Recent developments and applications of three-nucleon interactions

Kai Hebeler

Hirschegg, January 16, 2018

Hirschegg 2018:
Multiparticle resonances in hadrons, nuclei and ultracold gases

SFB 1245

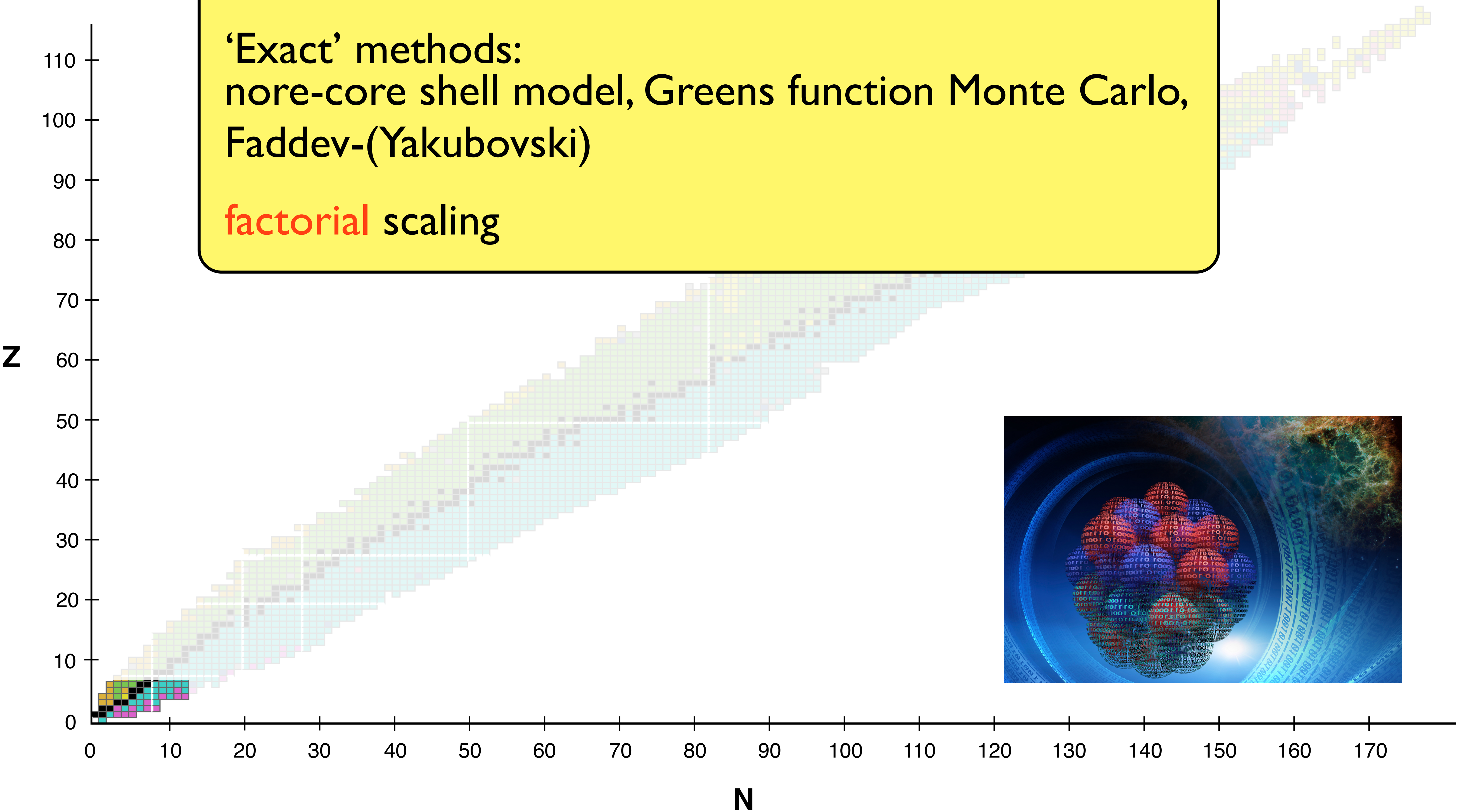
TECHNISCHE UNIVERSITÄT DARMSTADT

The theoretical nuclear landscape: Scope of ab initio methods for atomic nuclei

since 1980‘s

‘Exact’ methods:
nore-core shell model, Greens function Monte Carlo, Faddev-(Yakubovski)

factorial scaling

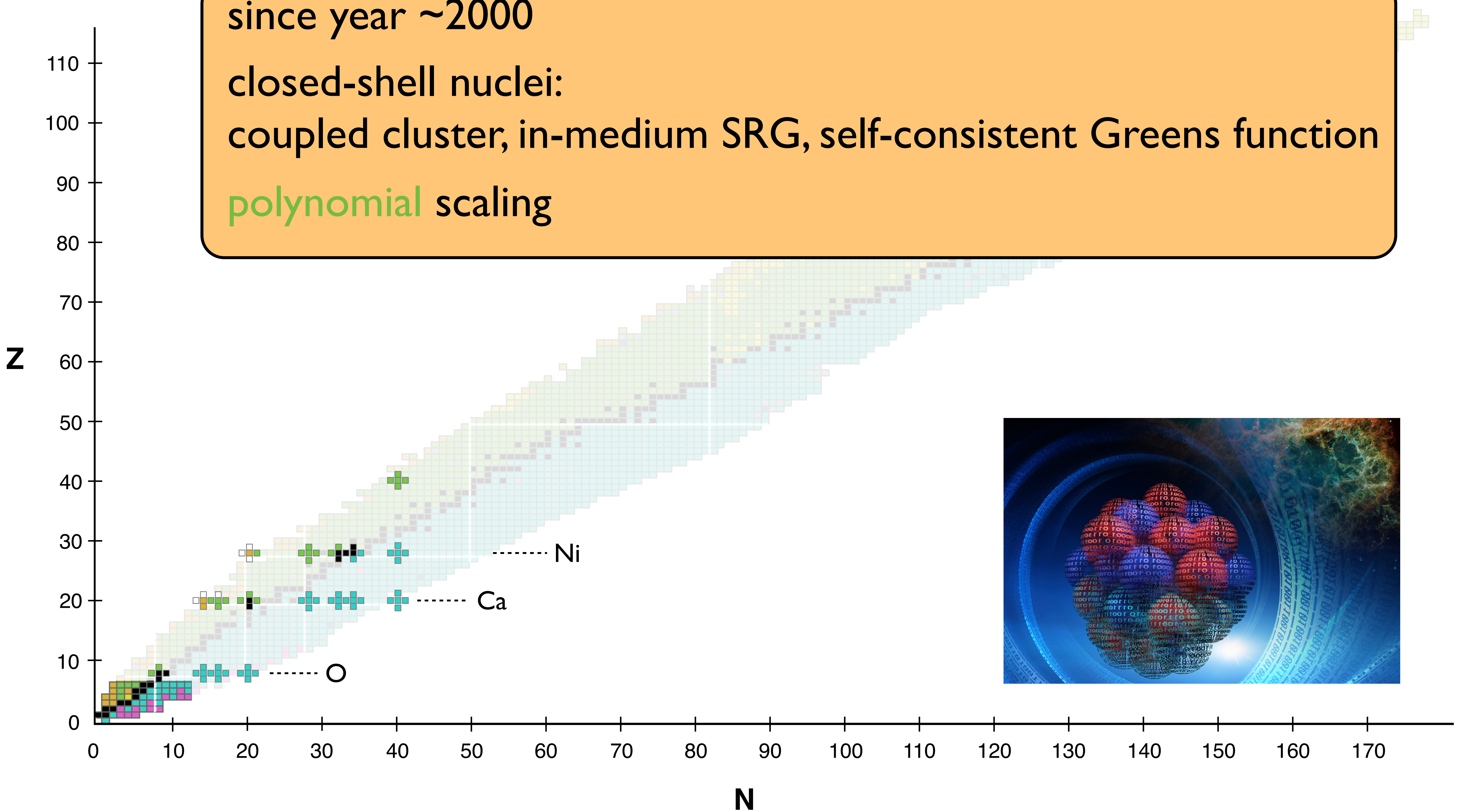


The theoretical nuclear landscape: Scope of ab initio methods for atomic nuclei

since year ~2000

closed-shell nuclei:
coupled cluster, in-medium SRG, self-consistent Greens function

