Calculations for p-shell Nuclei with SRG-evolved Chiral NN+3N Interactions

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Physical and Life Sciences/Physics

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Lawrence Livermore National Laboratory

Ab initio Nuclear Structure

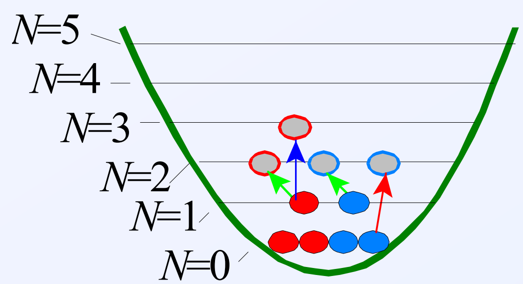
Goal: to compute properties of light nuclei using point-like protons and neutrons with two- and three-nucleon interactions

- We'll use a basis of harmonic oscillator slater determinants

$$\Psi_n = \sum_m c_{nm}\phi_m$$

$$\phi = \frac{1}{\sqrt{A}}\begin{vmatrix} \phi_i(r_1) & \phi_i(r_2) & \cdots & \phi_i(r_A) \\ \phi_j(r_1) & \phi_j(r_2) & & \phi_j(r_A) \\ \vdots & & \ddots & \vdots \\ \phi_l(r_1) & \phi_l(r_2) & \cdots & \phi_l(r_A) \end{vmatrix}$$

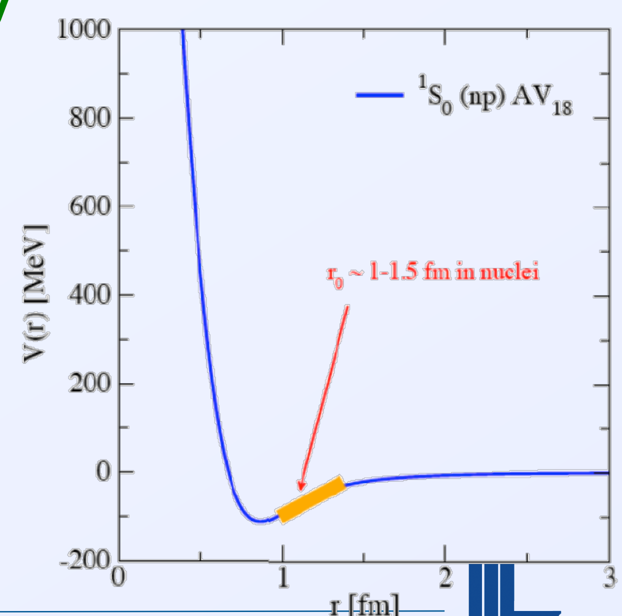
$$H\Psi_n = E_n\Psi_n$$



- Diagonalize to obtain eigenvalues

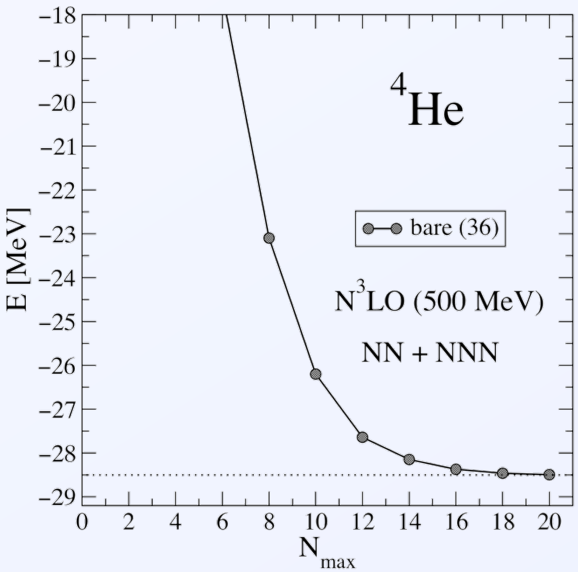
$$H = \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1k} \\ H_{21} & H_{22} & & H_{2k} \\ \vdots & & \ddots & \vdots \\ H_{k1} & H_{k2} & \cdots & H_{kk} \end{pmatrix}$$

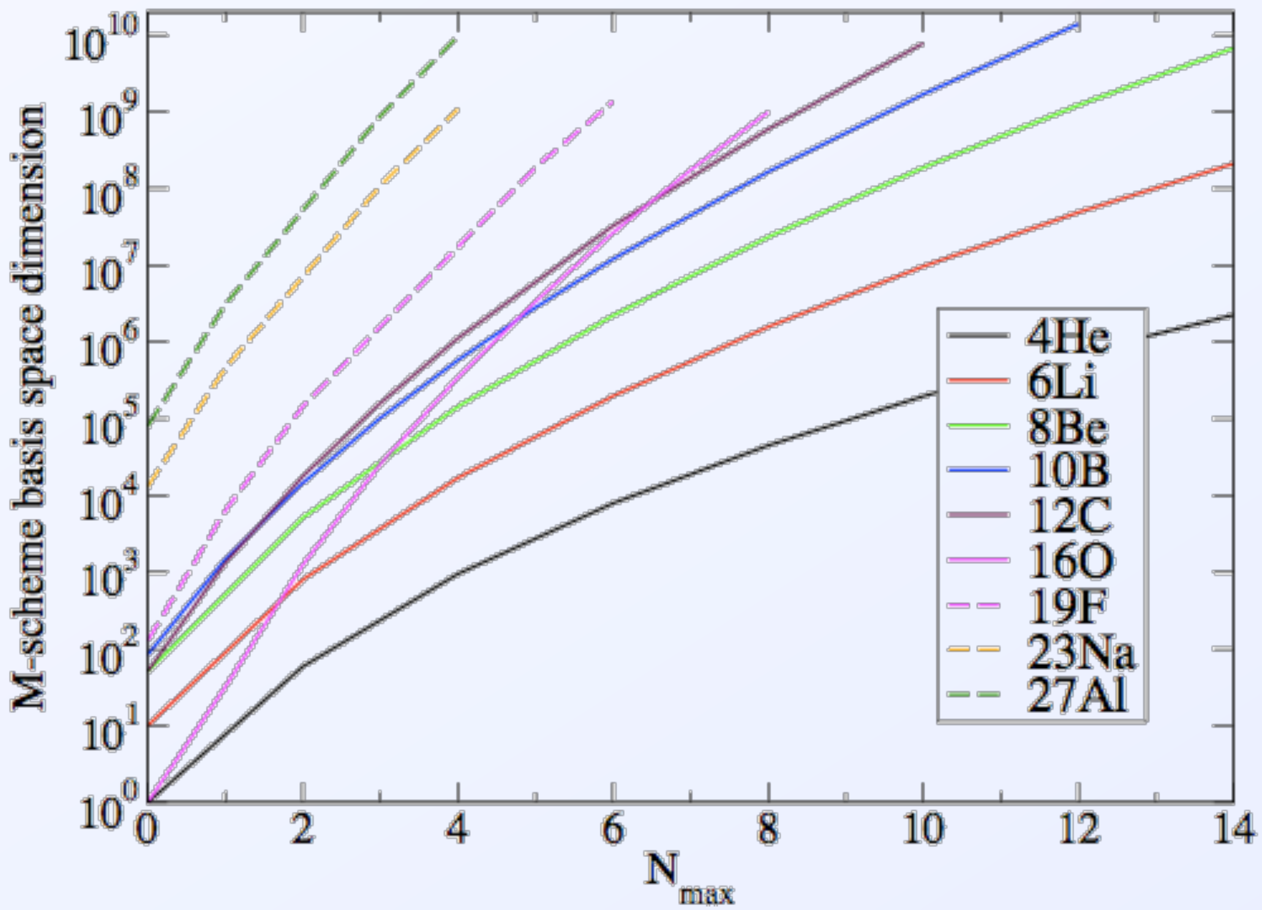
- These pathologies mean we need a large basis (hard core = high momenta)



Convergence in the oscillator basis

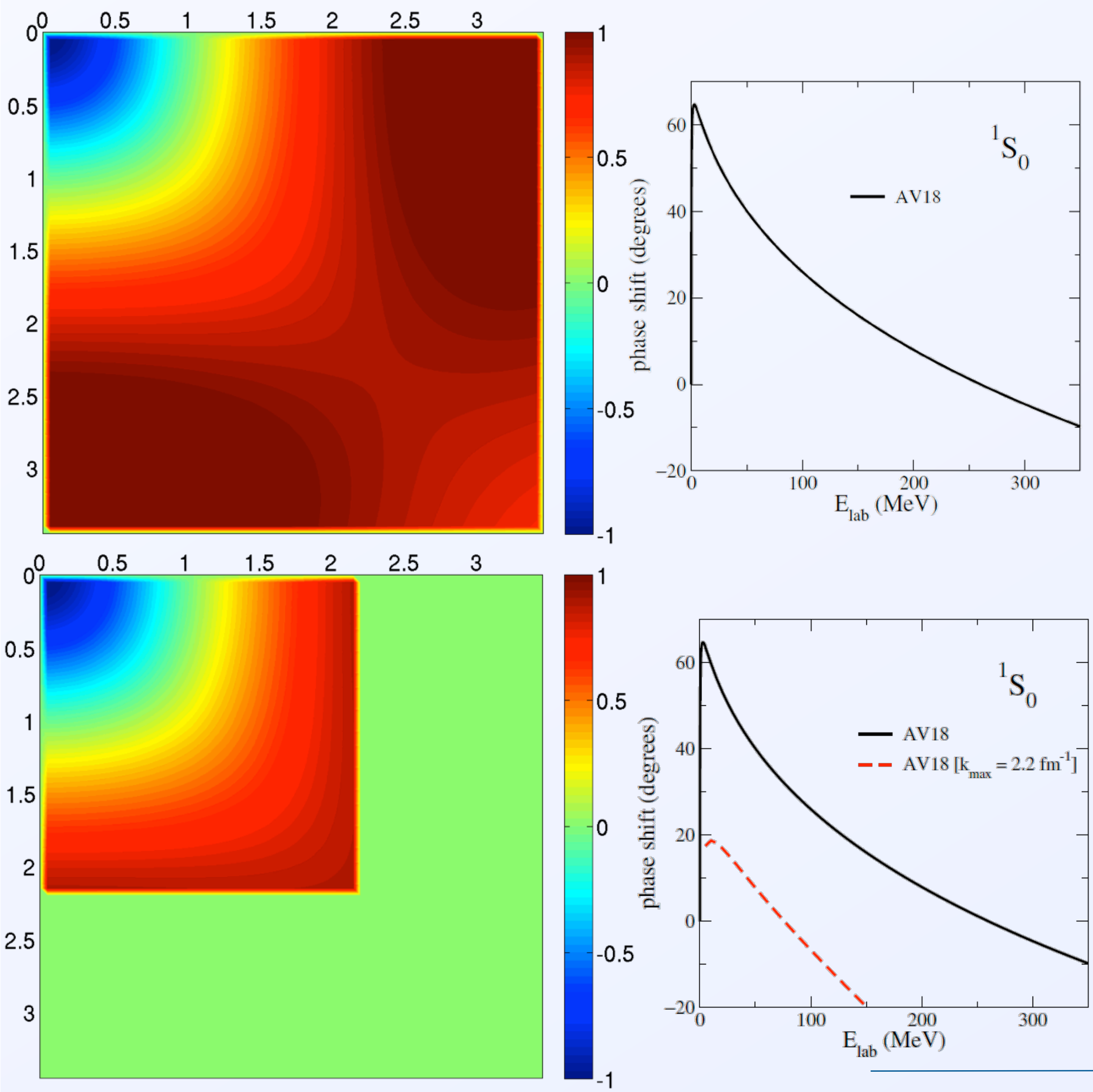
- Oscillator basis scaling is harsh
- ^{4}He is hard
- ^{12}C is intractable





- Need substantial reduction in required basis size
  - ➔ need smarter way to solve this problem!

Let's try a low-pass filter



- Start with bare
- Cut at $k=2.2\ fm^{-1}$
- Compute Observable
  (here: phase shift)
- Compare: fails
- High and low coupled
- Absorb high-energy
  ➔ Renormalization
  (unitary transformation)

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

SRG to the rescue

- Similarity Renormalization Group (SRG) is a series of Unitary Transformations:

K.Wilson & S.Glazek, PRD 48,5863 (1993)

PRC 75,061001 (2007) [arXiv: nucl-th/0611045]

$$H_s = U_s H U_s^+ \equiv T_{rel} + V_s$$

- Implement as flow equations:

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

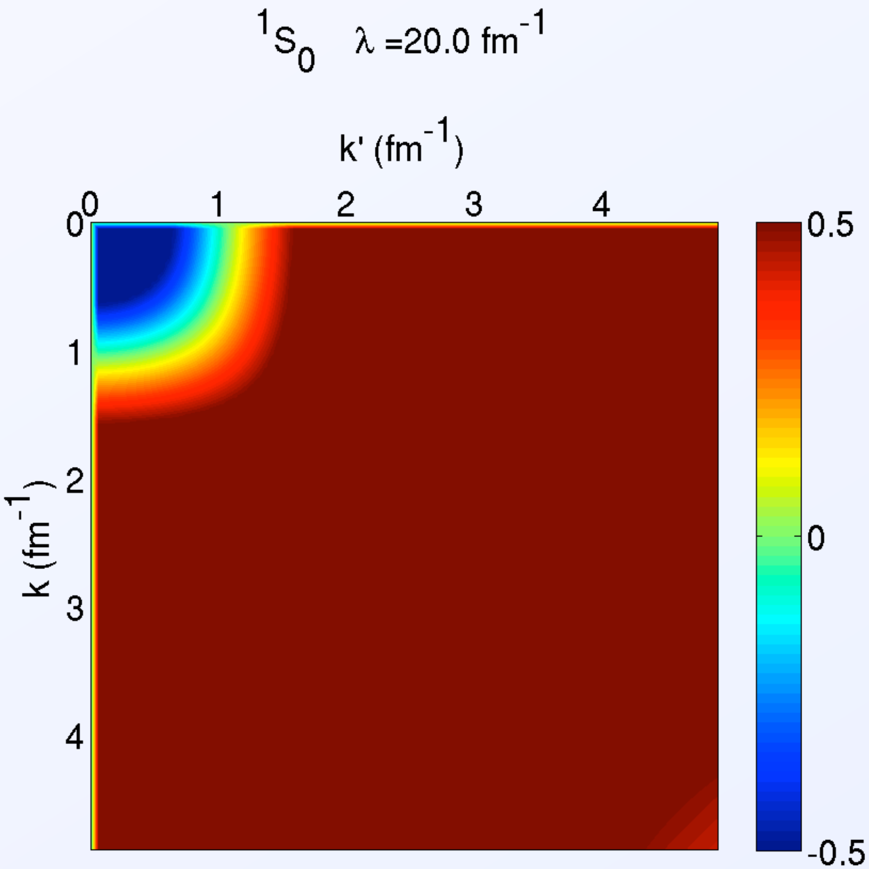
(usually with $G_s = T_{rel}$)

