Atomic nuclei: from fundamental interactions to structure and stars

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Mainz, April 7, 2016

TECHNISCHE UNIVERSITÄT DARMSTADT

SFB 1245

European Research Council
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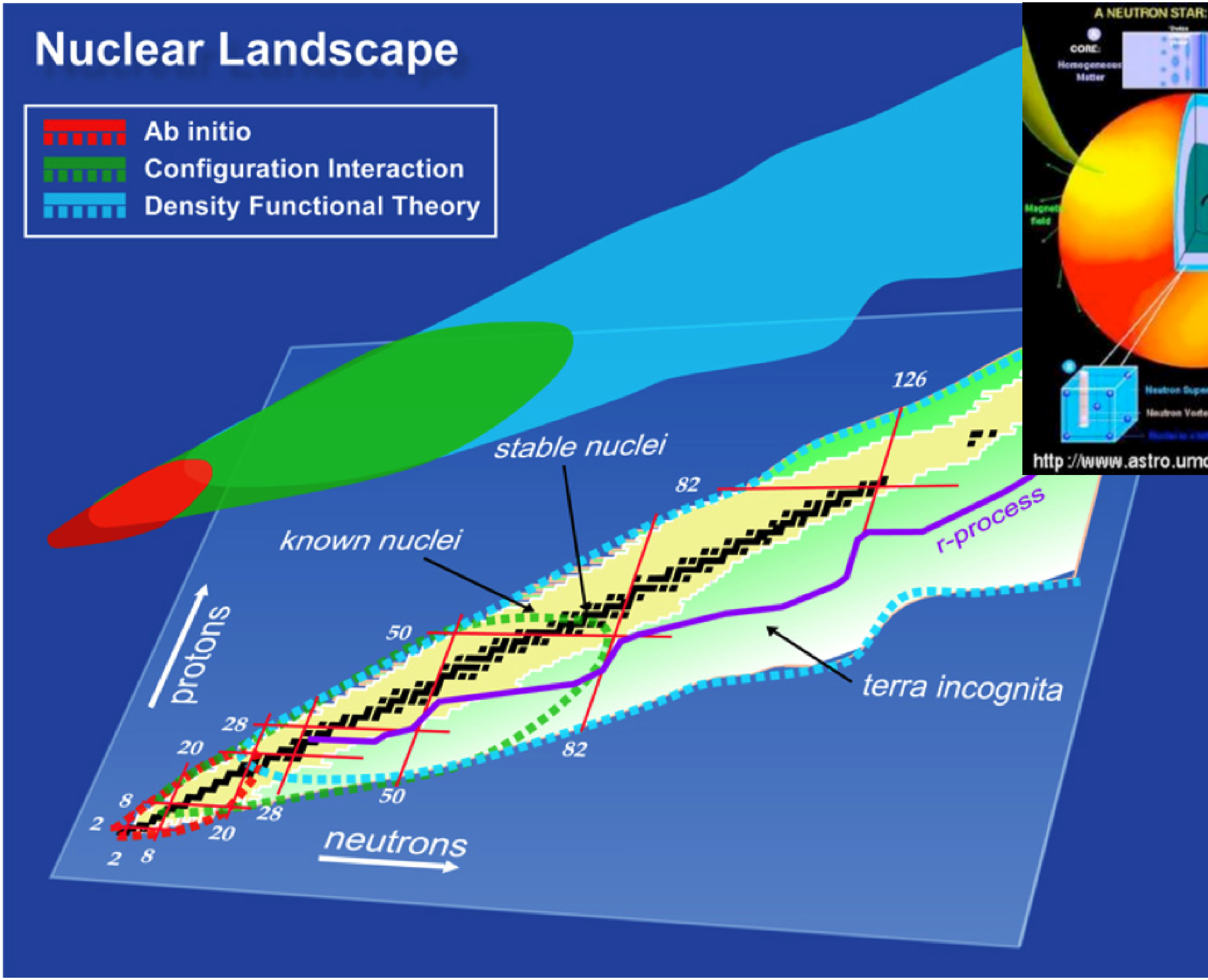
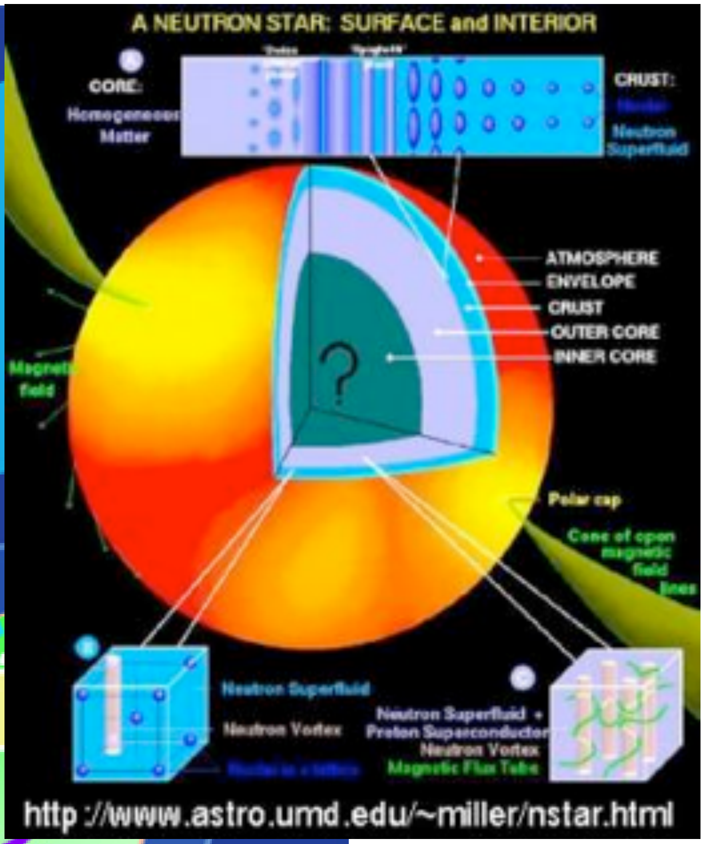
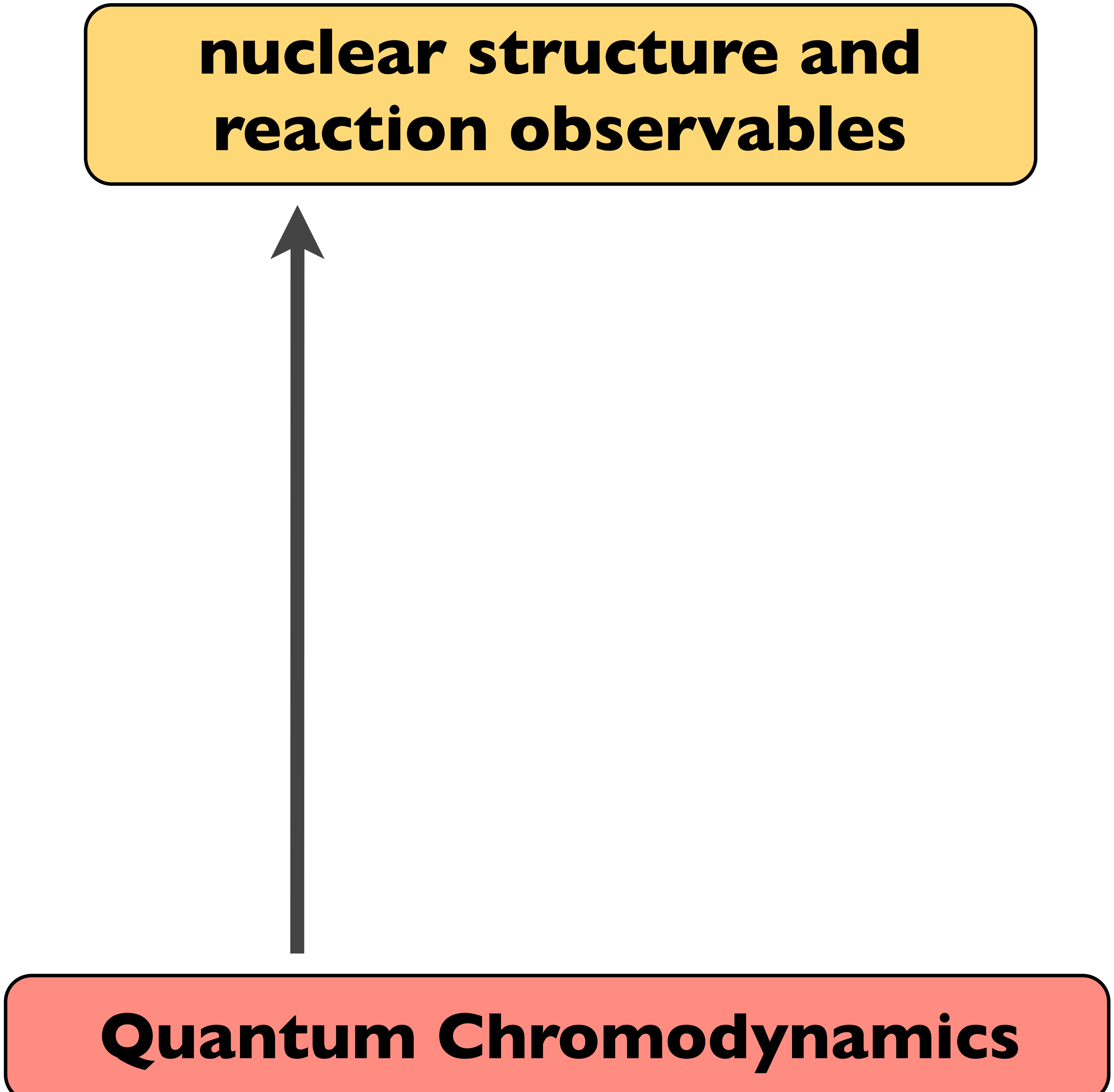
New Vistas in Low-Energy Precision Physics (LEPP)

The theoretical nuclear landscape several years ago...





Ab initio nuclear structure theory



Ab initio nuclear structure theory

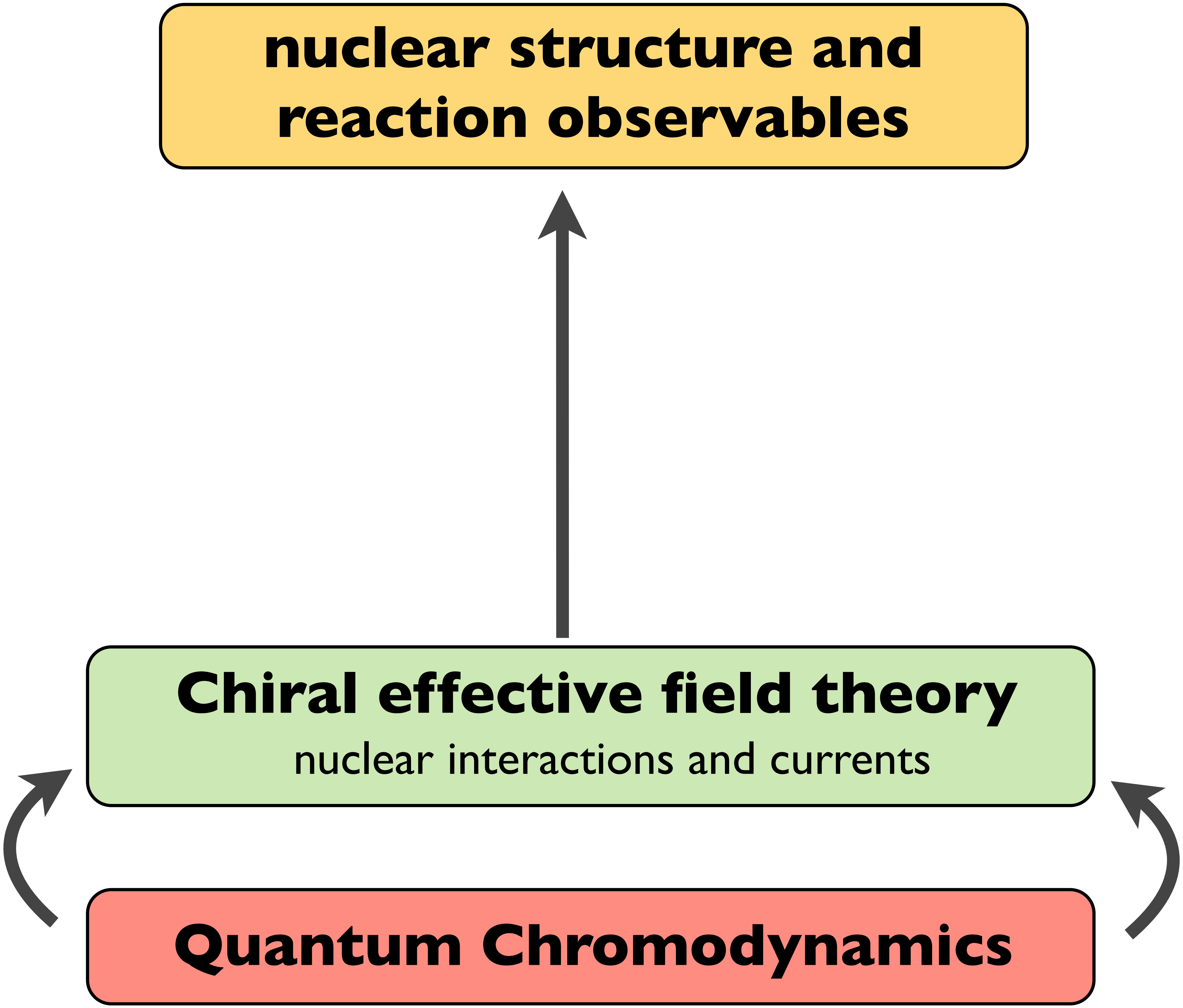
nuclear structure and reaction observables

Lattice QCD

- requires extreme amounts of computational resources
- currently limited to 1- or 2-nucleon systems
- current accuracy insufficient for precision nuclear structure

Quantum Chromodynamics

Ab initio nuclear structure theory



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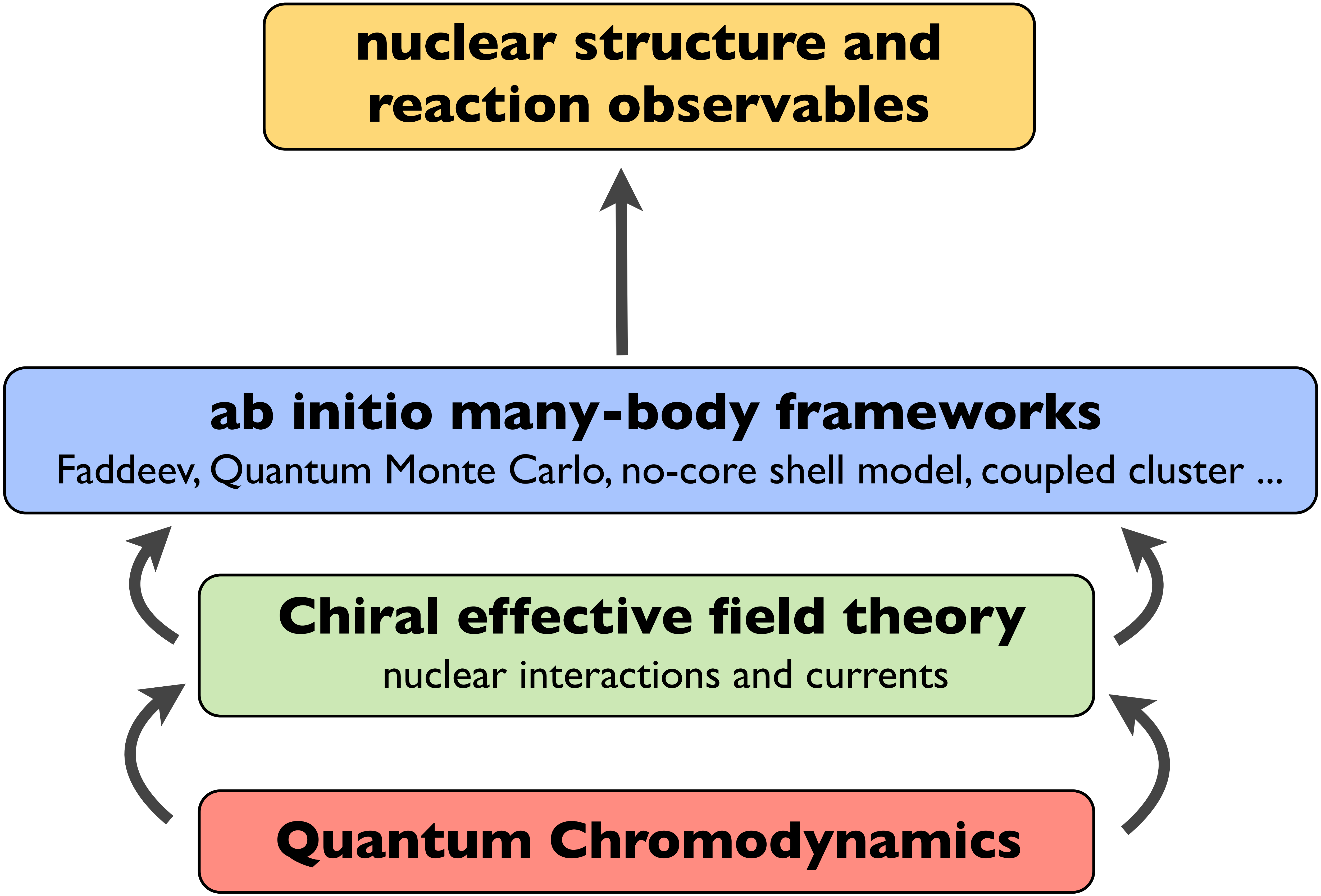

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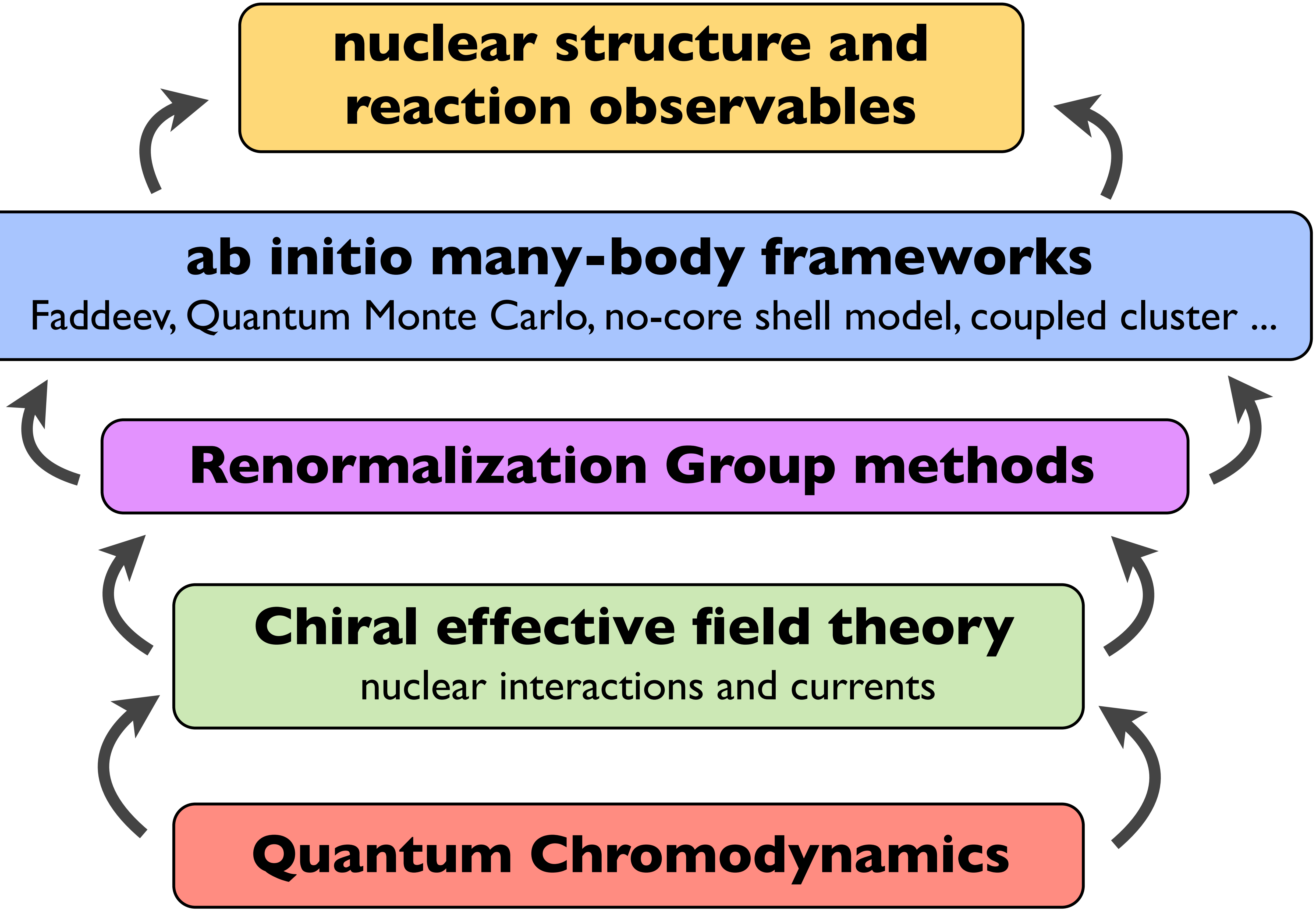
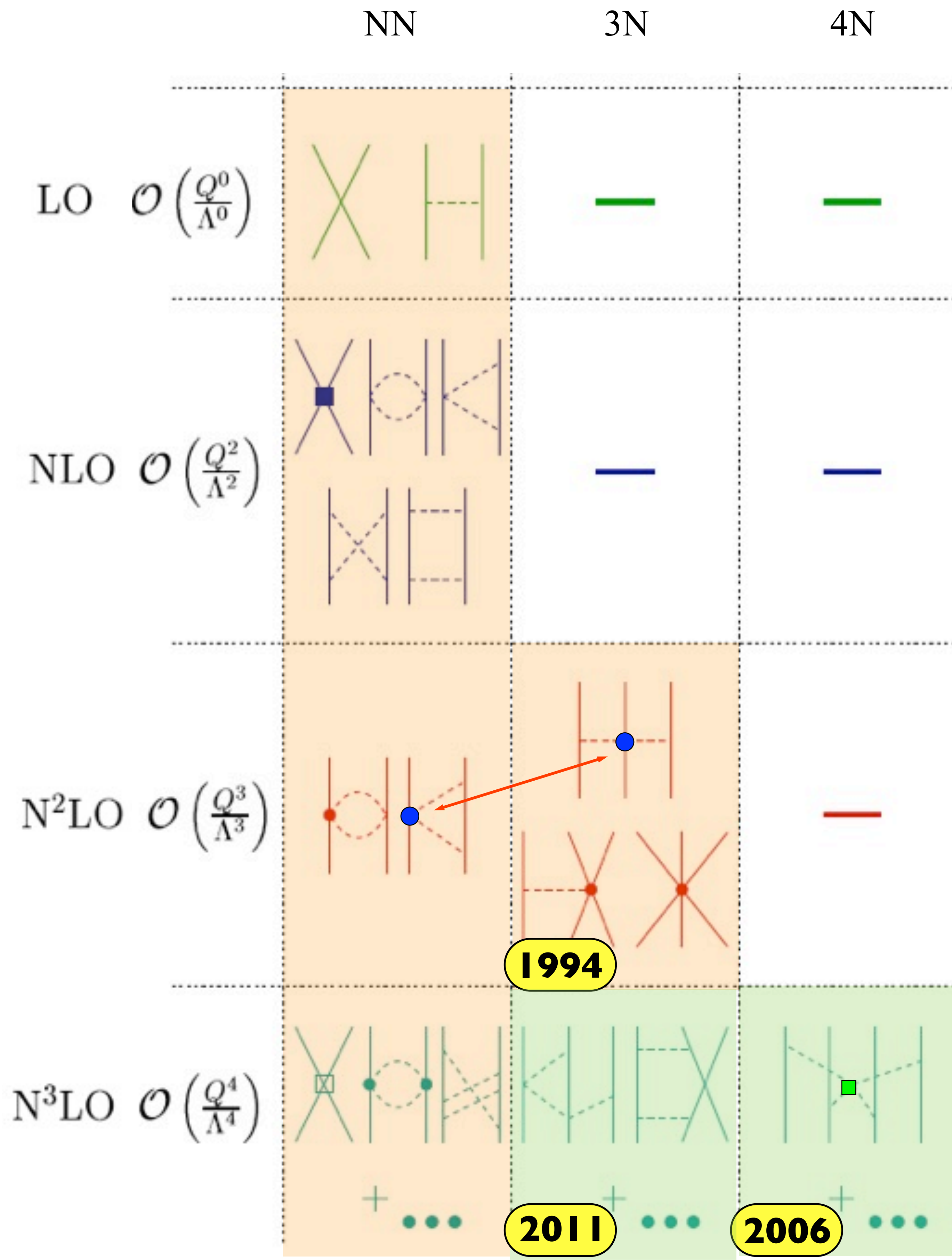
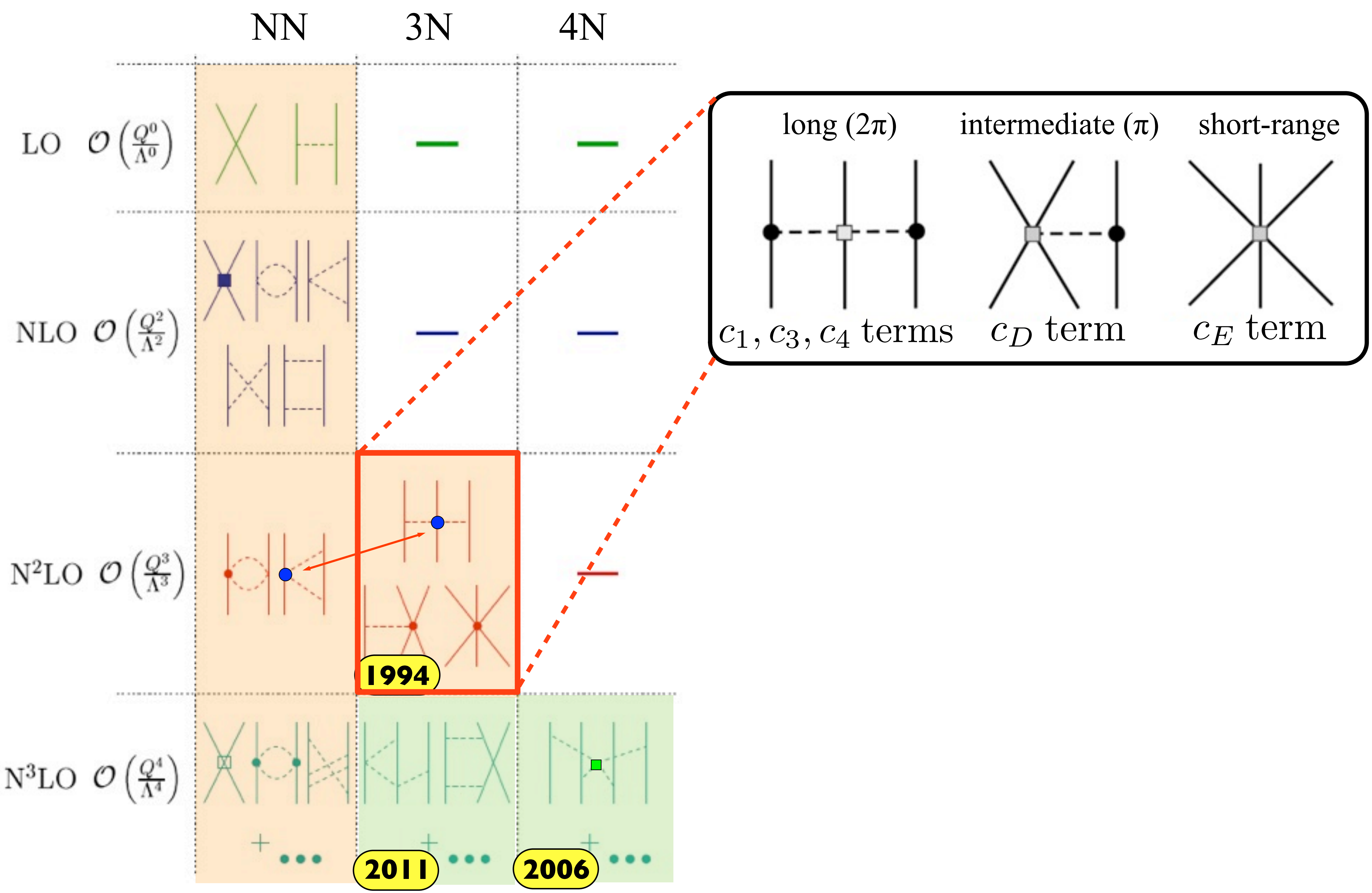


Chiral effective field theory for nuclear forces

- choose relevant degrees of freedom: here nucleons and pions
- operators constrained by symmetries of QCD
- short-range physics captured in few short-range couplings
- separation of scales: $Q << \Lambda_b$, breakdown scale Λ_b~500 MeV
- power-counting: expand in powers Q/Λ_b
- systematic: work to desired accuracy, obtain error estimates



Many-body forces in chiral EFT



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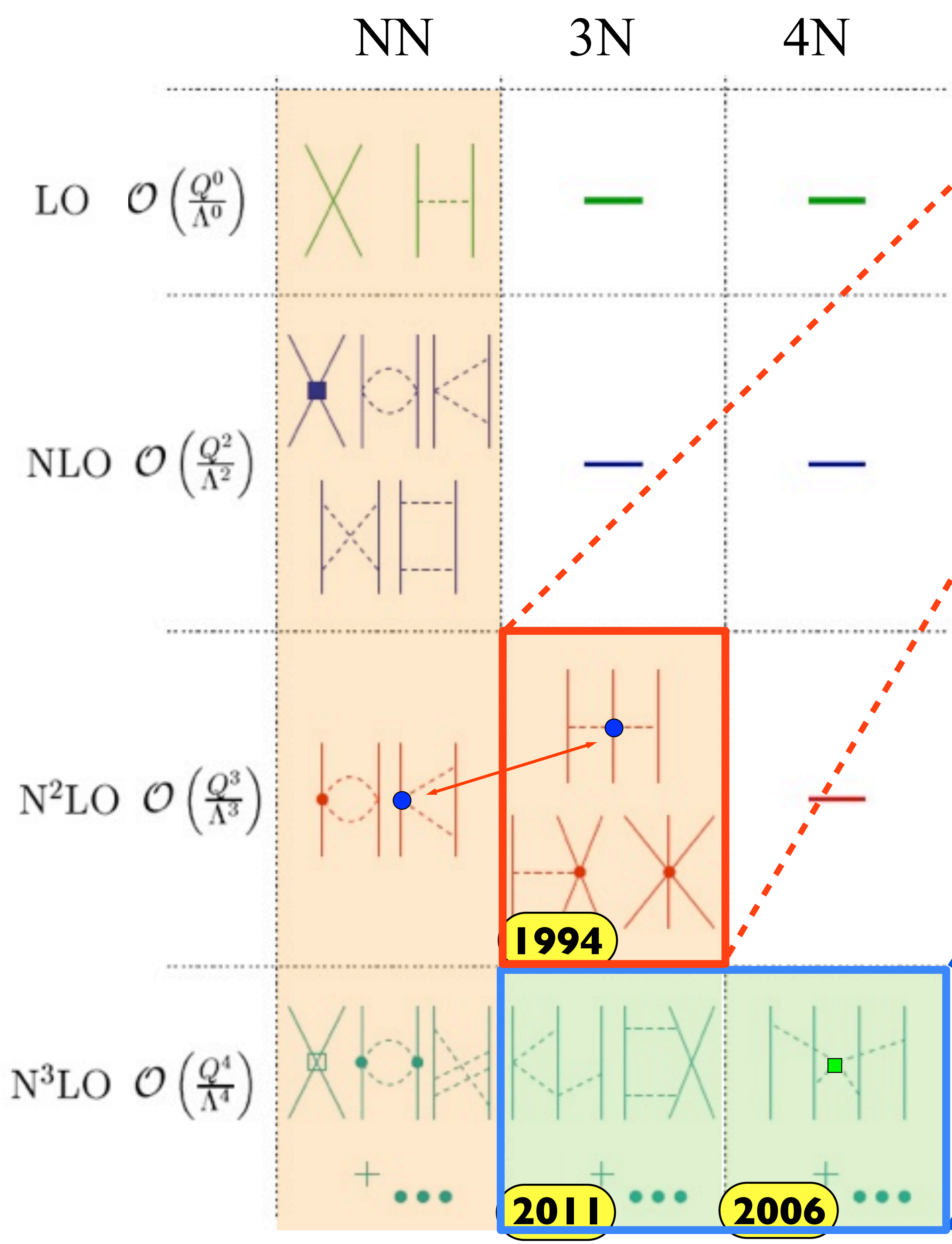
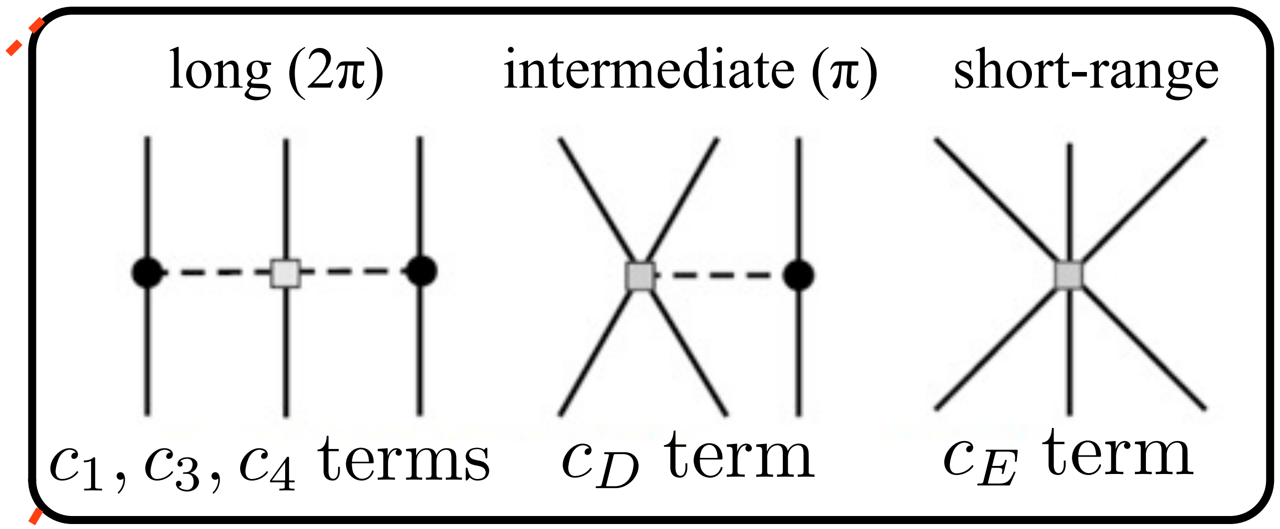


