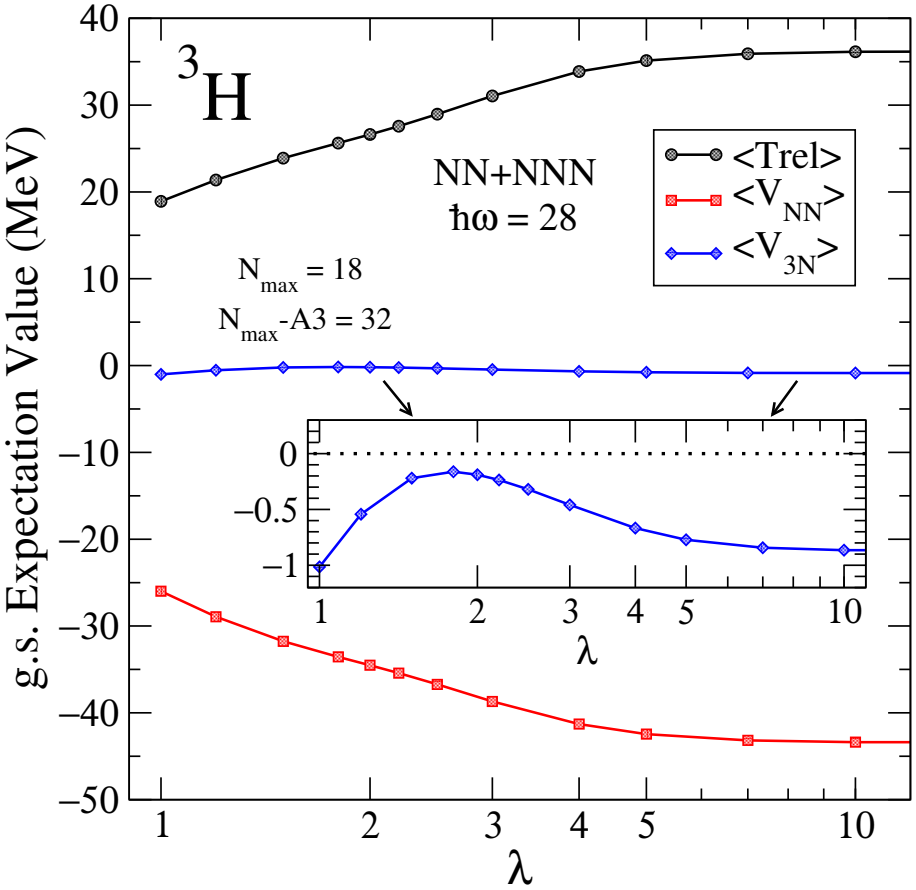


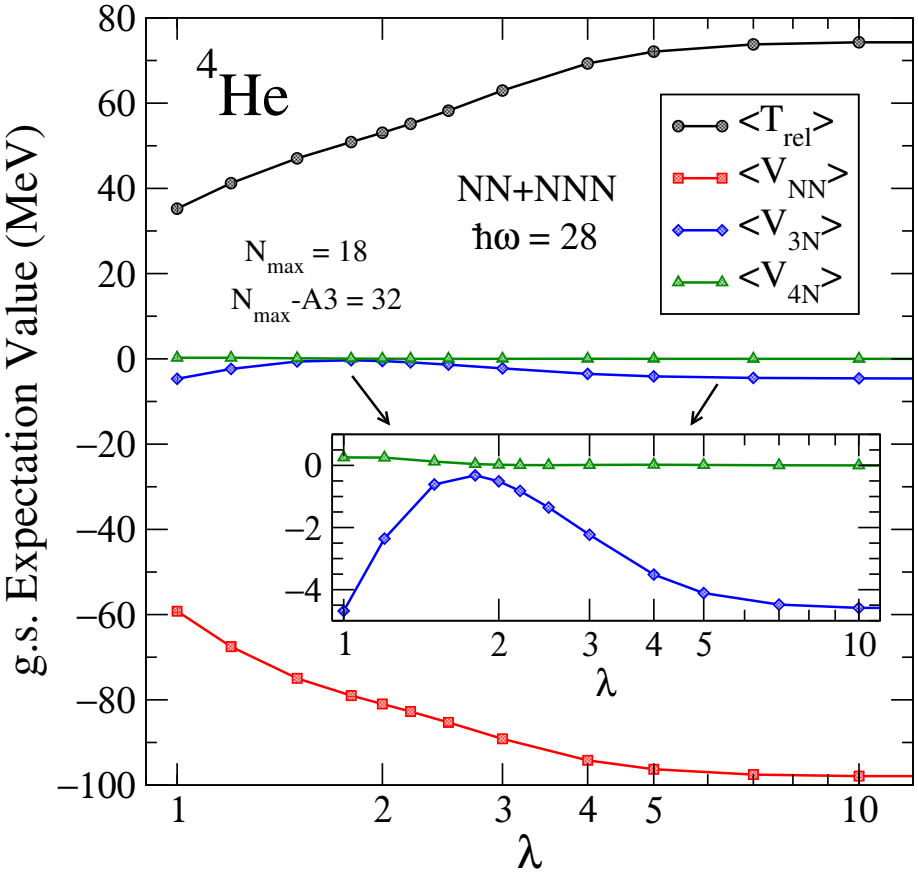
Tjon line revisited



Contributions to the ground-state energy

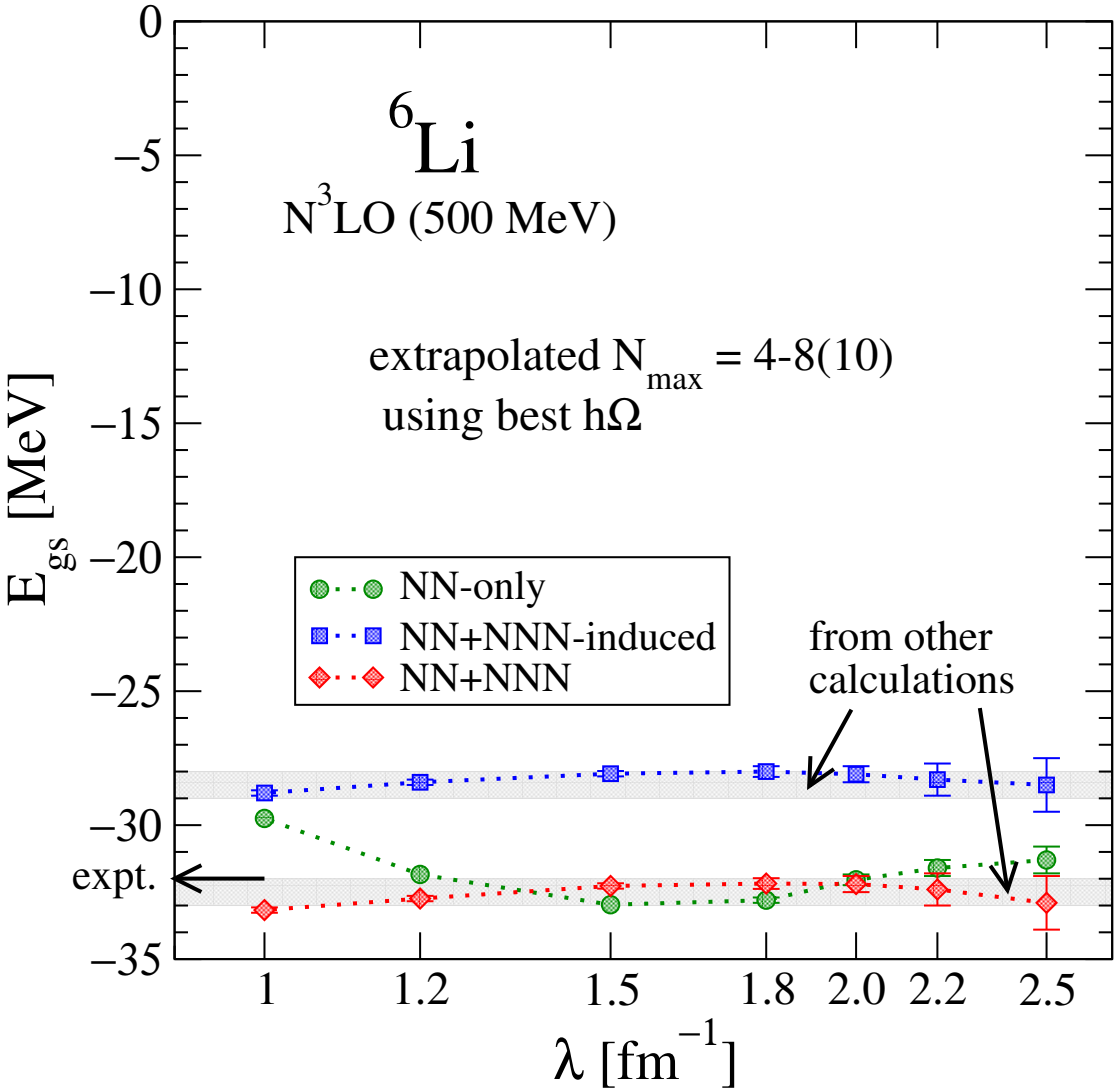
- Look at ground-state matrix elements of KE, NN, 3N, 4N





- Clear hierarchy, but also strong cancellations at NN level
- What about the *A* dependence?

SRG running in Lithium-6 [E. Jurgenson, P. Navrátil, rjf]



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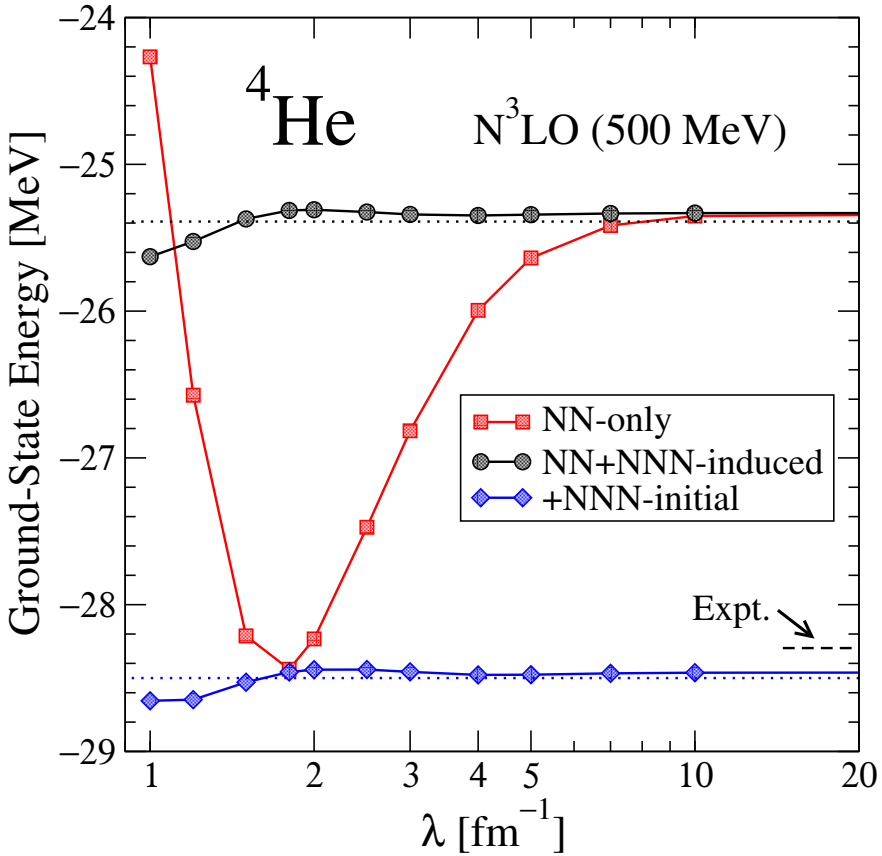
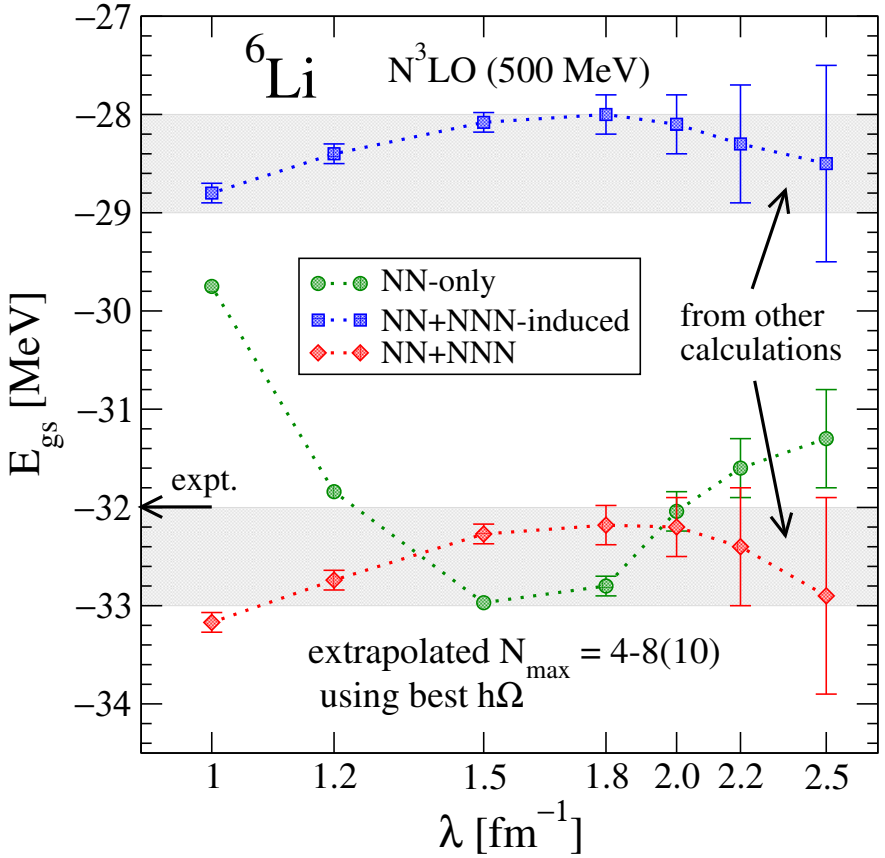




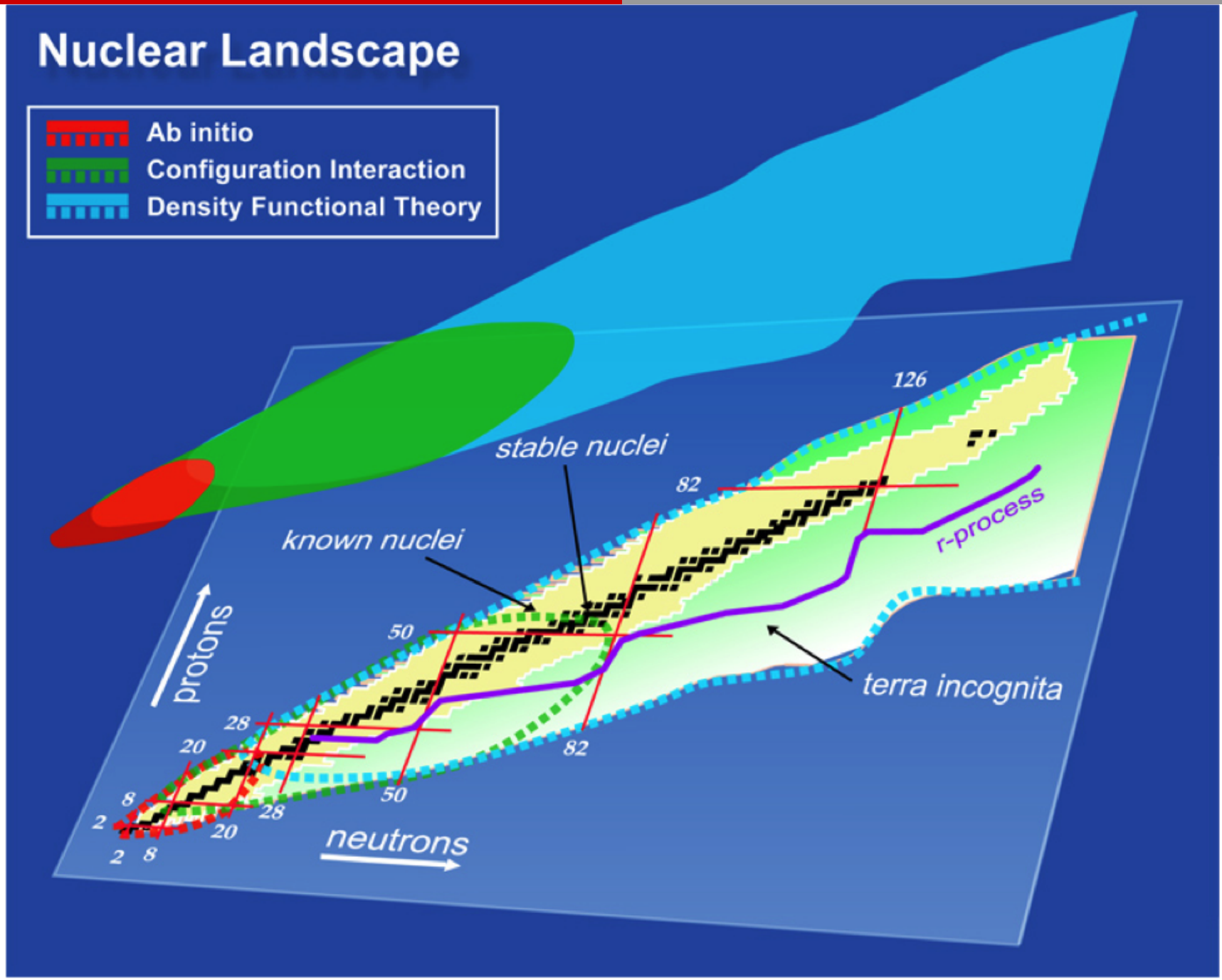
- Coming soon:
  - More p-shell nuclei (using “m-scheme” codes with Maris, Vary)
  - See also R. Roth and collaborators using ITNCSM

Outline

Overview: Goals of low-energy nuclear physics

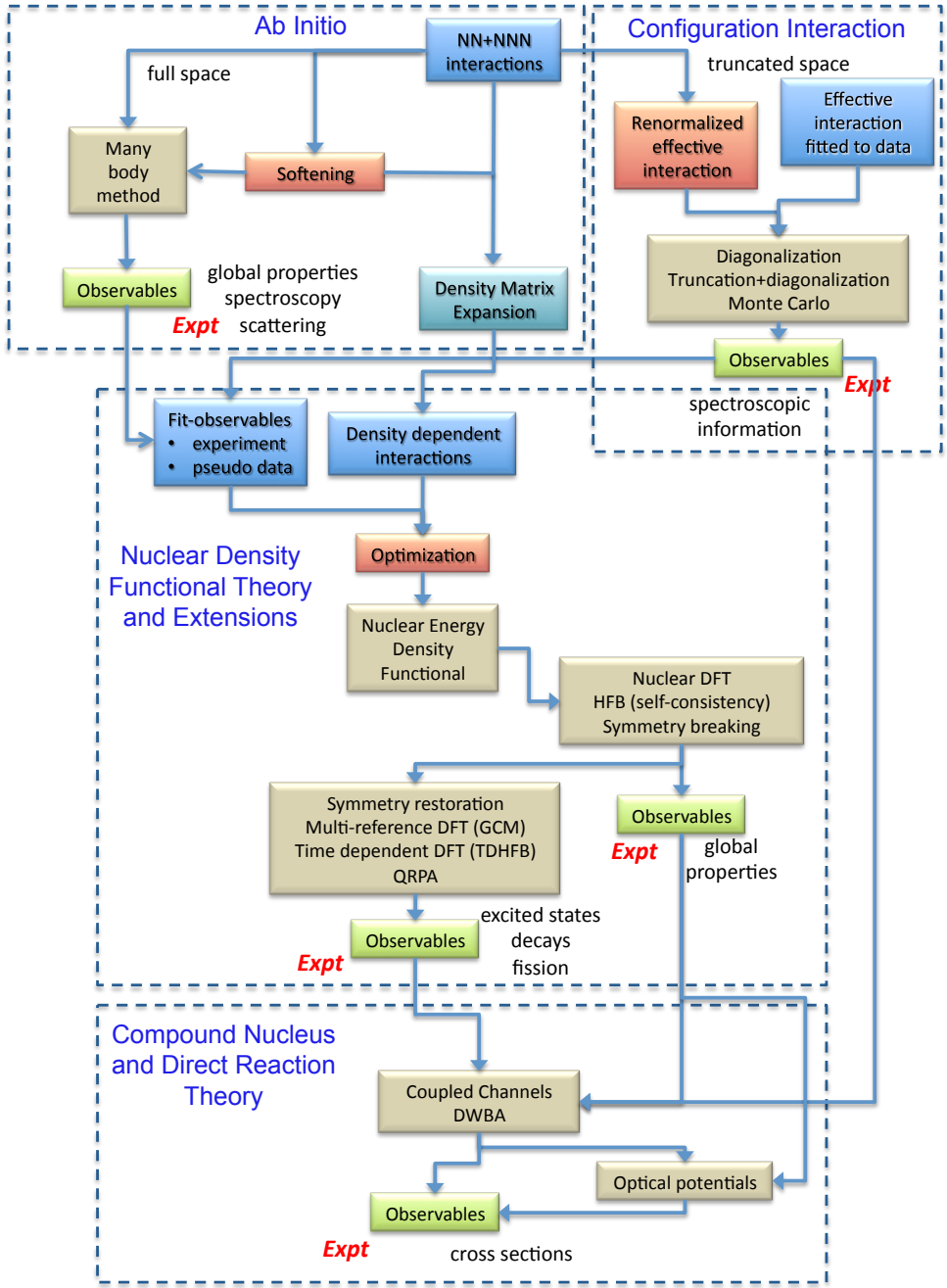
Lowering the resolution with RG

Implications of low resolution for nuclear calculations


Nuclear Landscape
Ab initio
Configuration Interaction
Density Functional Theory
stable nuclei
known nuclei
r-process
terra incognita
protons
neutrons
2
8
20
28
50
82
126

- SciDAC UNEDF project
- Universal Nuclear Energy Density Functional
- Collaboration of physicists, applied mathematicians, and computer scientists
- US funding but international collaborators also
- See unedf.org for highlights!

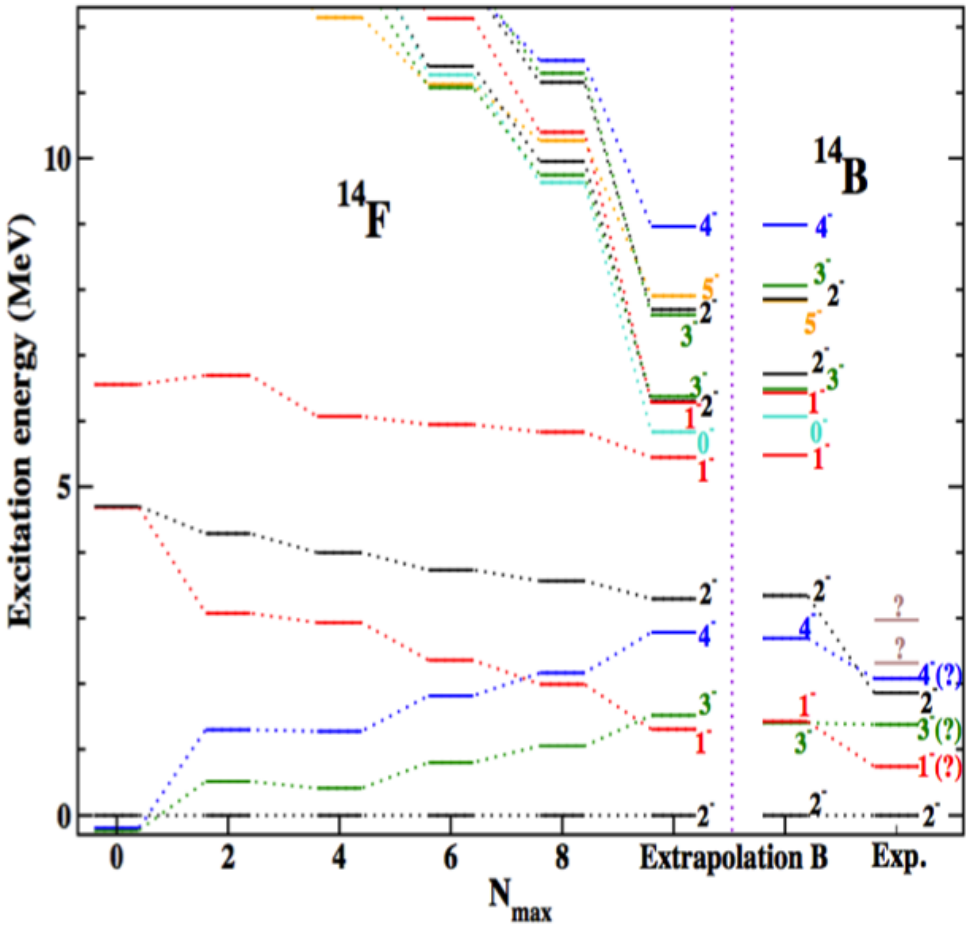
Many non-UNEDF developments as well!