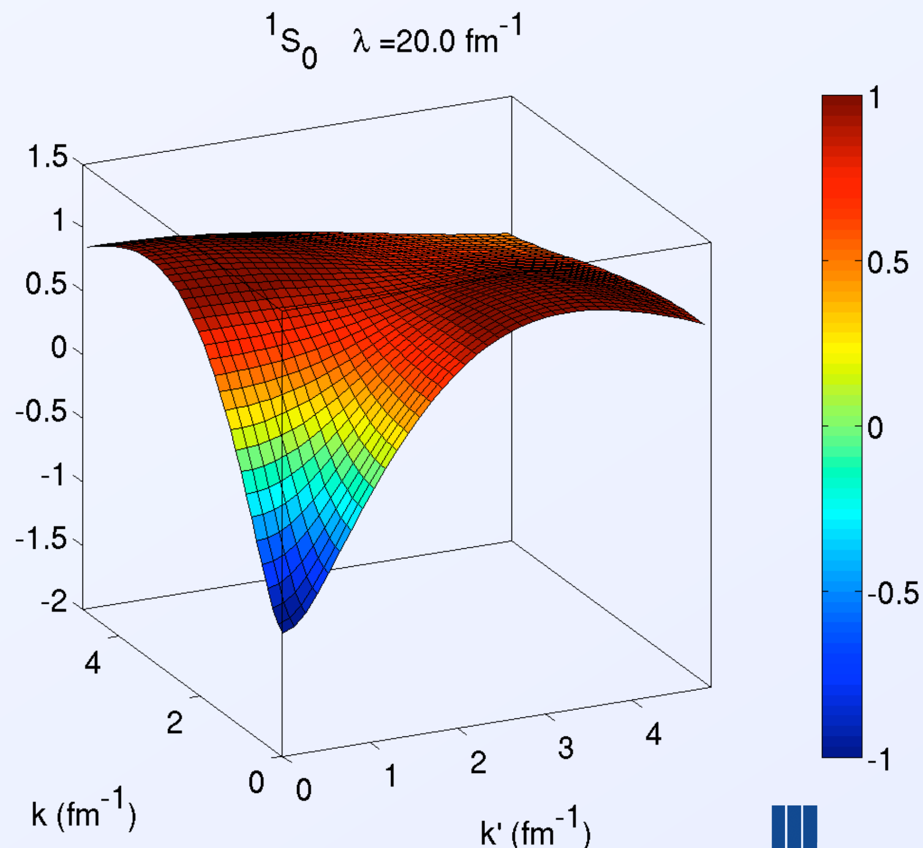
- G_s can be any Hermitian operator

$$G_s = T_{rel}, H_{diag}, H_{osc}, H_{BD}, T + V_{NN}, \exp[-T], \cdots$$

SRG evolves Hamiltonians unitarily

$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$





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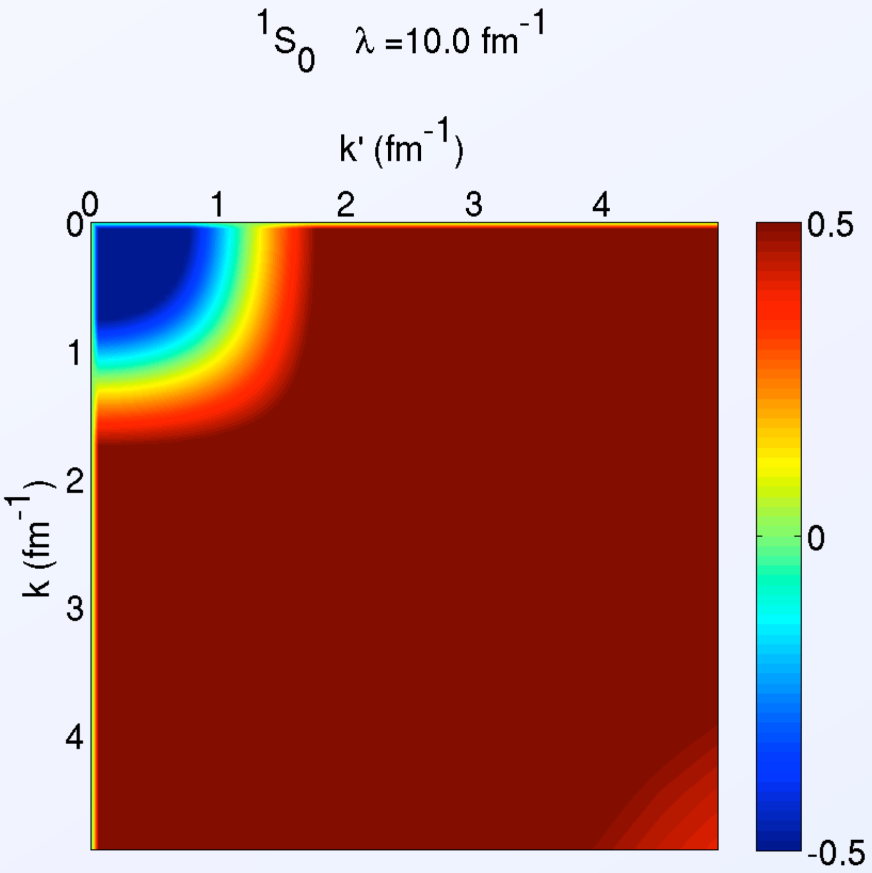

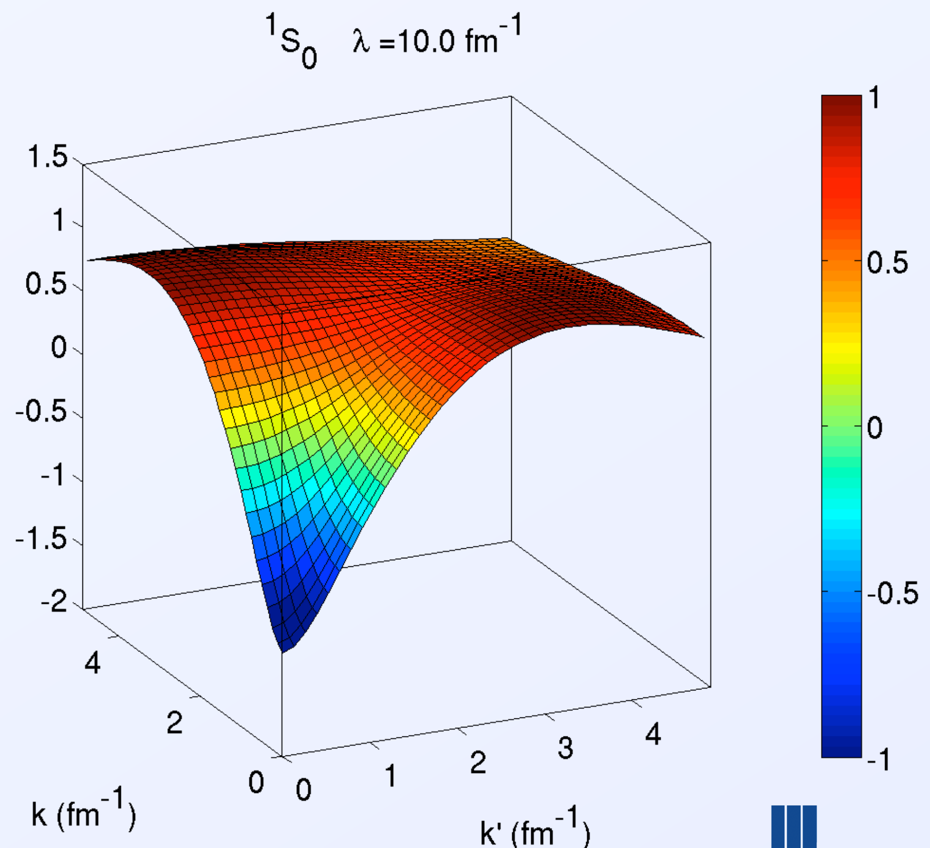

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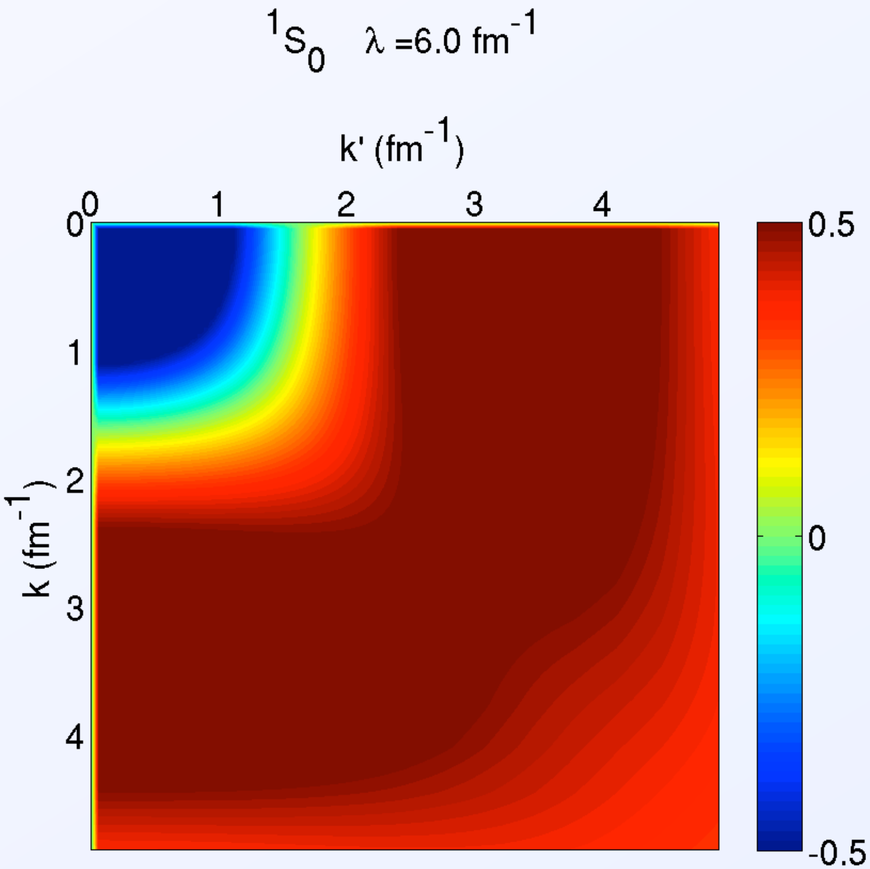

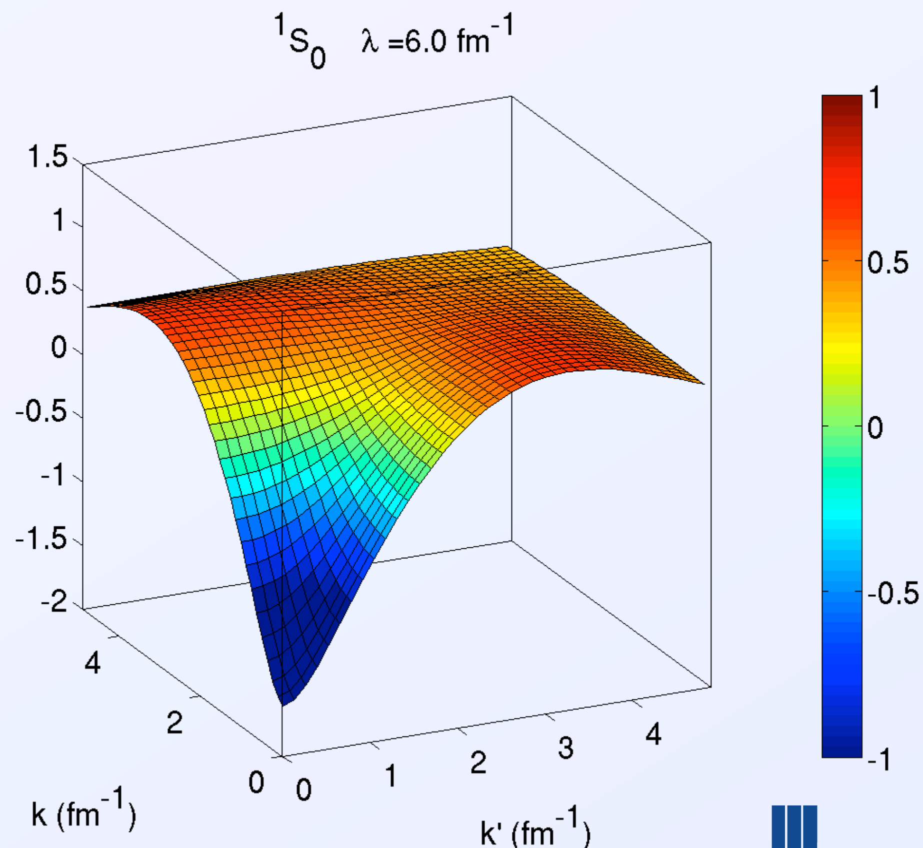

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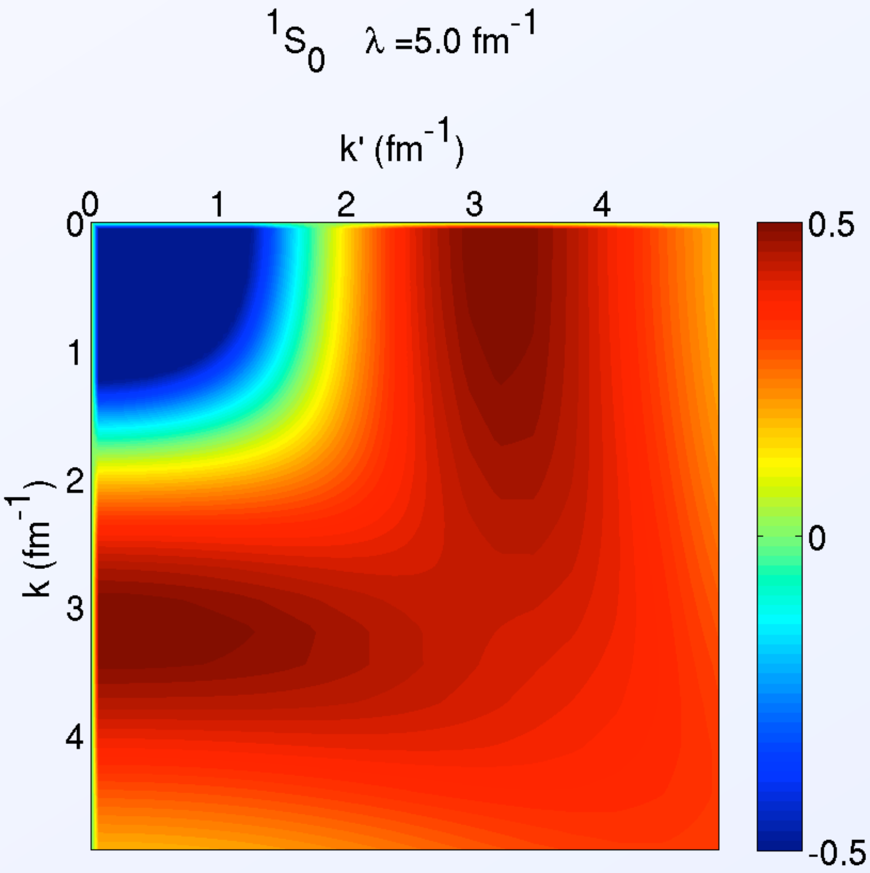

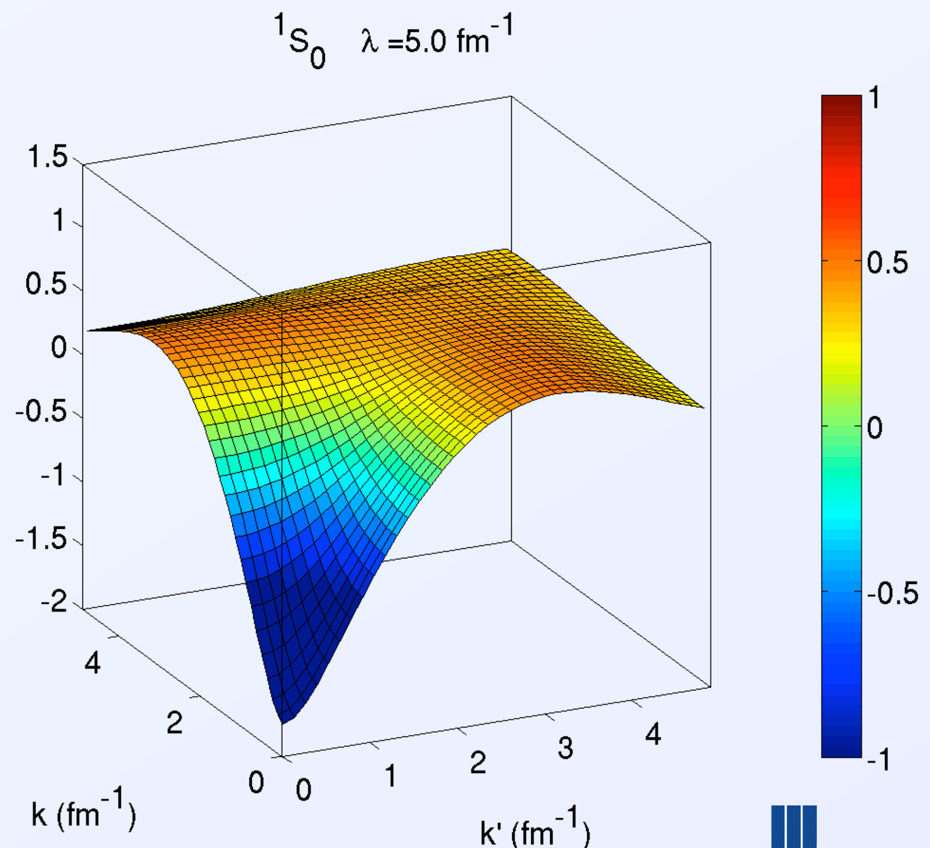

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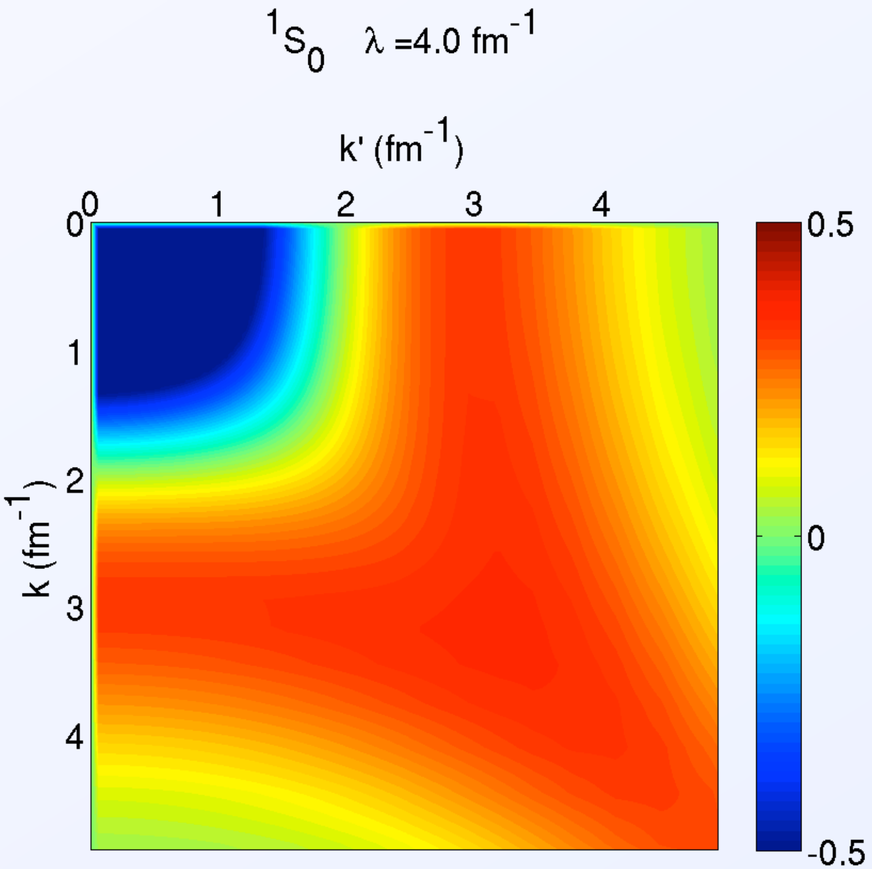

