Chiral Effective Field Theory and Nuclear Forces: The SRG and applications in many-body calculations

Kai Hebeler

Mainz, August 1, 2022

TALENT school @MITP:
Effective field theories in light nuclei

SFB 1245

TECHNISCHE UNIVERSITÄT DARMSTADT

Basis function expansion methods

$$H\left|\psi_i\right\rangle = T + V\left|\psi_i\right\rangle = E_i\left|\psi_i\right\rangle$$

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most common choice: harmonic oscillator basis functions

$$\left|n\right\rangle = \left|n_1 l_1 m_1\right\rangle \otimes \left|n_2 l_2 m_2\right\rangle \otimes \ldots \otimes \left|n_A l_A m_A\right\rangle$$

with $\left\langle \mathbf{r}|nlm\right\rangle = R_{nl}(r)Y_{lm}(\hat{\mathbf{r}})$

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eigen energies E_i and eigenstates $|\psi_i\rangle$ can then be determined by ordinary matrix diagonalization (no-core shell model)

$$\langle m|E_i|\psi_i\rangle = E_i c_i^m = \langle m|H|\psi_i\rangle = \sum_n \langle m|H|n\rangle c_i^n$$

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N_{max} N_{max}

$\left|\psi_i\right\rangle$

skipped details:

- transformation to single-particle coordinates
- isospin
- antisymmetrization
- decoupling of center-of-mass motion

most comm

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Basis function expansion methods

transformation of NN interactions from momentum to HO basis:

$$\langle n'(L'S)J\,|V_{NN}|\,n(LS)J\rangle = \int dpp^2 \int dp'p'^2 R_{n'L'}\,(p',b)\,\langle p'(L'S)J\,|V_{NN}|\,p(LS)J\rangle\,R_{nL}(p,b)$$

with the radial wave functions of 3d harmonic oscillator

$$R_{nl}(p,b) = \sqrt{\frac{2n!b^3}{\Gamma\left(n+l+\frac{3}{2}\right)}}(pb)^l e^{-p^2b^2/2} L_n^{l+\frac{1}{2}}\left(p^2b^2\right)$$

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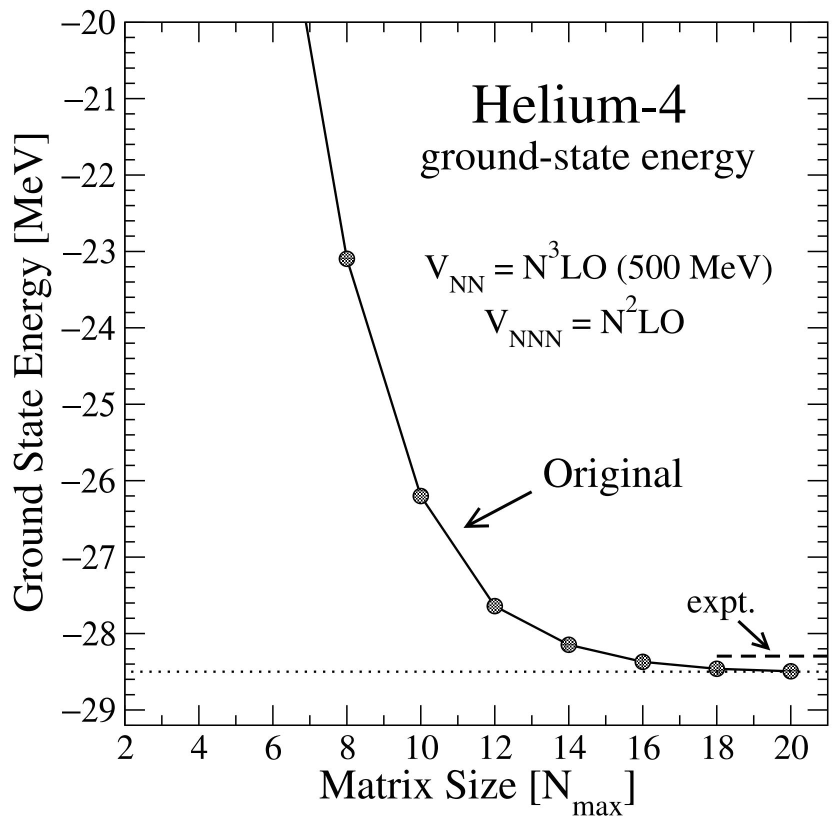
in practice many-body frameworks are typically formulated in a single-particle basis:

$$\langle n_1'(l_1'1/2)j_1', n_2'(l_2'1/2)j_2', \ldots|\, H\, |n_1(l_1 1/2)j_1, n_2(l_2 1/2)j_2, \ldots\rangle$$

this transformation involves the Talmi-Moshinski overlap brackets

$$\langle n_1 l_1, n_2 l_2 | n_{\mathrm{rel}} L_{\mathrm{rel}}, N_{\mathrm{cm}} L_{\mathrm{cm}}\rangle$$

Basis size and matrix dimensions



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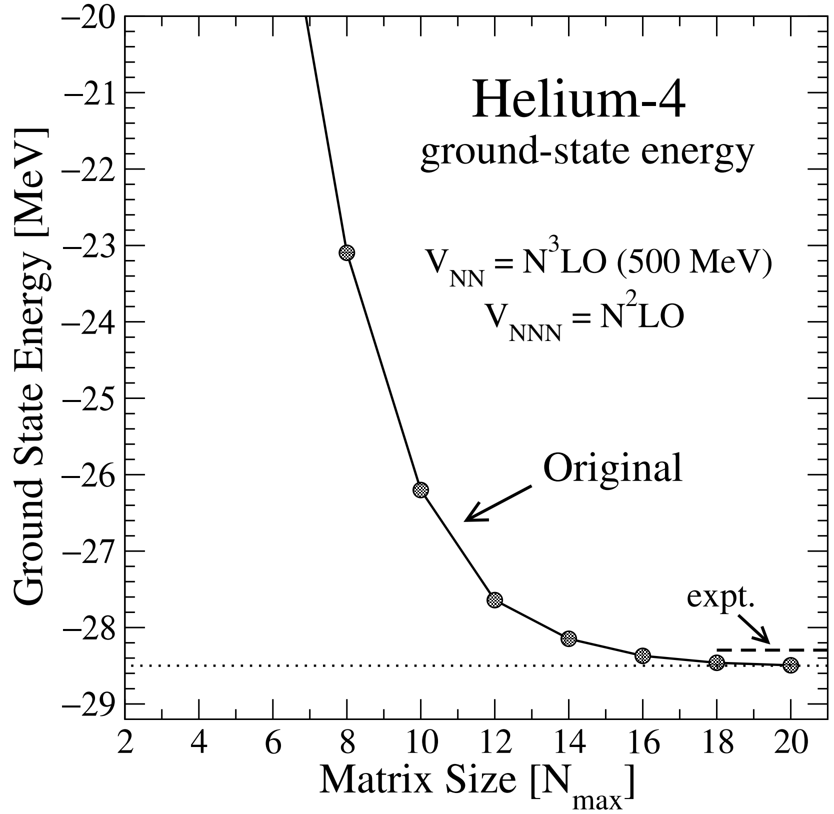

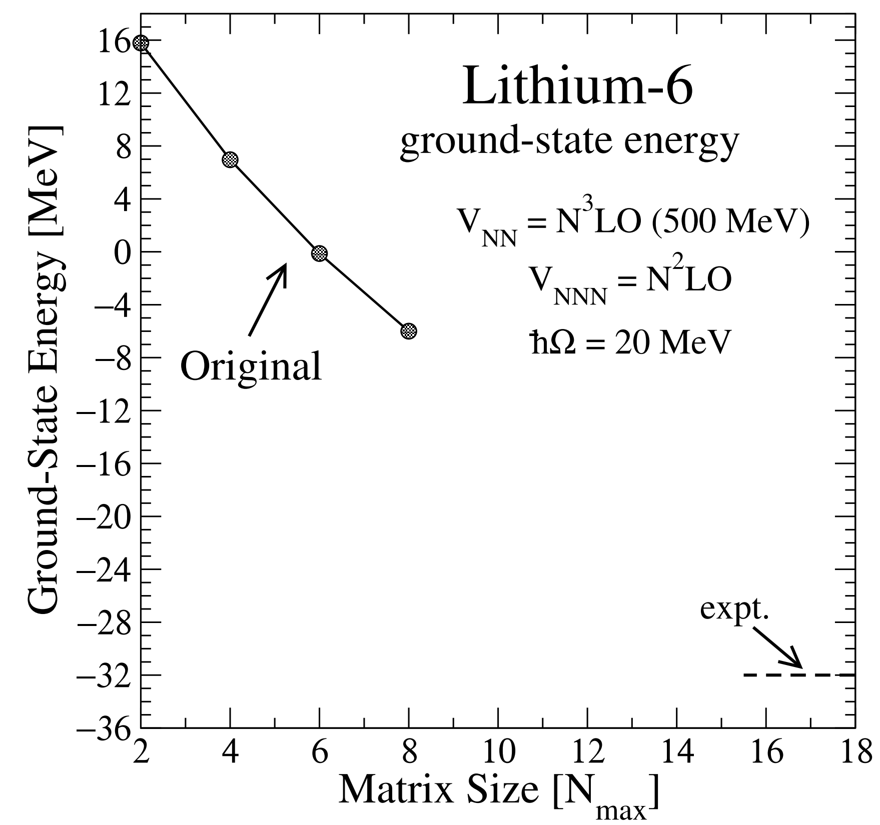

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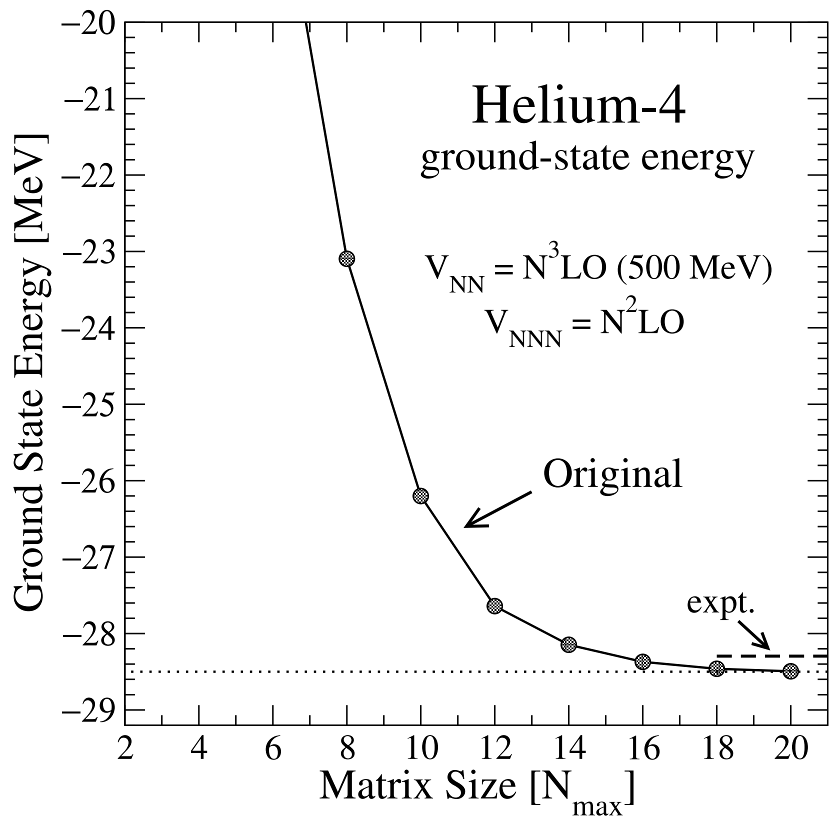