polynomial scaling

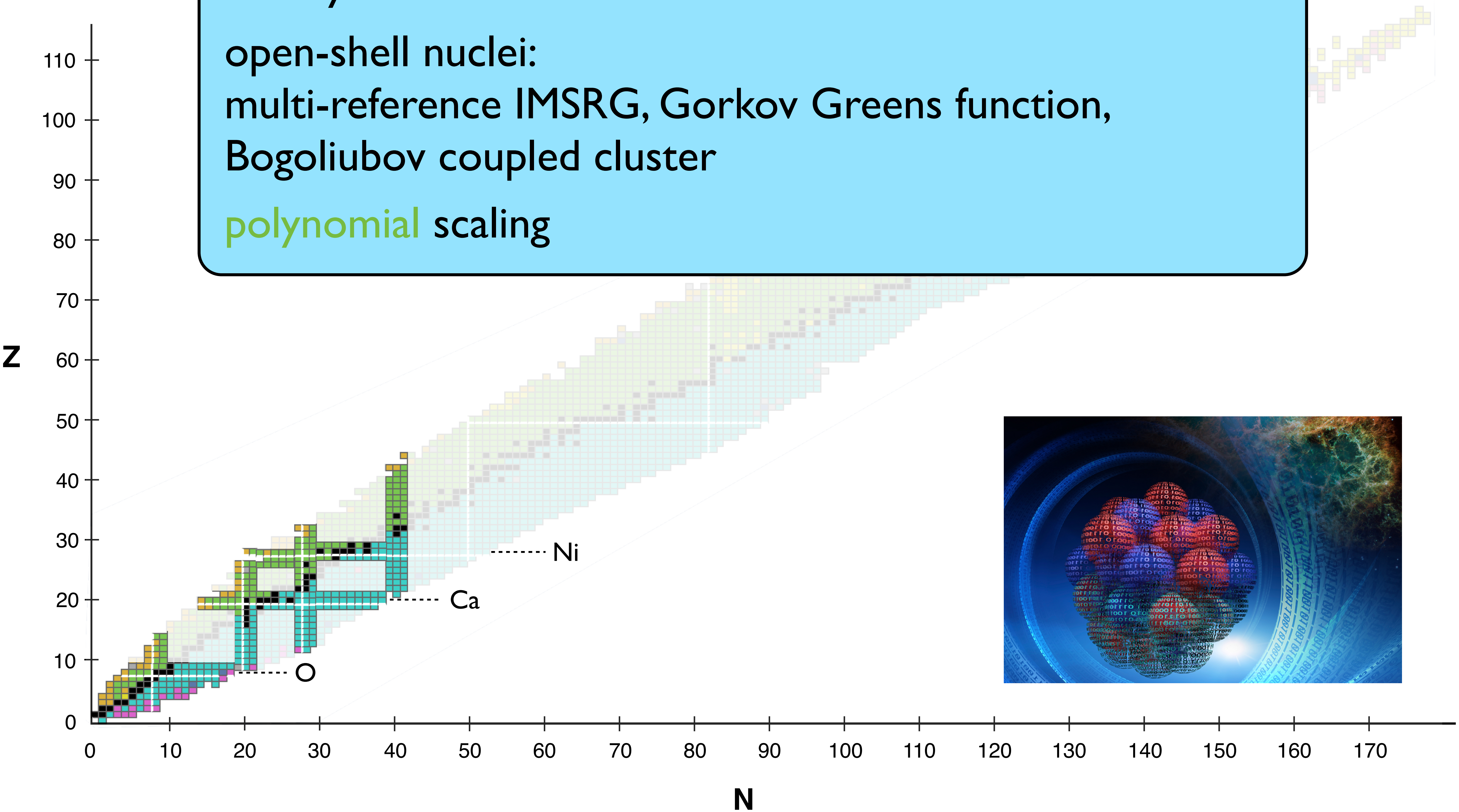


The theoretical nuclear landscape: Scope of ab initio methods for atomic nuclei

since year ~2010

open-shell nuclei:
multi-reference IMSRG, Gorkov Greens function, Bogoliubov coupled cluster

polynomial scaling

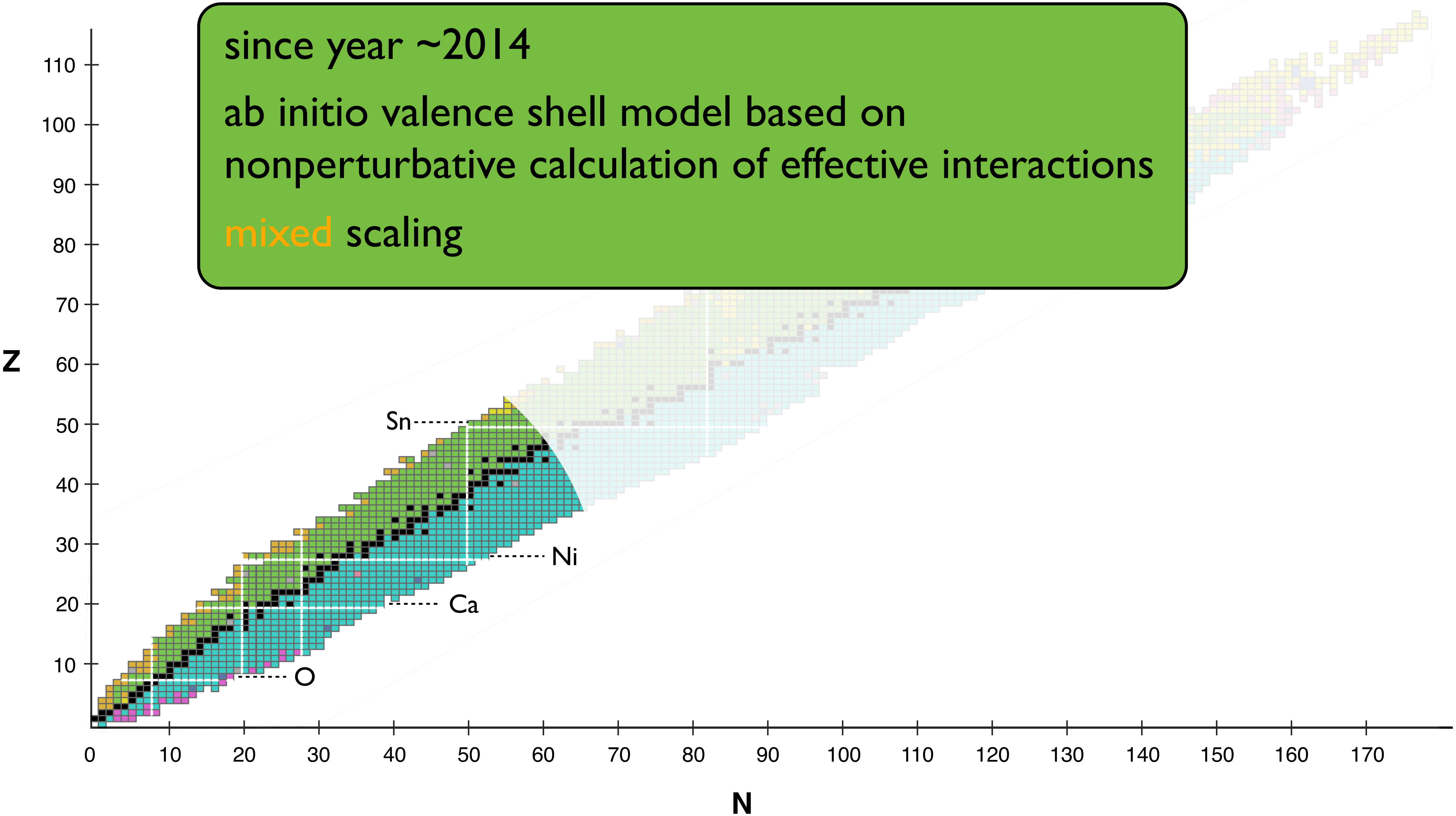


The theoretical nuclear landscape: Scope of ab initio methods for atomic nuclei

since year ~2014

ab initio valence shell model based on nonperturbative calculation of effective interactions