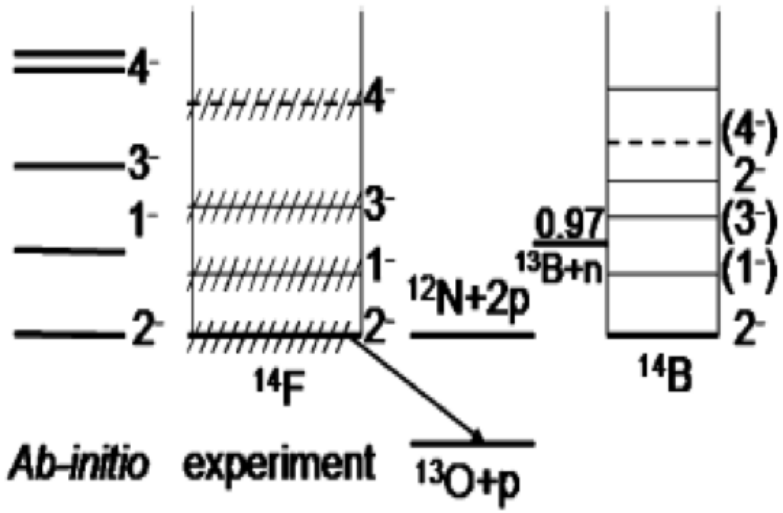
Unstable "proton-dripping" fluorine-14

- Ab initio calculation using low-k inverse-scattering potential
- NCFC theory preceded recent experimental measurement

P. Maris et al., PRC **81**, 021301(R) (2010)



V.Z. Goldberg et al., Phys. Lett. B **692**, 307 (2010)

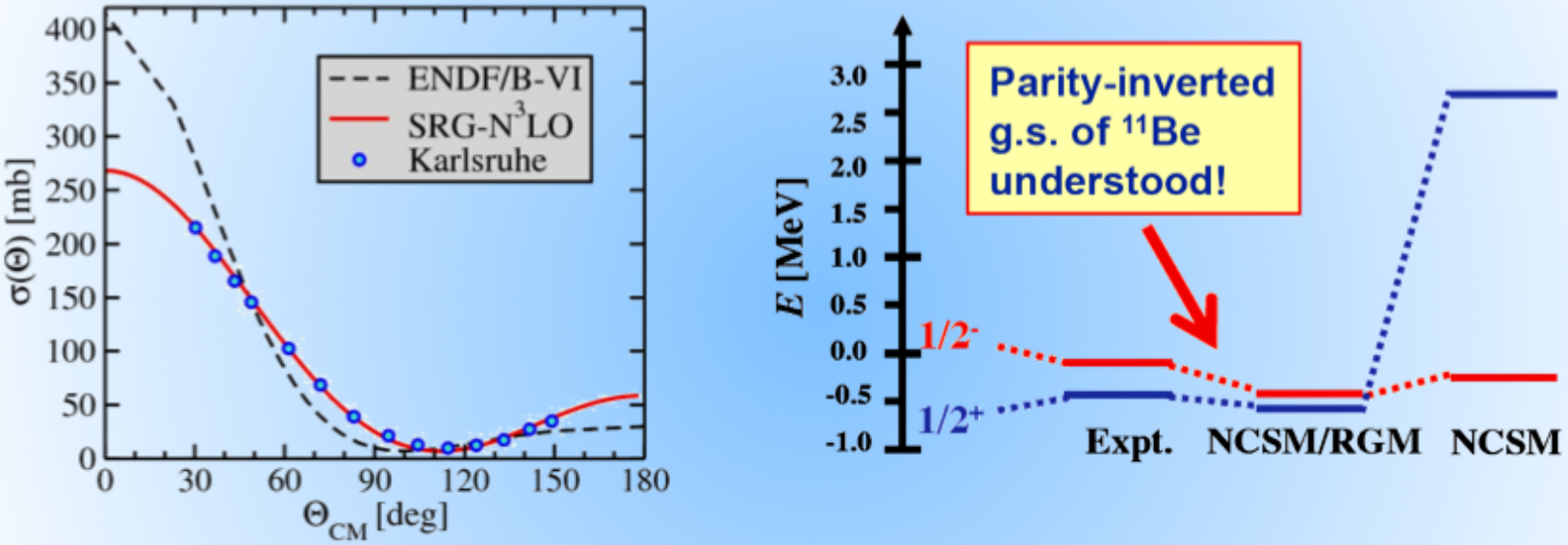


- Matrix dimension 2×10^9, 2.5 hours on 30,000 cores

Ab initio approach to light-ion reactions

- NCSM/RGM using low momentum SRG NN interactions
- See, e.g., Navrátil, Roth, Quaglioni, PRC **82**, 034609 (2010) for nucleon-nucleus scattering

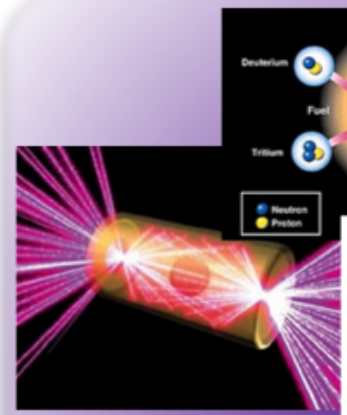
S.Quaglioni and P. Navrátil, PRL101, 092501 (2008); PRC79, 044606 (2009)

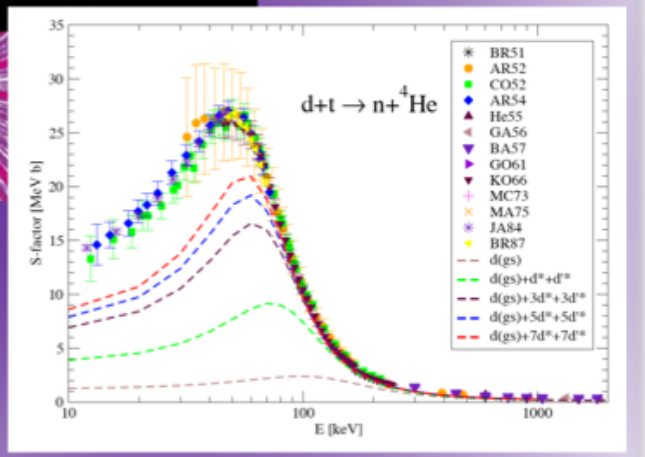


The n-^{4}He differential cross section for 17 MeV neutrons (left) and ^{11}Be bound spectrum (right) obtained within the NCSM/RGM compared to experimental data

Ab initio approach to light-ion reactions

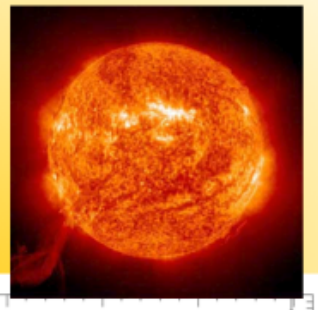
- Applications to fusion energy systems and stellar evolution

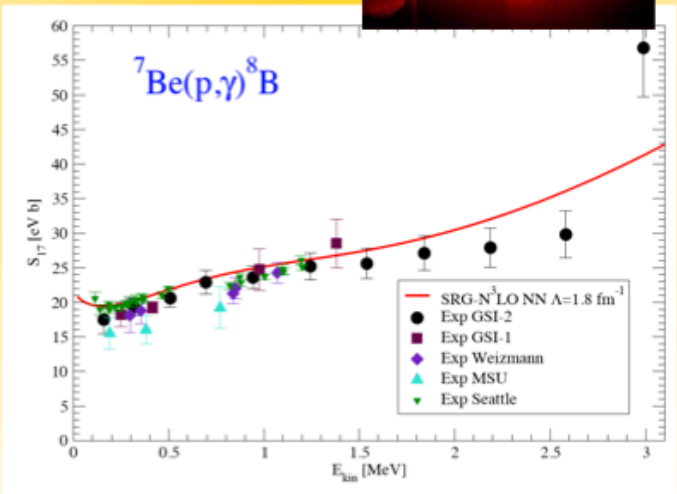




First principles calculations for d+T reaction can lead to a fundamental understanding of thermonuclear fusion

Thermonuclear reactions power stars, ^{7}Be(p,γ)^{8}B is the principal source of observed solar neutrinos





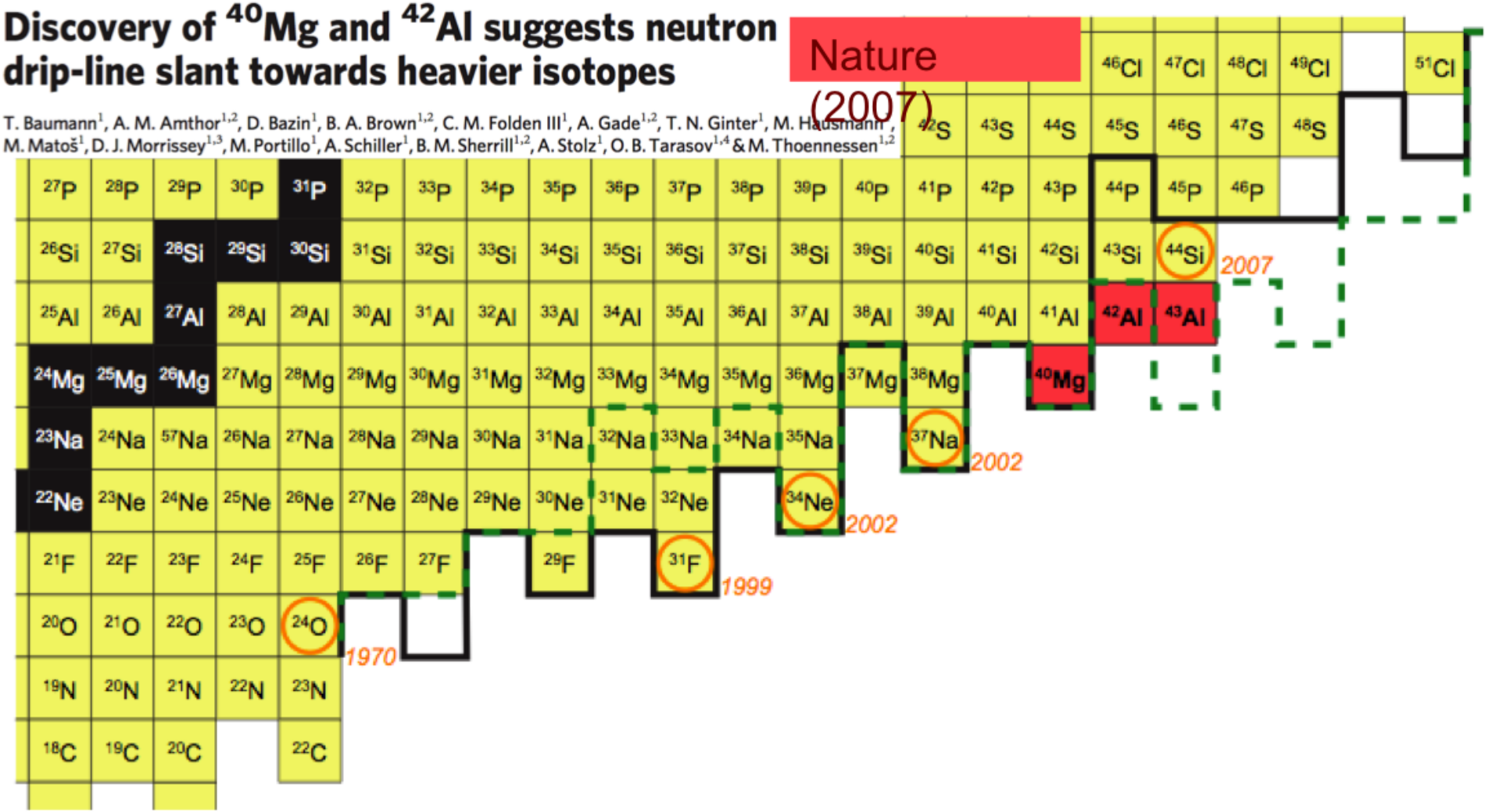
- Still to do: including SRG-evolved NNN interactions

Finding the "driplines" — limits of existence!

Discovery of ^{40}Mg and ^{42}Al suggests neutron drip-line slant towards heavier isotopes

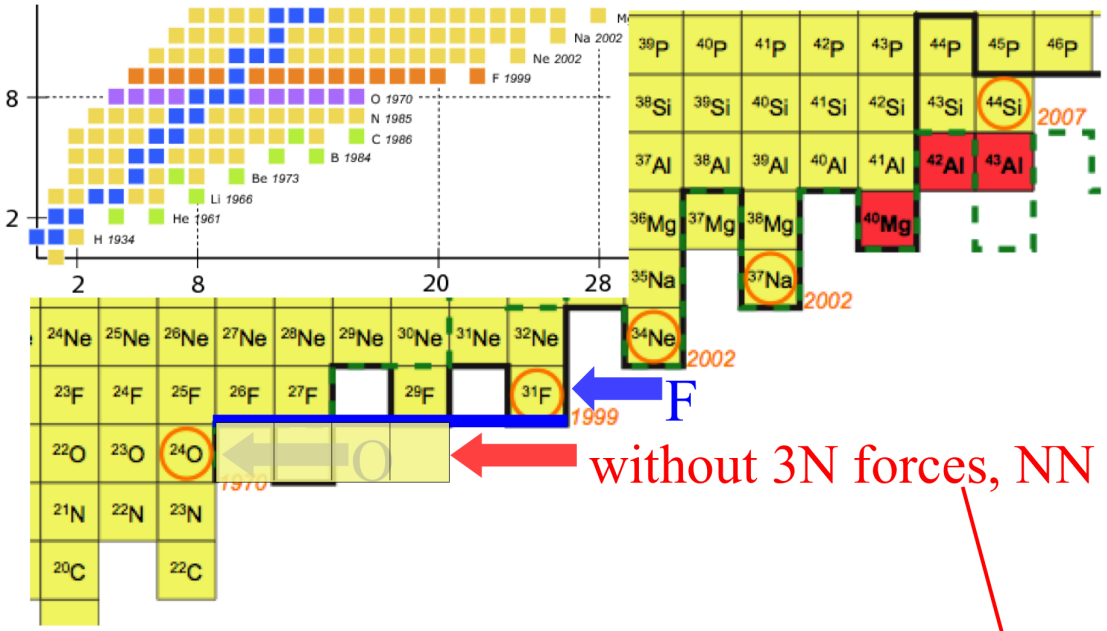
Nature (2007)

T. Baumann[1], A. M. Amthor[1,2], D. Bazin[1], B. A. Brown[1,2], C. M. Folden III[1], A. Gade[1,2], T. N. Ginter[1], M. Hausmann[1], M. Matoš[1], D. J. Morrissey[1,3], M. Portillo[1], A. Schiller[1], B. M. Sherrill[1,2], A. Stolz[1], O. B. Tarasov[1,4] & M. Thoennessen[1,2]



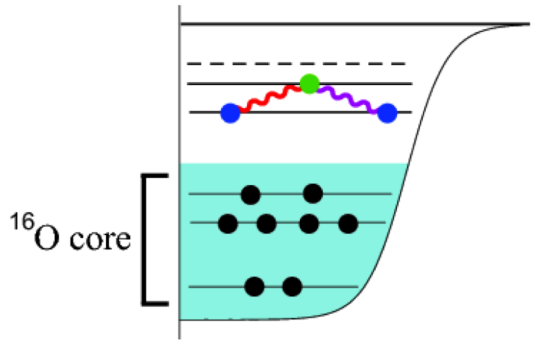
- Oxygen-24 is doubly magic $\Longrightarrow$ Why is it on limit of stability?
- Why do microscopic calculations fail to predict magic $N = 28$?

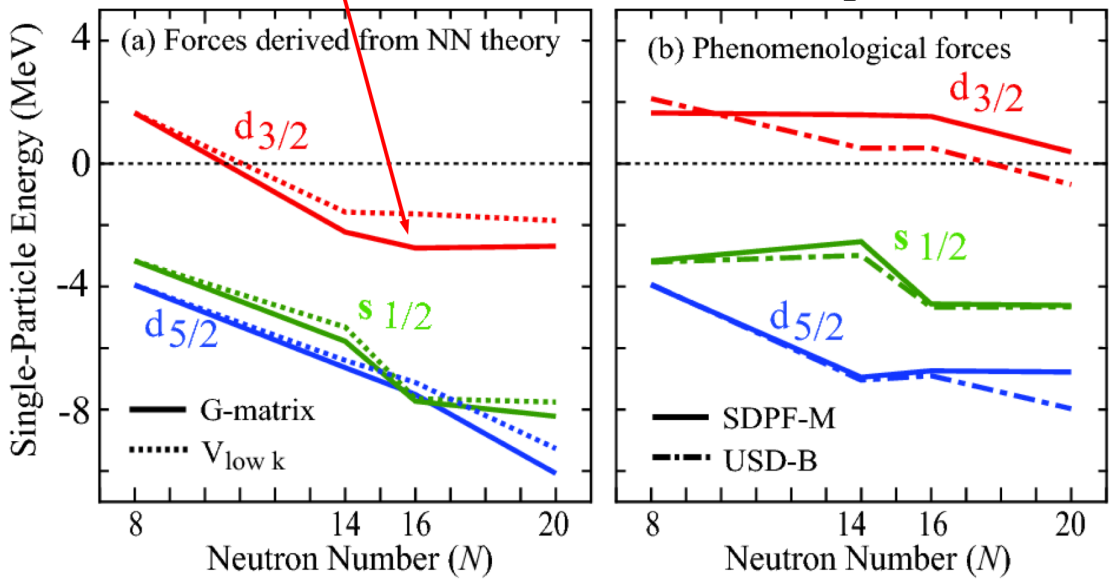
The oxygen anomaly - not reproduced without 3N forces



fit to experiment

many-body theory based on two-nucleon forces:
drip-line incorrect at ^{28}O

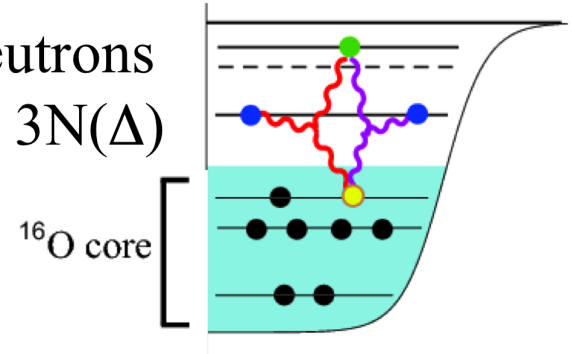




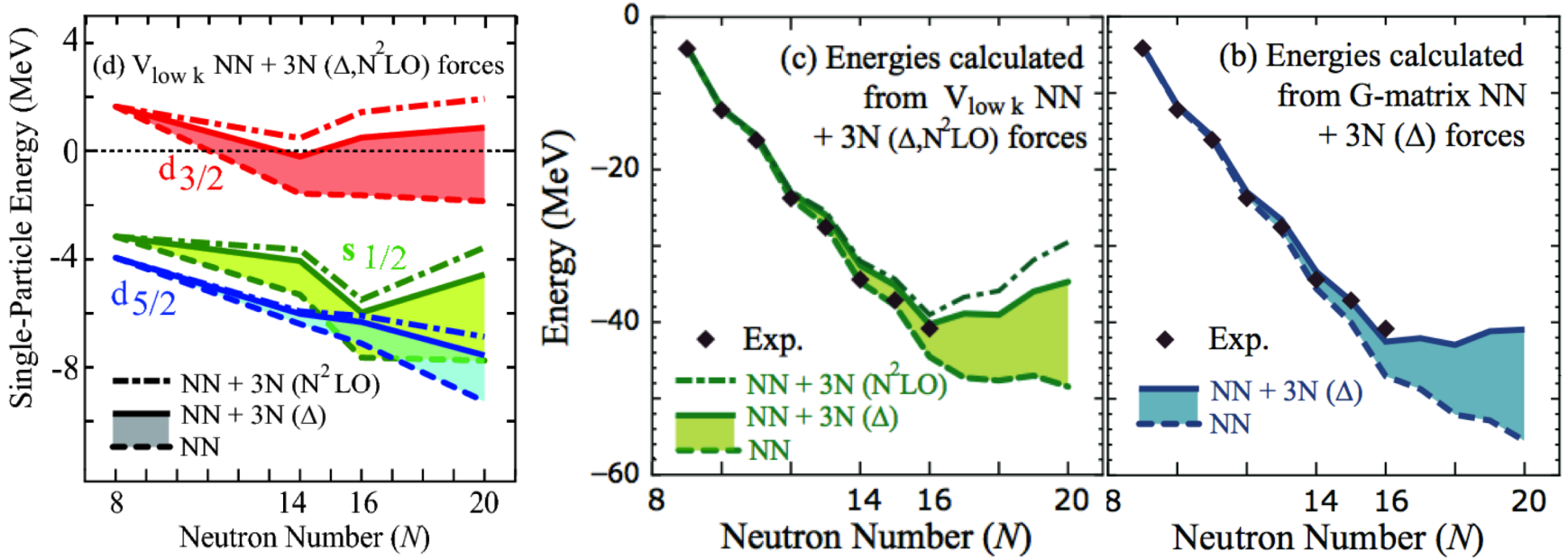
The oxygen anomaly - impact of 3N forces

include "normal-ordered" 2-body part of 3N forces (enhanced by core A)

leads to repulsive interactions between valence neutrons
can understand partly based on Pauli principle for 3N(Δ)



$d_{3/2}$ orbital remains unbound from ^{16}O to ^{28}O



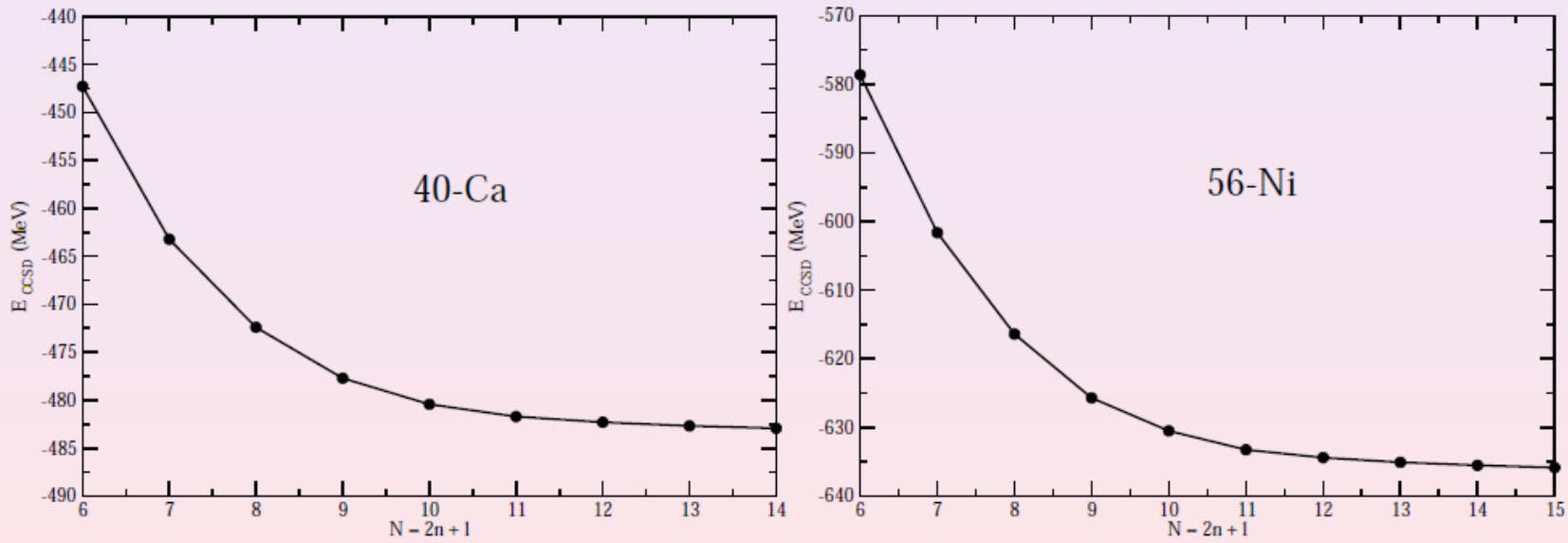
first microscopic explanation of the oxygen anomaly

Otsuka, Suzuki, Holt, Schwenk, Akaishi (2010)

More perturbative $\Longrightarrow$ like quantum chemistry

- Powerful coupled cluster method works! (figure from G. Hagen)

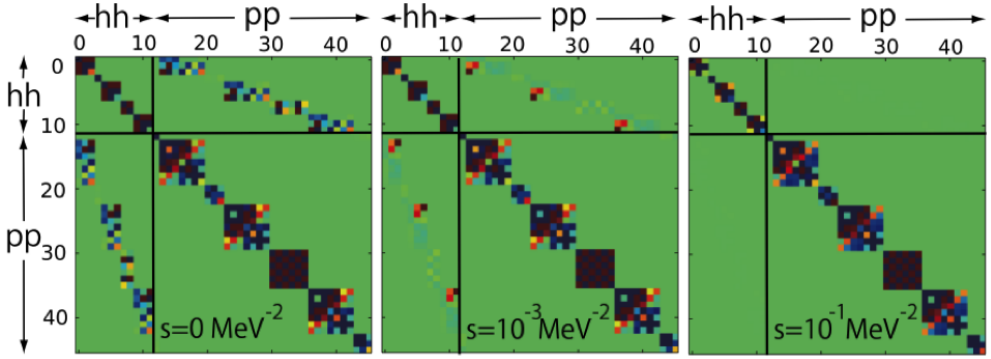
Converged results for ^{40}Ca and ^{56}Ni, using N^{3}LO evolved down to $\lambda = 2.5\mathrm{fm}^{-1}$ from similarity renormalization group theory.

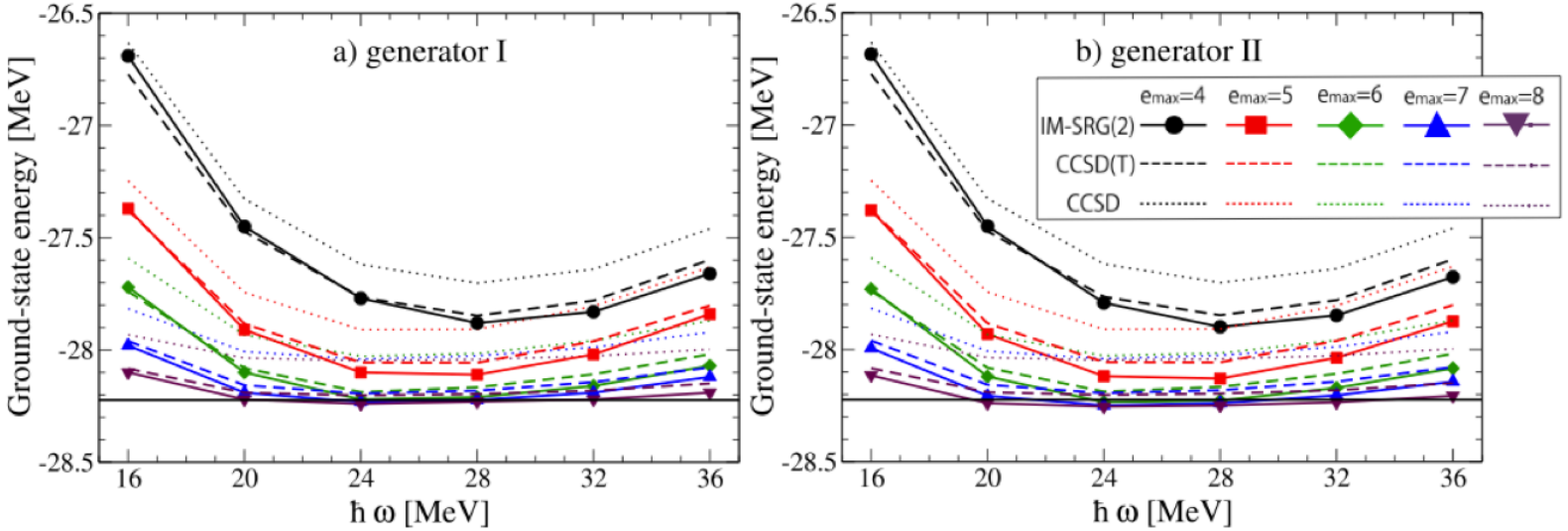


- Improved convergence with low-resolution SRG potentials
- CC extended to 3-body forces by Hagen et al. . . .

In-medium SRG for nuclei [Tsukiyama, Bogner, Schwenk]

- SRG in *A*-body system using normal-ordering
- Decouple 1p1h, 2p2h, . . . sectors from (HF) reference state



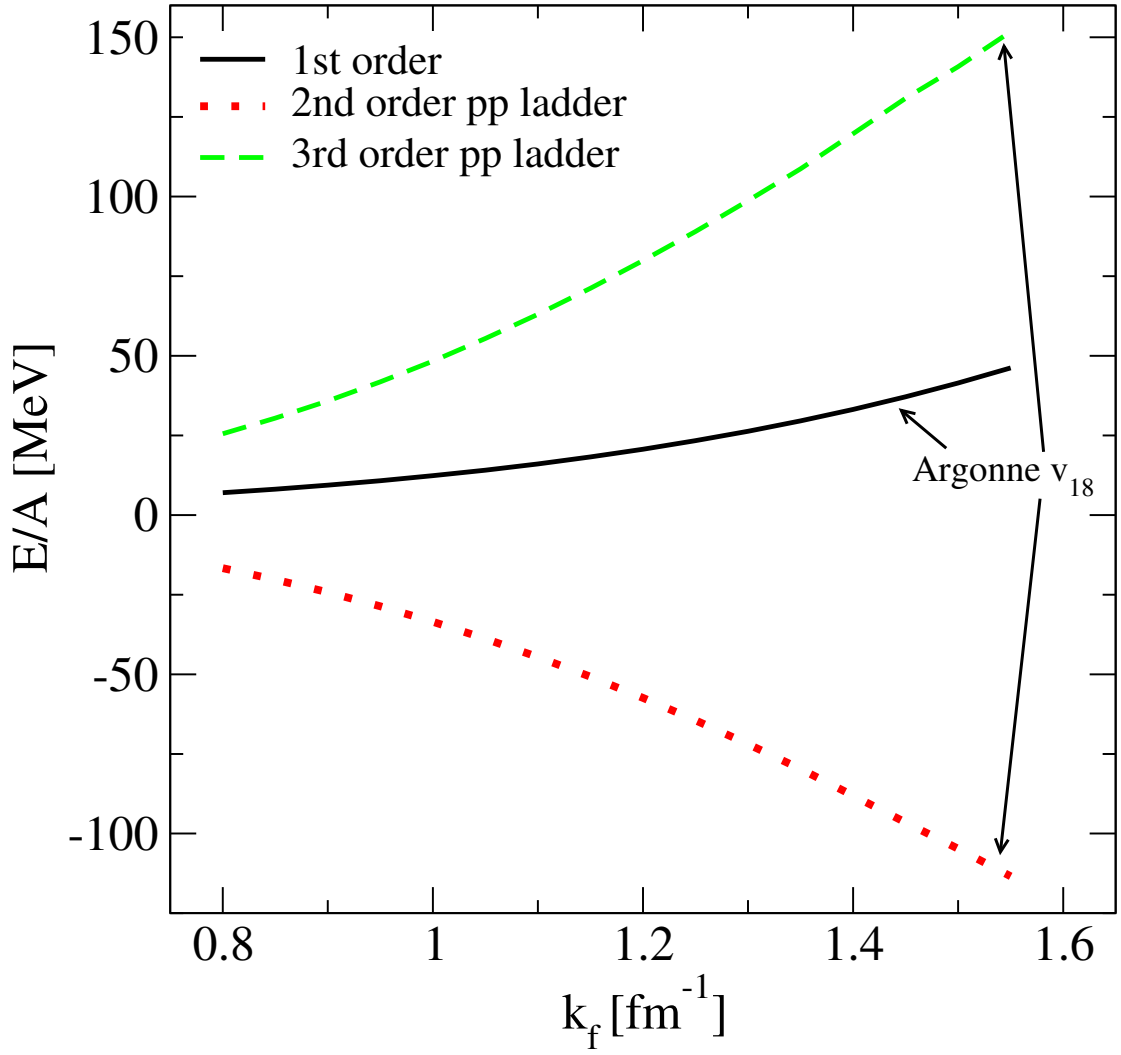


- Promising results for closed-shell nuclei: ^{4}He, ^{16}O, ^{40}Ca
- Energies between coupled cluster CCSD and CCSD(T)
- Two-body valence shell-model effective interactions

Low resolution $\Longrightarrow$ MBPT is feasible!