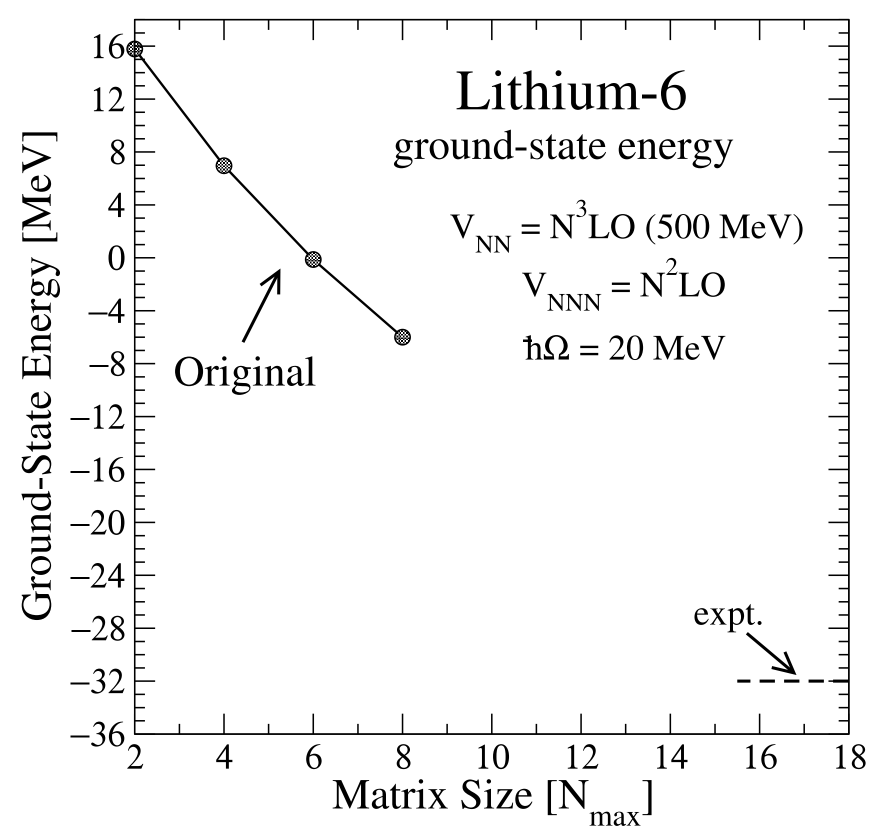

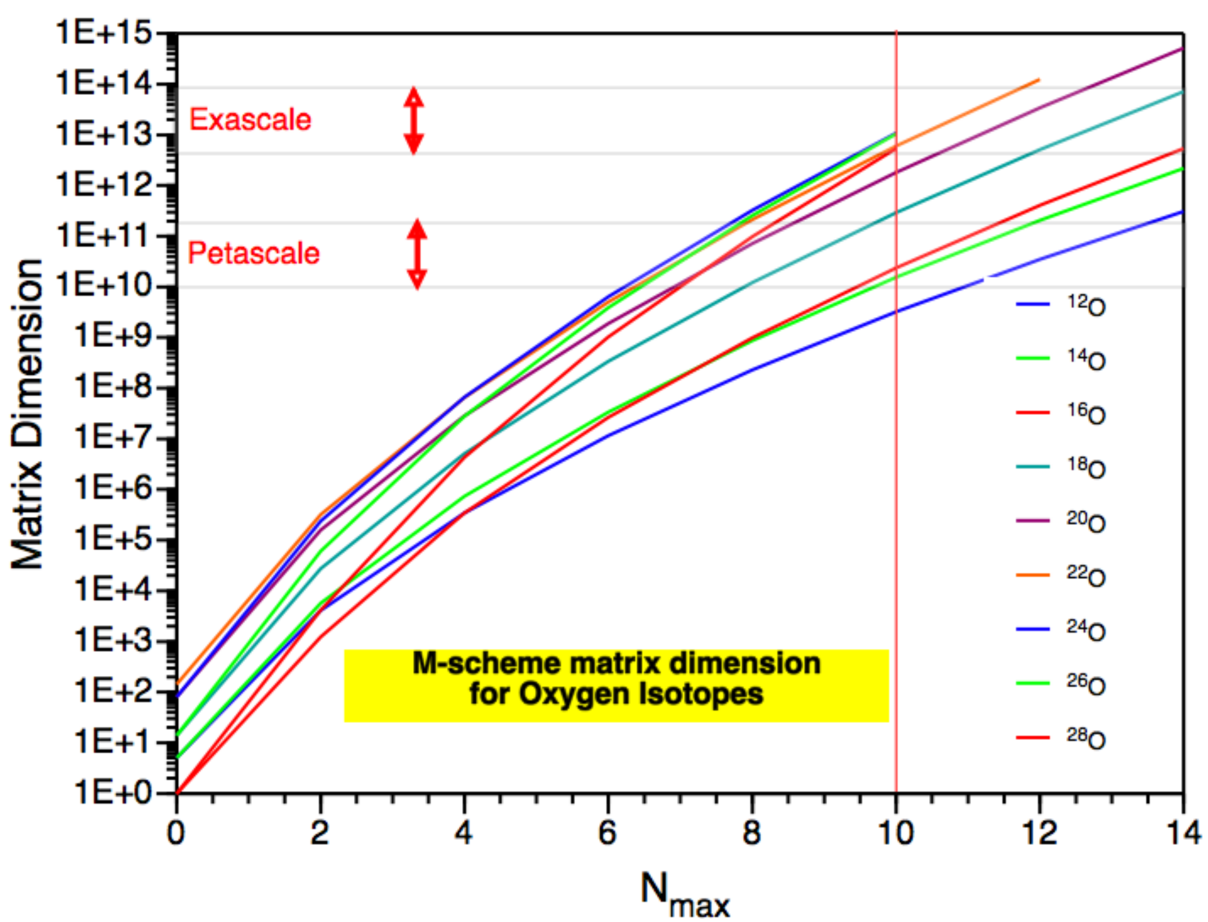

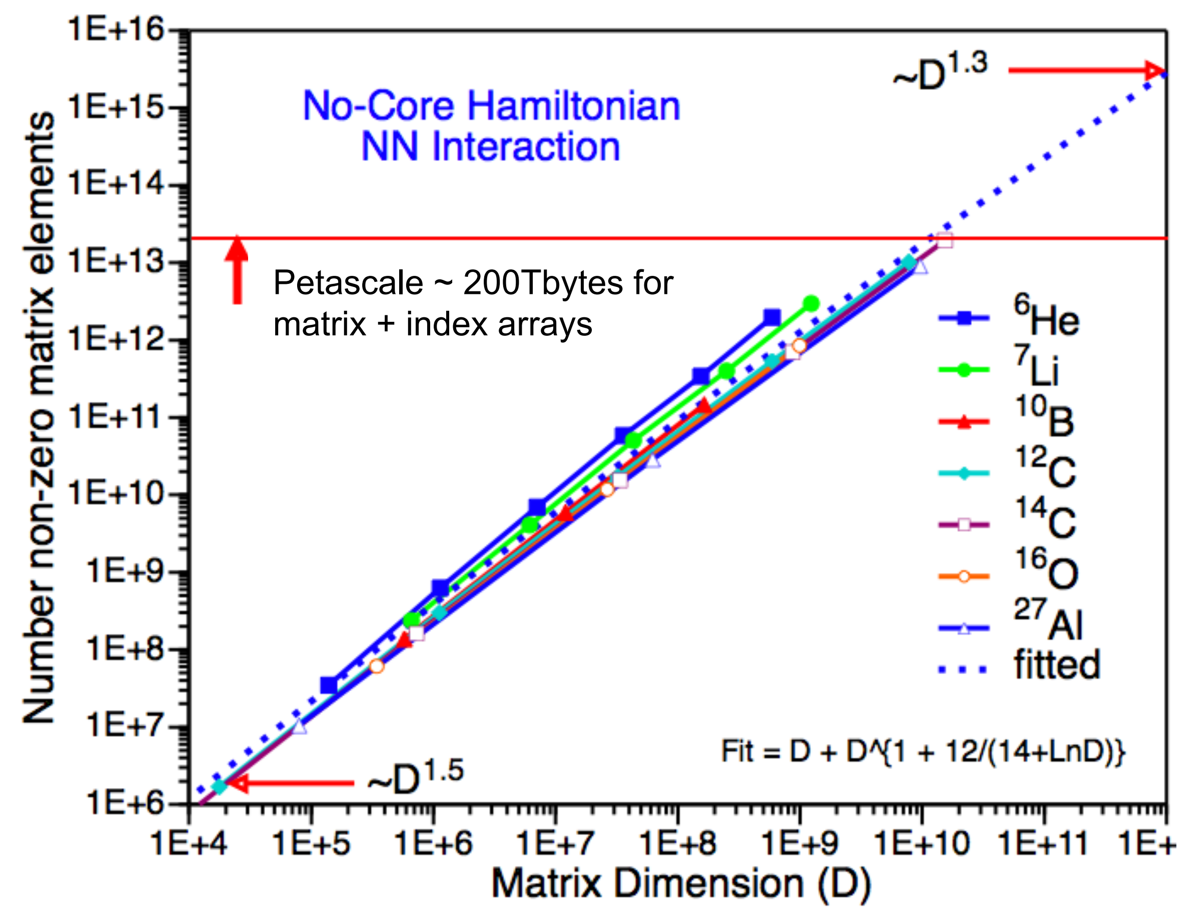

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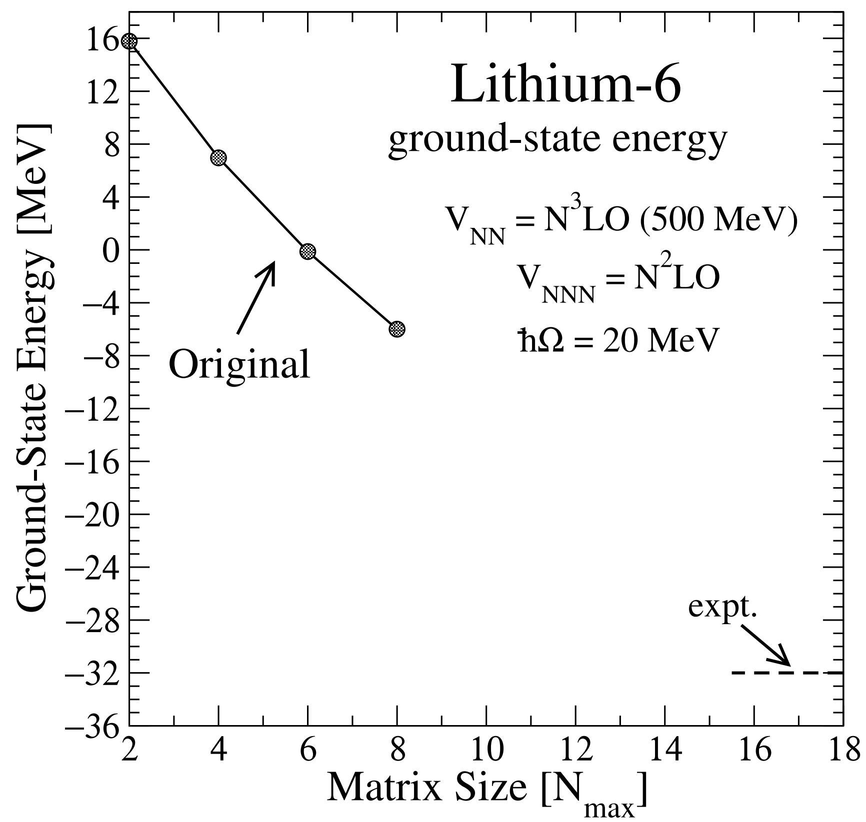
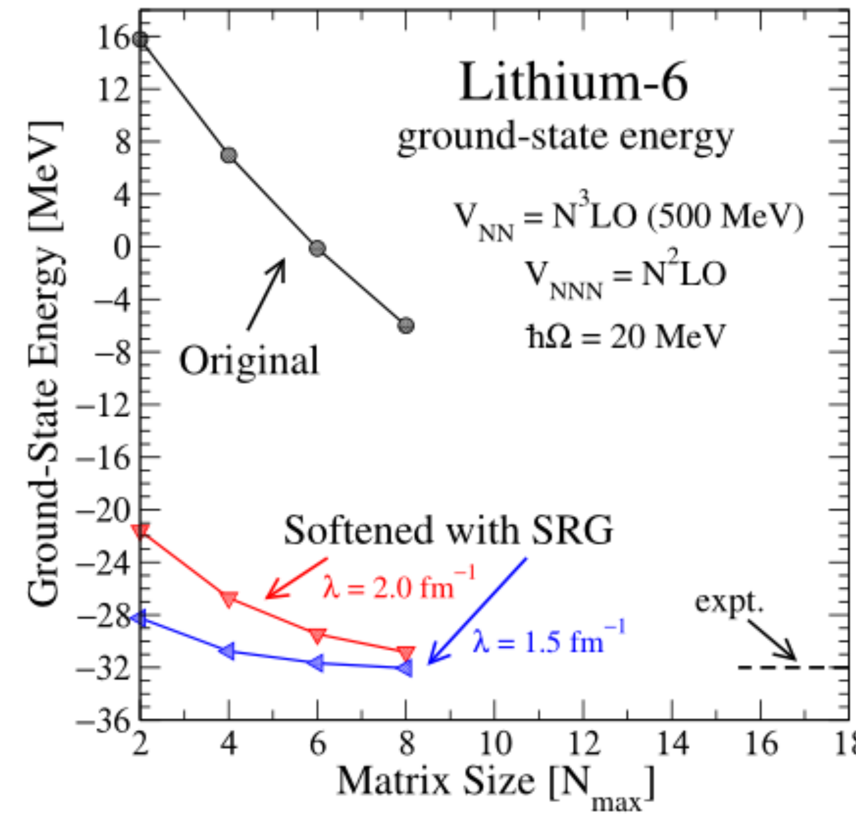
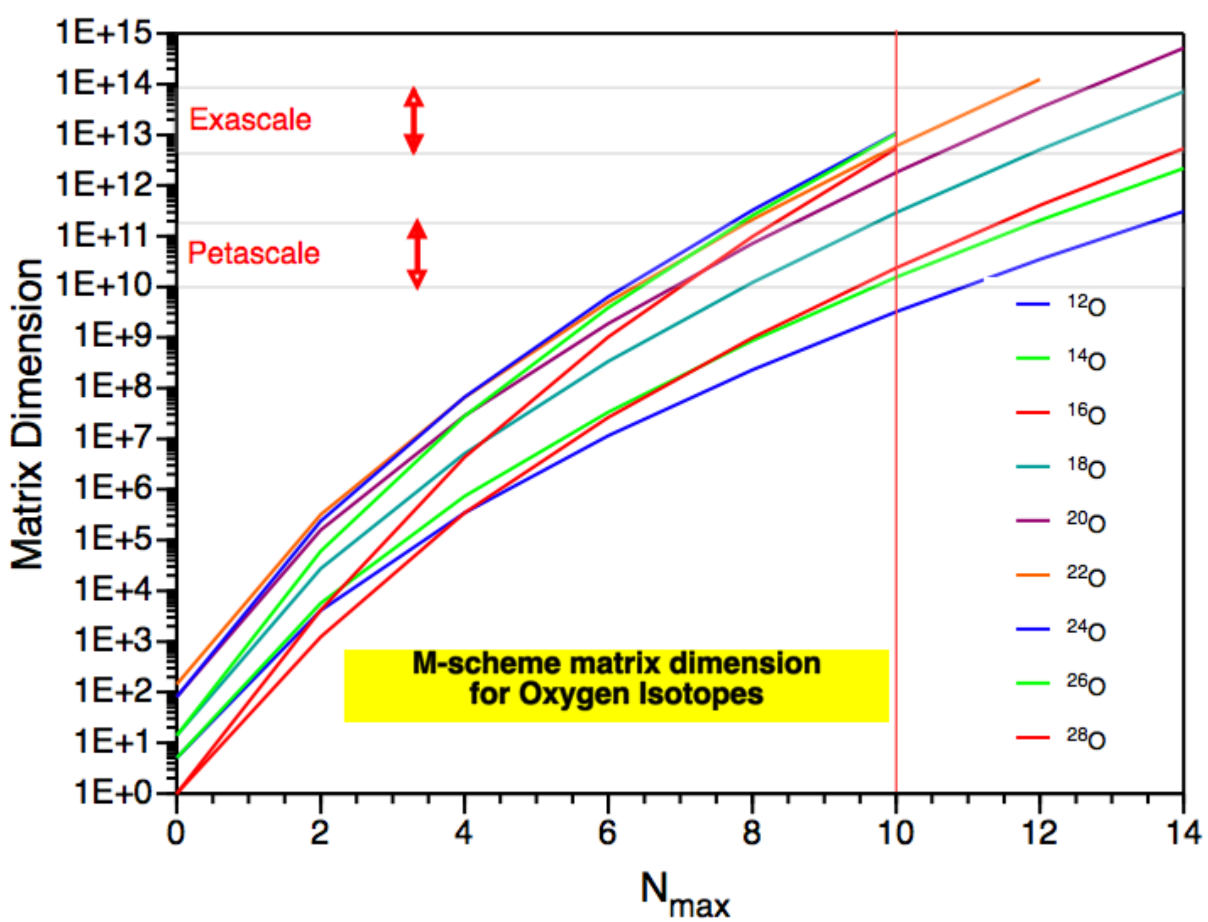
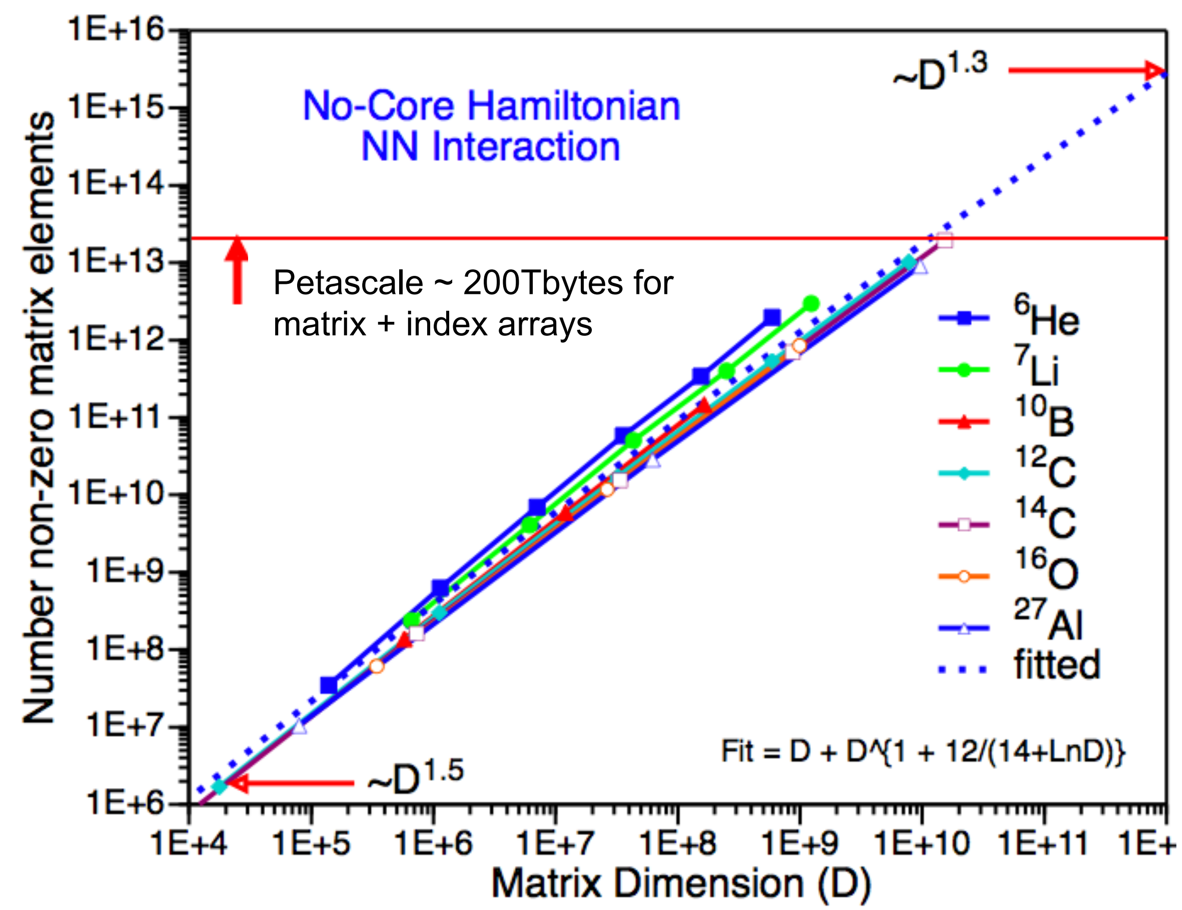


SRG
evolution





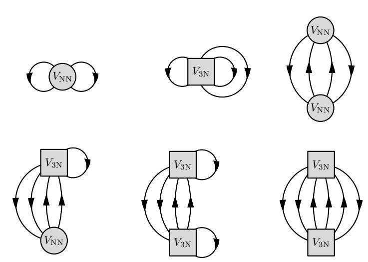


Nuclear forces for different ab-initio many-body frameworks

Hyperspherical harmonics

no-core shell model

Many-body
perturbation theory



Faddeev,
Faddeev-Yakubovski

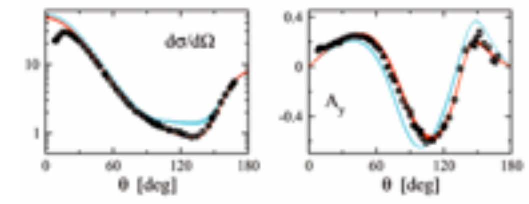
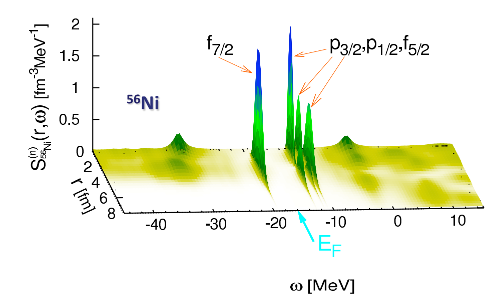


FIG. 4: Nd elastic observables at 65 MeV.

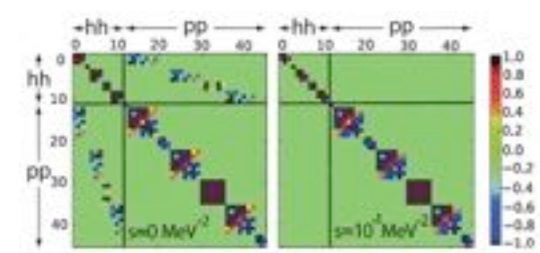
coupled cluster method

$$|\Psi\rangle = e^{T}|\Phi_0\rangle = \left(1 + T + \frac{1}{2}T^2 + \frac{1}{3!}T^3 + \cdots\right)|\Phi_0\rangle,$$

Self-consistent
Greens function



In-medium SRG

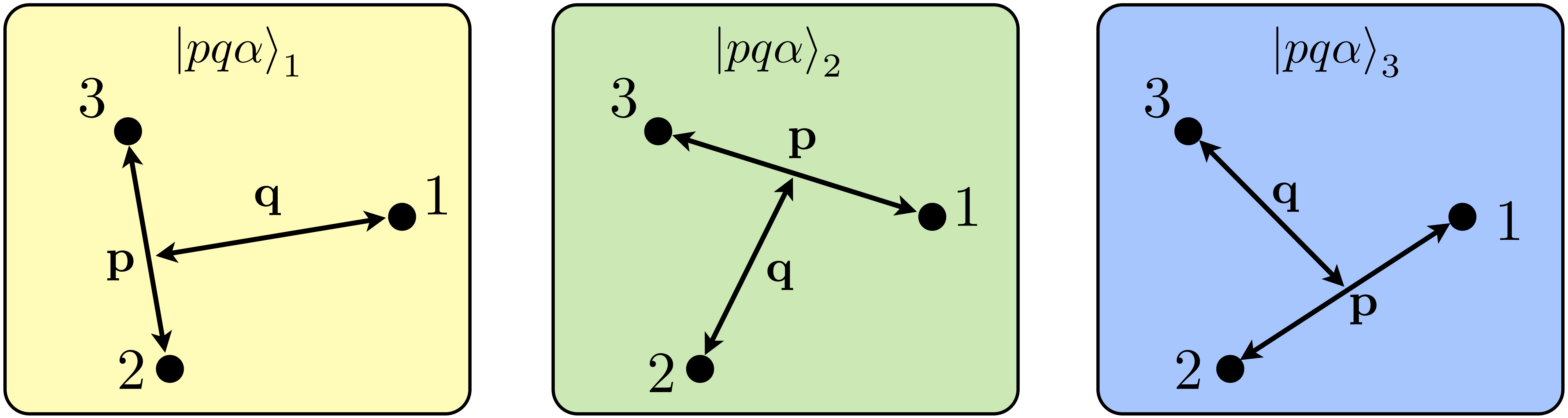


Required inputs:

1. consistent NN and 3N forces in partial-wave-decomposed form
2. softened forces for judging approximations and pushing to heavier nuclei

Calculation of 3N interactions for many-body frameworks

$$|pq\alpha\rangle_i \equiv |p_i q_i; [(LS)J(ls_i)j]\,\mathcal{J}\mathcal{J}_z(Tt_i)\mathcal{T}\mathcal{T}_z\rangle$$



Due to the large number of matrix elements, the traditional way of computing matrix elements requires extreme amounts of computer resources.

$$N_p \simeq N_q \simeq 15$$
$$N_\alpha \simeq 30 - 180$$

$\longrightarrow$ $\dim[\langle pq\alpha|V_{123}|p'q'\alpha'\rangle] \simeq 10^7 - 10^{10}$

Optimized algorithm allows an efficient calculation for large basis spaces

KH, Krebs, Epelbaum, Golak, Skibinski, PRC 91, 044001(2015)

Calculation of 3N forces in momentum partial-wave representation

$$\langle pq\alpha|V_{123}|p'q'\alpha'\rangle \sim \sum_{m_i}\int d\hat{\mathbf{p}}\,d\hat{\mathbf{q}}\,d\hat{\mathbf{p}}'\,d\hat{\mathbf{q}}' Y_l^m(\hat{\mathbf{p}})Y_{\bar{l}}^{\bar{m}}(\hat{\mathbf{q}})\,\langle\mathbf{pq}ST|V_{123}|\mathbf{p}'\mathbf{q}'S'T'\rangle\,Y_{l'}^{m'}(\hat{\mathbf{p}}')Y_{\bar{l}'}^{\bar{m}'}(\hat{\mathbf{q}}')$$

traditional method:

- reduce dimension of angular integrals from 8 to 5 by using symmetry
- discretize angular integrals and perform all sums numerically

much more efficient method:

- use that all interaction contributions (except rel. corr.) are local:

$$\begin{aligned}\langle\mathbf{pq}|V_{123}|\mathbf{p}'\mathbf{q}'\rangle &= V_{123}(\mathbf{p}-\mathbf{p}',\mathbf{q}-\mathbf{q}')\\ &= V_{123}(p-p',q-q',\cos\theta)\end{aligned}$$

$\longrightarrow$ allows to perform all except for 3 integrals analytically

- only a few small discrete internal sums need to be performed for each external momentum and angular momentum

KH, Phys. Rept. 890, 1 (2021)

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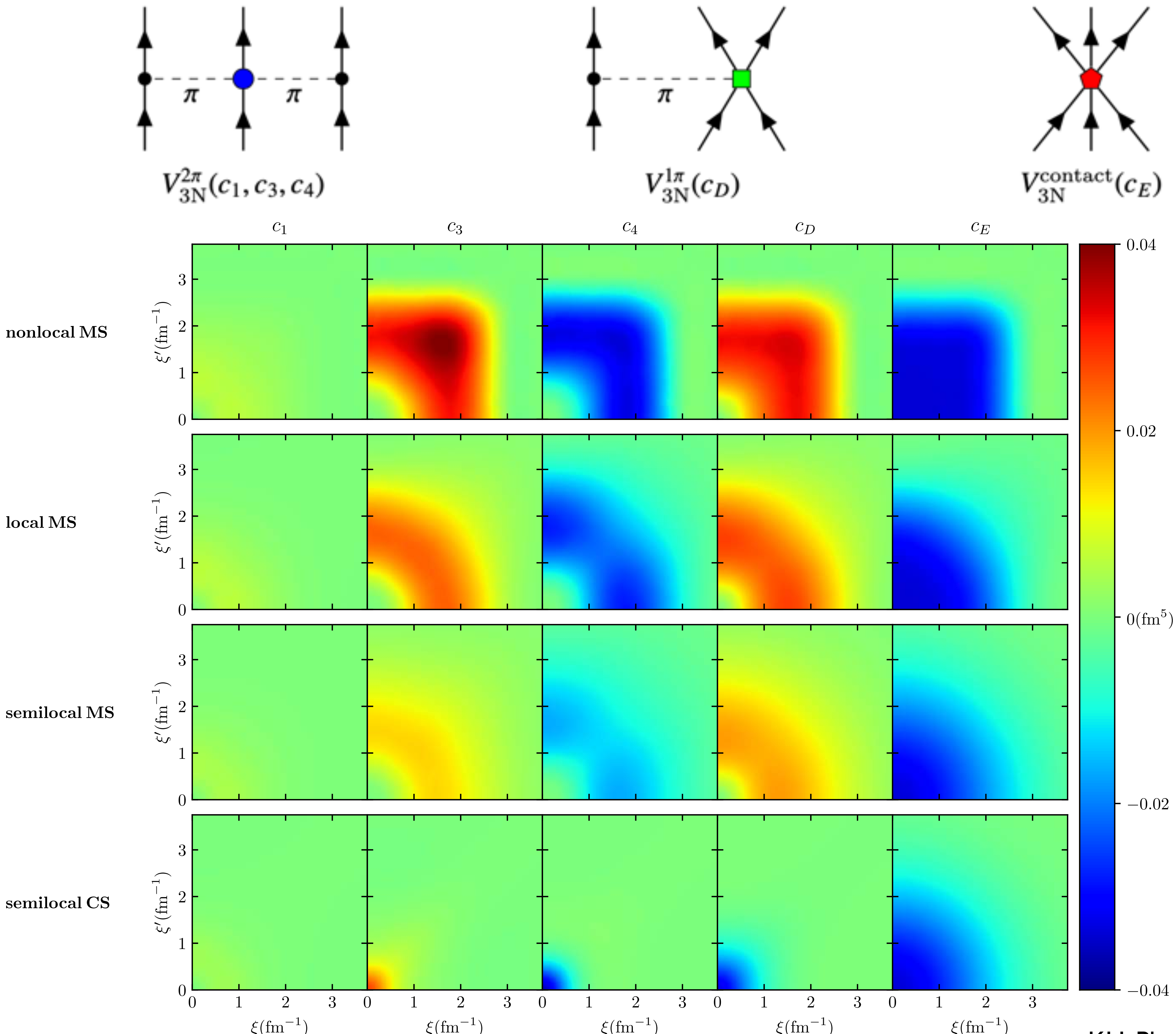

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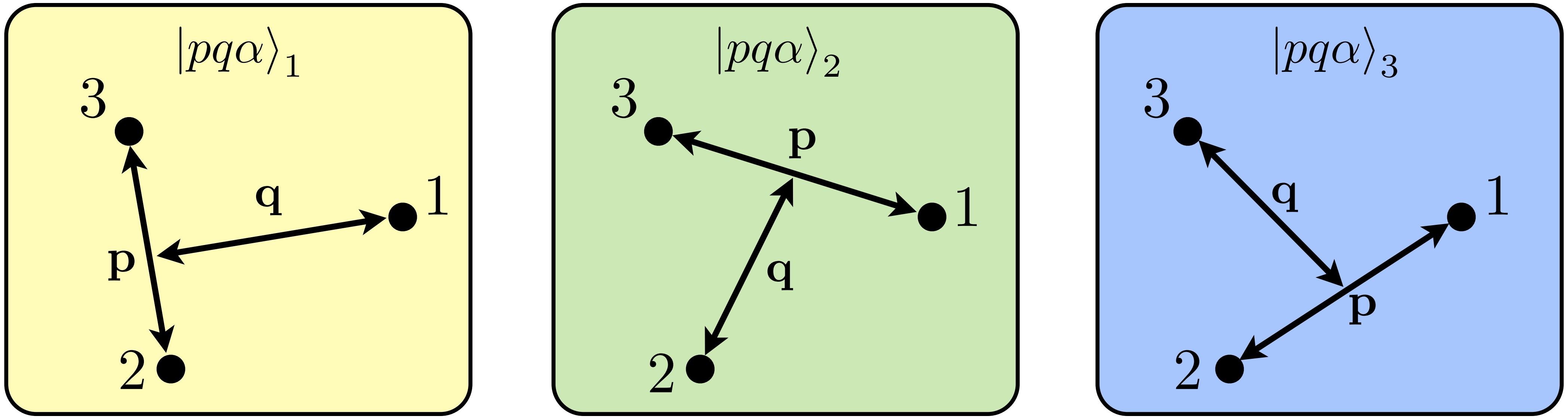
RG evolution of 3N interactions in momentum space



- represent interaction in basis $|pq\alpha\rangle_i \equiv |p_i q_i; [(LS)J(ls_i)j]\,\mathcal{J}\mathcal{J}_z(Tt_i)\mathcal{T}\mathcal{T}_z\rangle$
- explicit equations for NN and 3N flow equations

$$\frac{dV_{ij}}{ds} = [[T_{ij}, V_{ij}], T_{ij} + V_{ij}],$$

$$\begin{aligned}\frac{dV_{123}}{ds} &= [[T_{12}, V_{12}], V_{13} + V_{23} + V_{123}] \\ &+ [[T_{13}, V_{13}], V_{12} + V_{23} + V_{123}] \\ &+ [[T_{23}, V_{23}], V_{12} + V_{13} + V_{123}] \\ &+ [[T_{\rm rel}, V_{123}], H_s]\end{aligned}$$

Bogner, Furnstahl, Perry PRC 75, 061001(R) (2007)

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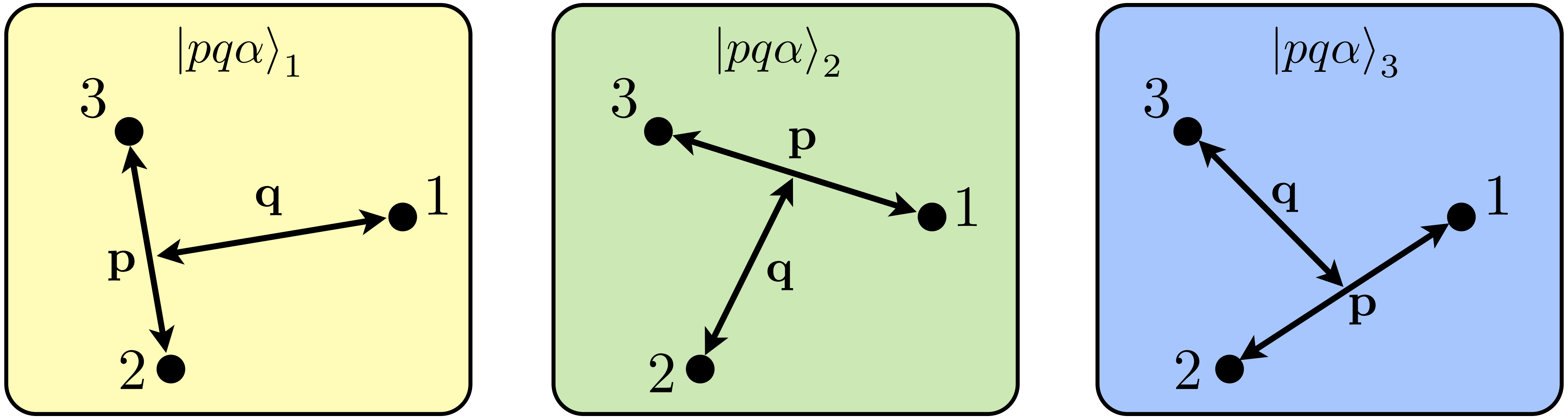

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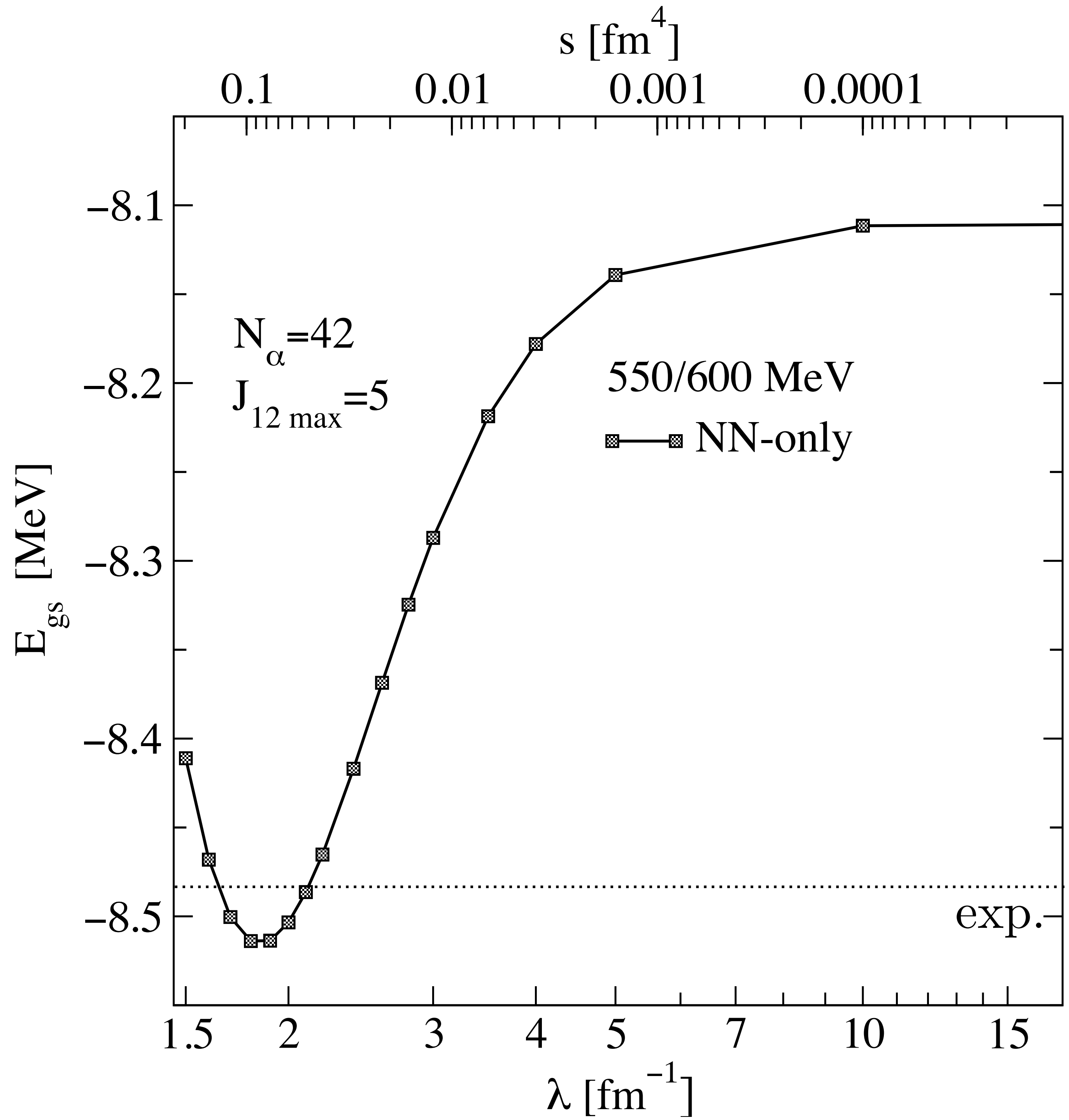
details in the SRG exercise session!

Bogner, Furnstahl, Perry PRC 75, 061001(R) (2007)

SRG evolution of 3N interactions in momentum space: Results for the Triton



KH PRC(R) 85, 021002 (2012)

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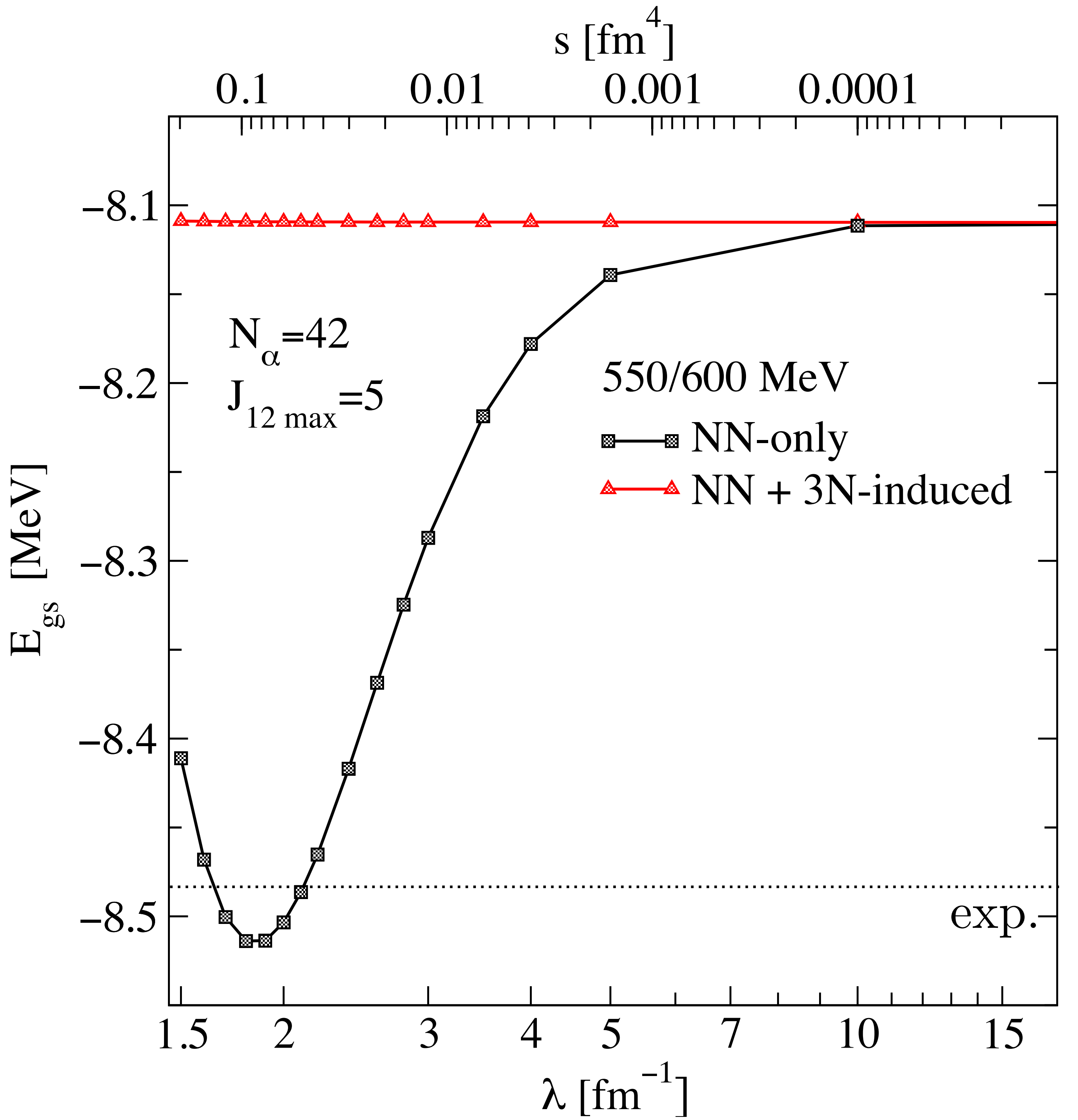