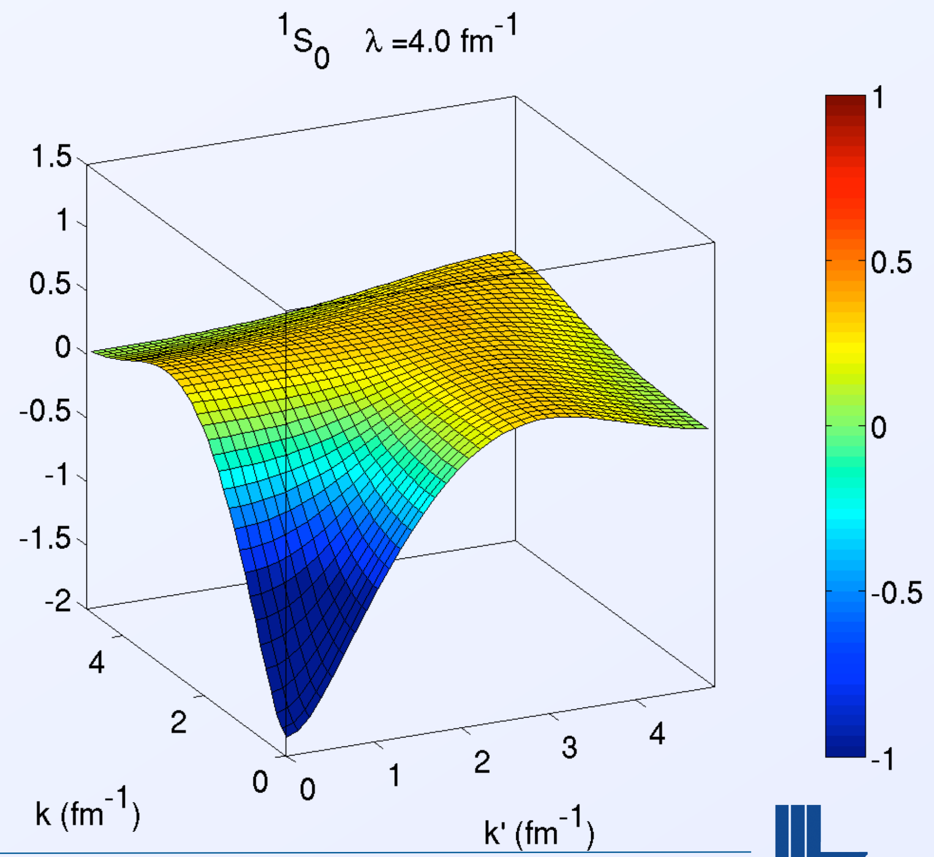

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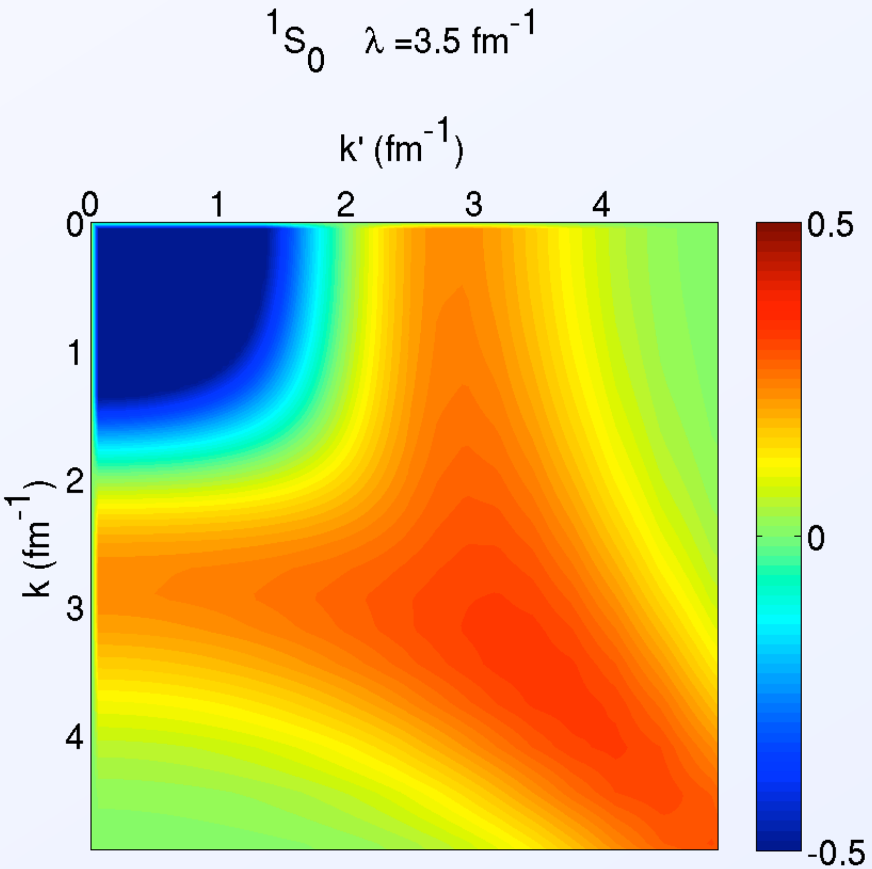

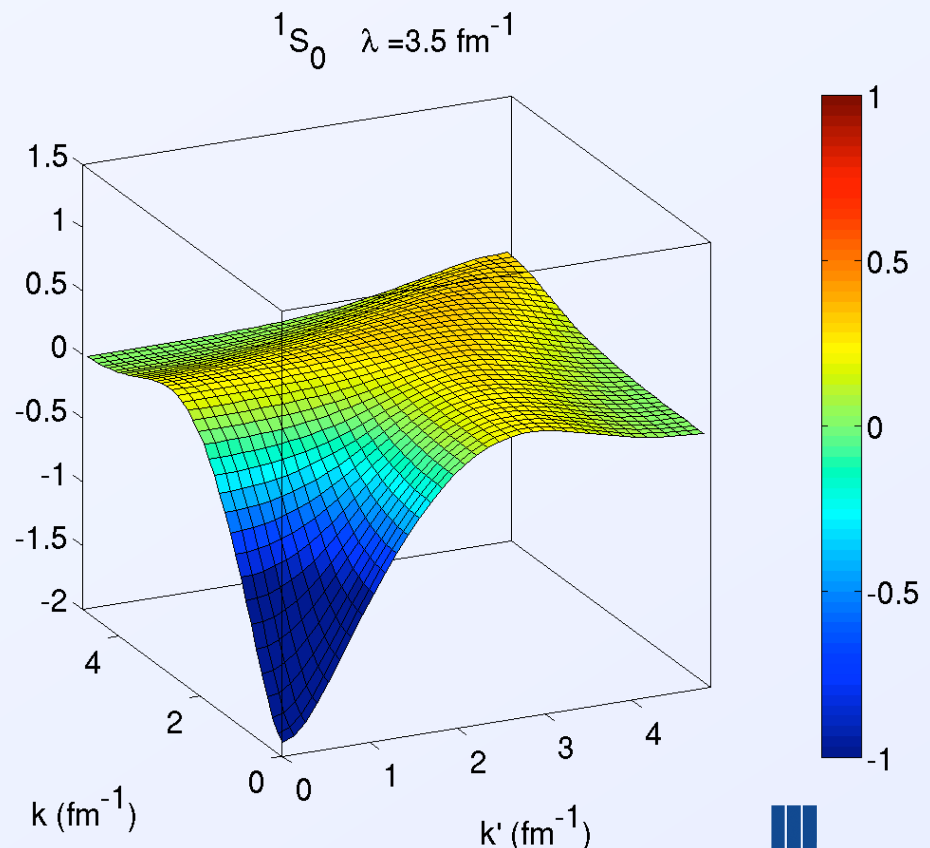

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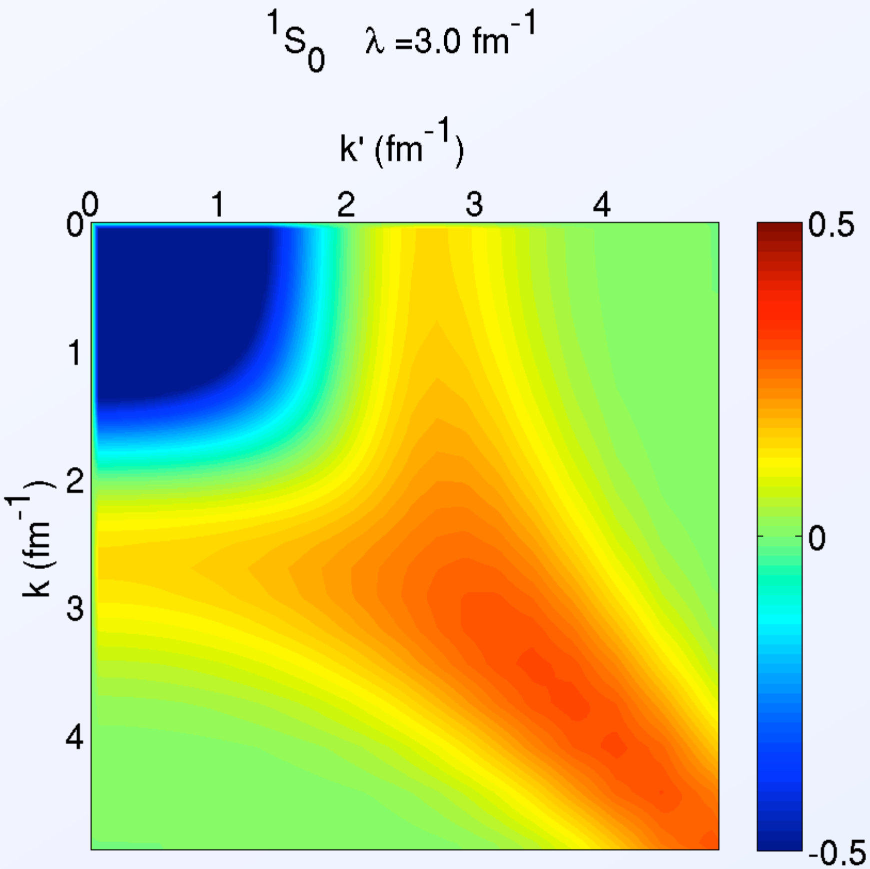

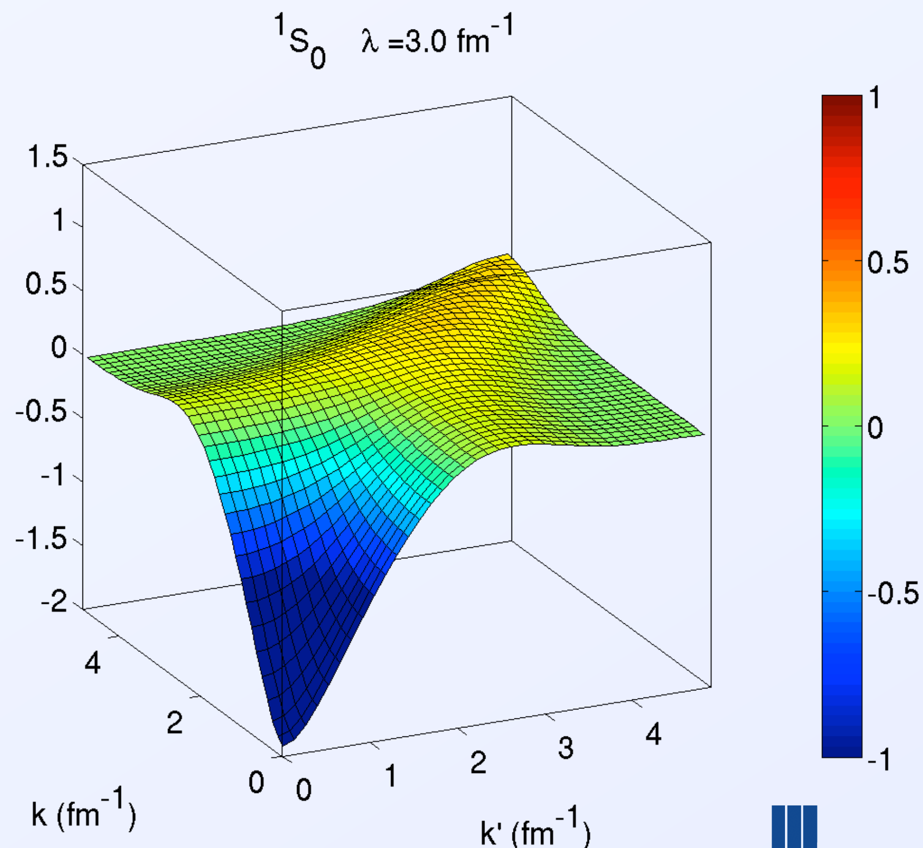

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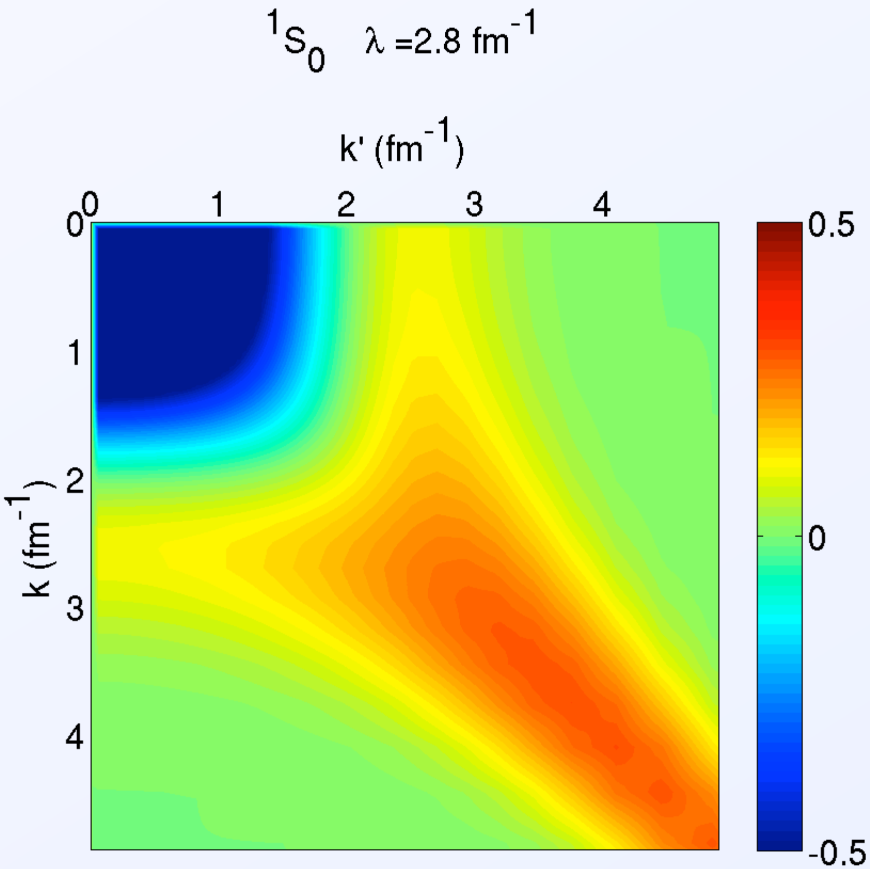