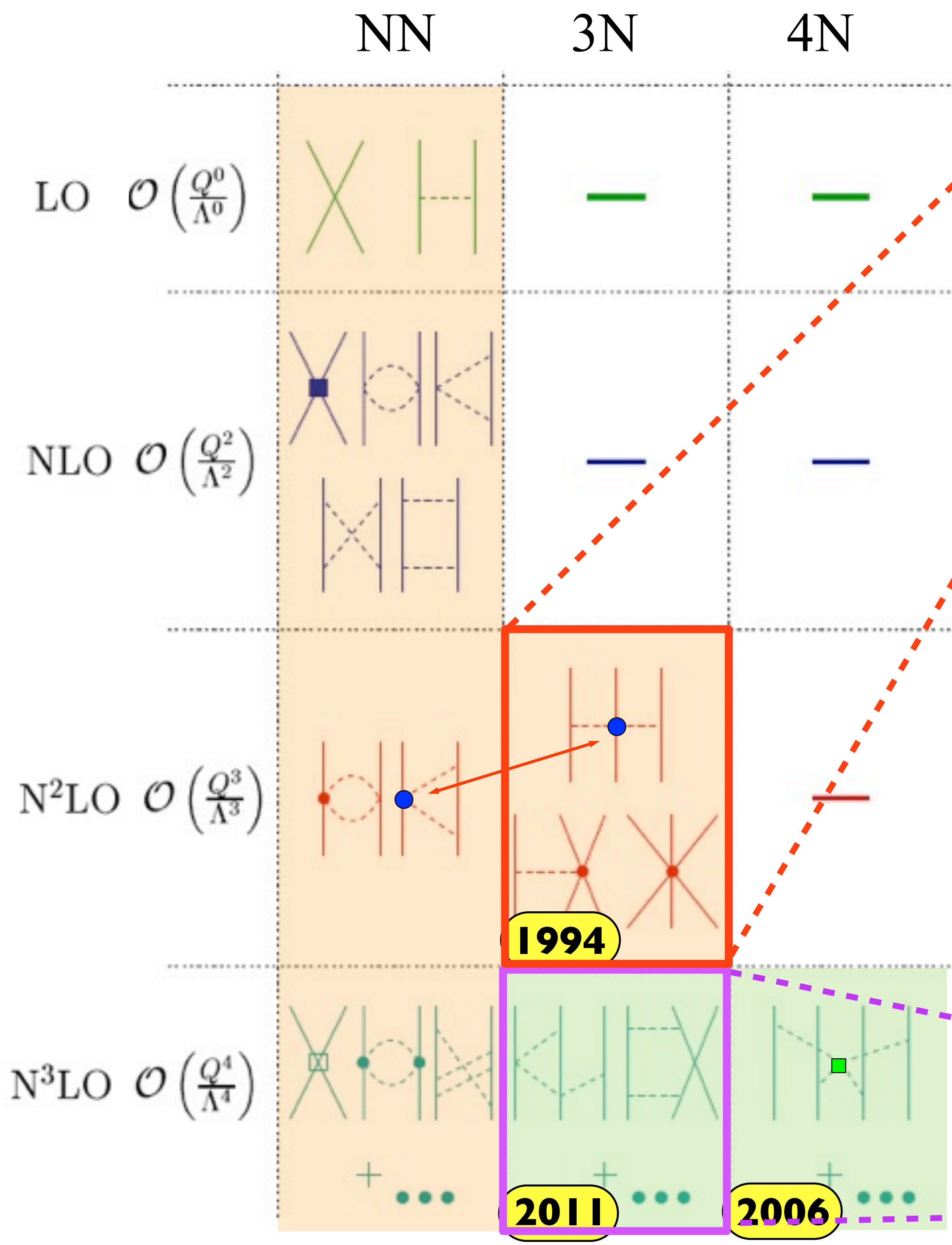


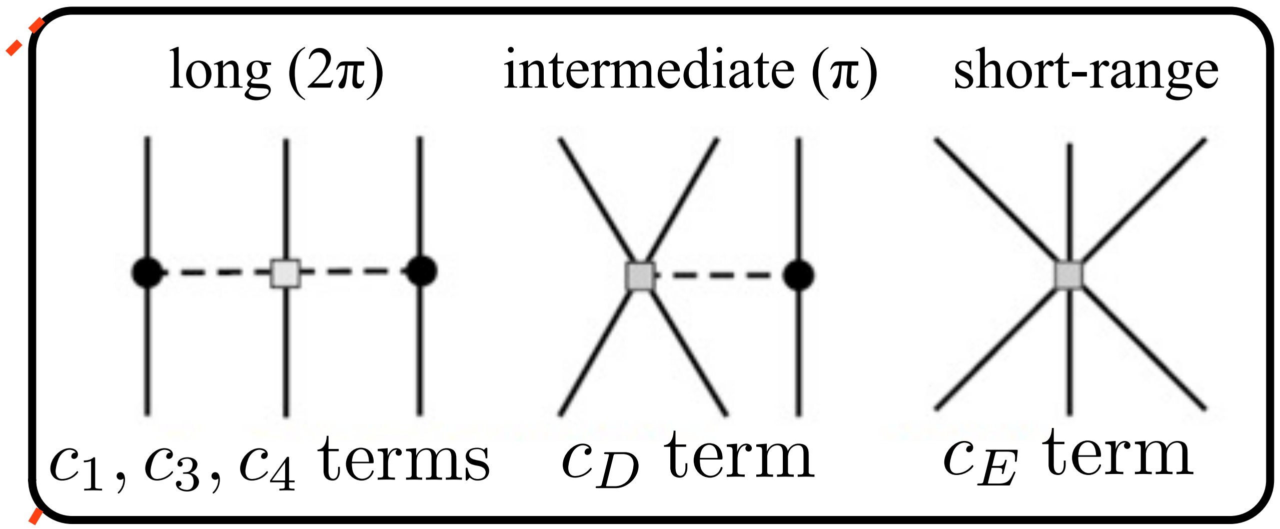
first incorporation in calculations of neutron and nuclear matter

Tews, Krueger, KH, Schwenk, PRL 110, 032504 (2013)
Krueger, Tews, KH, Schwenk, PRC 88, 025802 (2013)

all terms predicted

Many-body forces in chiral EFT





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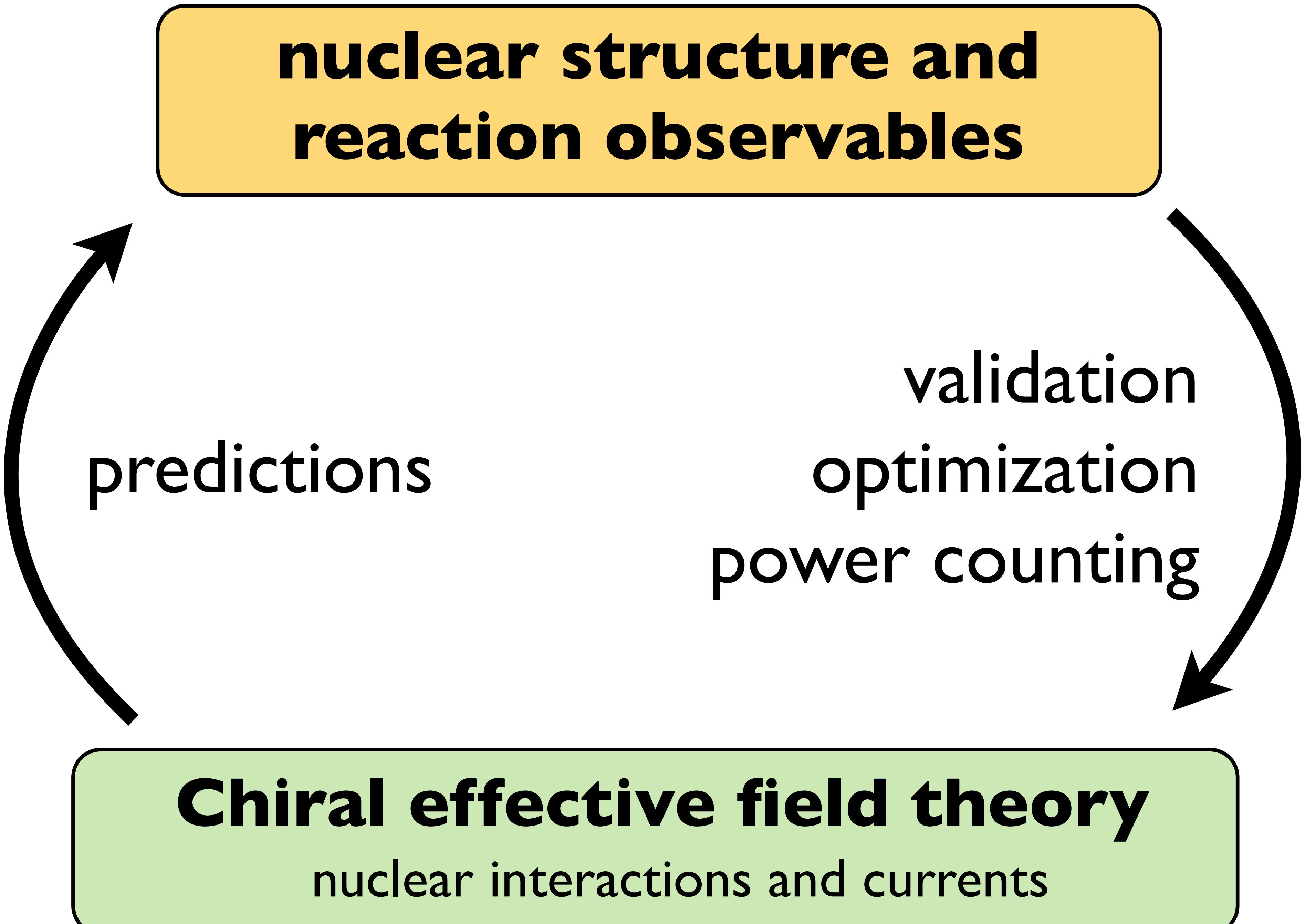
first calculation of matrix elements for ab initio studies of matter and nuclei

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

Development of nuclear interactions



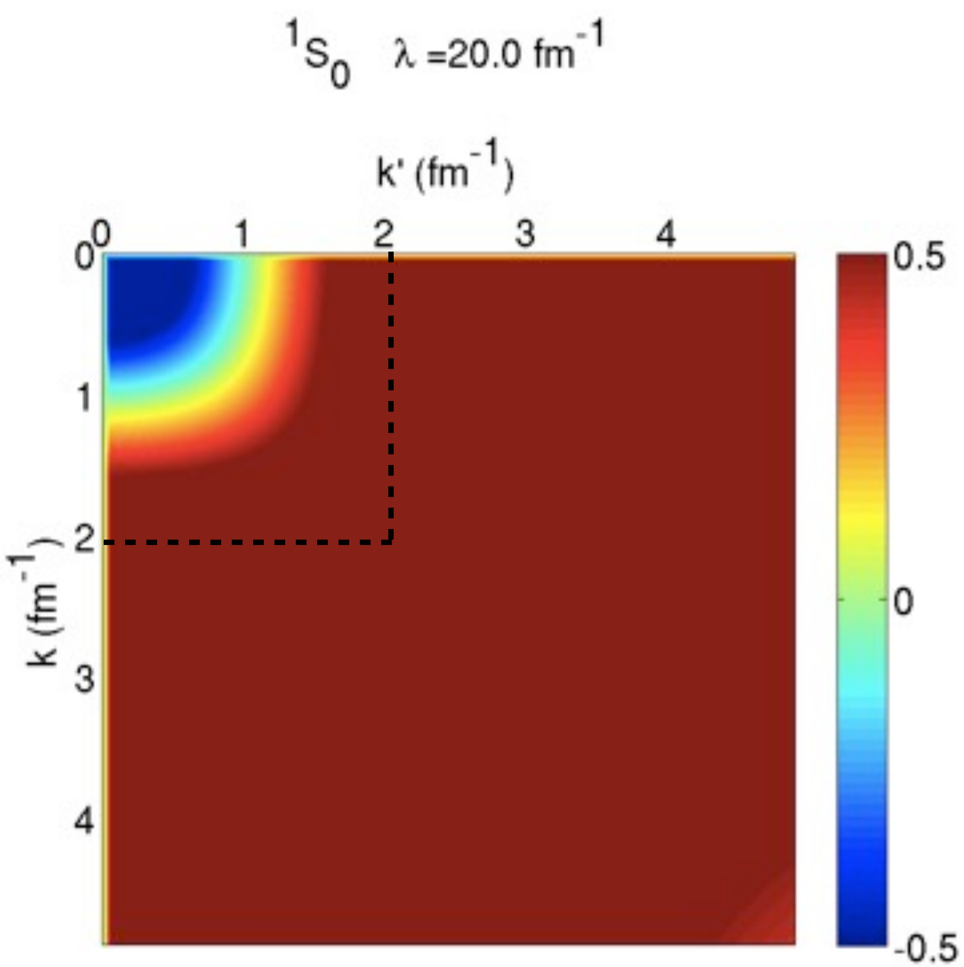
LENPIC

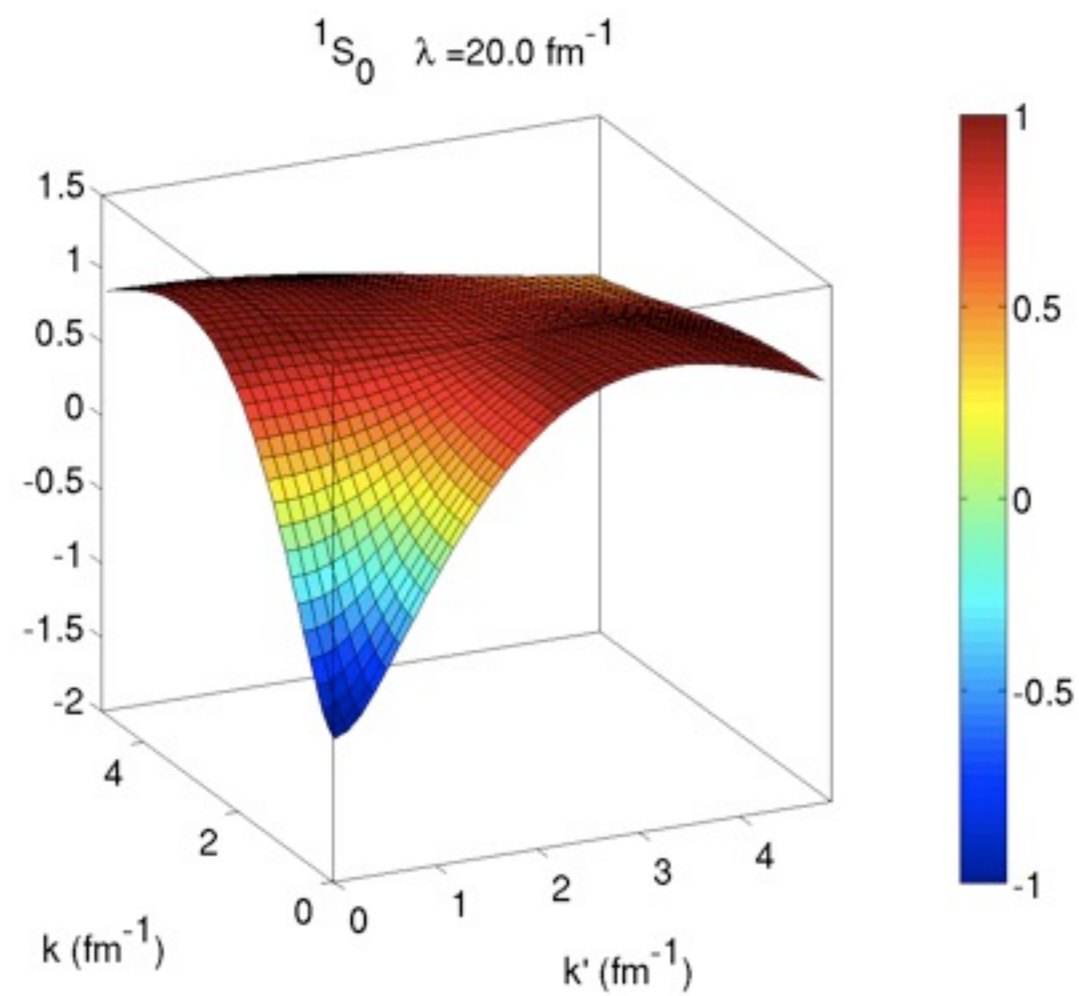
The Similarity Renormalization Group

- generate unitary transformation which decouples low- and high momenta

$$H_\lambda = U_\lambda H U_\lambda^\dagger$$ with the resolution parameter λ

- basic idea: change resolution successively in small steps: $\frac{dH_\lambda}{d\lambda} = [\eta_\lambda, H_\lambda]$
- generator η_λ can be chosen and tailored to different applications
- observables are preserved due to unitarity of transformation





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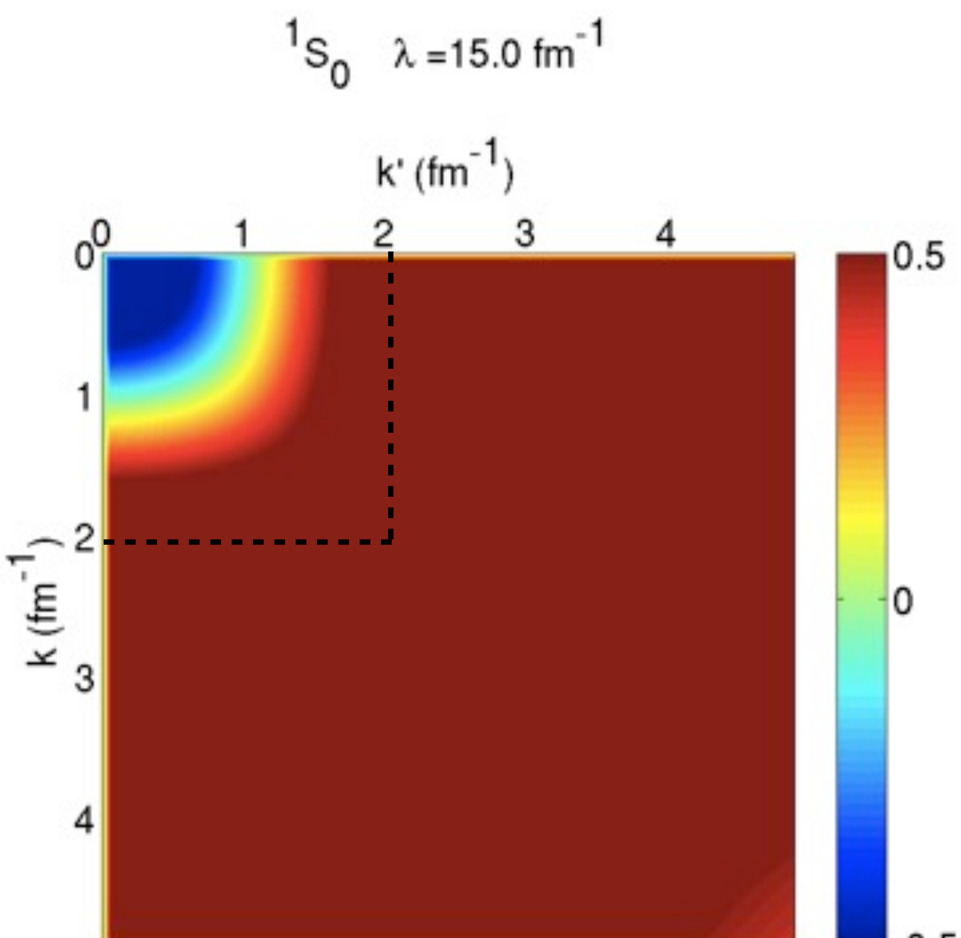

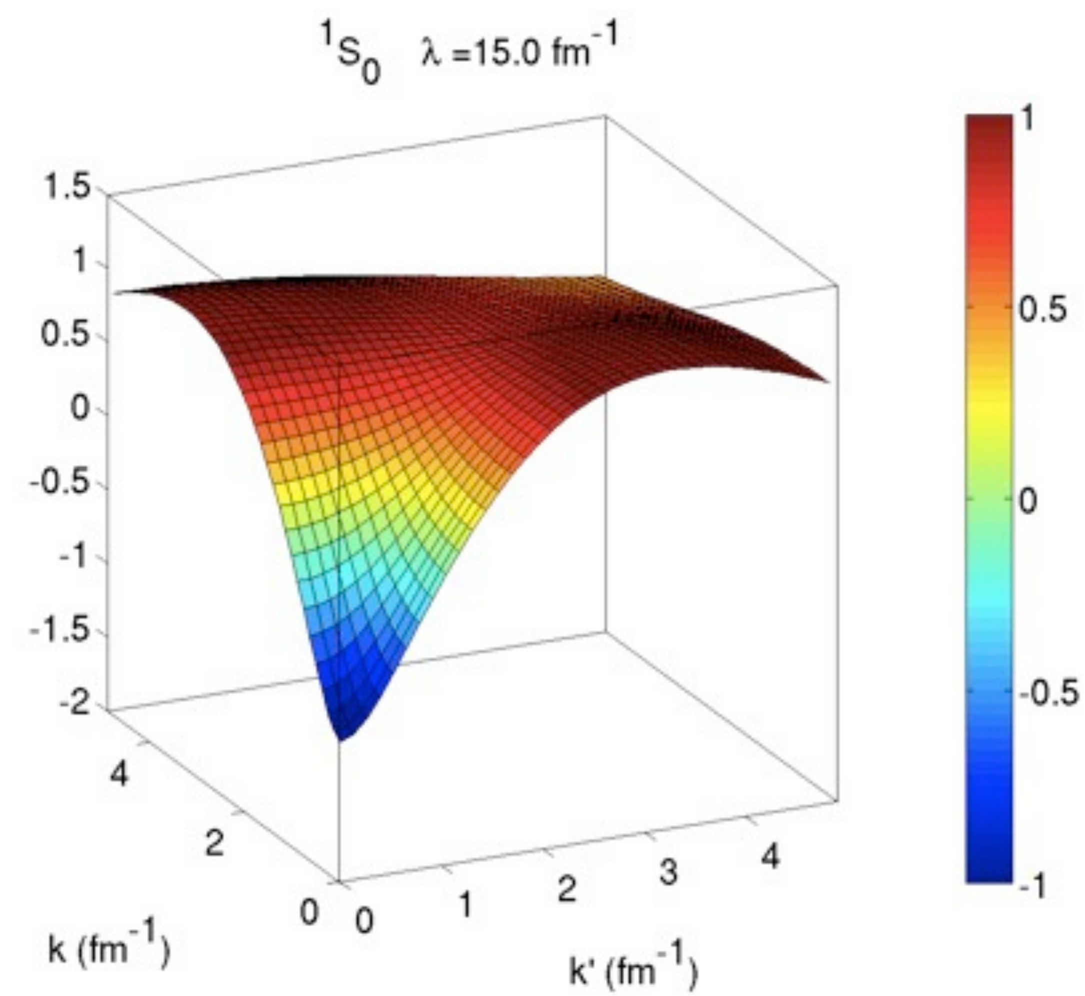

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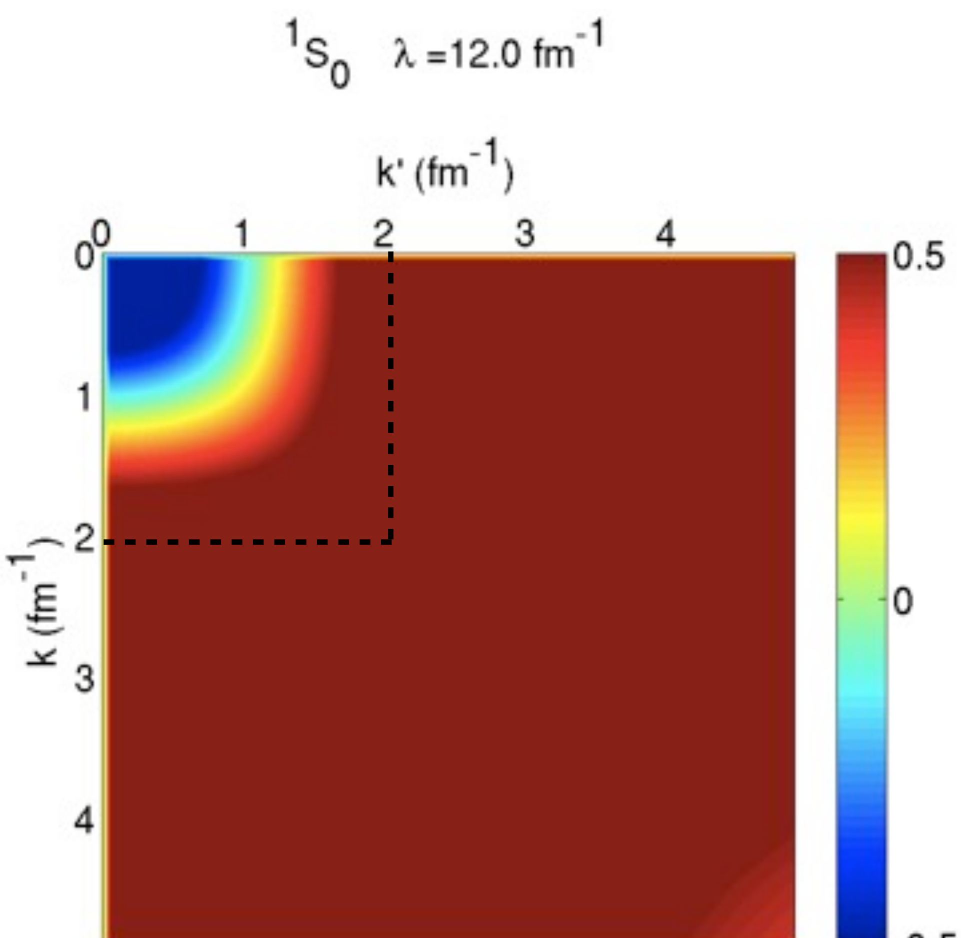

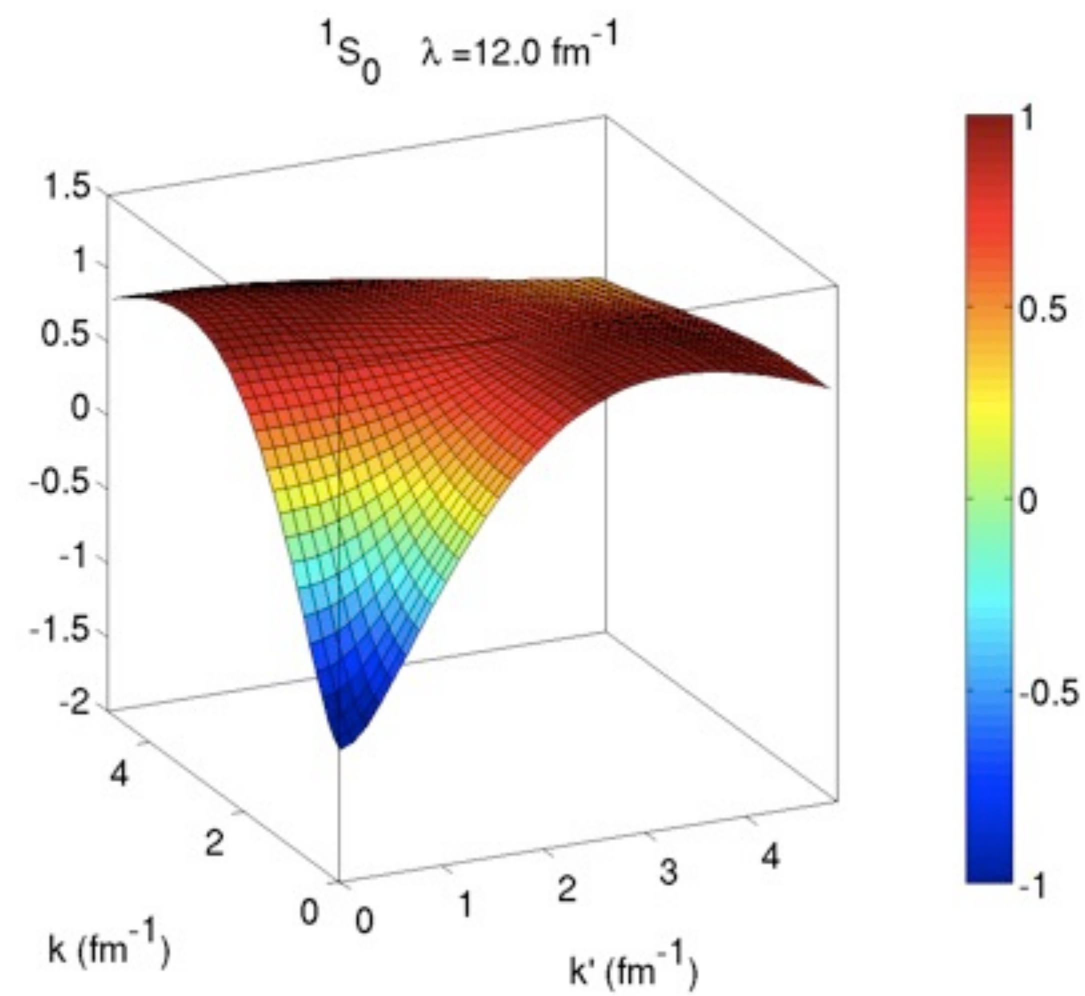

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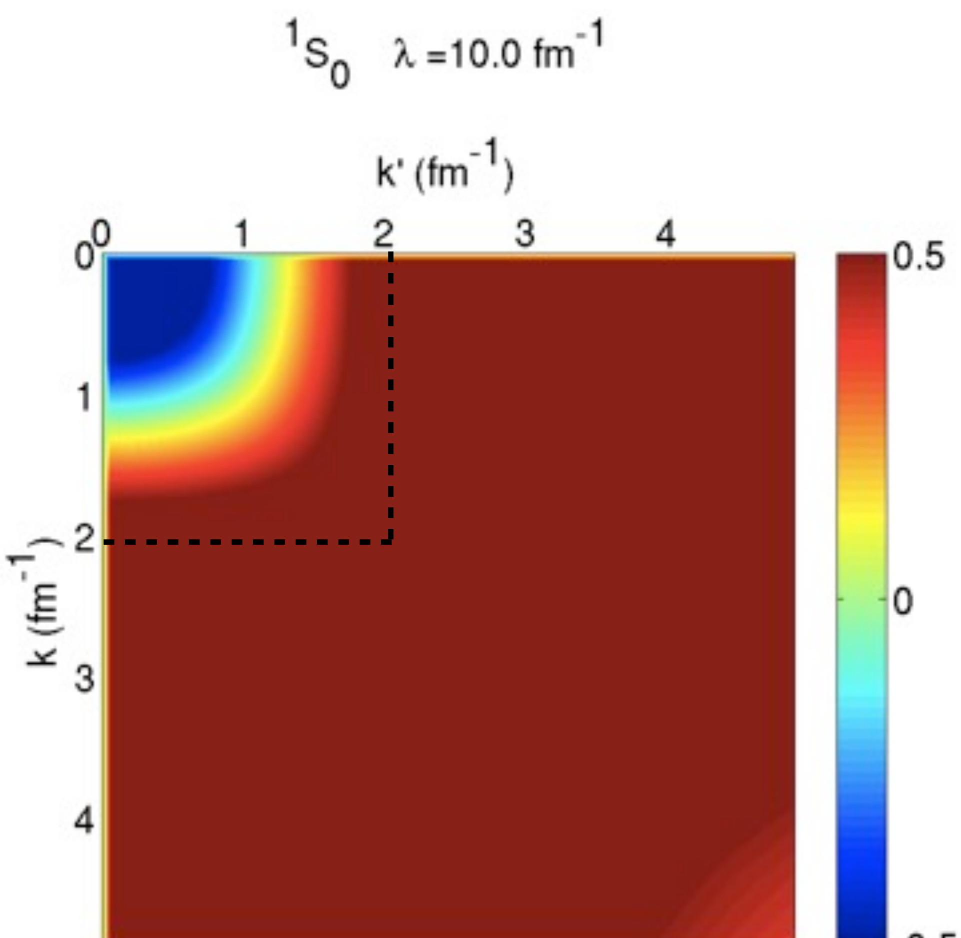

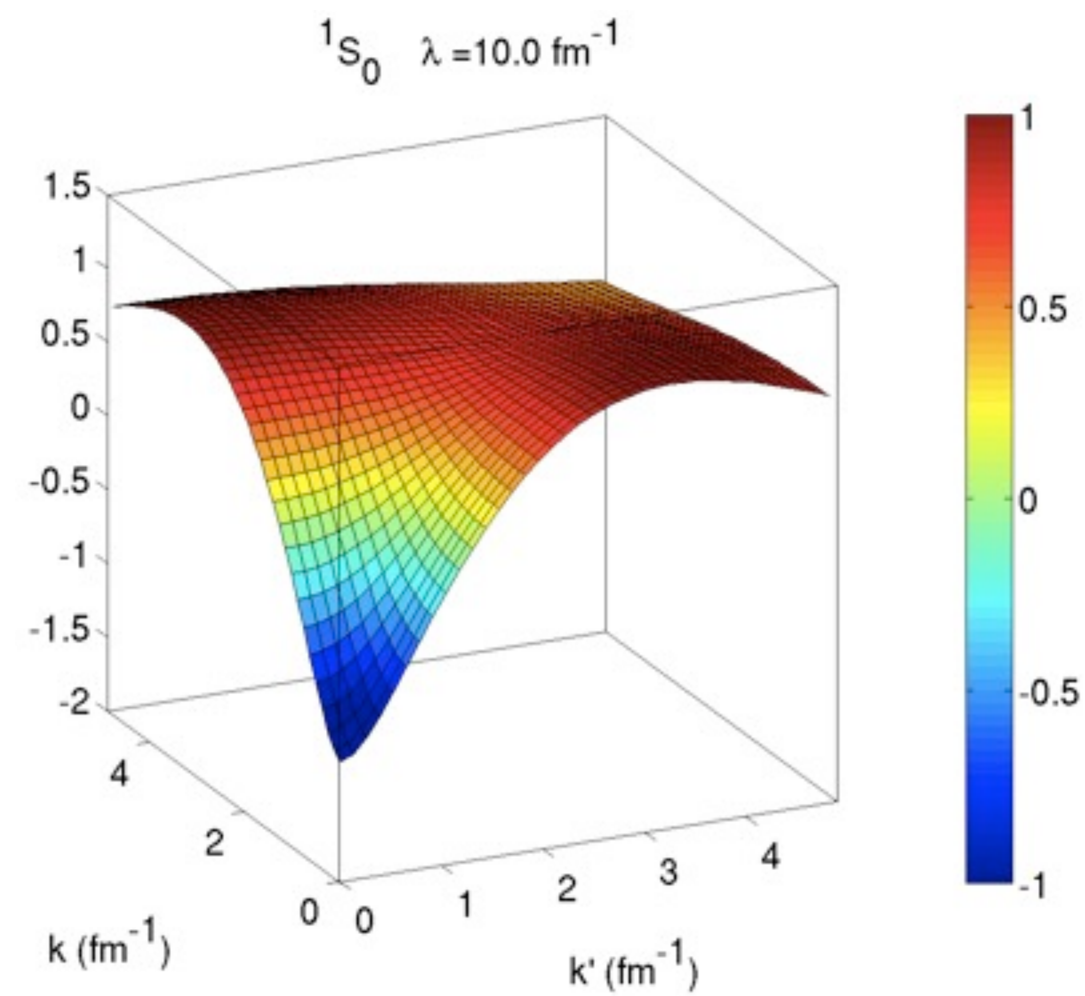

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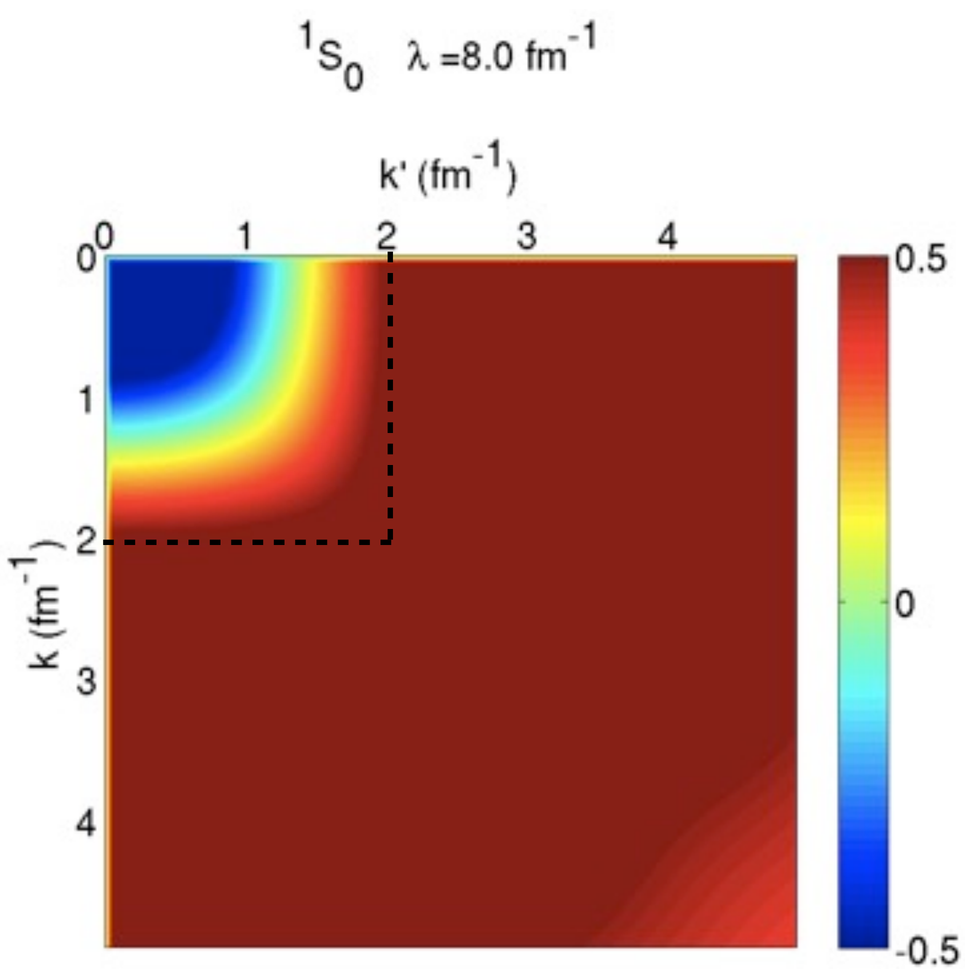