- MBPT $\equiv$ Many-Body Perturbation Theory

- Compare high resolution to low resolution
- pp MBPT converges!
- Roth et al. $\Longrightarrow$ apply to finite nuclei (4NF?)



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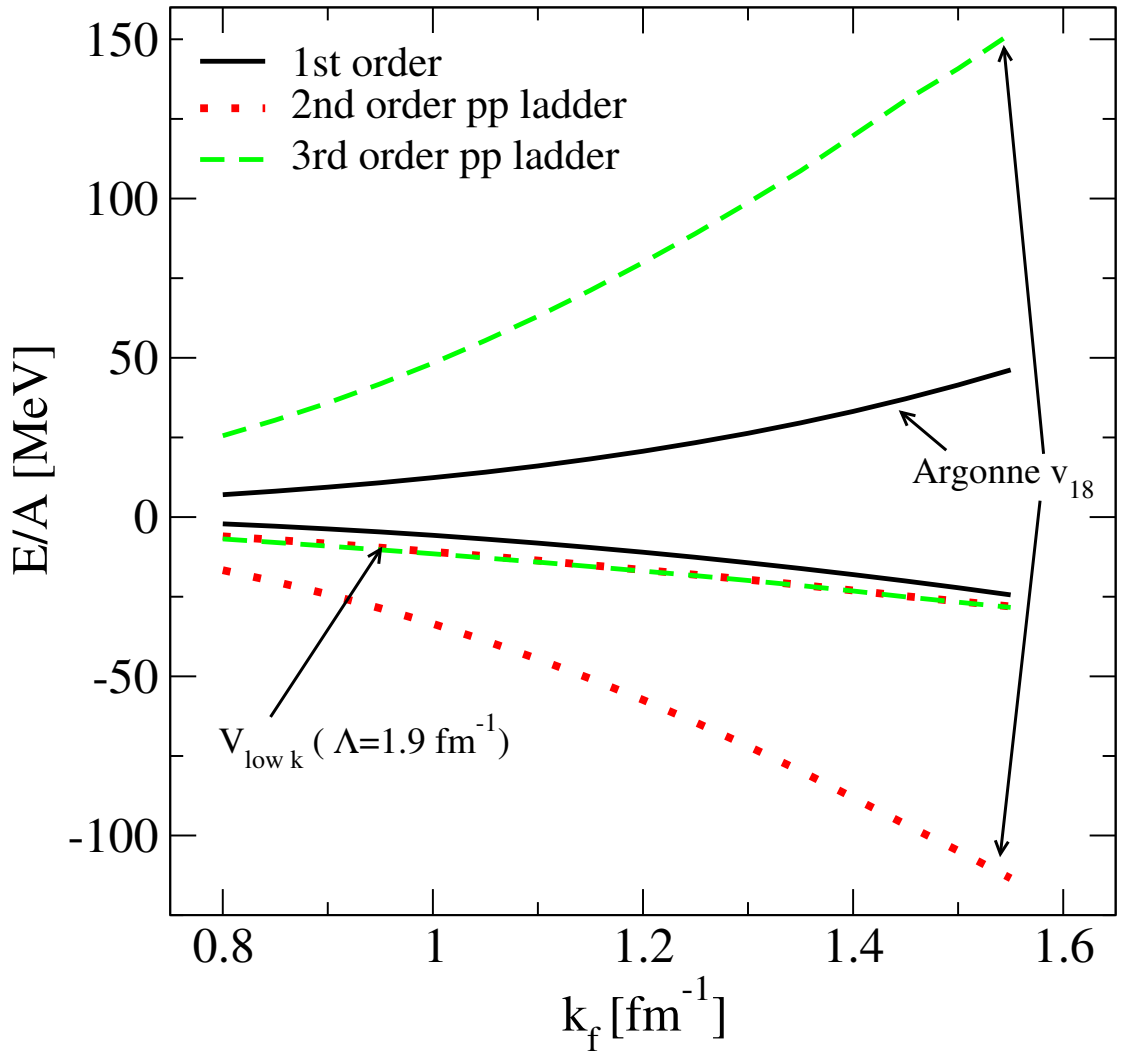
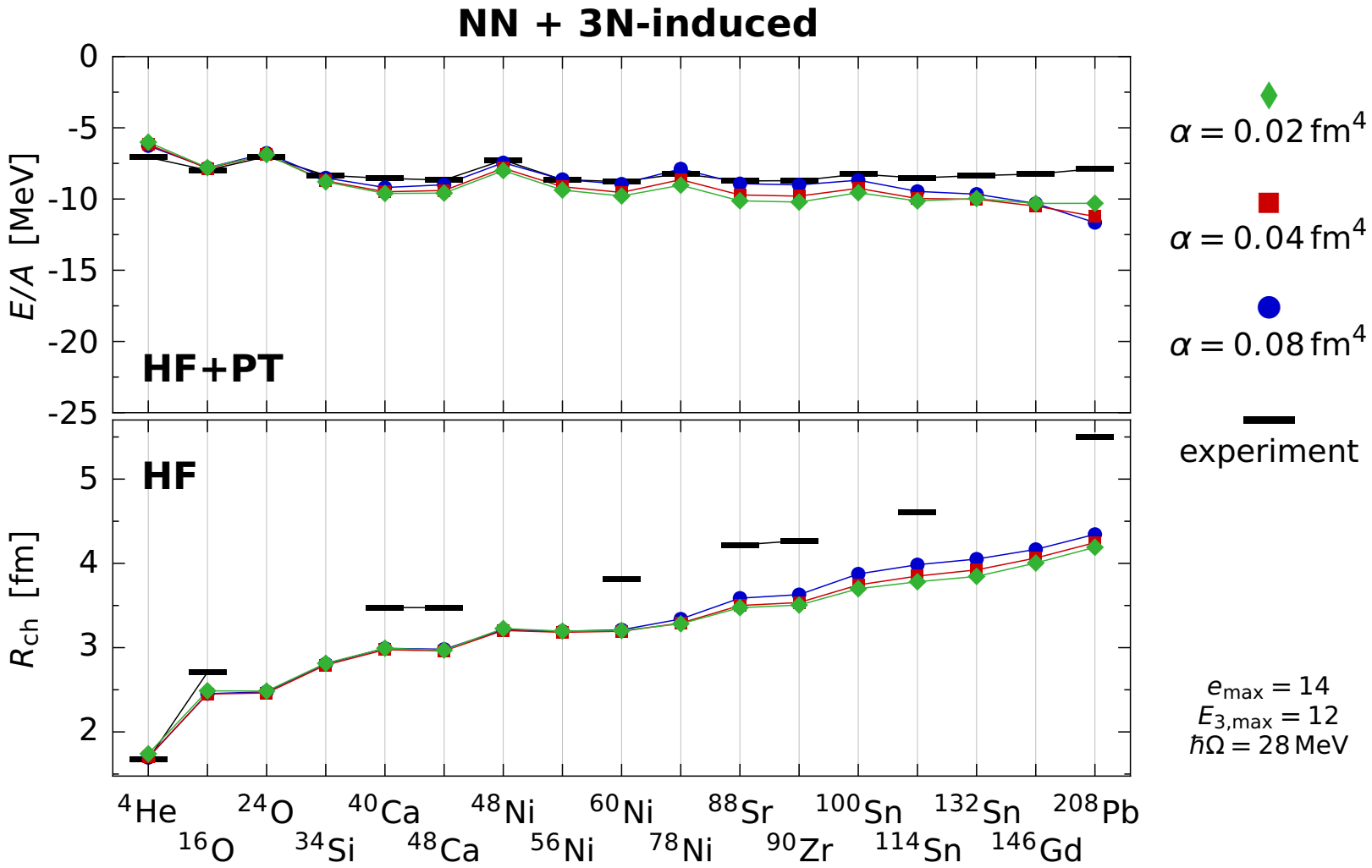
- Need evolved 3-body force for saturation



R. Roth et al. N^{3}LO(500) E/A and $R_{\rm ch}$ in MBPT

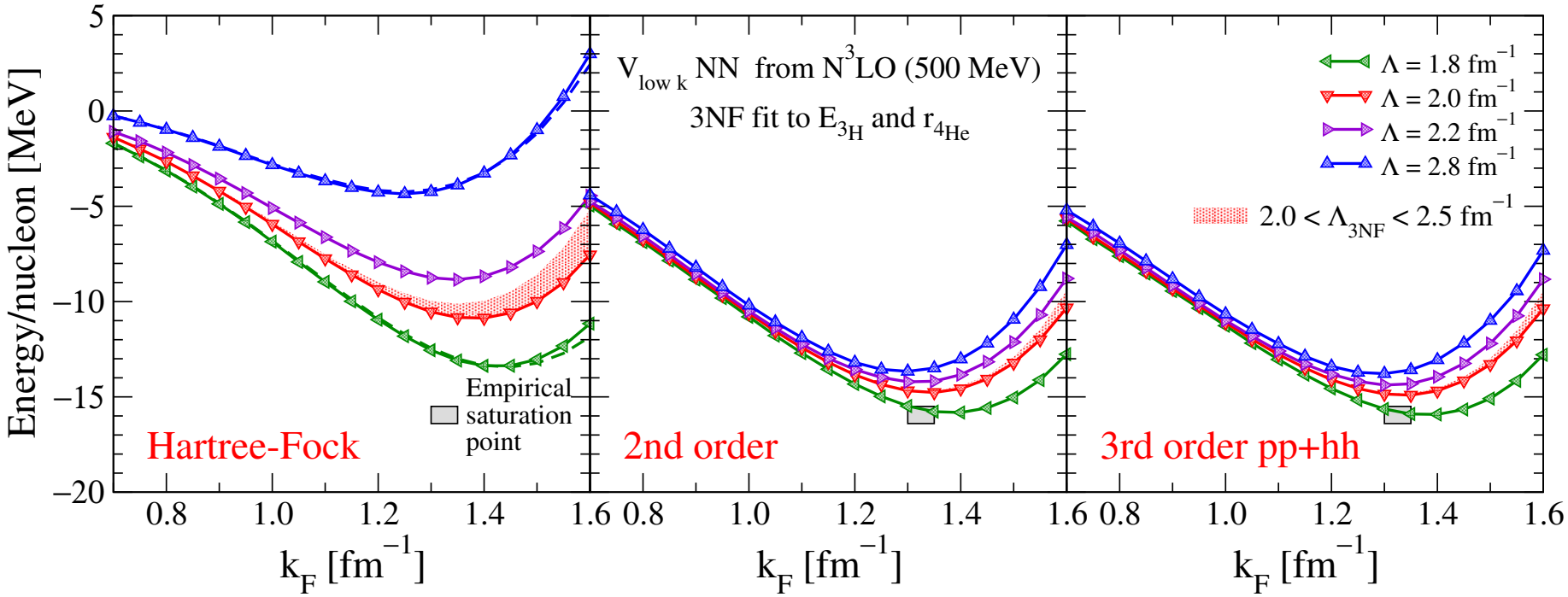
- Coupled cluster NN-only results:

^{16}O	7.7 MeV	2.3 fm^{-1}
^{40}Ca	8.6 MeV	2.8 fm^{-1}
^{48}Ca	8.3 MeV	2.9 fm^{-1}



One of the paths to microscopic nuclear DFT

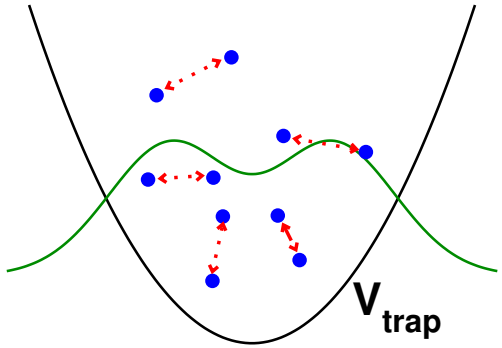
- Construct a chiral EFT to a given order (N^3LO at present)
- Evolve Λ down with RG (to $\Lambda \approx 2\,\mathrm{fm}^{-1}$ for ordinary nuclei)
  - NN interactions fully, NNN interactions approximately (fit)
- Generate density functional in MBPT
  - Hartree-Fock plus "≈ second order", use "DME" in *k*-space

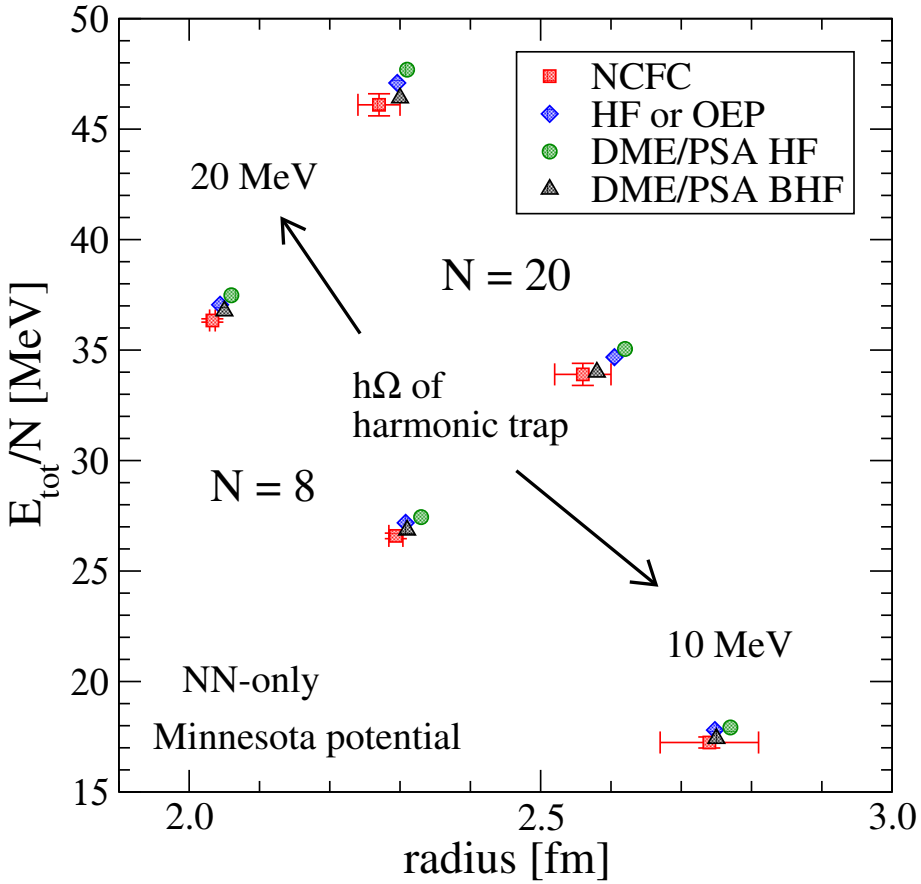


Bogner et al., (2009); Hebeler et al., (2010); Gebremariam et al., (2010)

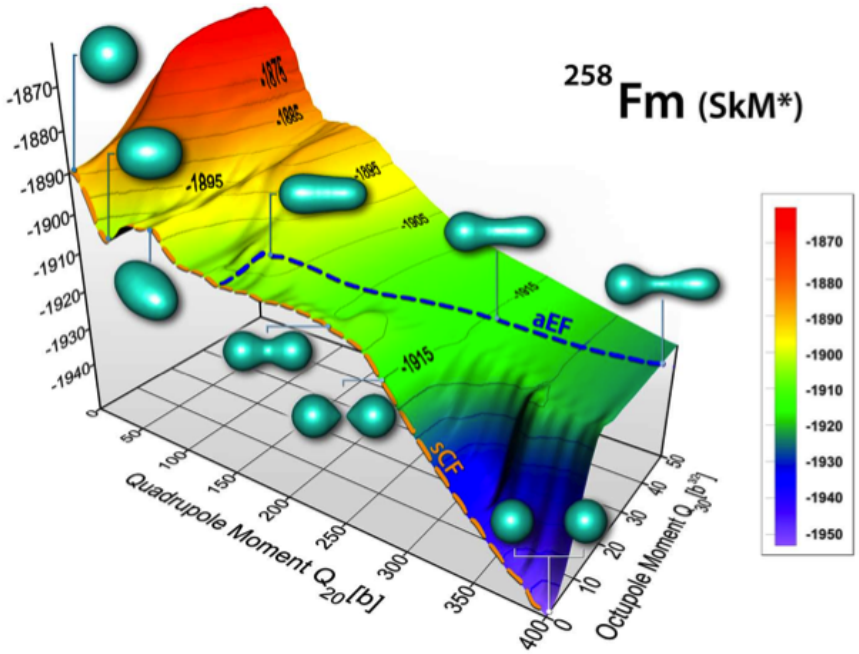
Hybrid DFT: Merge chiral EFT and Skyrme

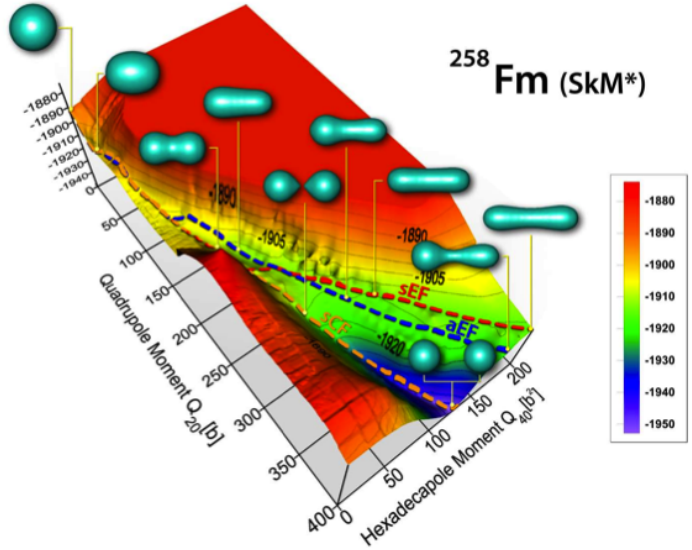
- Include long-range pion physics via density matrix expansion (DME/PSA)
- Refit short-range physics in Skyrme EDF form
- Validate against ab initio NCFC calculations [Maris]
- Controlled tests for neutrons in trap $\Longrightarrow$ constraints on neutron-rich nuclei
  - UNEDF sub-collaboration
  - Tests with simplified interaction promising!

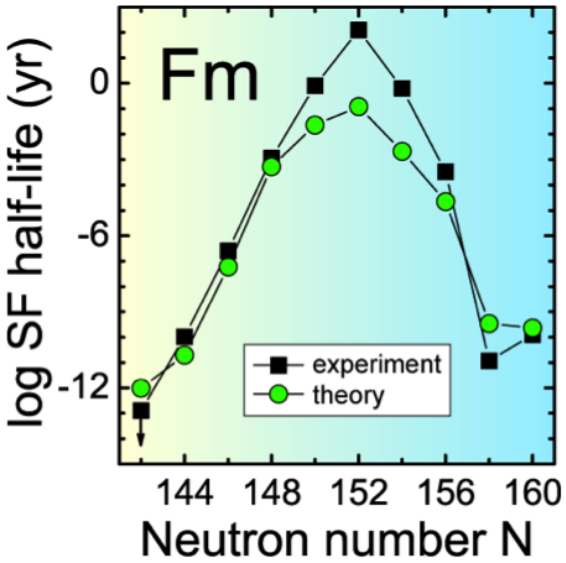




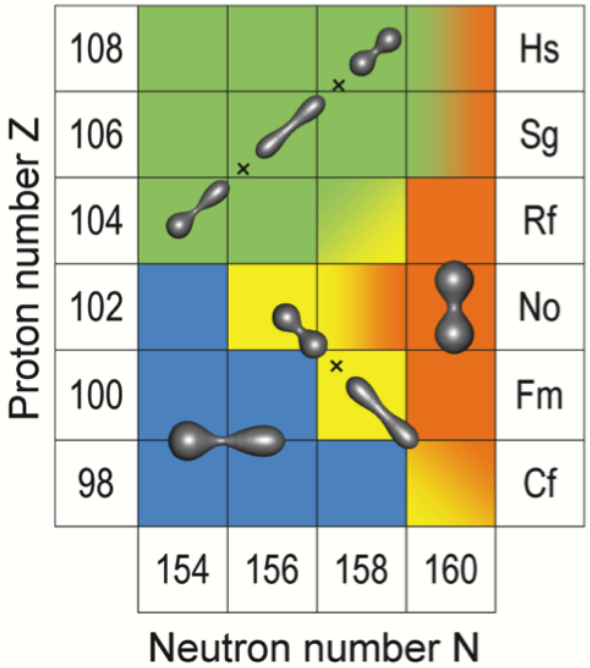
Spontaneous fission: Energy surfaces from DFT





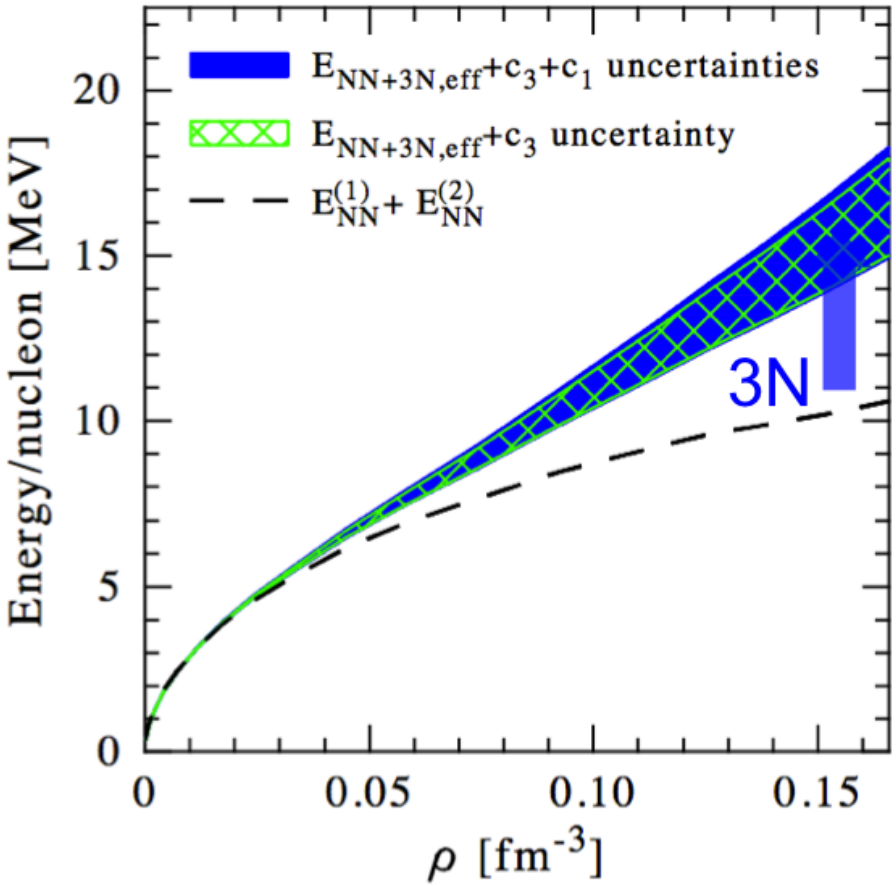


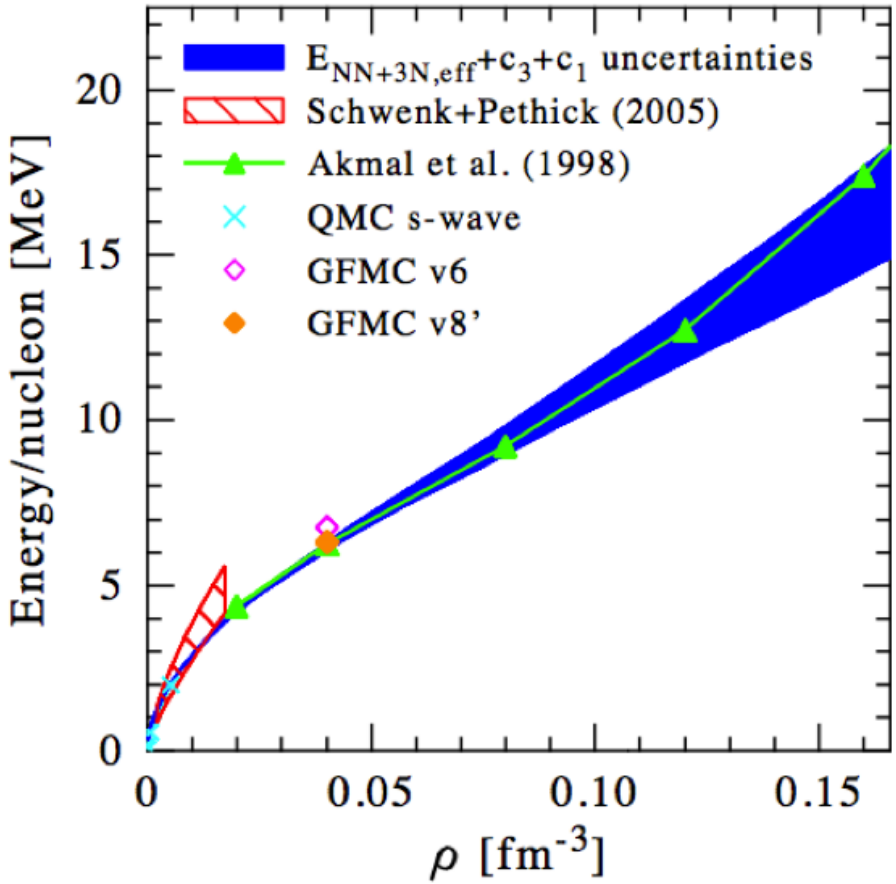
A. Staszczak et al.,
PRC 80, 014309 (2009)



Low resolution calculations of neutron matter

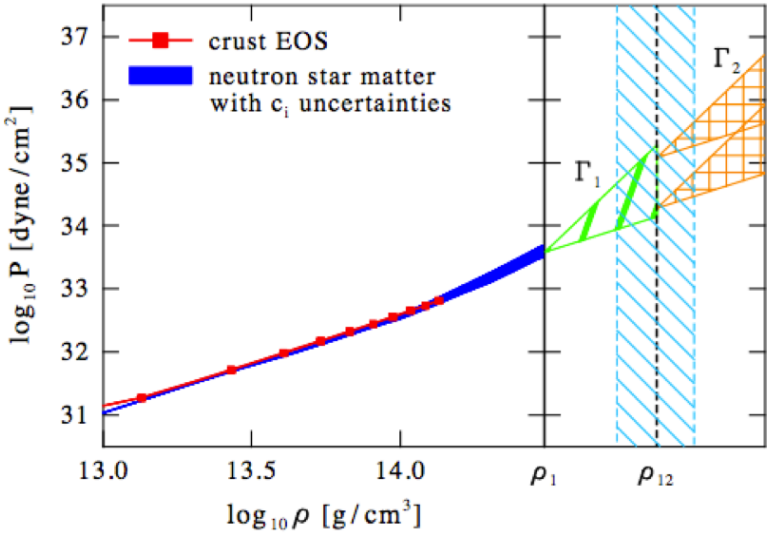
- Evolve NN to low momentum, fit NNN to $A = 3, 4$
- Neutron matter in perturbation theory [Hebeler, Schwenk (2010)]