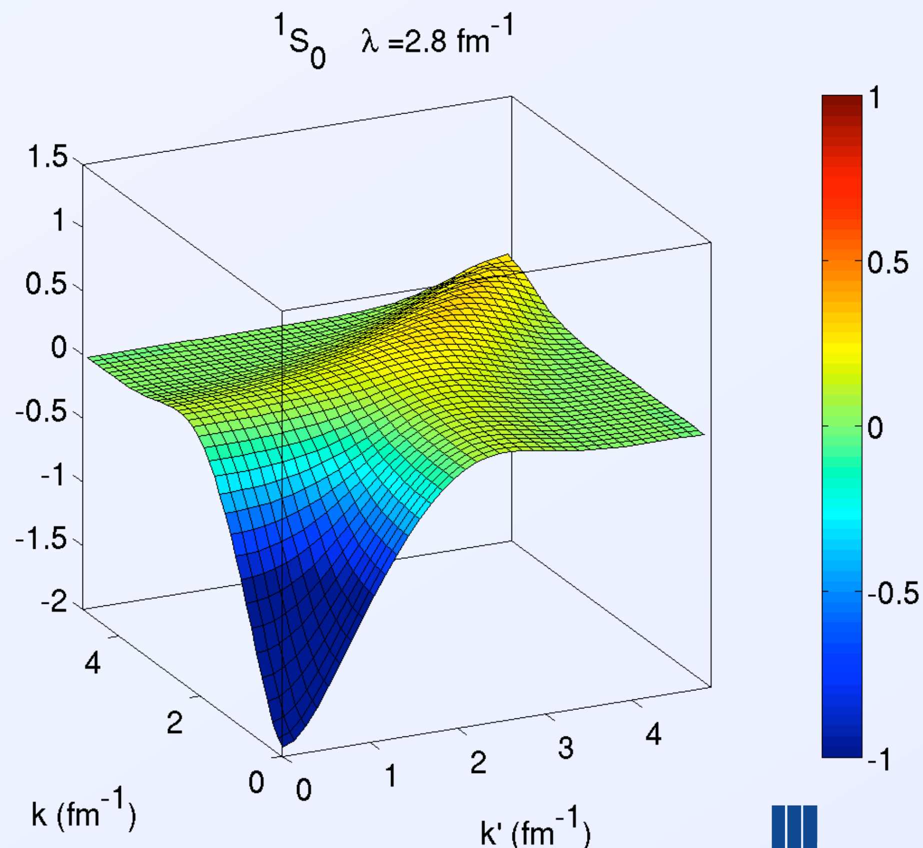

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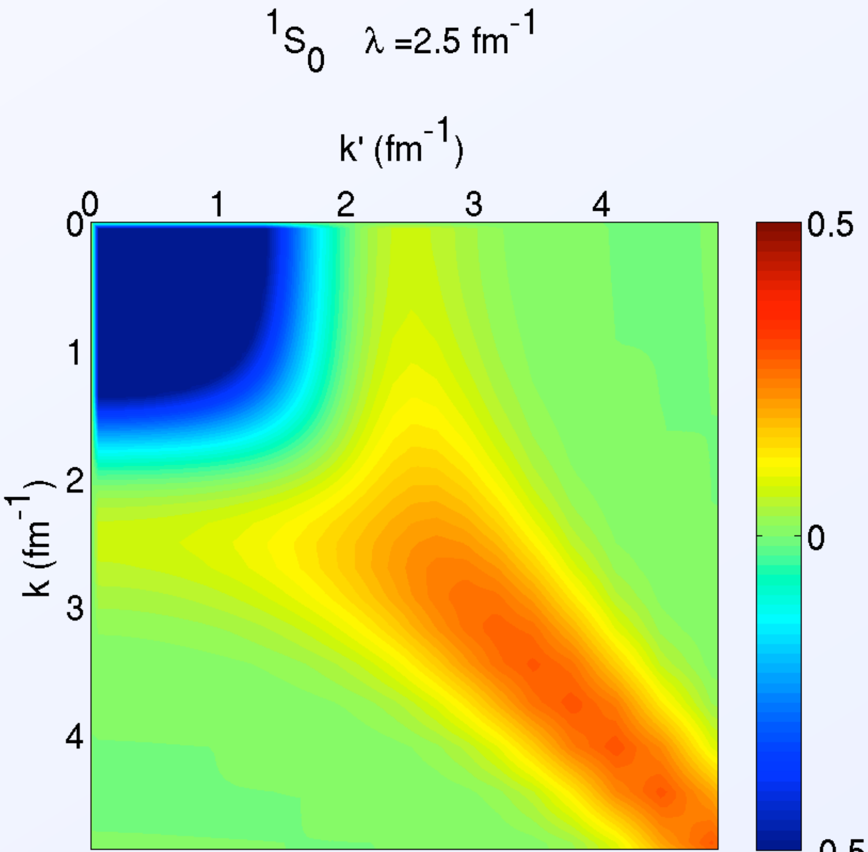

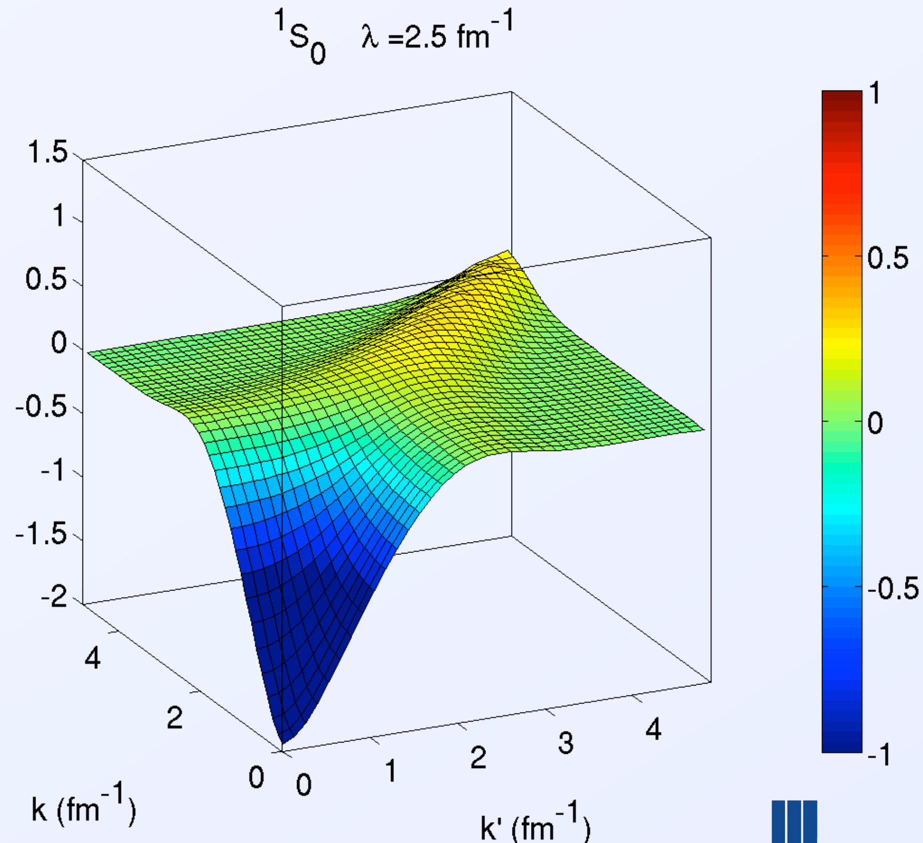

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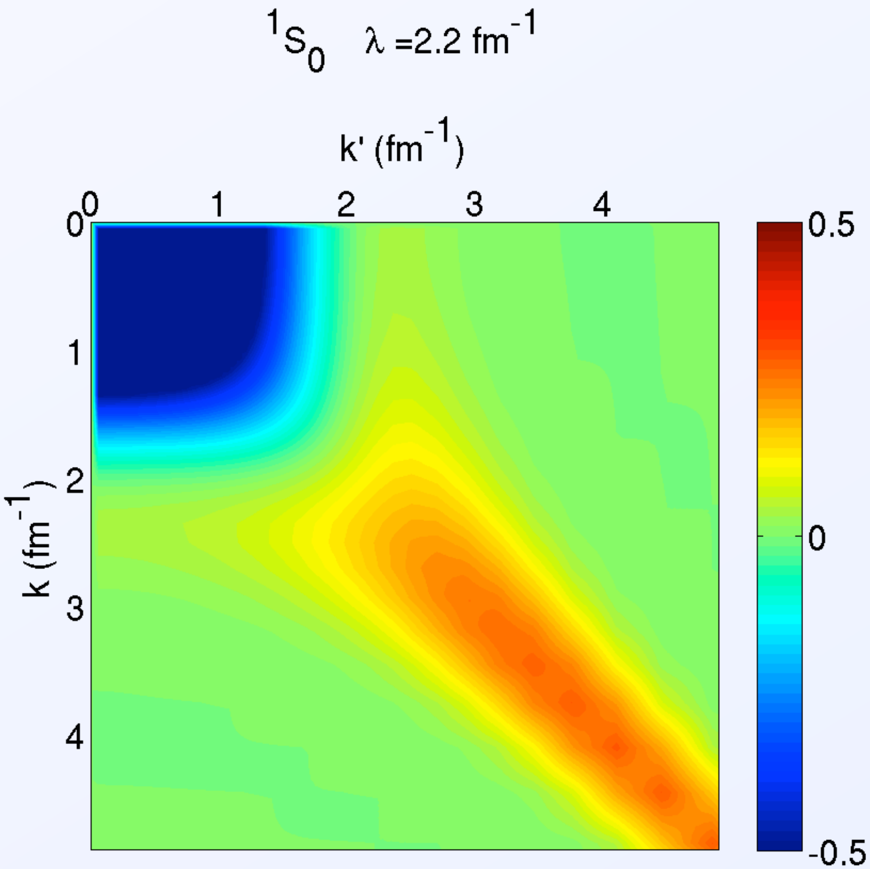

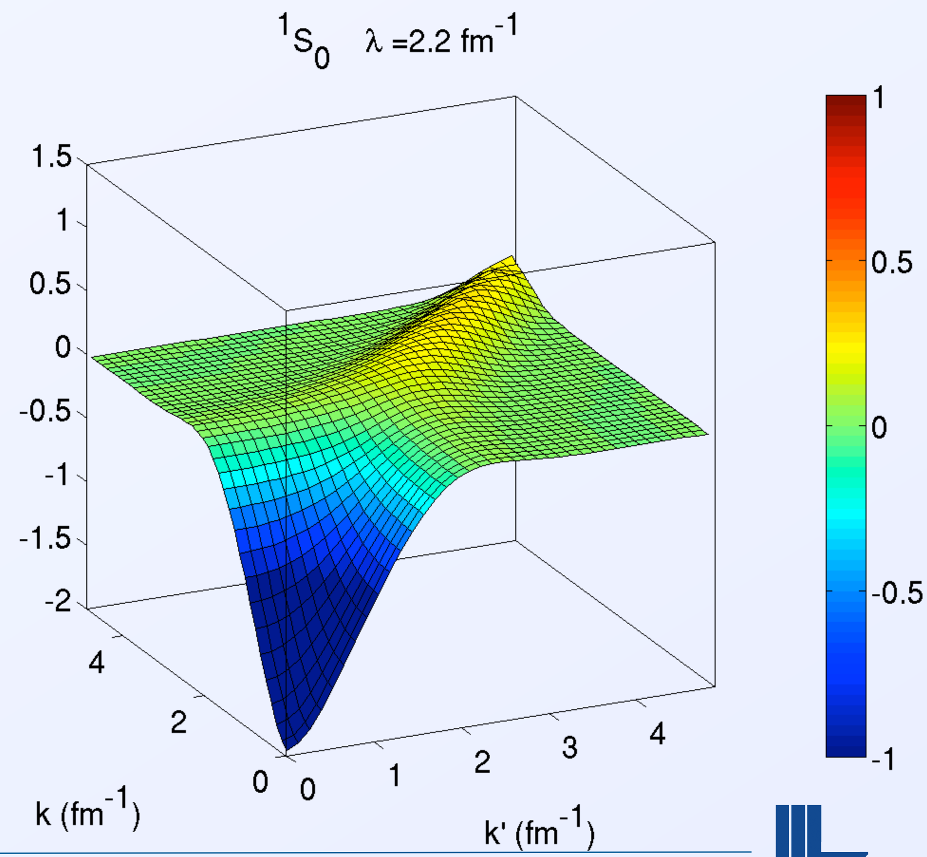

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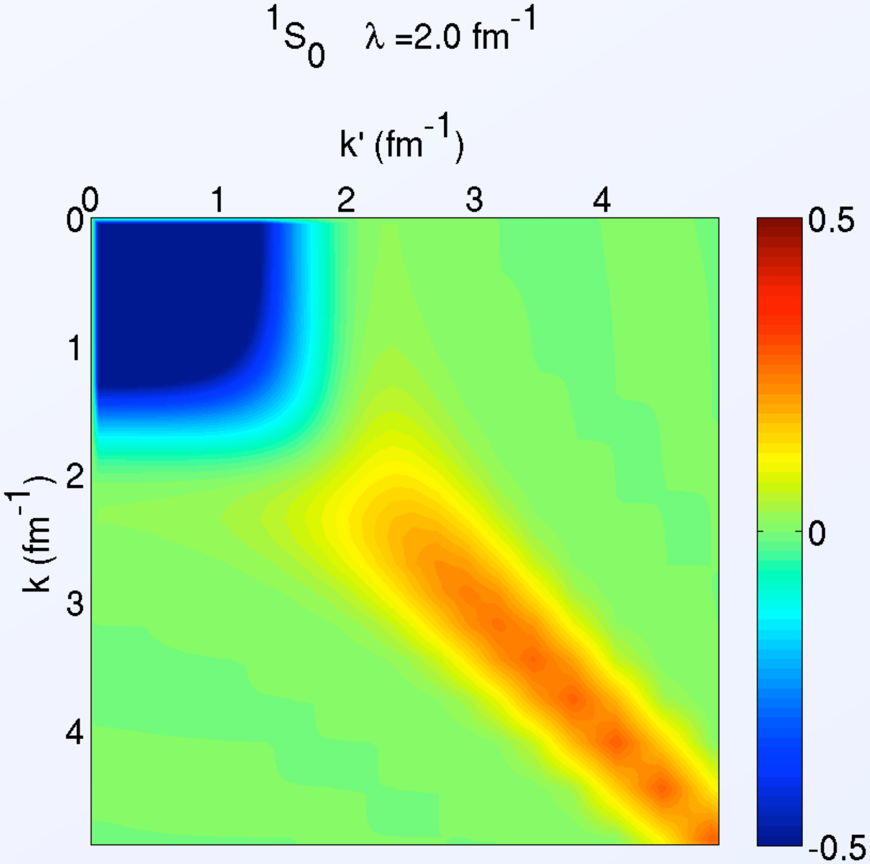
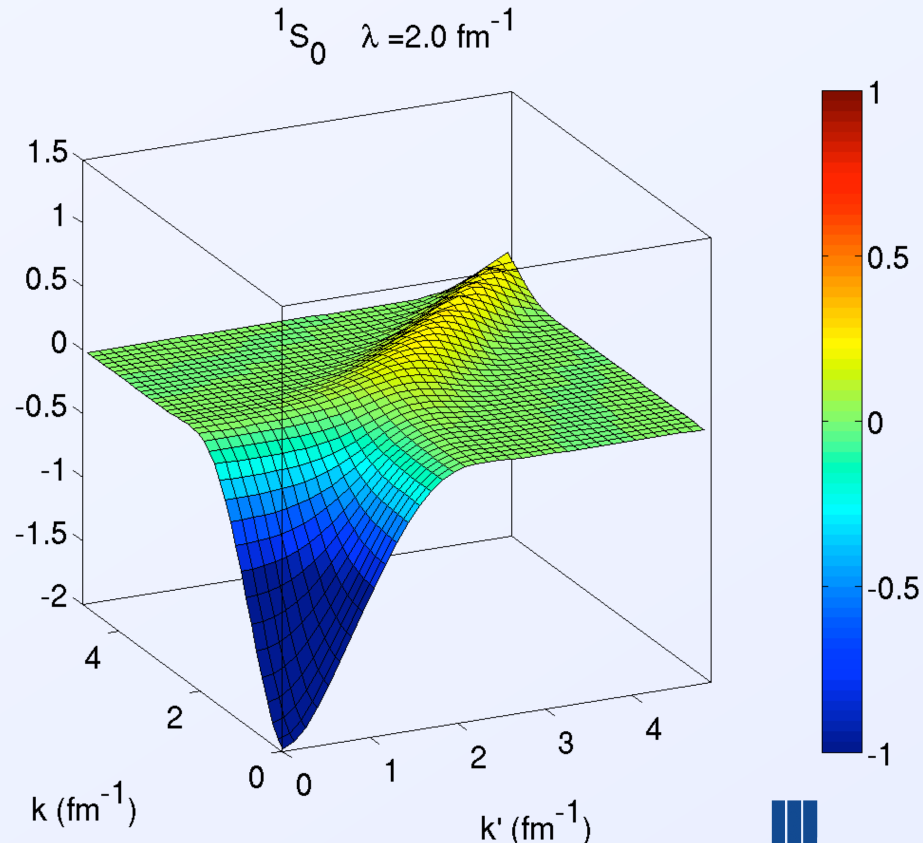
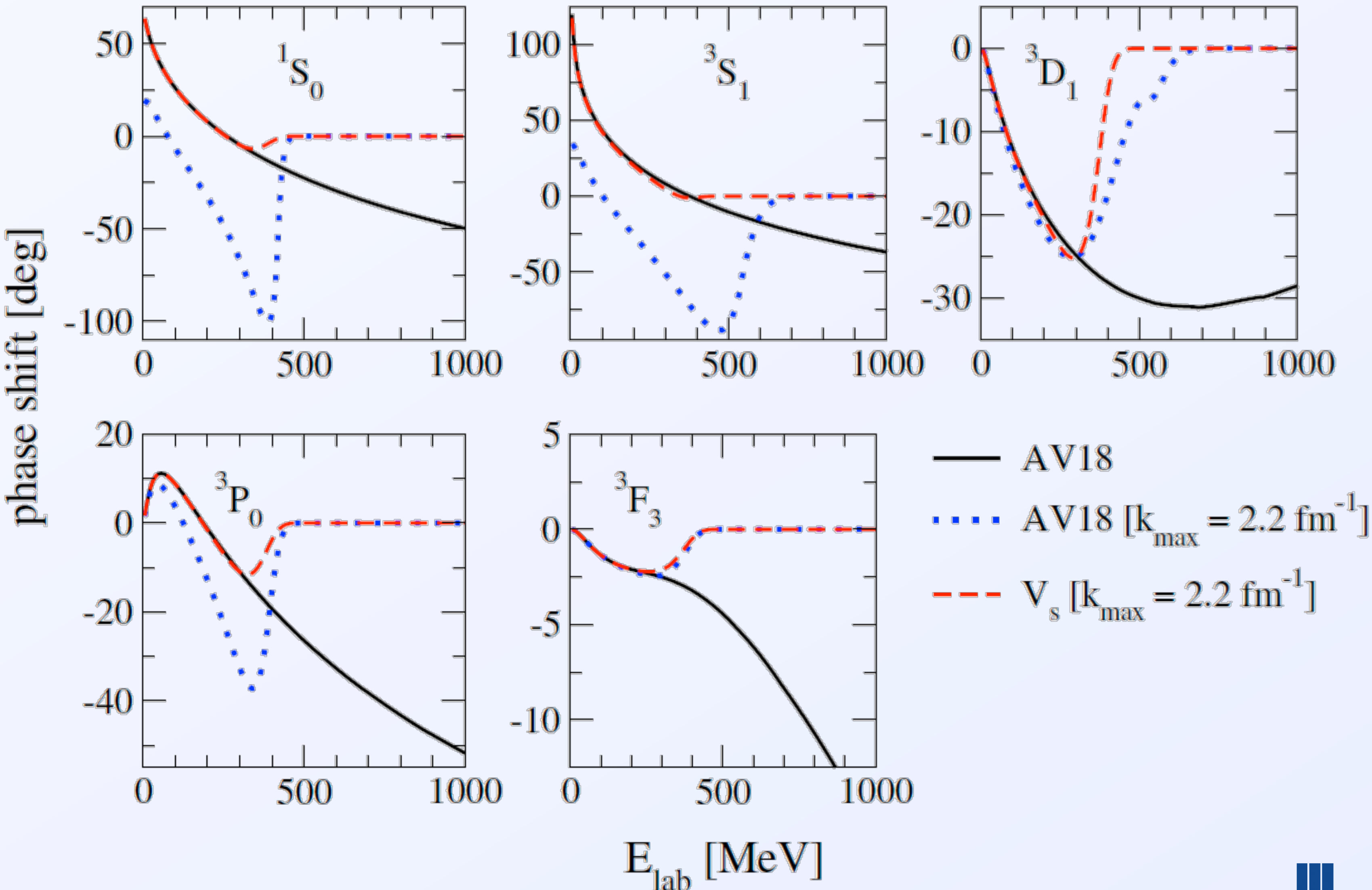