mixed scaling



The theoretical nuclear landscape:
Scope of ab initio methods for atomic nuclei

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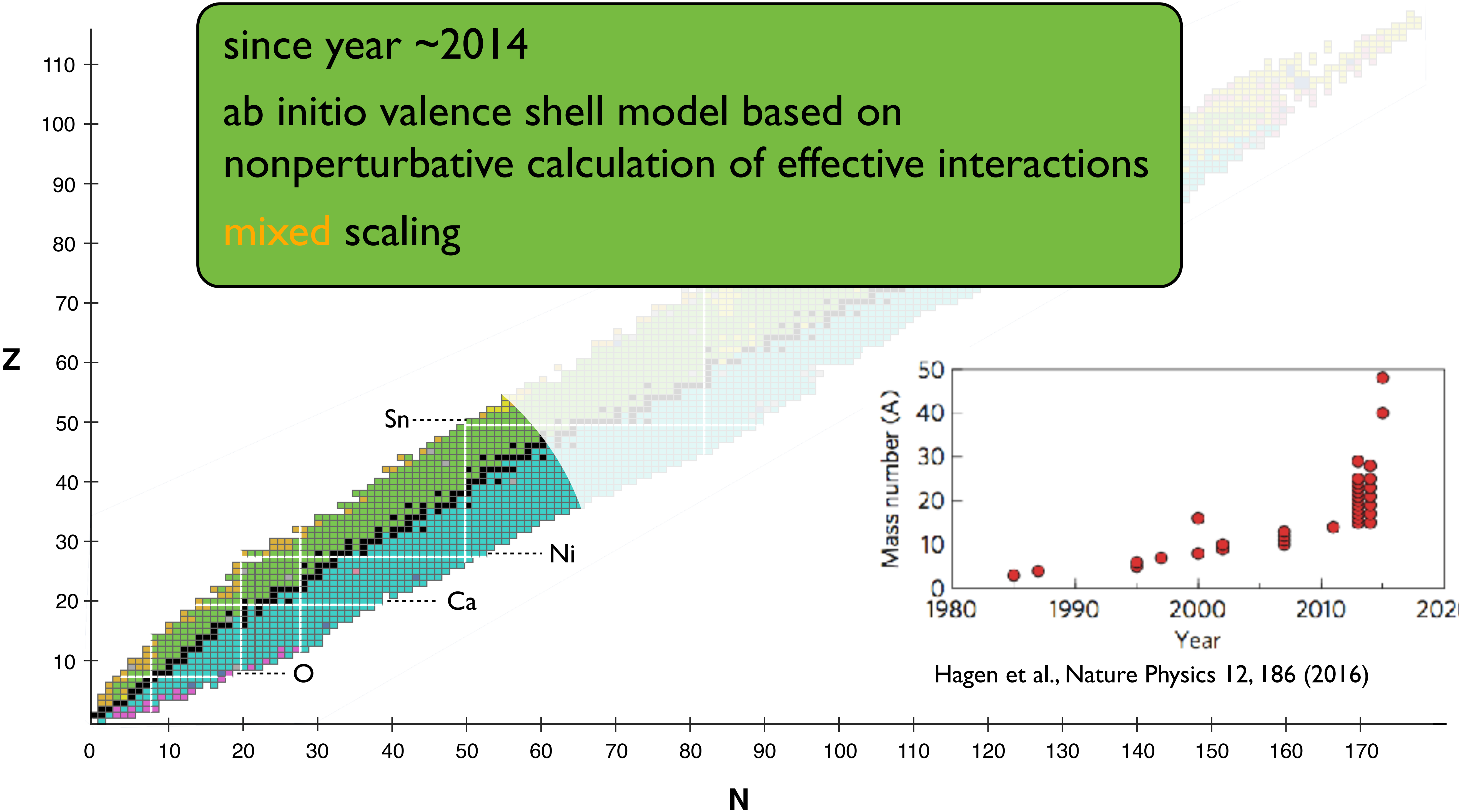
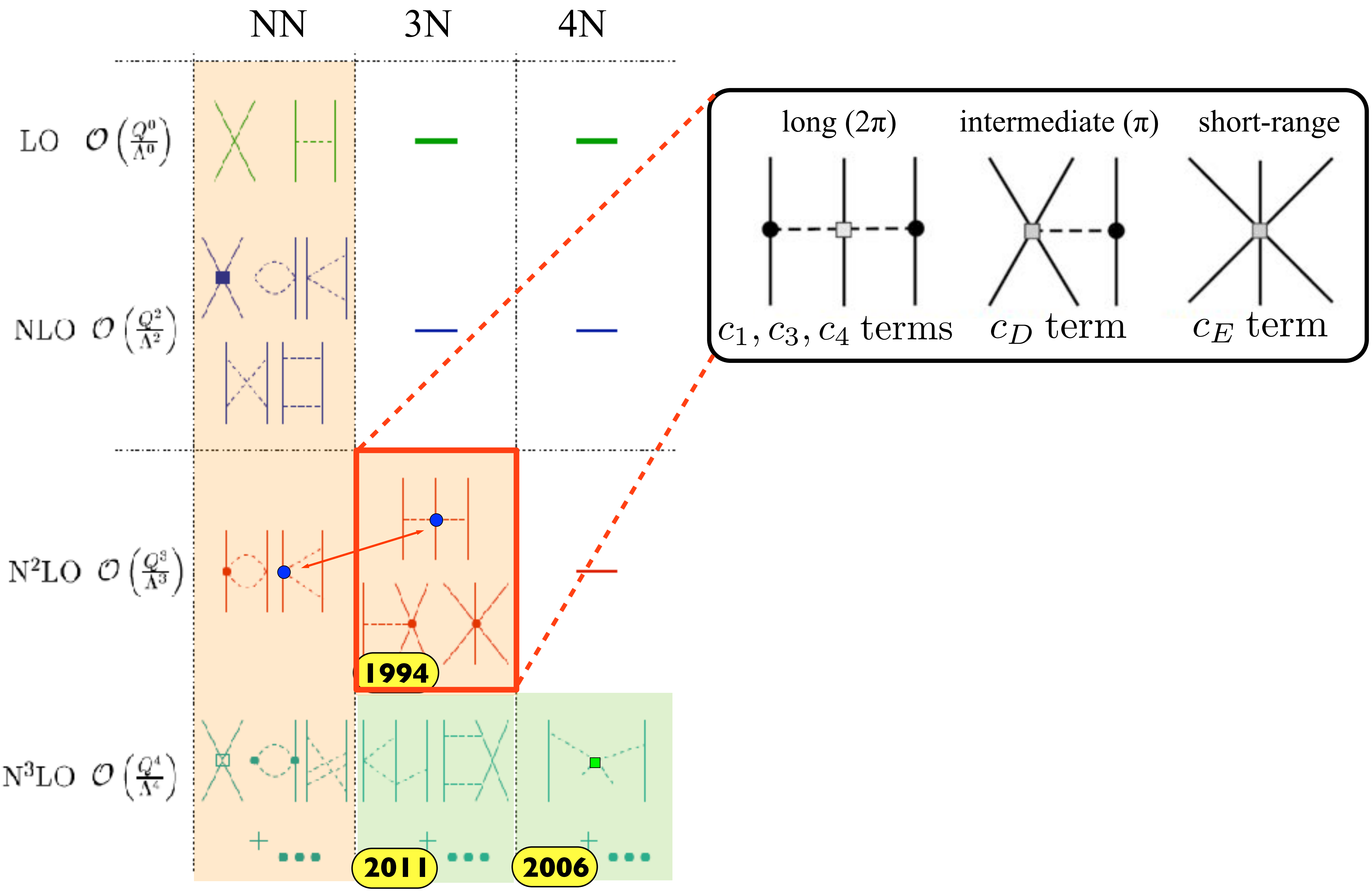