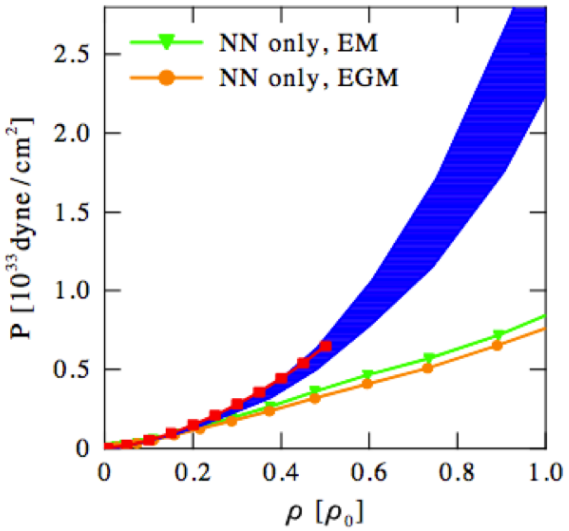




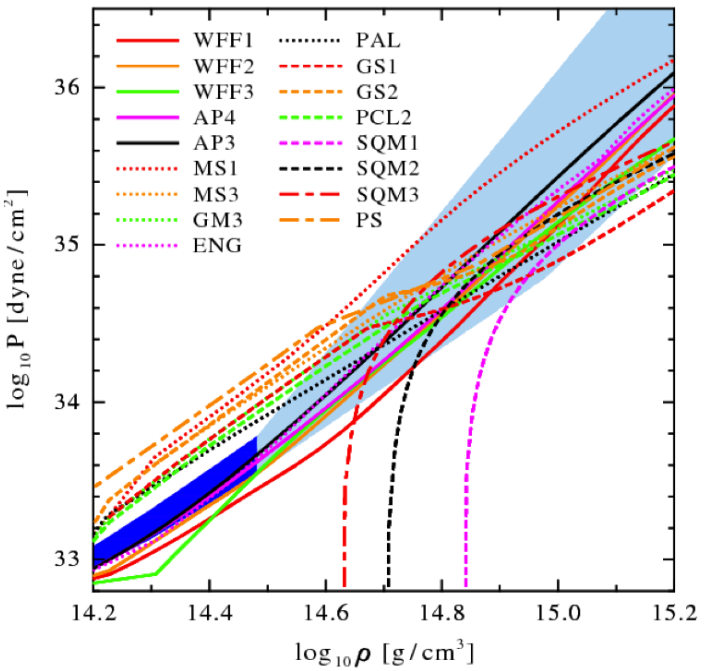
- Use cutoff dependence to estimate many-body uncertainty
- Uncertainties from long-range NNN constants are greatest

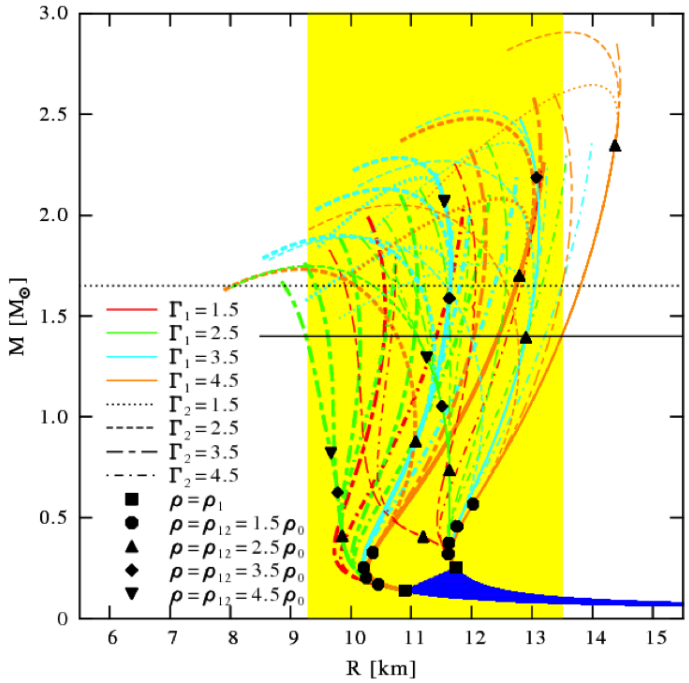
Constraining neutron stars: $R = 9.7$–13.9 km for $1.4\,M_{\rm sun}$





Hebeler, Lattimer, Pethick, Schwenk (2010)





- Extrapolate EOS to higher density
- Solve for M vs. R $\Longrightarrow$ yellow band constrains radius

Summary: Atomic Nuclei at Low Resolution

- Strategy: Lower the resolution and track dependence
  - High resolution $\Longrightarrow$ high momenta can be painful!
    (“It hurts when I do this.” “Then don’t do that.”)
  - Correlations in wave functions reduced dramatically
  - Non-local potentials and many-body operators “induced”

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  - Band (or block) diagonalizing Hamiltonian matrix (or . . .)
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    but physics interpretation may change!
  - Nuclear case: evolve until few-body forces start to explode
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  - Nuclear case: evolve until few-body forces start to explode
    or use in-medium SRG
- Applications to nuclei and beyond
  - CI, coupled cluster, . . . converge faster $\Longrightarrow$ new possibilities
  - Microscopic shell model $\Longrightarrow$ role of 3-body forces
  - MBPT works $\Longrightarrow$ constructive nuclear density functional theory

Thanks: collaborators and others at low resolution

- Darmstadt: R. Roth, A. Schwenk
- INT / Chalmers: L. Platter
- Iowa State: P. Maris, J. Vary
- Jülich: A. Nogga
- Michigan State: S. Bogner, H. Hergert
- LLNL: E. Jurgenson, N. Schunck
- Ohio State: E. Anderson, M. Bettencourt, K. Hebeler, W. Li, R. Perry, K. Wendt
- ORNL / UofT: M. Kortelainen, W. Nazarewicz, M. Stoitsov
- TRIUMF: S. Bacca, P. Navratil
- Warsaw: S. Glazek
- many others in UNEDF

Some open questions and issues for SRG

- Power counting for evolved many-body interactions
  - Need analytic estimates plus more numerical tests
  - Can the SRG help with constructing/analyzing EFT's?
- Operator issues (SRG evolves operators, too!)
  - Scaling of many-body operators
  - Technical issues (e.g., boosting)
  - Test factorization for few- and many-body systems
- Can different choices for G_s ...
  - control the growth of many-body forces?
  - improve convergence in HO basis?
  - drive a non-local potential to local form?
- Use of different basis for SRG evolution
  - Need $A = 3$ momentum-space implementation
  - Hyperspherical coordinates? (also for visualization)
- How can we use Monte Carlo methods?

Every operator flows [see Anderson et al., arXiv:1008.1569]

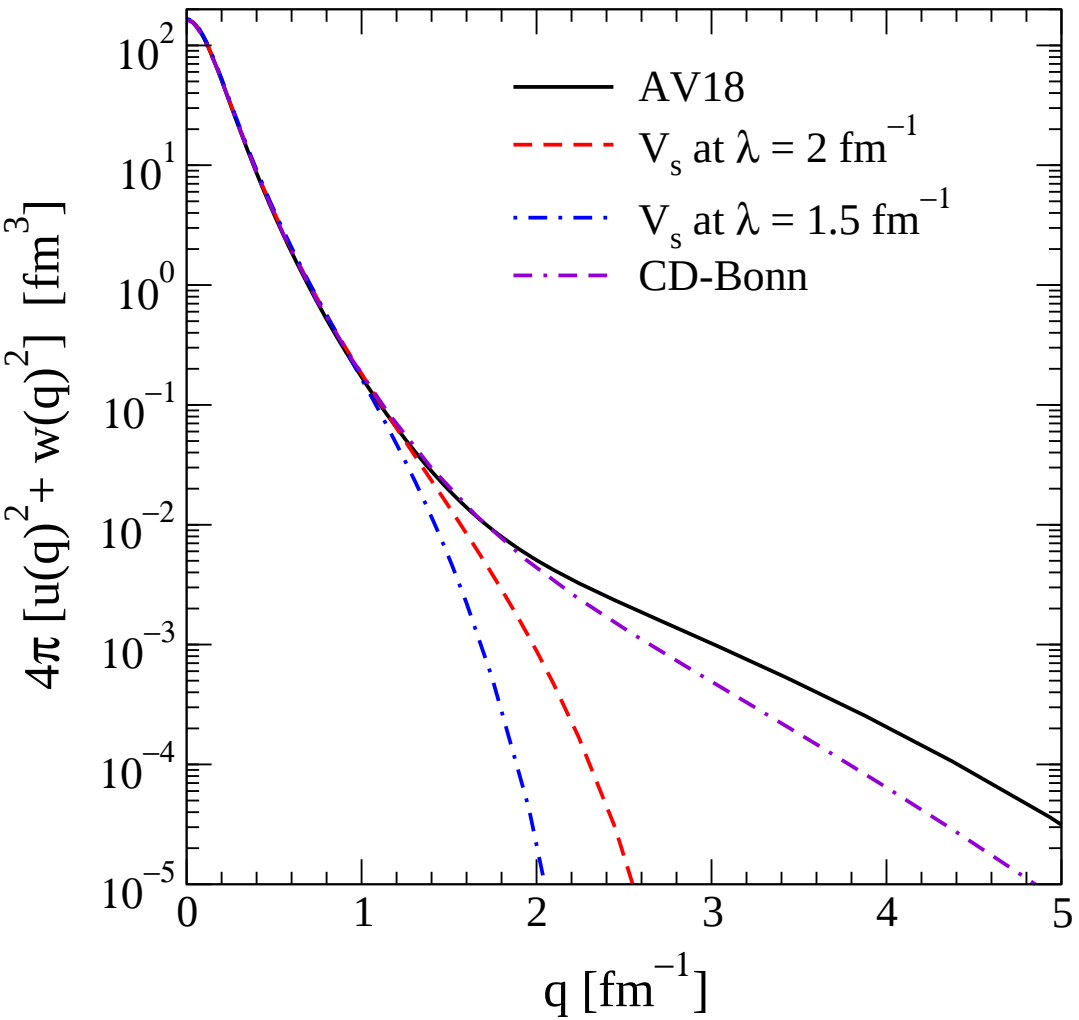
- Evolution with s of any operator O is given by:

$$O_s = U_s O U_s^\dagger$$

so O_s evolves via

$$\frac{dO_s}{ds} = [[G_s, H_s], O_s]$$

- $U_s = \sum_i |\psi_i(s)\rangle\langle\psi_i(0)|$
- Matrix elements of evolved operators are unchanged
- Consider momentum distribution $< \psi_d | a_q^\dagger a_q | \psi_d >$ at $q = 0.34$ and $3.0\,\mathrm{fm}^{-1}$ in deuteron



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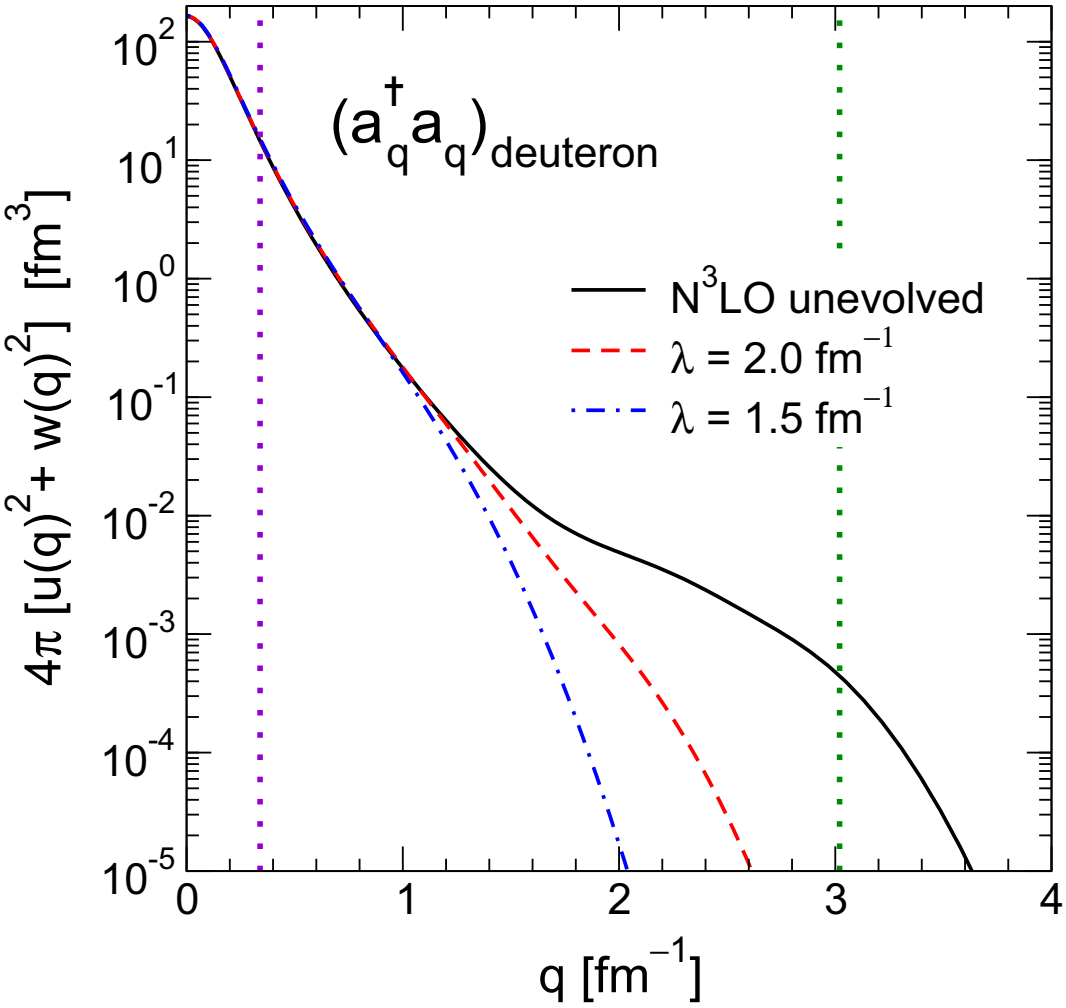
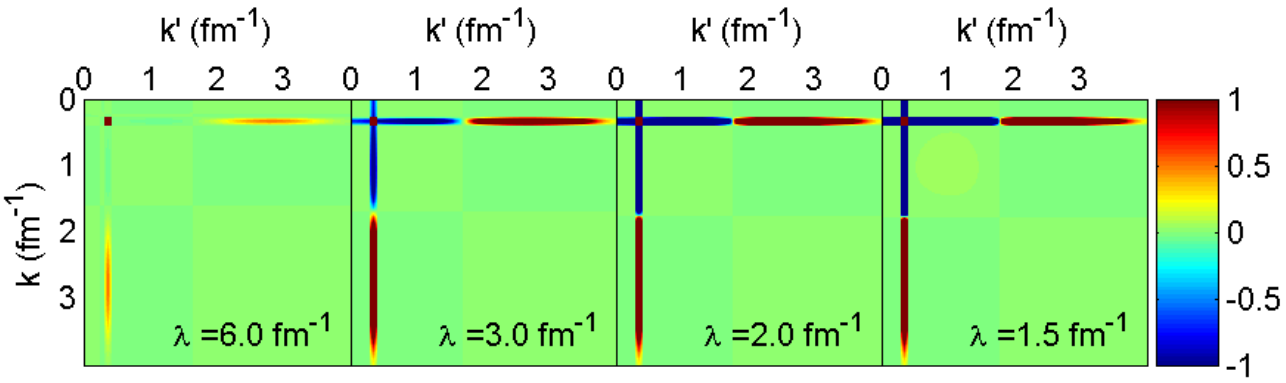
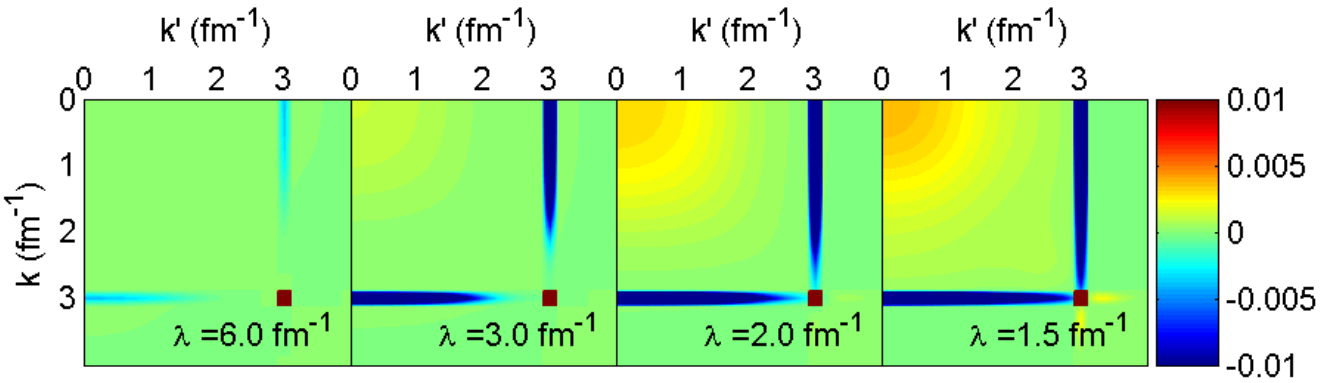


High and low momentum operators in deuteron

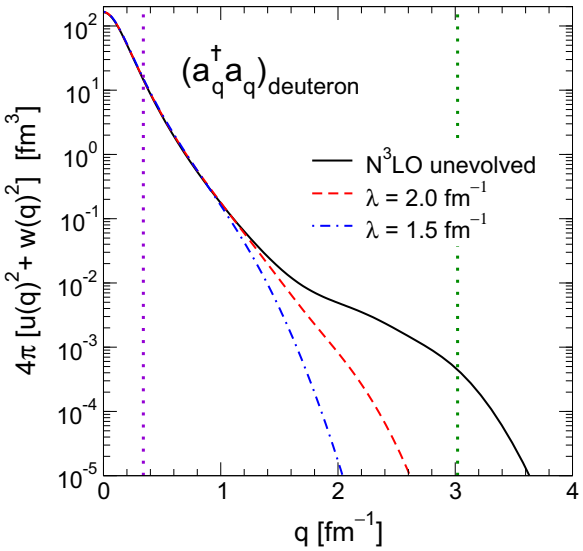
- **Integrand** of $(U a_q^\dagger a_q U^\dagger)$ for $q = 0.34\,\mathrm{fm}^{-1}$



- **Integrand** for $q = 3.02\,\mathrm{fm}^{-1}$



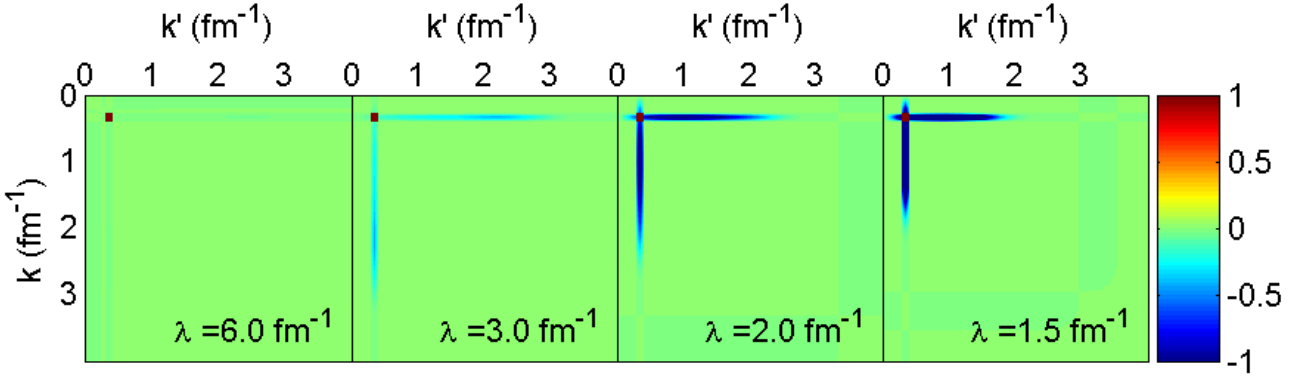
- Momentum distribution



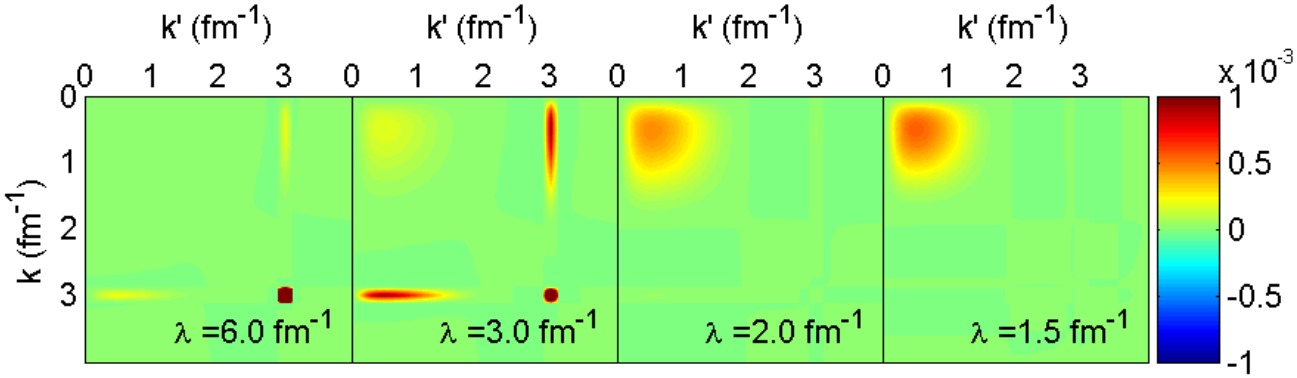
- **Decoupling** $\Longrightarrow$ High momentum components suppressed
- Integrated value does not change, but nature of operator does
- Similar for other operators: $\langle r^2 \rangle$, $\langle Q_d \rangle$, $\langle 1/r \rangle$ $\left\langle \frac{1}{r} \right\rangle$, $\langle G_C \rangle$, $\langle G_Q \rangle$, $\langle G_M \rangle$

High and low momentum operators in deuteron

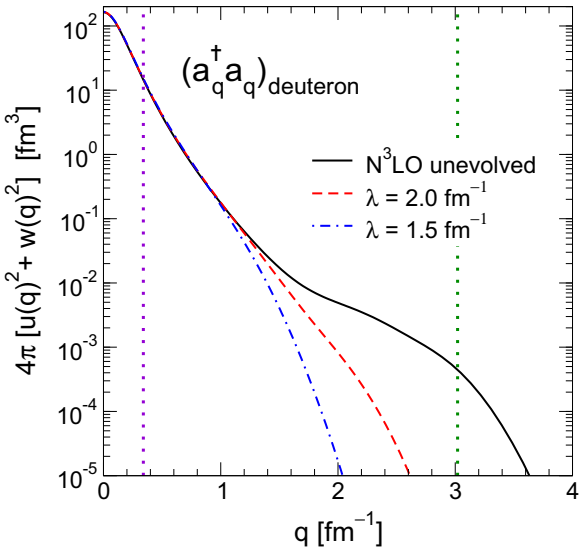
- **Integrand** of $\langle\psi_d|\left(U a_q^\dagger a_q U^\dagger\right)|\psi_d\rangle$ for $q = 0.34\,\mathrm{fm}^{-1}$



- **Integrand** for $q = 3.02\,\mathrm{fm}^{-1}$



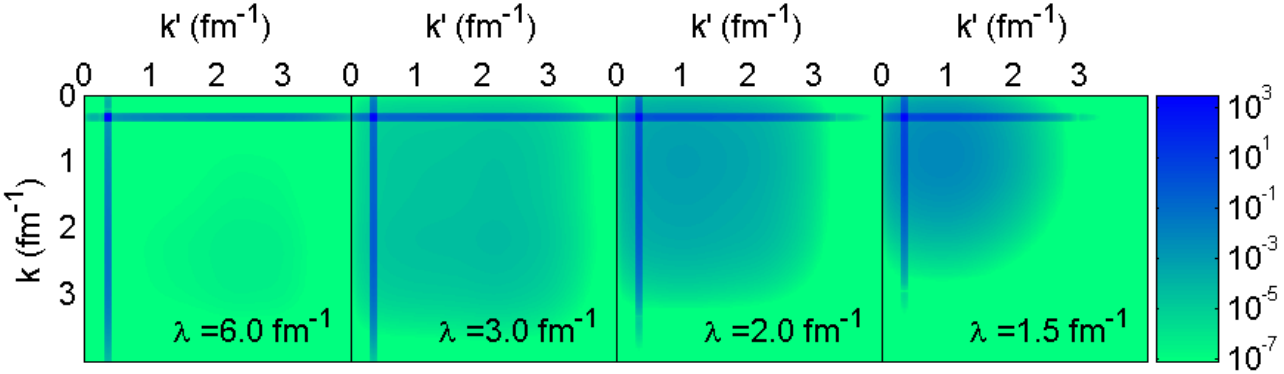
- Momentum distribution



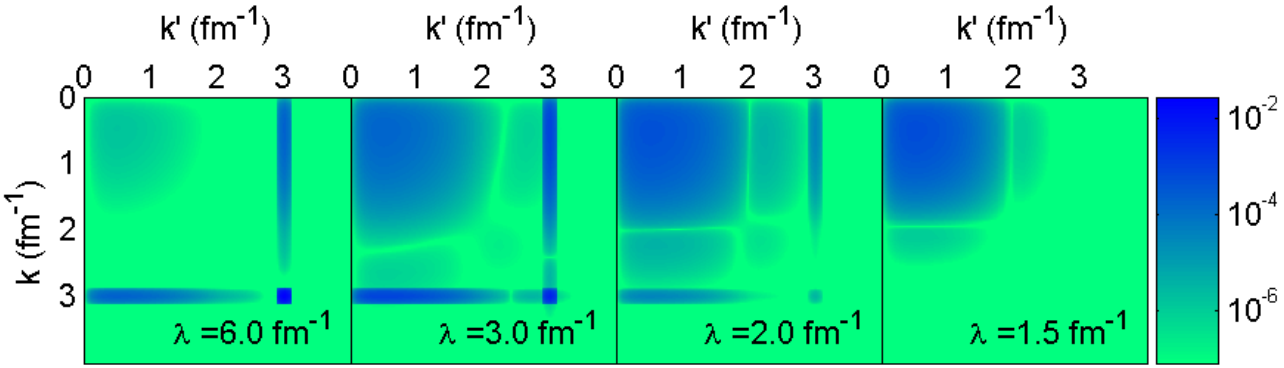
- **Decoupling** $\Longrightarrow$ High momentum components suppressed
- Integrated value does not change, but nature of operator does
- Similar for other operators: $\langle r^2\rangle$, $\langle Q_d\rangle$, $\langle 1/r\rangle$ $\left\langle\frac{1}{r}\right\rangle$, $\langle G_C\rangle$, $\langle G_Q\rangle$, $\langle G_M\rangle$

High and low momentum operators in deuteron

- **Integrand** of $\langle\psi_d|\left(U a_q^\dagger a_q U^\dagger\right)|\psi_d\rangle$ for $q = 0.34\,\mathrm{fm}^{-1}$



- **Integrand** for $q = 3.02\,\mathrm{fm}^{-1}$



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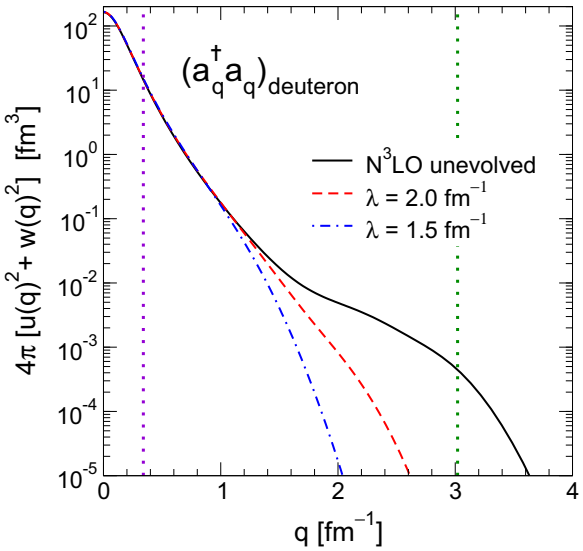