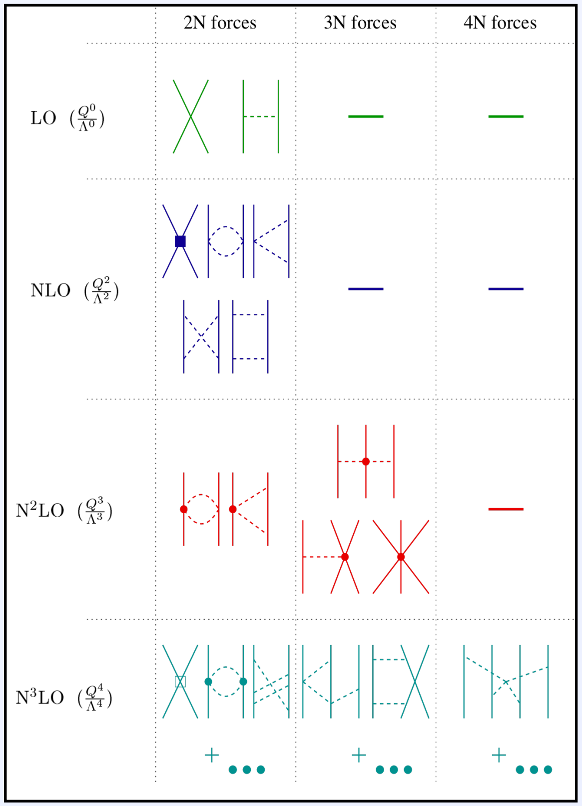


Now Low-Pass Filters Work!



Many-Nucleon Forces

- Two sources:
- Initial:
  - NN is not enough
    - But NNN is dependent on NN



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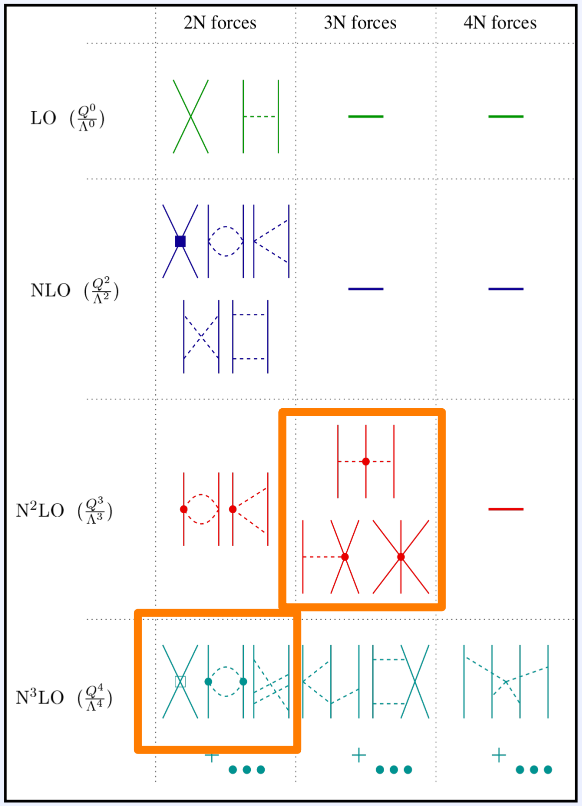


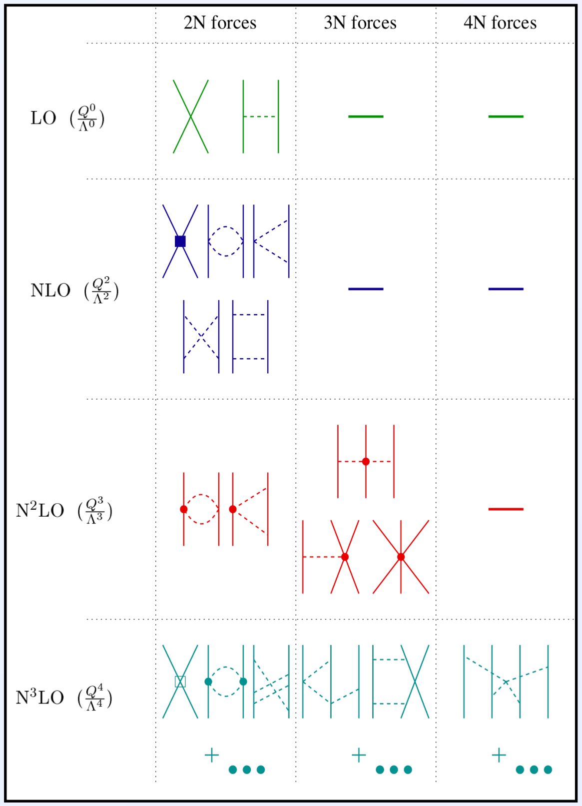
Chrial EFT
NN at N^{3}LO
NNN at N^{2}LO

Many-Nucleon Forces

- Two sources:
- Initial:
  - NN is not enough
    - But NNN is dependent on NN
- Induced:
  - SRG flow equations lead to induced many-body interactions

$$\frac{dH_s}{ds} = \left[\left[\sum a^+a, \sum a^+a + \underbrace{a^+a^+aa}_{2-body}\right], \sum a^+a + \underbrace{a^+a^+aa}_{2-body}\right]$$

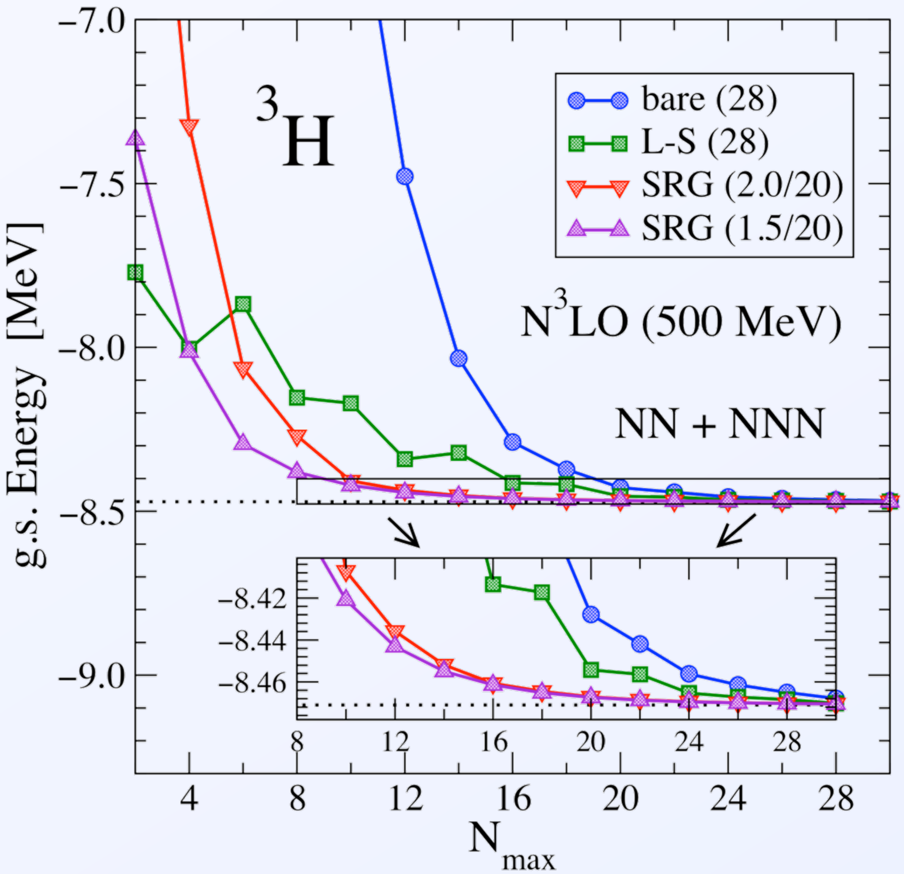
$$= \sum a^+a + \sum a^+a^+aa + \underbrace{a^+a^+a^+aaa}_{3-body} + \ldots$$

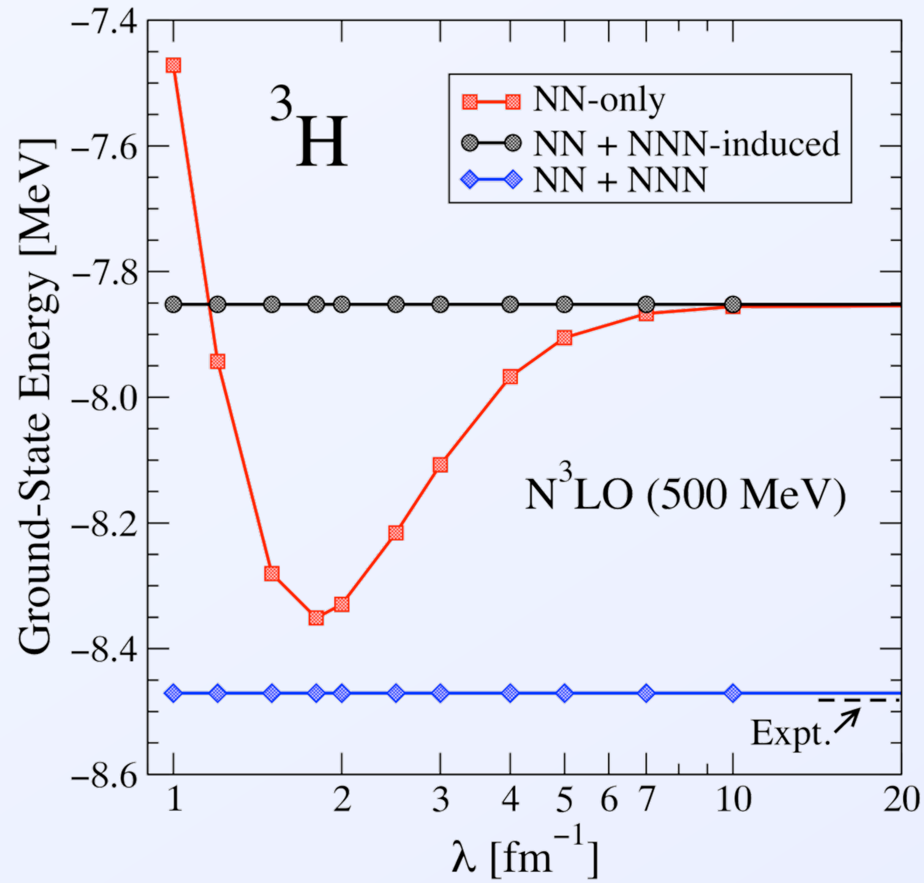


Is there a natural hierarchy? Is 2N > 3N > 4N, etc? How important are 4NI terms?

Triton

- SRG improves convergence, Unitary transformation for A=3





PRL **103**, 82501 (2009) [arXiv: 09005.1873]

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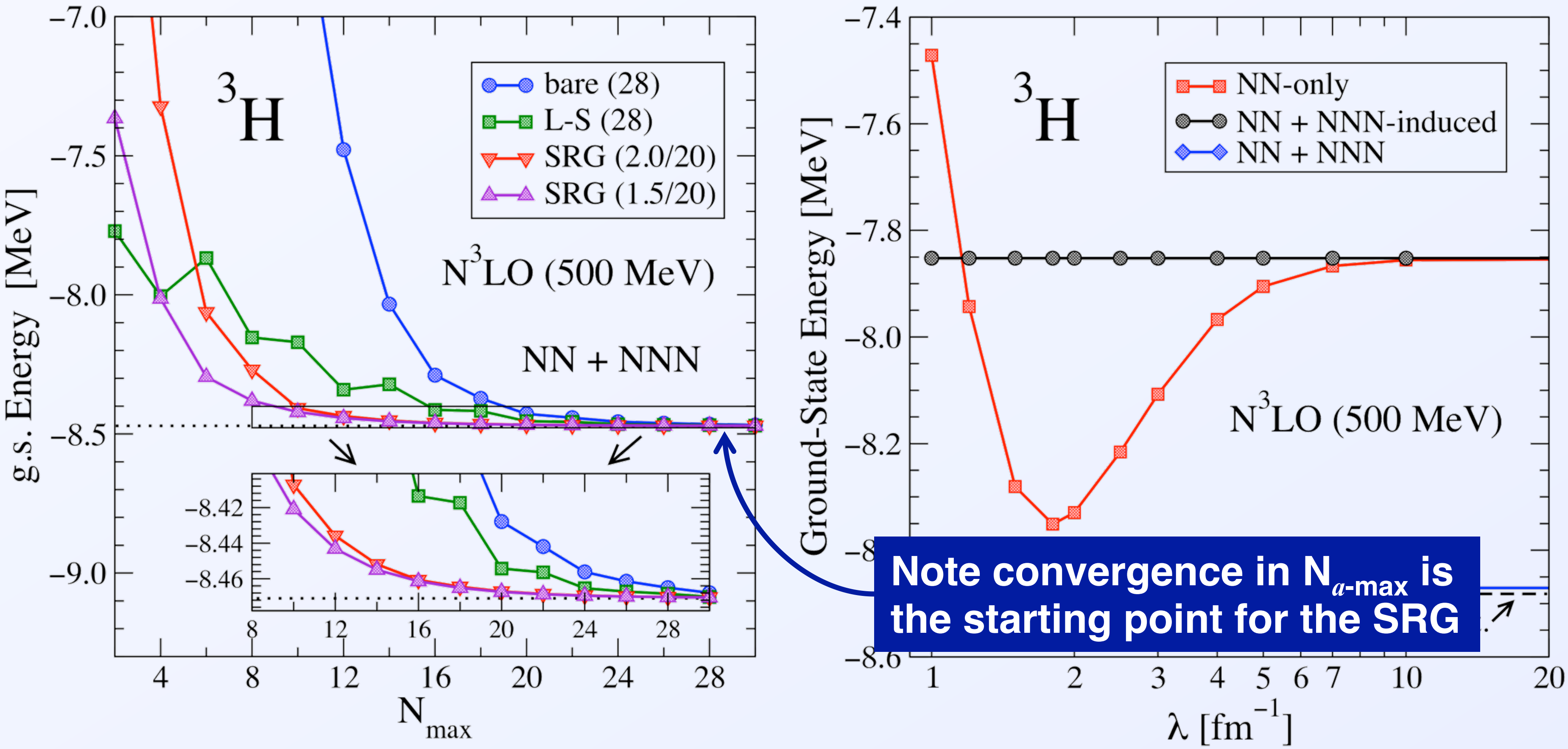