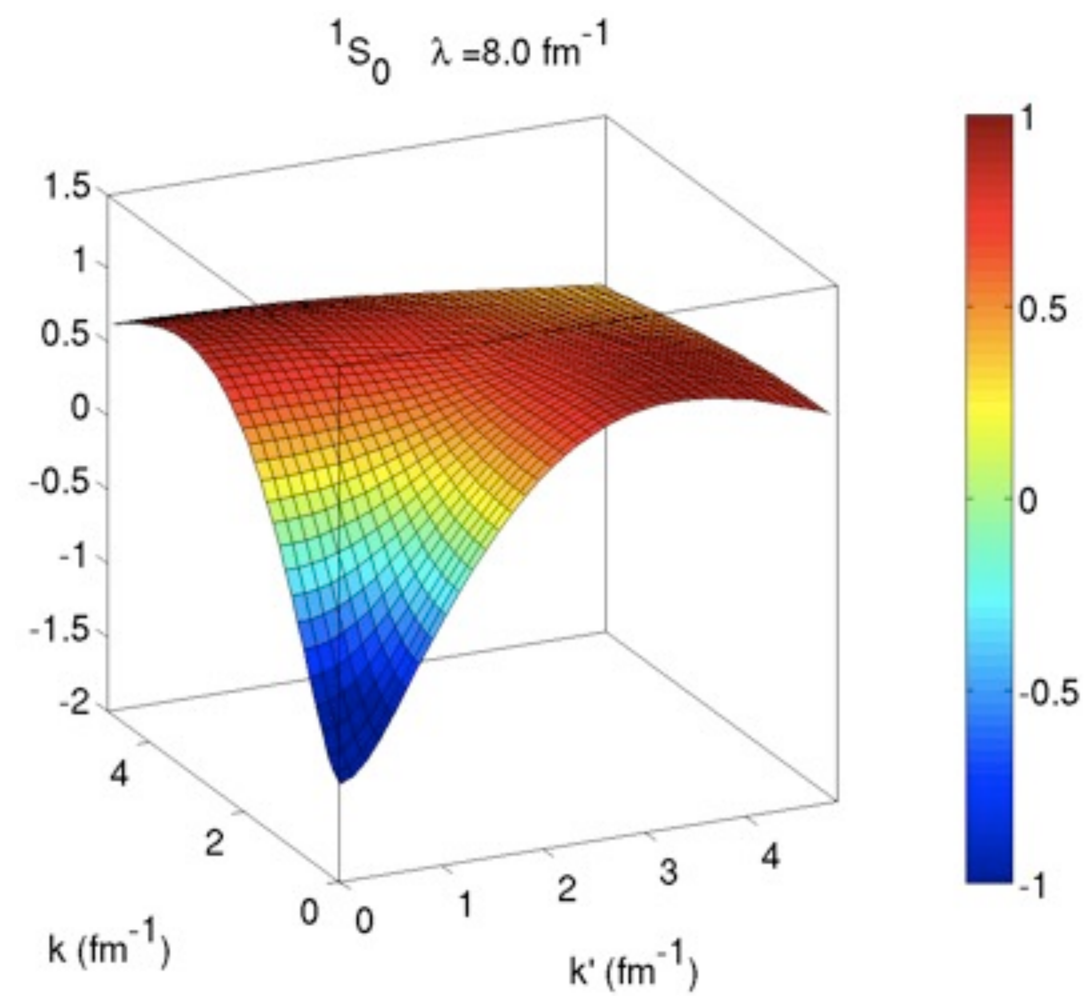

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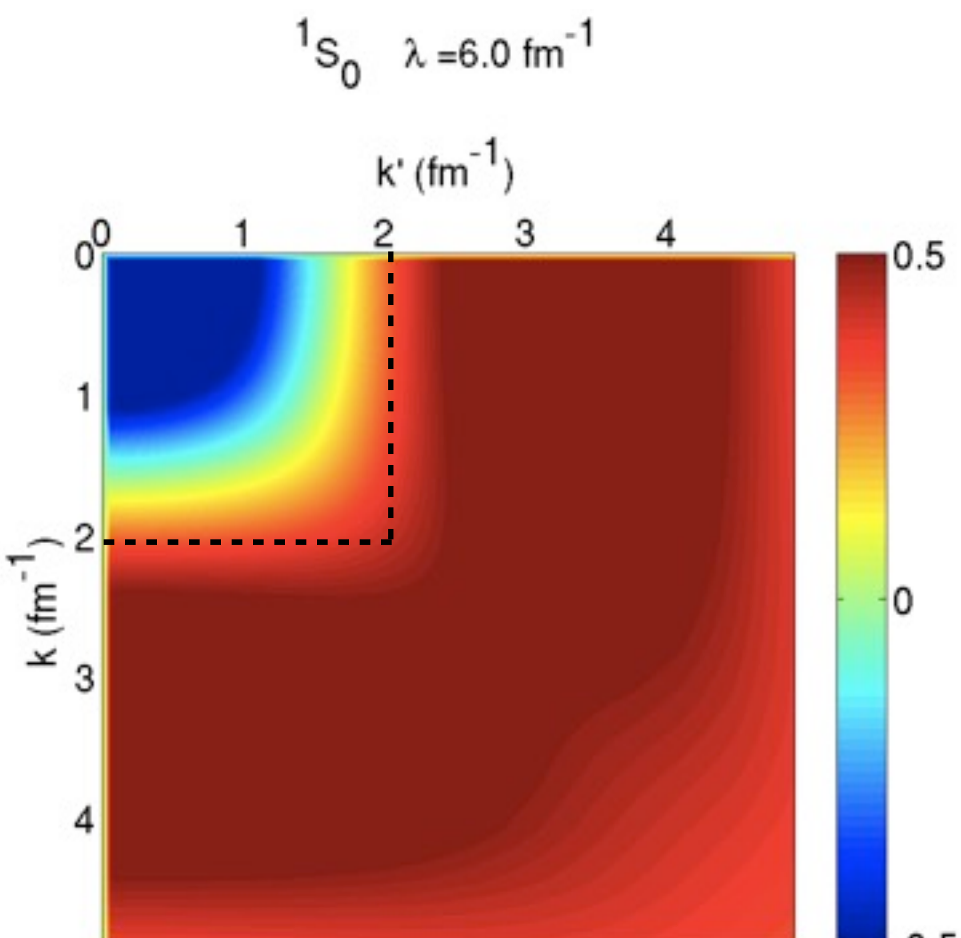

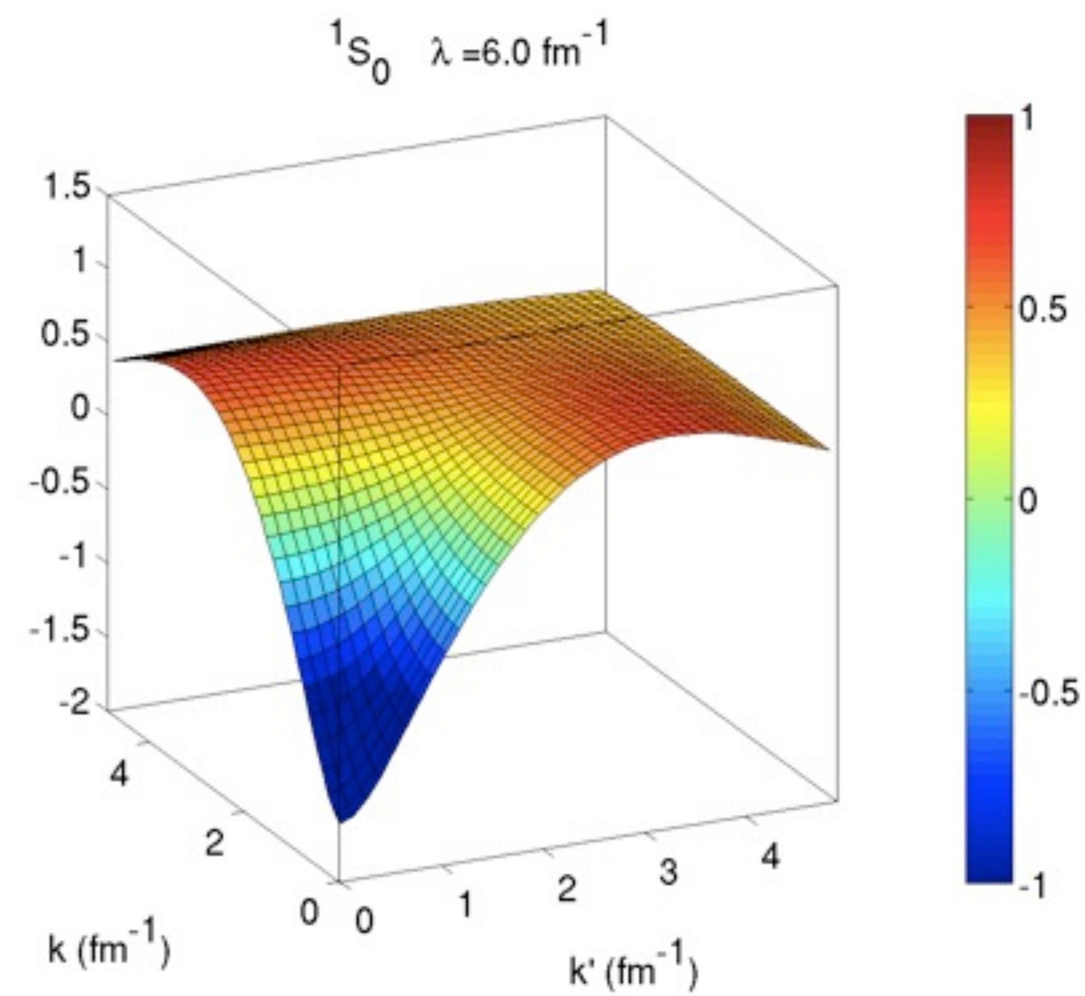

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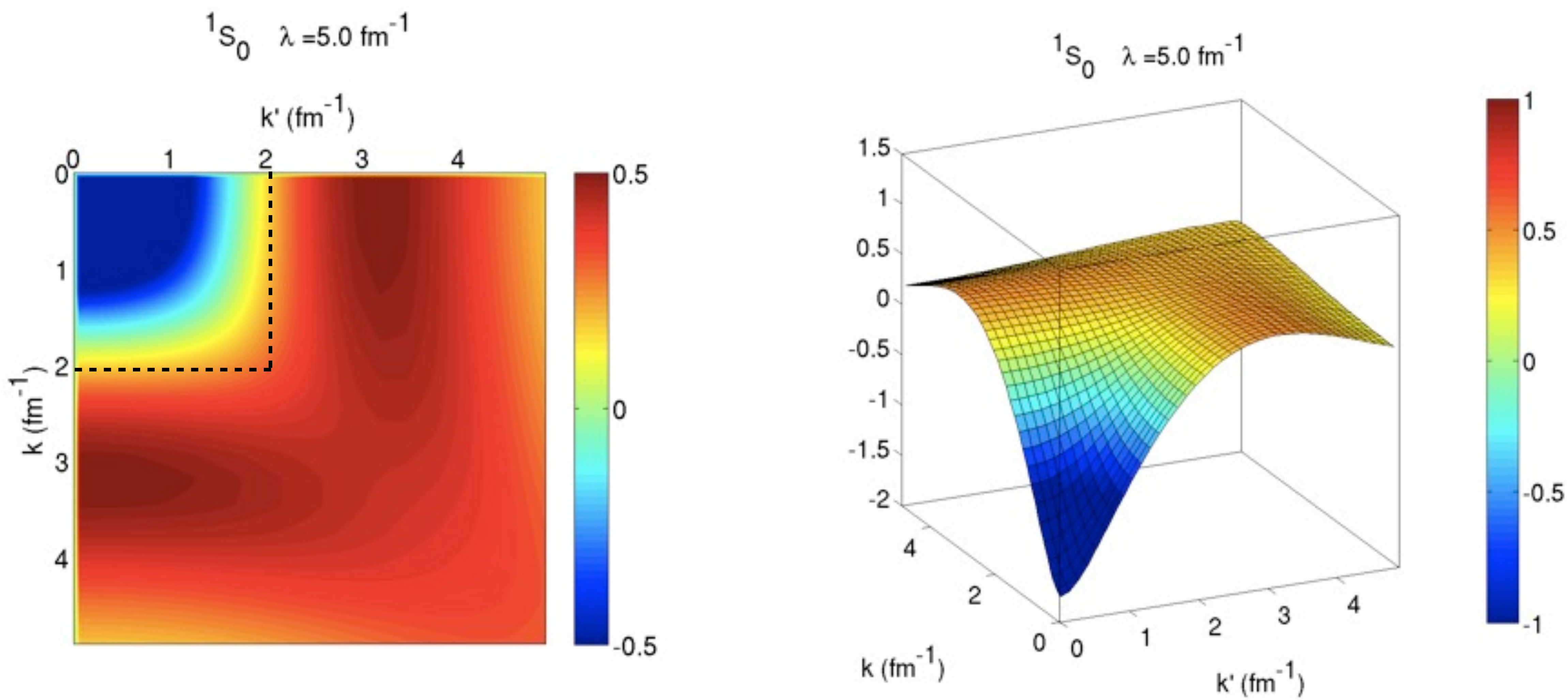

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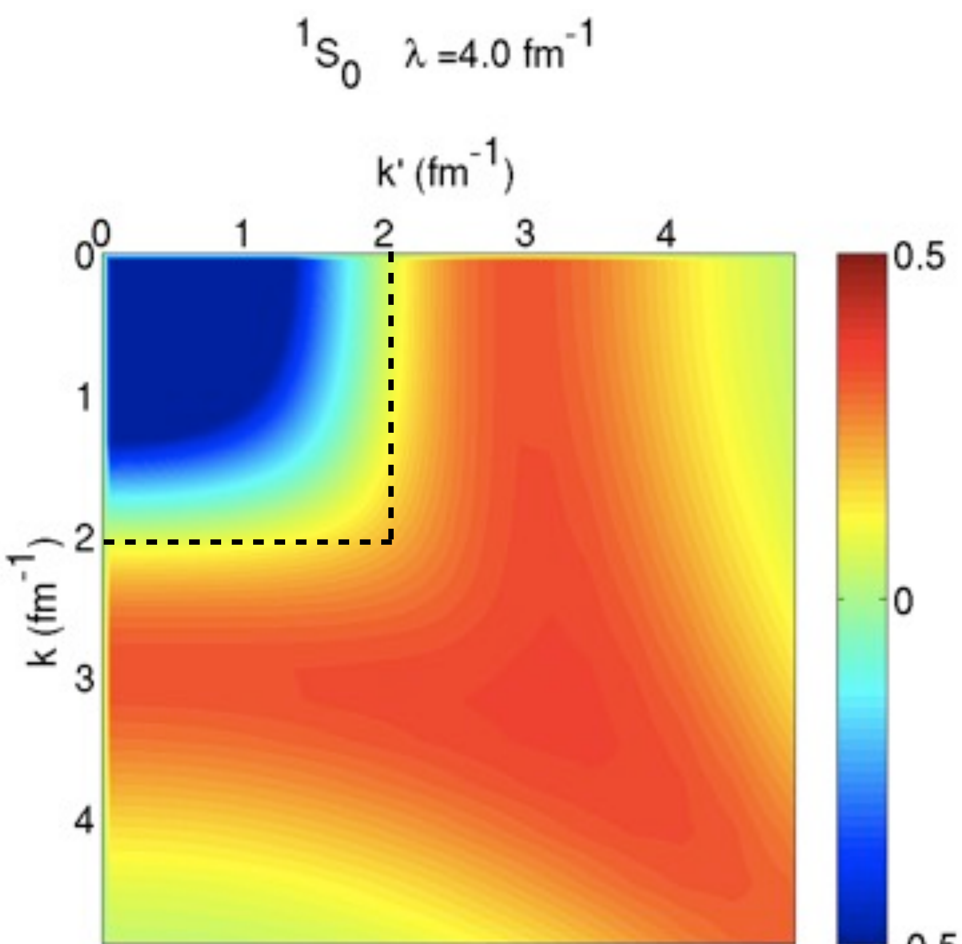

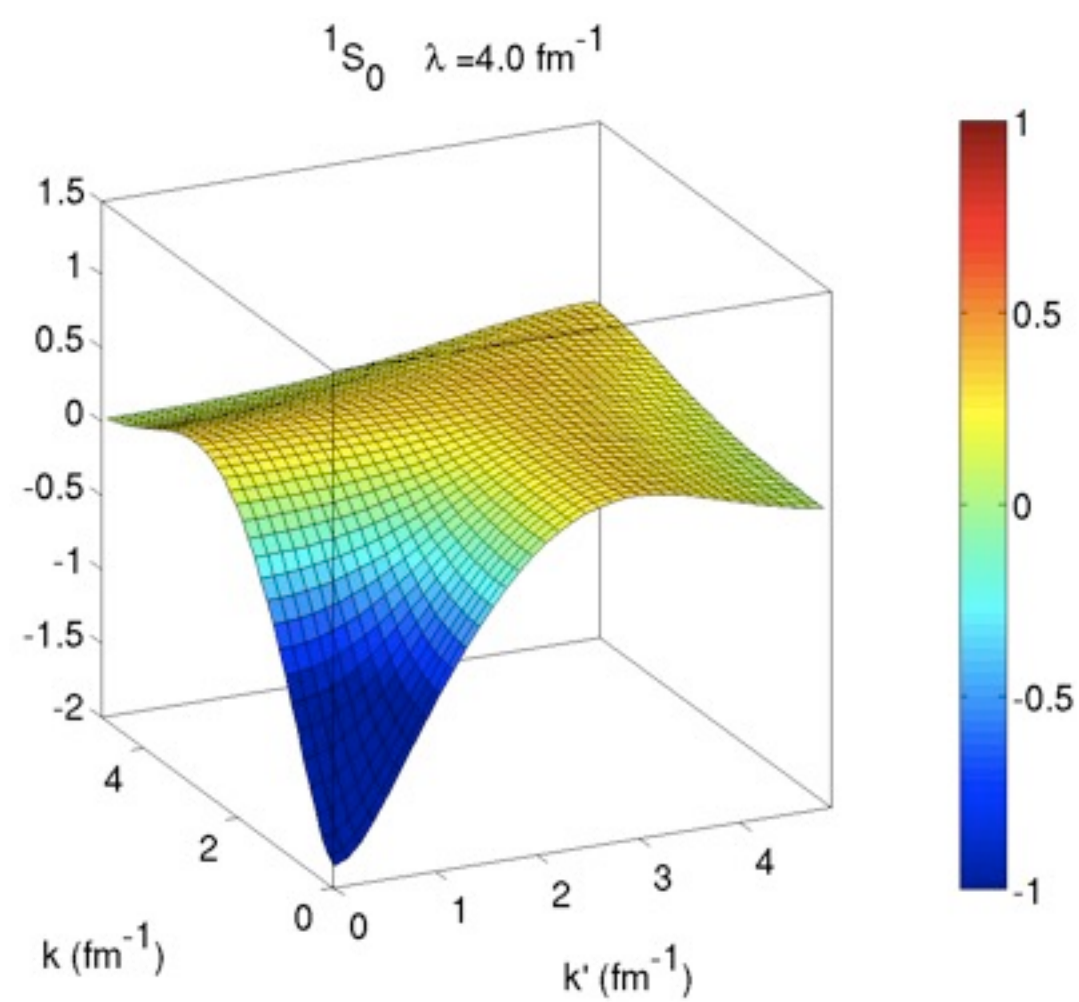

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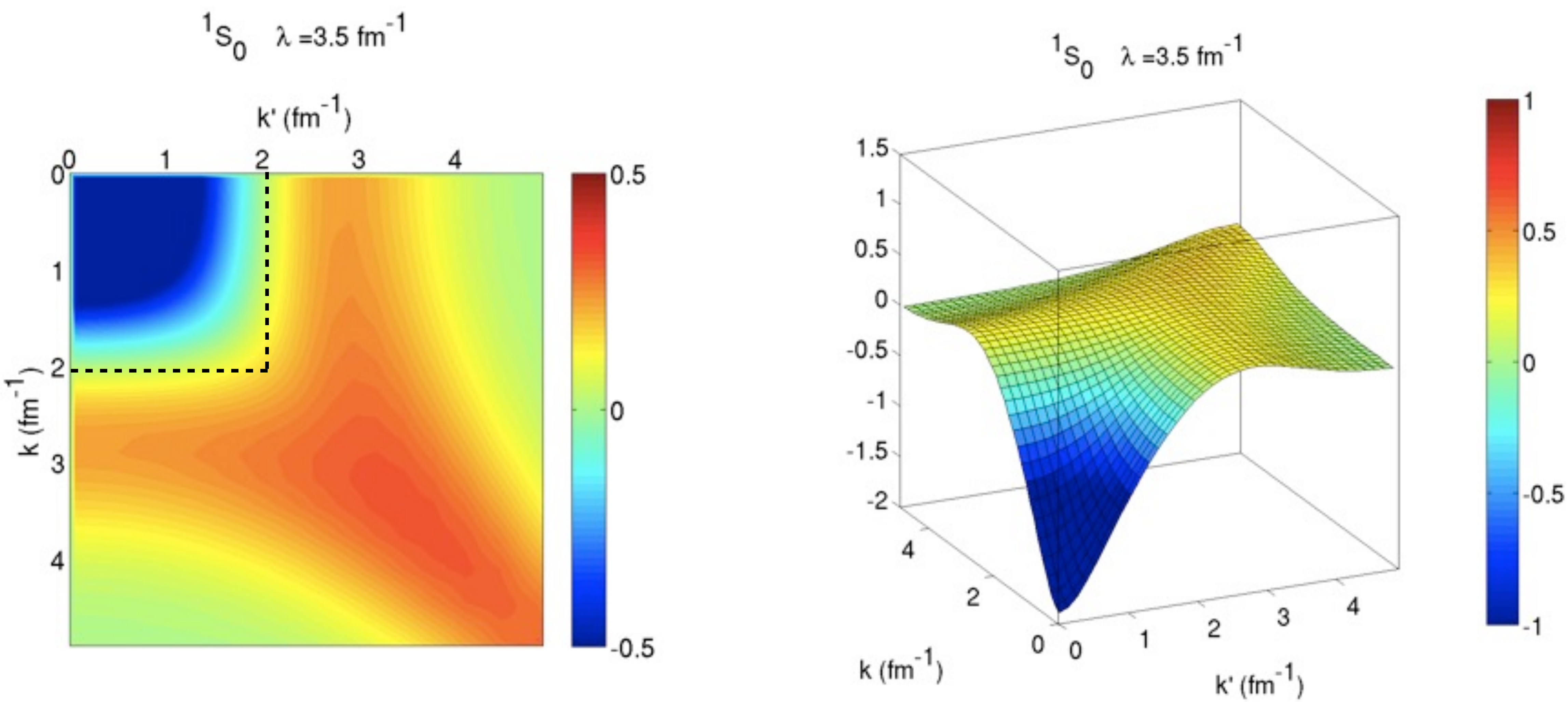

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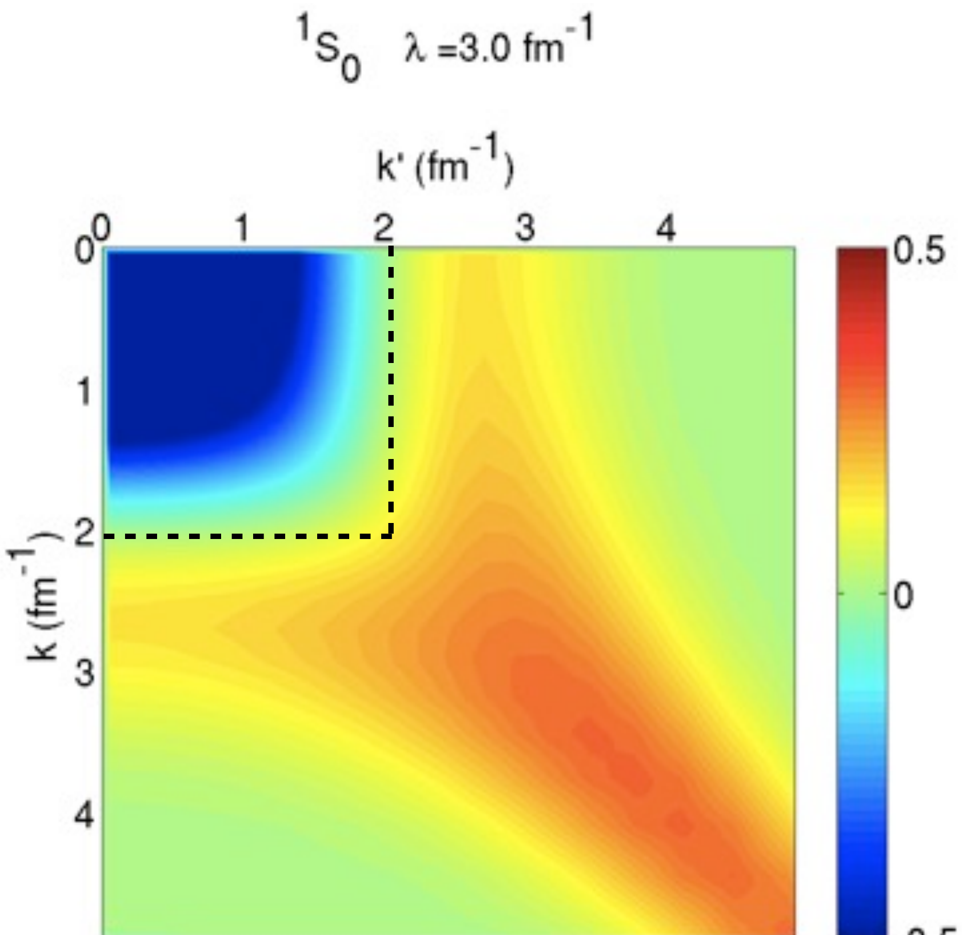

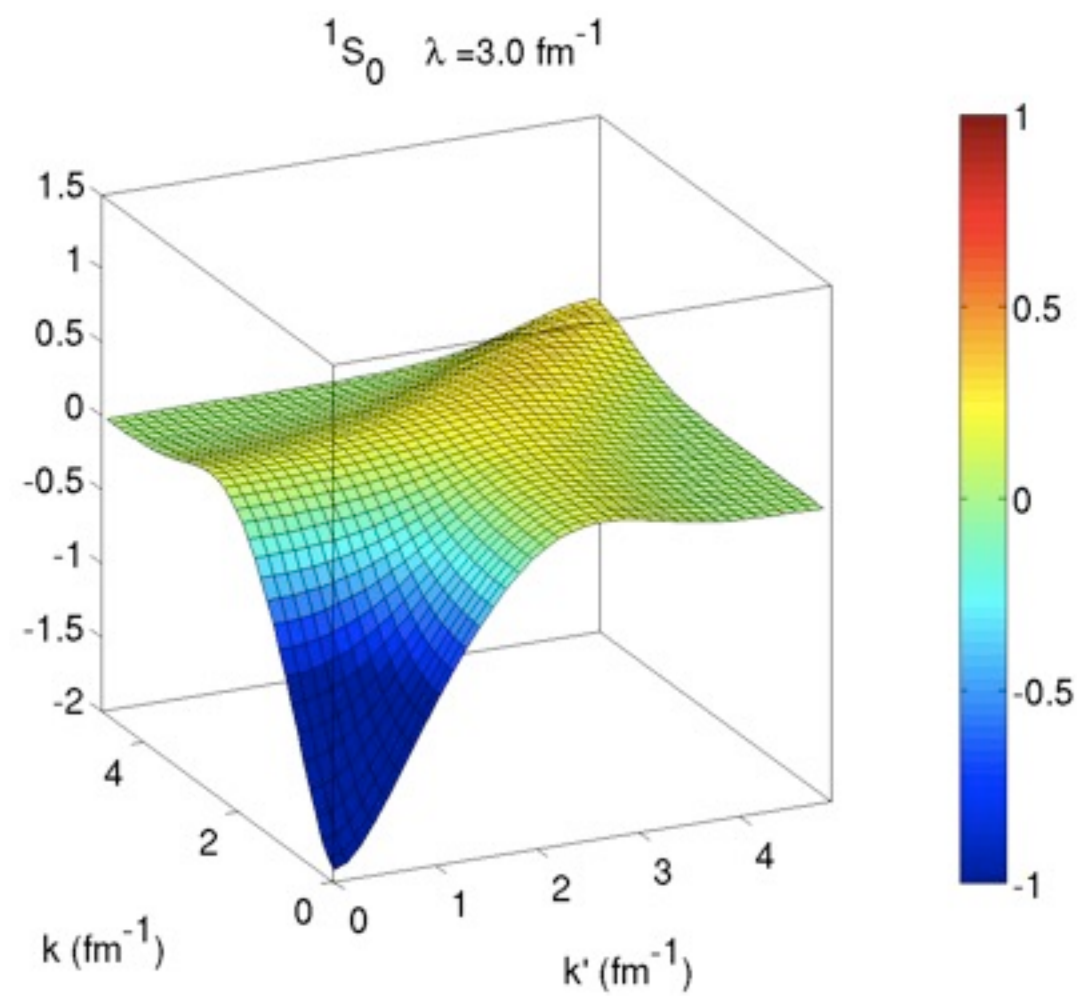

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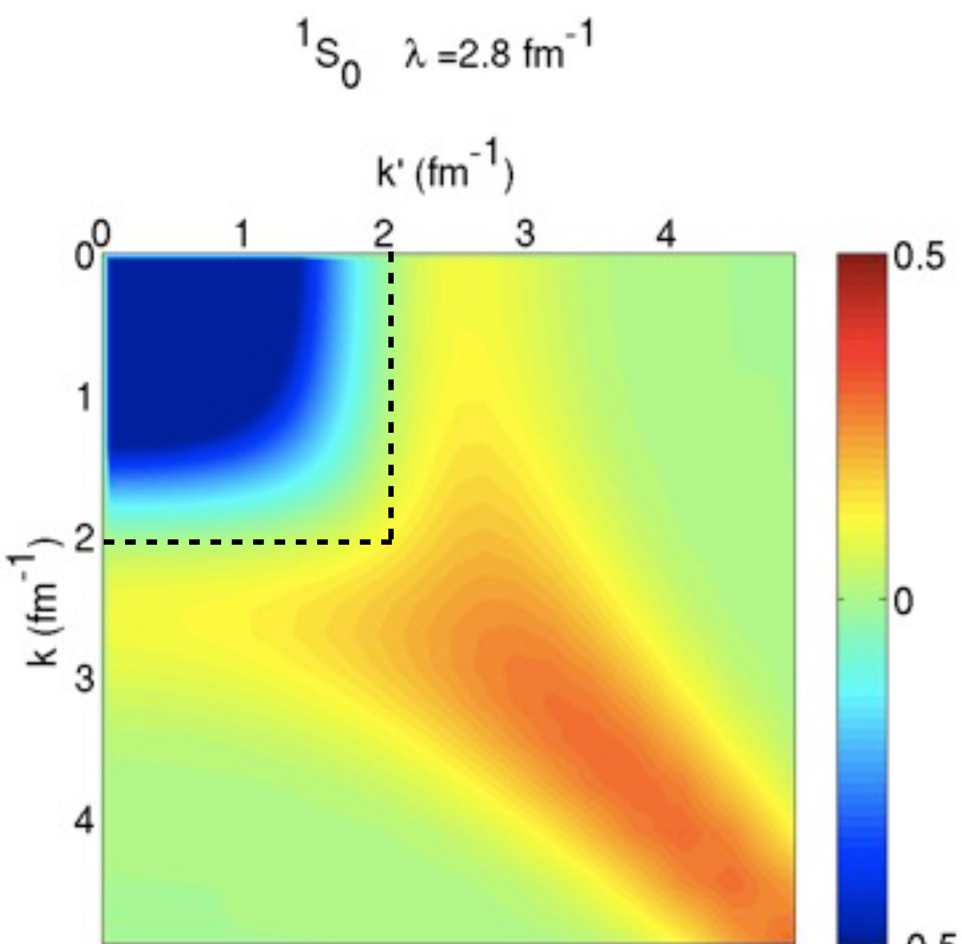

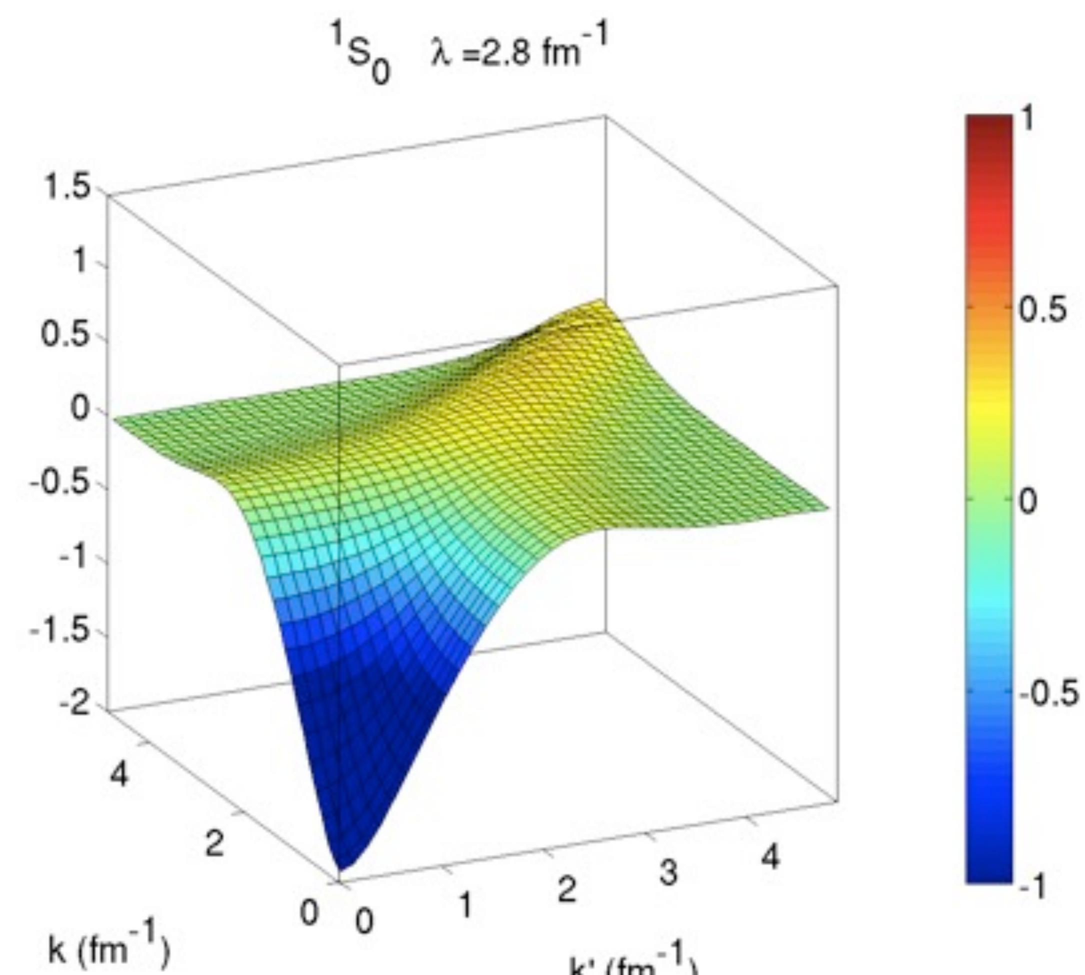

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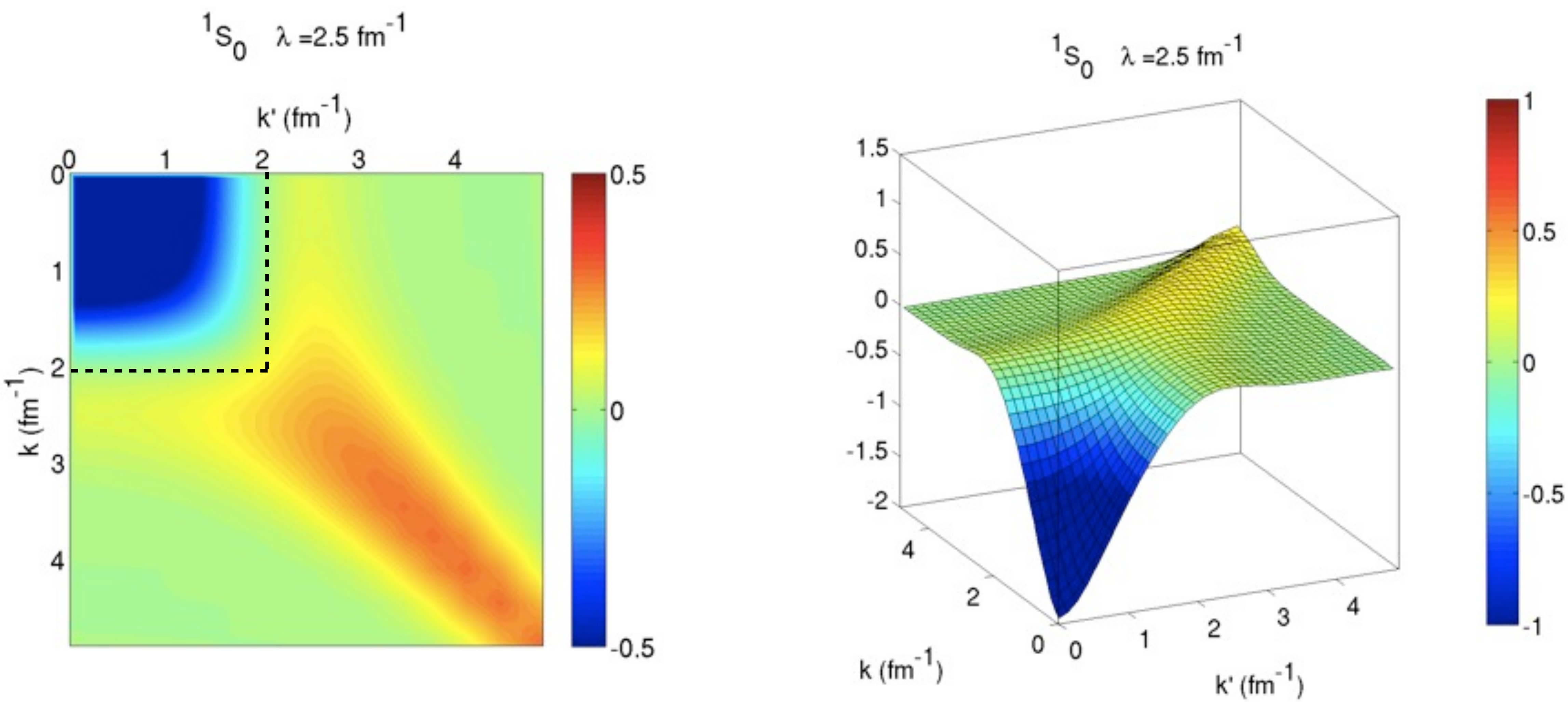