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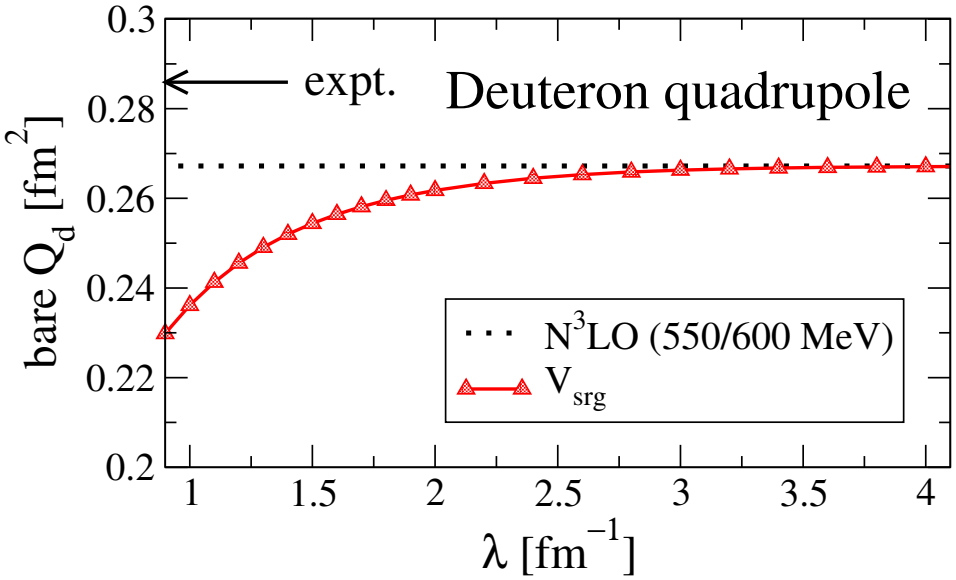
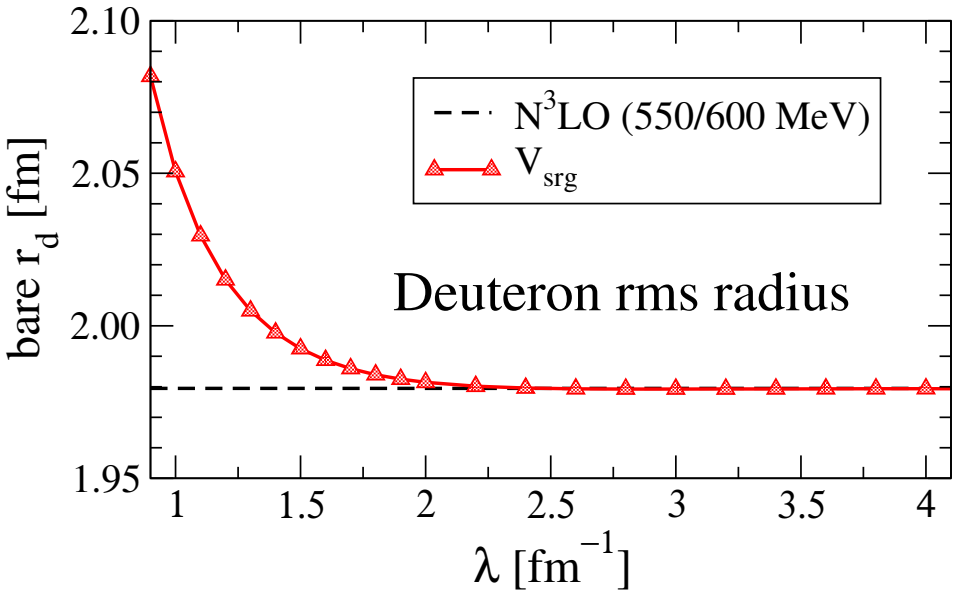
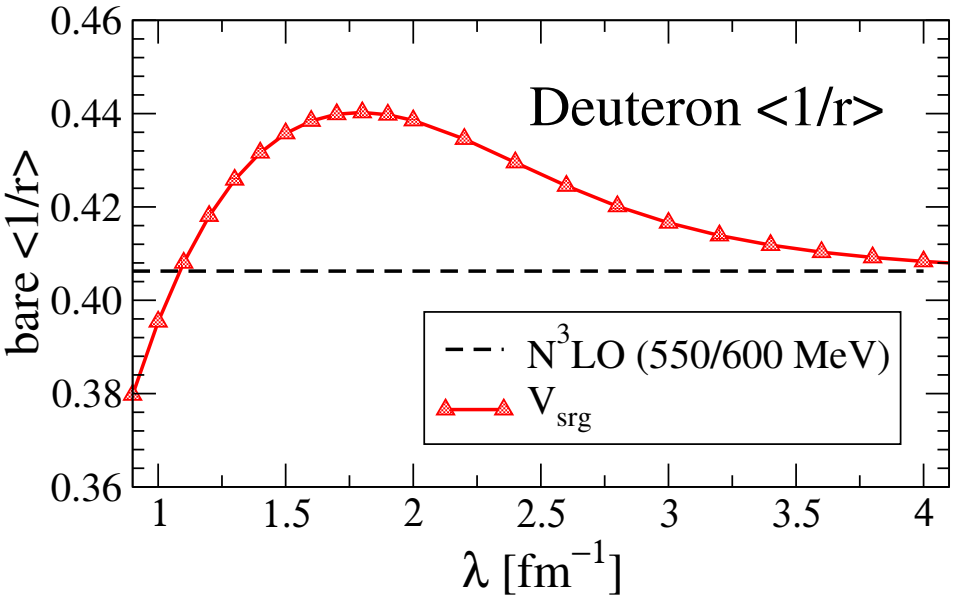
Long-distance physics largely unchanged

- Matrix elements dominated by long range run slowly for $\lambda \gtrsim 2\,\mathrm{fm}^{-1}$
- Here: examples from deuteron (compressed scales)

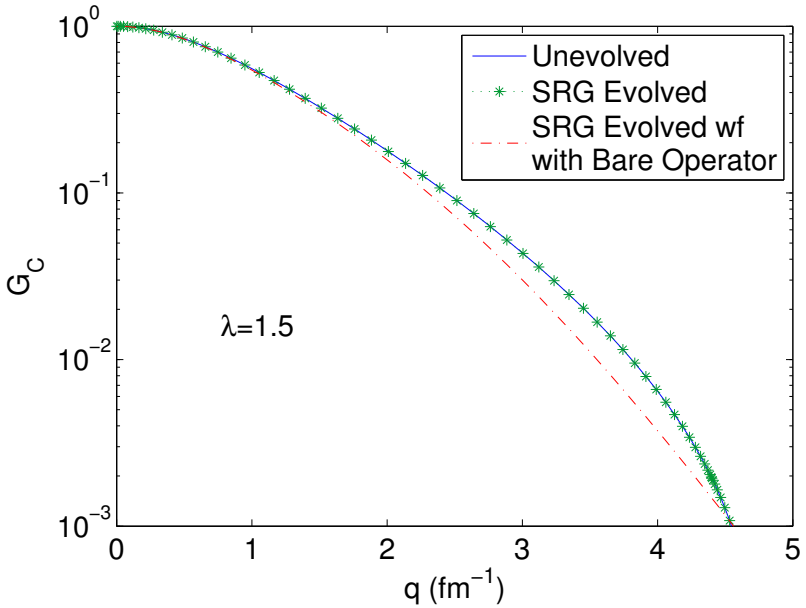


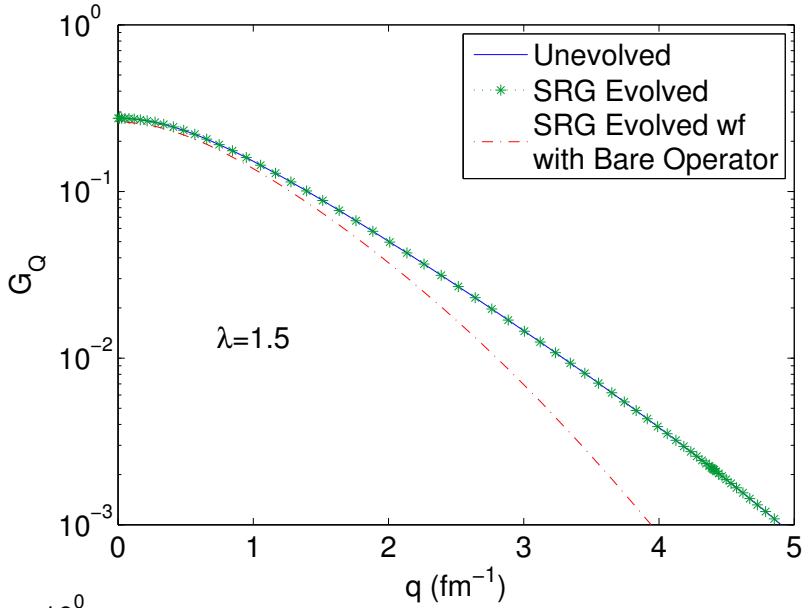


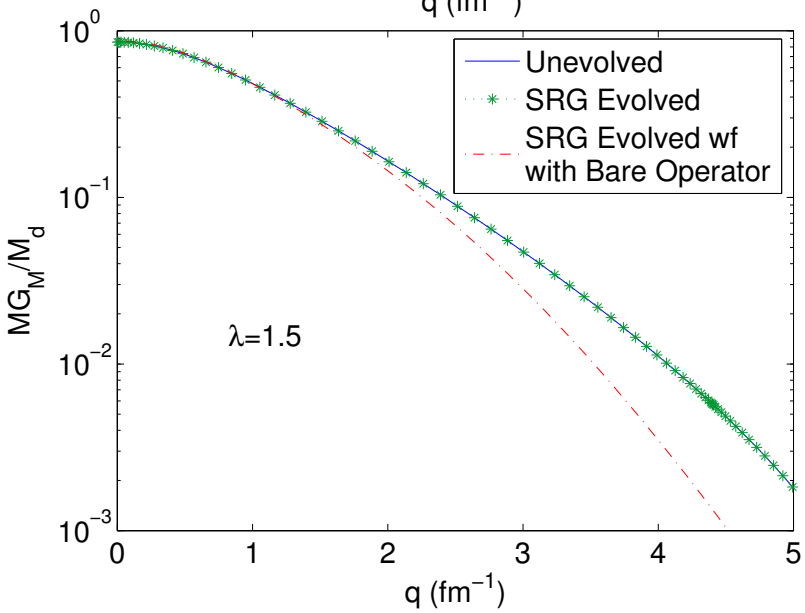


Deuteron electromagnetic form factors

- G_C, G_Q, G_M in deuteron with chiral EFT at leading order (Valderrama et al.)
- NNLO 550/600 MeV potential

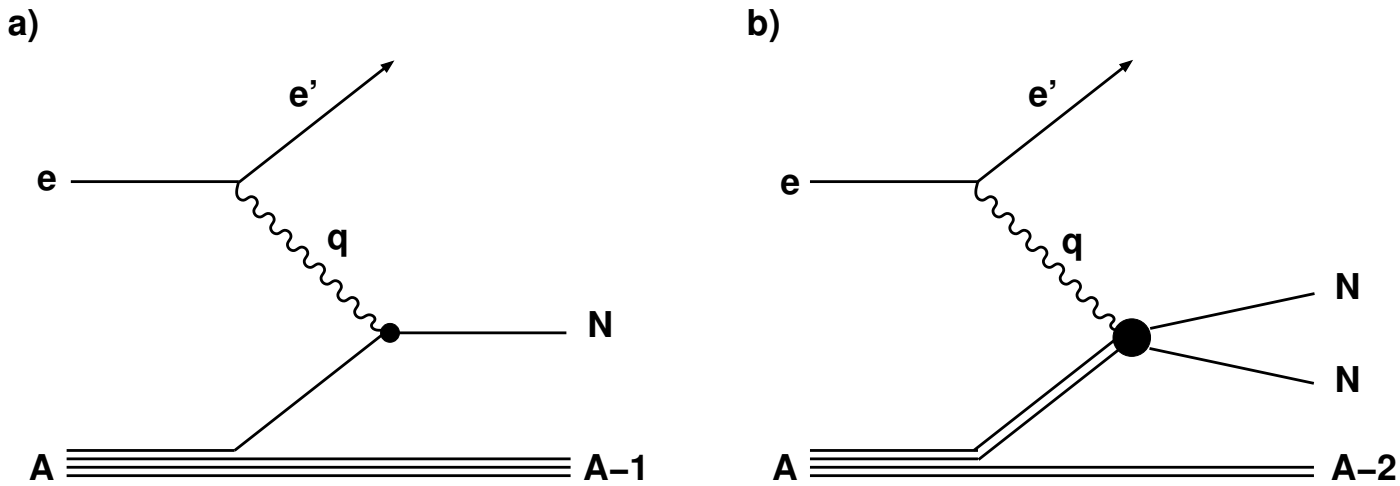






Changing resolution shifts physics: Not unique!

- From D. Higinbotham, arXiv:1010.4433

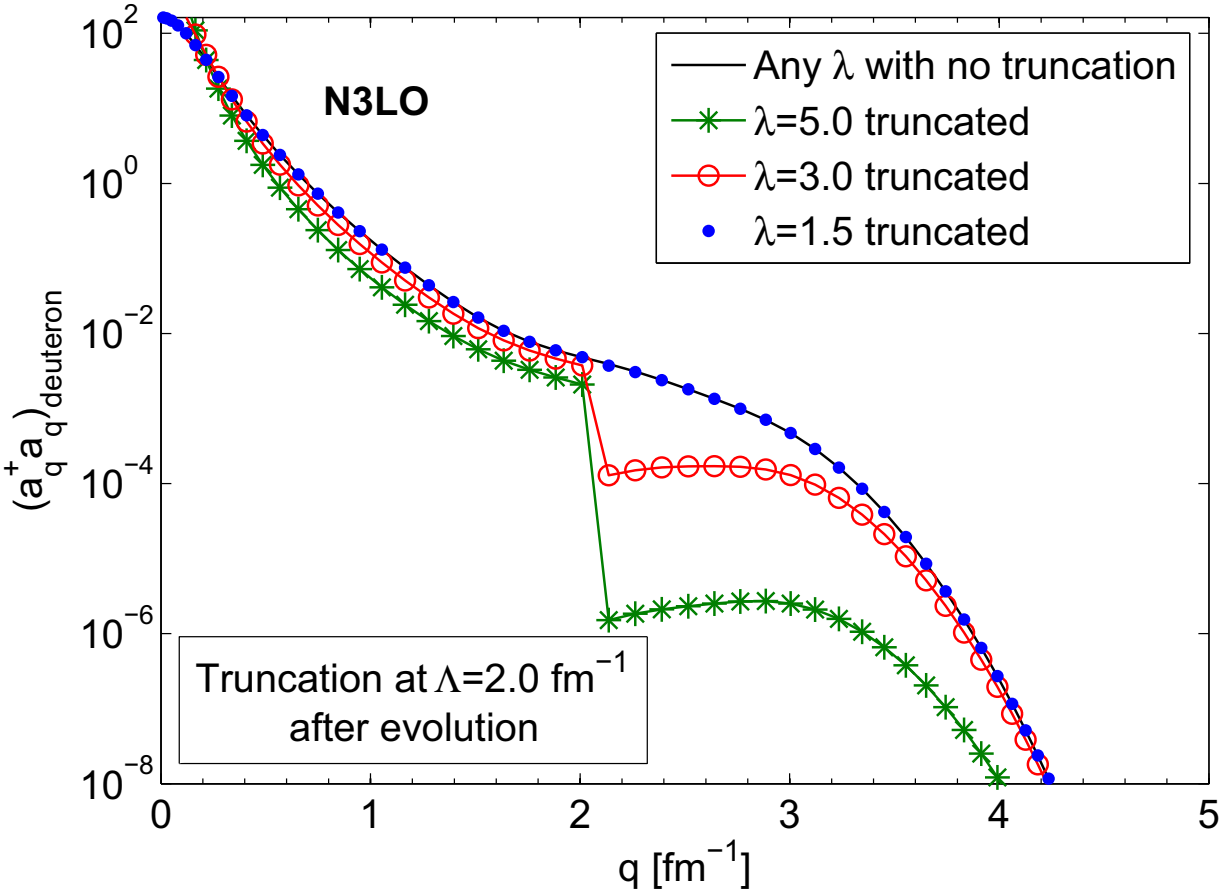


"The simple goal of short-range nucleon-nucleon correlation studies is to cleanly isolate diagram b) from a). Unfortunately, there are many other diagrams, including those with final-state interactions, that can produce the same final state as the diagram scientists would like to isolate. If one could find kinematics that were dominated by diagram b) it would finally allow electron scattering to provide new insights into the short-range part of the nucleon-nucleon potential."

- What is in the blob in b)? A one-body vertex and an SRC, or a two-body vertex? Depends on the resolution! (Also FSI+ will mix.)

Test decoupling in operator expectation values

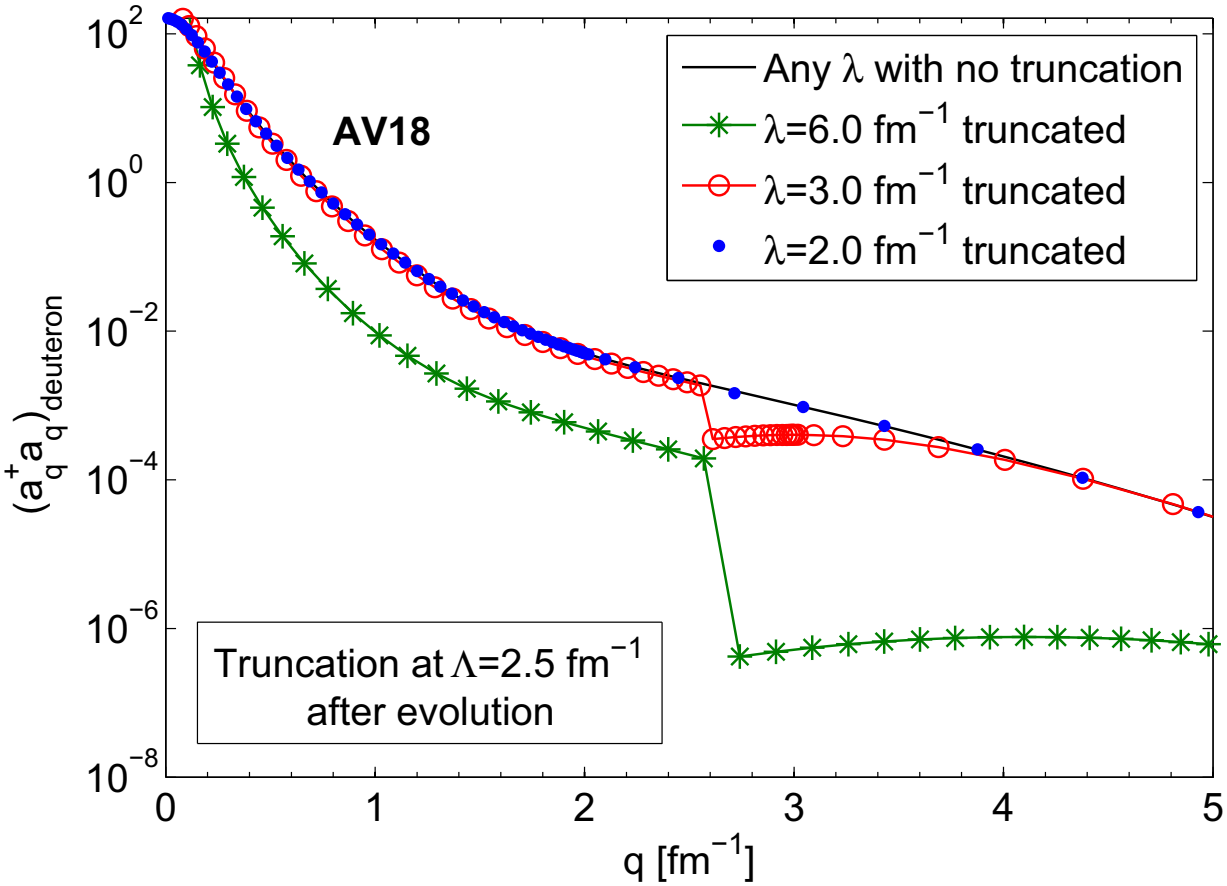
- Evolve to λ in full space $\rightarrow$ **TRUNCATE at** $\Lambda = 2.0\,\mathbf{fm}^{-1}$:



- Here: momentum distribution $a^\dagger_q a_q$
- Decoupling for all q works when $\lambda < \Lambda_{\text{truncate}}$

Test decoupling in operator expectation values

- Evolve to λ in full space $\rightarrow$ **TRUNCATE at** $\Lambda = 2.5\,\mathbf{fm}^{-1}$:



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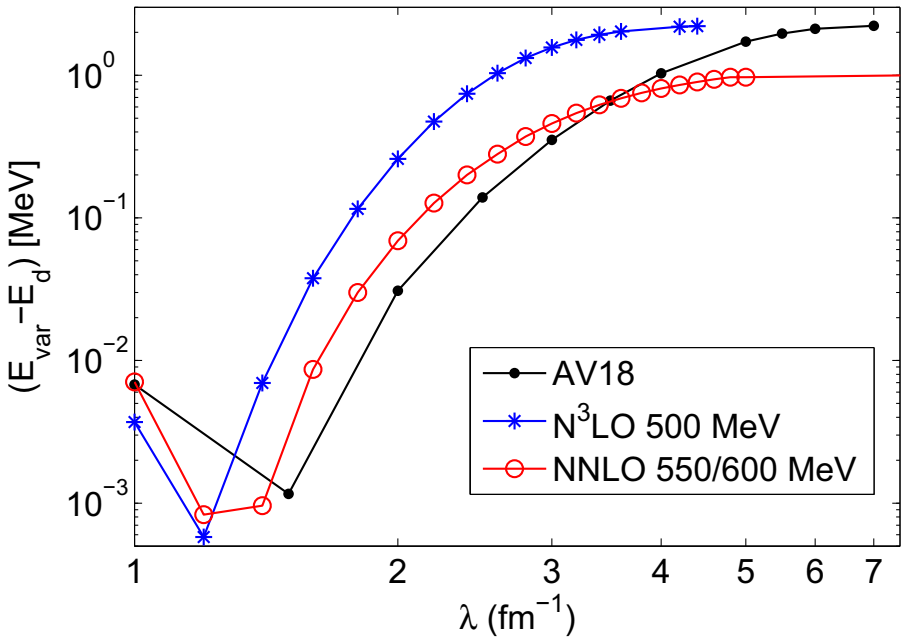
Variational calculations in the deuteron

- Test whether operators are fine-tuned
- Try a simple variational ansatz (from k-space S-eqn)

$$u(k) = \frac{1}{(k^2+\gamma^2)(k^2+\mu^2)} e^{-\left(\frac{k^2}{\lambda^2}\right)^2} \qquad w(k) = \frac{ak^2}{(k^2+\gamma^2)(k^2+\nu^2)^2} e^{-\left(\frac{k^2}{\lambda^2}\right)^2}$$

- error in energy for different starting potentials
- small λ works great!
- no fine-tuning



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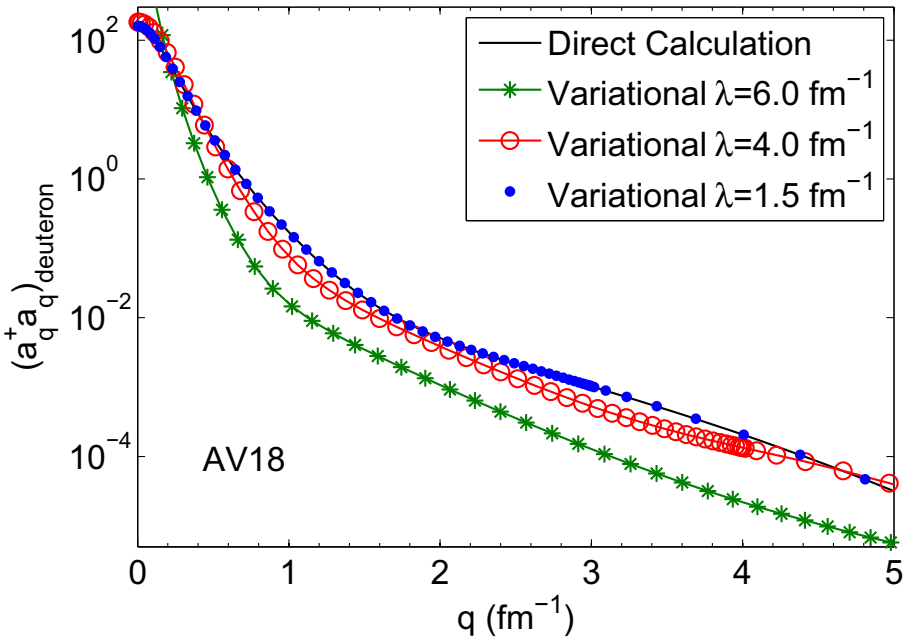
- momentum distribution for AV18 at several λ's
- small λ works great!
- no fine-tuning



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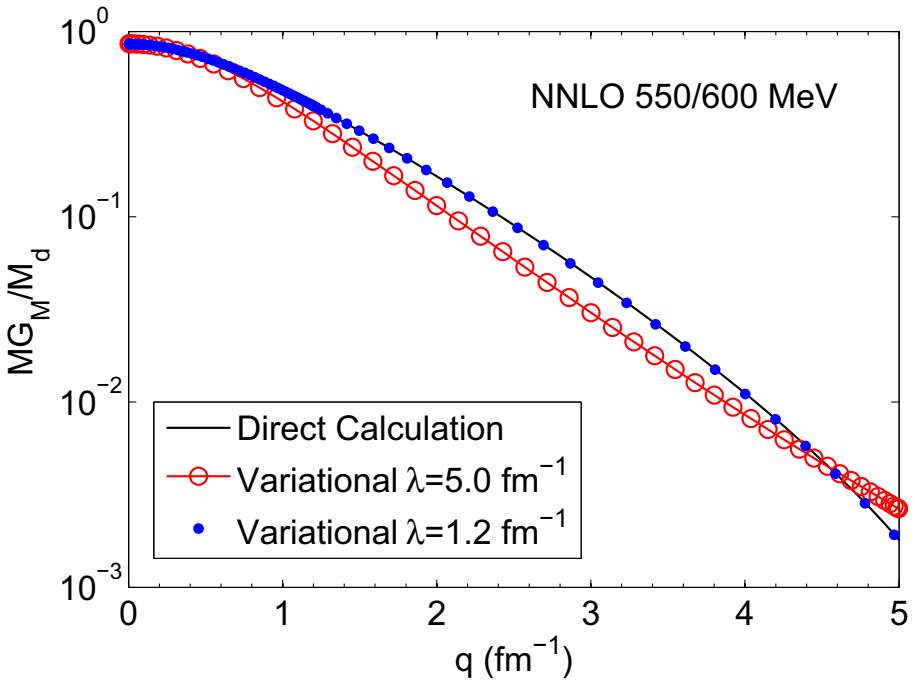
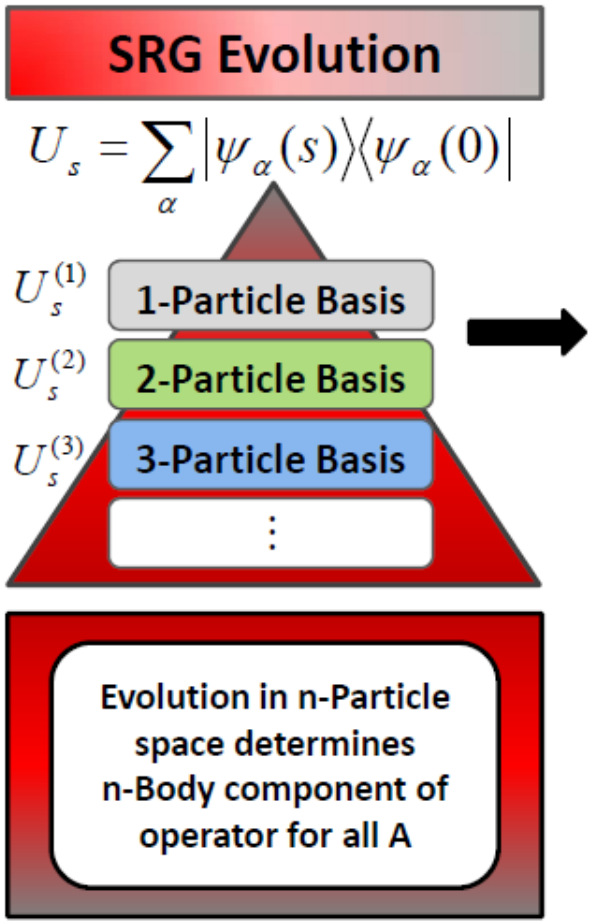
- form factor G_M for NNLO at two λ's vs. direct
- small λ works great!
- no fine-tuning