Hagen et al., Nature Physics 12, 186 (2016)

Many-body forces in chiral EFT



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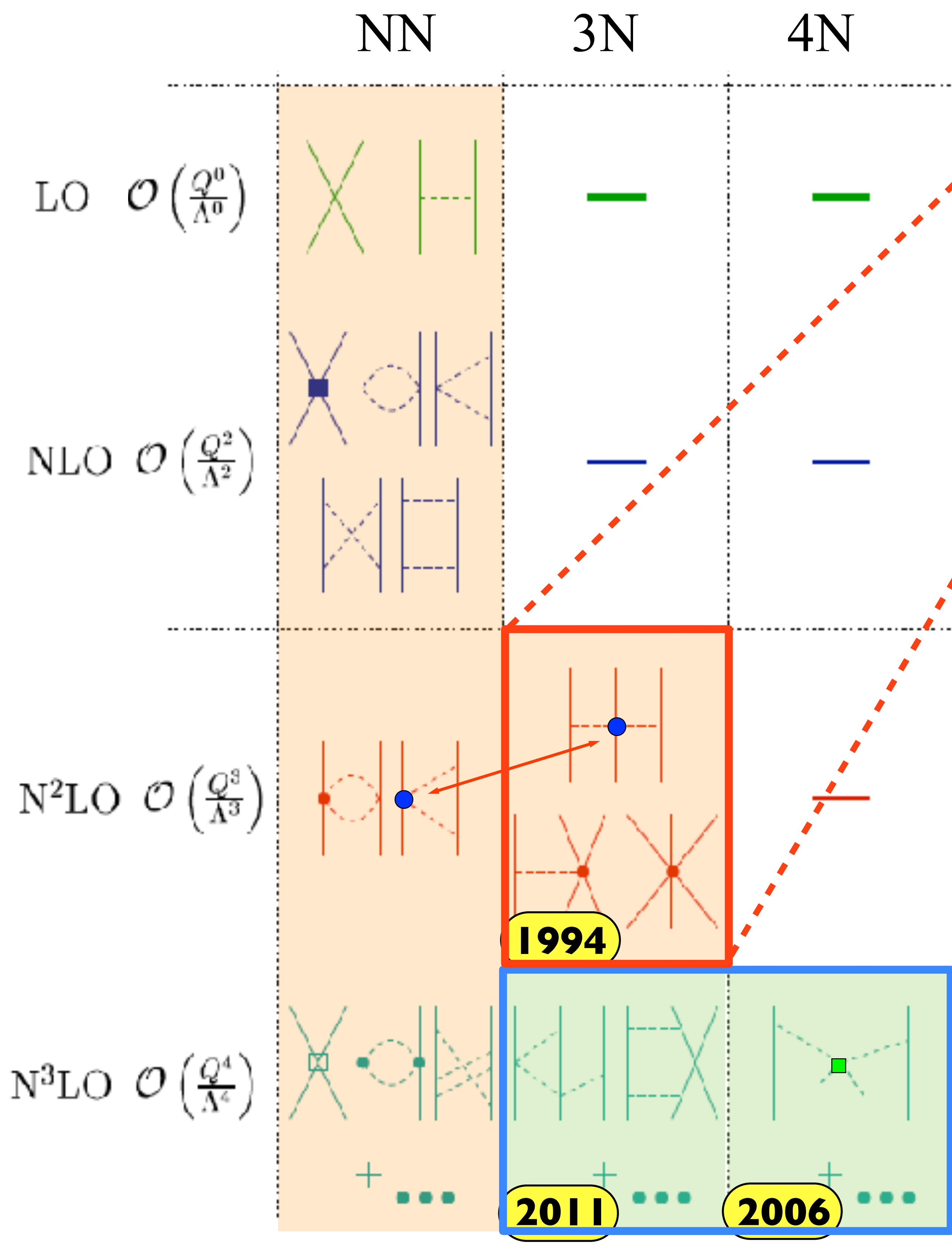
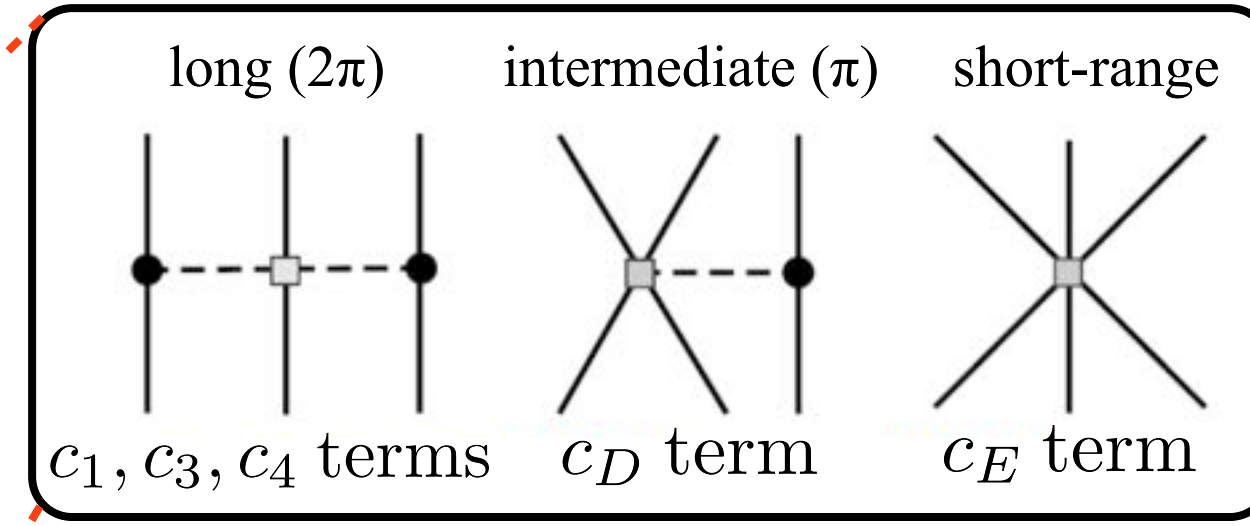