Note convergence in $N_{a\text{-}max}$ is the starting point for the SRG

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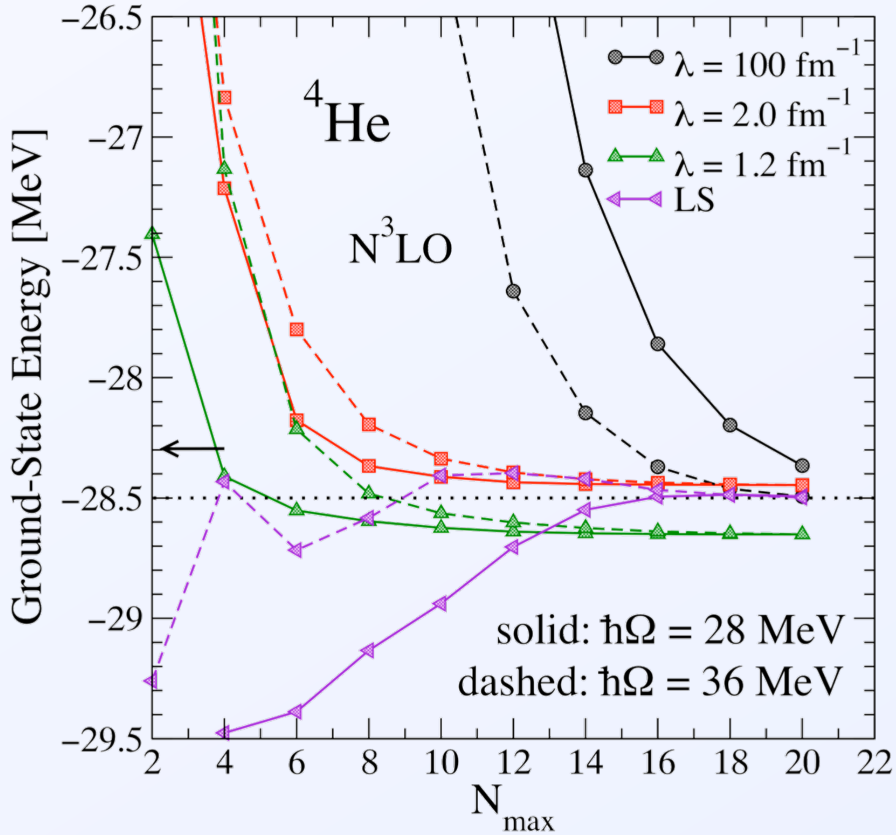
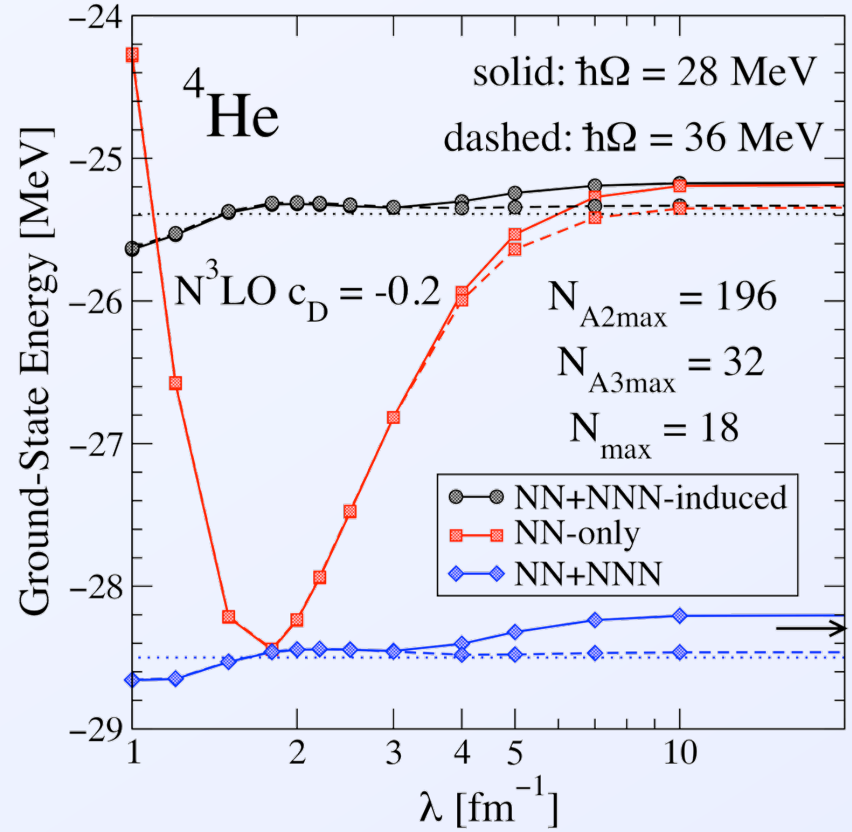
Helium

- SRG induces many-body forces – how big are they?





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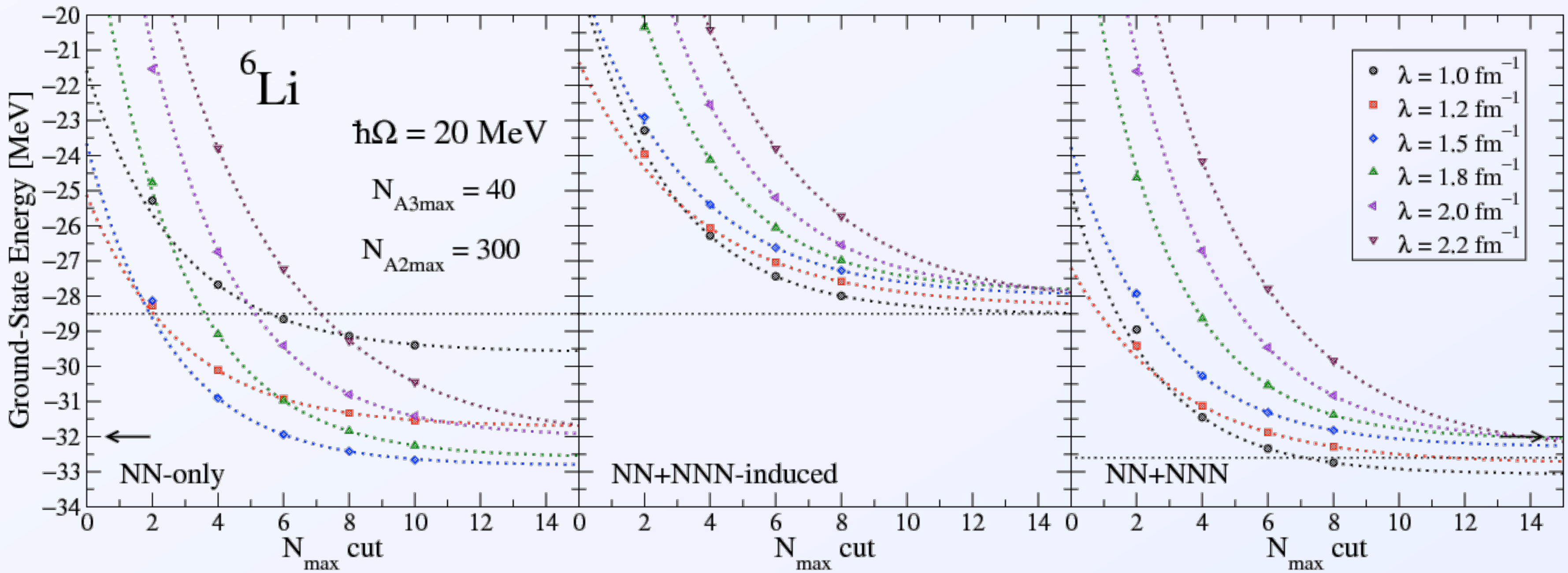
Convergence in ^{6}Li

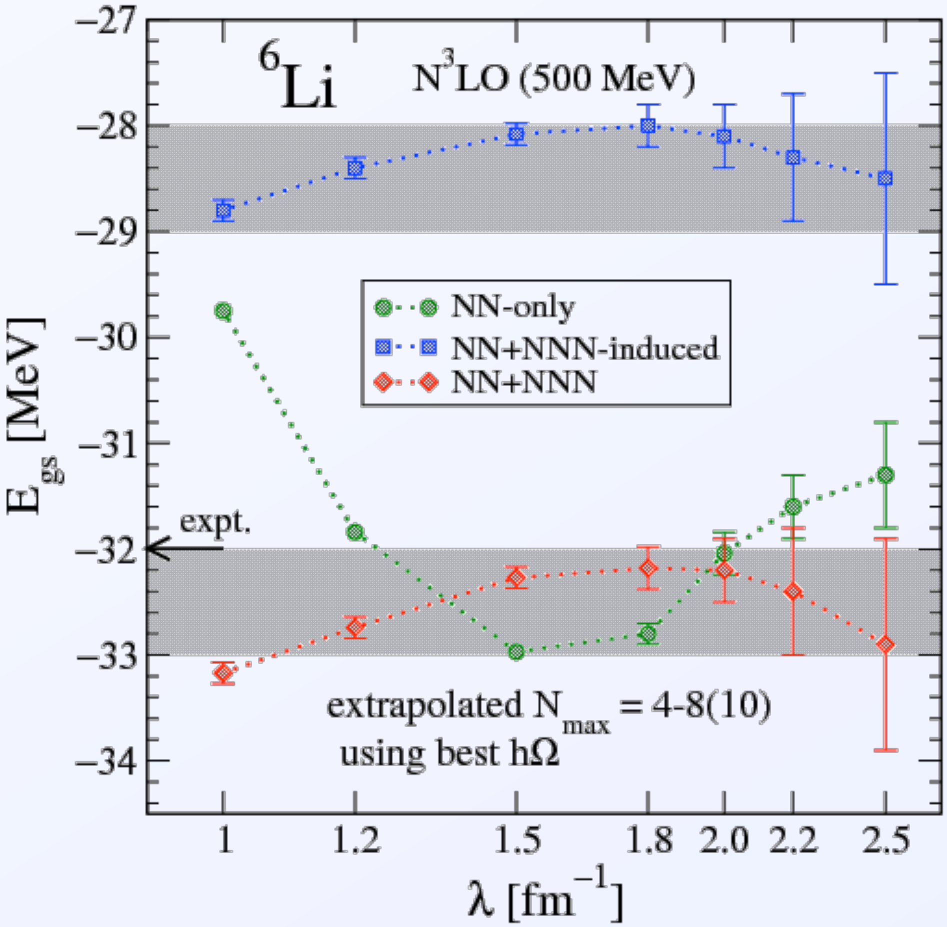
PRC **83**:034301, 2011 [arXiv: 1011.4085]

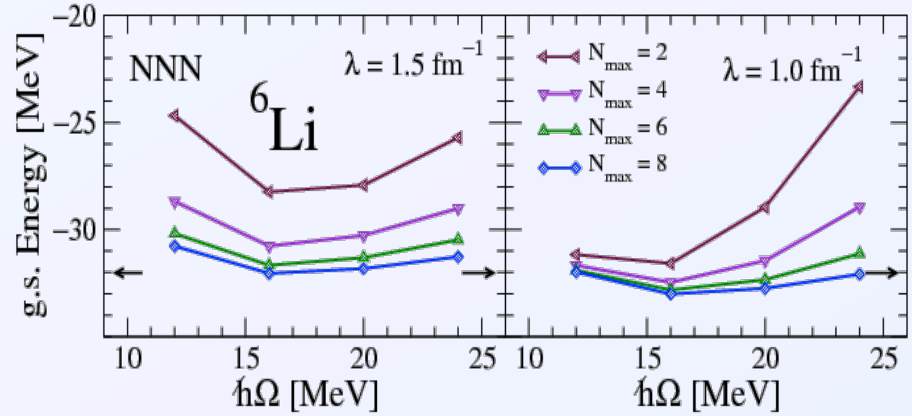


- Increased N_{A2max} to 300 and N_{A3max} to 40
- Simple extrapolations show spread in λ
- Example here for one ħΩ – need optimal for each λ

Lithium

PRC **83**:034301, 2011 [arXiv: 1011.4085]

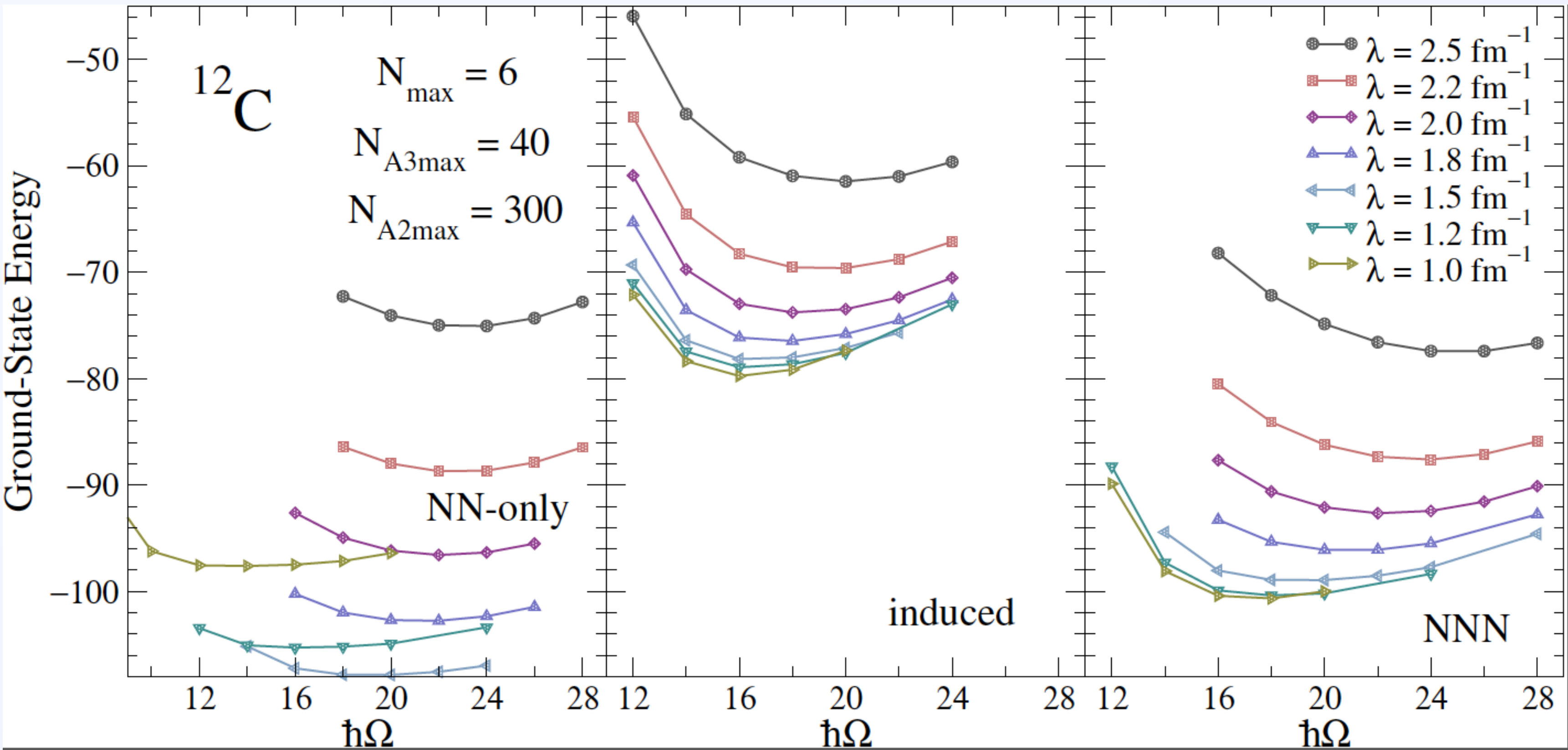




- Optimal ħΩ shifts with evolution
- Extrapolations use this info
- Error bars are consistent with previous work