Operator evolution & extraction process



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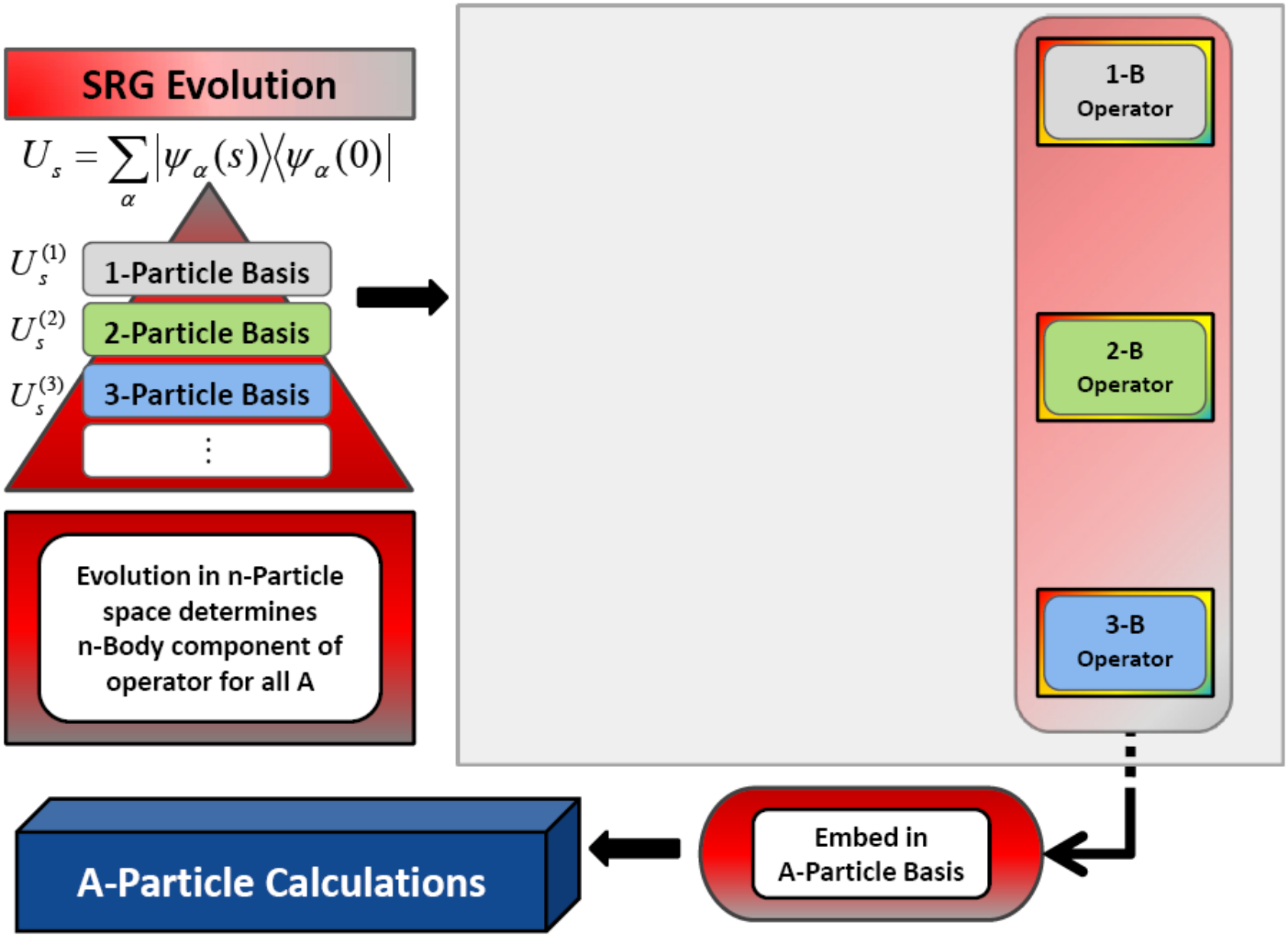

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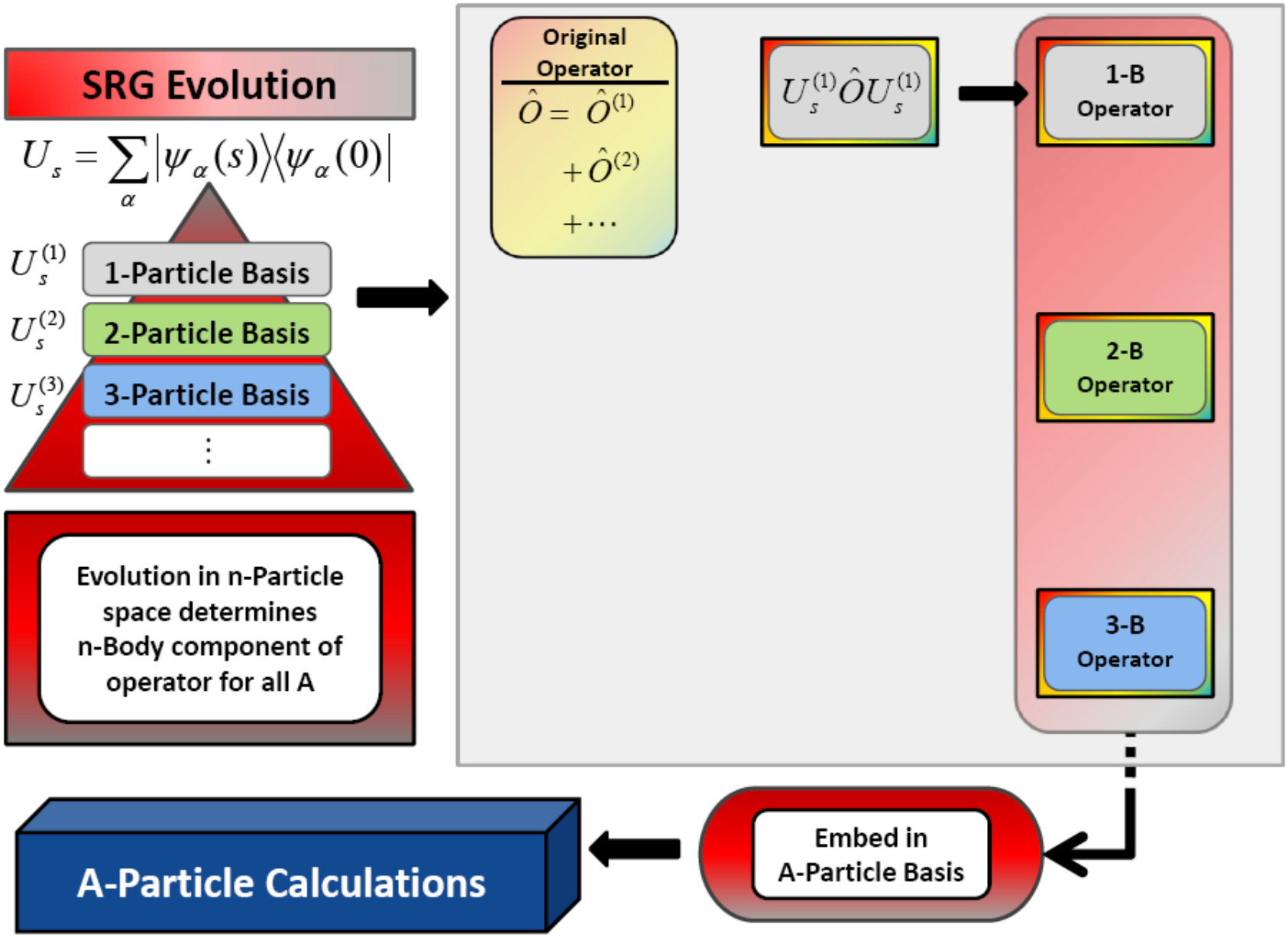

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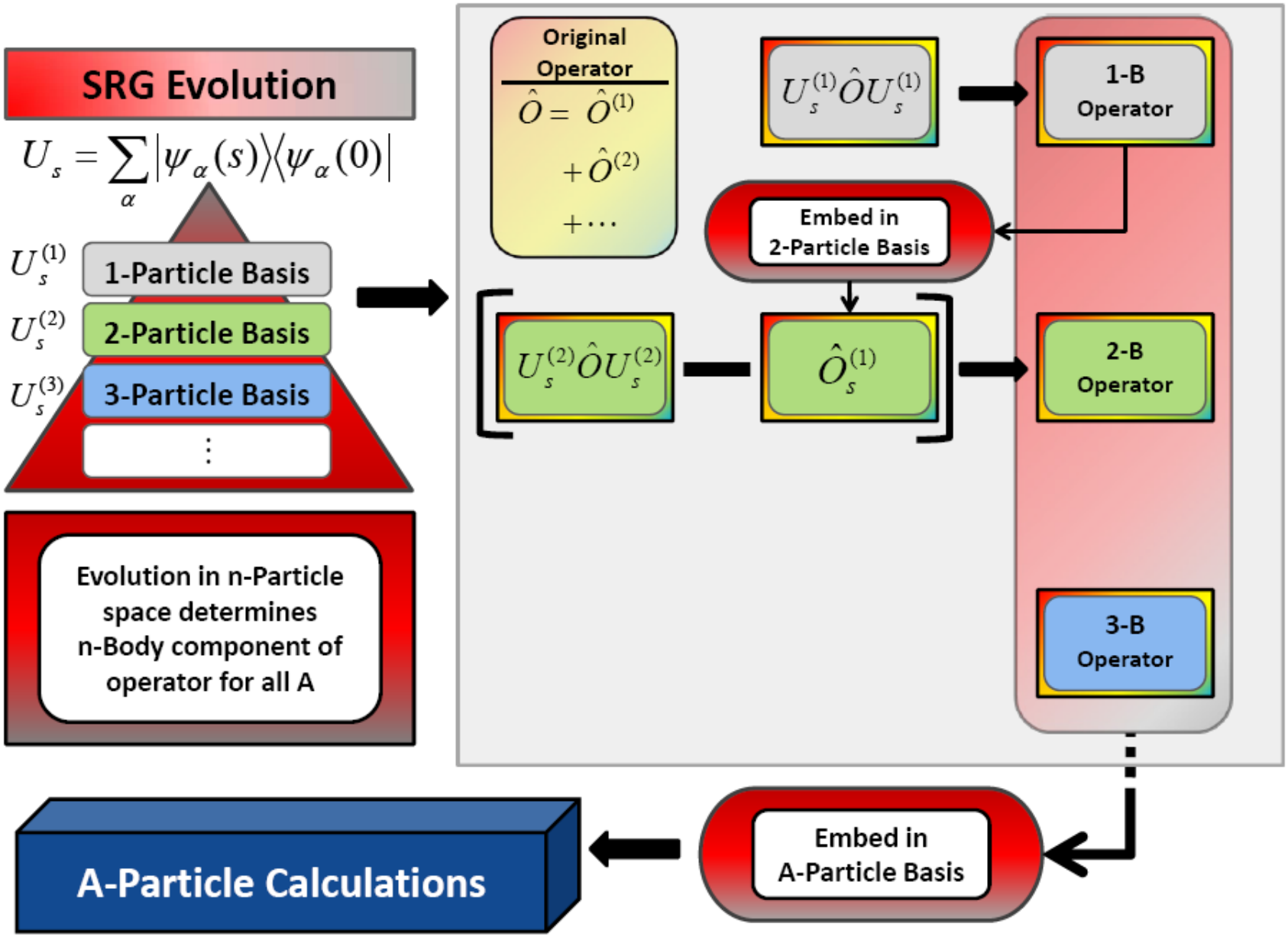

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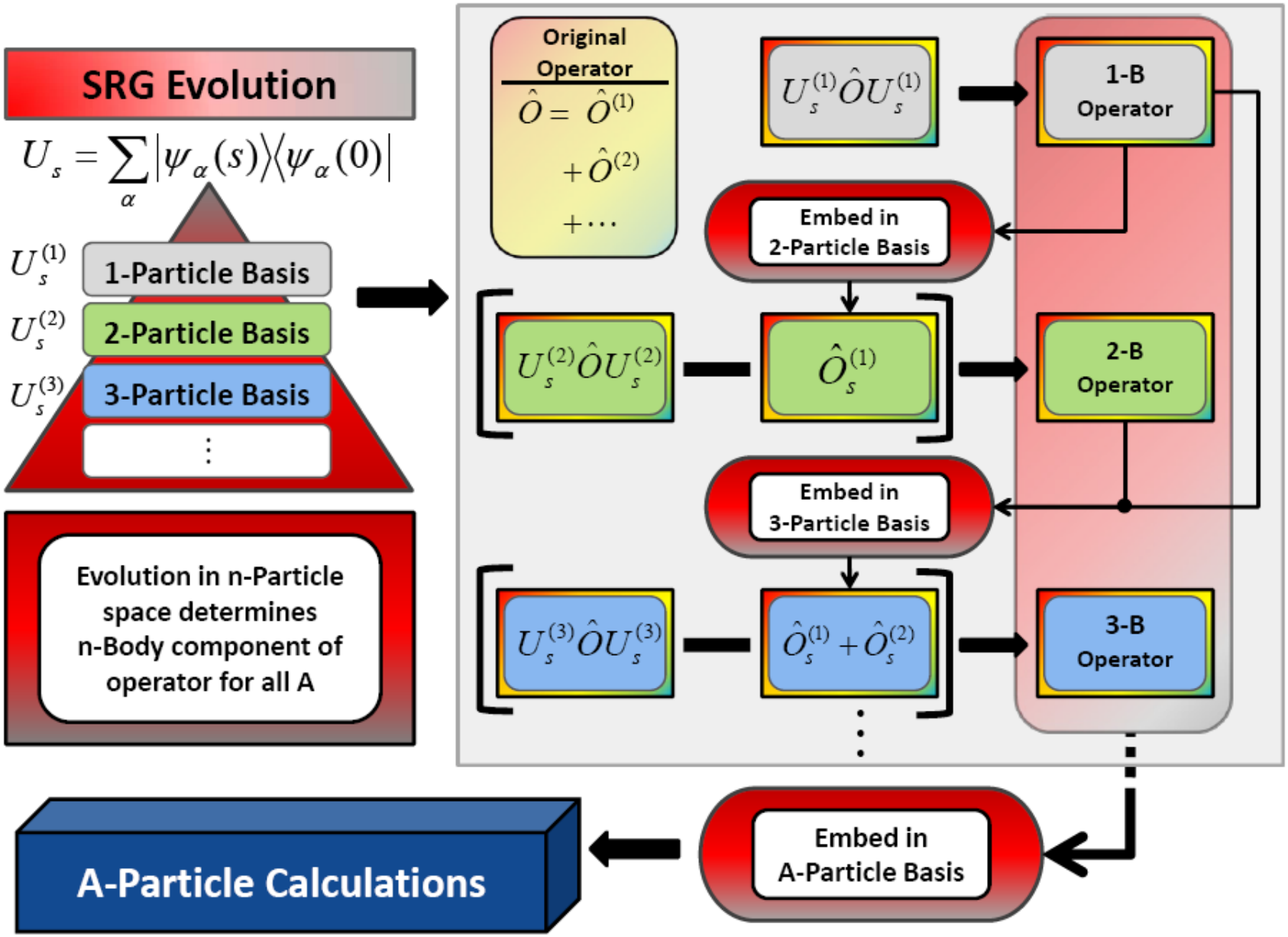

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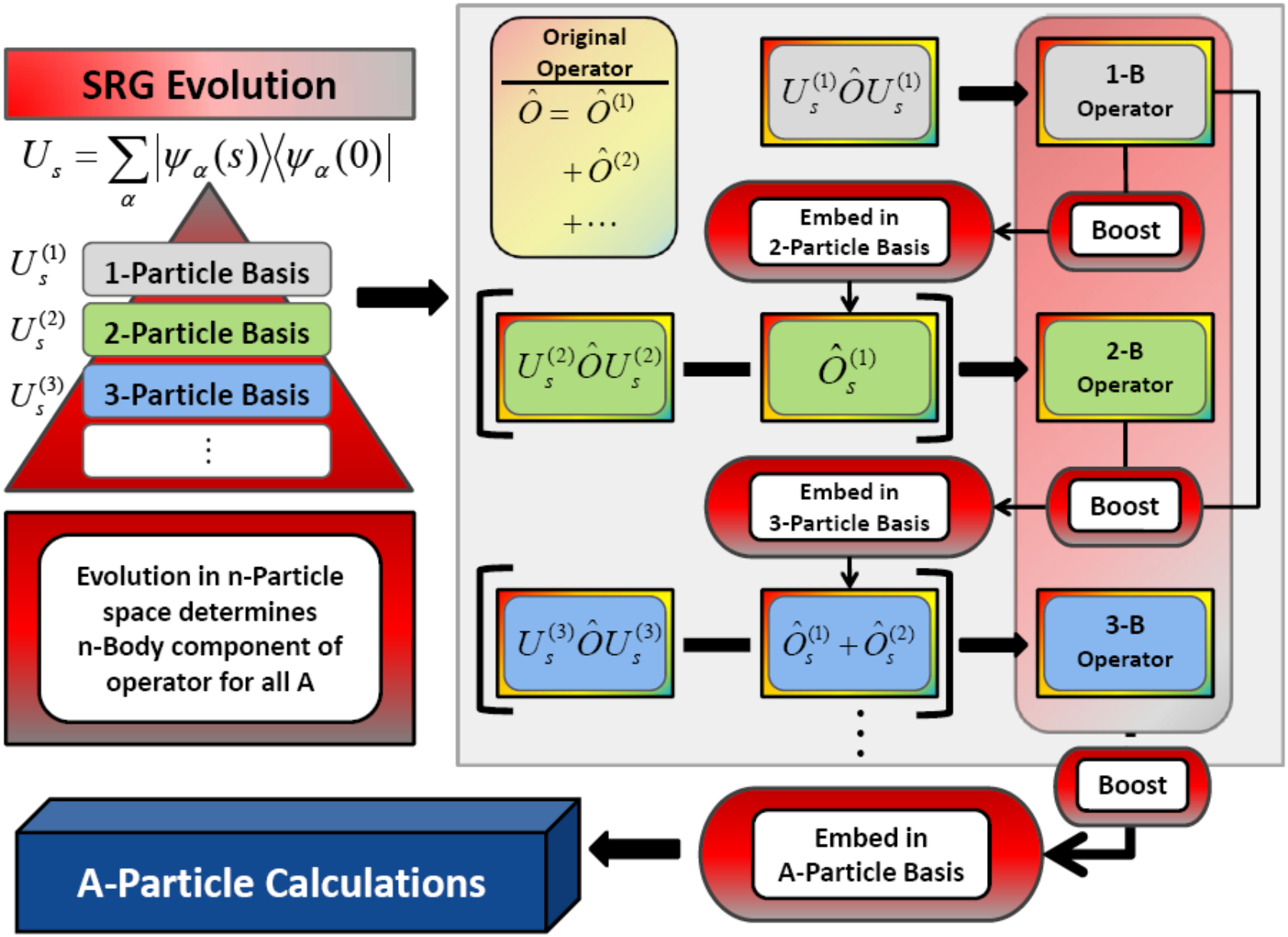
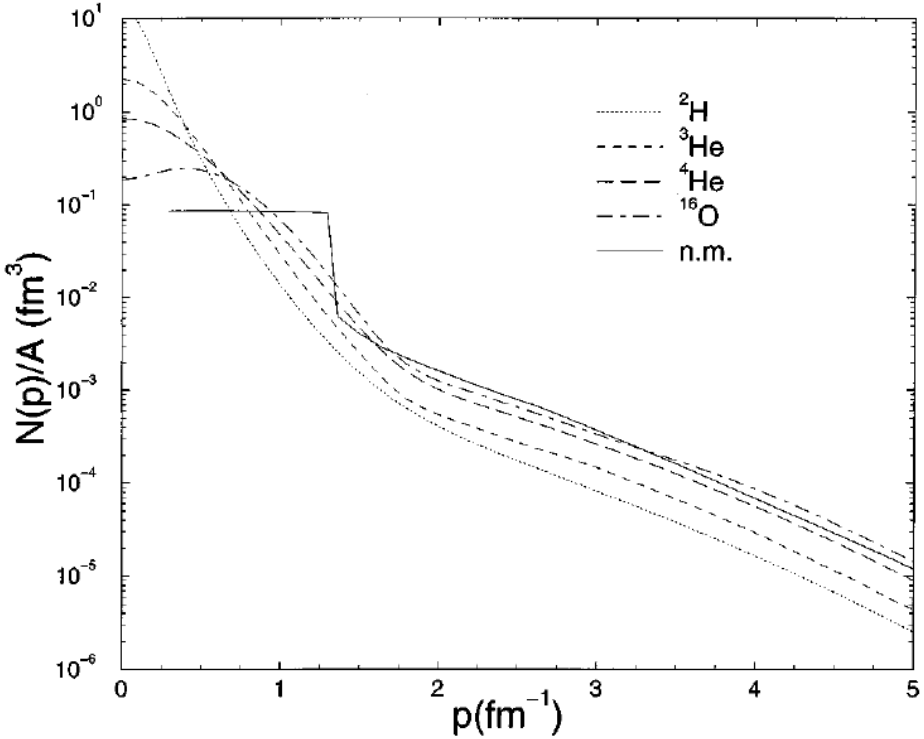


Nuclear scaling: $n_A(p) \approx C_A n_D(p)$ at large p

- AV14 NN with VMC



From Pieper, Wiringa, and Pandharipande (1992).

- Conventional explanation: Dominance of NN potential and short-range correlations (Frankfurt et al.)

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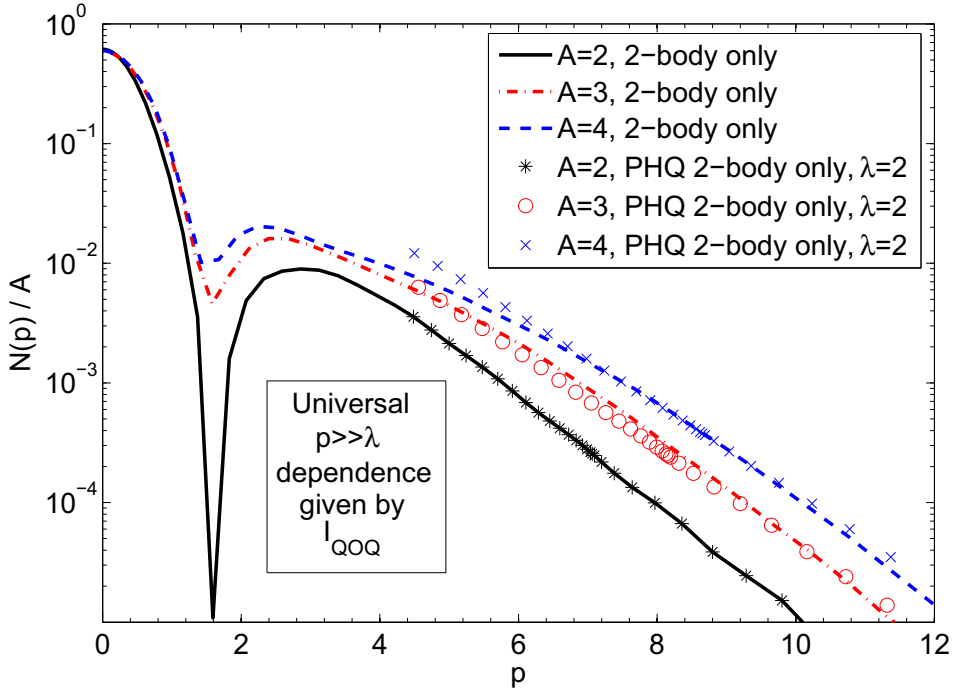

- Alternative: *factorization*

$$\int_0^\lambda \int_0^\lambda \psi_\lambda^\dagger(k') \left[I_{QOQ} K_\lambda(k') K_\lambda(k) \right] \psi_\lambda(k)$$

- universal p dependence from I_{QOQ}
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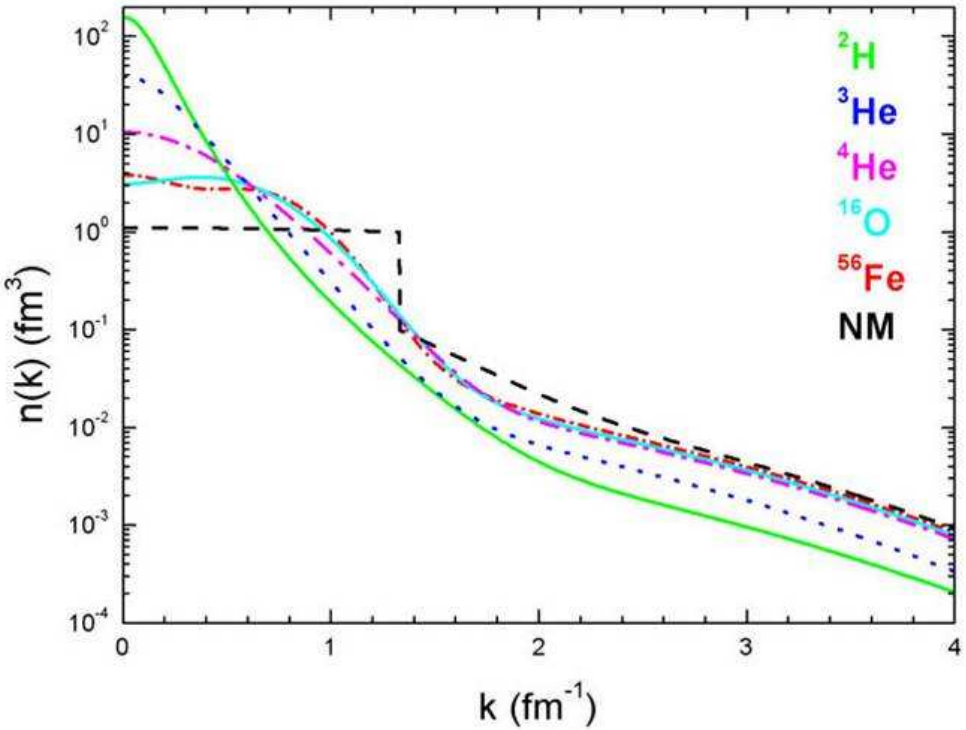
- Two-nucleon correlation model



From C. Ciofi degli Atti and S. Simula.