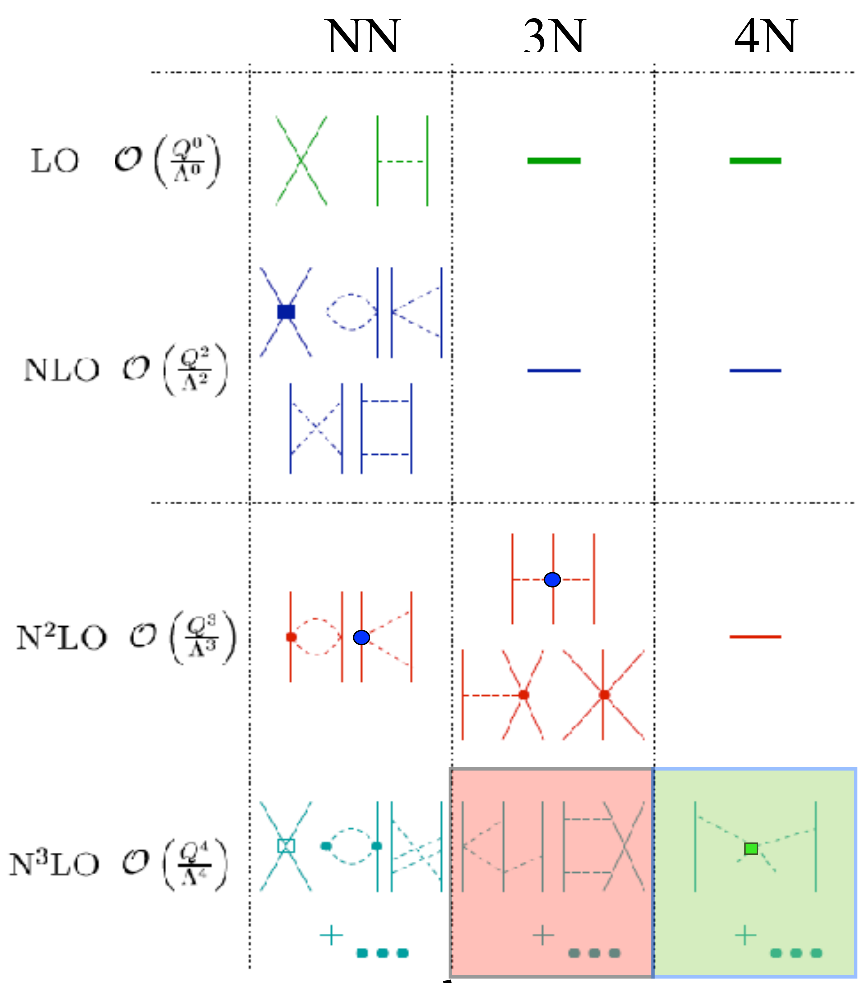
first incorporation in calculations of neutron and nuclear matter

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

Krueger, Tews, KH, Schwenk, PRC 88, 025802 (2013)

all terms predicted (no new low-energy couplings)

Contributions of many-body forces at N³LO in neutron matter



- first calculations of N³LO 3NF and 4NF contributions to EOS of neutron matter
- found large contributions in Hartree Fock appr., comparable to size of N²LO contributions

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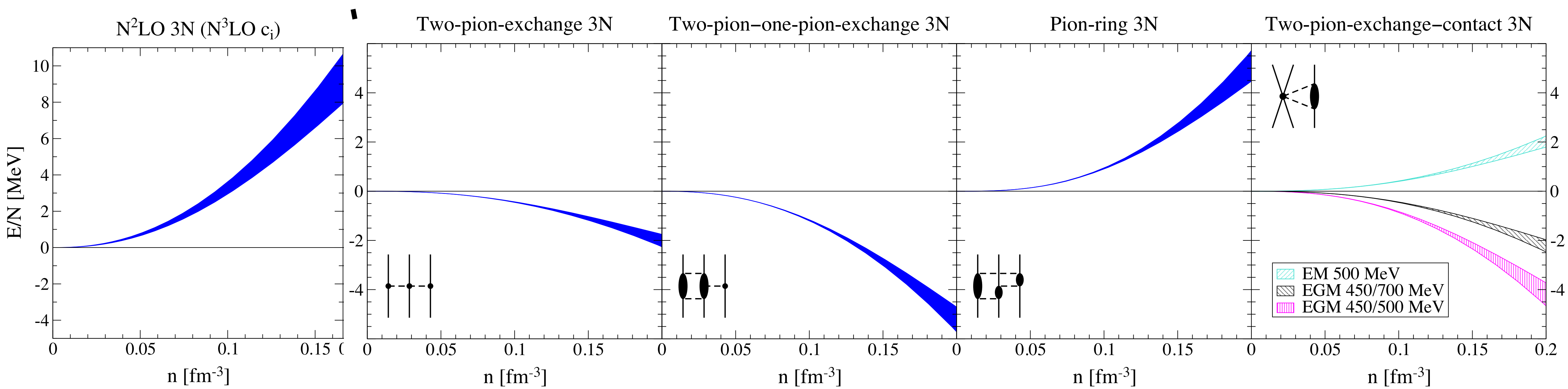
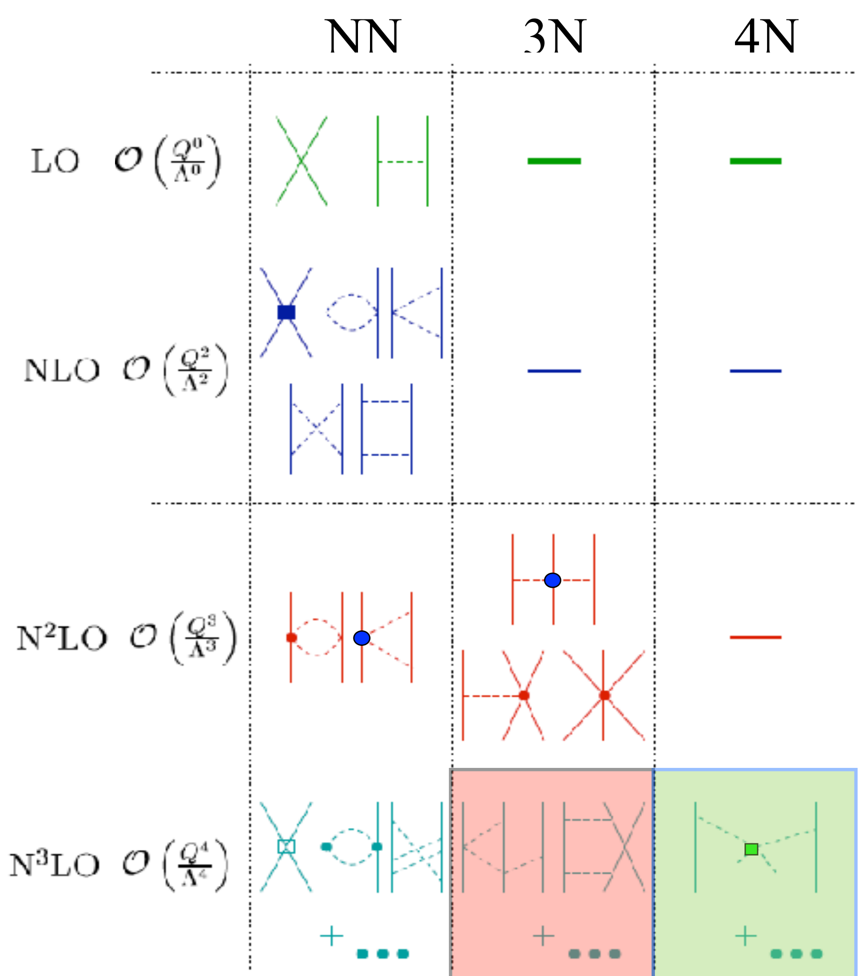


Contributions of many-body forces at N^{3}LO in neutron matter



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

Krüger, Tews, KH, Schwenk, PRC 88, 025802 (2013)