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It works:

Invariance of $E_{\rm gs}^{^3H}$ within $\leq 1\,\mathrm{eV}$ for consistent chiral interactions at $\mathrm{N^2LO}$

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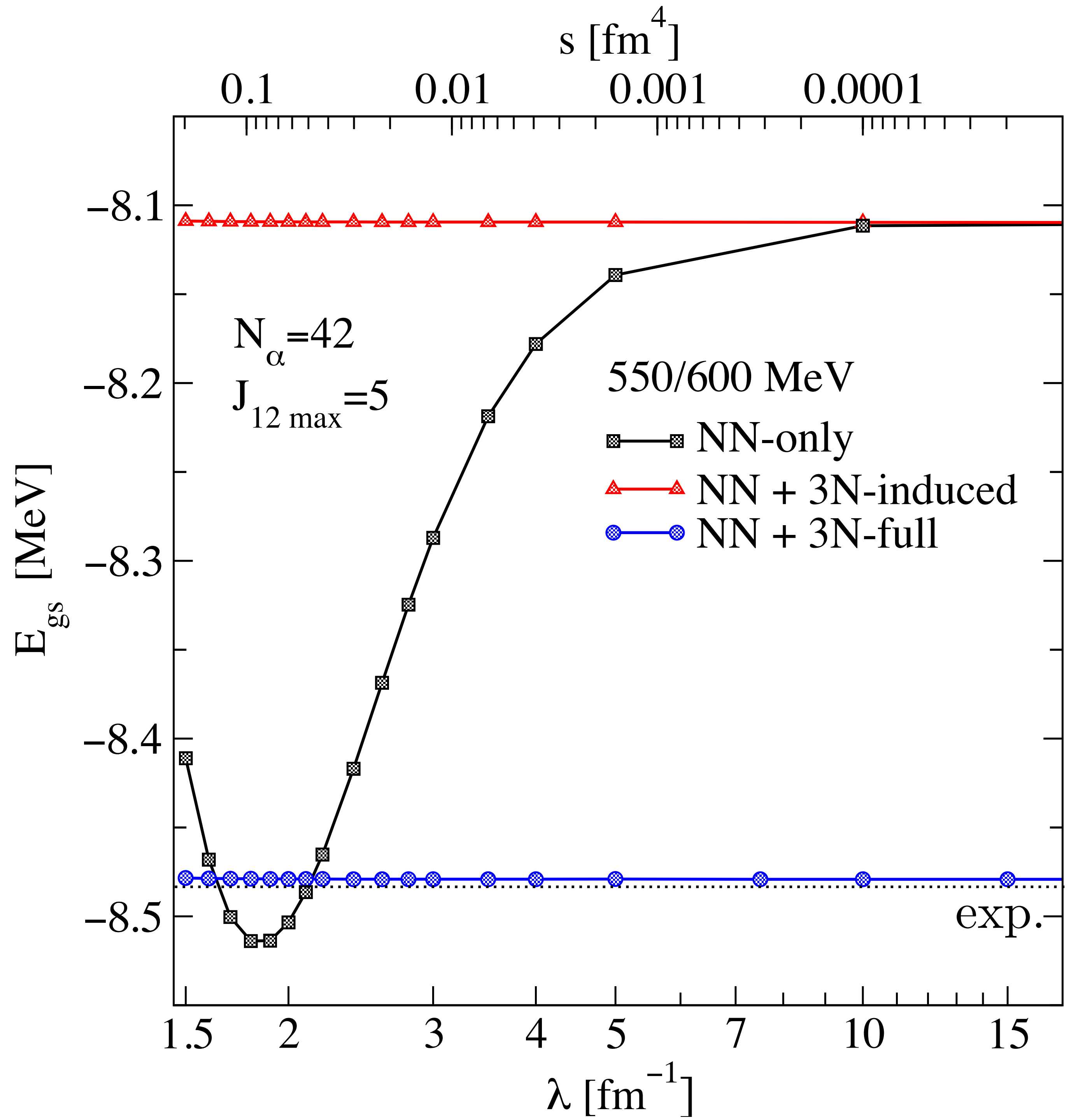

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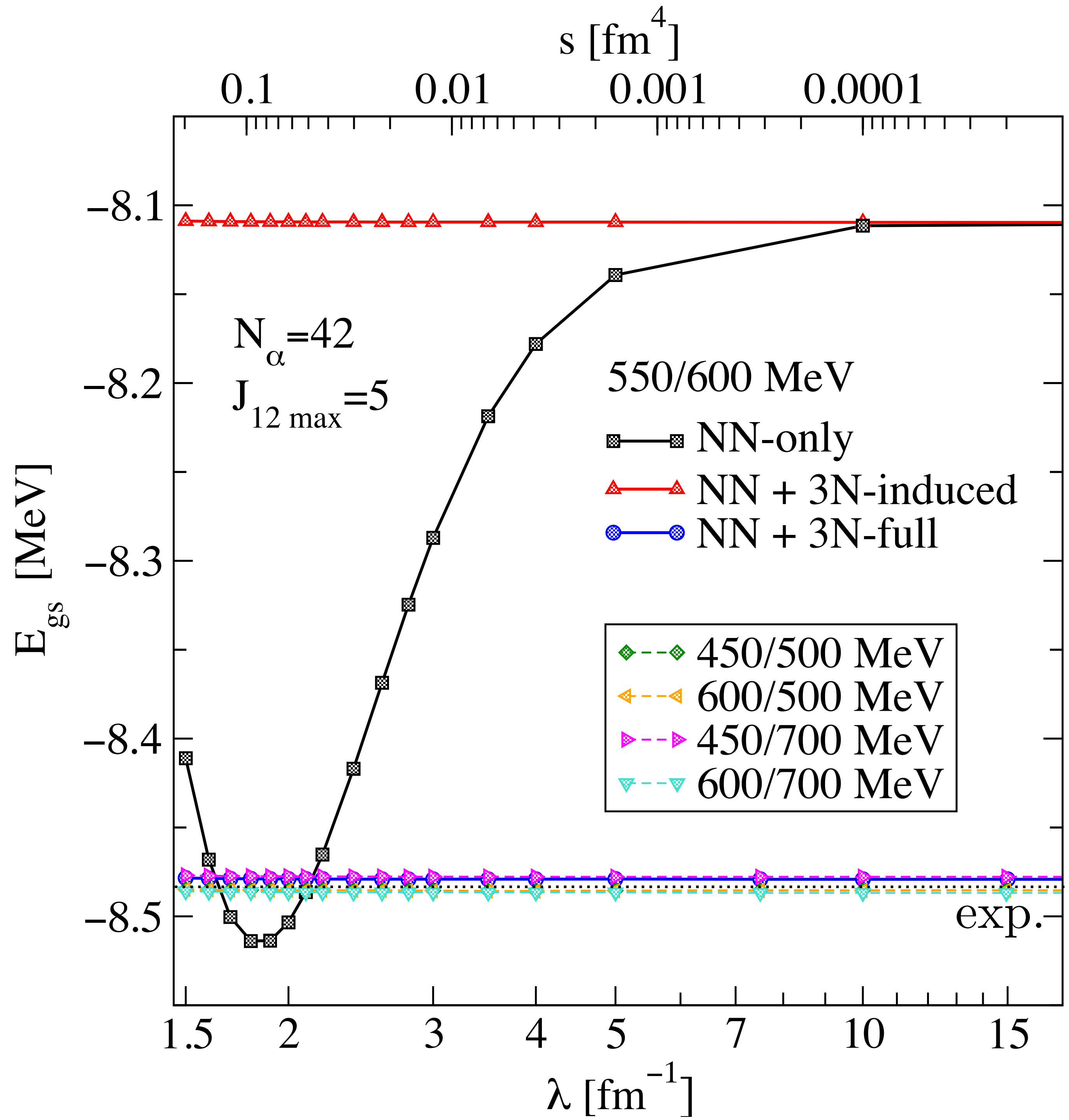

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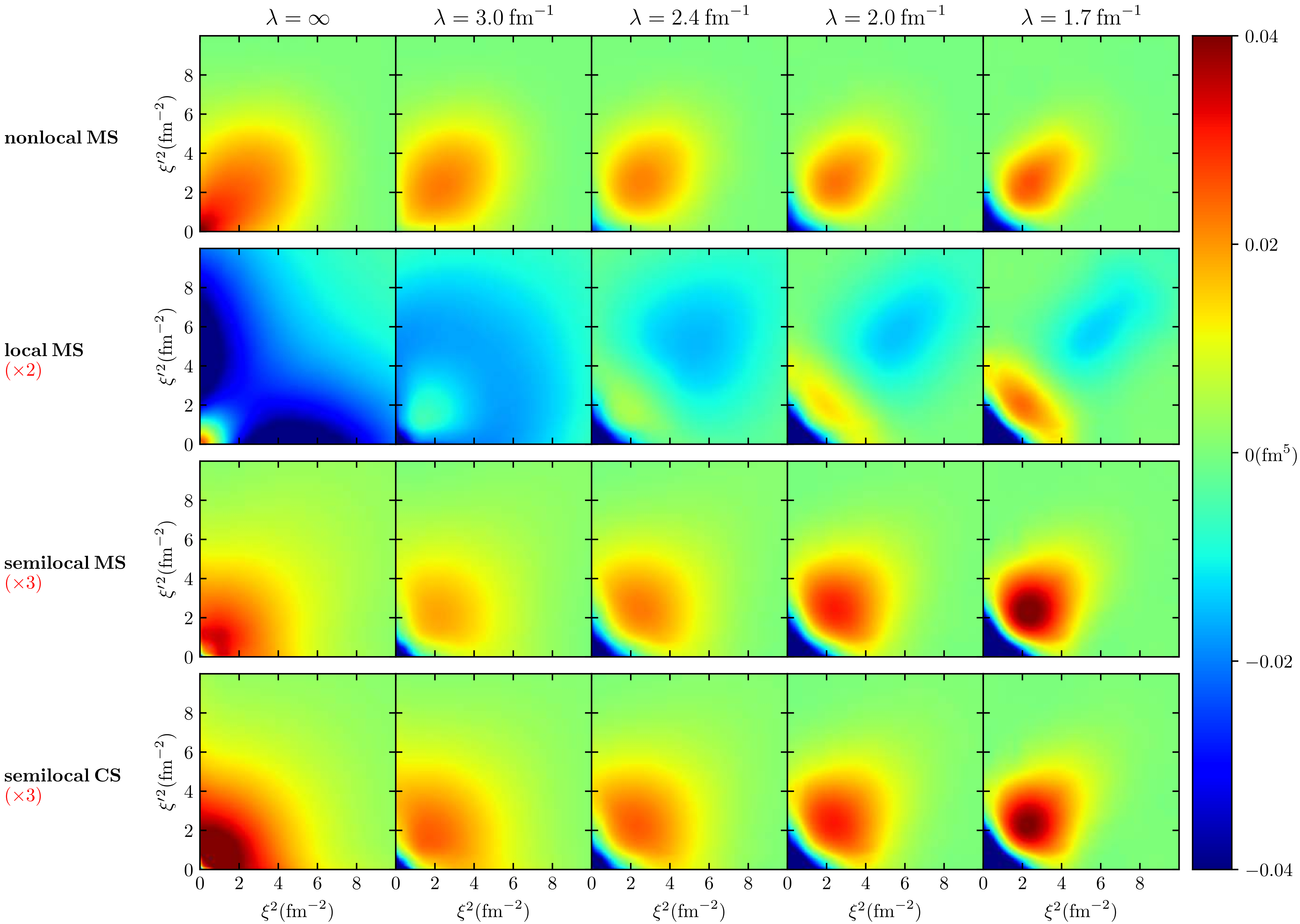

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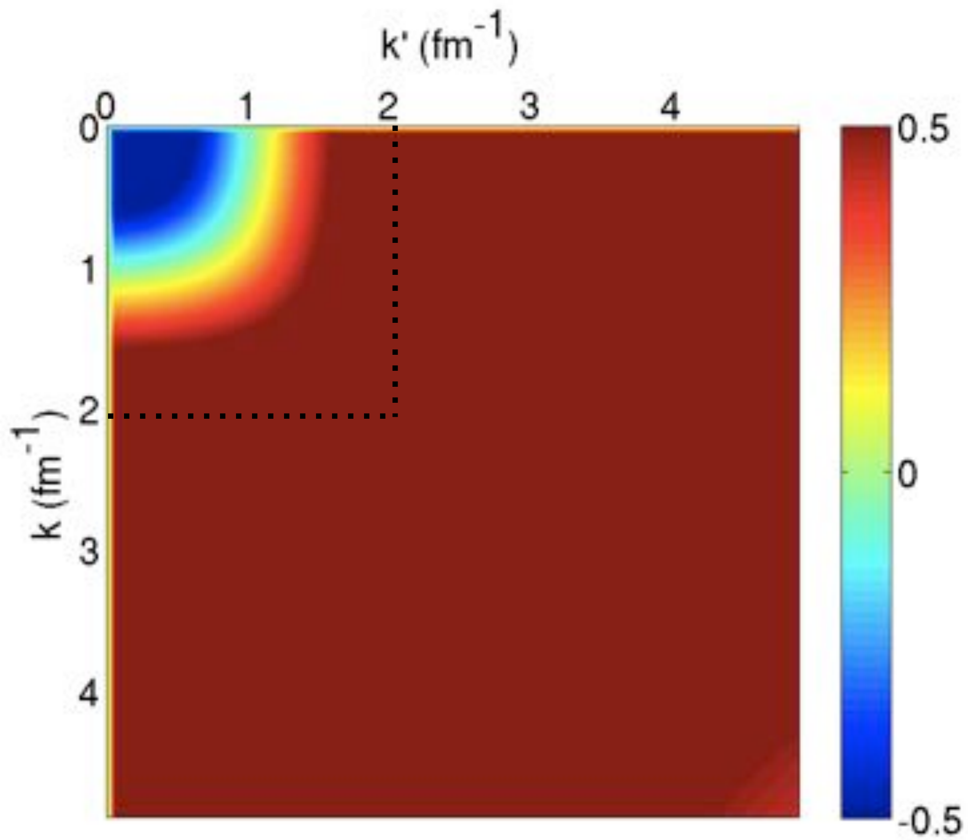
Systematically changing the resolution: the Similarity Renormalization Group



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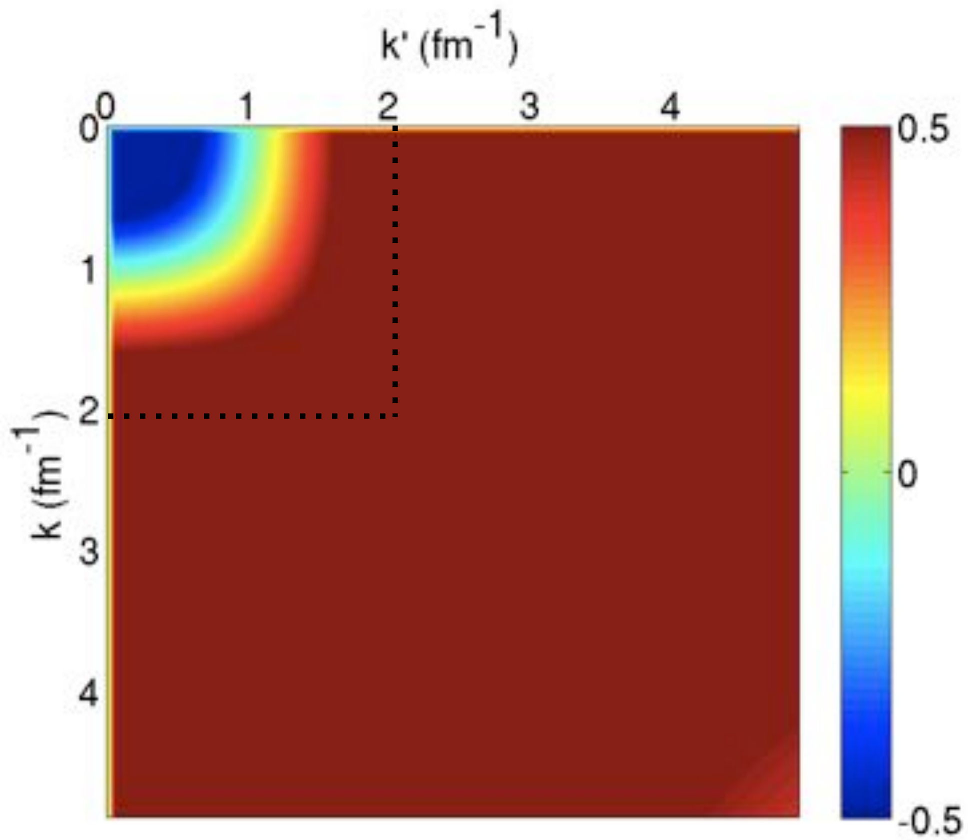