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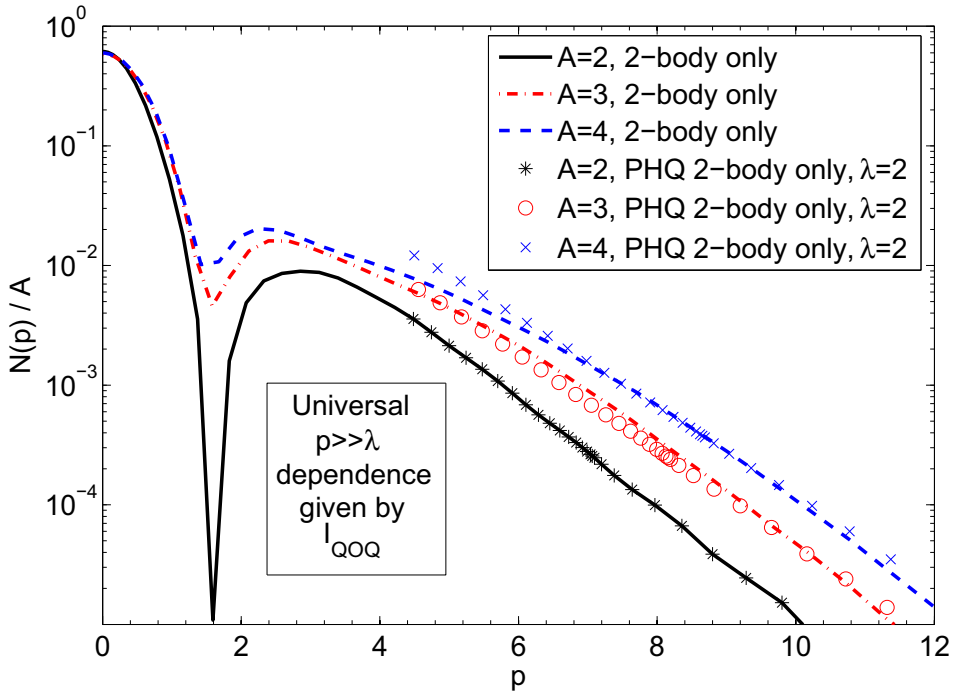

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Factorization [Anderson et al., arXiv:1008.1569]

- If $k < \lambda$ and $q \gg \lambda \Longrightarrow$ factorization: $U_\lambda(k,q) \to K_\lambda(k) Q_\lambda(q)$
- Operator product expansion for nonrelativistic wf's (see Lepage)

$$\Psi_{true}(r) = \overline{\gamma}(r) \int dr'\, \Psi_{eff} \delta_a(r') + \overline{\eta}(r) a^2 \int dr'\, \Psi_{eff} \nabla^2 \delta_a(r') + \mathcal{O}(a^4)$$

- Similarly, in momentum space

$$\Psi^\infty_\alpha(q) \approx \gamma^\lambda(q) \int_0^\lambda p^2 dp\; Z(\lambda) \Psi^\lambda_\alpha(p) + \eta^\lambda(q) \int_0^\lambda p^2 dp\, p^2\, Z(\lambda)\, \Psi^\lambda_\alpha(p) + \cdots$$

- By projecting potential in momentum subspace, recover OPE via:

$$\gamma^\lambda(q) \equiv -\int_\lambda^\infty q'^2 dq' \,\langle q| \frac{1}{\widehat{Q}_\lambda H^\infty \widehat{Q}_\lambda} |q'\rangle V^\infty(q',0)$$

$$\eta^\lambda(q) \equiv -\int_\lambda^\infty q'^2 dq' \,\langle q| \frac{1}{\widehat{Q}_\lambda H^\infty \widehat{Q}_\lambda} |q'\rangle \frac{\partial^2}{\partial p^2} V^\infty(q',p)|_{p^2=0}$$

- Construct unitary transformation to get $U_\lambda(k,q) \approx K_\lambda(k) Q_\lambda(q)$

$$U_\lambda(k,q) = \sum_\alpha \langle k|\psi^\lambda_\alpha\rangle\langle\psi^\infty_\alpha|q\rangle \to \left[\sum_\alpha^{\alpha_{low}} \langle k|\psi^\lambda_\alpha\rangle \int_0^\lambda p^2 dp\; Z(\lambda)\Psi^\lambda_\alpha(p)\right]\gamma^\lambda(q) + \cdots$$

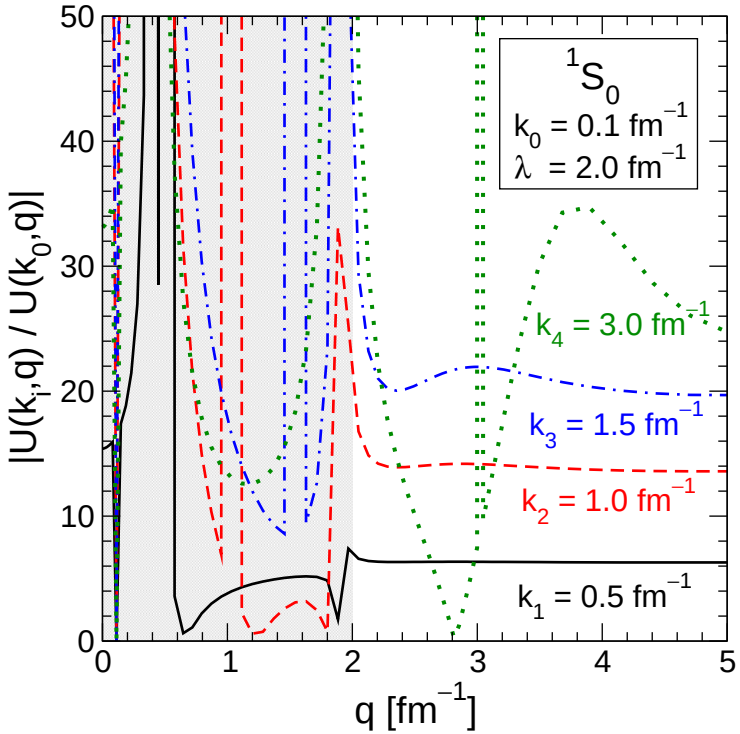
Numerical factorization [Anderson et al., arXiv:1008.1569]

- Test of factorization of U:

$$\frac{U_\lambda(k_i,q)}{U_\lambda(k_0,q)} \to \frac{K_\lambda(k_i)Q_\lambda(q)}{K_\lambda(k_0)Q_\lambda(q)},$$

so for $q \gg \lambda \Rightarrow \frac{K_\lambda(k_i)}{K_\lambda(k_0)}$.

- Look for plateaus: $k_i \lesssim 2\,\mathrm{fm}^{-1} \lesssim q$



- Singular value decomposition
  - quantitatively analyze the extent to which U factorizes
  - outer product expansion

$$G = \sum_{i=1}^{r} d_i \mathbf{u}_i \mathbf{v}_i^t$$

where r is the rank and the d_i are decreasing singular values

- Example: results for $\lambda = 2\,\mathrm{fm}^{-1}$, for $q > \lambda$ and $k < \lambda$

	$^1S_0$		
Potential	d_1	d_2	d_3
AV18	0.763	0.033	0.007
N3LO 500 MeV	1.423	0.221	0.015
N3LO 550/600 MeV	3.074	0.380	0.061
	$^3S_1$–$^3S_1$		
AV18	0.671	0.015	0.008
N3LO 500 MeV	1.873	0.225	0.044
N3LO 550/600 MeV	4.195	0.587	0.089

Practical use of factorization

- Decoupling implies

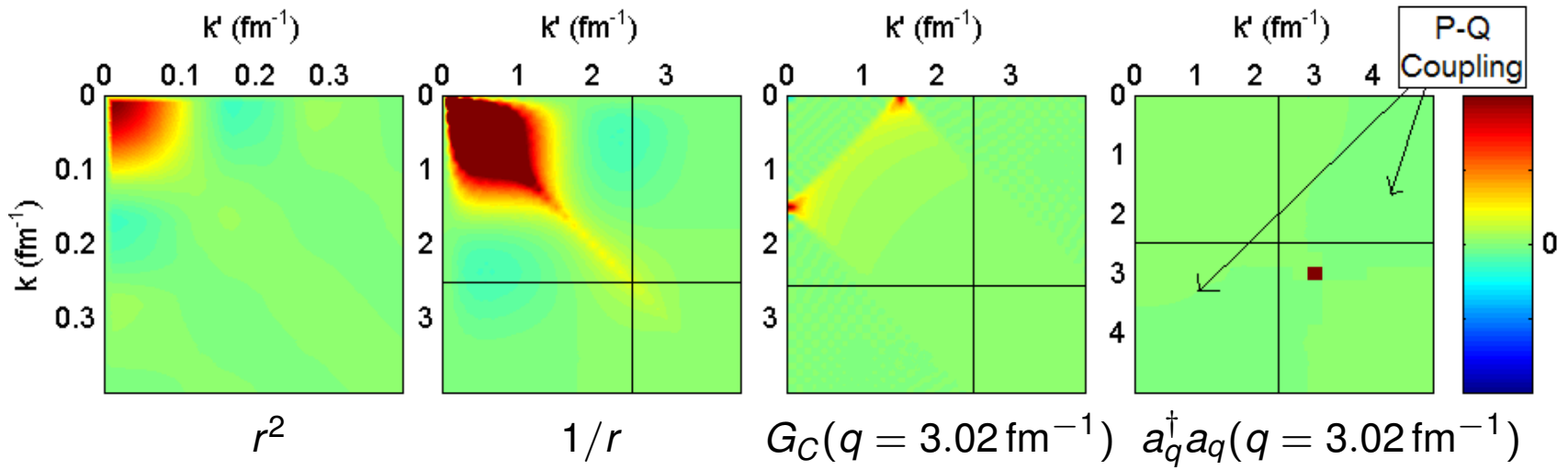
$$\langle\psi_\lambda|\, U_\lambda \widehat{O}\, U_\lambda^\dagger \,|\psi_\lambda\rangle \cong \int_0^\lambda dk' \int_0^\infty dq' \int_0^\infty dq \int_0^\lambda dk\; \psi_\lambda^\dagger(k') U_\lambda(k',q') \widehat{O}(q',q) U_\lambda^\dagger(q,k) \psi_\lambda(k)$$

- Factorization: set $U_\lambda(k,q) \to K_\lambda(k) Q_\lambda(q)$, where $k < \lambda$ and $q \gg \lambda$

$$\Longrightarrow \int_0^\lambda \int_0^\lambda \psi_\lambda^\dagger(k') \left[\int_0^\lambda \int_0^\lambda \underbrace{U_\lambda(k',q') \widehat{O}(q',q) U_\lambda^\dagger(q,k)}_{\text{Low Momentum Structure}} + I_{QOQ}\, \underbrace{K_\lambda(k') K_\lambda(k)}_{\text{Low Momentum Structure}} \right] \psi_\lambda(k)$$

where $I_{QOQ} \equiv \int_\lambda^\infty dq' \int_\lambda^\infty dq \left[Q_\lambda(q') \widehat{O}(q',q) Q_\lambda(q) \right]$ ← *Universal*

– Valid when initial operators weakly couple high and low momentum:



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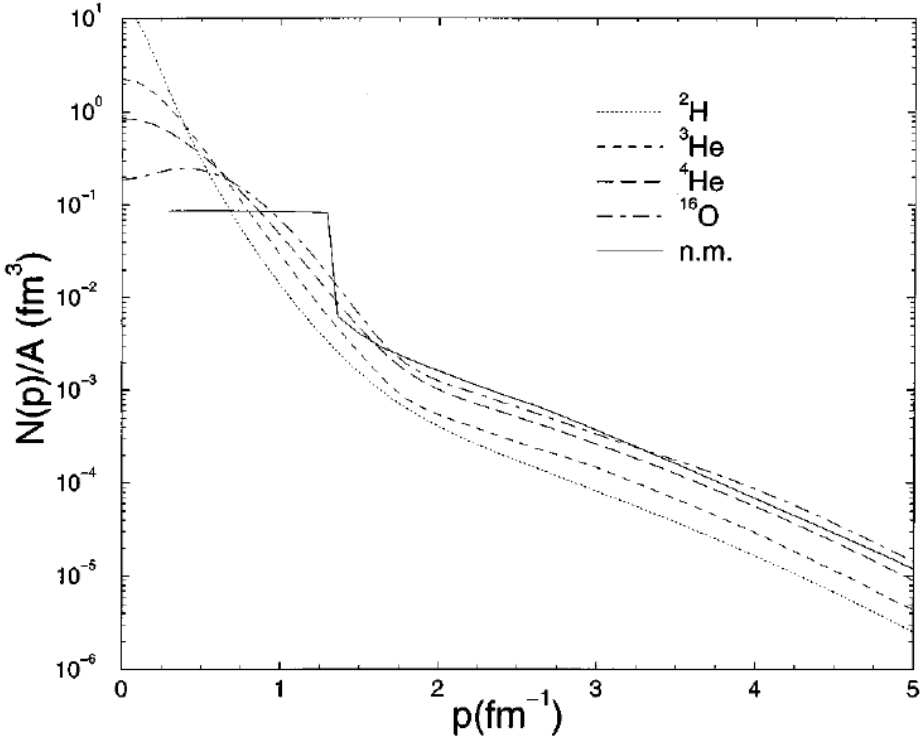

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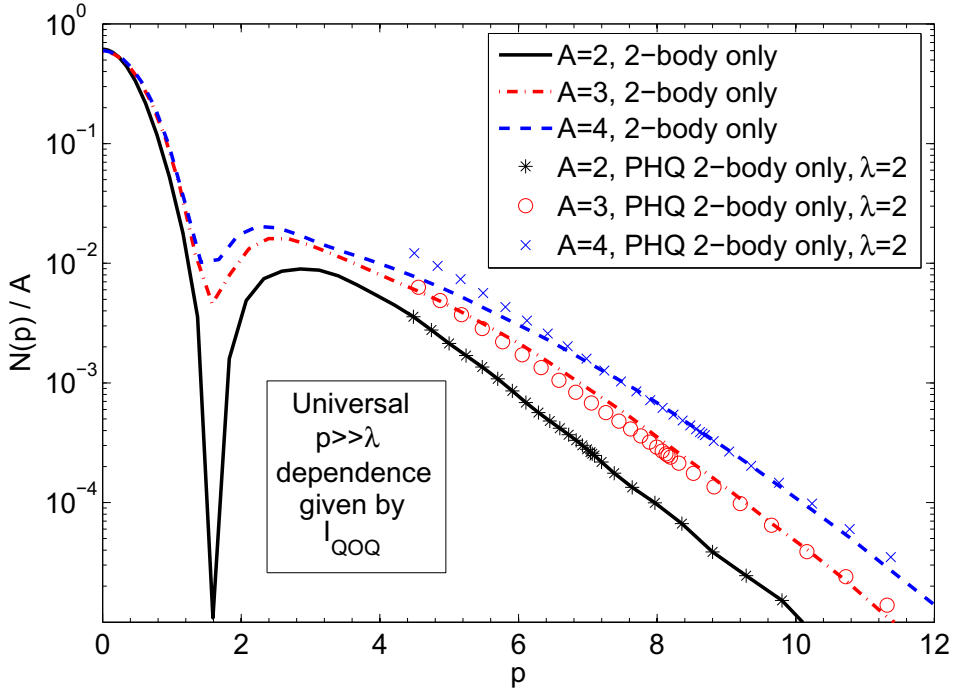

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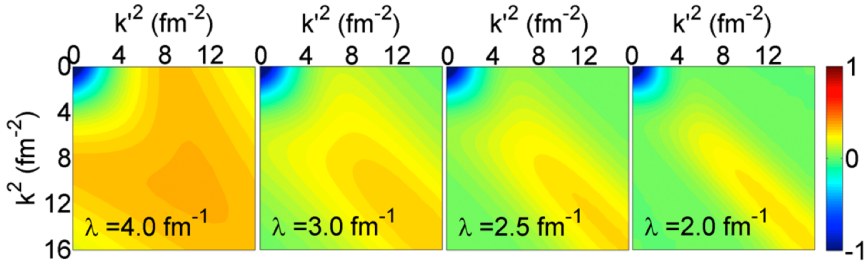
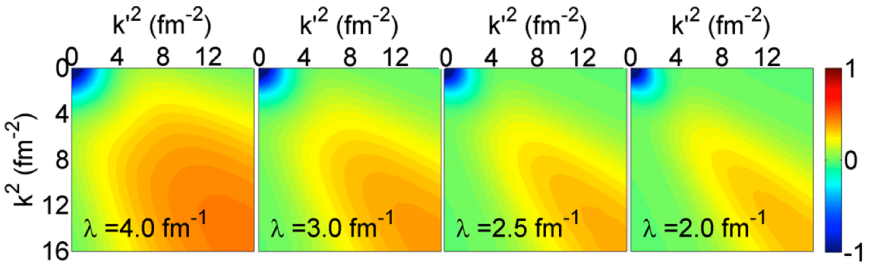
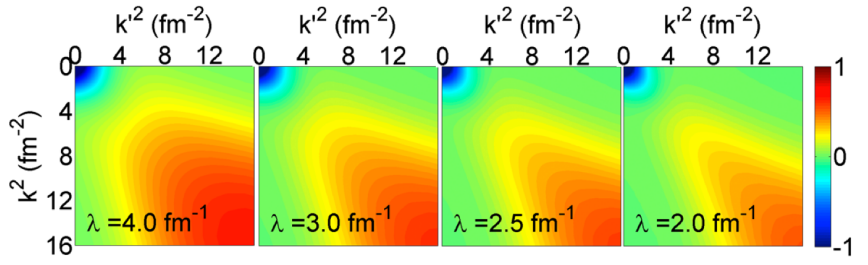
Novel generators [Shirley Li, OSU physics major]



$$G_s = T$$

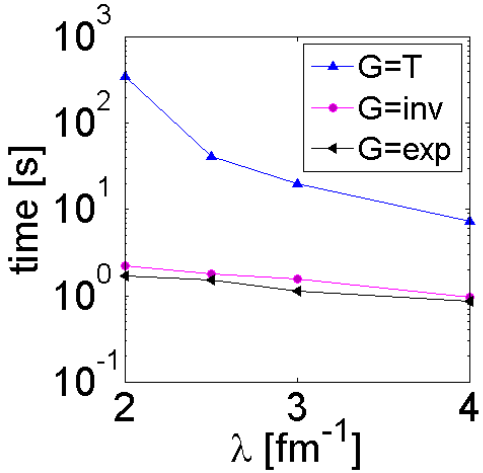


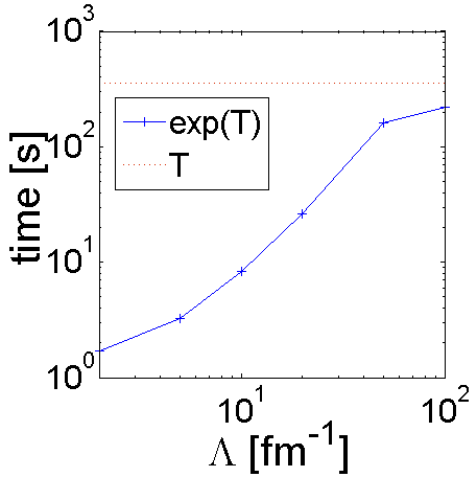
$$G_s = -\Lambda^2/(1 + T/\Lambda^2) \approx c + T + \cdots$$



$$G_s = -\Lambda^2 e^{-T/\Lambda^2} \approx c + T + \cdots$$

- For $\Lambda = 2\,\mathrm{fm}^{-1}$, low E part of V still decoupled
- Much less evolution at high E $\Longrightarrow$ much faster!





- Allows evolution to low λ
- Application to $A > 2$ evolution
- Other useful generators?

Custom Potentials Via the SRG

- Can we tailor the potential to other shapes with the SRG?
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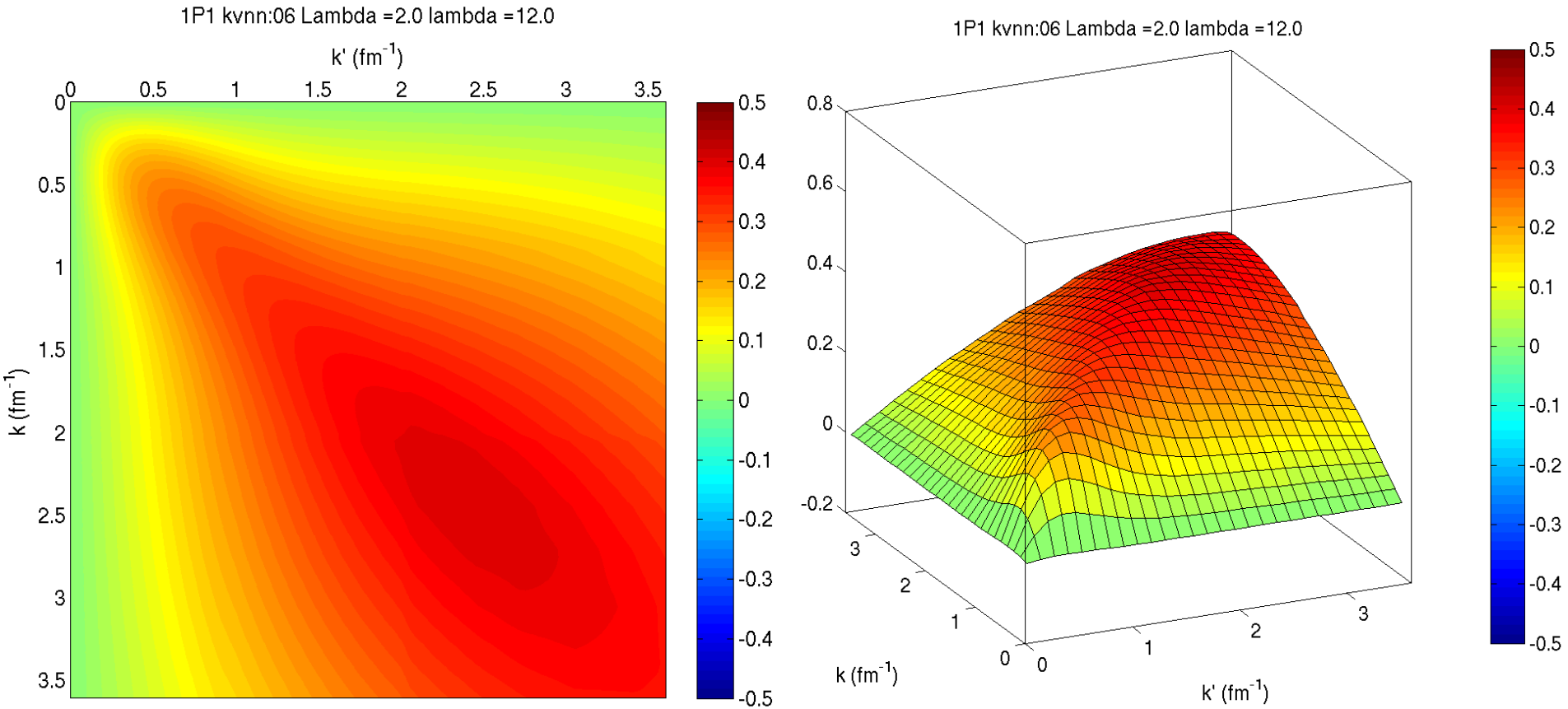

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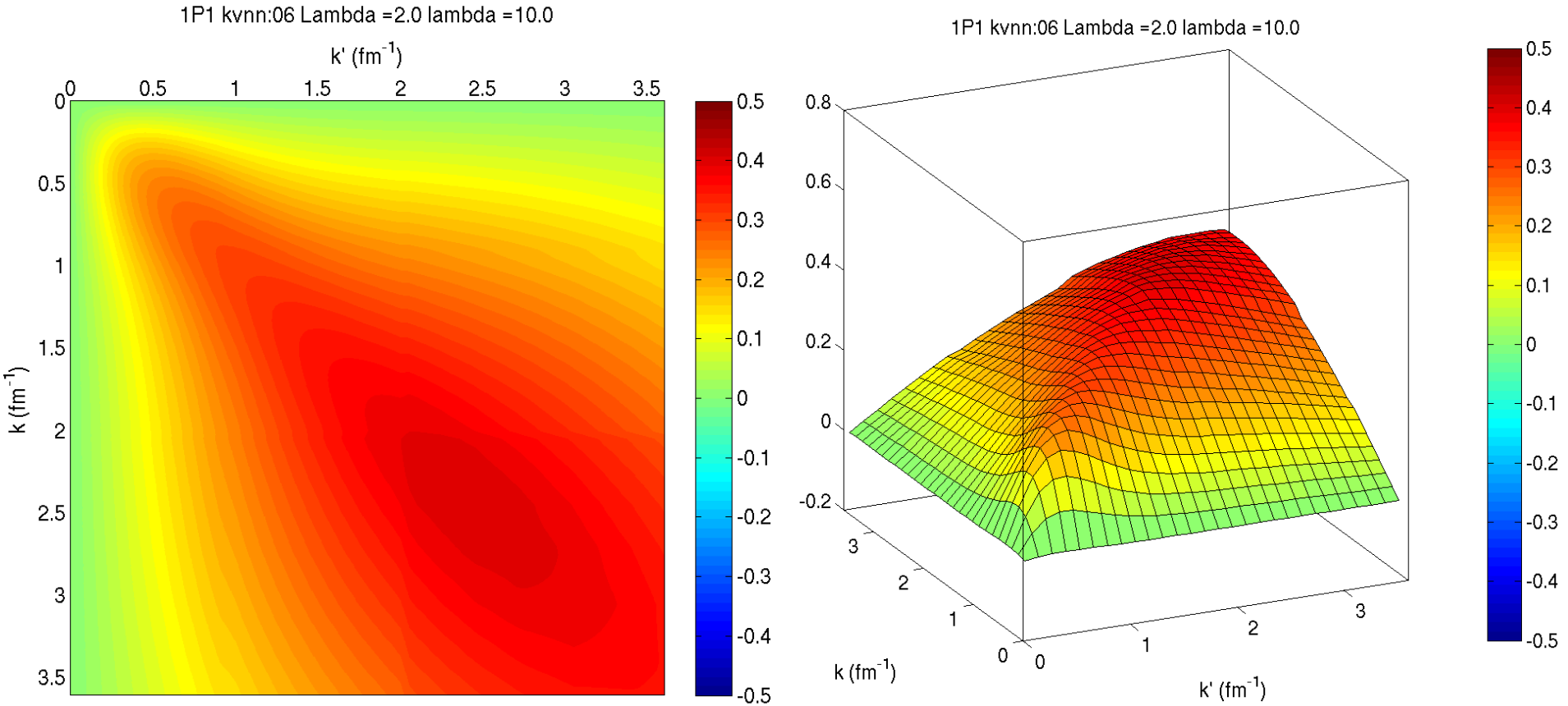

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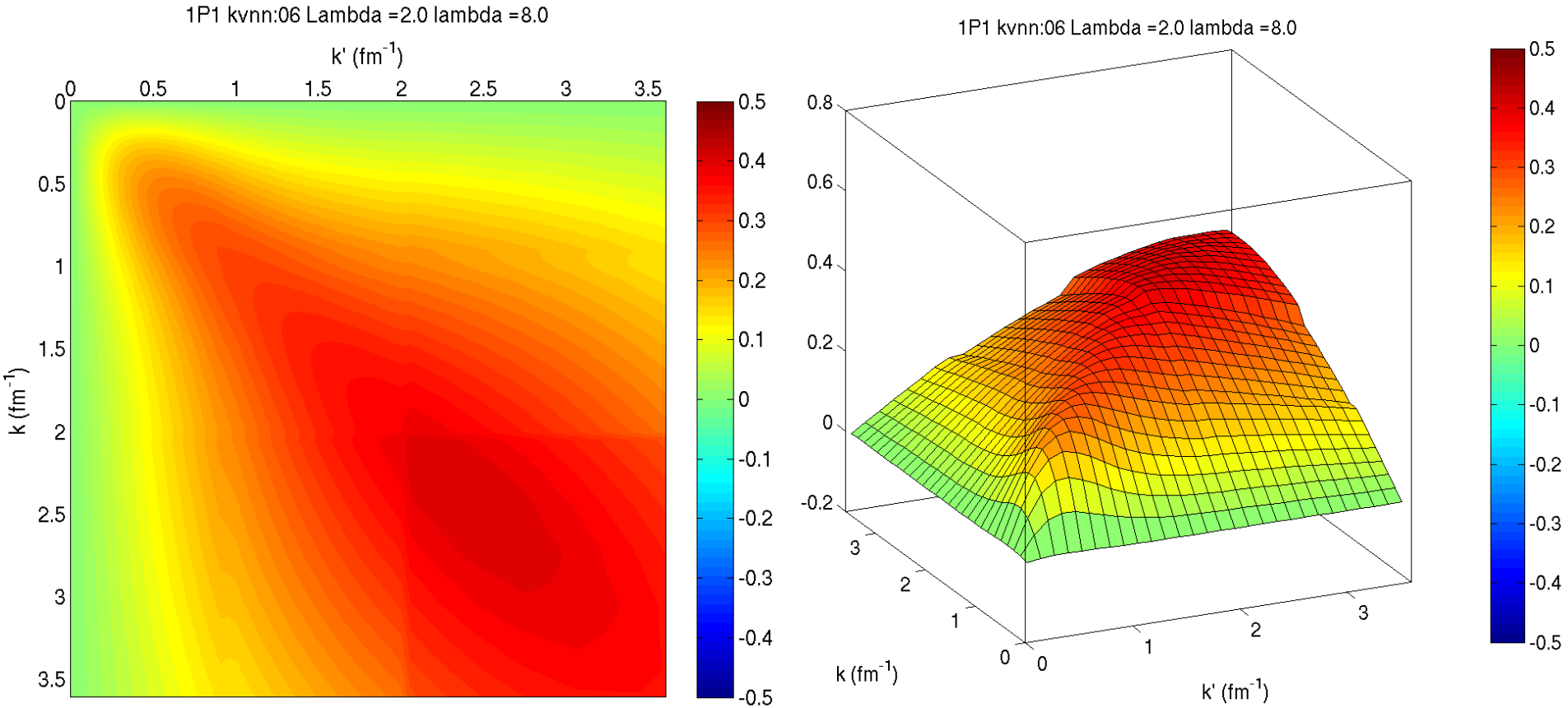