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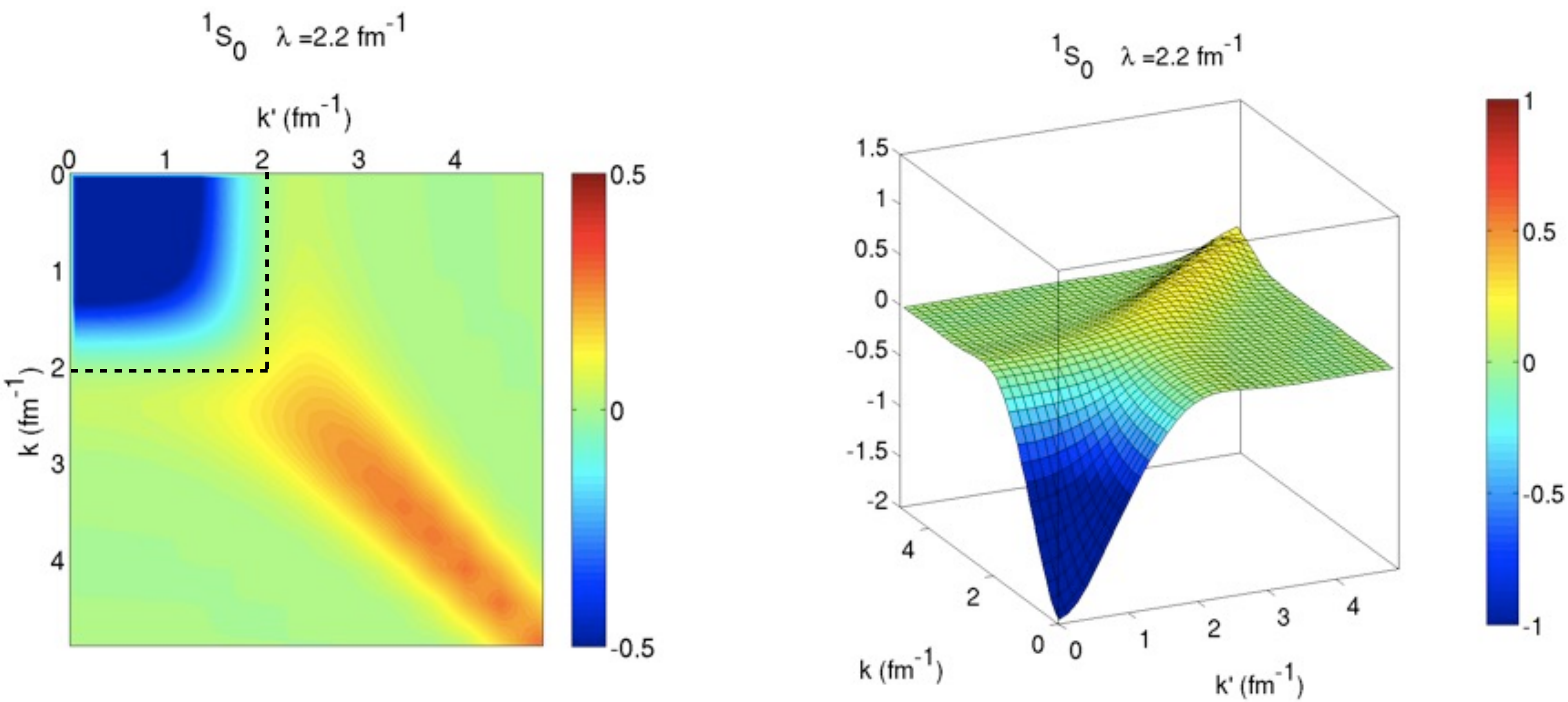

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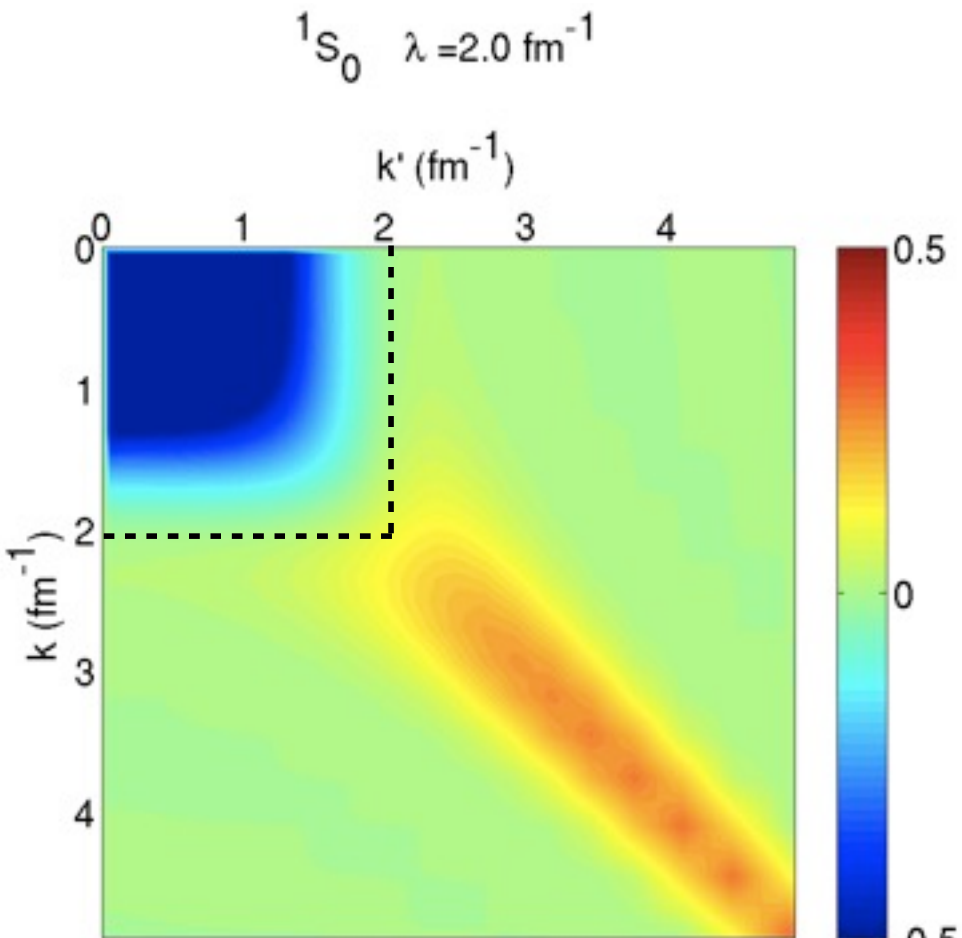
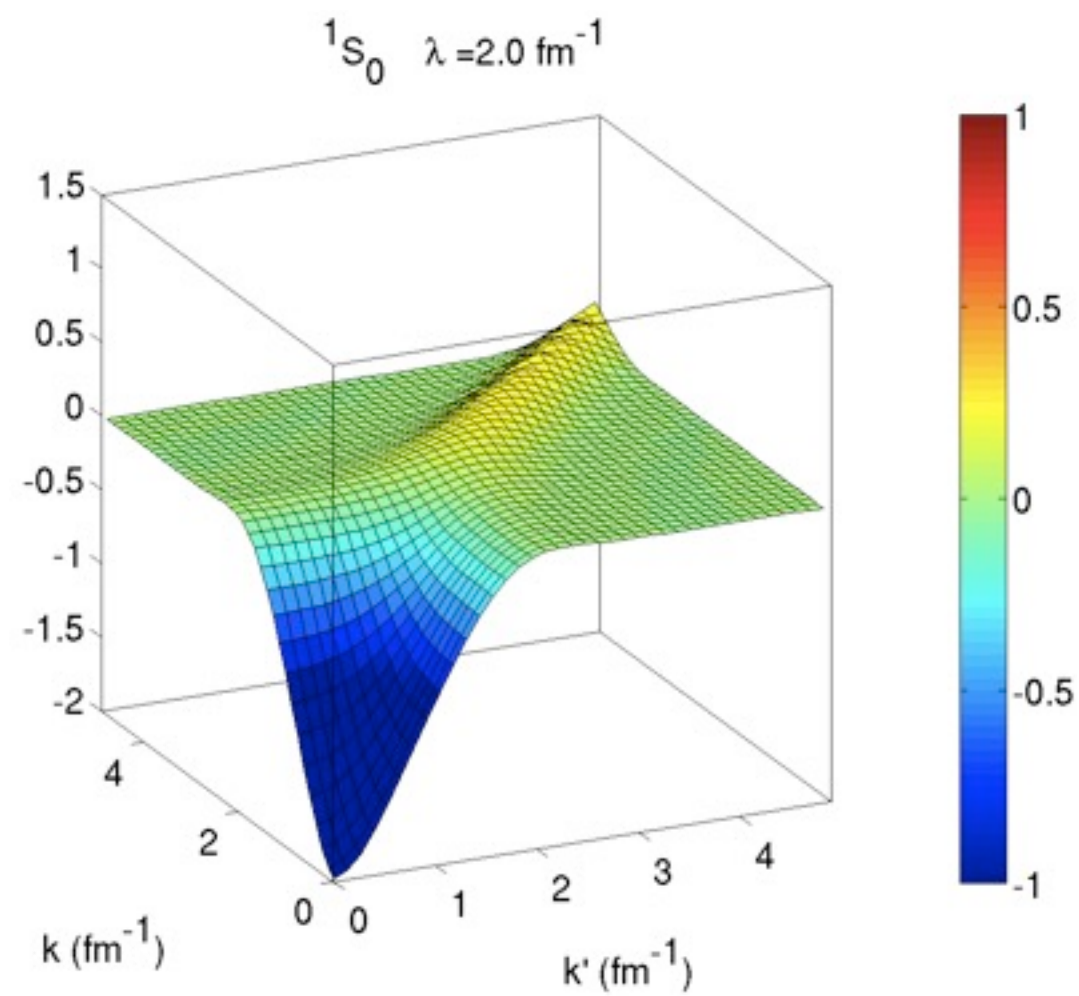
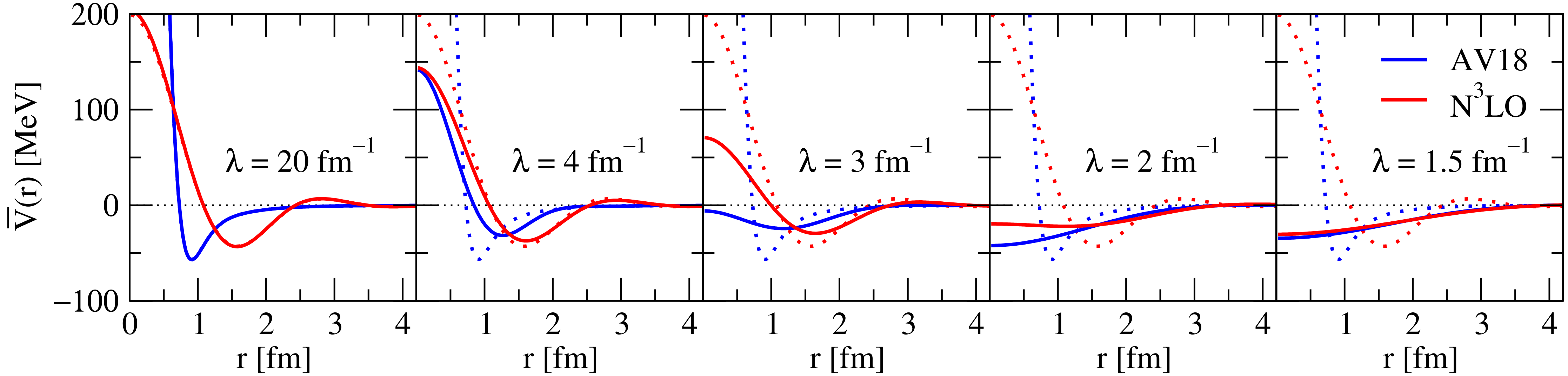
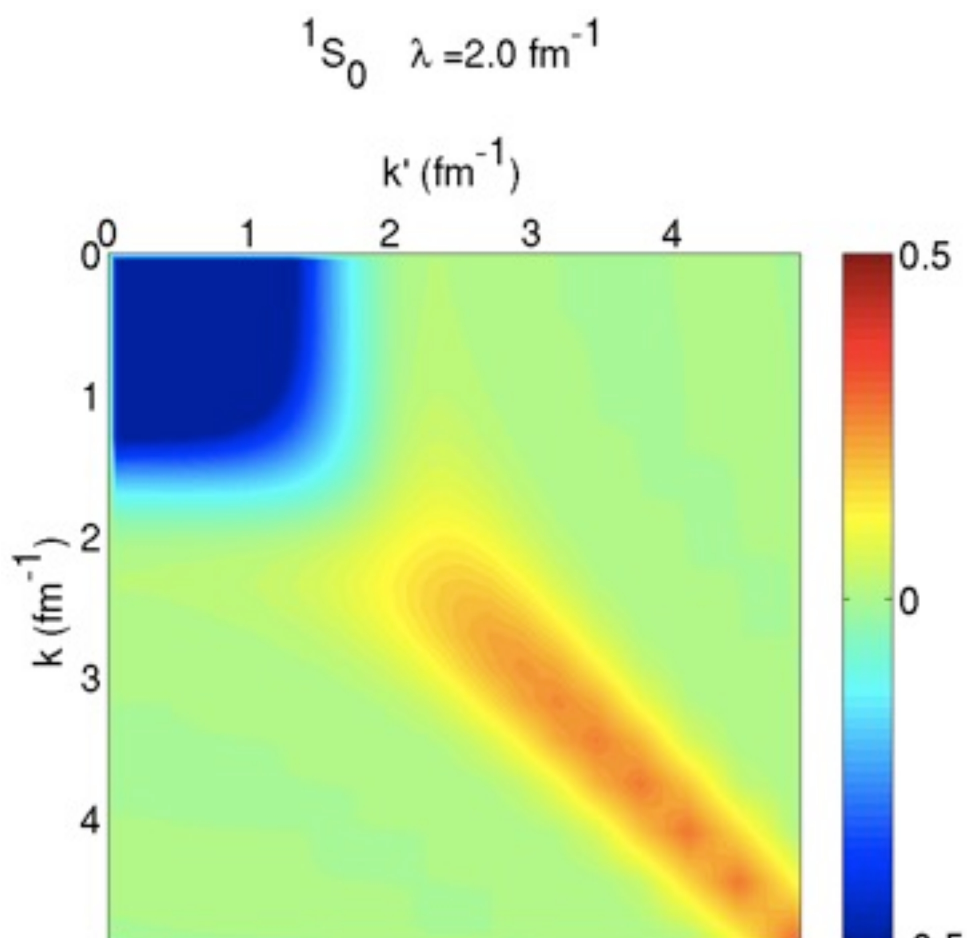


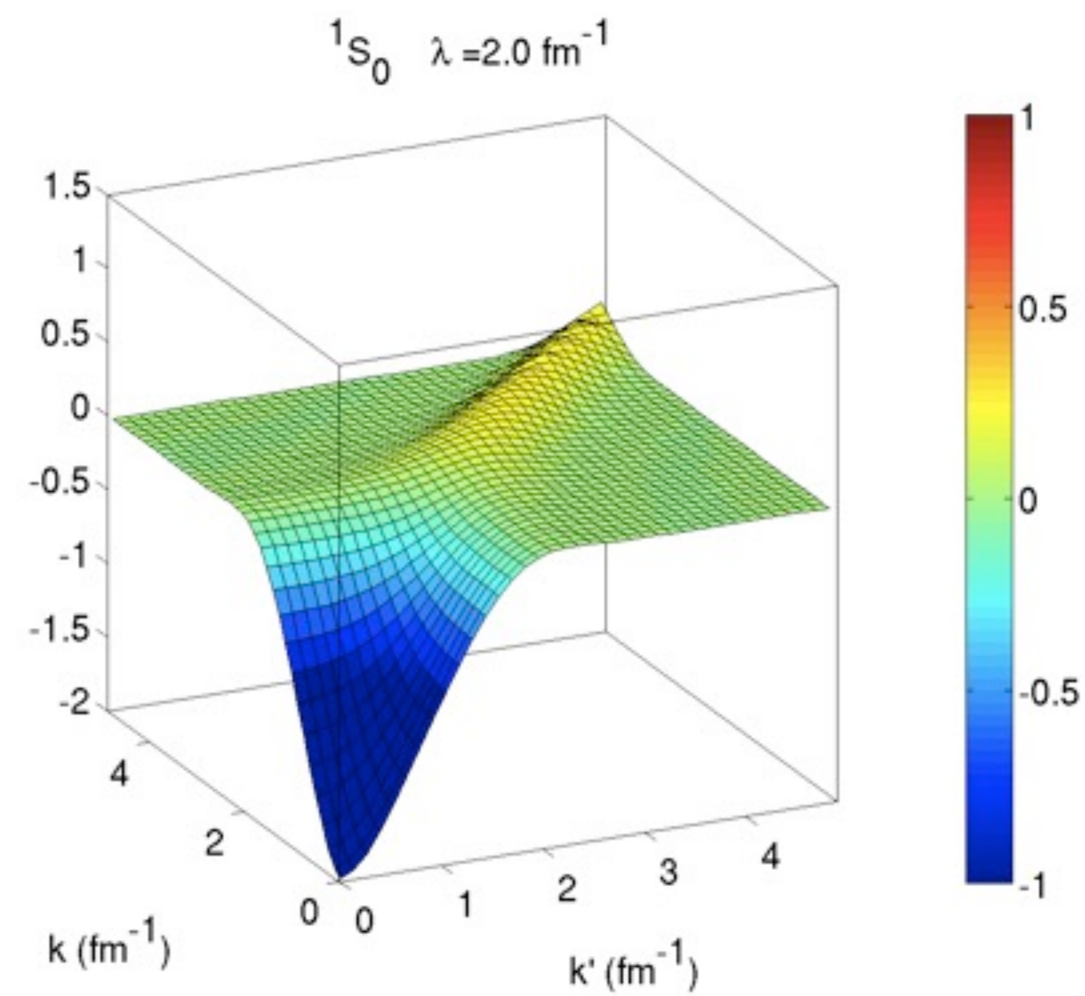


Systematic decoupling of high-momentum physics: The Similarity Renormalization Group

$$\overline{V}_\lambda(r) = \int dr' r'^2 V_\lambda(r, r')$$







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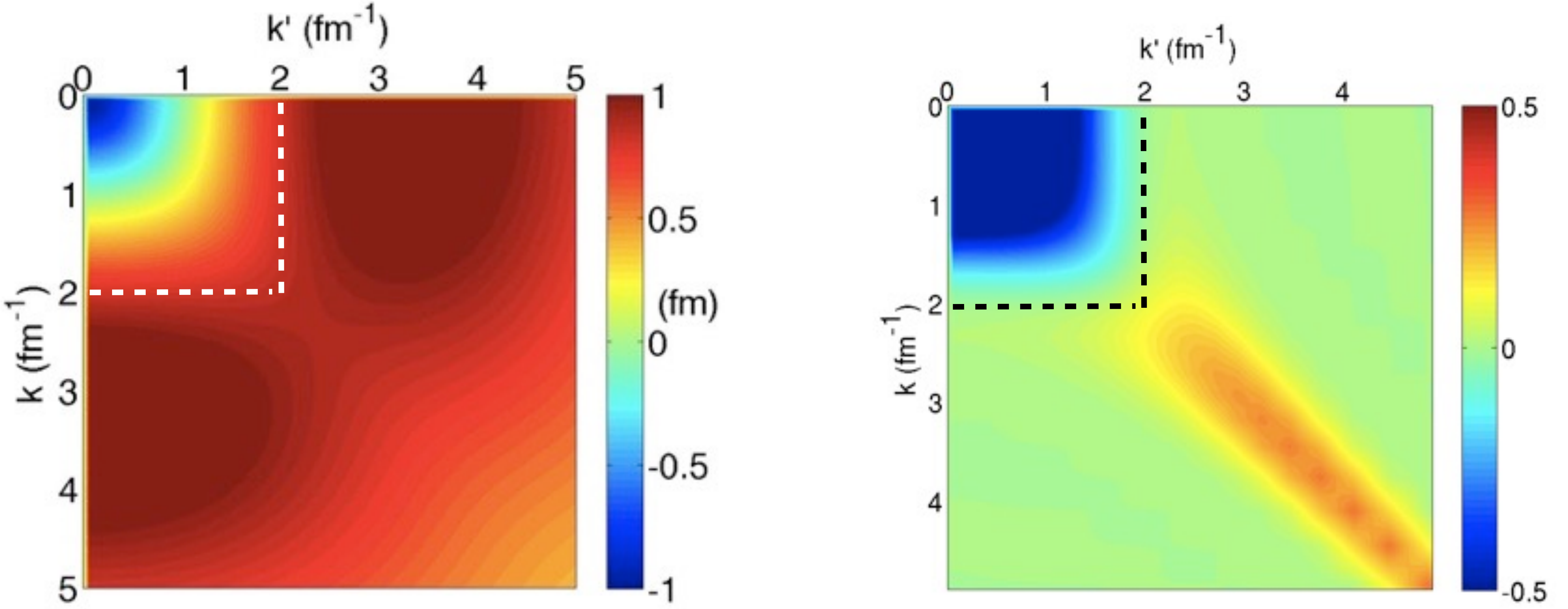
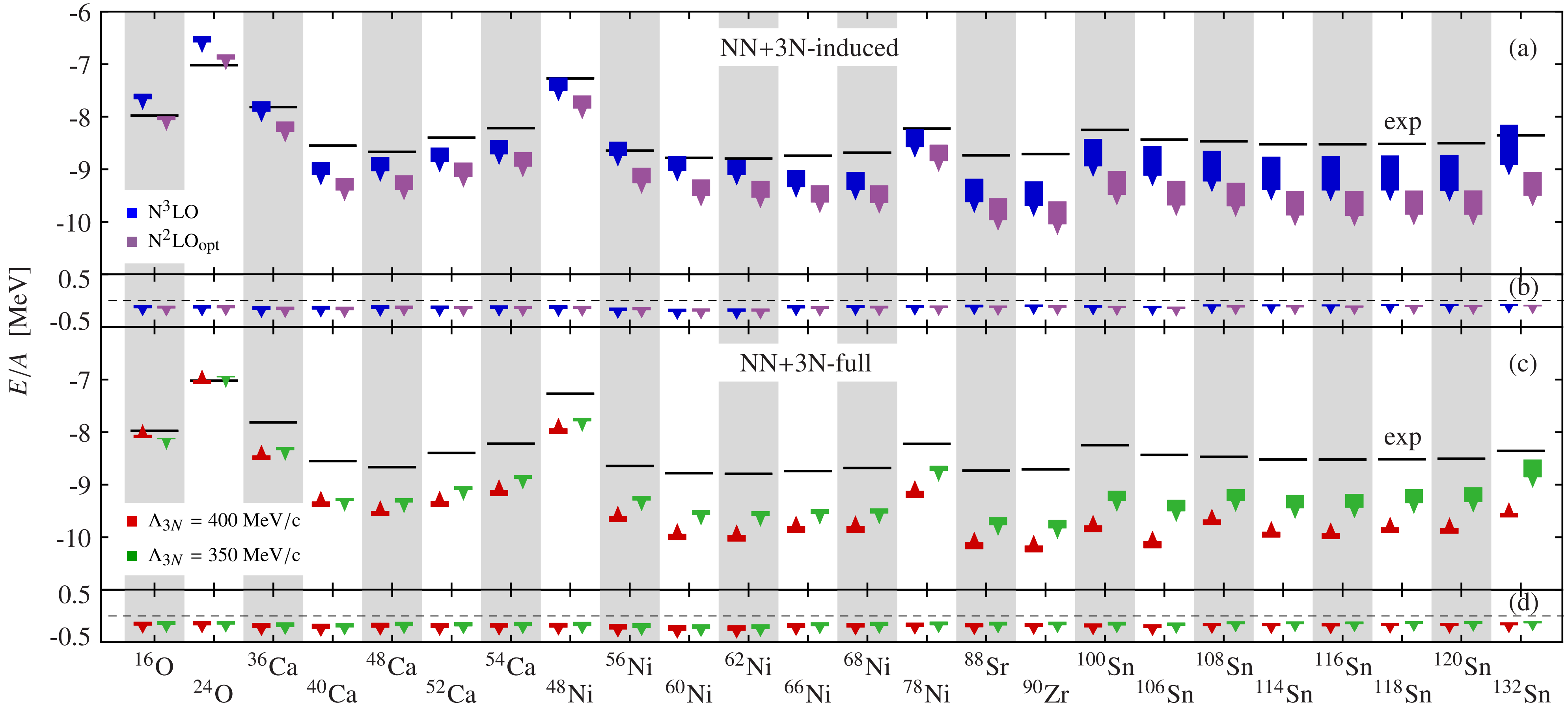
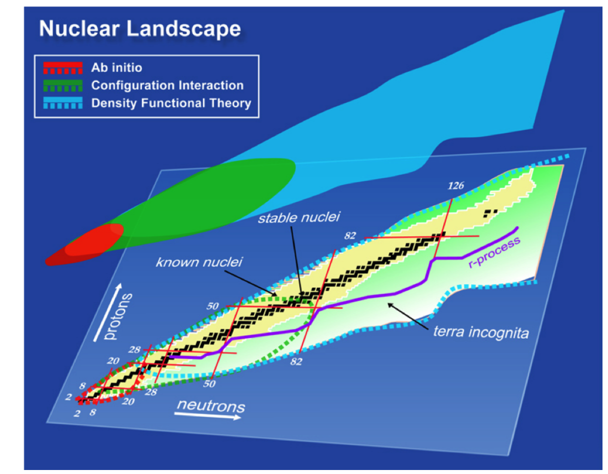


- elimination of coupling between low- and high momentum components,
  ⟶ simplified many-body calculations, smaller required model spaces
- observables unaffected by resolution change (for exact calculations)
- residual resolution dependences can be used as tool to test calculations

Not the full story:
RG transformation also changes three-body (and higher-body) interactions.

Recent advances in ab-initio many-body theory





Binder et al. , Phys. Lett B 736, 119 (2014)

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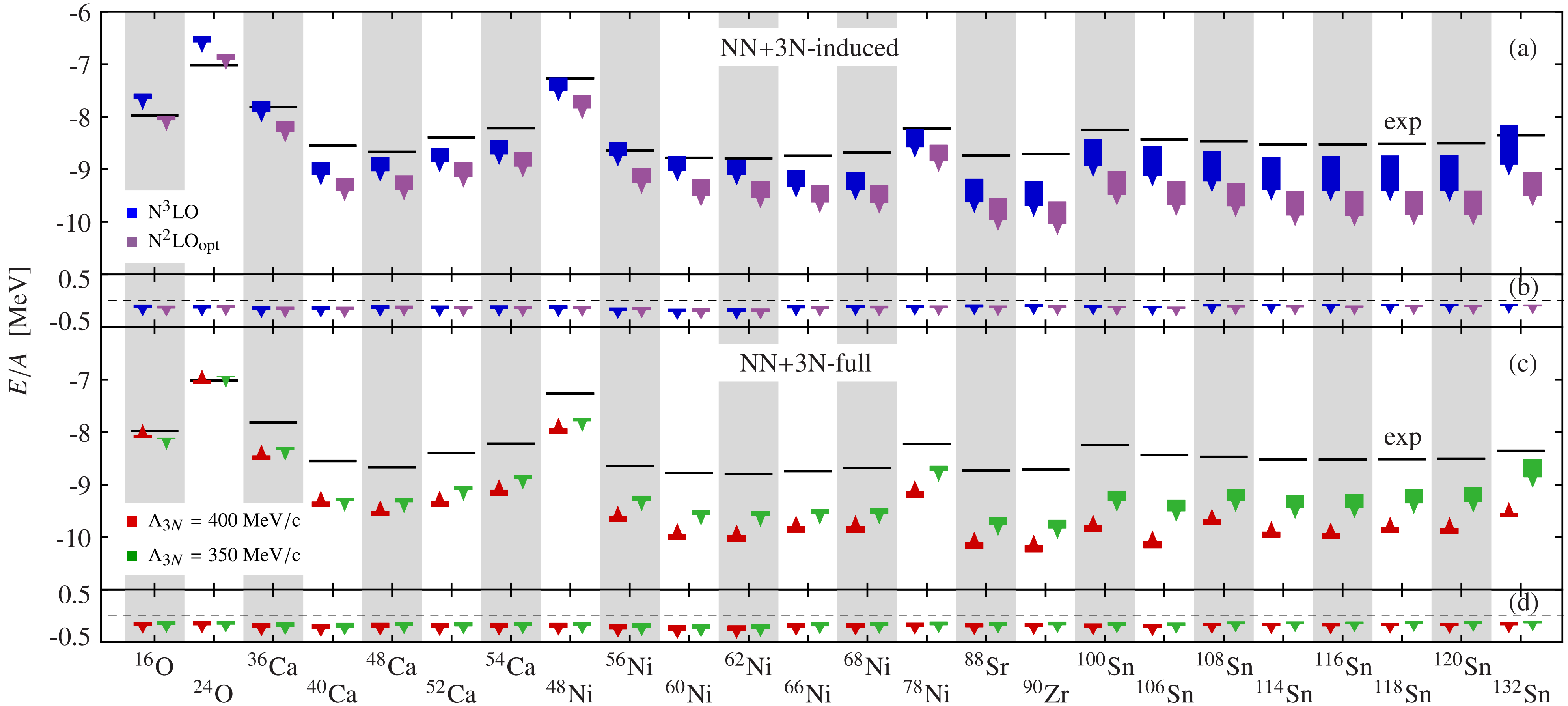

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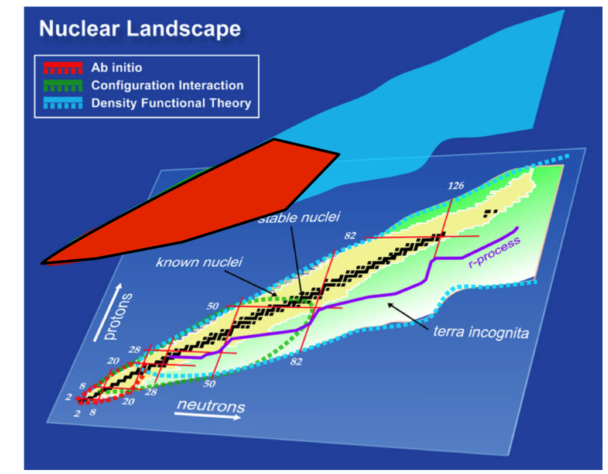
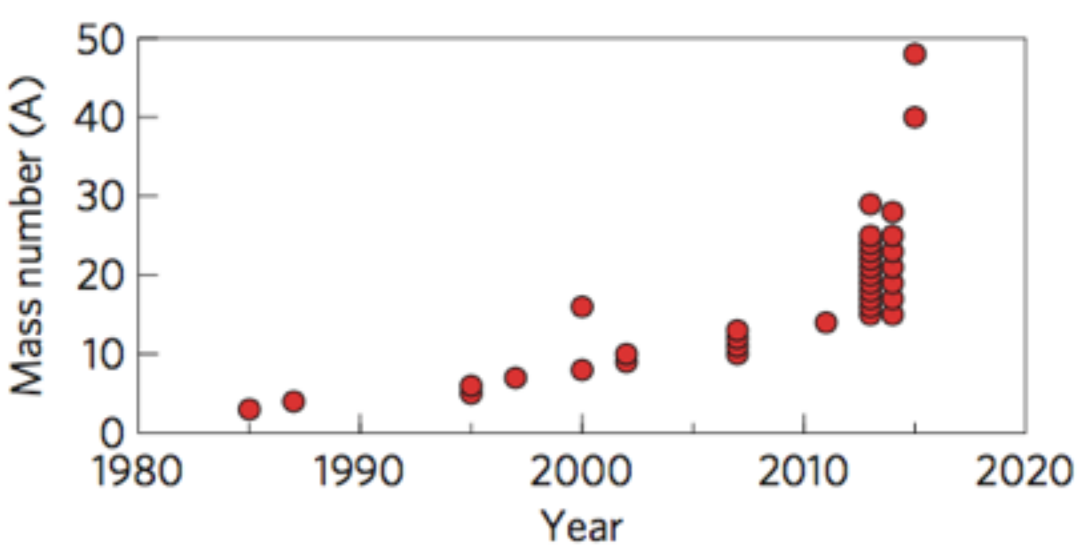
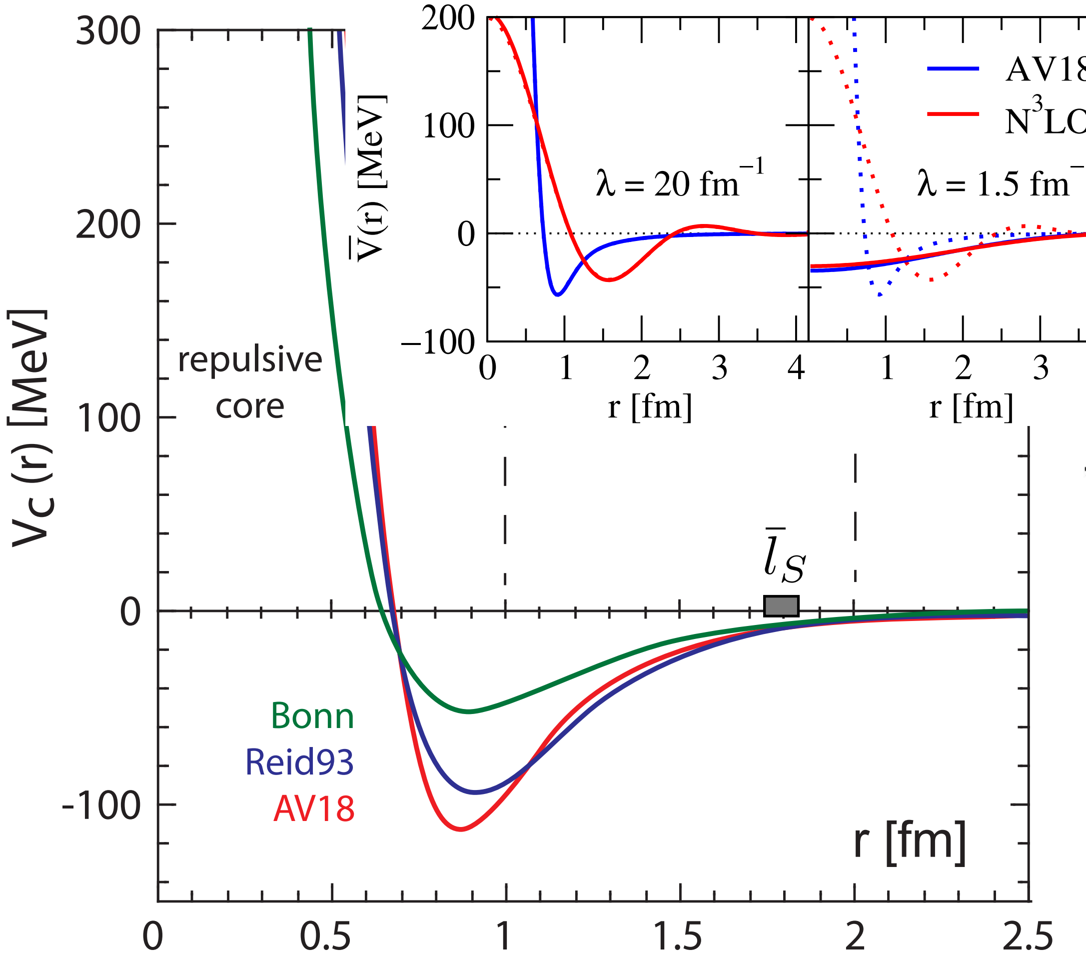