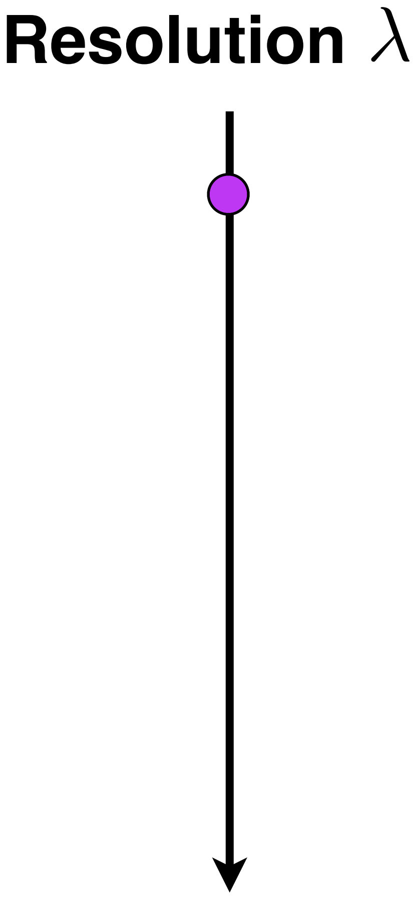

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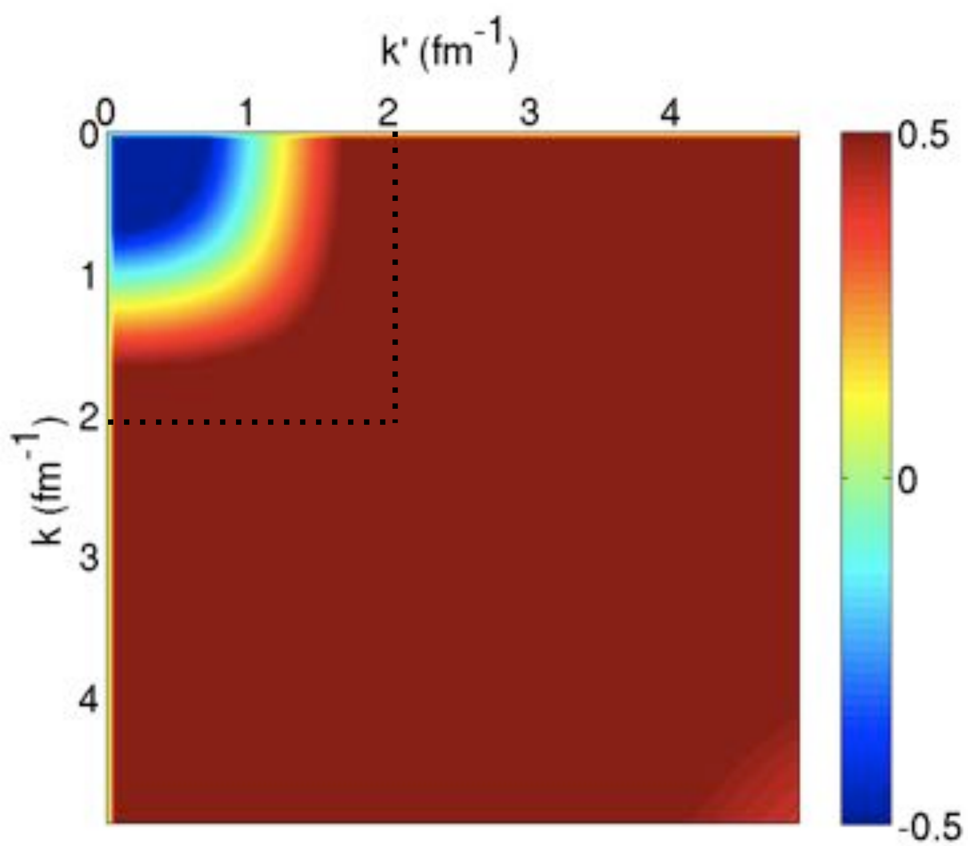

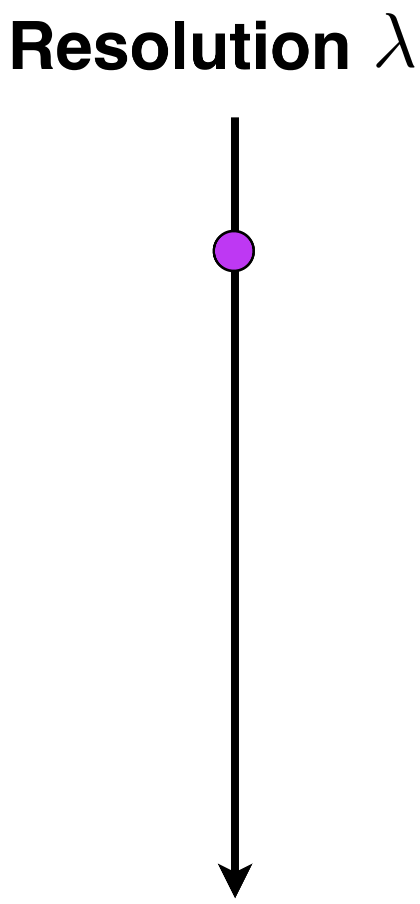

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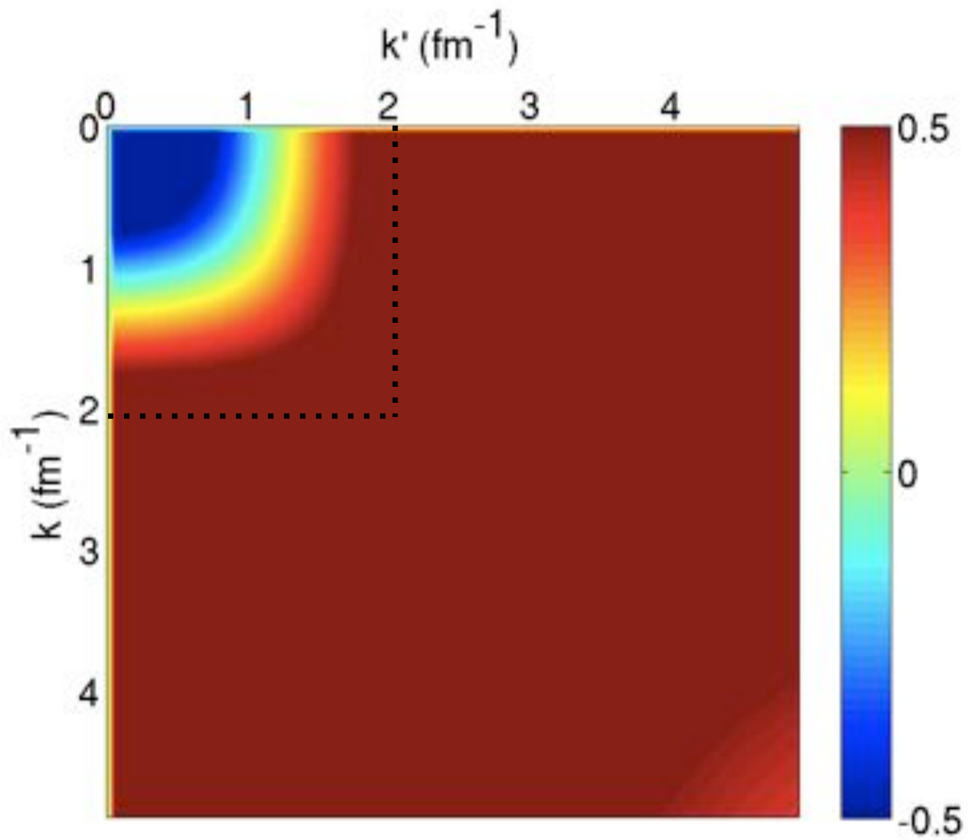

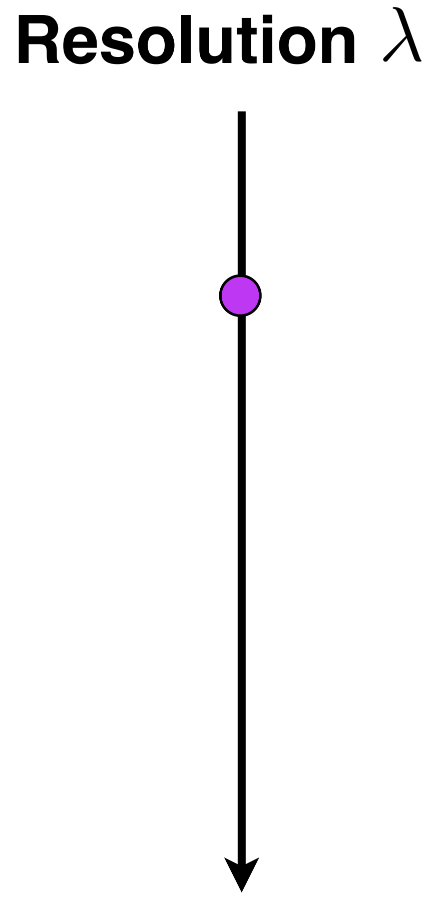

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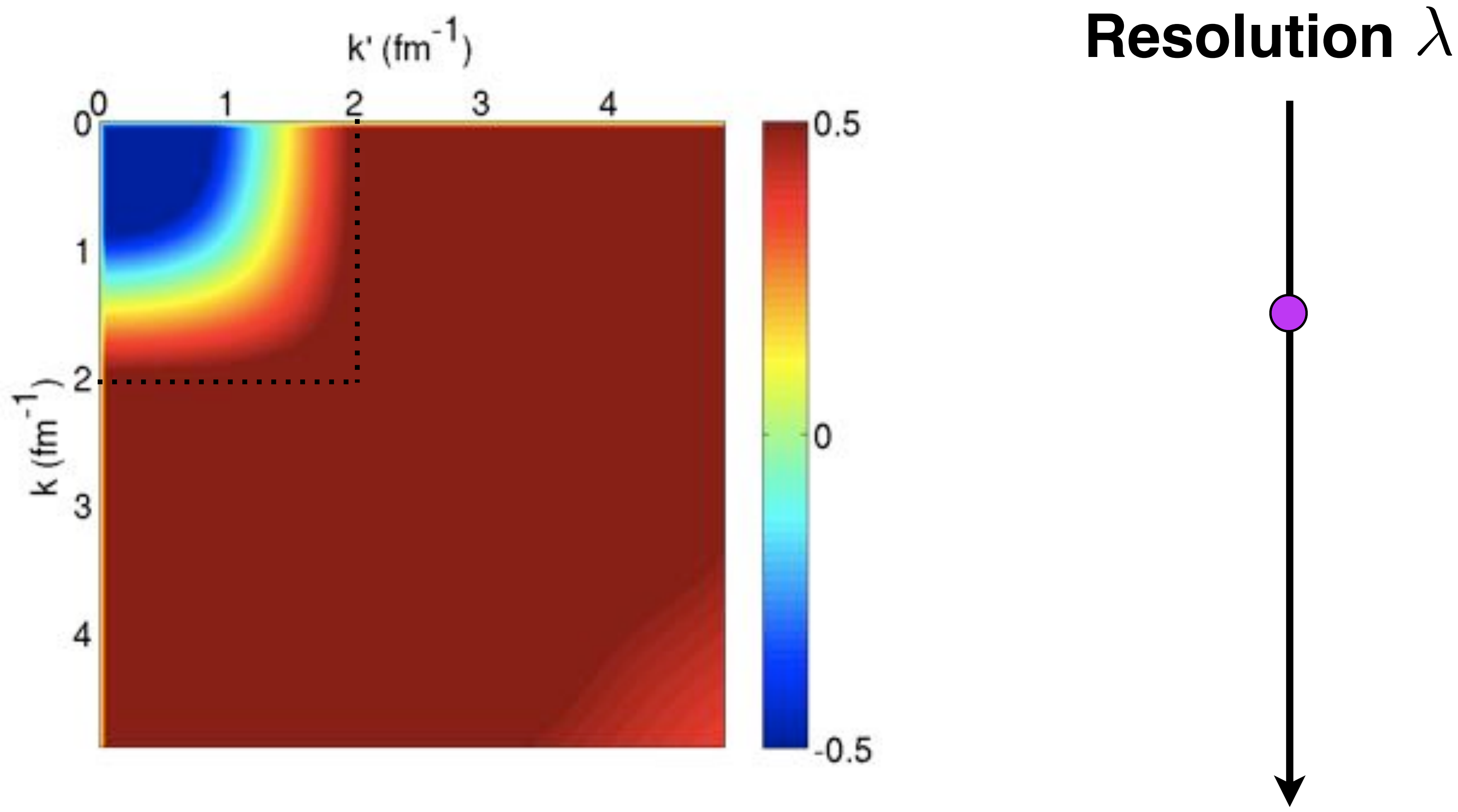

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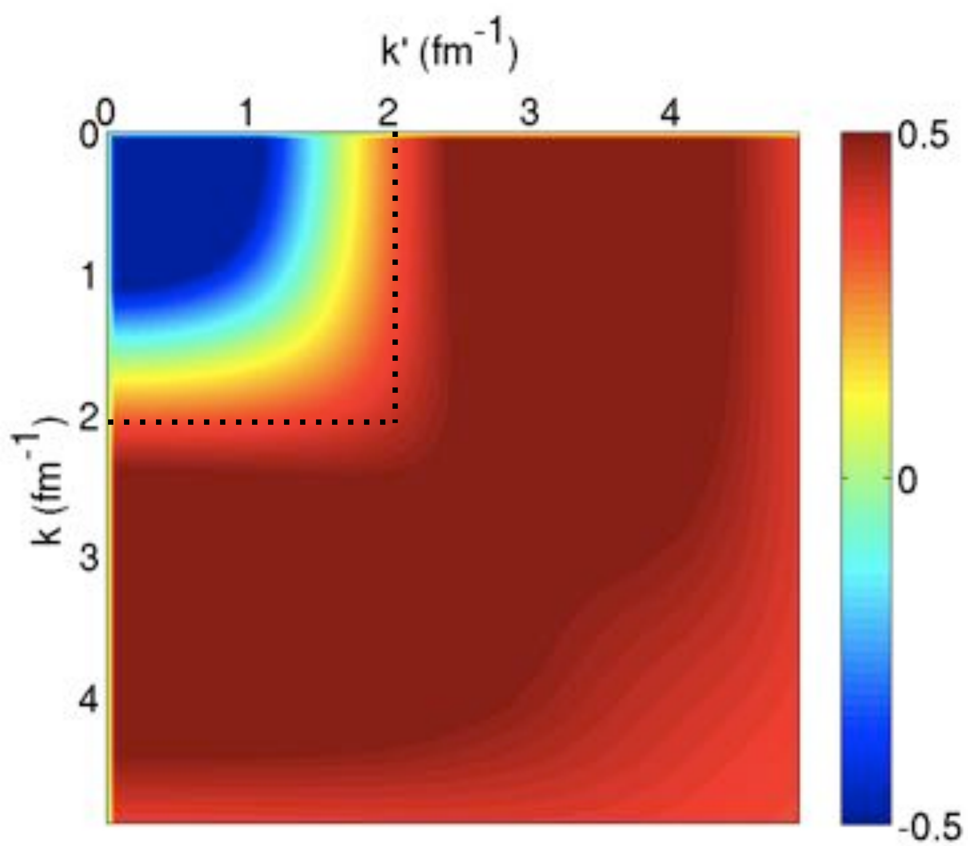

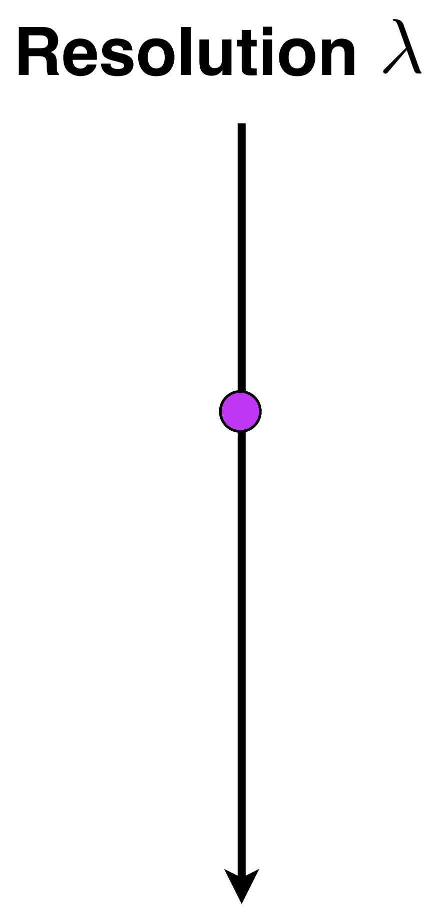

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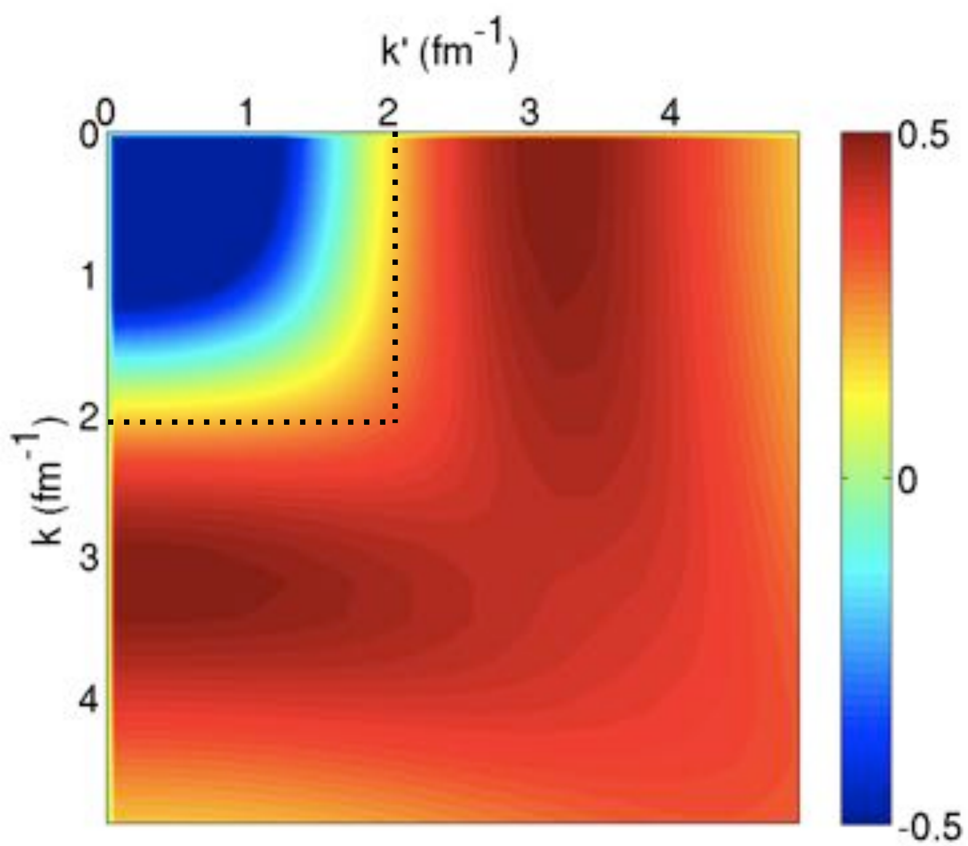