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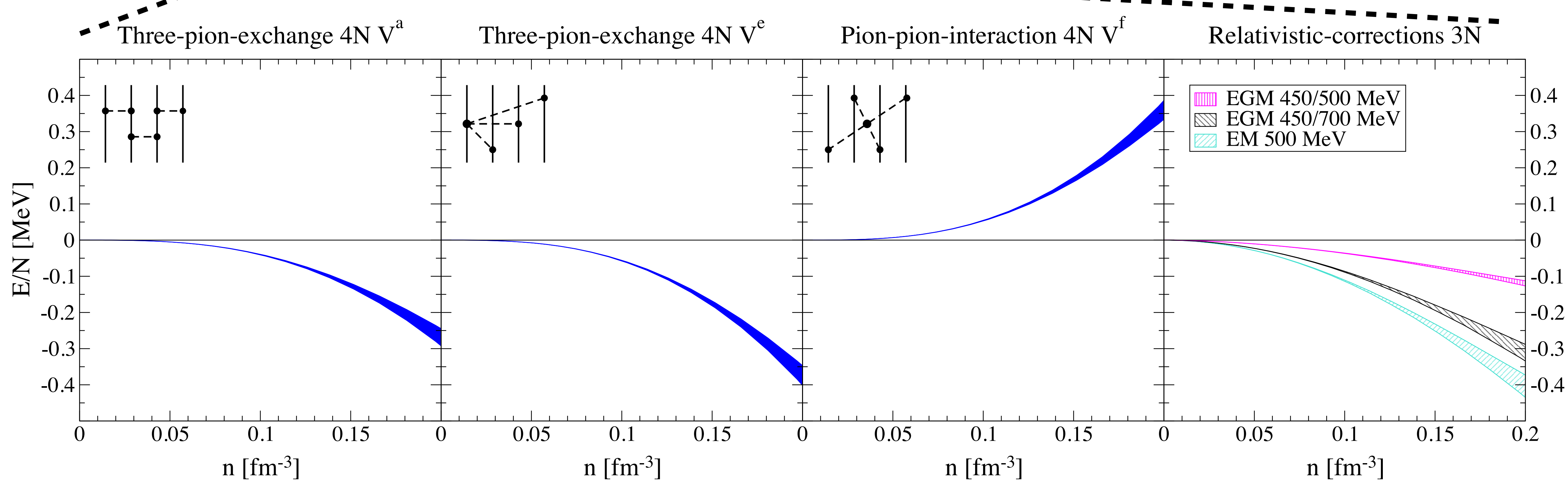
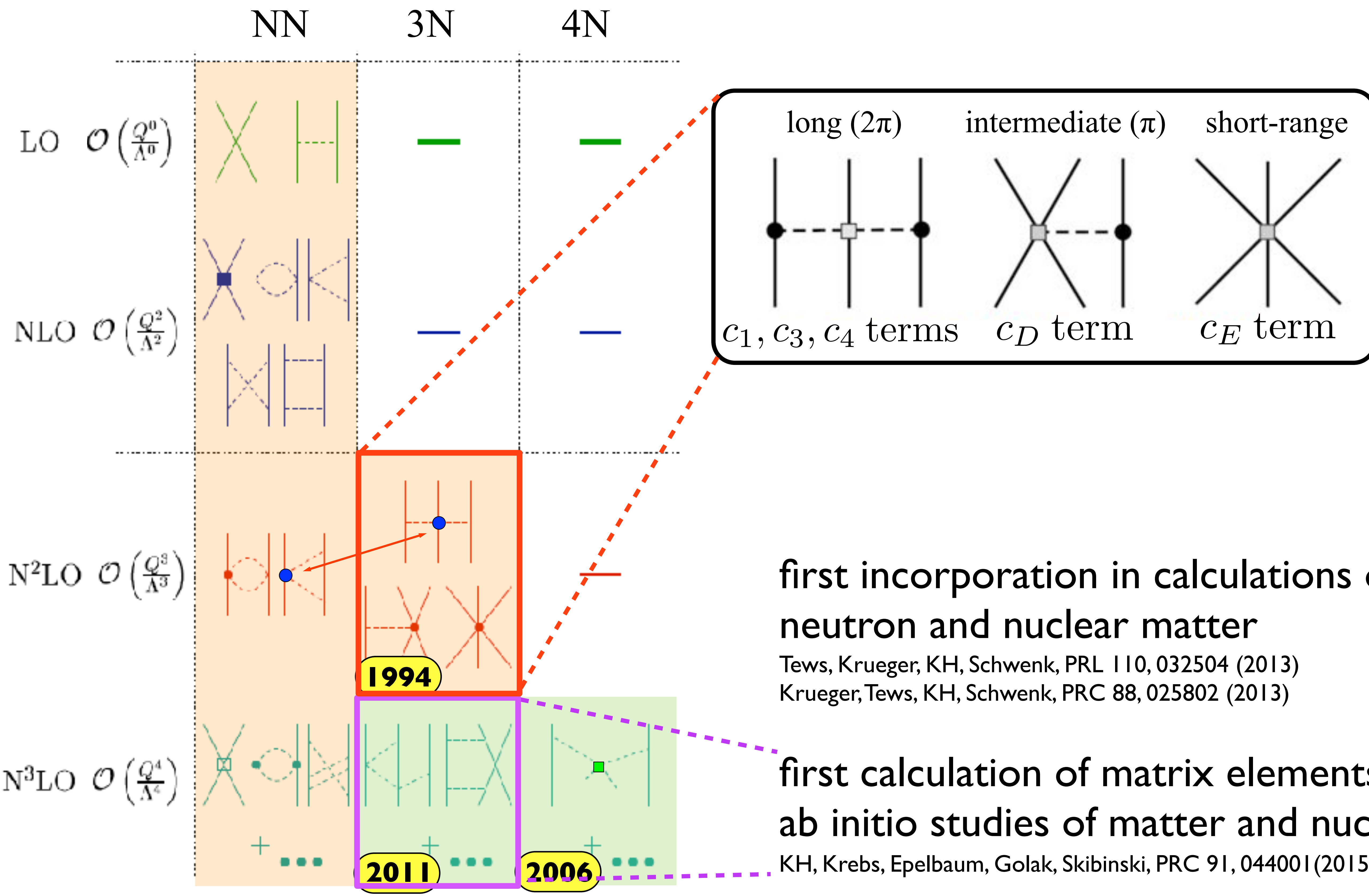


Many-body forces in chiral EFT



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

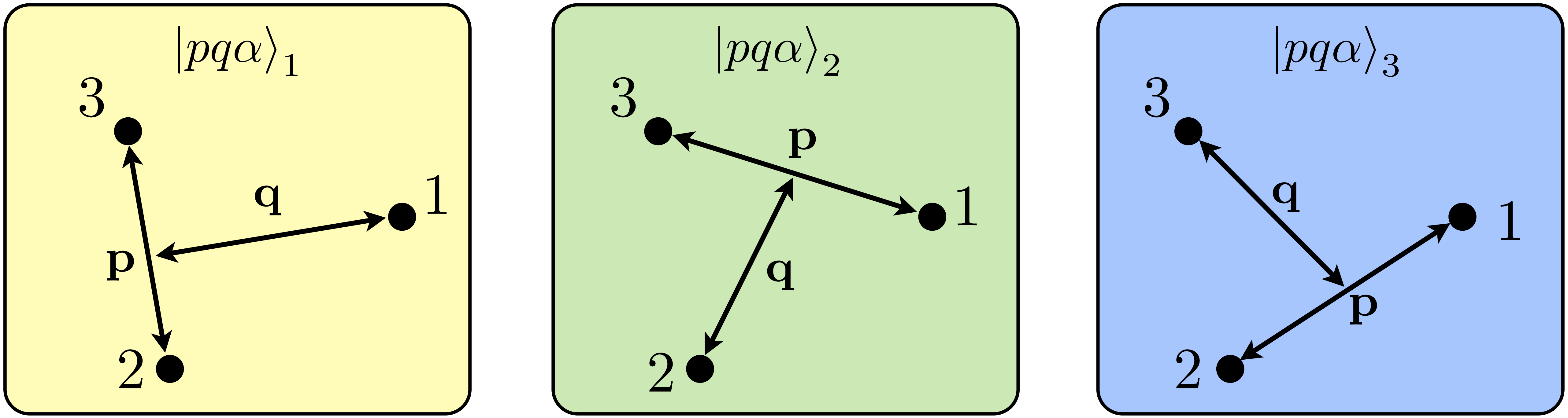
Krueger, Tews, KH, Schwenk, PRC 88, 025802 (2013)

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

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

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.