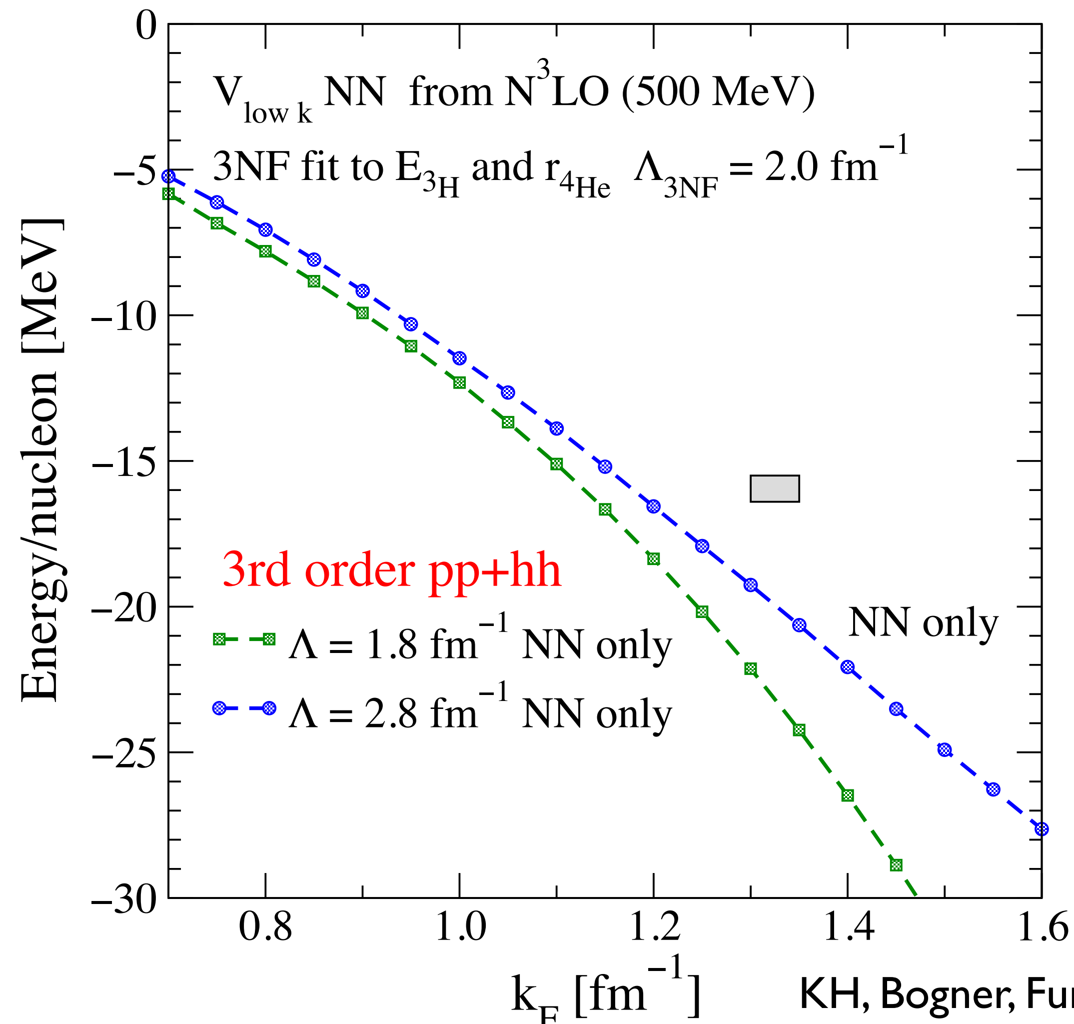


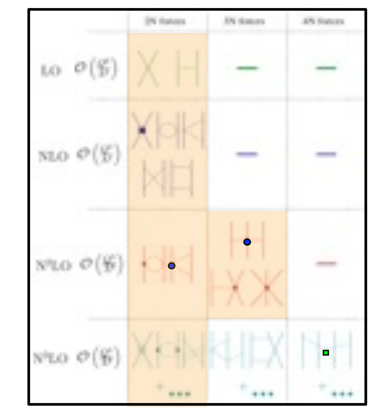
Hagen et al., Nature Physics 12, 186 (2016)

- spectacular increase in range of applicability of *ab initio* many body frameworks
- significant overbinding in heavy nuclei for presently used nuclear interactions

Fitting the 3NF LECs at low resolution scales







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

"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)

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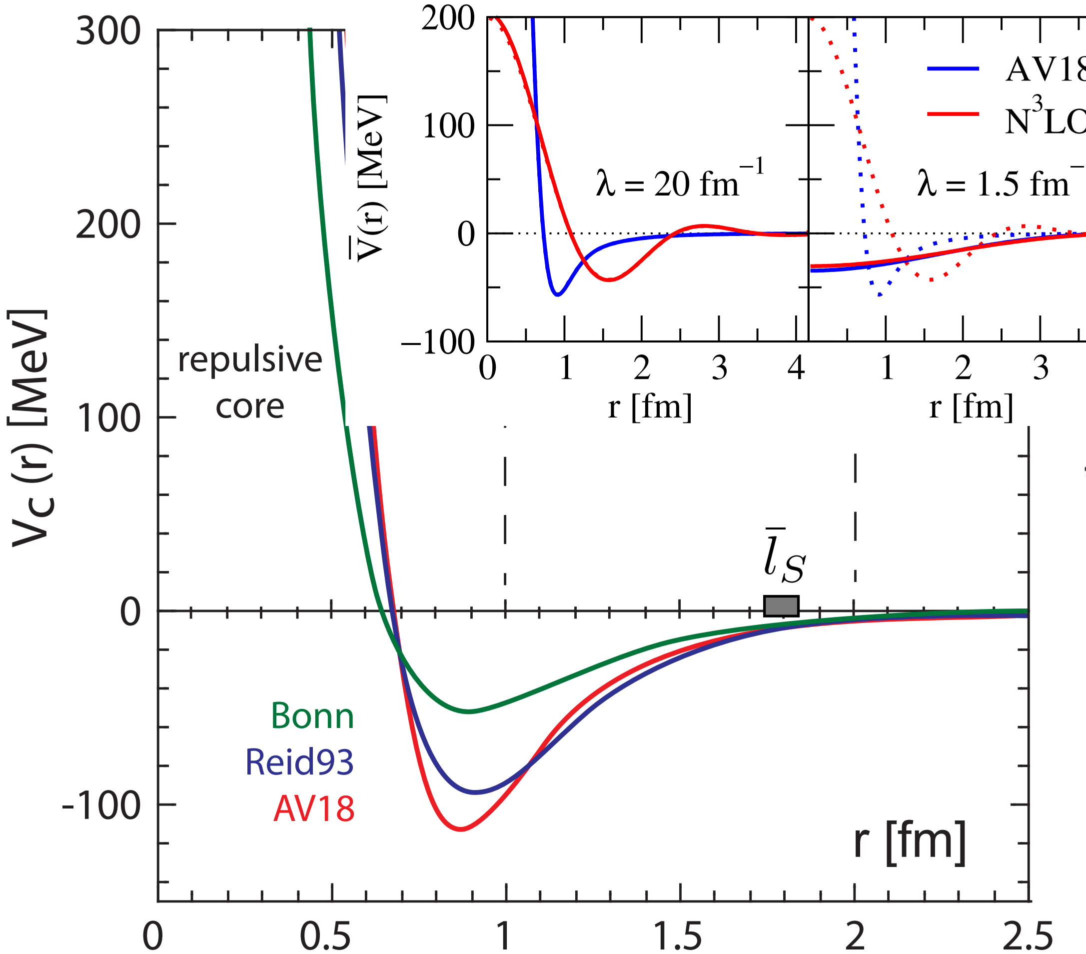

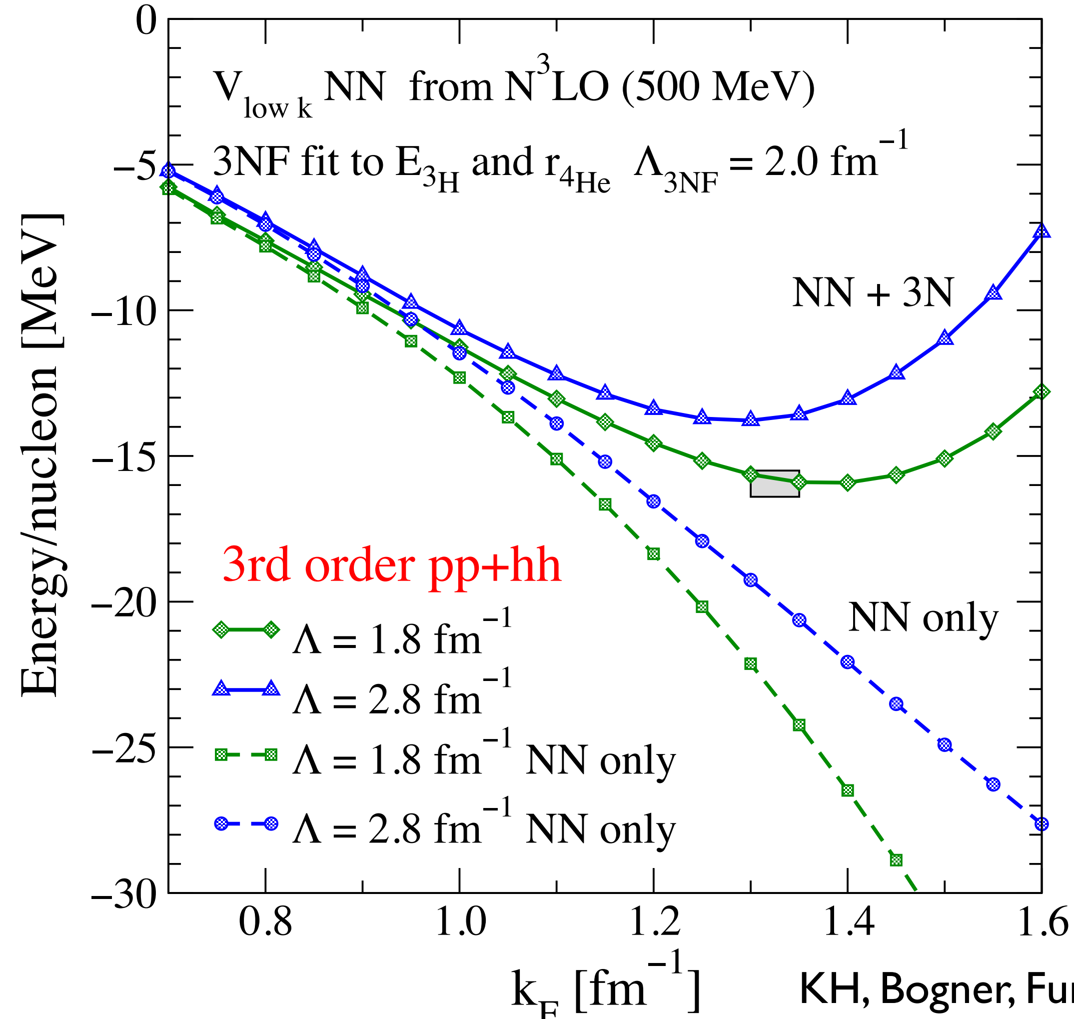

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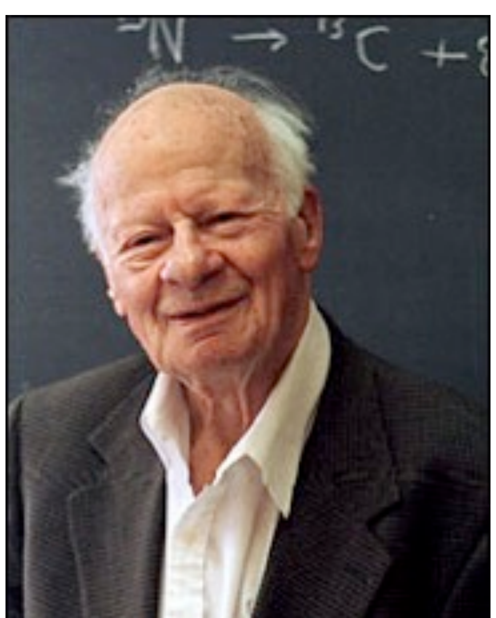

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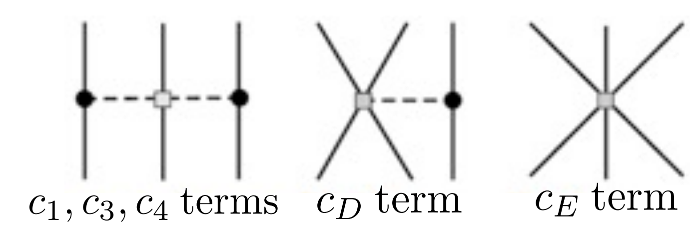
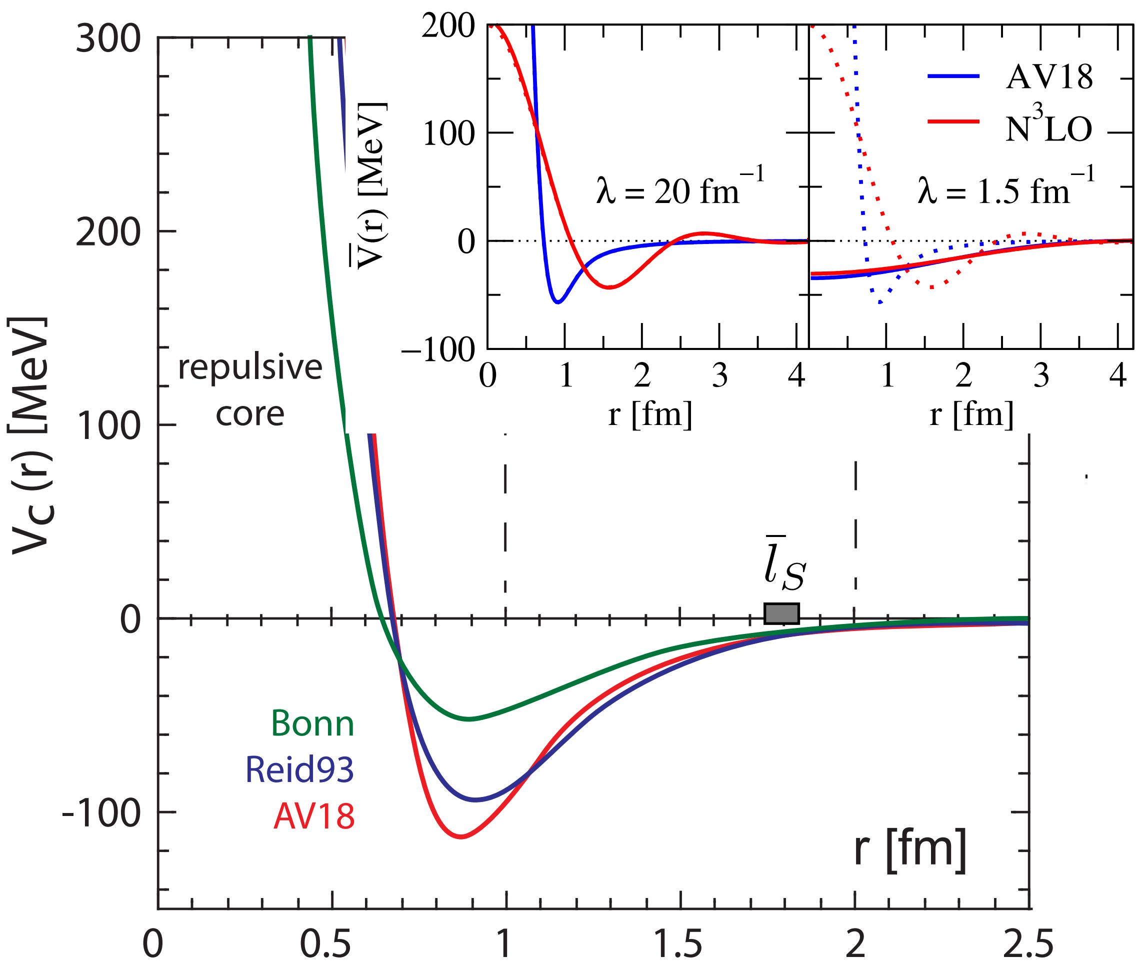
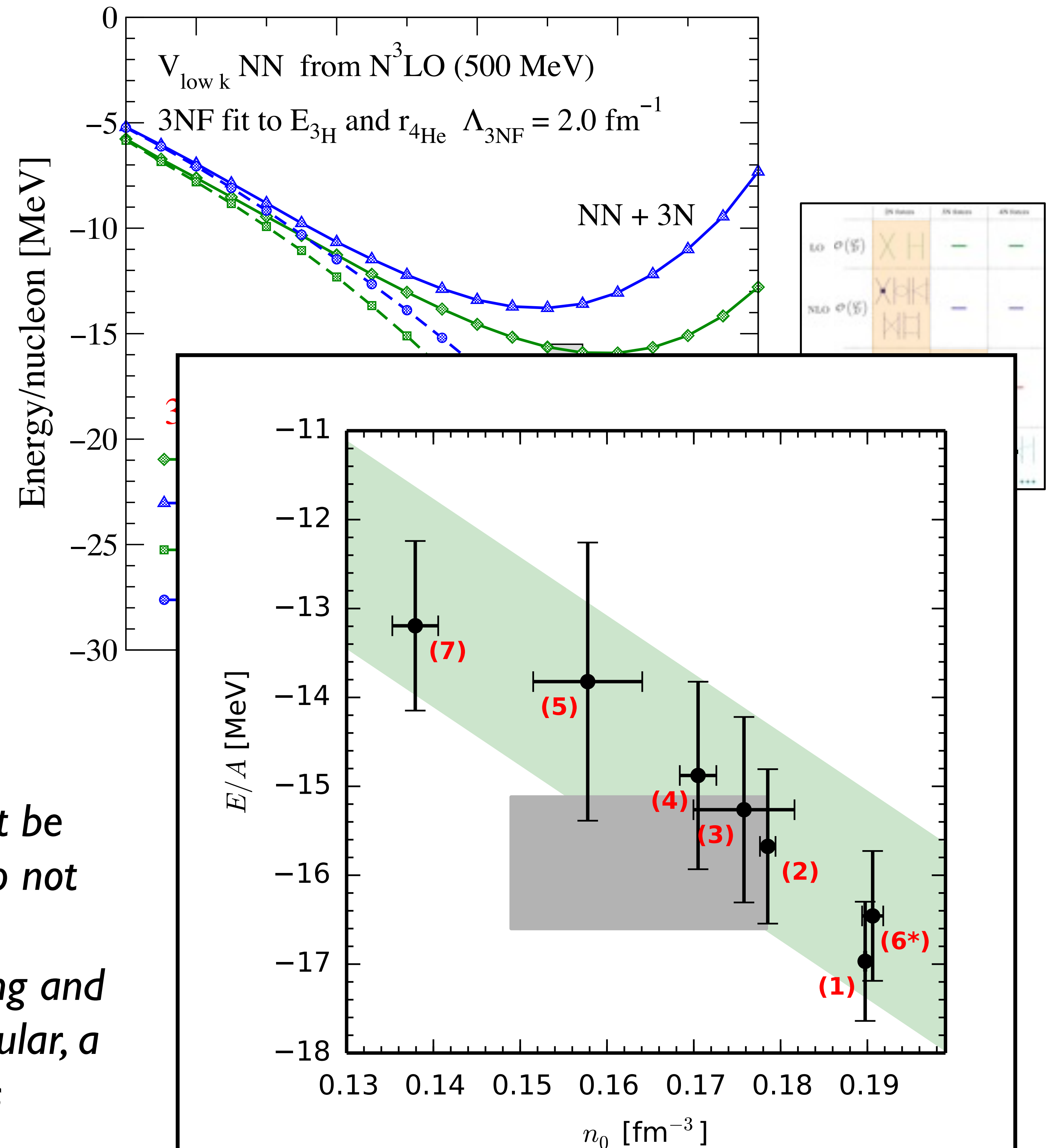
intermediate (c_D) and short-range (c_E) 3NF couplings fitted to few-body systems at different resolution scales:

$$E_{^3\mathrm{H}} = -8.482\,\mathrm{MeV} \qquad r_{^4\mathrm{He}} = 1.464\,\mathrm{fm}$$



Fitting the 3NF LECs at low resolution scales



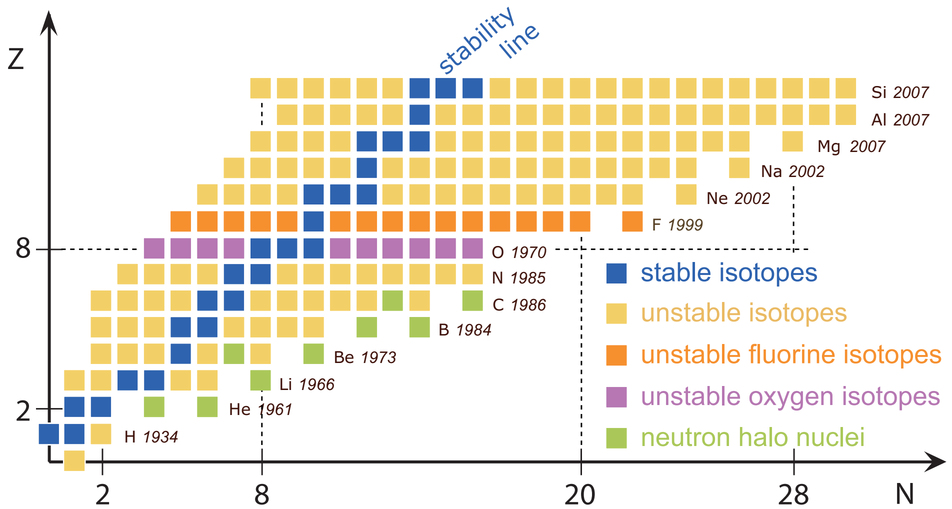


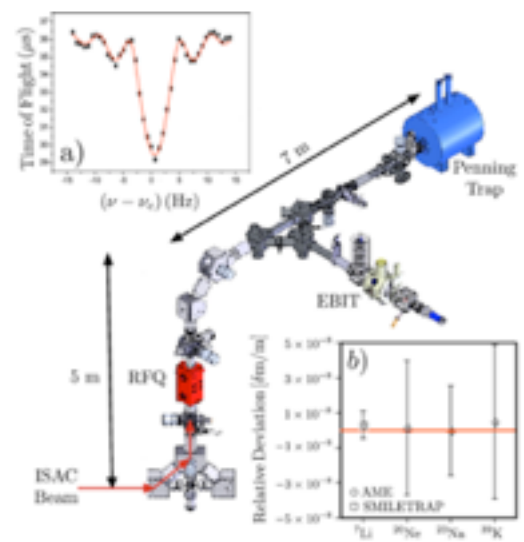
Drischler, KH, Schwenk, arXiv:1510.06728

"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)

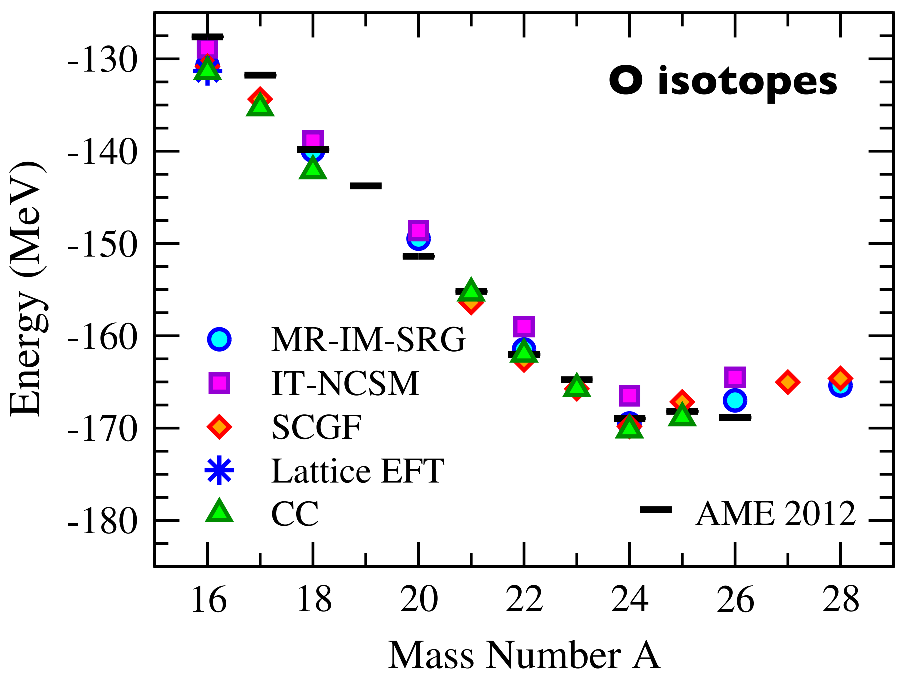
Studies of neutron-rich nuclei

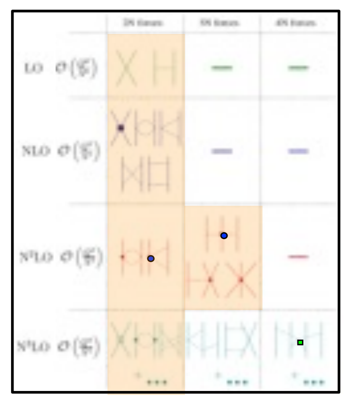


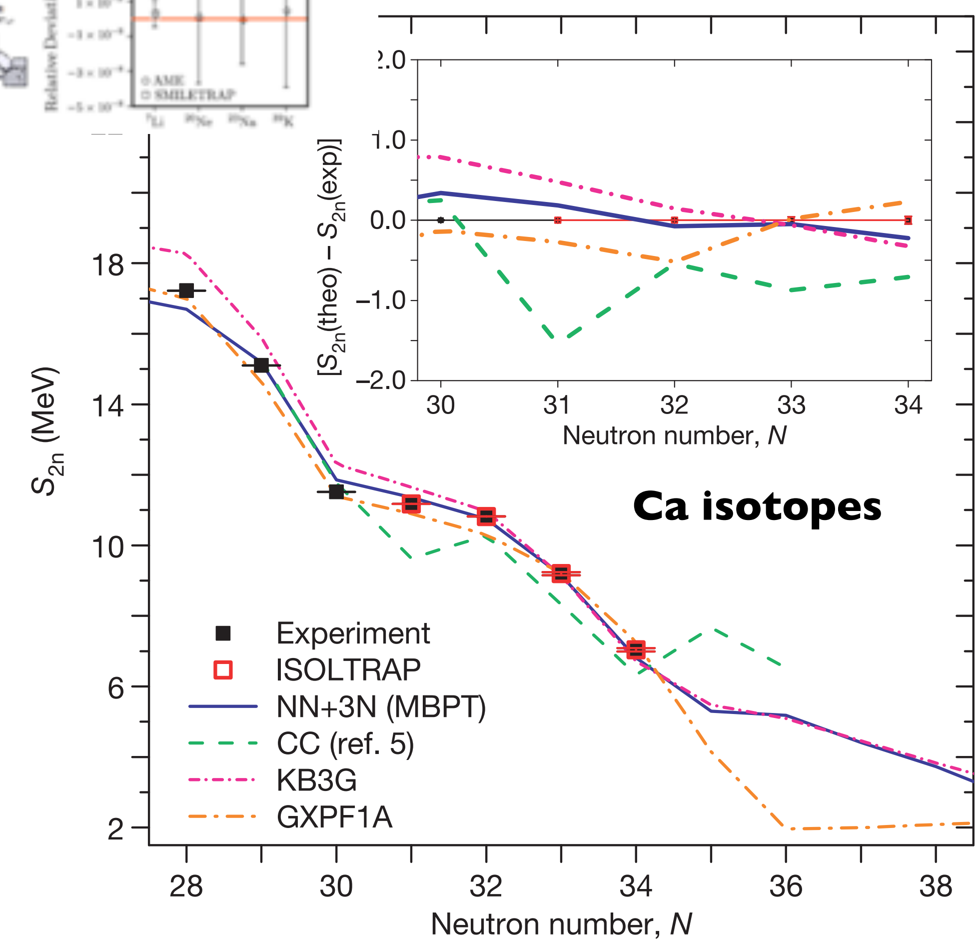


Gallant et al.
PRL 109, 032506 (2012)

Wienholtz et al.
Nature 498, 346 (2013)



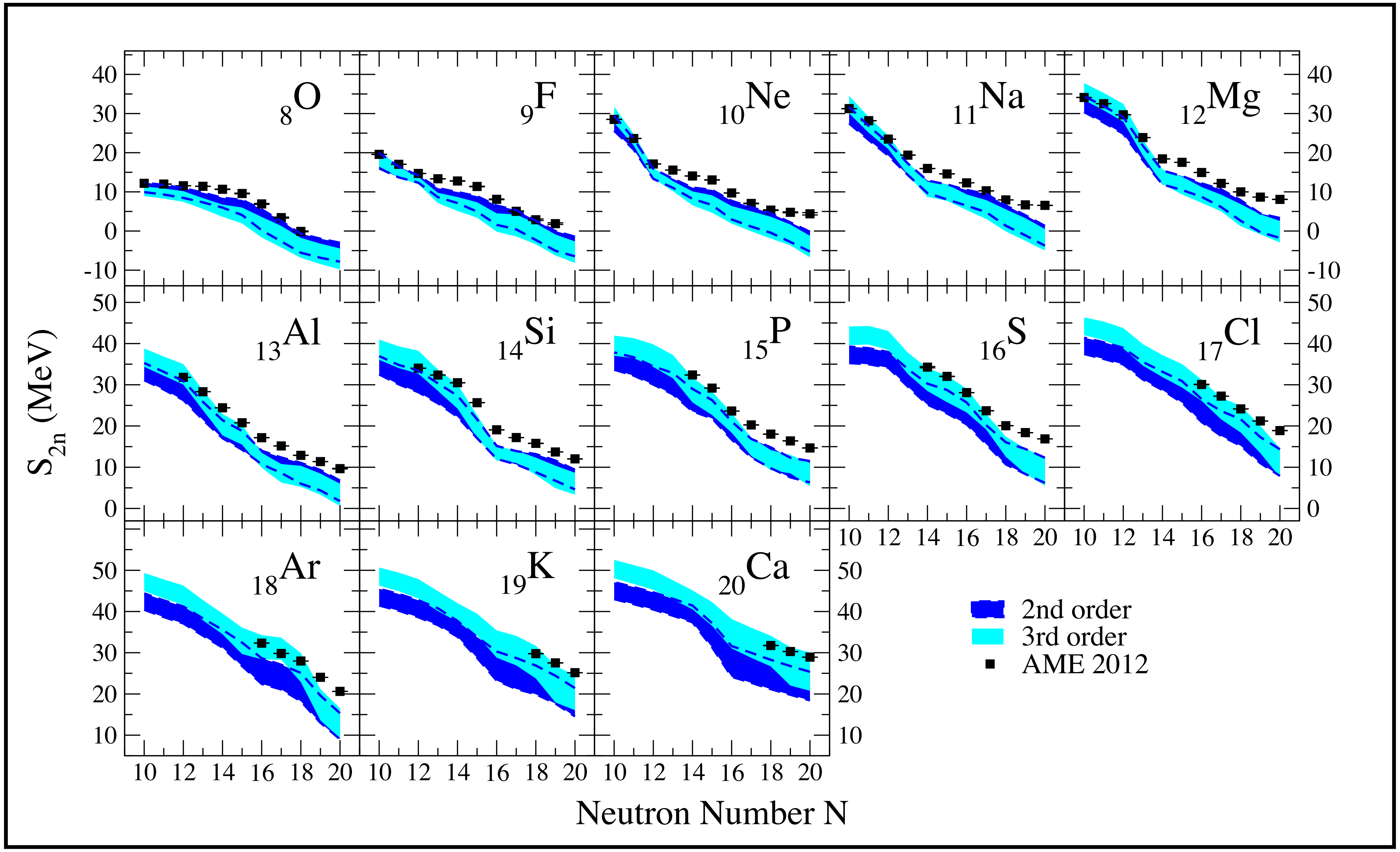




KH et al., Ann. Rev. Nucl. Part. Sci. 165, 457 (2015)

- remarkable agreement between different many-body frameworks
- excellent agreement between theory and experiment for masses of oxygen and calcium isotopes based on specific chiral interactions
- need to quantify theoretical uncertainties

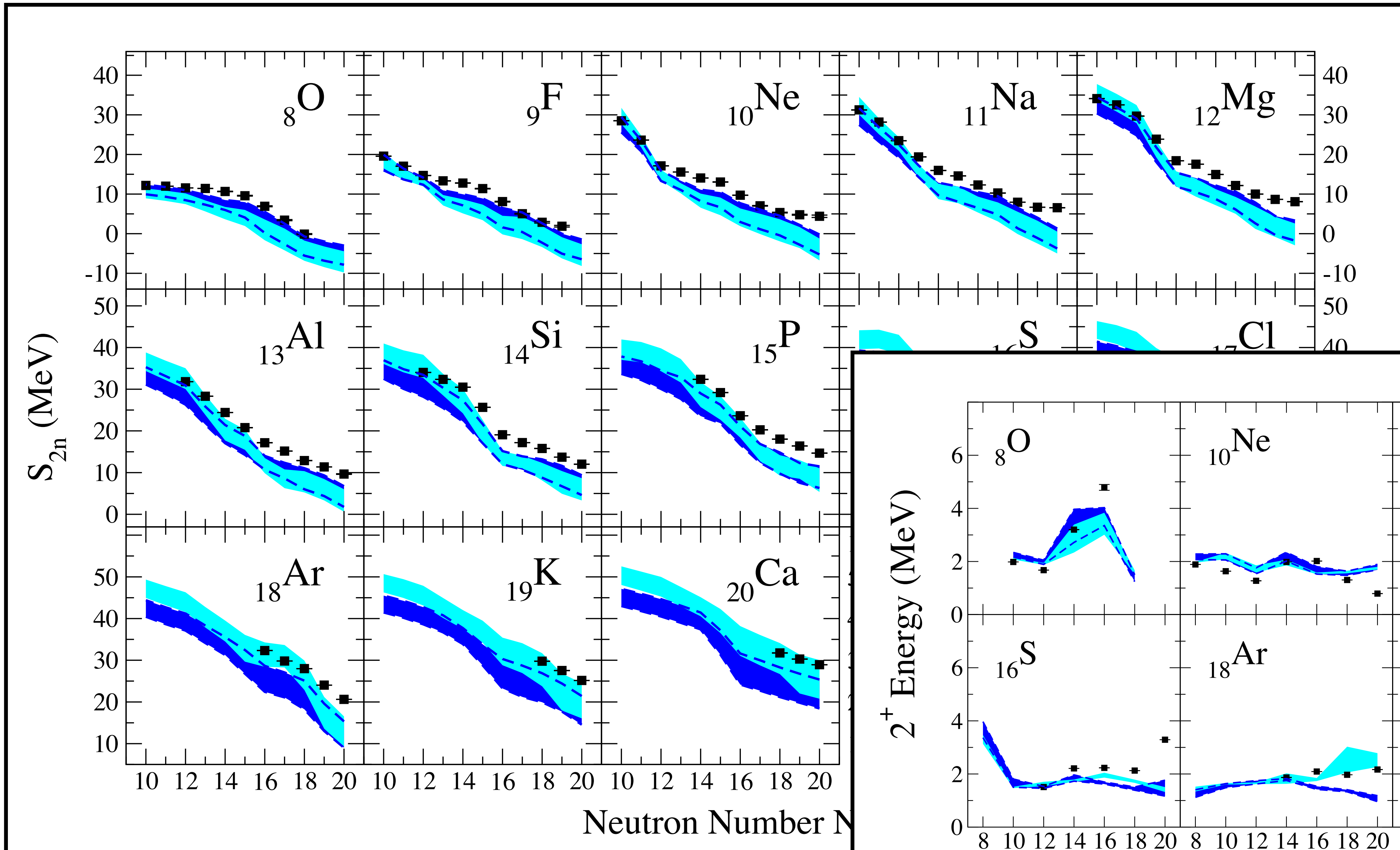
Towards theoretical uncertainty quantification

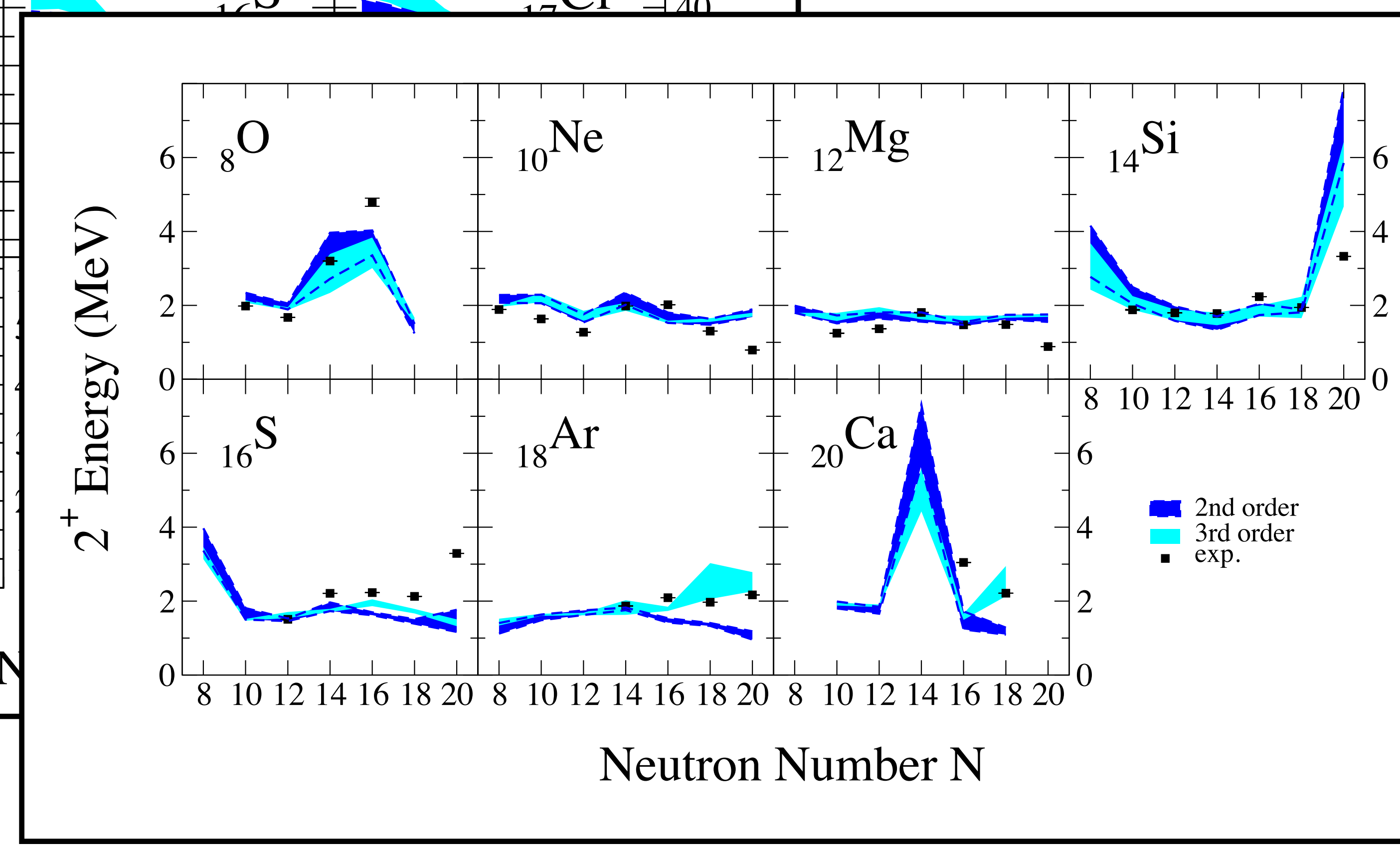


Simonis, KH, Holt, Menendez, Schwenk,
Phys. Rev. C93, 011302(R) (2016)