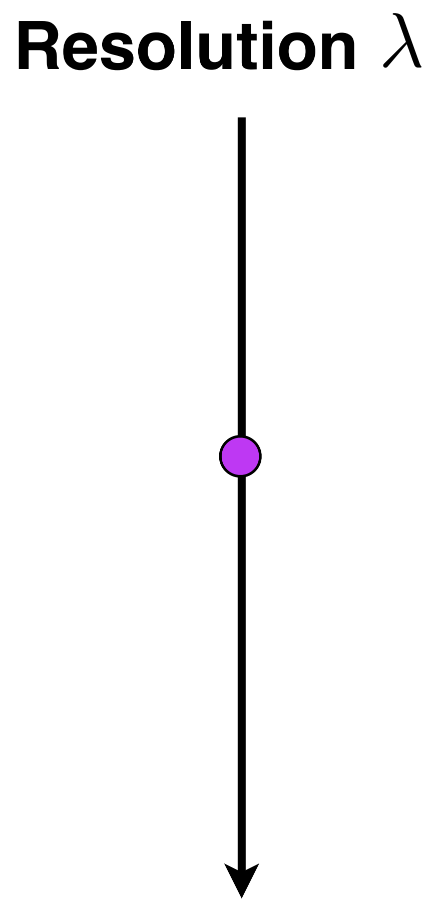

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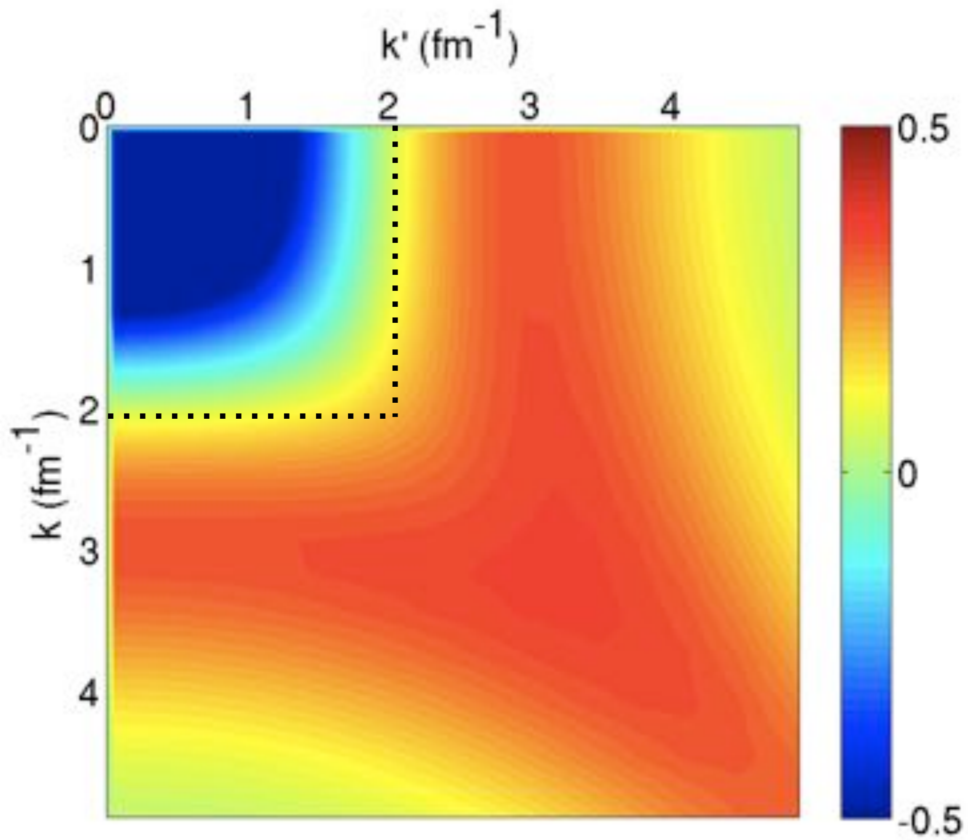

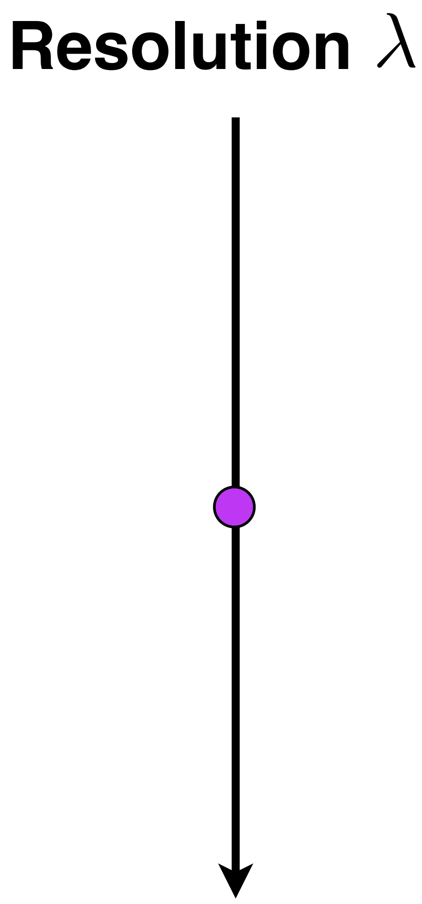

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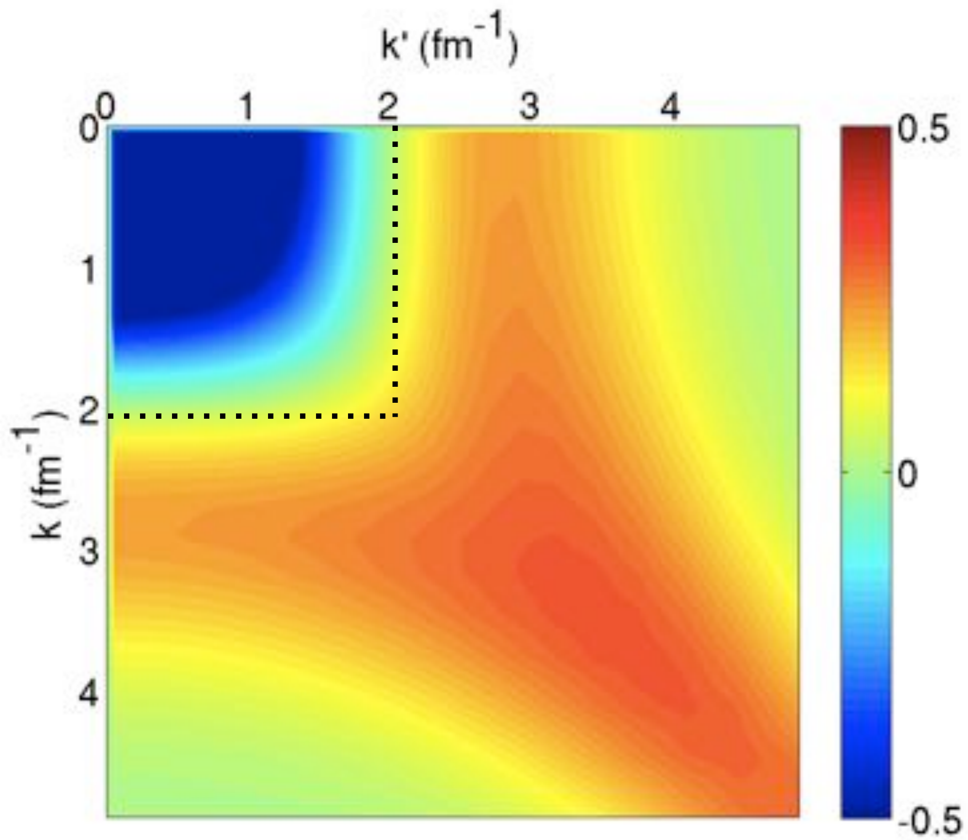

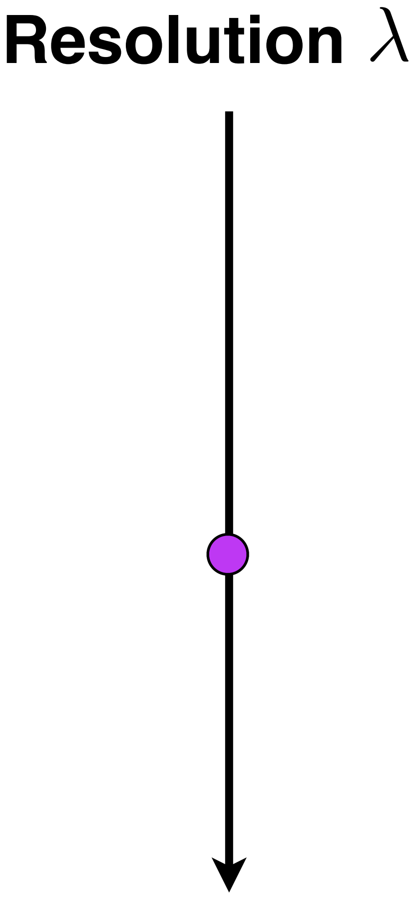

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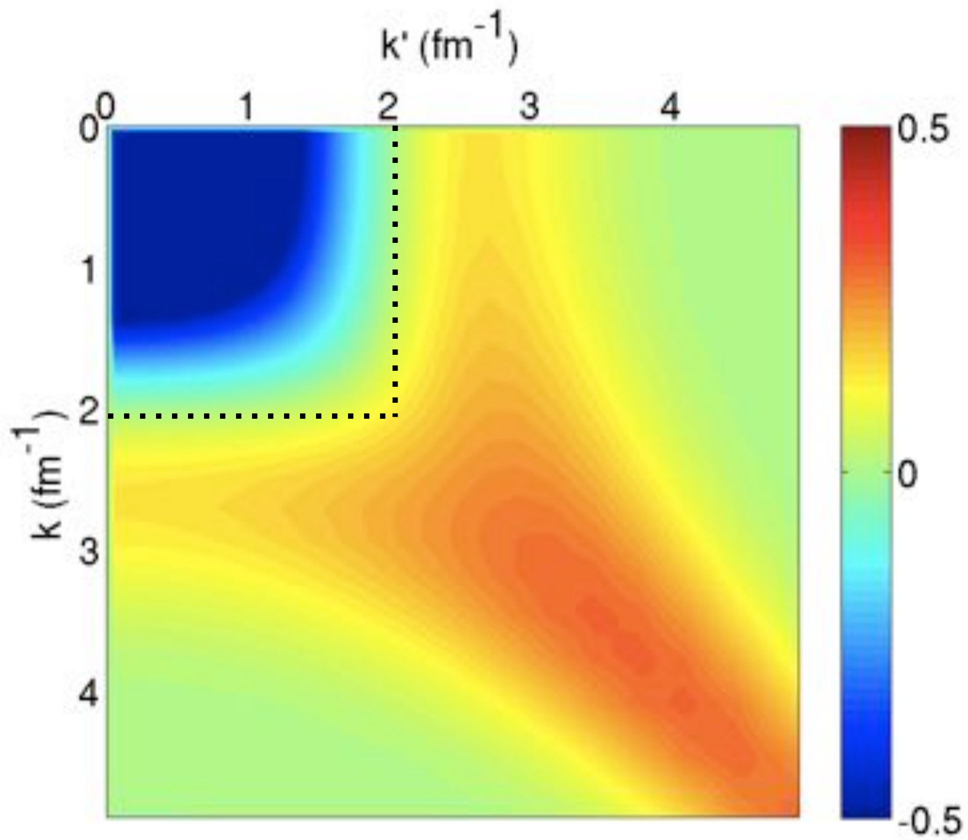

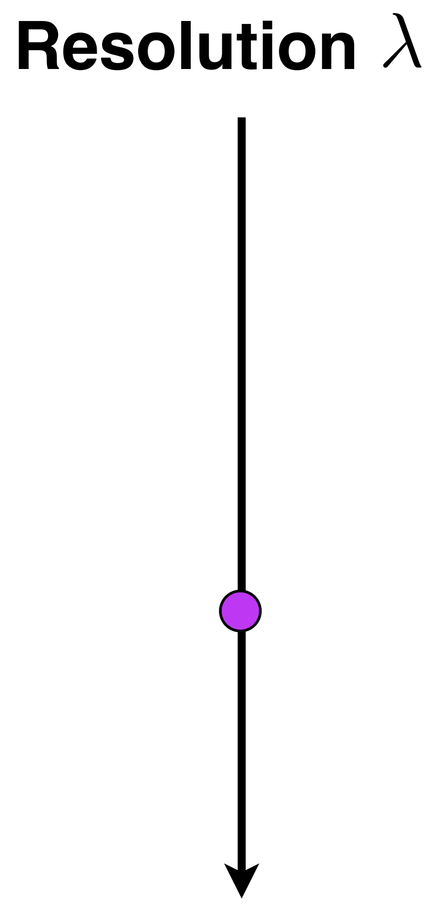

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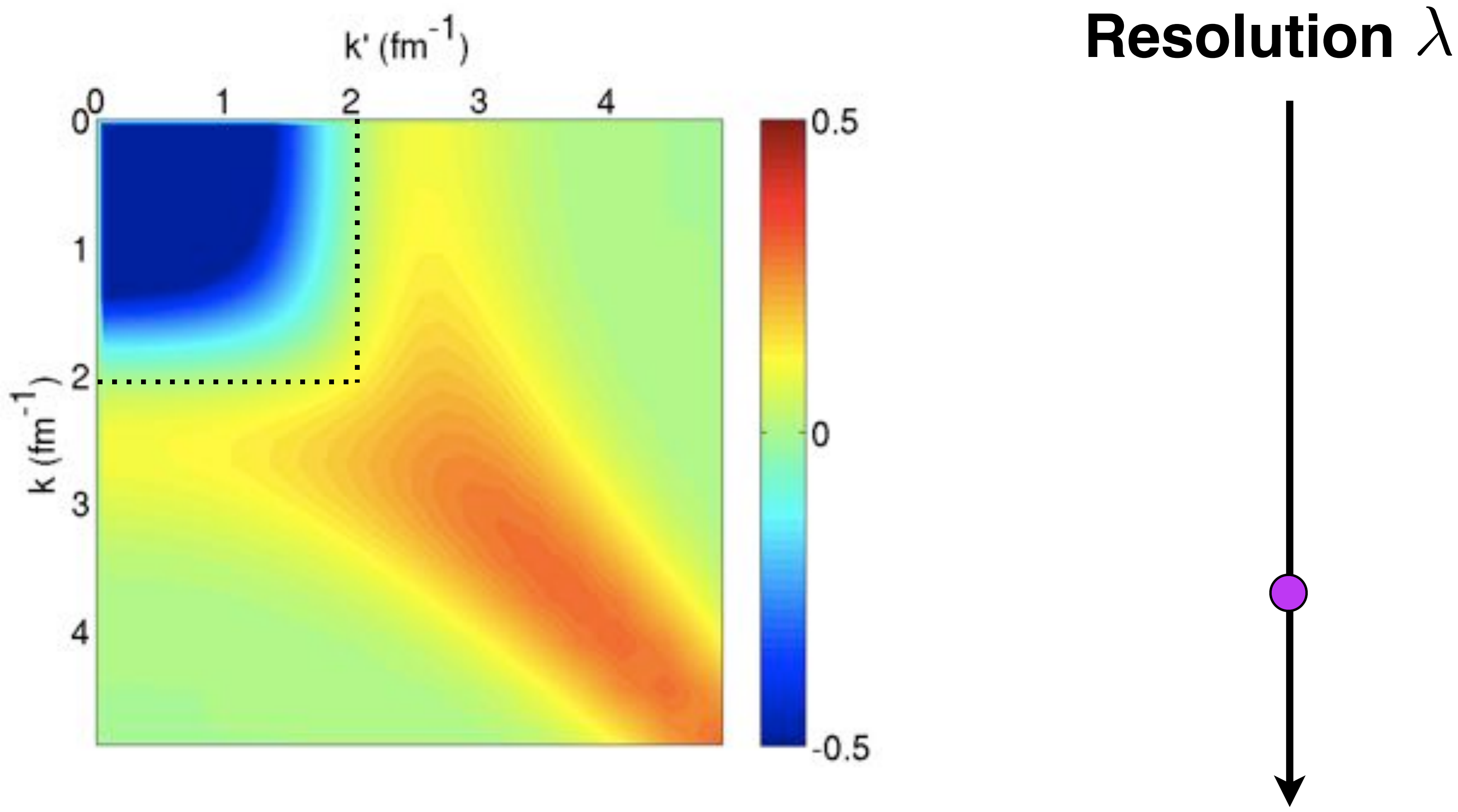

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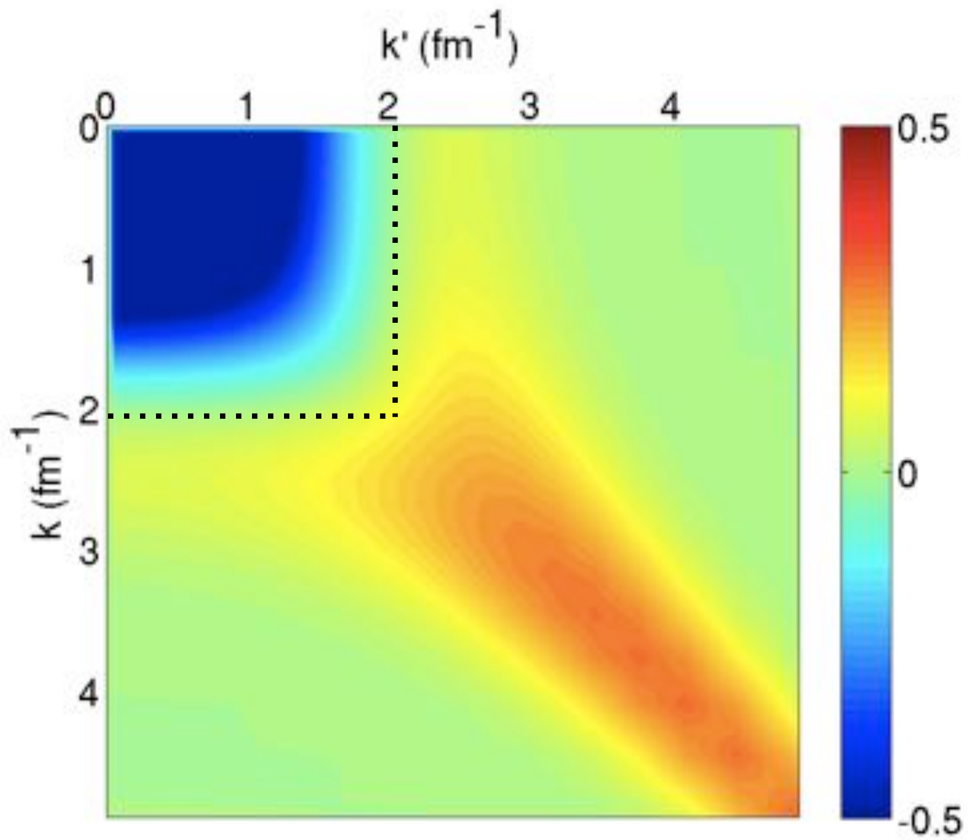