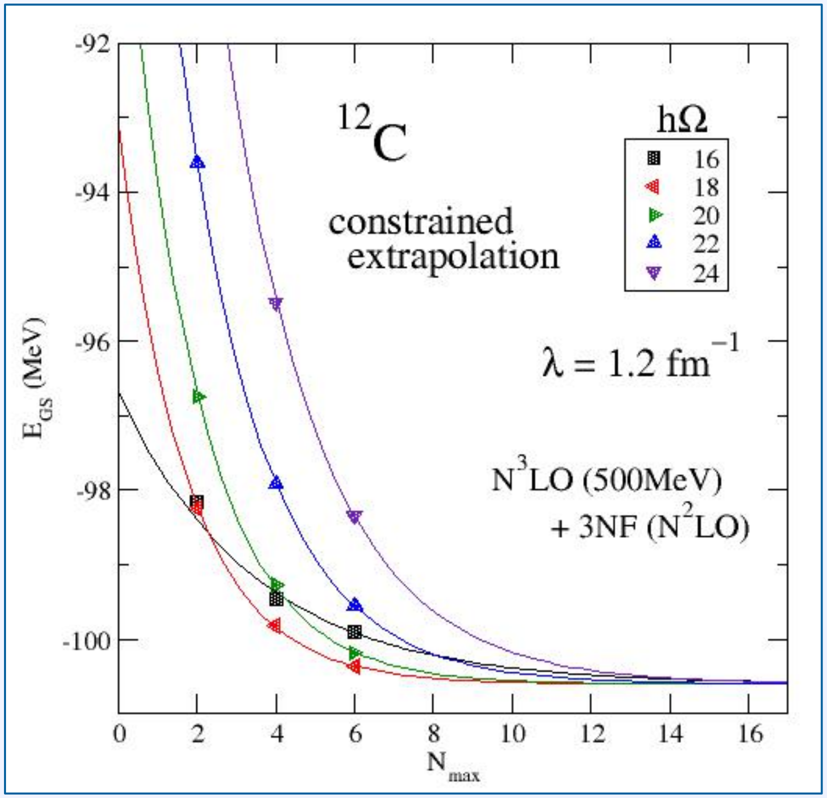
- λ dependence reduced from 4 to <1 MeV

Carbon-12



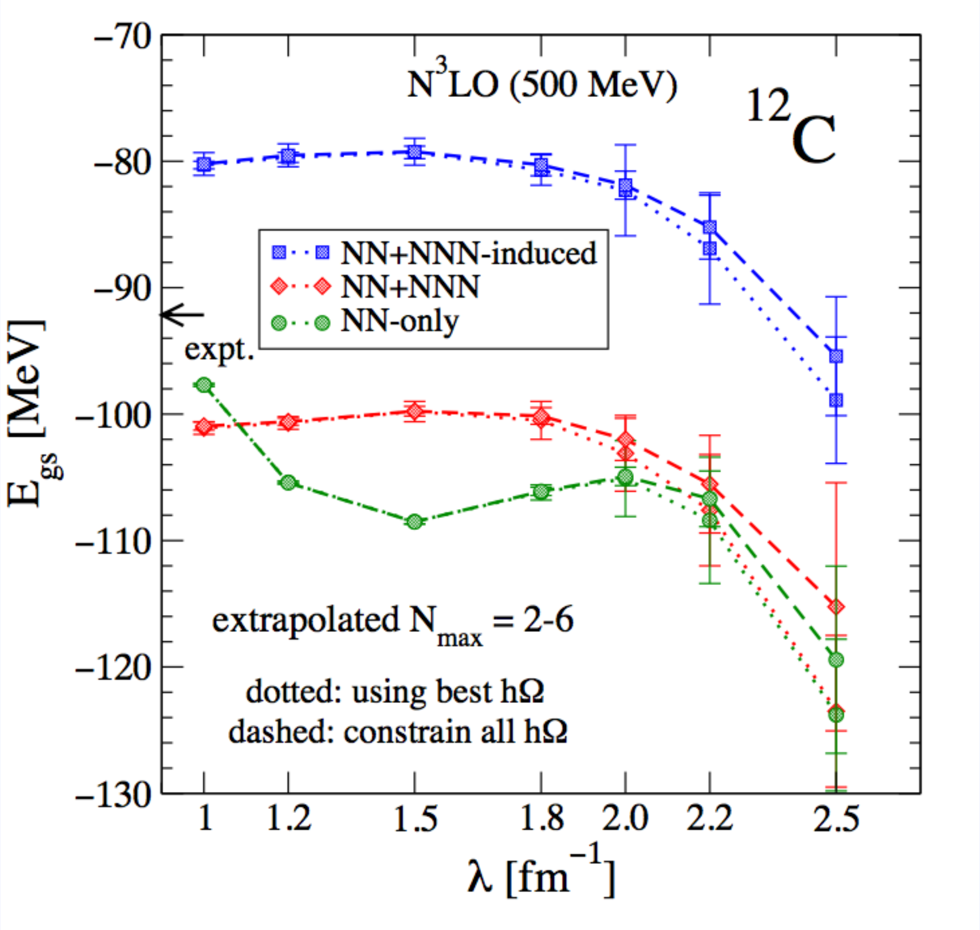
Optimal hbar Ω depends on λ and the interaction
Hbar Ω influences the extrapolation to "full" space

Carbon-12



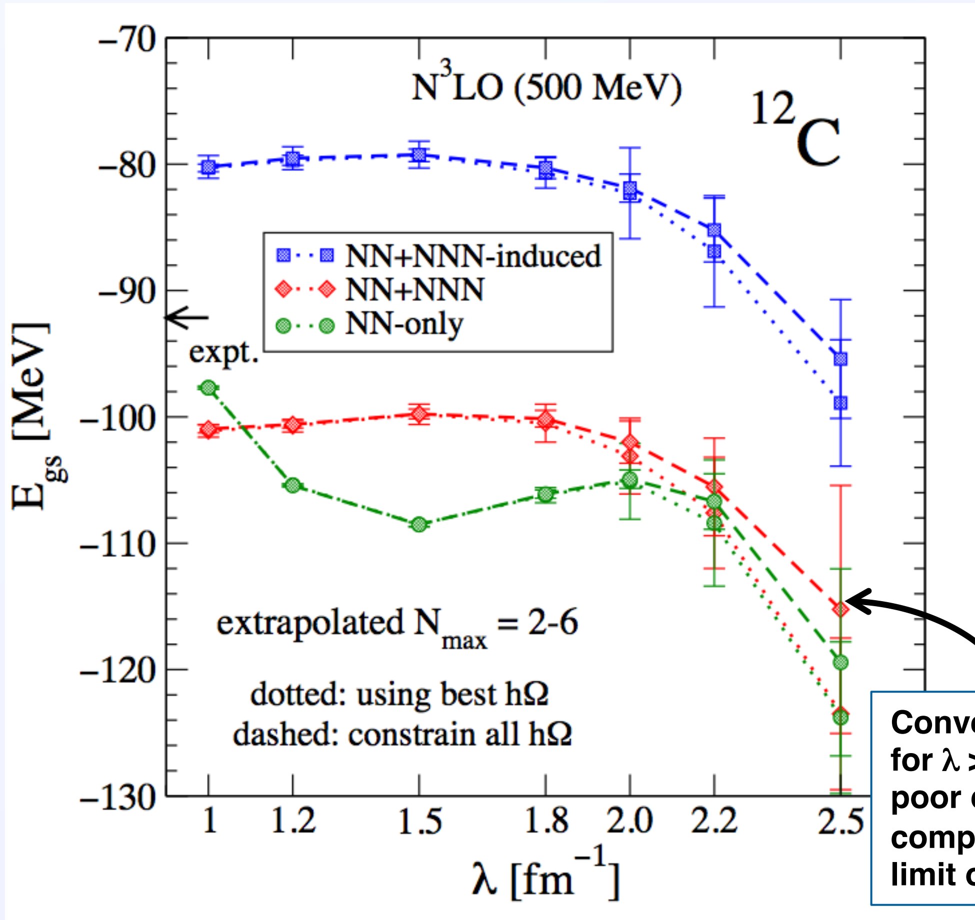
Simultaneous extrapolation with all hbar Ω

Carbon-12



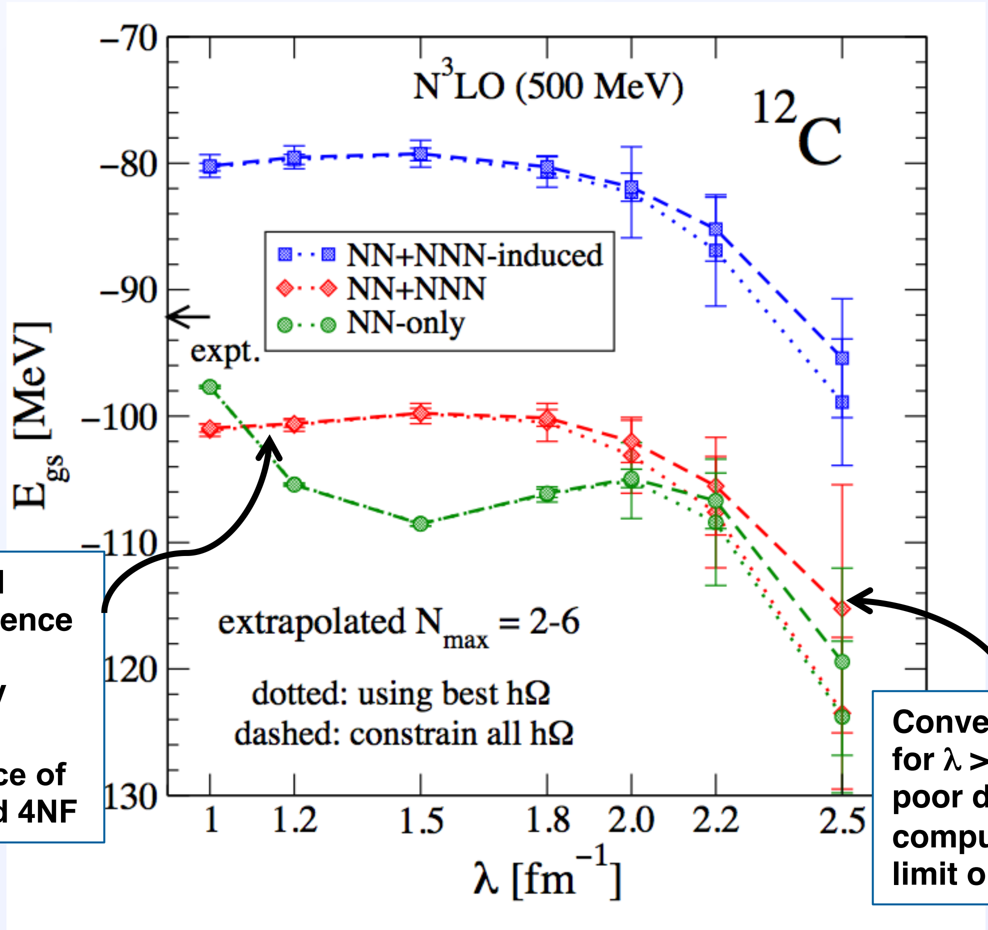
N^3LO (500 MeV)
12C
NN+NNN-induced
NN+NNN
NN-only
expt.
extrapolated Nmax = 2-6
dotted: using best hΩ
dashed: constrain all hΩ
Egs [MeV]
λ [fm^-1]
−70
−80
−90
−100
−110
−120
−130
1
1.2
1.5
1.8
2.0
2.2
2.5

Carbon-12



Convergence for $\lambda > 2.0$ is poor due to computational limit on N_{max}

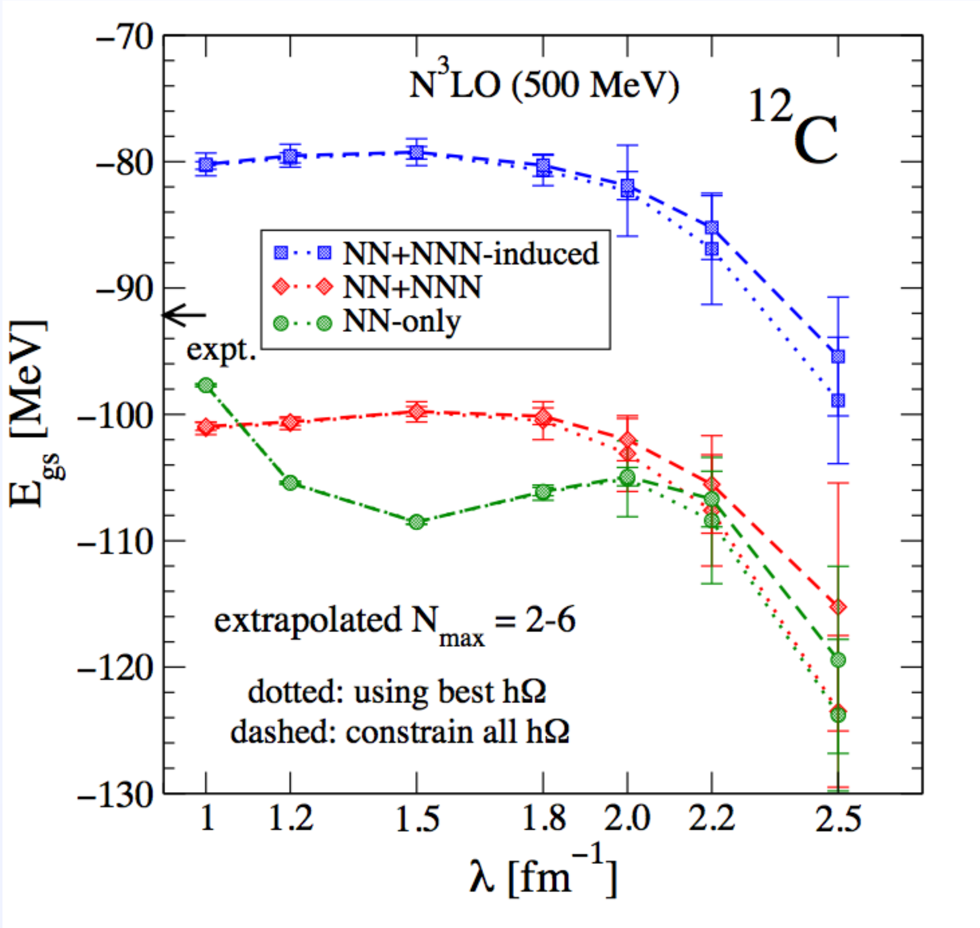
Carbon-12



Minimal dependence on λ
~ 1 MeV spread; influence of induced 4NF

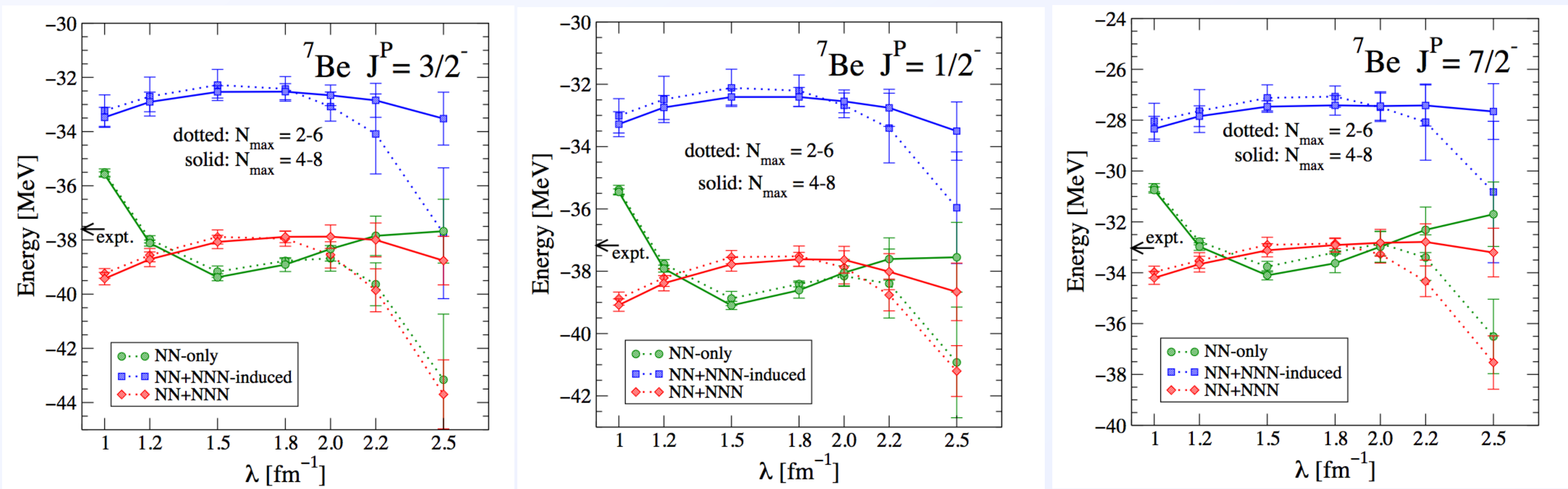
Convergence for λ > 2.0 is poor due to computational limit on N_{max}

Carbon-12



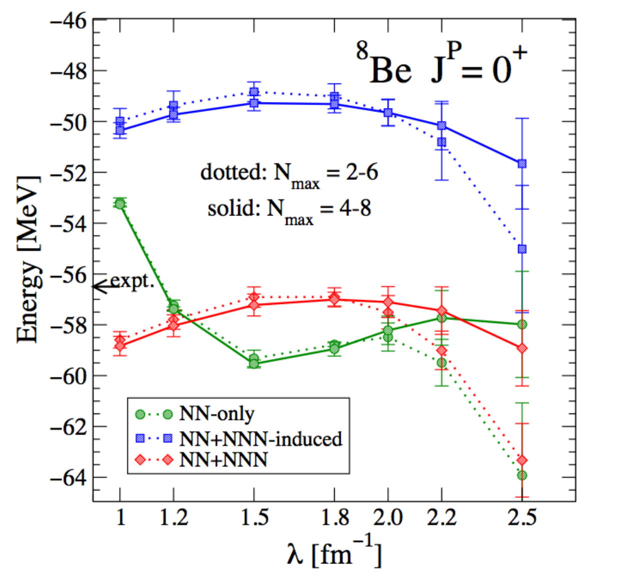
NN (N^3LO) + NNN (N^2LO) overbinds ^{12}C by ~ 8 MeV

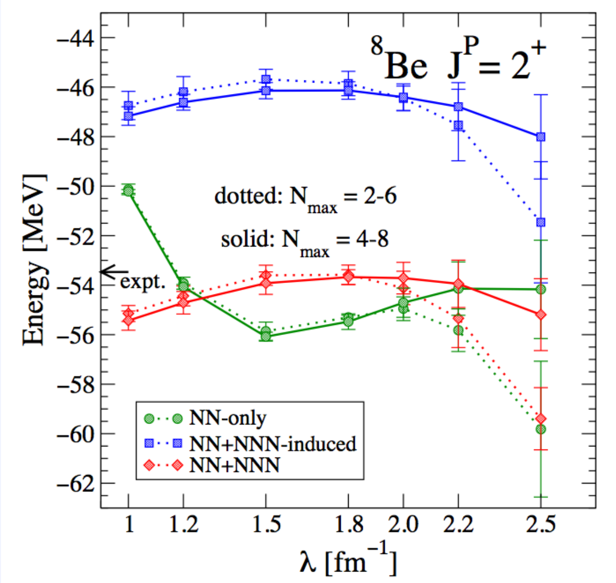
^{7}Be

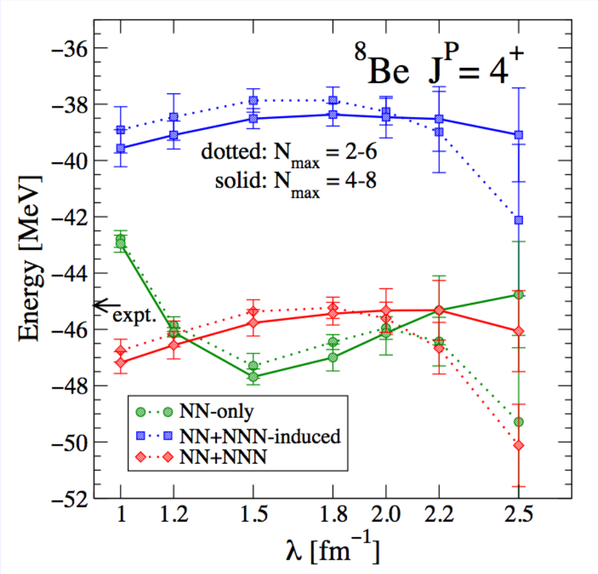


2-8 and 2-6 Extrapolations are in agreement for $\lambda < 2.0$
NNN calculations stable to within ~ 1-1.5 MeV