- calculations based on NN+3N interactions fitted to NN, 3N and 4N systems
- reasonable reproduction of experimental trends
- uncertainties dominated by differences in nuclear Hamiltonians

Towards theoretical uncertainty quantification





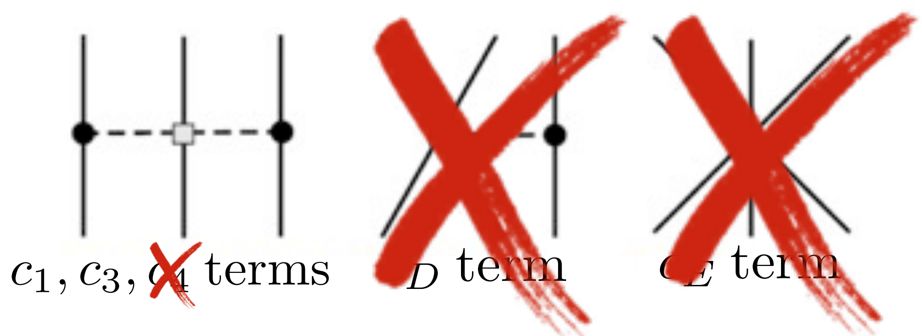
Simonis, KH, Holt, Menendez, Schwenk,
Phys. Rev. C93, 011302(R) (2016)

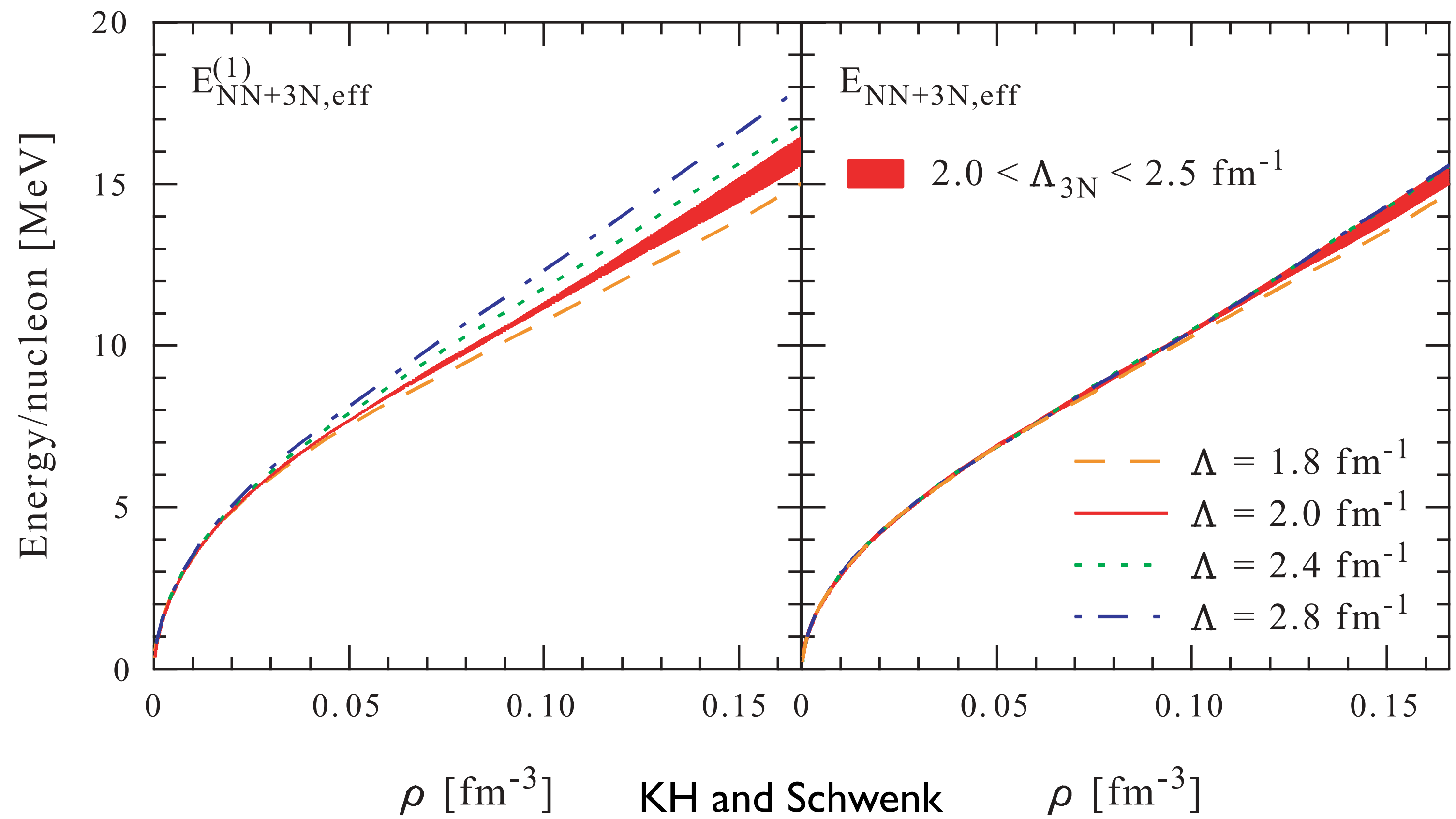
- calculations based on NN+3N interactions fitted to NN, 3N and 4N systems
- reasonable reproduction of experimental trends
- uncertainties dominated by differences in nuclear Hamiltonians

Results for the neutron matter equation of state

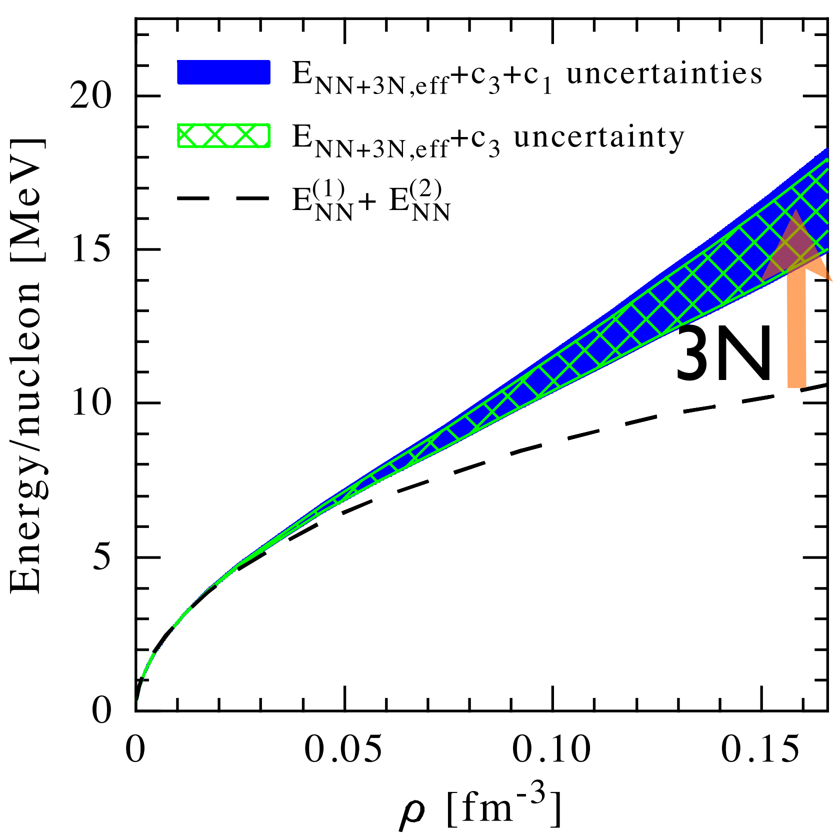
neutron matter is a **unique system** for chiral EFT:

only long-range 3NF contribute in leading order



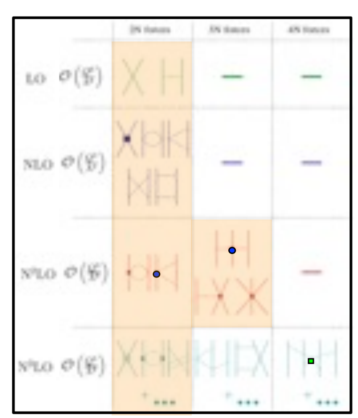


KH and Schwenk
PRC 82, 014314 (2010)



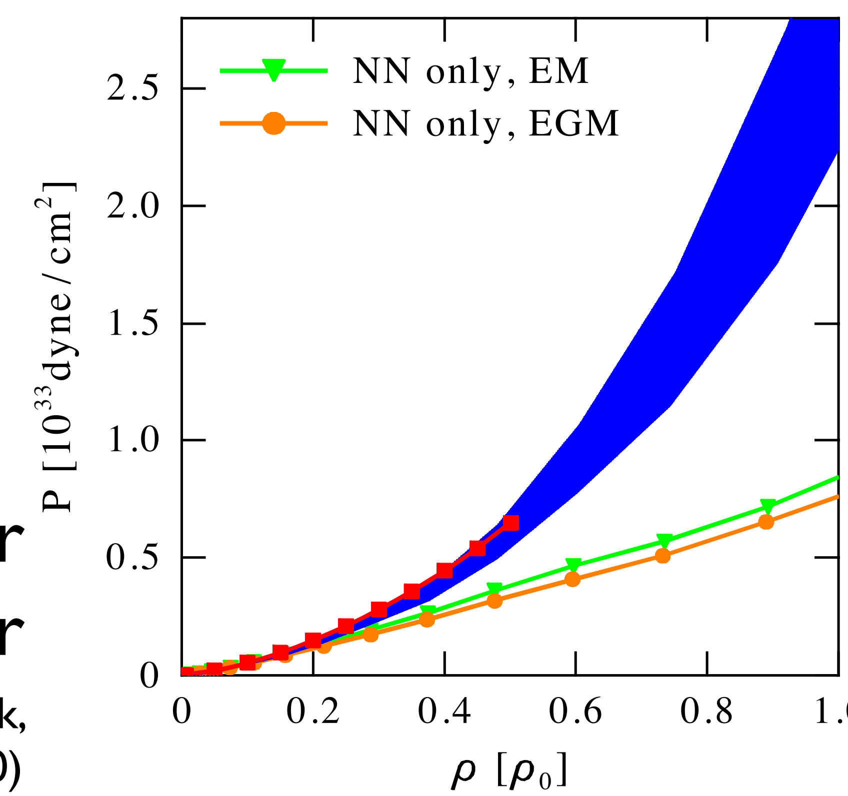
pure neutron matter

KH and Schwenk PRC 82, 014314 (2010)

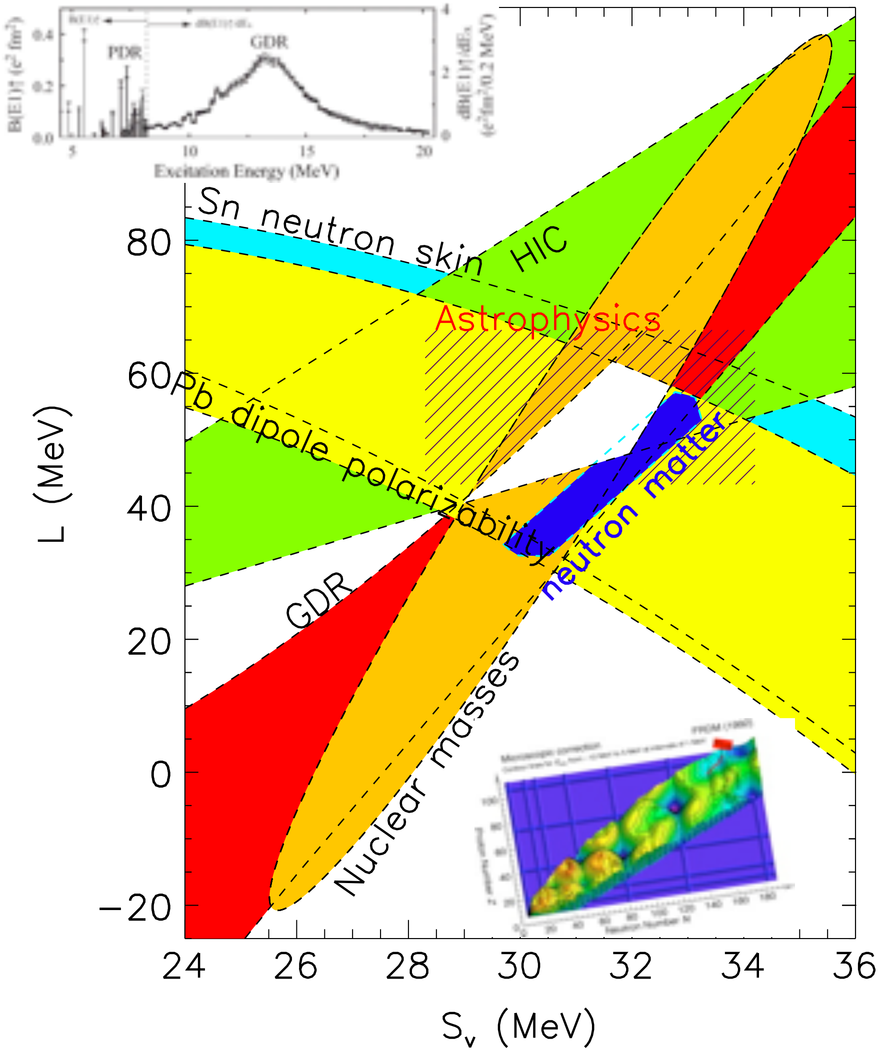


neutron star matter

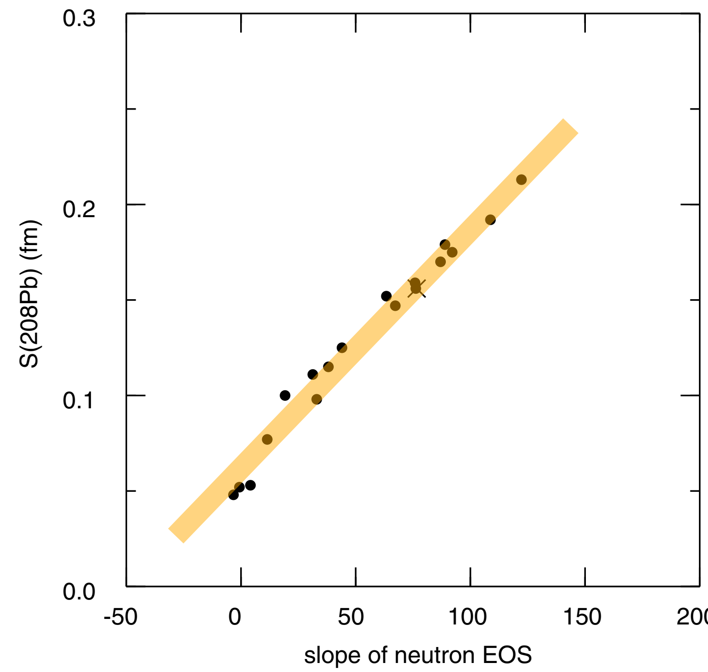
KH, Lattimer, Pethick, Schwenk,
PRL 105, 161102 (2010)



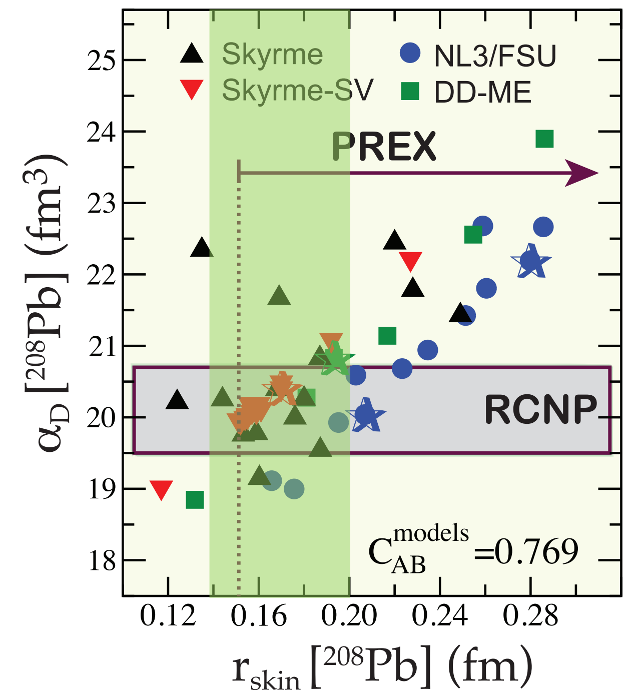
Symmetry energy and neutron skin constraints



KH, Lattimer, Pethick, Schwenk, ApJ 773, 11 (2013)



Brown,
PRL 85, 5296 (2000)



Piekarewicz,
PRC 85, 041302 (2012)

$$S_v = \left.\frac{\partial^2 E/N}{\partial^2 x}\right|_{\rho=\rho_0, x=1/2}$$

$$L = \frac{3}{8}\left.\frac{\partial^3 E/N}{\partial\rho\partial^2 x}\right|_{\rho=\rho_0, x=1/2}$$

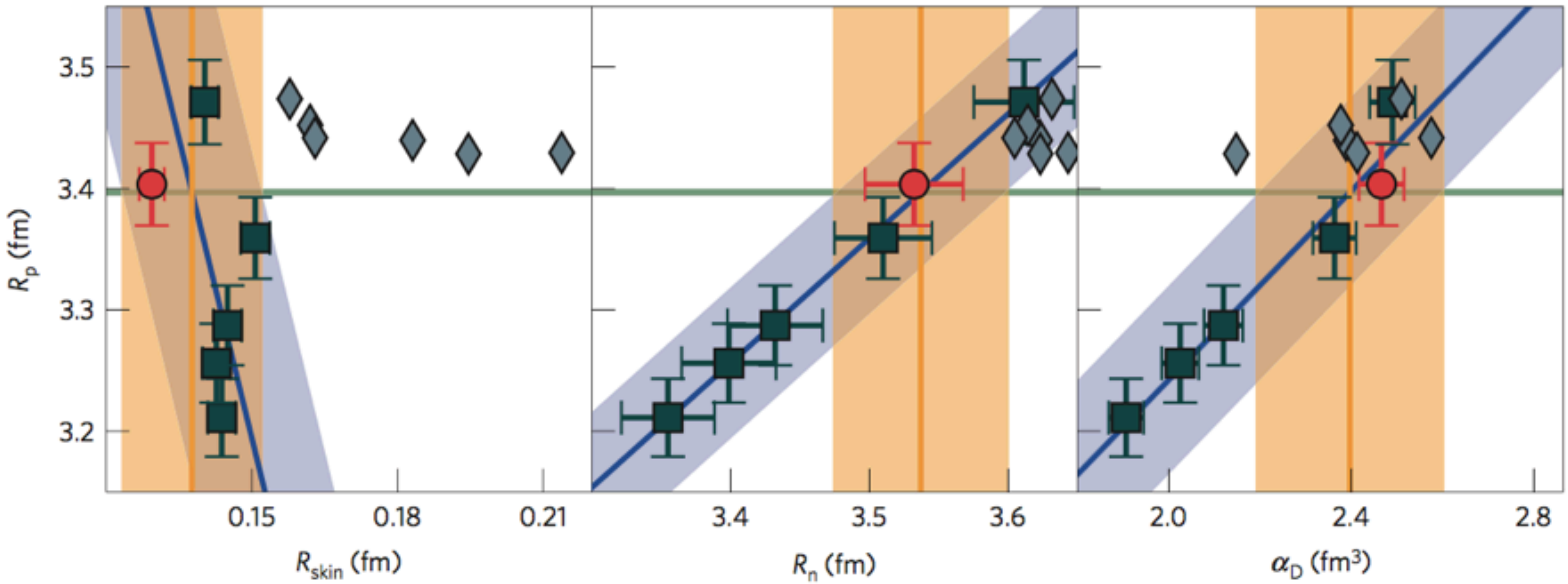
neutron skin constraint from neutron matter results:

$$r_{\mathrm{skin}}[^{208}\mathrm{Pb}] = 0.14 - 0.2 \text{ fm}$$

KH, Lattimer, Pethick, Schwenk, PRL 105, 161102 (2010)

- neutron matter give tightest constraints
- in agreement with all other constraints

Predictions for the neutron skin of ^{48}Ca

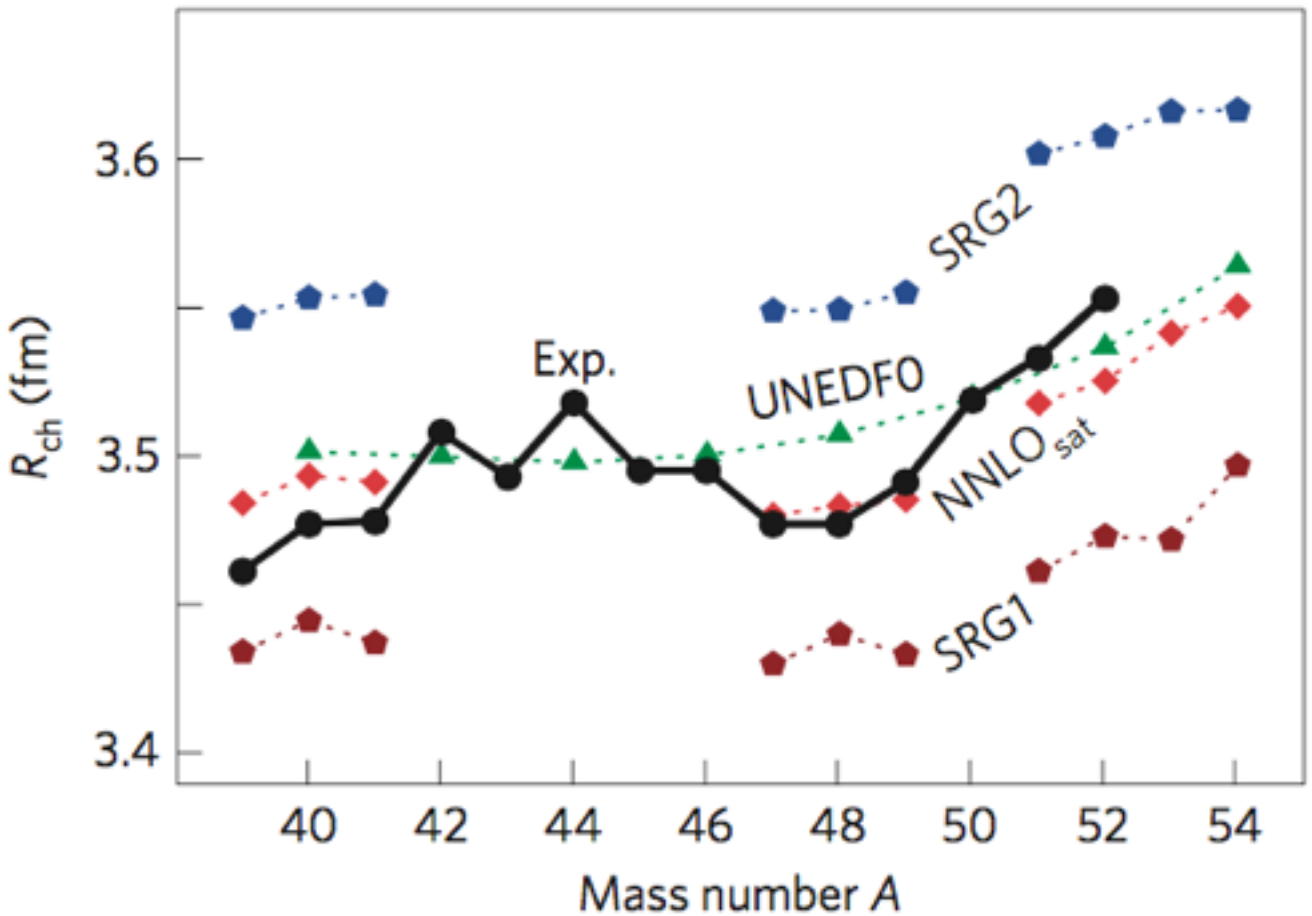


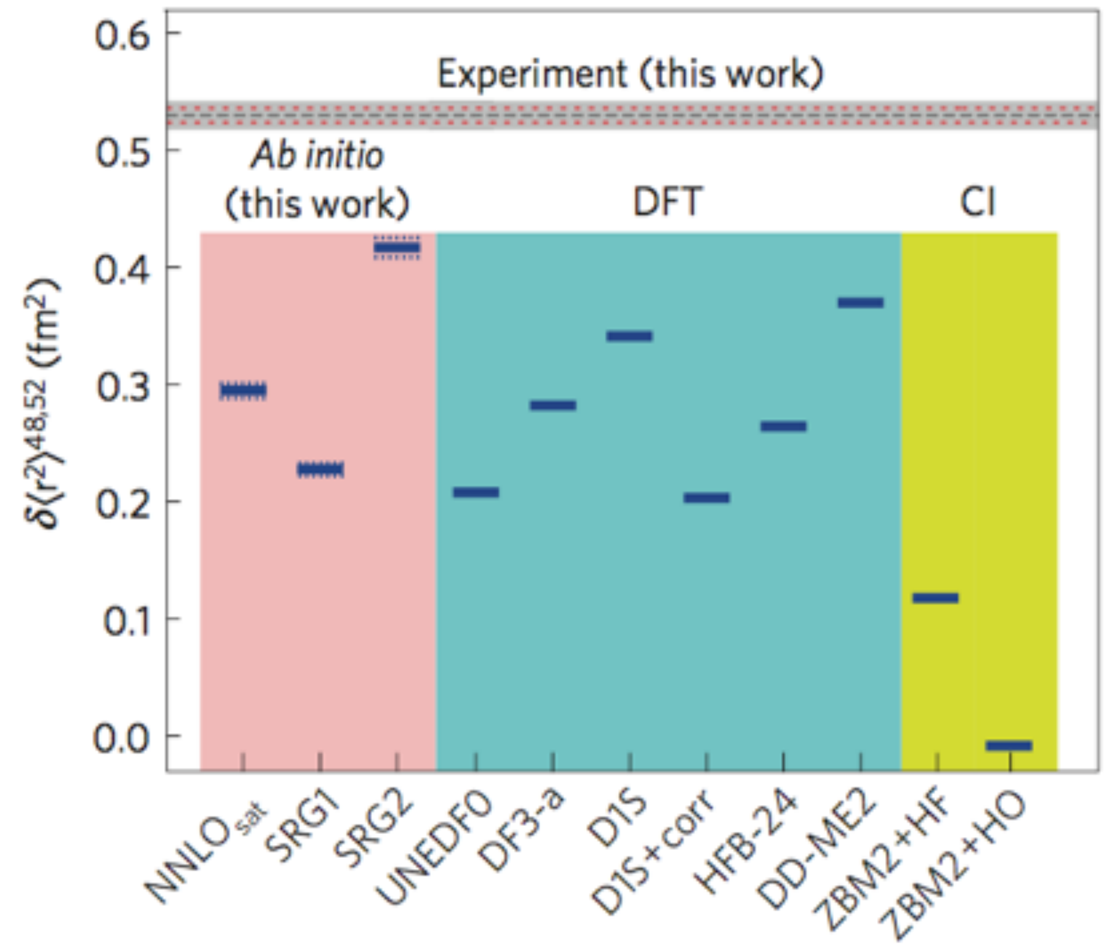
Hagen et al., Nature Physics 12, 186 (2016)

- microscopic coupled cluster results based on a set of different nuclear NN+3N interactions (see also Phys. Rev. C91, 051301 (2015))
- correlations between different observables and the precisely measured R_p
- prediction of significantly smaller neutron skin compared to EDF results:

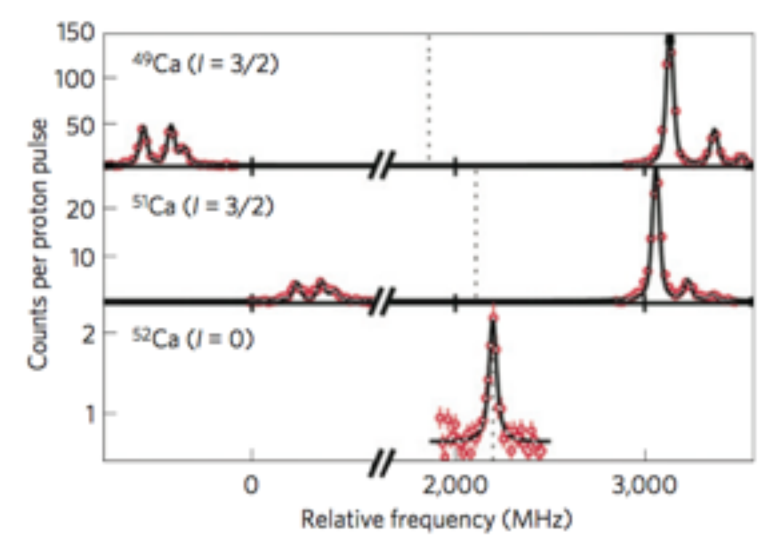
$$0.12 \lesssim R_{\text{skin}} \lesssim 0.15\,\text{fm}$$

Charge radii of calcium isotopes





Garcia Ruiz at al., Nature Physics (advanced online, 2016)



- novel precise measurements of Ca isotope shifts
- unexpectedly large radii of neutron-rich isotopes
- reasonable theoretical reproduction of radius trends

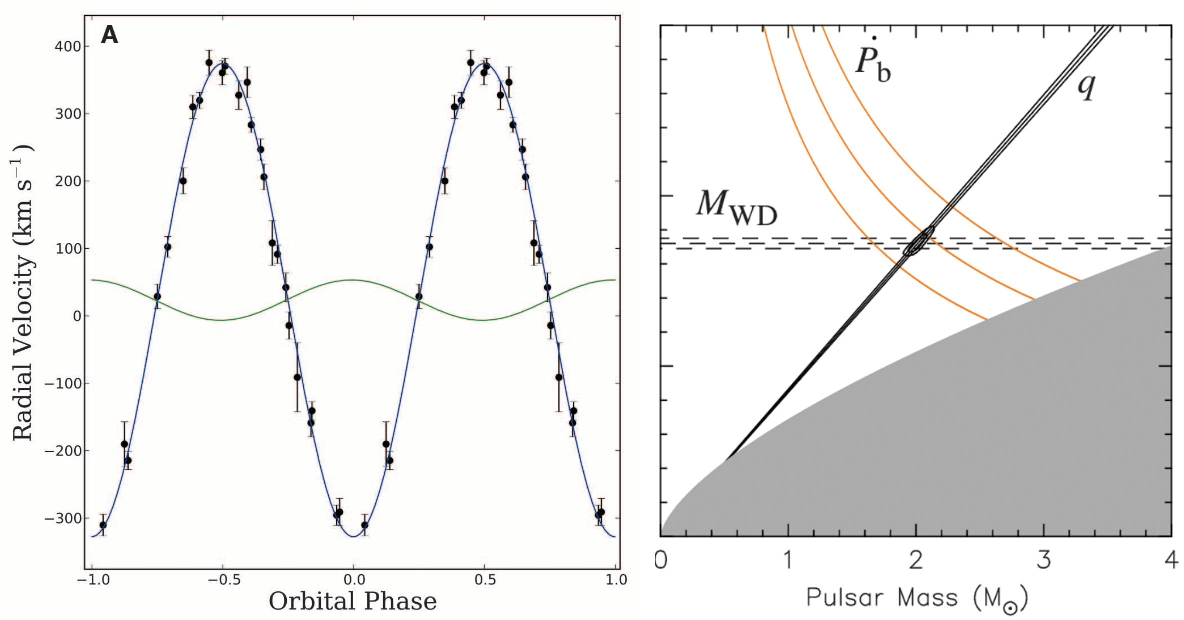
in coupled cluster calculations based on chiral EFT interactions

- radius increase quantitatively underestimated in all theoretical studies

Constraints on the nuclear equation of state (EOS)

Science

A Massive Pulsar in a Compact Relativistic Binary

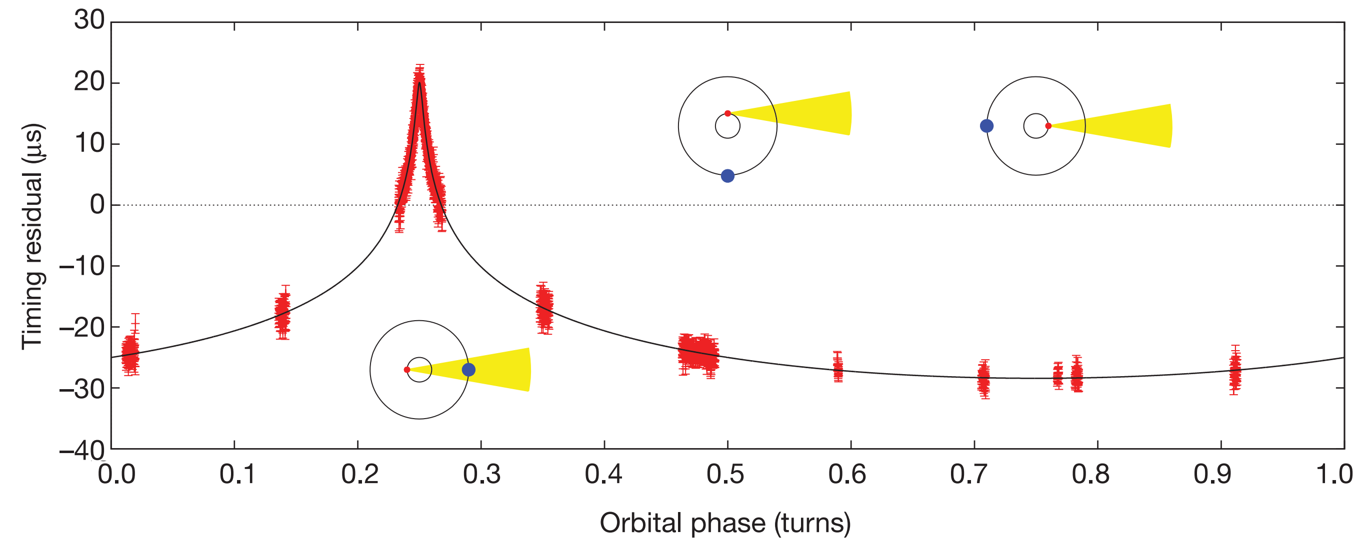


Antoniadis et al., Science 340, 448 (2013)

nature

A two-solar-mass neutron star measured using Shapiro delay

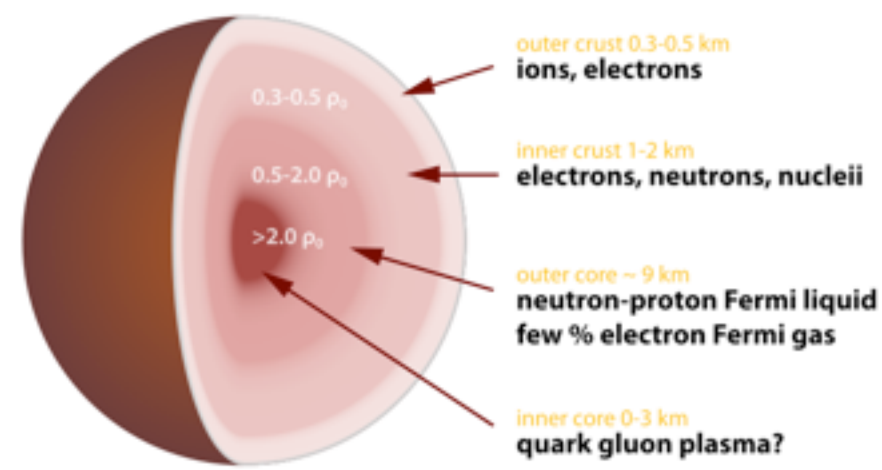
P. B. Demorest[1], T. Pennucci[2], S. M. Ransom[1], M. S. E. Roberts[3] & J. W. T. Hessels[4,5]



Demorest et al., Nature 467, 1081 (2010)

New constraints from recent observations:

$$M_{\max} = 1.65 M_\odot \rightarrow 1.97 \pm 0.04\, M_\odot$$
$$\rightarrow 2.01 \pm 0.04\, M_\odot$$



Calculation of neutron star properties require EOS up to high densities.