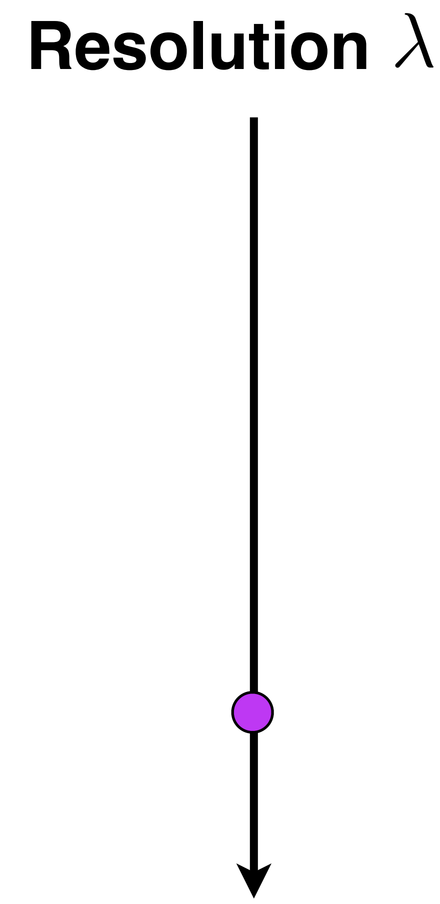

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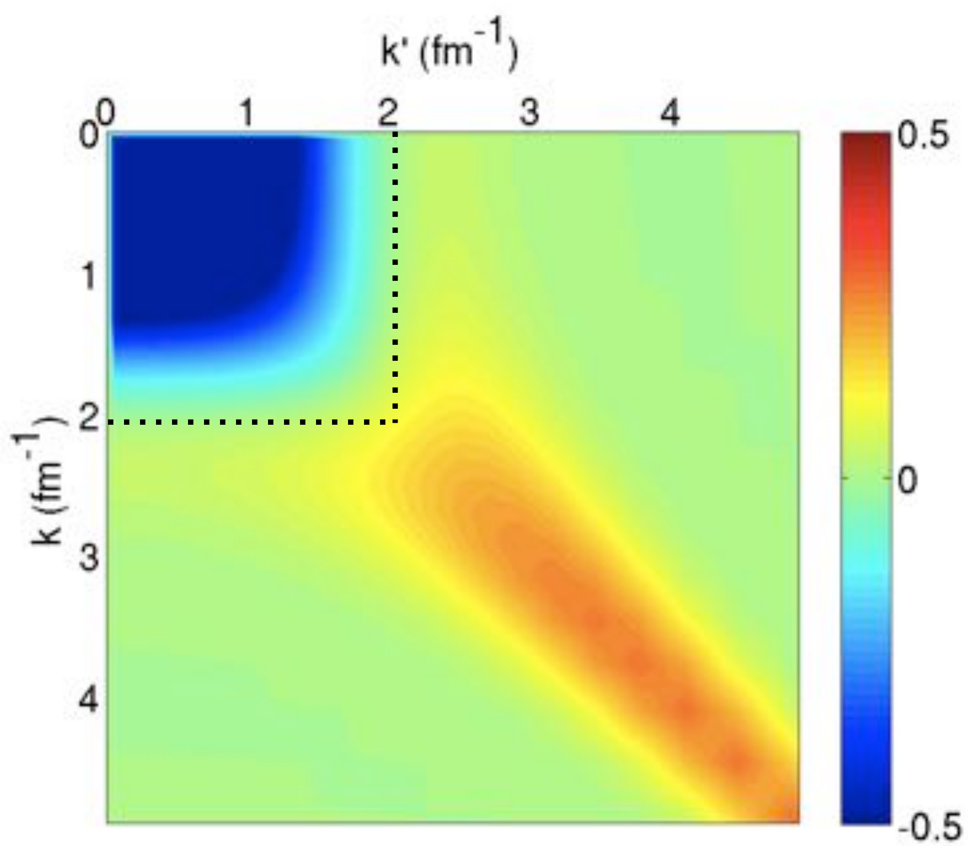
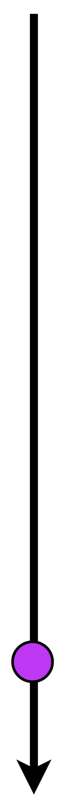


Resolution λ



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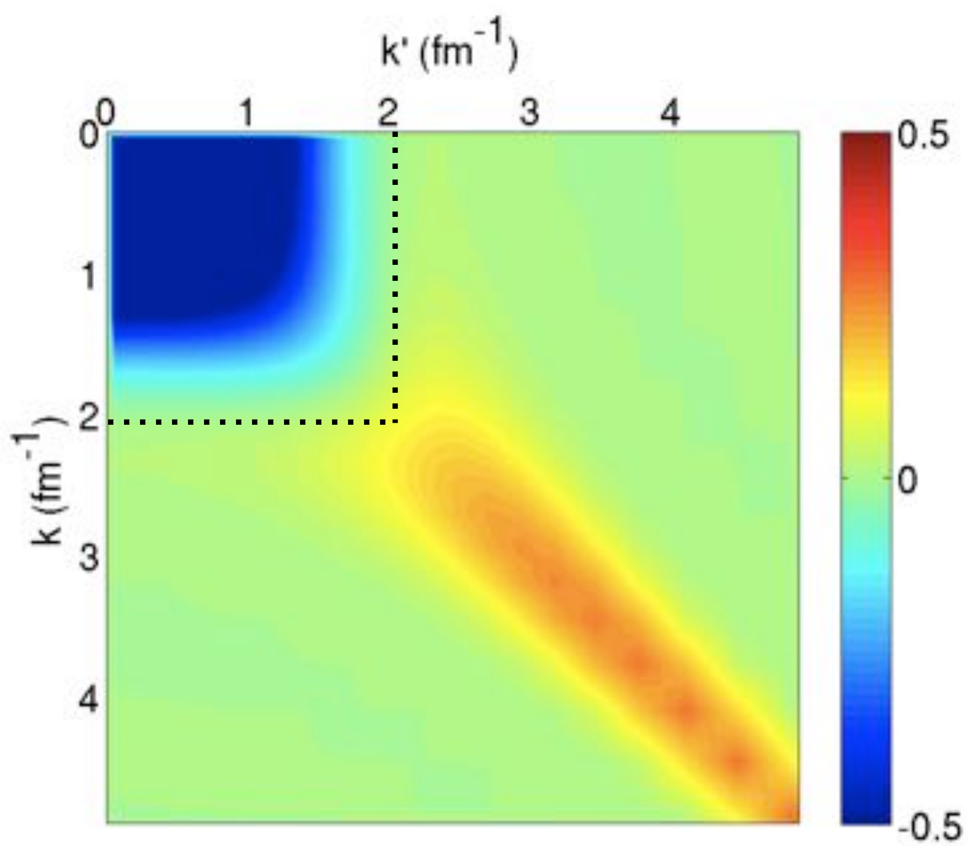
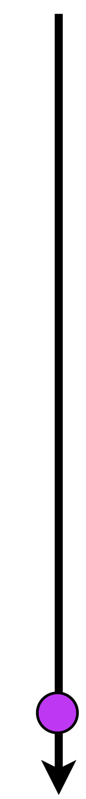
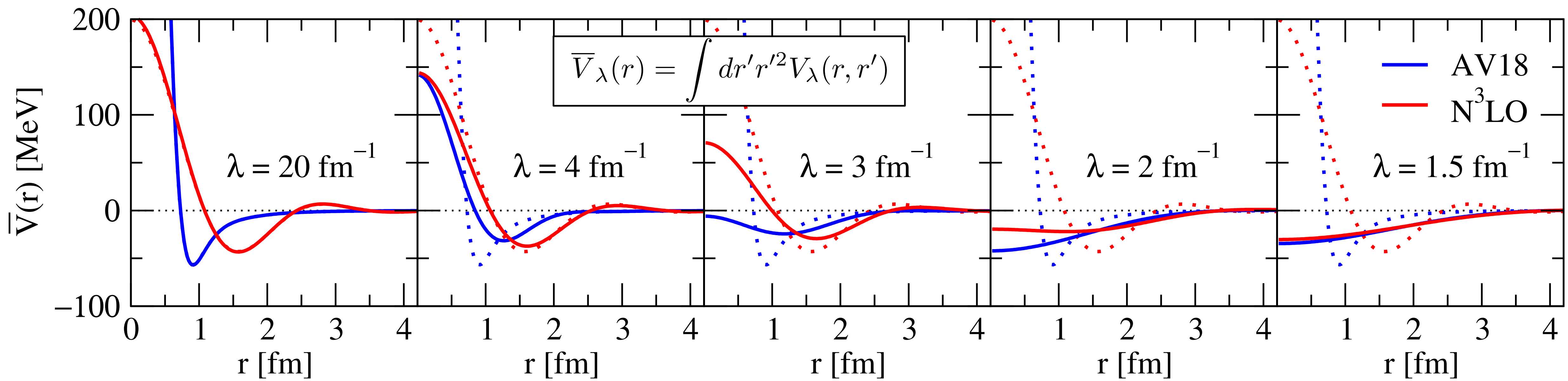
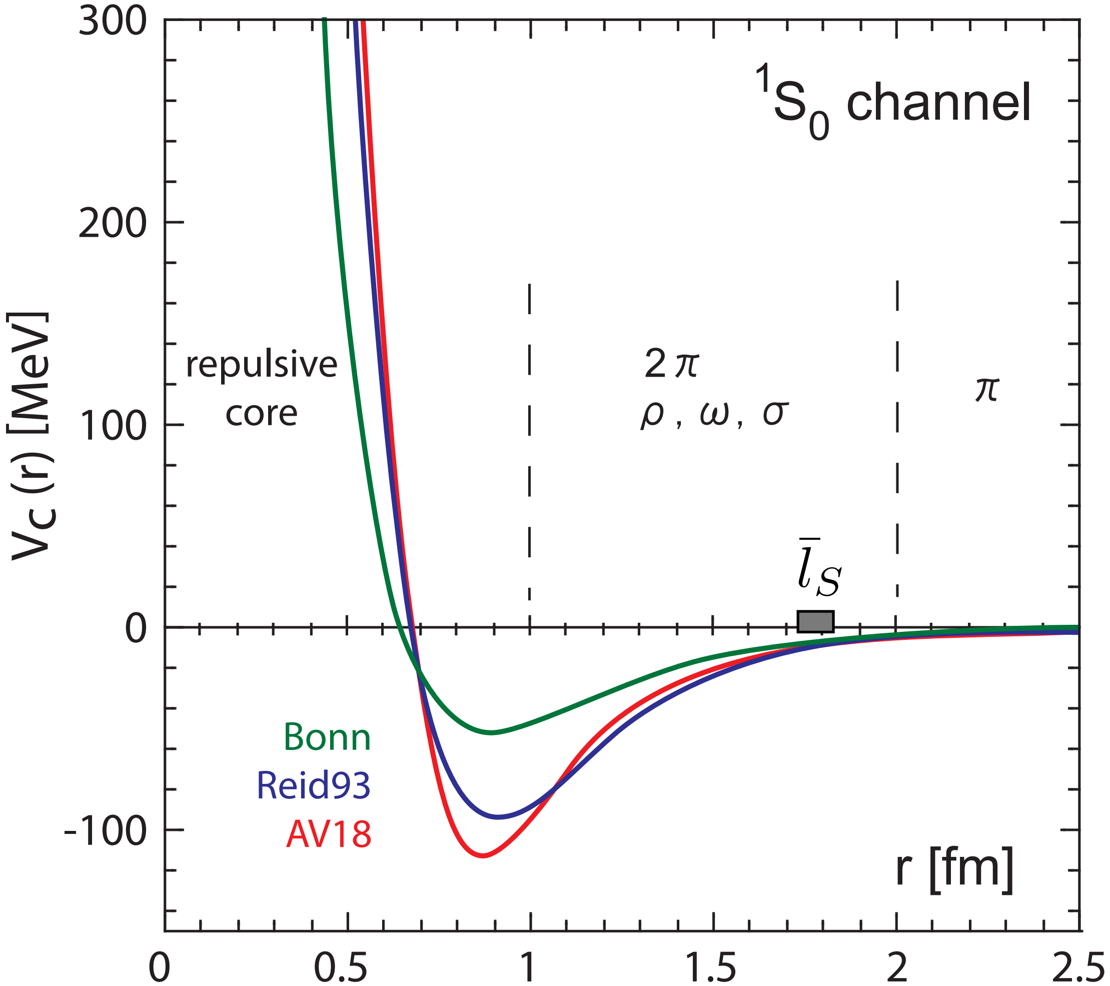




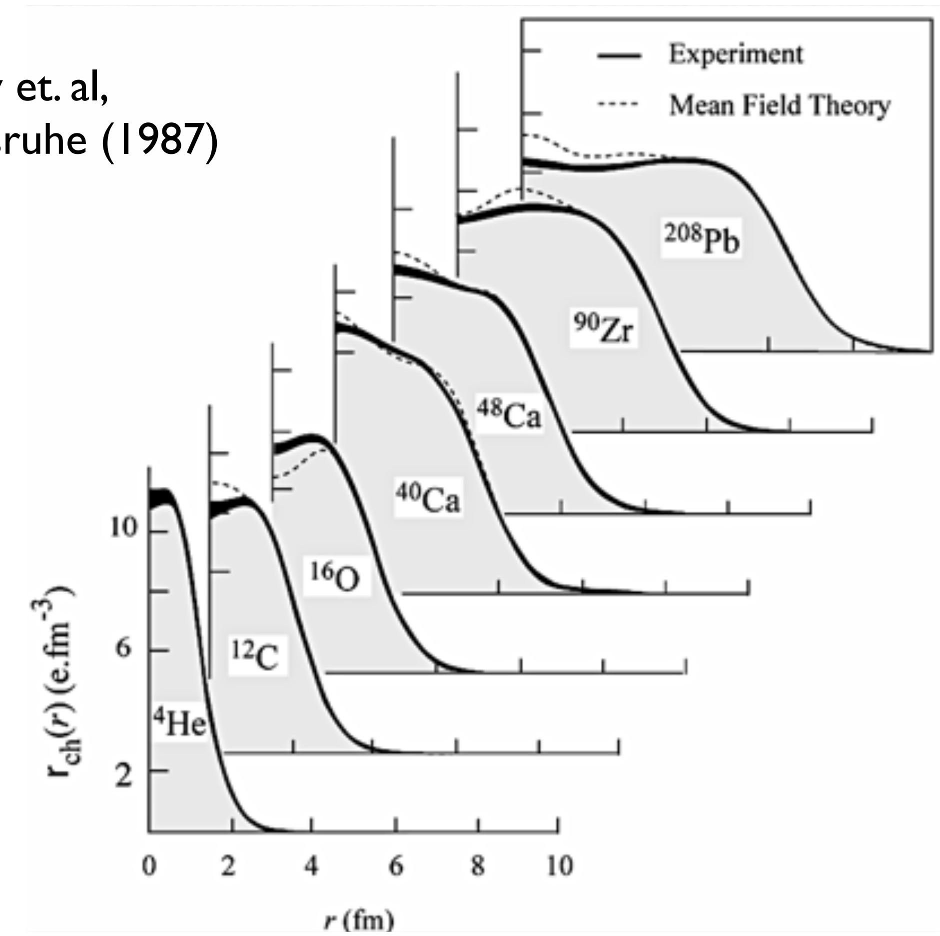


Wendt et al., PRC 86, 014003 (2012)

Equation of state of symmetric nuclear matter, nuclear saturation



Batty et. al, Karlsruhe (1987)



KH, Bogner, Furnstahl, Nogga, PRC(R) 83, 031301 (2011)