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

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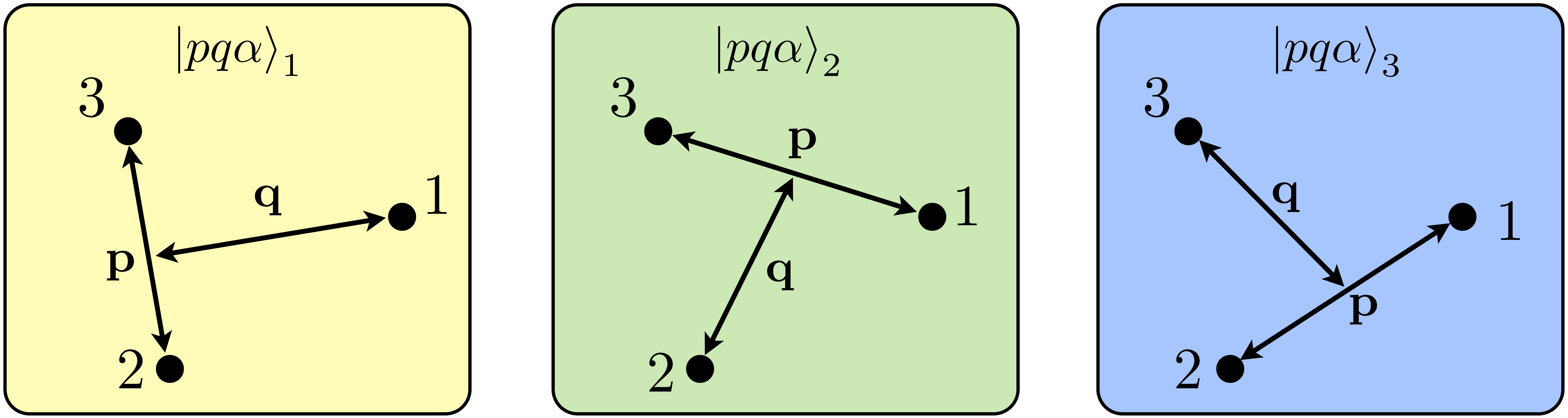

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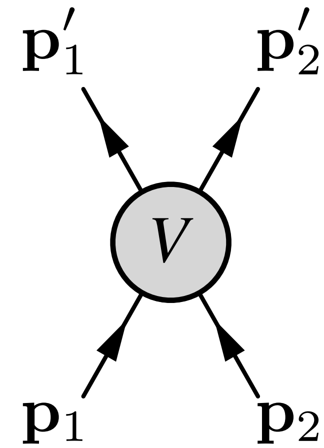
A new algorithm allows much more efficient calculations.

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

Regularization schemes for nuclear interactions (here: NN)

Separation of long- and short-range physics



$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2$$
$$\mathbf{p}' = (\mathbf{p}_1' - \mathbf{p}_2')/2$$
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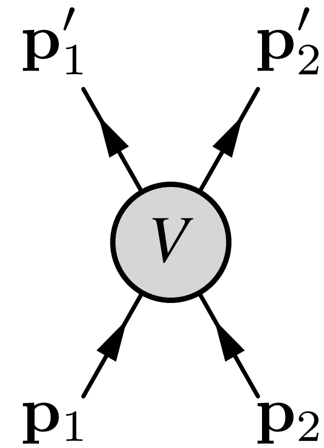

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nonlocal
$$V_{\mathrm{NN}}(\mathbf{p}, \mathbf{p}') \to \exp\left[-\left((p^2 + p'^2)/\Lambda^2\right)^n\right] V_{\mathrm{NN}}(\mathbf{p}, \mathbf{p}')$$

Epelbaum, Glöckle, Meissner, NPA 747, 362 (2005)
Entem, Machleidt, PRC 68, 041001 (2003)

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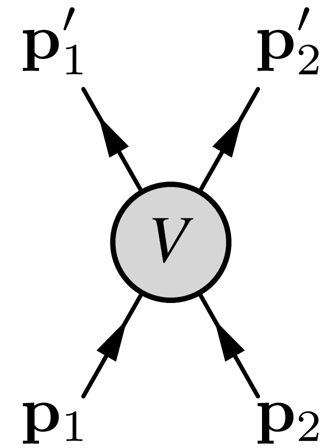

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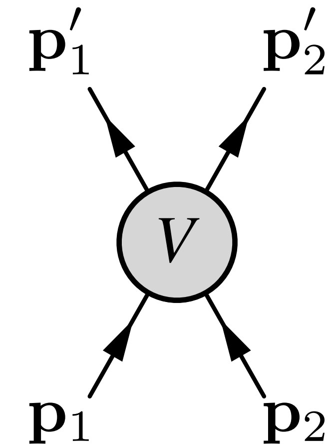
cf. Navratil, Few-body Systems 41, 117 (2007)

Regularization schemes for nuclear interactions (here: NN)

Separation of long- and short-range physics



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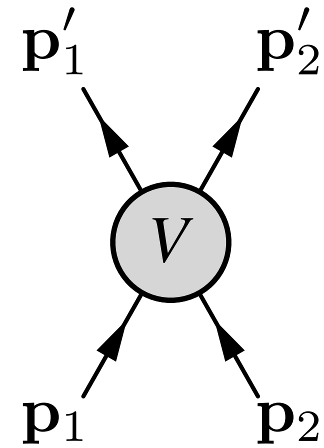
local (coordinate space)

$$V_{\mathrm{NN}}^{\pi}(\mathbf{r}) \to \left(1 - \exp\left[-\left(r^2/R^2\right)^n\right]\right) V_{\mathrm{NN}}^{\pi}(\mathbf{r})$$
$$\delta(\mathbf{r}) \to \alpha_n \exp\left[-(r^2/R^2)^n\right]$$

Gezerlis et. al, PRL, 111, 032501 (2013)

Regularization schemes for nuclear interactions (here: NN)

Separation of long- and short-range physics



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semi-local

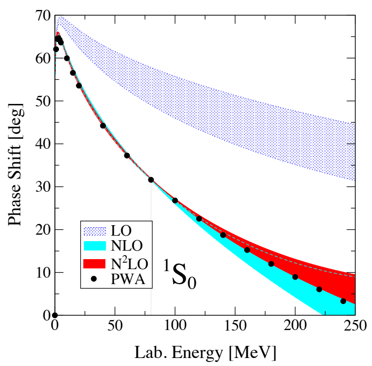
$$V_{\rm NN}^{\pi}(\mathbf{r}) \to \left(1-\exp\left[-\left(r^2/R^2\right)\right]\right)^n V_{\rm NN}^{\pi}(\mathbf{r})$$
$$\delta(\mathbf{r}) \to C \to \exp\left[-\left((p^2+p'^2)/\Lambda^2\right)^n\right] C$$

Epelbaum et. al, PRL, 115, 122301 (2015)

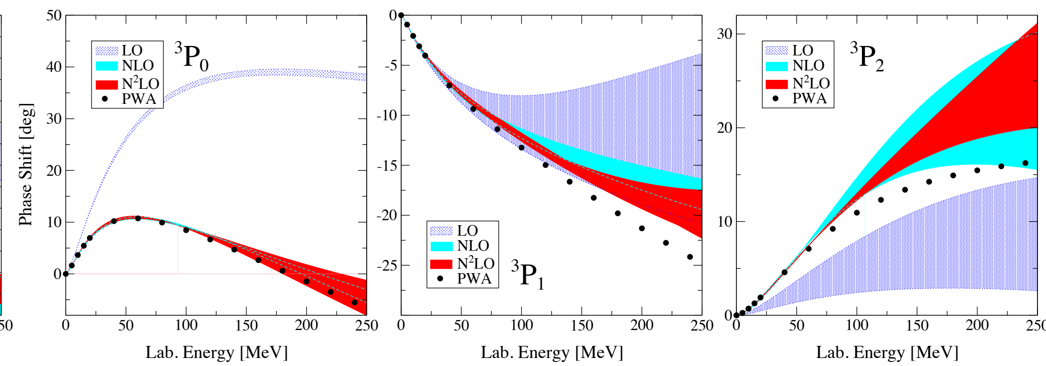
Recent and current developments of novel nuclear interactions