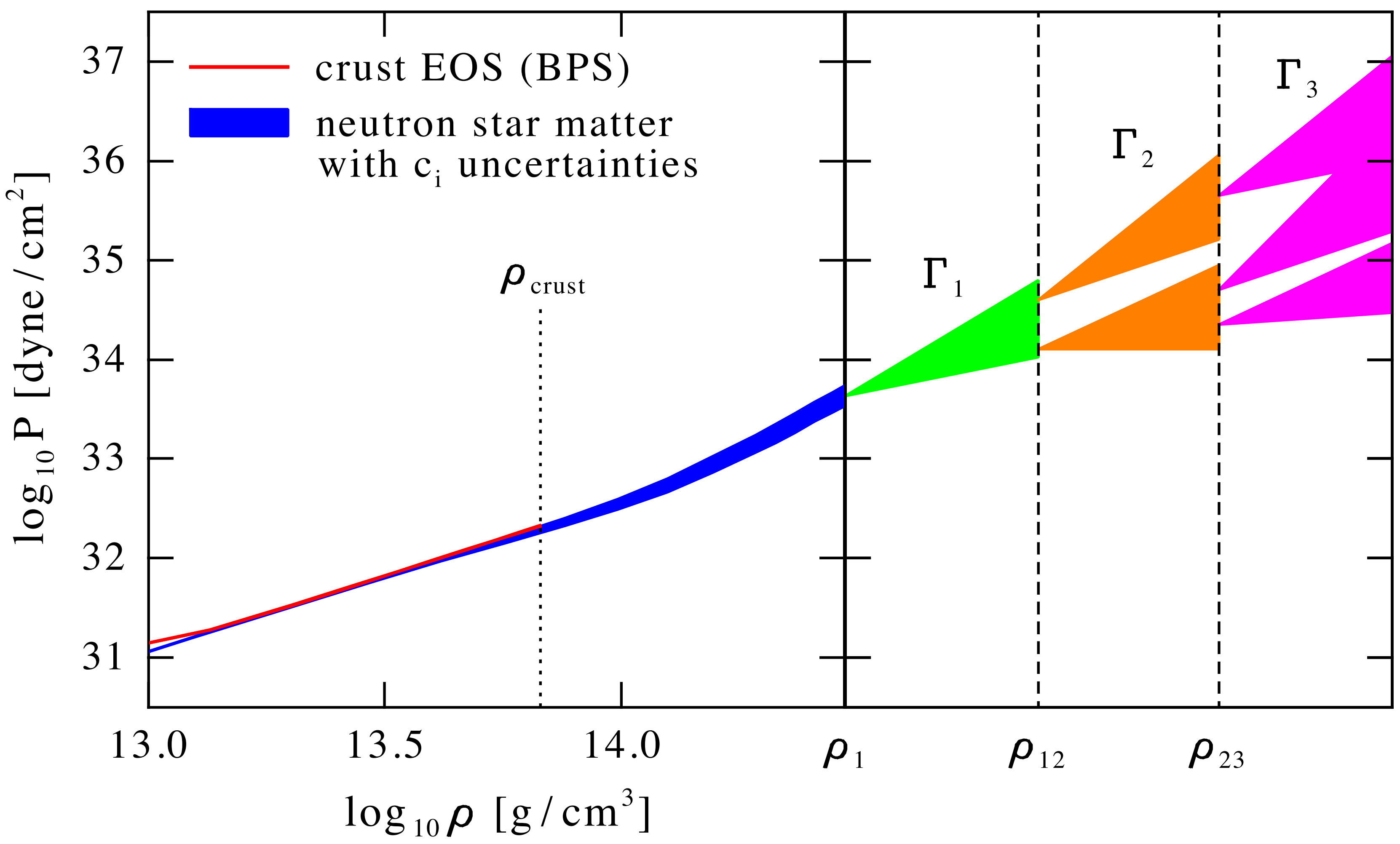
Strategy:
Use observations to constrain the high-density part of the nuclear EOS.

Neutron star radius constraints

incorporation of beta-equilibrium: neutron matter $\longrightarrow$ neutron star matter

parametrize piecewise high-density extensions of EOS:

- use polytropic ansatz $p \sim \rho^{\Gamma}$
- range of parameters $\Gamma_1, \rho_{12}, \Gamma_2, \rho_{23}, \Gamma_3$ limited by physics



KH, Lattimer, Pethick, Schwenk, ApJ 773, 11 (2013)
KH, Lattimer, Pethick, Schwenk, PRL 105, 161102 (2010)

Constraints on the nuclear equation of state

use the constraints:

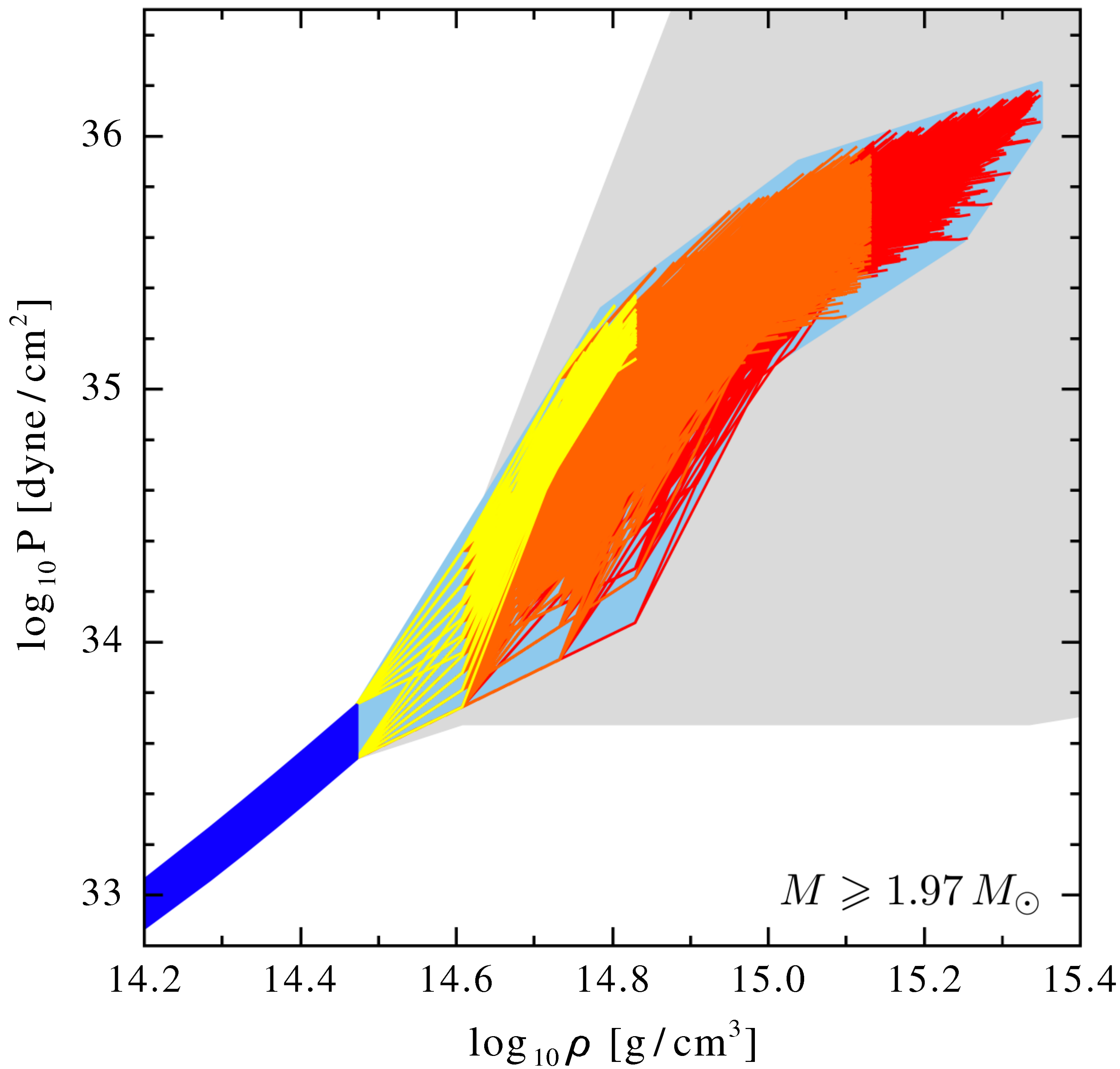
recent NS observations

$$M_{\max} > 1.97\, M_{\odot}$$

causality

$$v_s(\rho) = \sqrt{dP/d\varepsilon} < c$$

KH, Lattimer, Pethick, Schwenk, ApJ 773, 11 (2013)



constraints lead to significant reduction of EOS uncertainty band

Constraints on the nuclear equation of state

use the constraints:

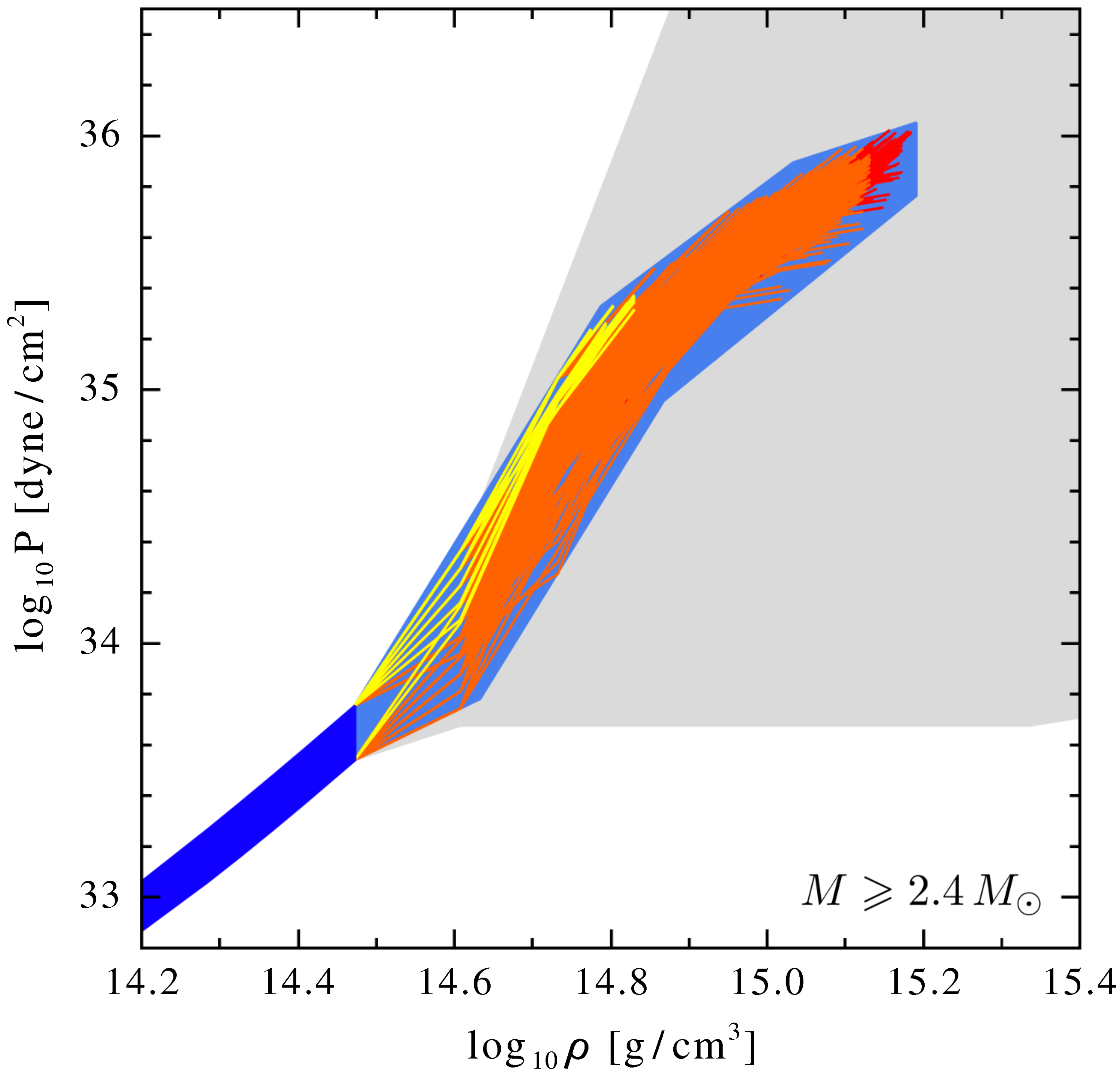
fictitious NS mass

$M_{\max} > 2.4\,M_\odot$

causality

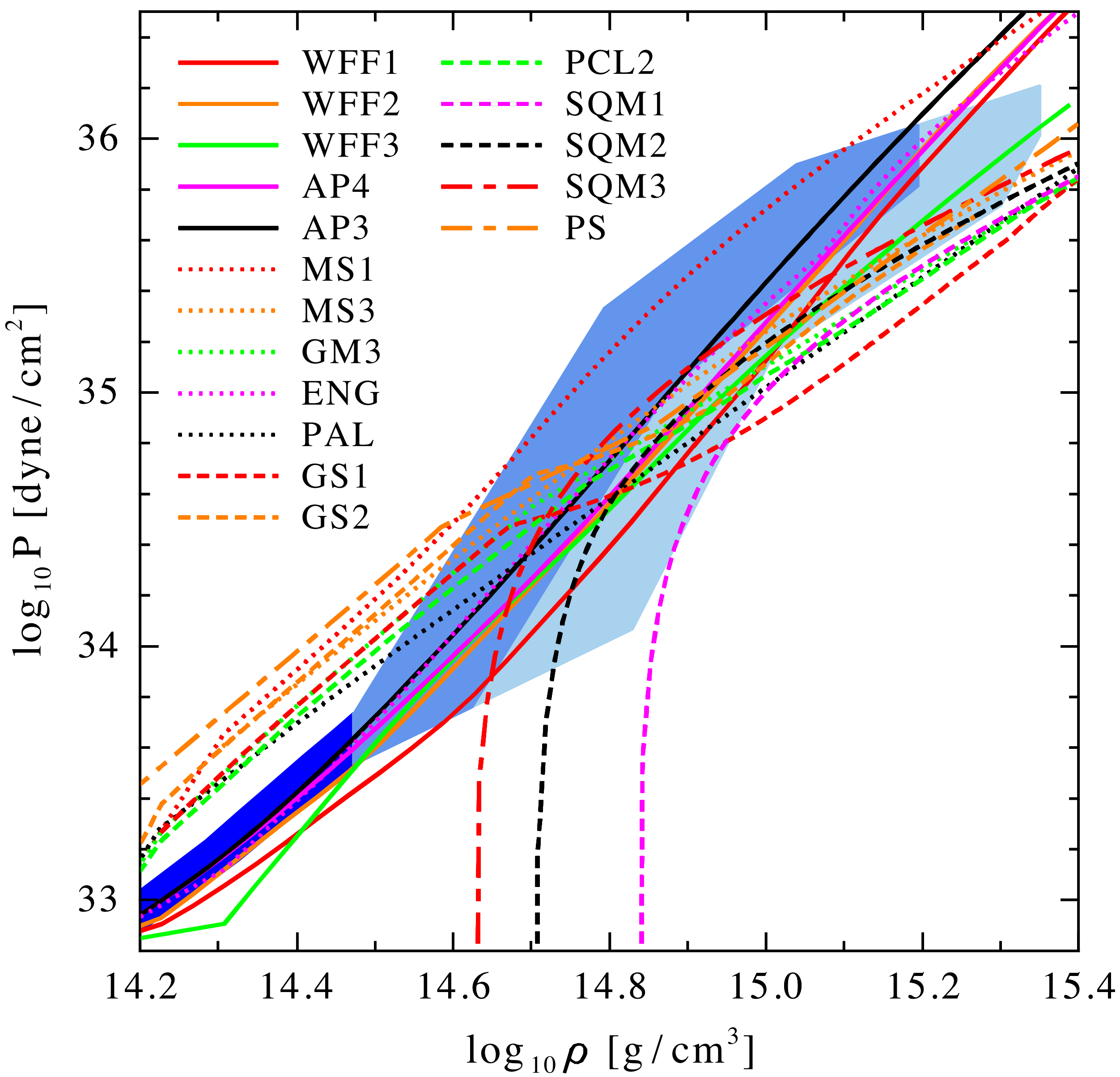
$v_s(\rho) = \sqrt{dP/d\varepsilon} < c$

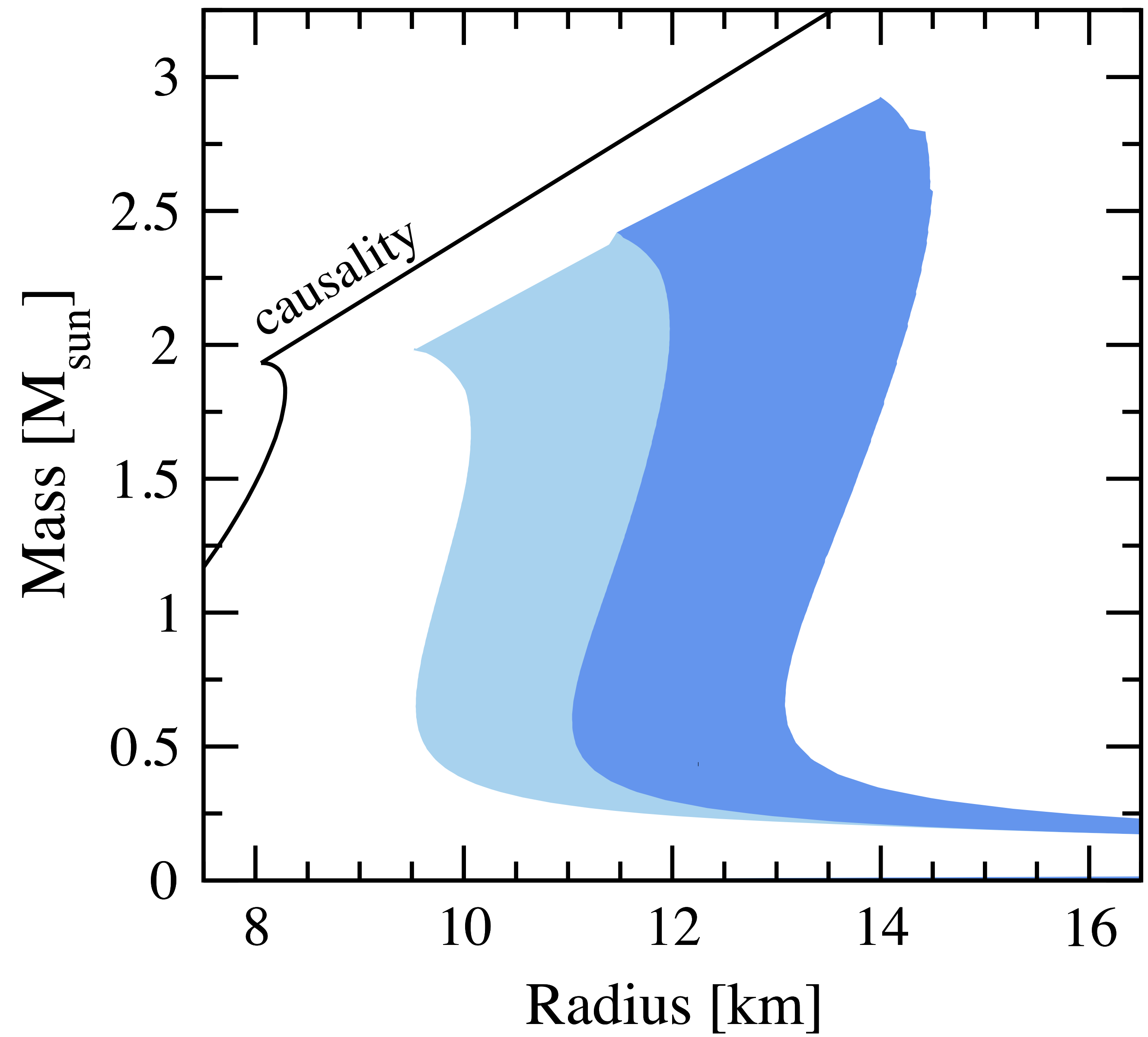
KH, Lattimer, Pethick, Schwenk, ApJ 773, 11 (2013)



increased $M_{\max}$ systematically reduces width of band

Constraints on neutron star radii

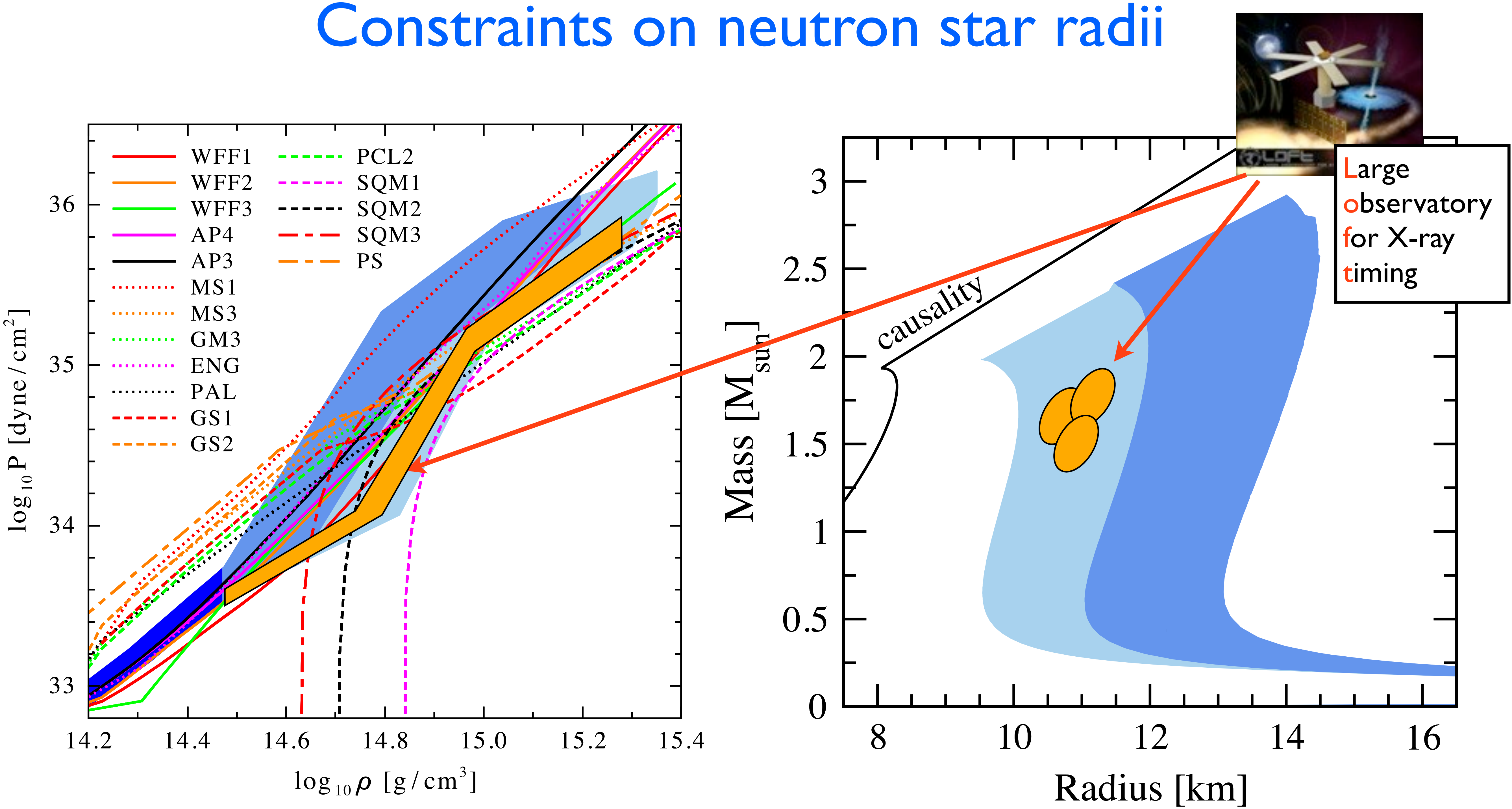




KH, Lattimer, Pethick, Schwenk, ApJ 773, 11 (2013)
see also KH, Lattimer, Pethick, Schwenk, PRL 105, 161102 (2010)

- low-density part of EOS sets scale for allowed high-density extensions
- current radius prediction for typical $1.4\,M_\odot$ neutron star: $9.7 - 13.9\,\mathrm{km}$

Constraints on neutron star radii



KH, Lattimer, Pethick, Schwenk, ApJ 773, 11 (2013)
see also KH, Lattimer, Pethick, Schwenk, PRL 105, 161102 (2010)

- low-density part of EOS sets scale for allowed high-density extensions
- current radius prediction for typical $1.4\,M_\odot$ neutron star: $9.7 - 13.9\,\mathrm{km}$
- radius measurements could significantly improve constraints

Summary

- recent advances allow ab initio studies of medium-mass nuclei
- remarkable agreement between different methods for given interaction, uncertainties dominated by differences in nuclear interactions
- results presented for properties of neutron-rich nuclei and matter based on sets of current chiral EFT NN+3N interactions

Future directions

- derivation of systematic uncertainty estimates for many-body observables, order-by-order convergence studies
- exploration of different fitting strategies, include bayesian analysis for statistical interpretation of uncertainties?
- role of regulators, clean separation of short- and long-range physics, naturalness of coupling constants, power counting schemes, inclusion of delta excitations...

In collaboration with:

TECHNISCHE UNIVERSITÄT DARMSTADT — C. Drischler, T. Krüger, R. Roth, A. Schwenk

The Ohio State University — R. Furnstahl, S. More

Michigan State University — S. Bogner

RUB — E. Epelbaum, H. Krebs

University of Guelph — A. Gezerlis

Jülich Forschungszentrum — A. Nogga

Stony Brook, State University of New York — J. Lattimer

NORDITA — C. Pethick

J. Golak, R. Skibinski

The University of Tennessee Knoxville — G. Hagen, T. Papenbrock

LENPIC — international collaborator in NUCLEI — Nuclear Computational Low-Energy Initiative

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computing support:

HRZ Hochschulrechenzentrum

Ohio Supercomputer Center

Jülich Forschungszentrum JUROPA

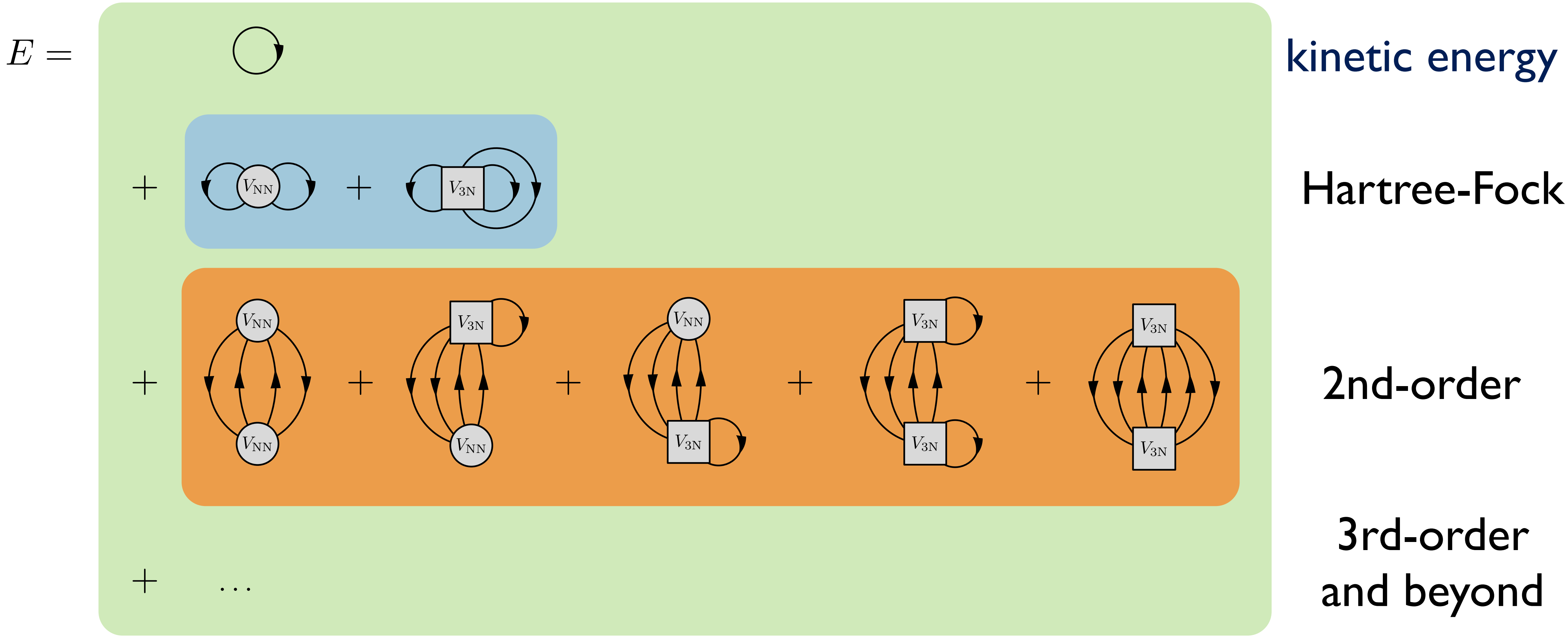
Thank you!

Backup slides

Equation of state: Many-body perturbation theory

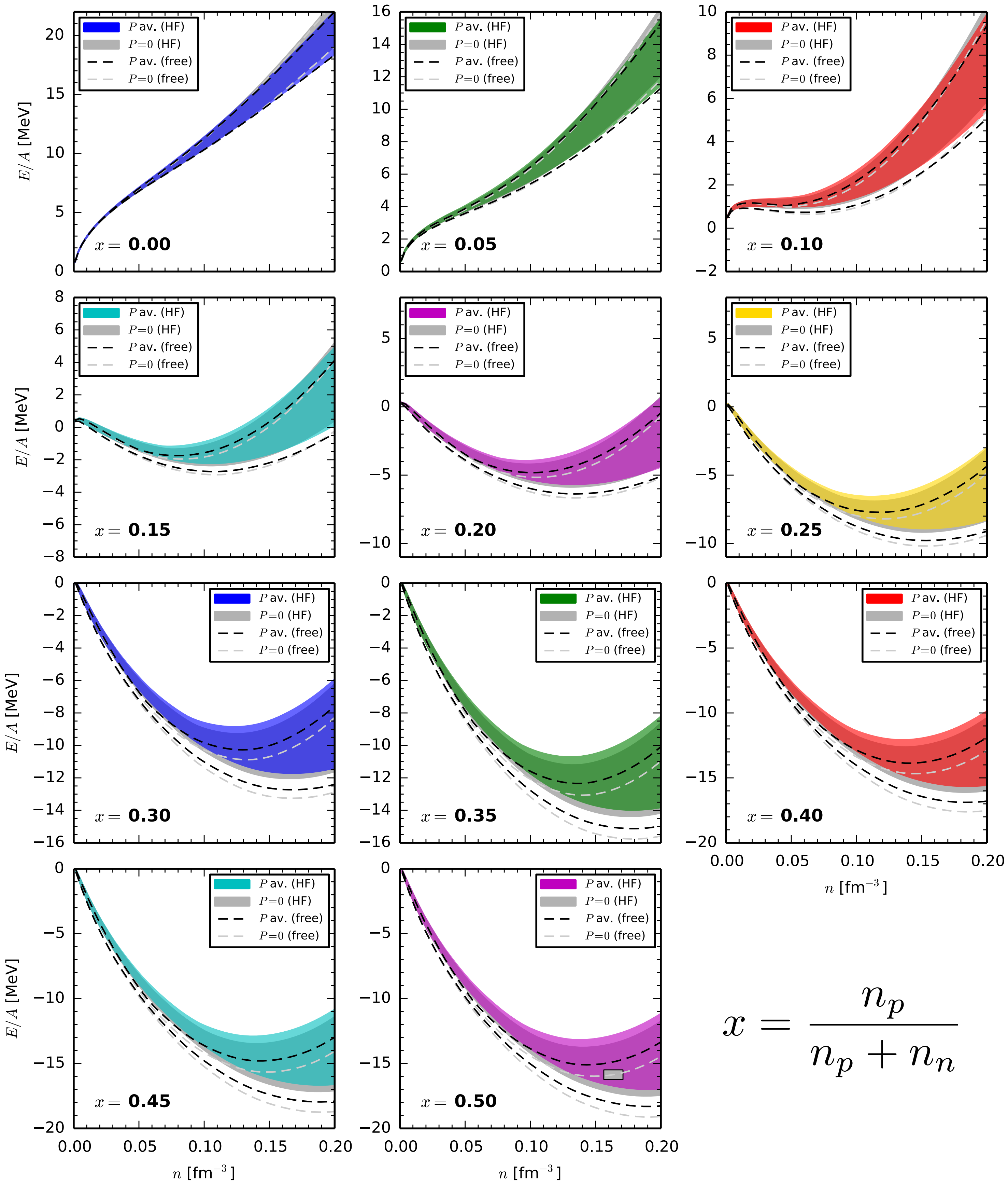
central quantity of interest: energy per particle E/N

$$H(\lambda) = T + V_{\mathrm{NN}}(\lambda) + V_{3\mathrm{N}}(\lambda) + \ldots$$

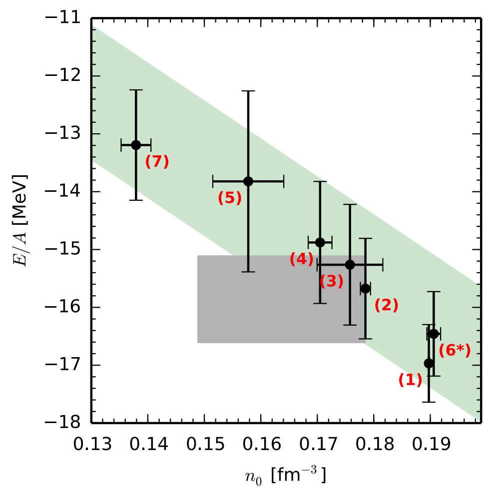


- “hard” interactions require non-perturbative summation of diagrams
- with low-momentum interactions much more perturbative
- inclusion of 3N interaction contributions crucial!