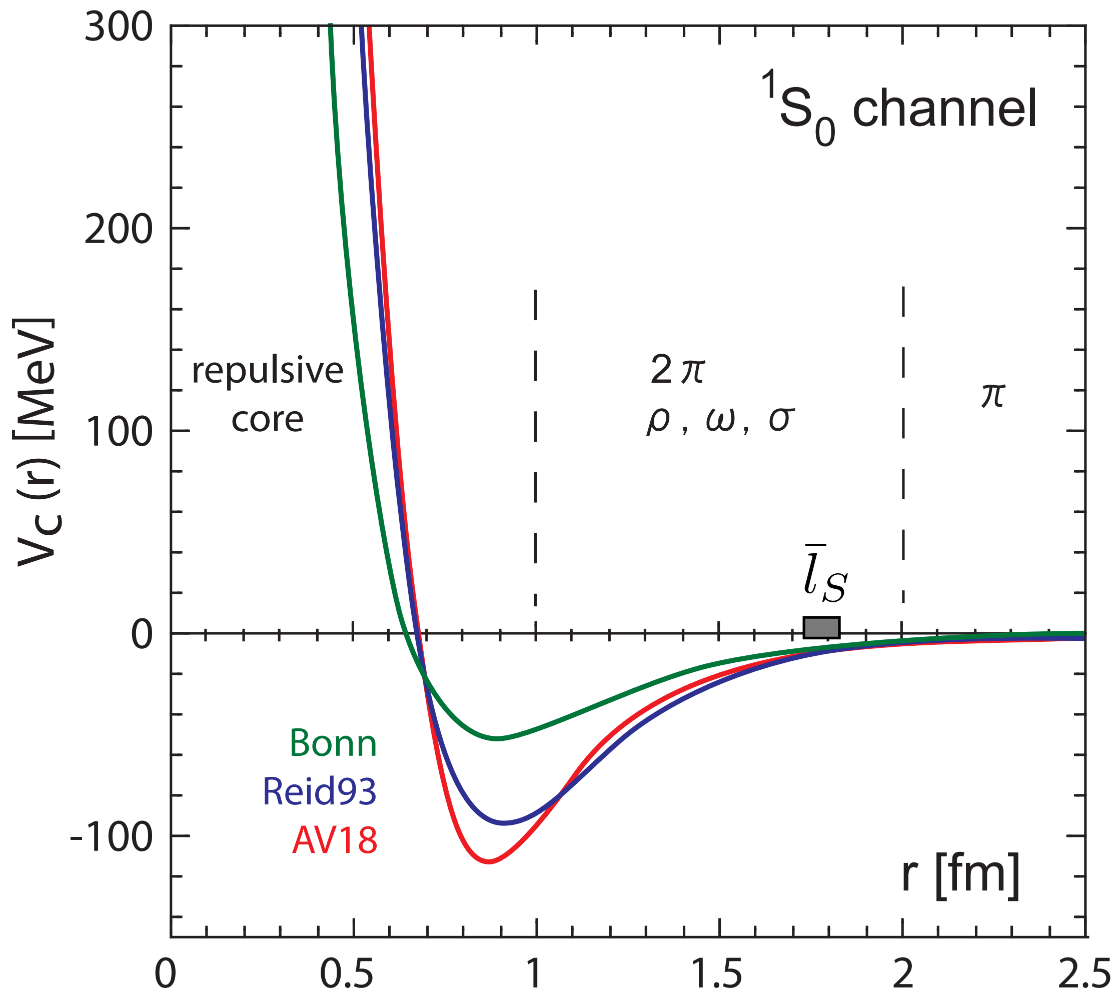
empirical nuclear saturation properties

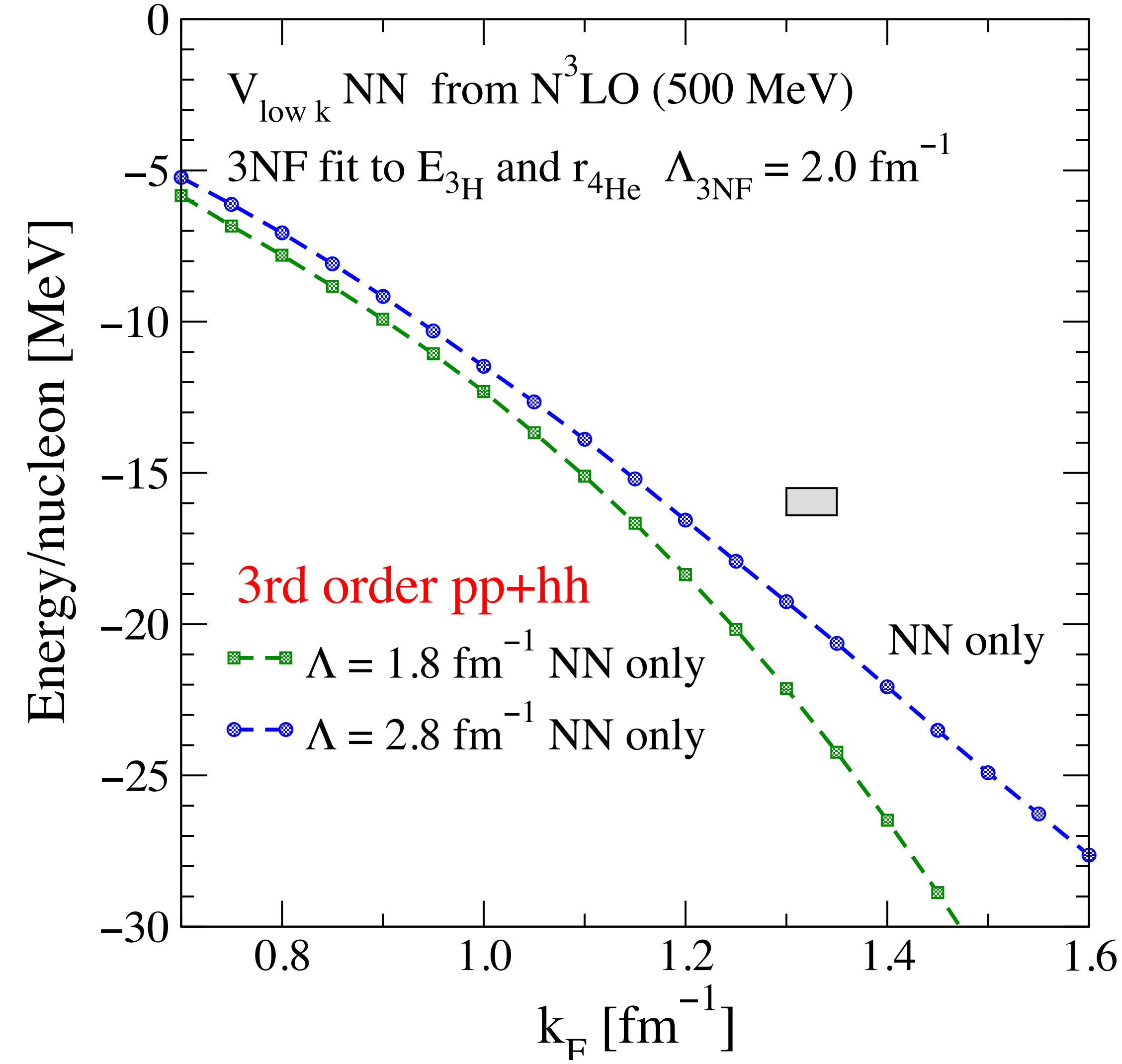
$$n_S \sim 0.16\,\mathrm{fm}^{-3}$$

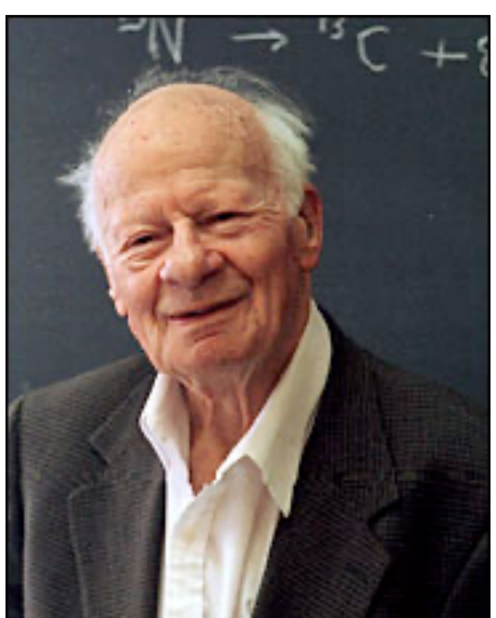
$$E_{\mathrm{binding}}/N \sim -16\,\mathrm{MeV}$$

$$\bar{l}_S \sim 1.8\,\mathrm{fm}$$

Equation of state of symmetric nuclear matter, nuclear saturation

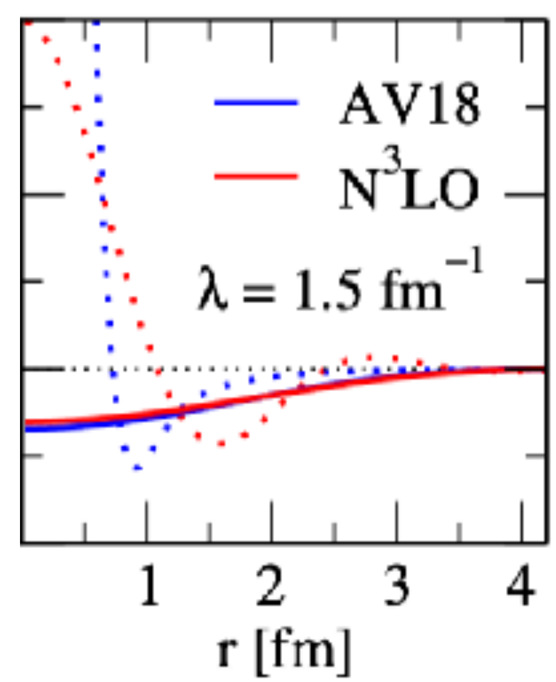




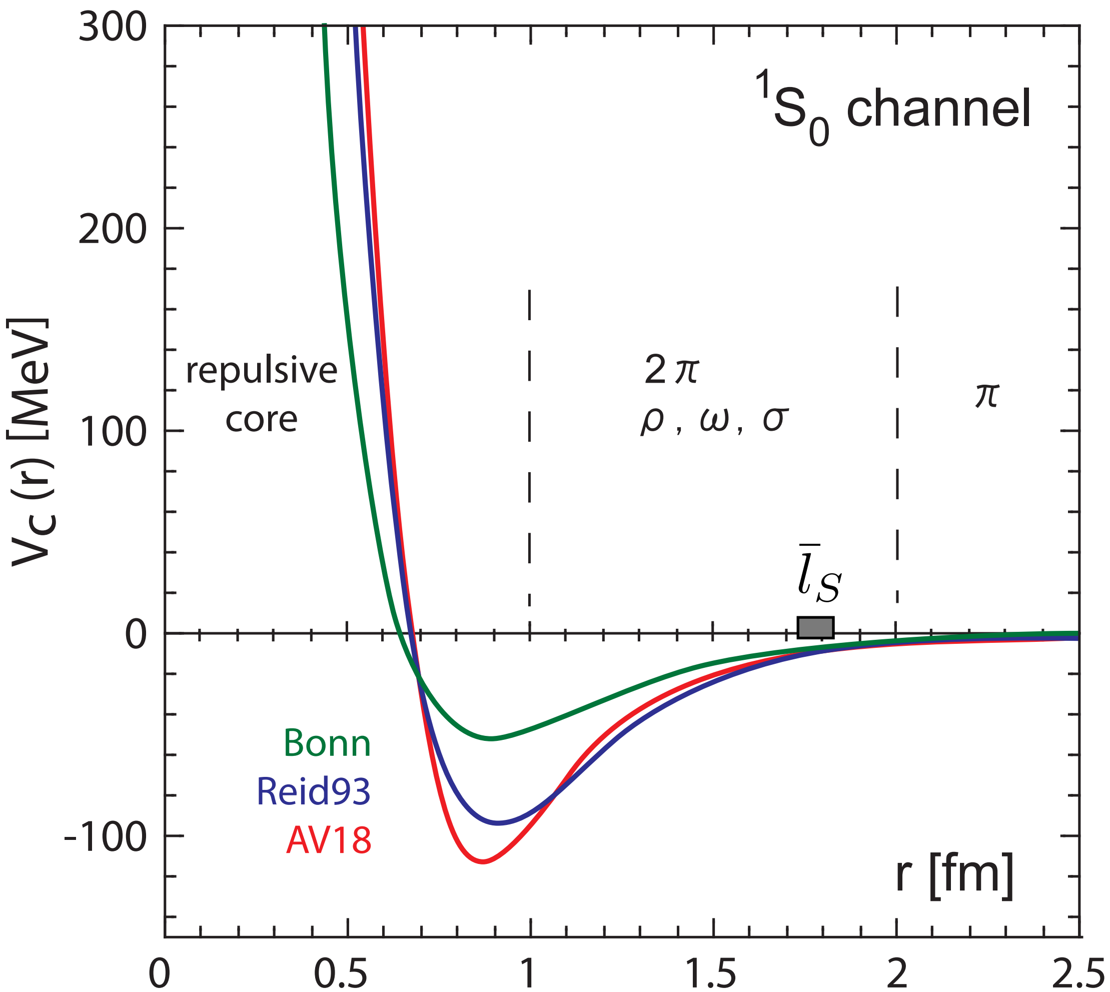


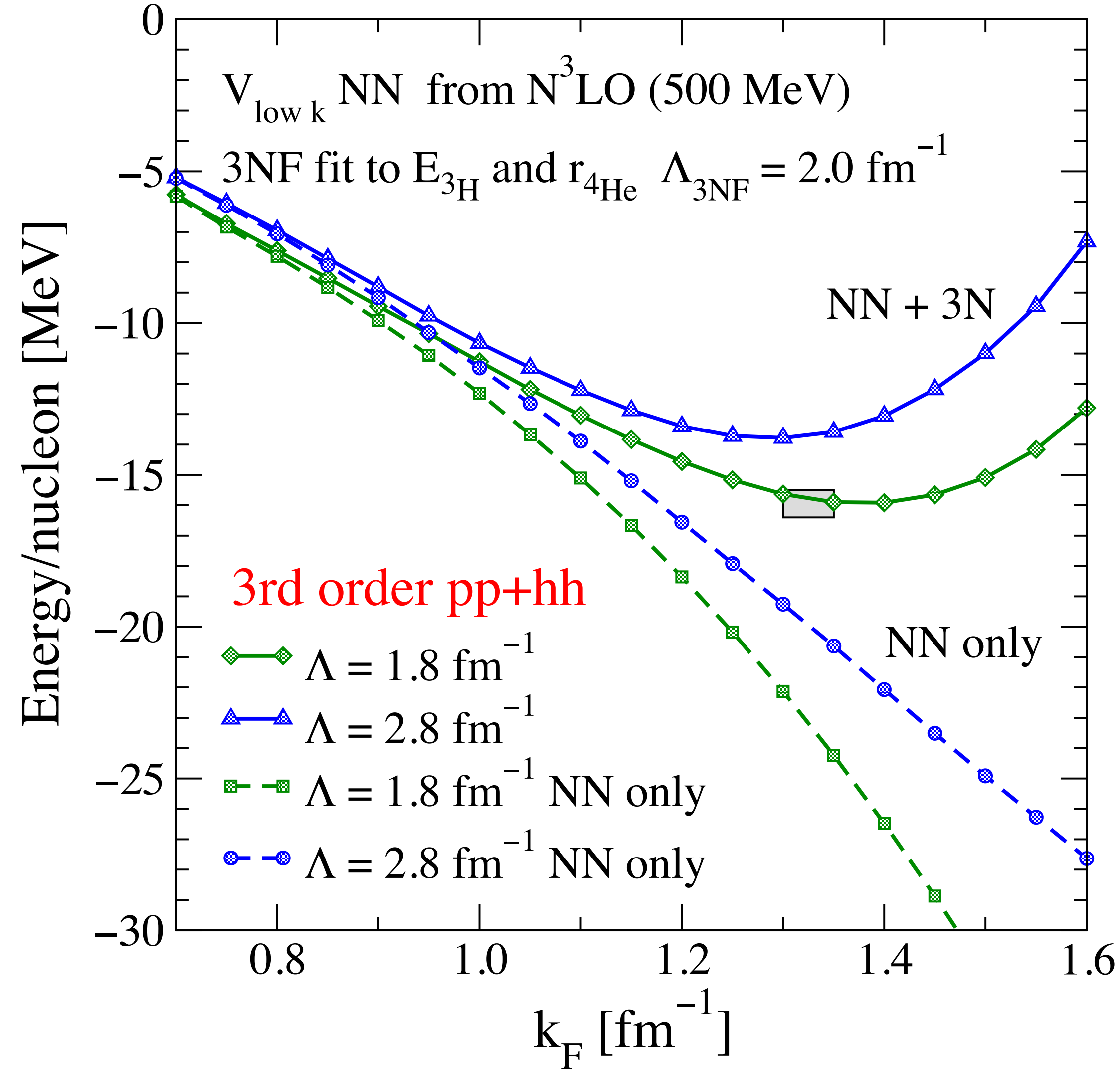
"Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."

Hans Bethe (1971)

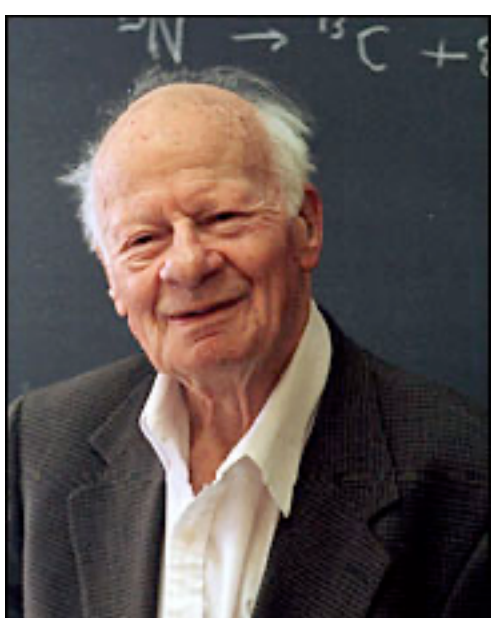


Equation of state of symmetric nuclear matter, nuclear saturation





KH, Bogner, Furnstahl, Nogga, PRC(R) 83, 031301 (2011)



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The SRG transformation of the Hamiltonian is defined by:

$$H(s) = U(s) H U^\dagger(s)$$

with the *unitary* operator $U(s)$, the Hamiltonian $H(s) = T_{rel} + V_{\rm NN}(s)$ and the resolution scale s .

Show that the flow equation is given by:

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

with the *anti-unitary* generator

$$\eta(s) = \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s)$$

The generator specifies the RG transformation and can be chosen suitably, such that the desired decoupling is achieved. The by far most common choice is:

$$\eta(s) = [T_{rel}, H(s)]$$

Where the kinetic energy operator is diagonal and hence hermitian. Show that the resulting generator is *anti-unitary*.

$$\frac{dH(s)}{ds} = [[T_{rel}, H(s)], H(s)]$$

1 Familiarize yourself with the first version of the code. This code allows you to read in matrix elements $V_{\rm NN}(s=0)$ and visualise them. Take a look at different coupled and uncoupled channels. In addition, a routine for computing the deuteron binding energy and phase shifts is included. Reproduce the experimental observables using the provided interaction matrix elements.

2 Implement a routine that allows to solve the SRG flow equations. For this you can use the NumPy routine **odeint**. You can use the upper limit $s \sim 0.1 \ {\rm fm}^4$ as an upper limit for the resolution scale.

3 Visualize the SRG-evolved interaction matrix elements using coloured contour plots and verify that the off-diagonal matrix elements get successively suppressed with increasing flow parameter. Verify that the deuteron binding energy remains invariant during the SRG evolution within numerical accuracy.

4 Modify the routine for the deuteron binding energy such that you can control the momentum range of the matrices. Show that you can reduce the dimensionality of the eigenvalue problem by cutting away high-momentum modes, without changing the binding energy for sufficiently large flow parameter values s .

5 Verify that also the phase shifts remain invariant under SRG transformations.

Compare the results and run times of the code for the two interactions AV18 und EM500.