^{8}Be







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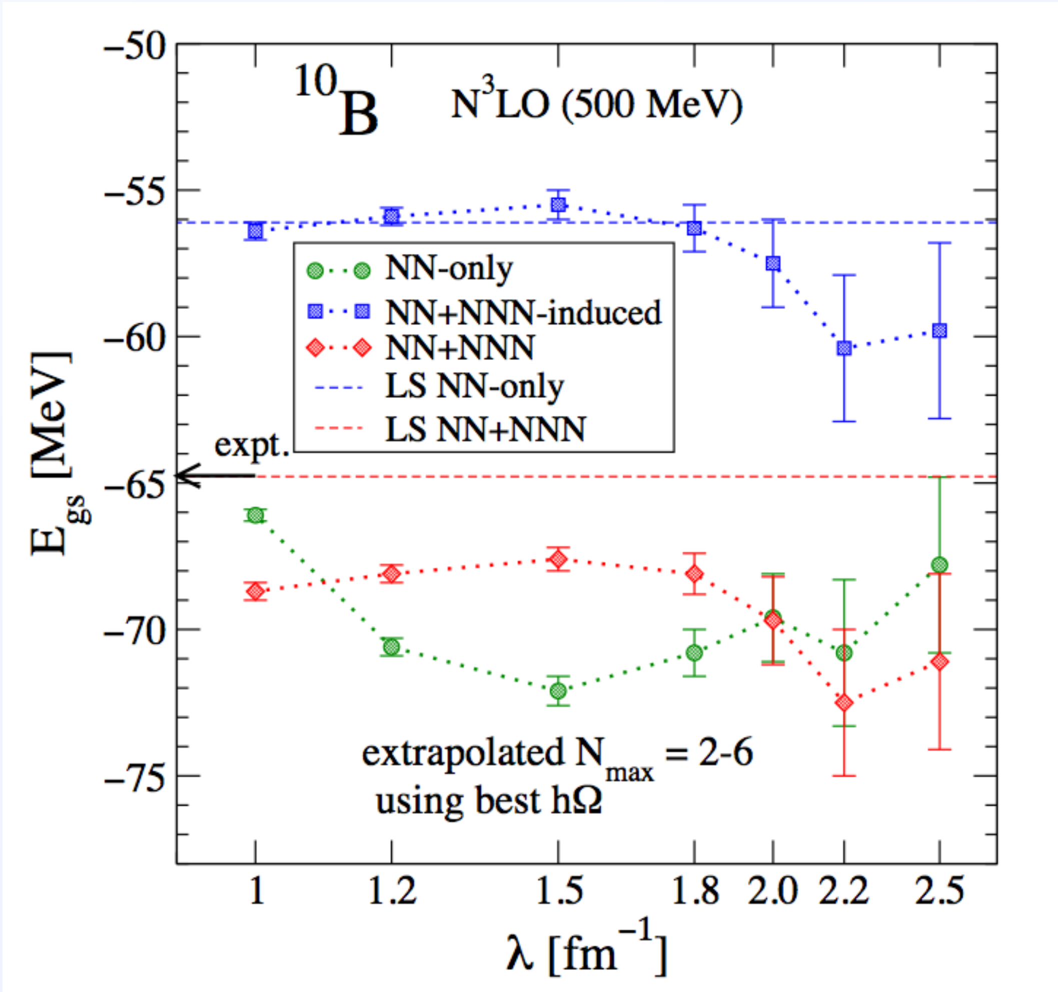
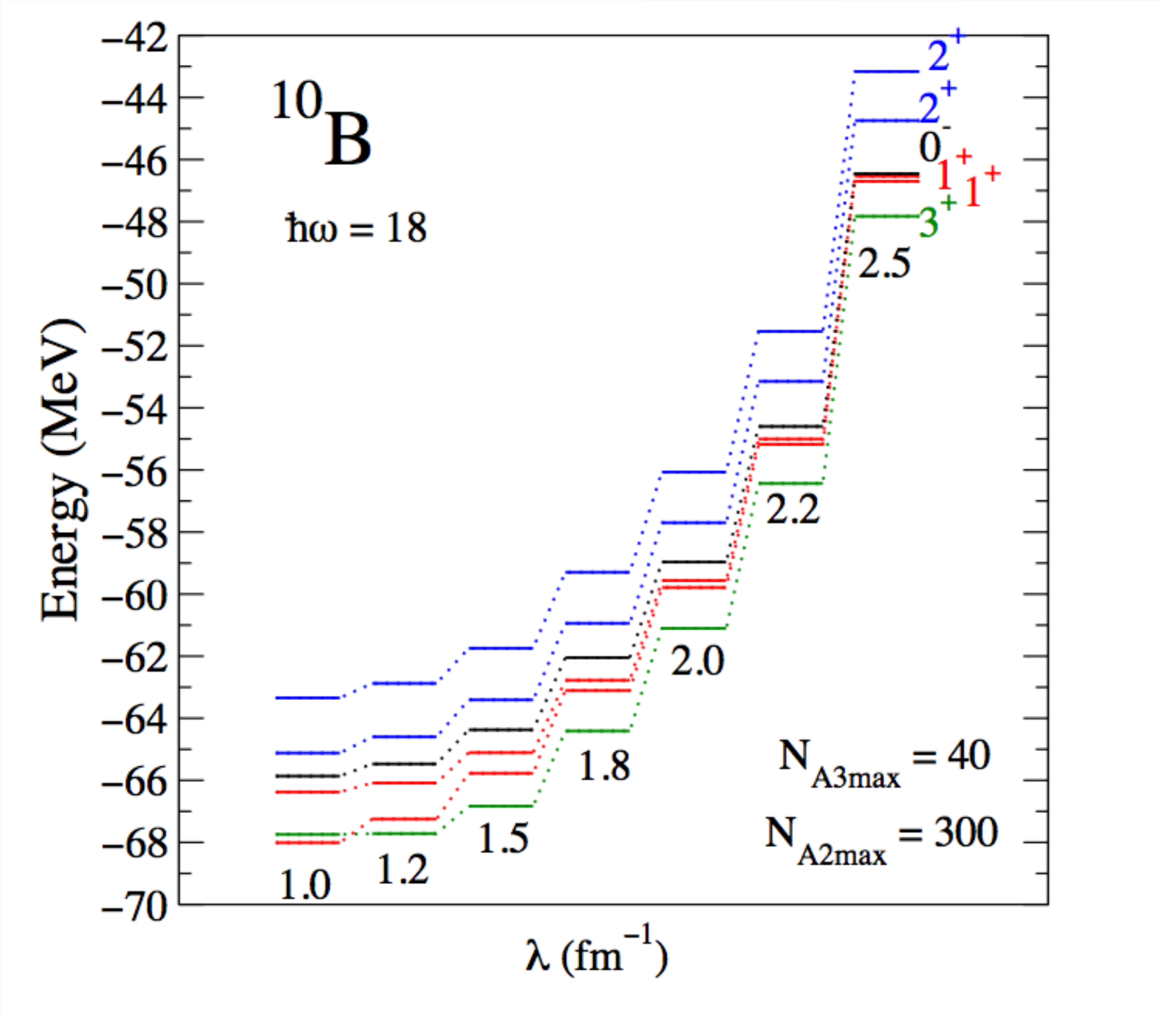
Boron-10



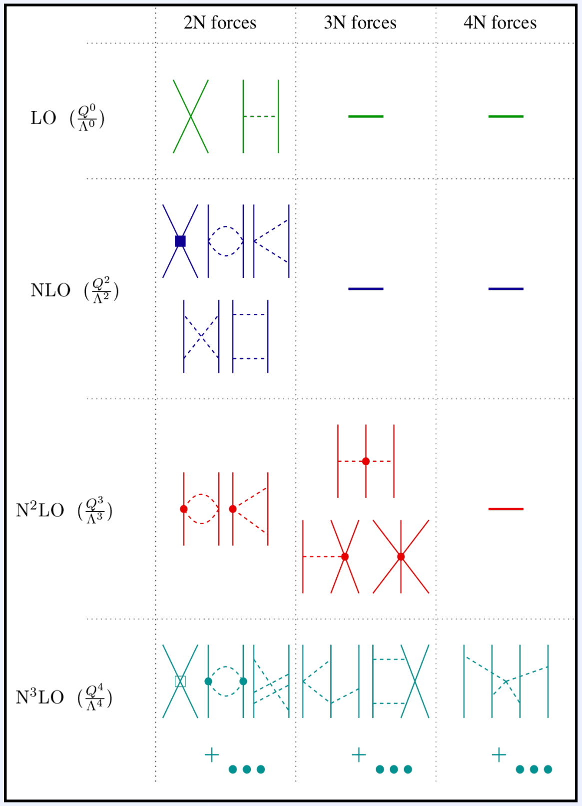
^{10}B
N^{3}LO (500 MeV)
NN-only
NN+NNN-induced
NN+NNN
LS NN-only
LS NN+NNN
expt.
extrapolated N$_{max}$ = 2-6
using best hΩ
−50
−55
−60
−65
−70
−75
E$_{gs}$ [MeV]
1
1.2
1.5
1.8
2.0
2.2
2.5
λ [fm^{-1}]

Boron-10 – spectrum λ dependence



Future

- EFT interactions have been derived to N^{3}LO



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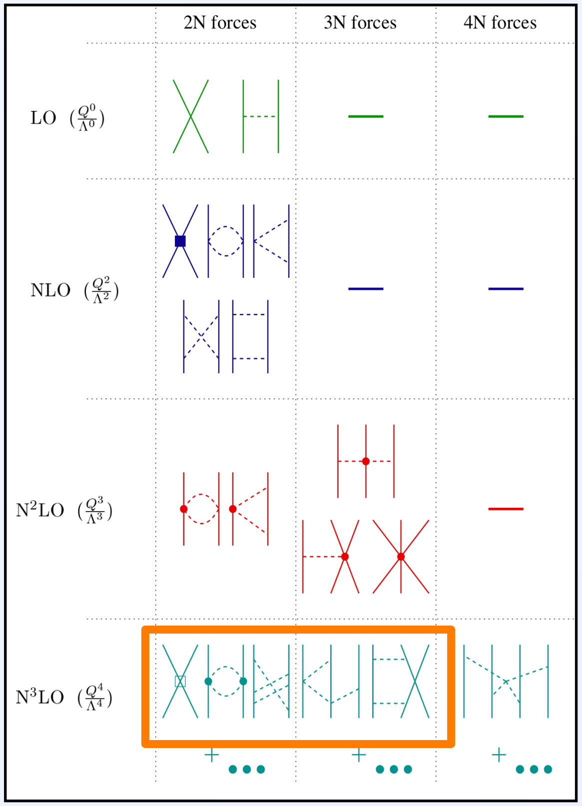

No new constants, but still need to constrain C_D and C_E

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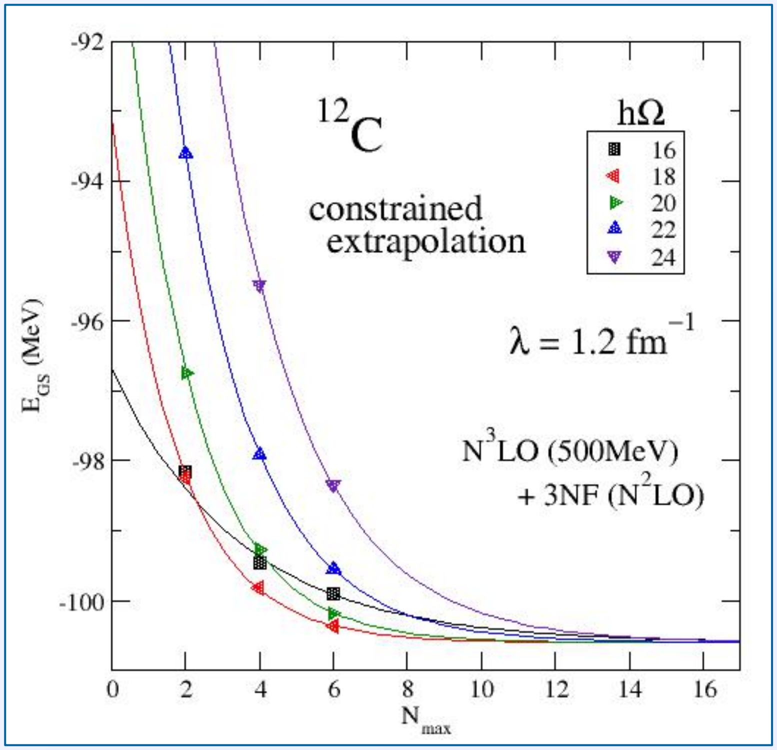
- Better convergence:
  - Importance truncation
  - But pretty good convergence for $1.2 \leq \lambda \leq 1.8$ at $N_{max} = 6$
    - $N_{max} = 8$ may be good enough for these λ values
  - 4NF terms are about 1 MeV
    - Include induced 4NF terms



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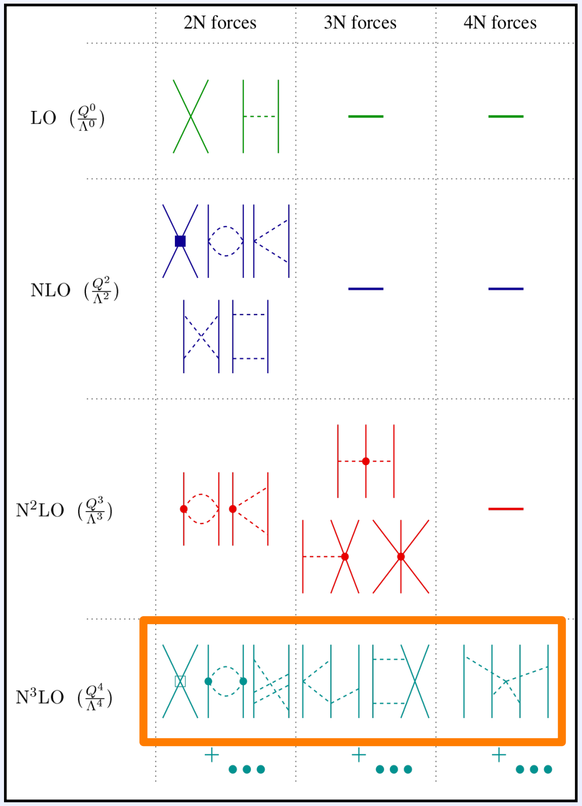

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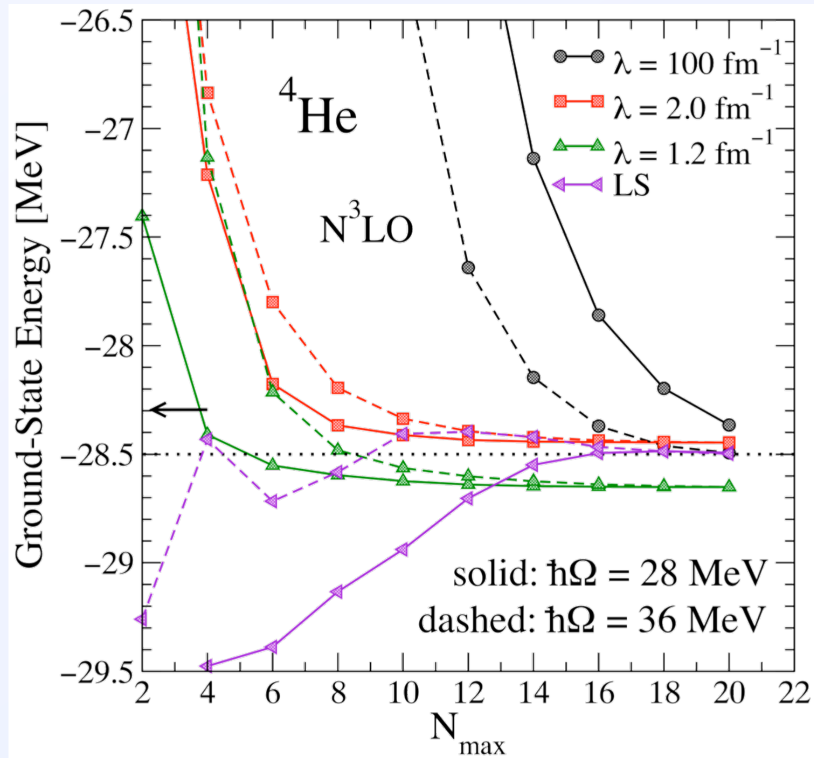

The catch is that convergence for needed hbar Ω will be difficult