First application to isospin asymmetric nuclear matter



- uncertainty bands determined by set of 7 Hamitonians

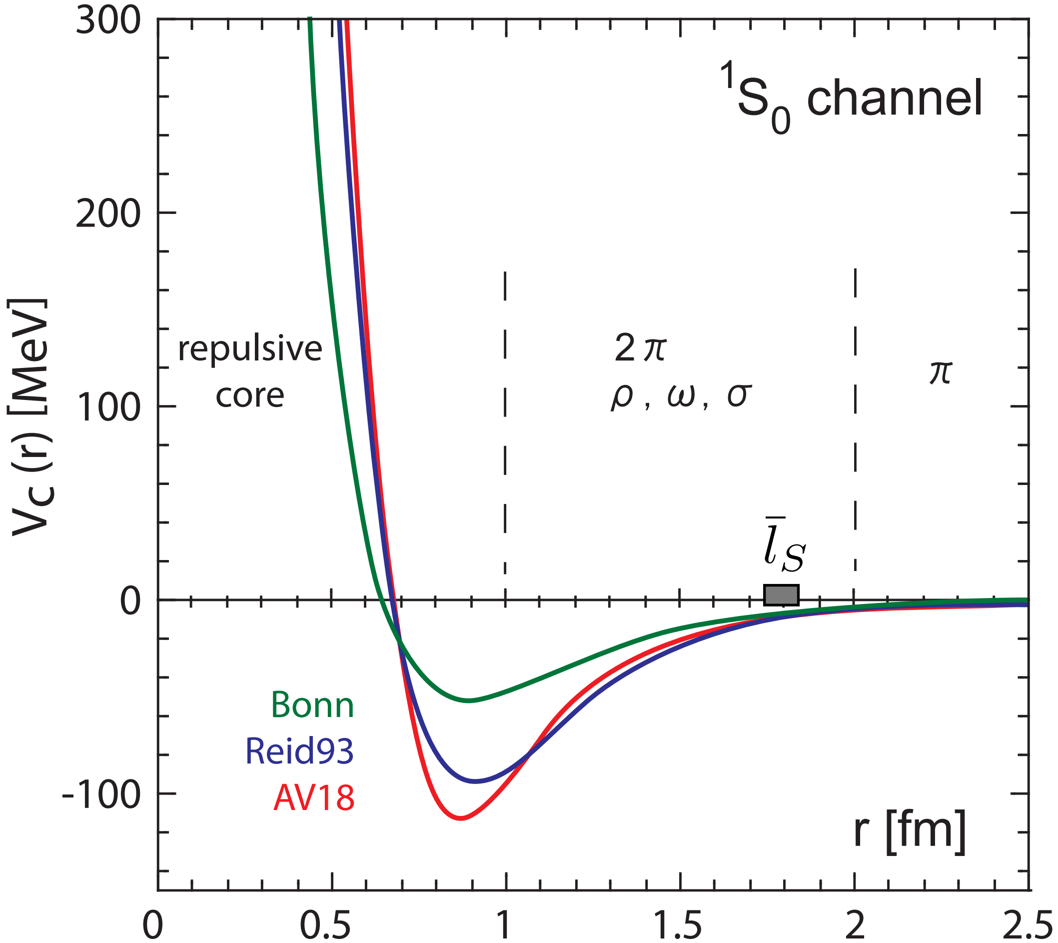


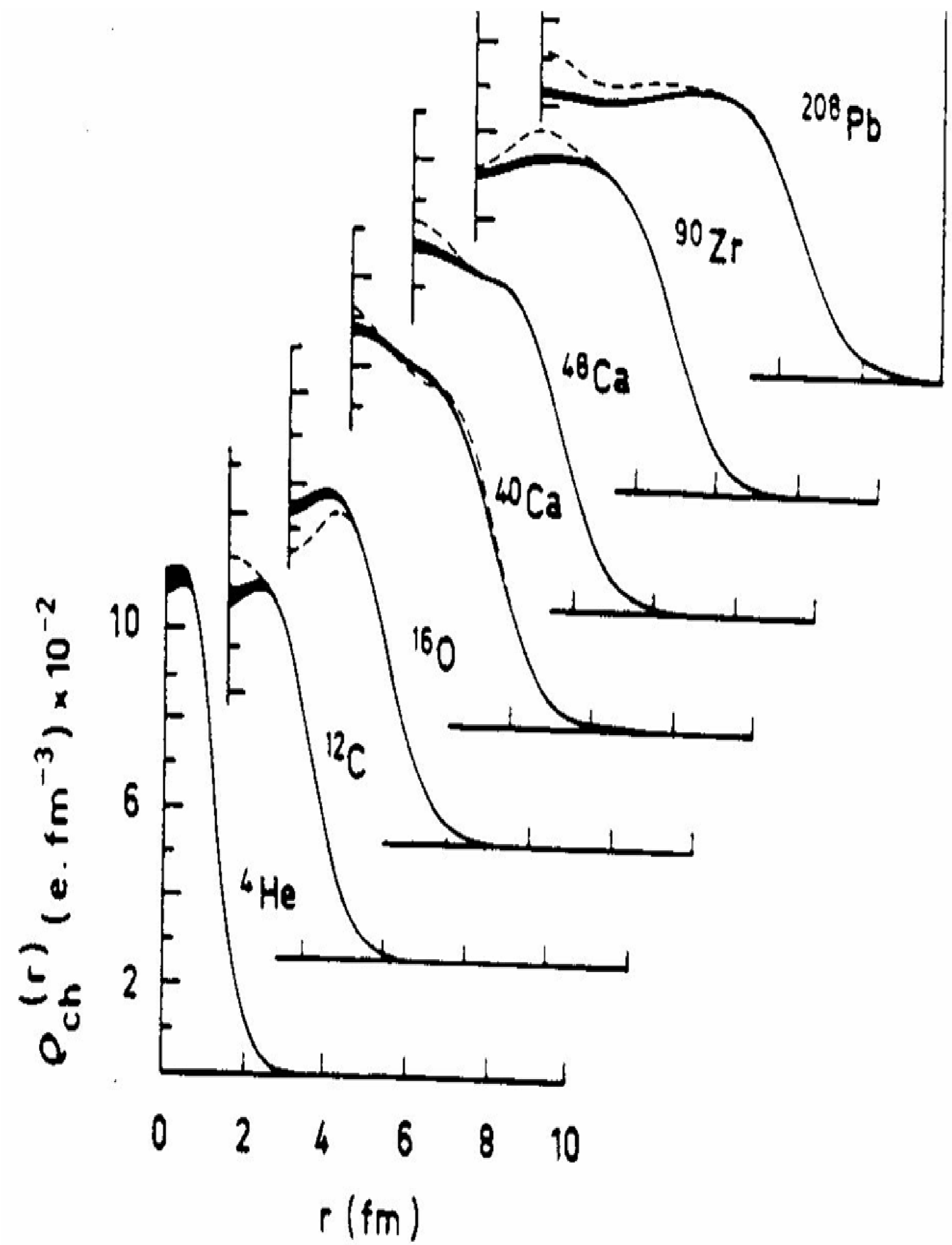
- many-body framework allows treatment of any decomposed 3N interaction

$$x = \frac{n_p}{n_p + n_n}$$

Drischler, KH, Schwenk, in preparation

Equation of state of symmetric nuclear matter, nuclear saturation

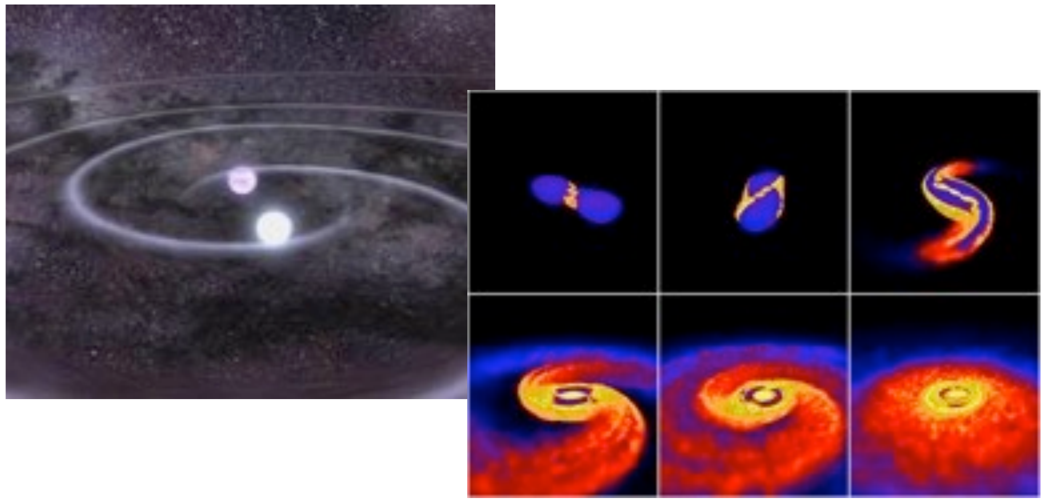


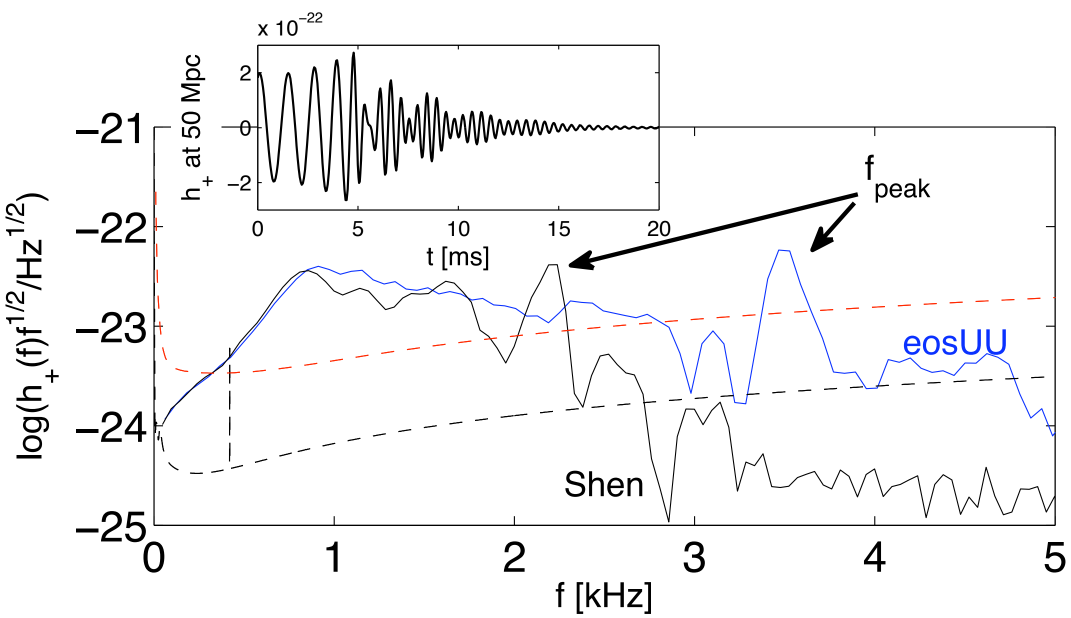


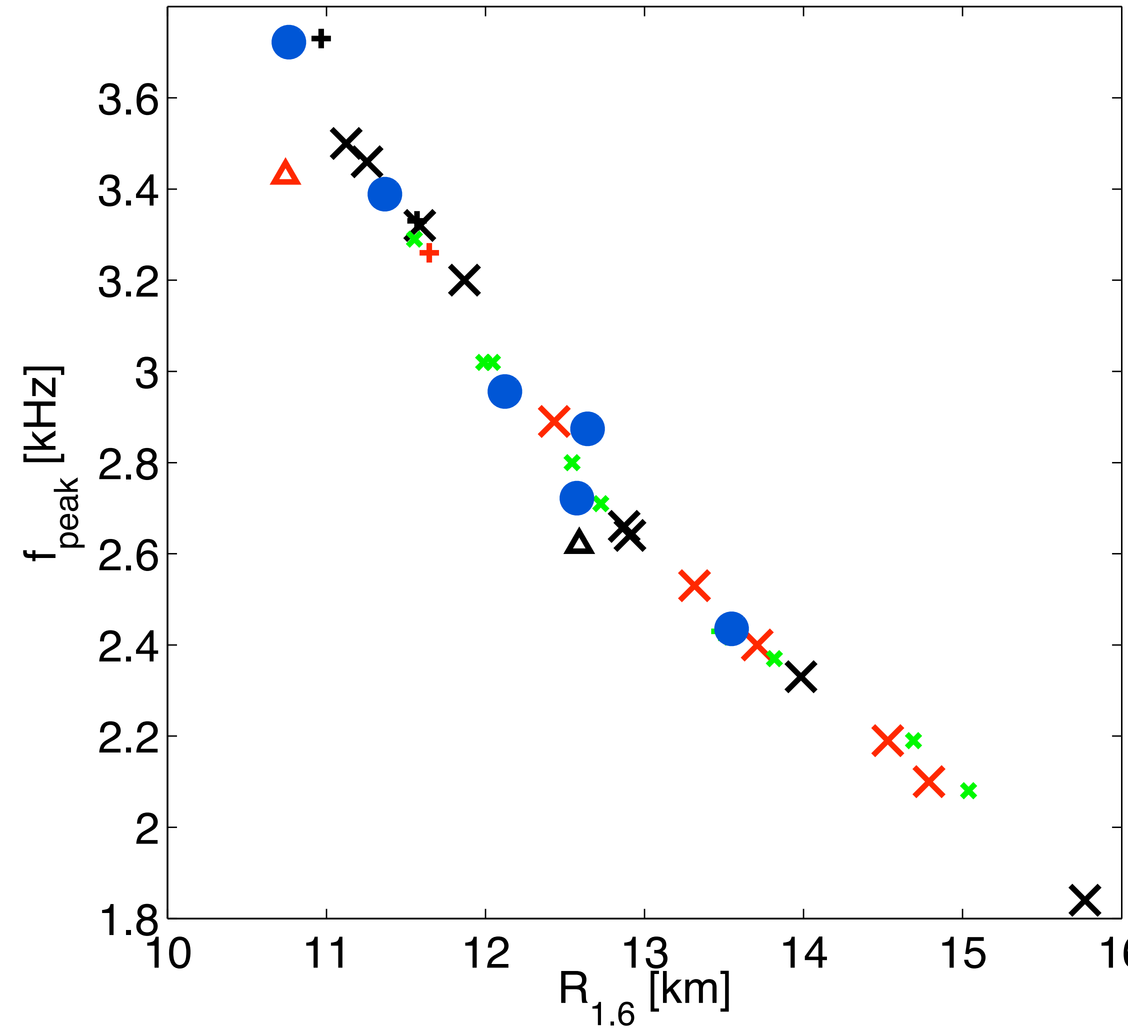
"Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."

Hans Bethe (1971)

Gravitational wave signals from neutron star binary mergers





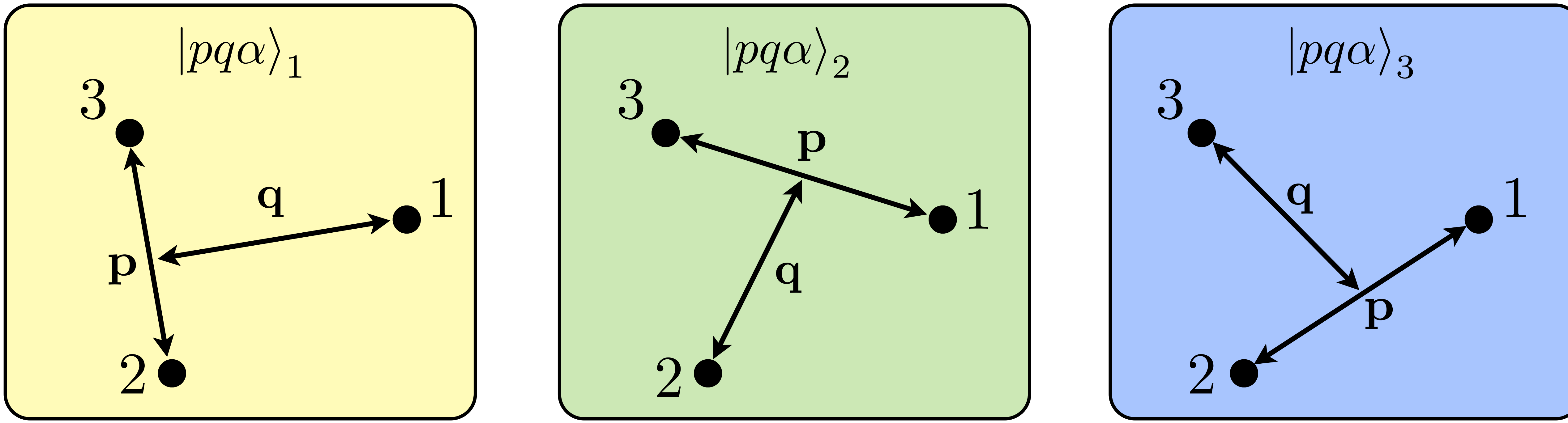


Bauswein and Janka, PRL 108, 011101 (2012),
Bauswein, Janka, KH, Schwenk, PRD 86, 063001 (2012)

- simulations of NS binary mergers show strong correlation between between $f_{\rm peak}$ of the GW spectrum and the radius of a NS
- measuring $f_{\rm peak}$ is key step for constraining EOS systematically at large ρ

Representation of 3N interactions in momentum space

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

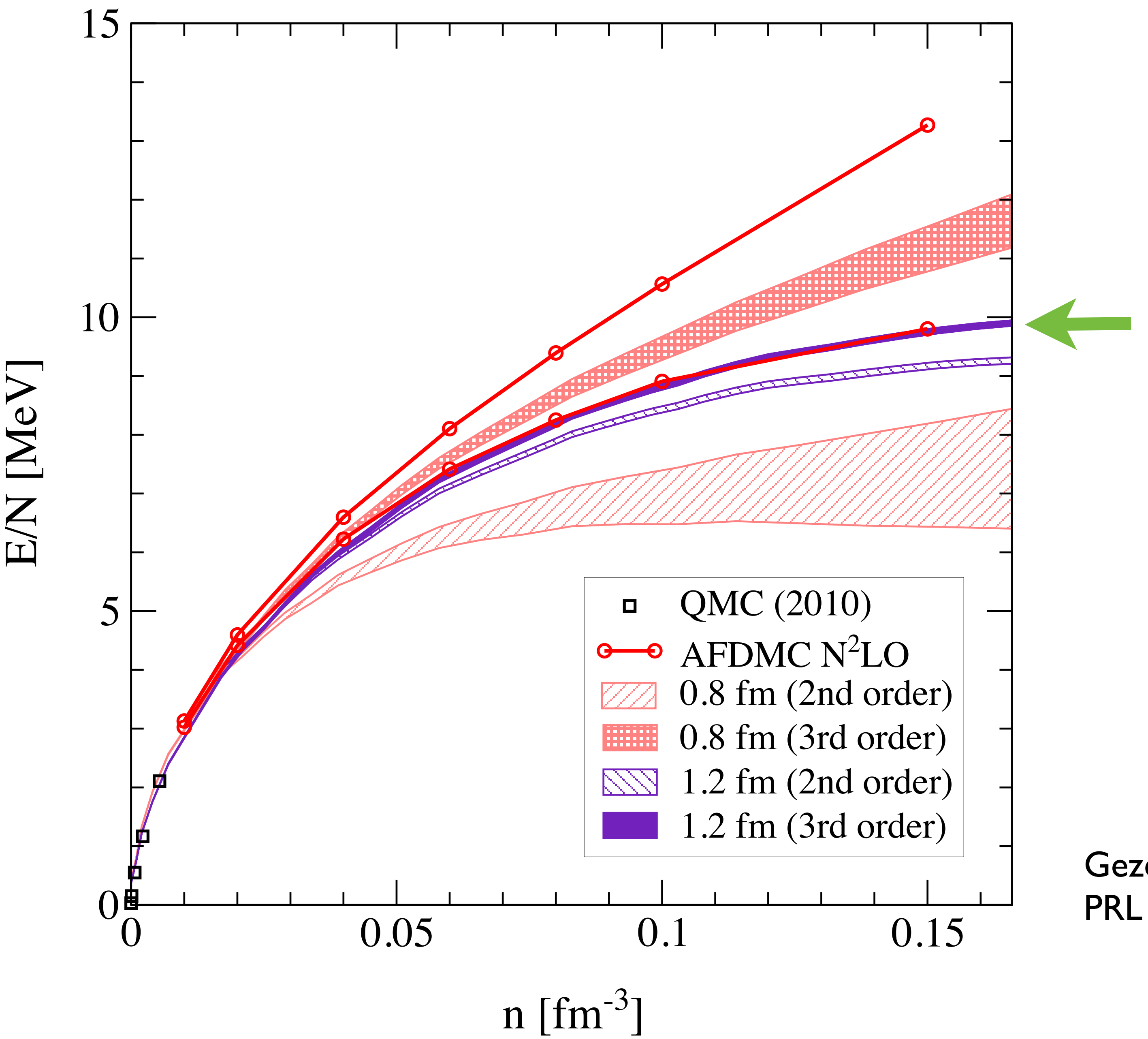


Due to the large number of matrix elements, the traditional way of computing matrix elements requires extreme amounts of computer resources.

$$N_p \simeq N_q \simeq 15$$
$$N_\alpha \simeq 30 - 180 \quad \longrightarrow \quad \dim[\langle pq\alpha|V_{123}|p'q'\alpha'\rangle] \simeq 10^7 - 10^{10}$$

Number of matrix elements was so far not sufficient for studies of $A \geq 4$ systems.

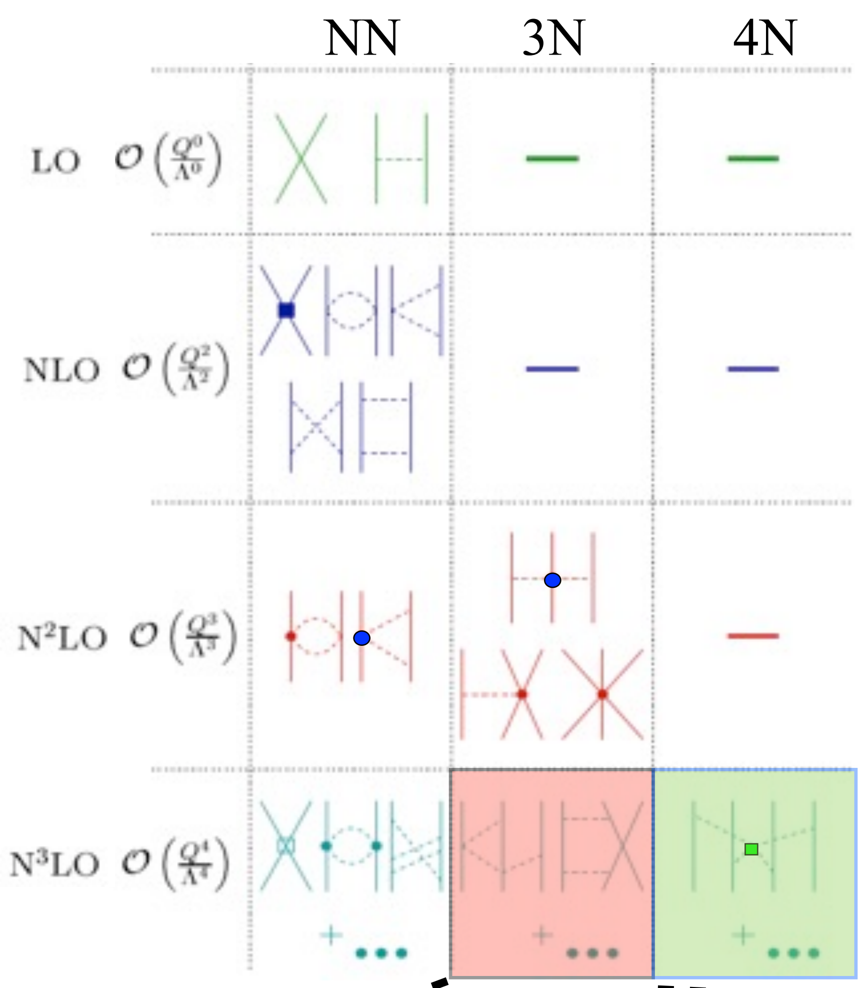
First Quantum Monte Carlo based on local chiral EFT interactions



perfect agreement for soft interactions, first direct validation of perturbative calculations

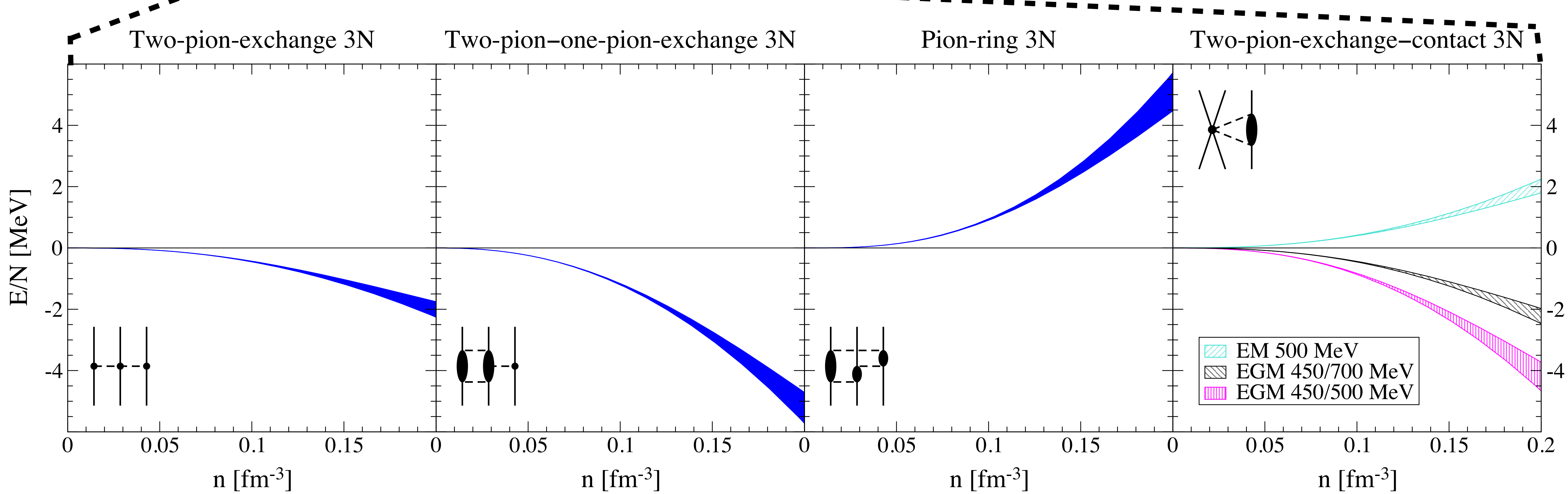
Gezerlis, Tews, Epelbaum, Gandolfi, KH, Nogga, Schwenk
PRL 111, 032501 (2013)

Contributions of many-body forces at N^3LO in neutron matter

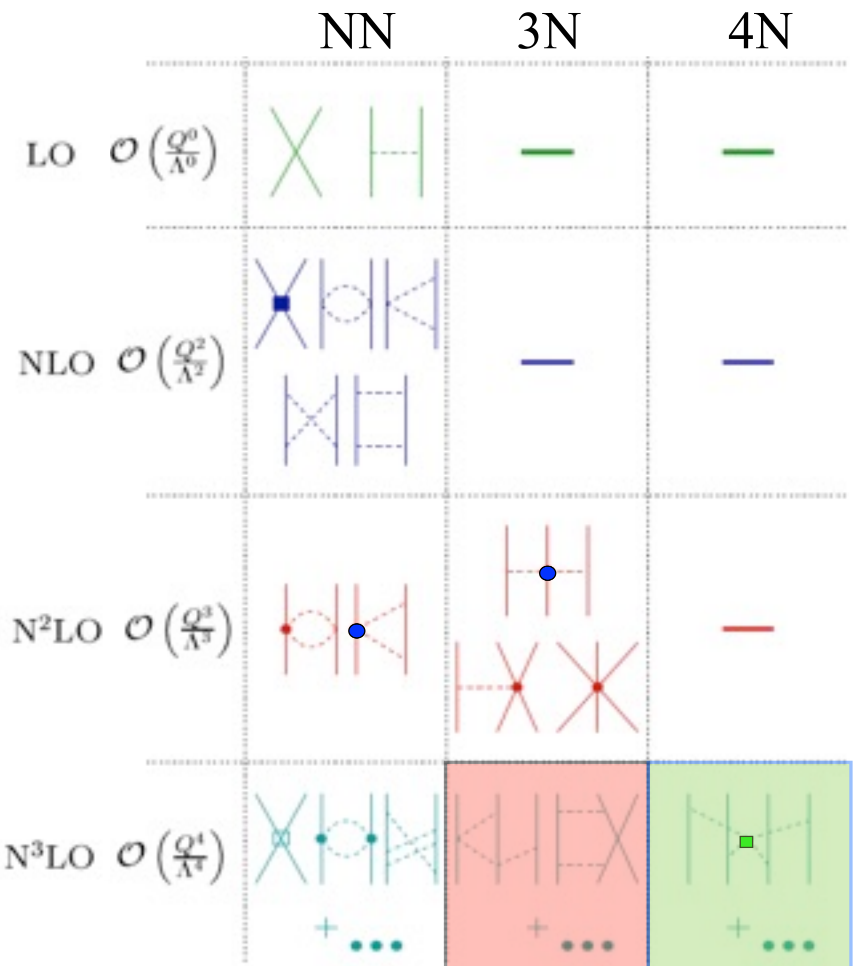


- first calculations of N^3LO 3NF and 4NF contributions to EOS of neutron matter
- found large contributions in Hartree Fock appr., comparable to size of N^2LO contributions

Tews, Krüger, KH, Schwenk
PRL 110, 032504 (2013)

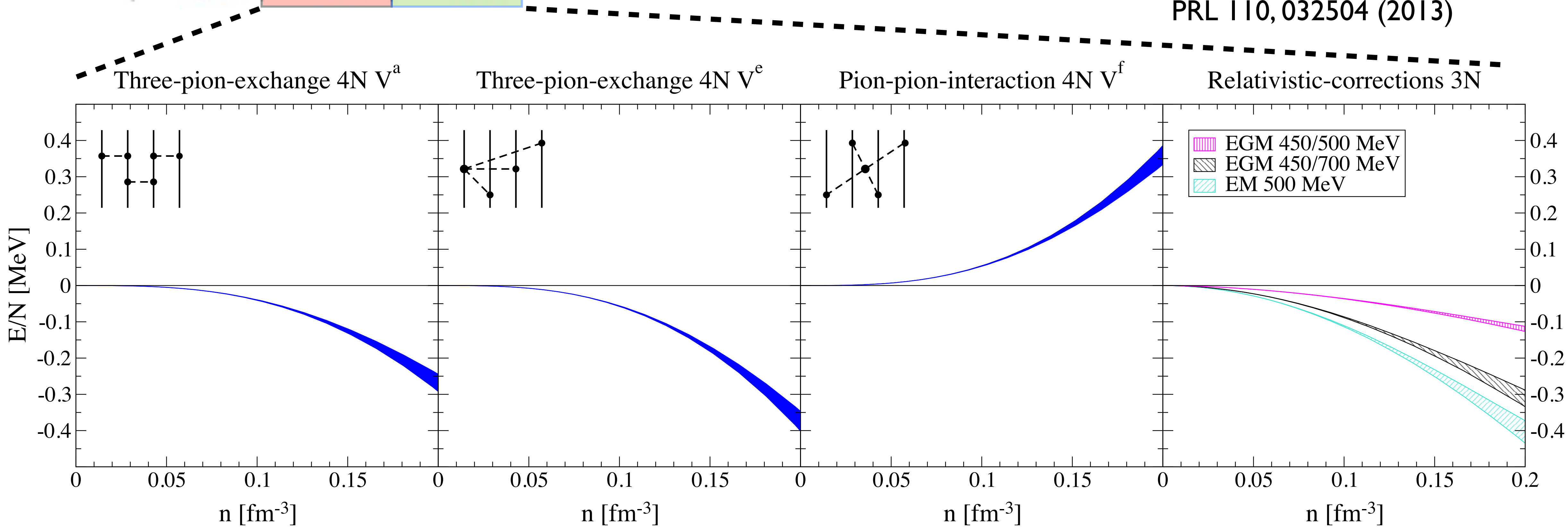


Contributions of many-body forces at N^3LO in neutron matter

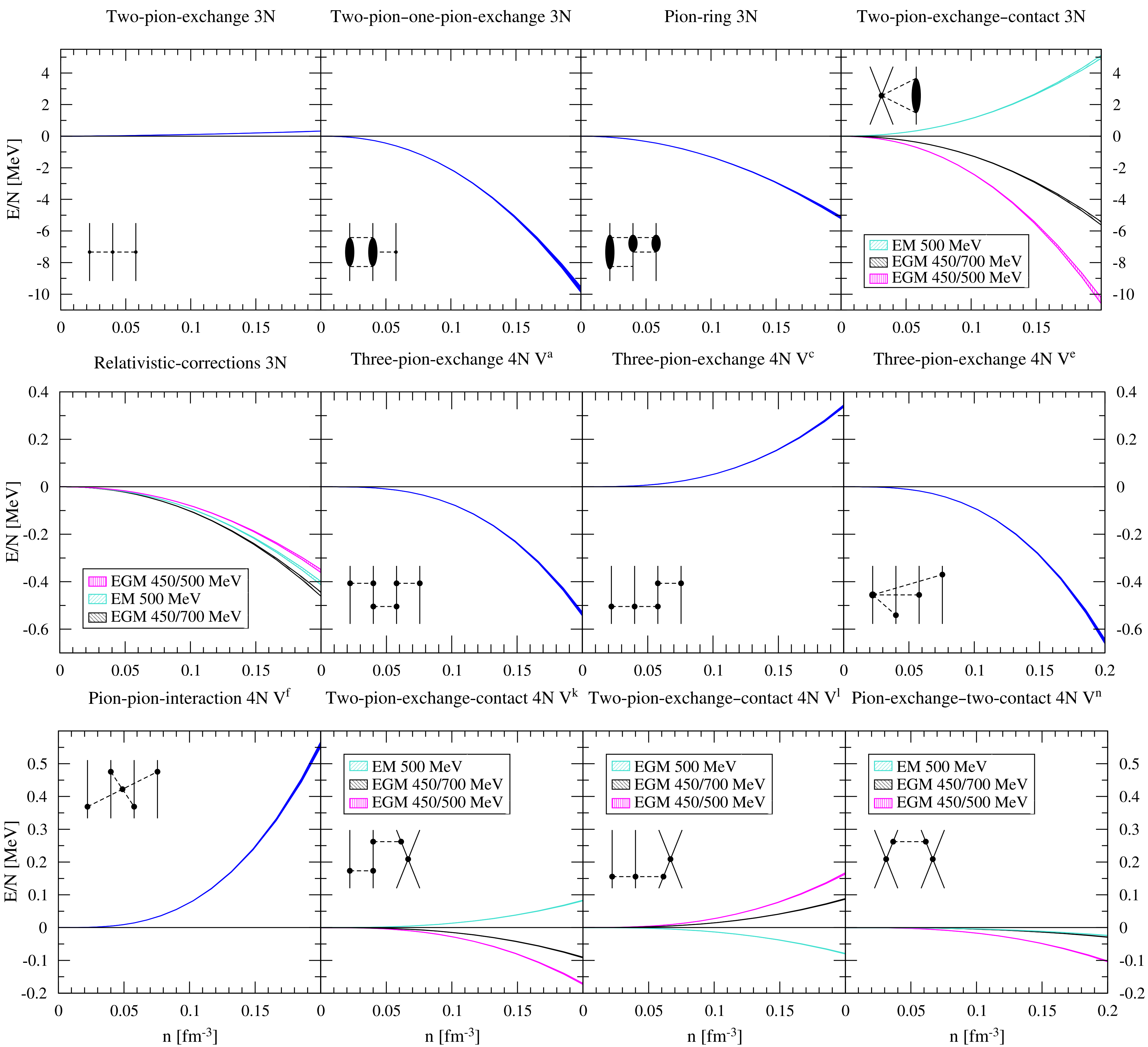


- first calculations of N^3LO 3NF and 4NF contributions to EOS of neutron matter
- found large contributions in Hartree Fock appr., comparable to size of N^2LO contributions
- 4NF contributions small

Tews, Krüger, KH, Schwenk
PRL 110, 032504 (2013)

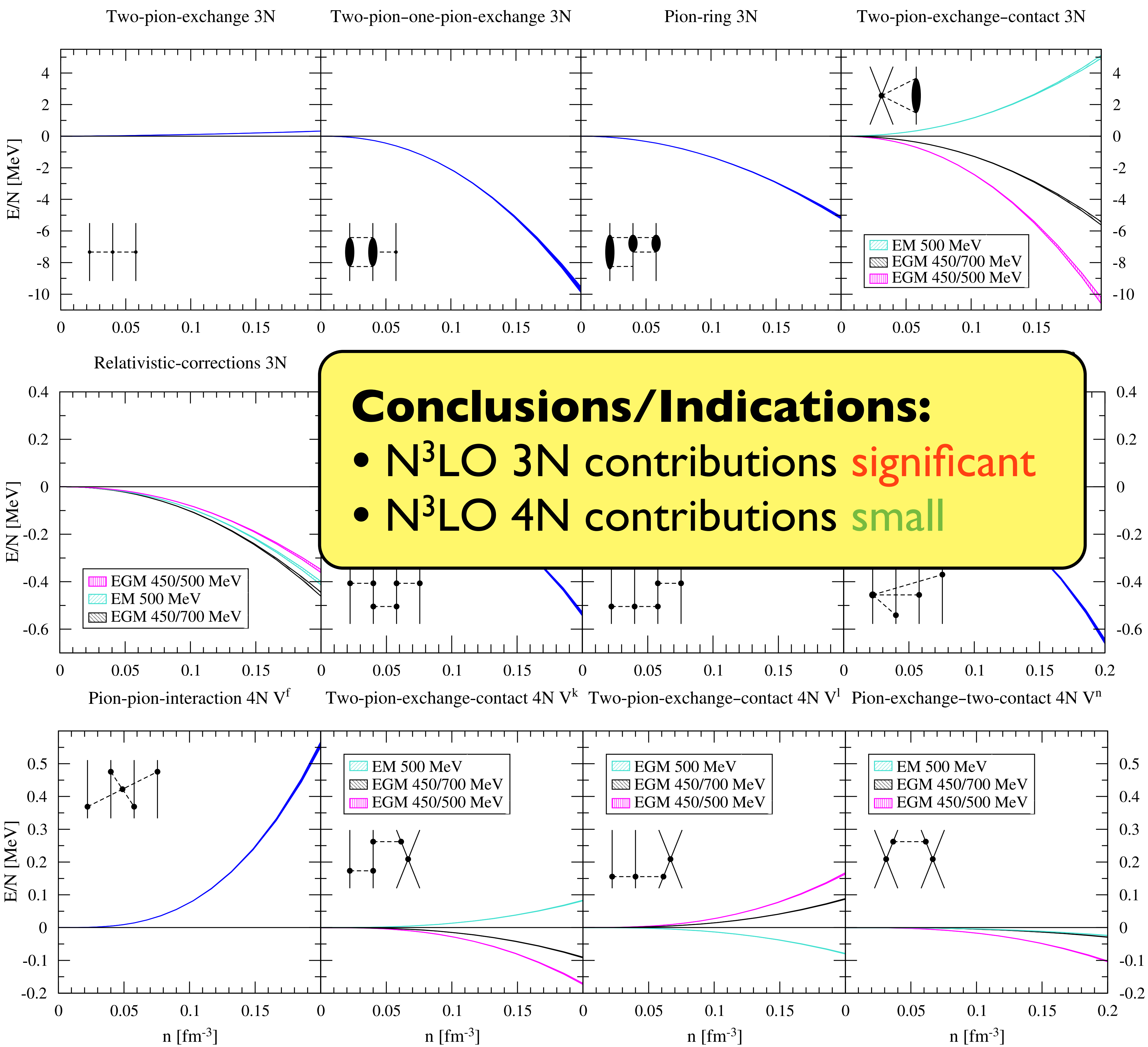


N^3LO contributions in nuclear matter (Hartree Fock)



Krüger, Tews, KH, Schwenk
PRC88, 025802 (2013)

N^3LO contributions in nuclear matter (Hartree Fock)



Conclusions/Indications:

- N^3LO 3N contributions significant
- N^3LO 4N contributions small

Krüger, Tews, KH, Schwenk
PRC88, 025802 (2013)