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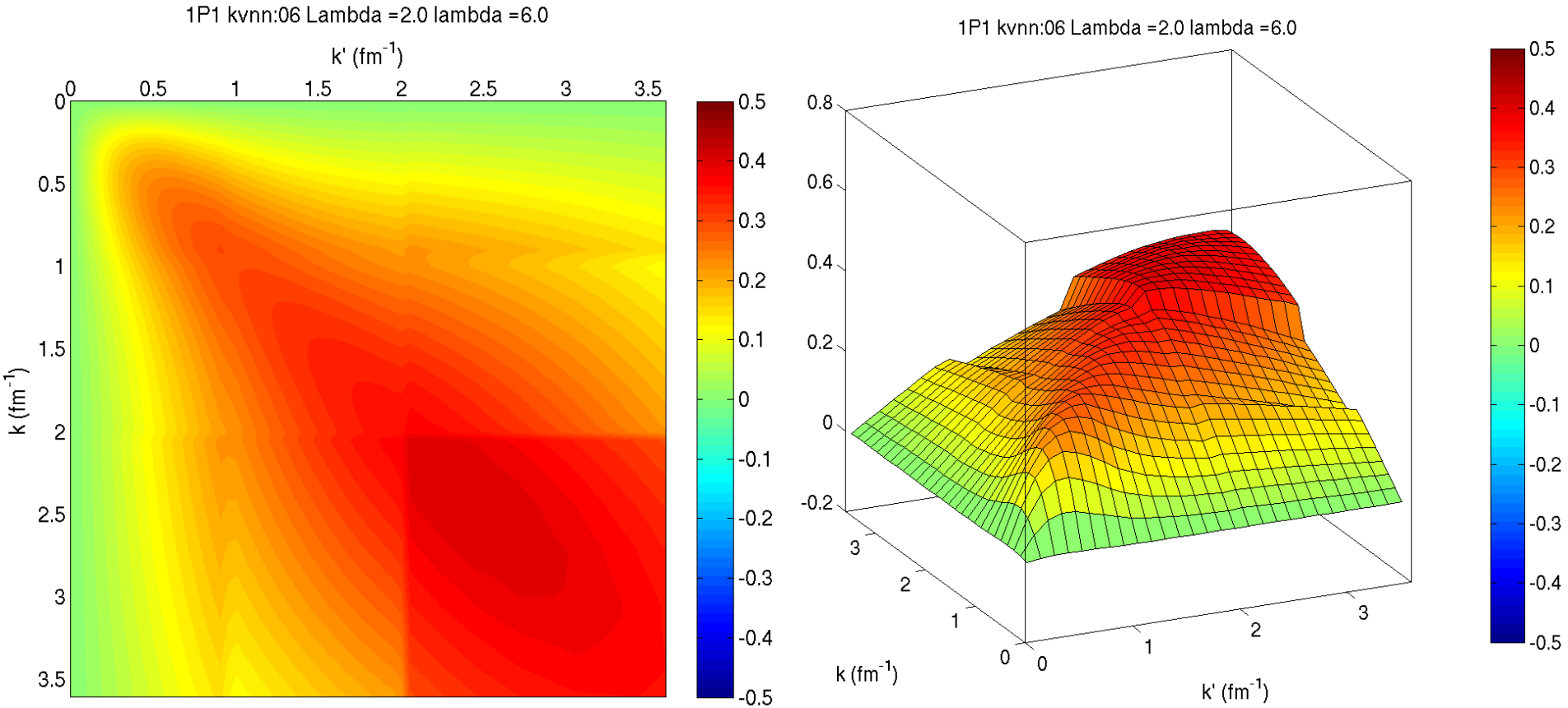

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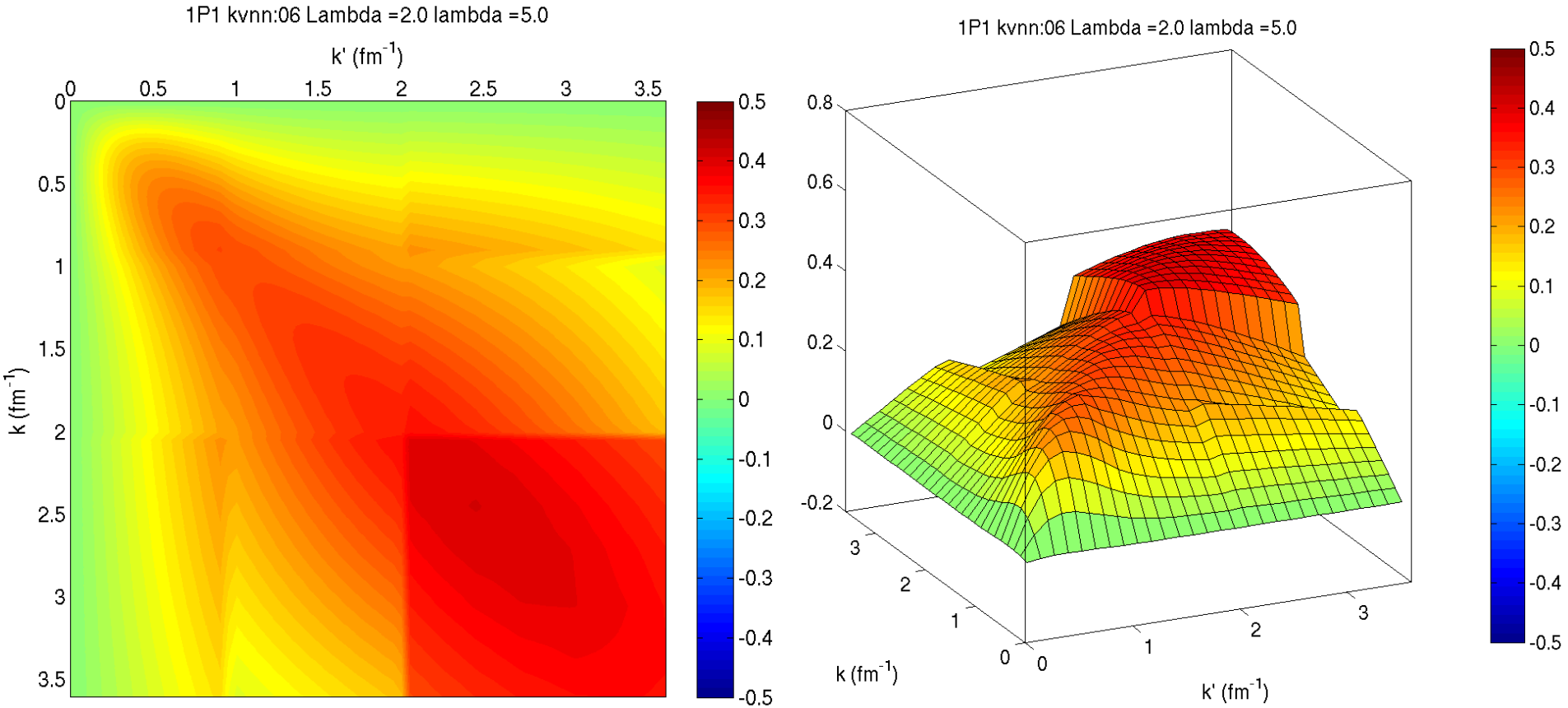

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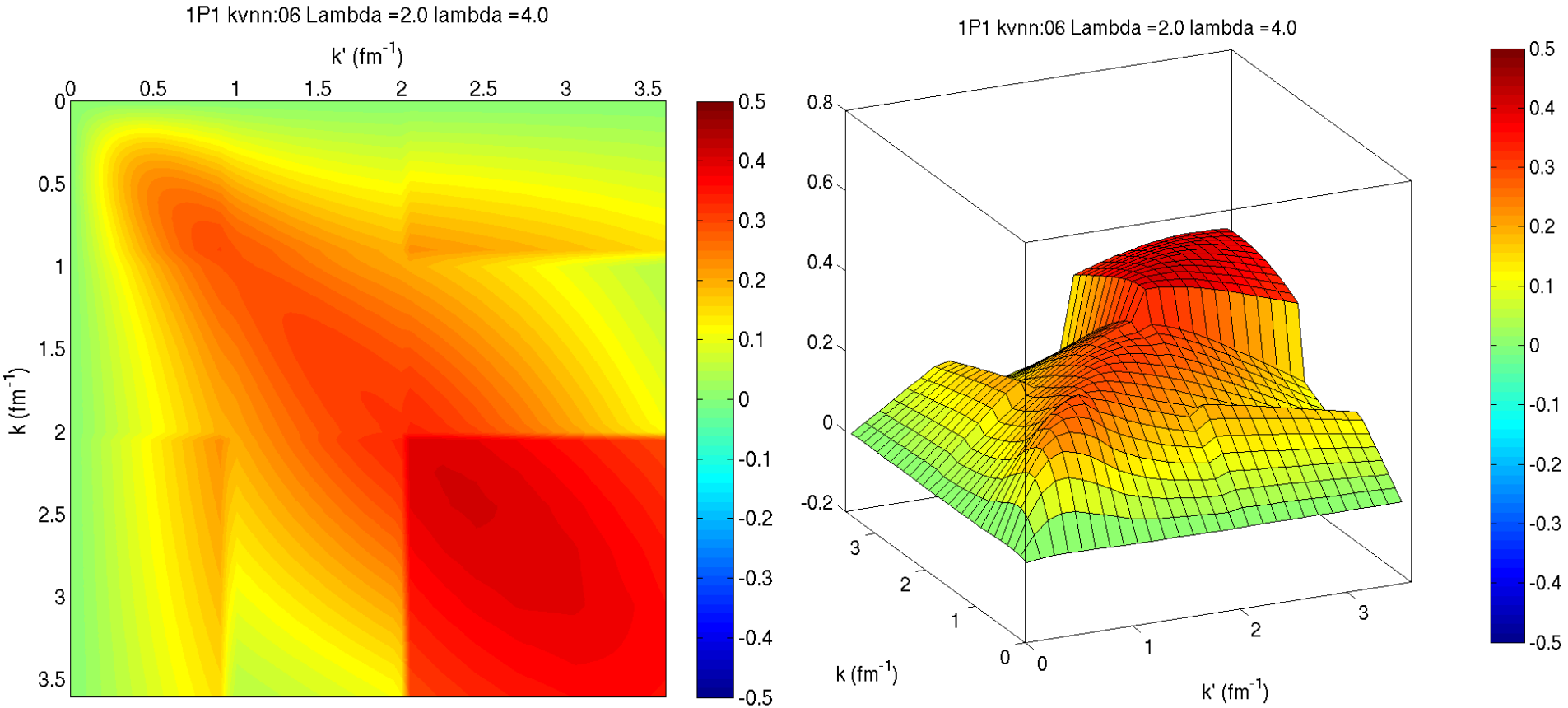

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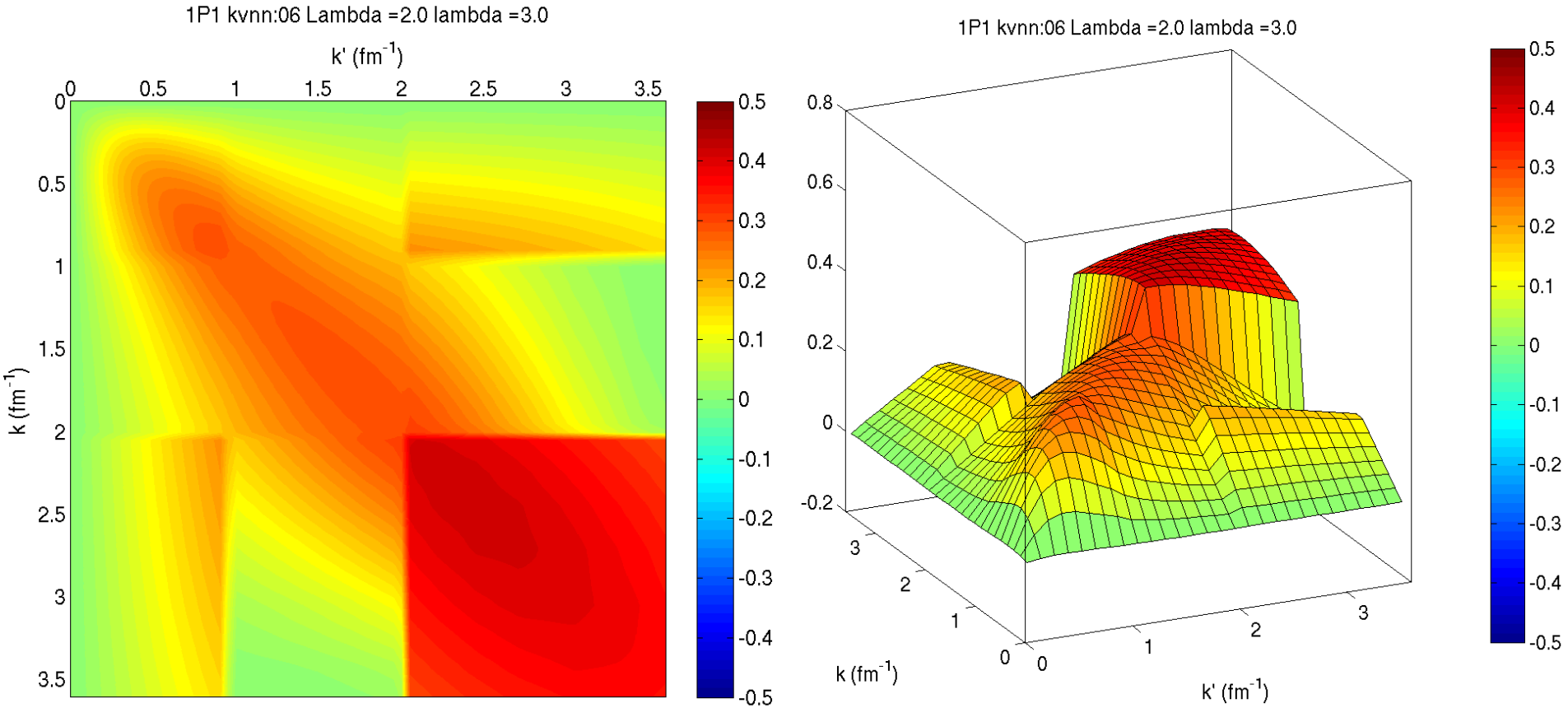

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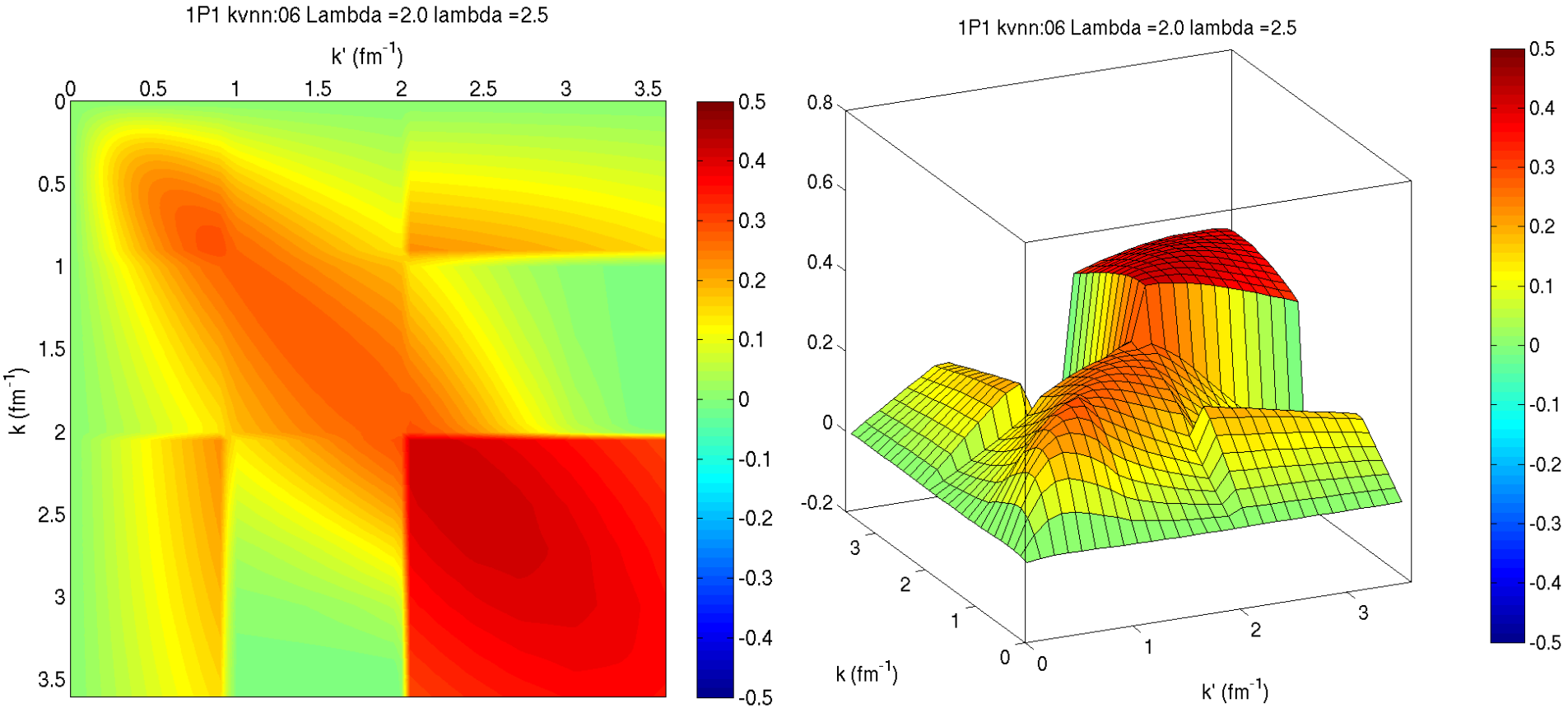

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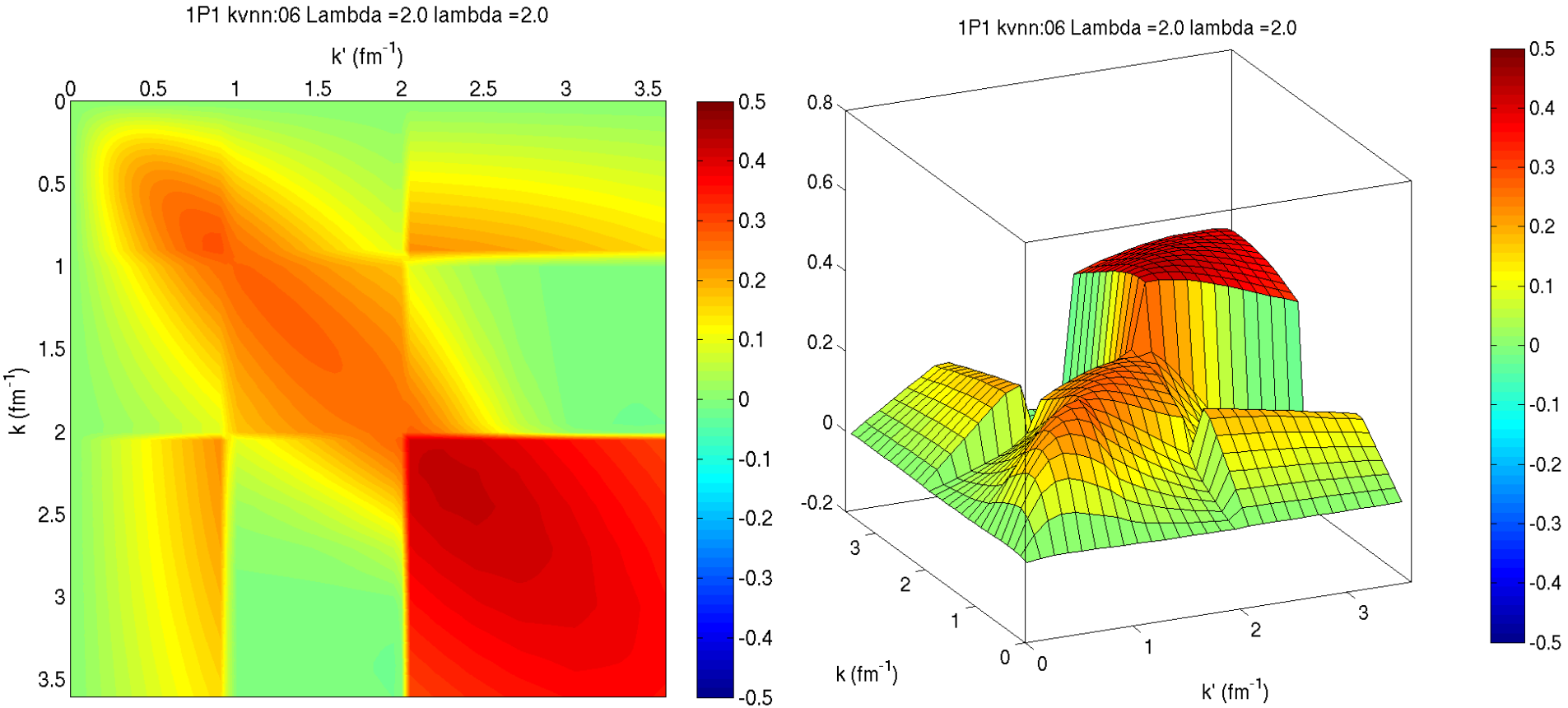

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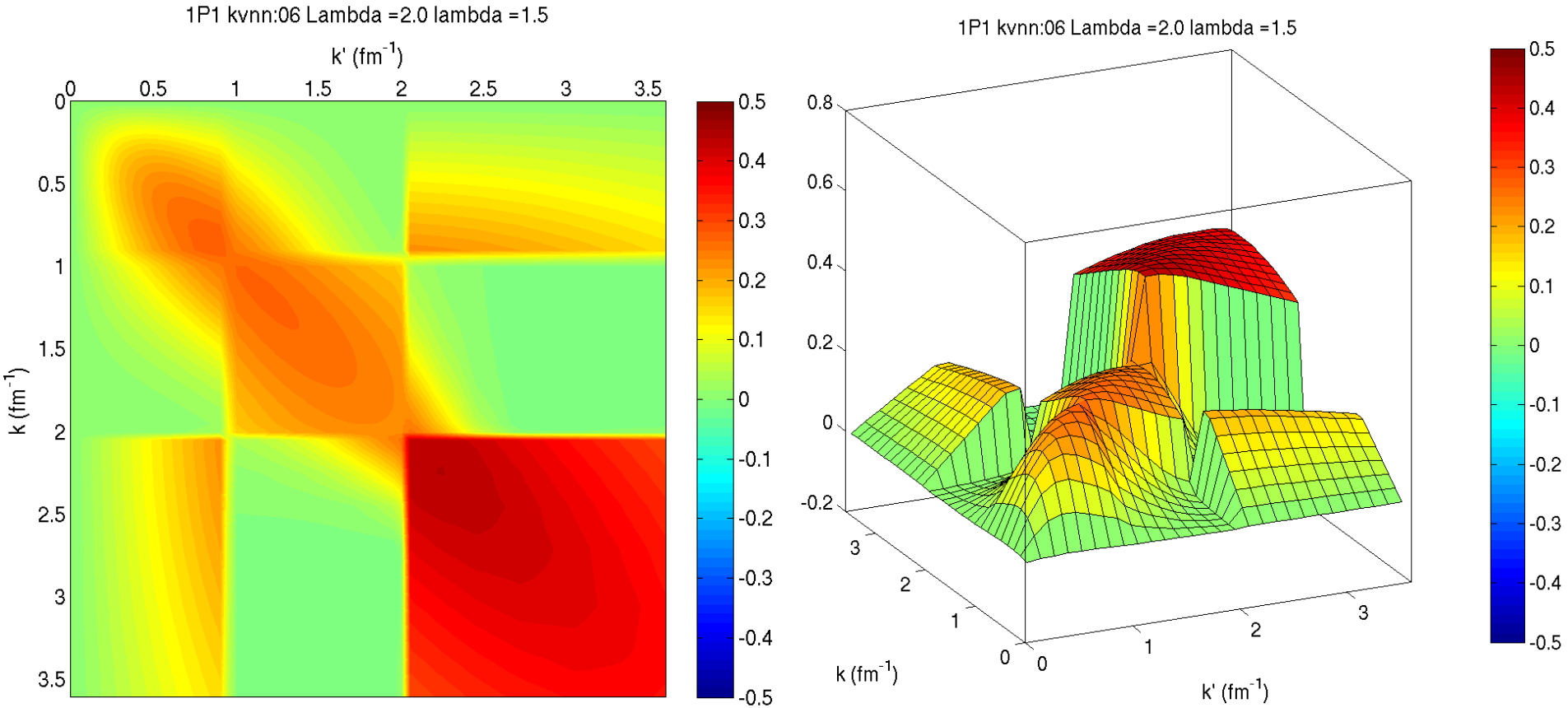

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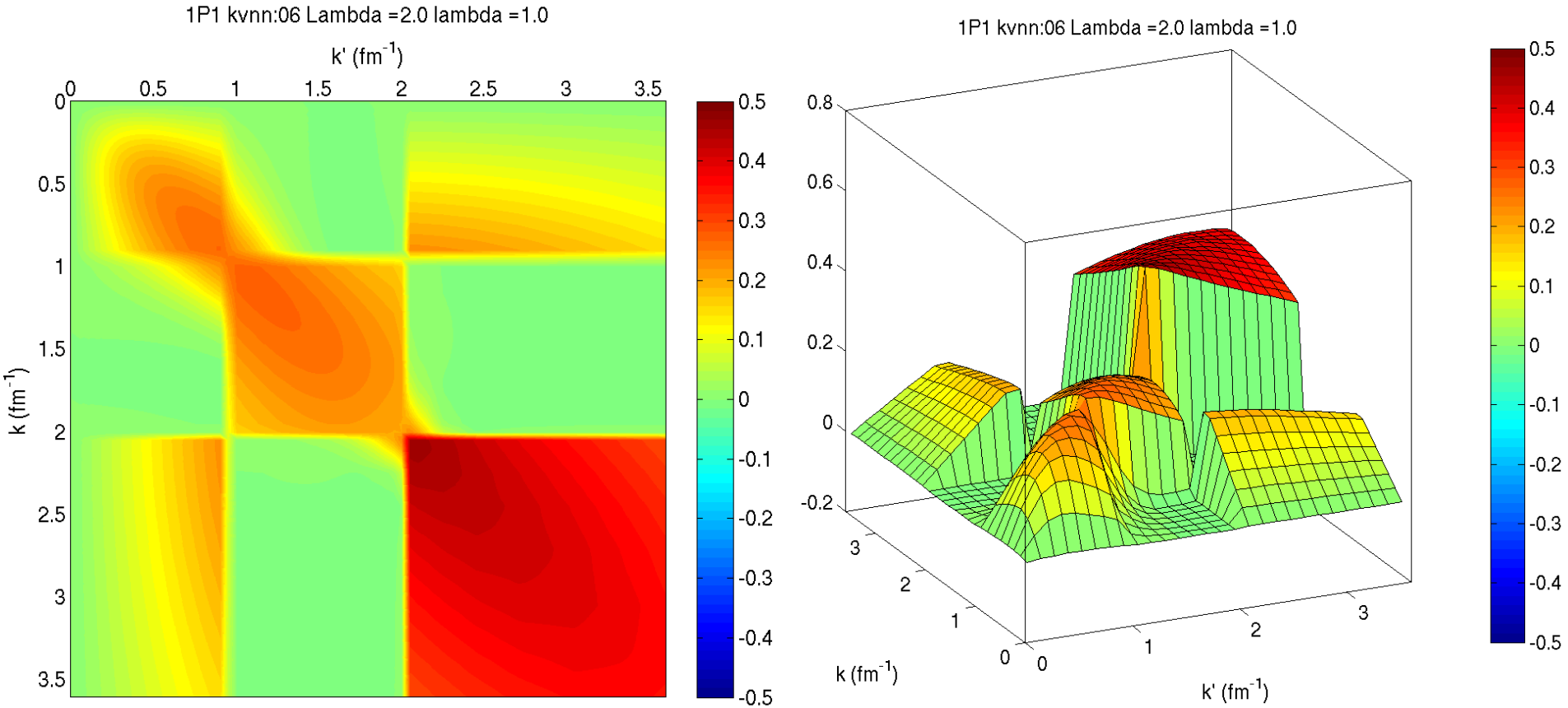
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