1. local EFT interactions, suitable for Quantum Monte Carlo calculations

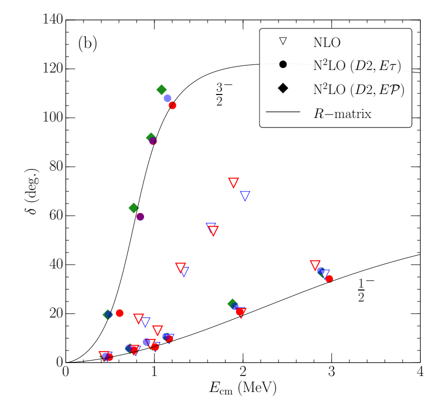
status: NN plus 3N up to N2LO, calculations of few-body systems and neutron matter

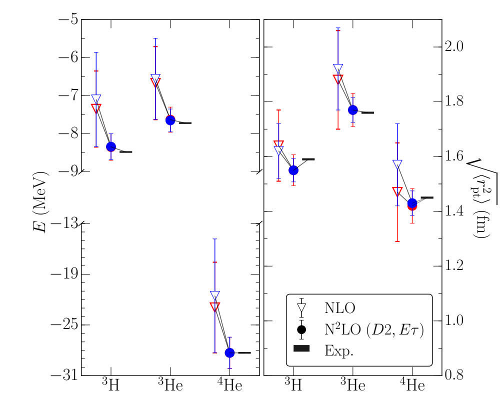


Gezerlis et al.,
PRL 111, 032501 (2013)



Gezerlis et al.,
PRC 90, 054323 (2014)





Lynn et al.,
PRL 116, 062501 (2016)

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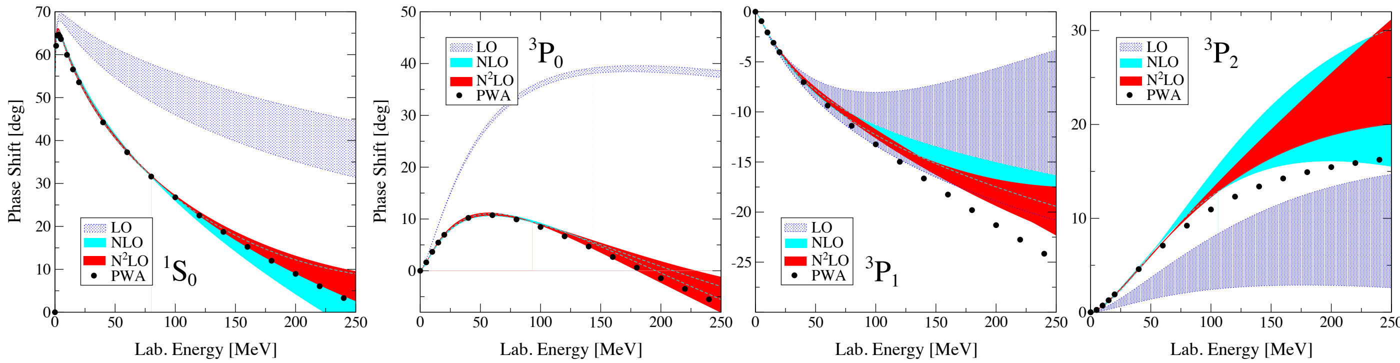

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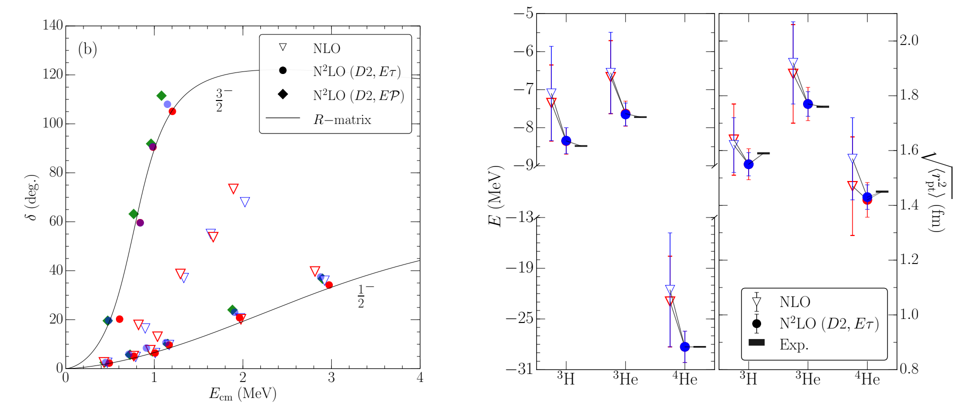
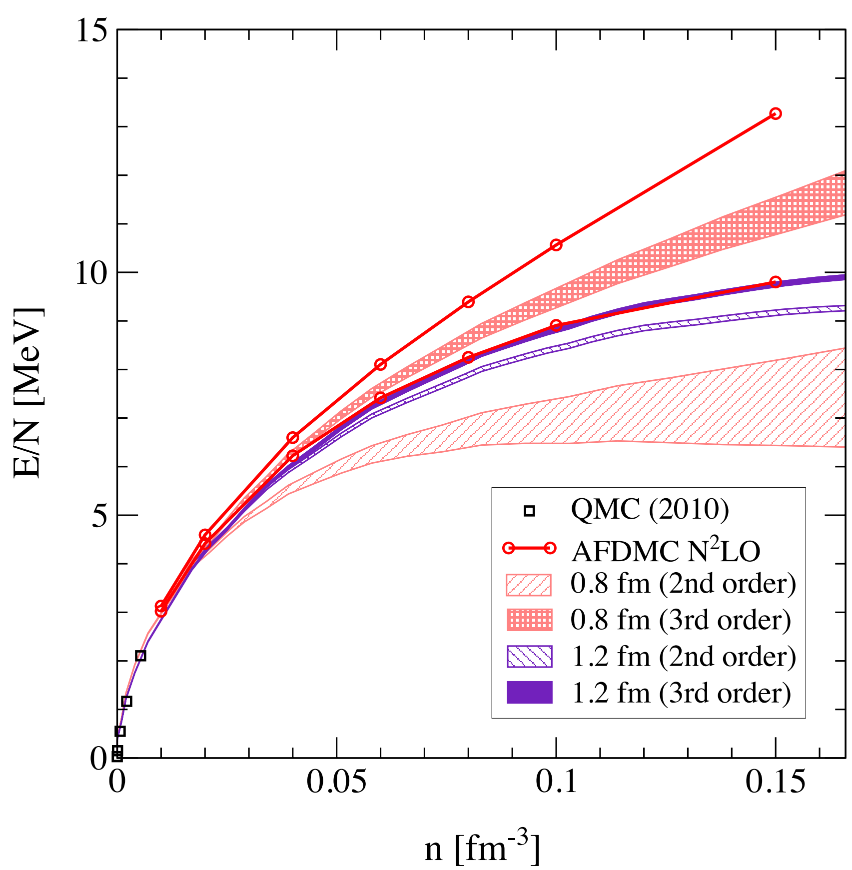


Lynn et al.,
PRL 116, 062501 (2016)



first Quantum Monte Carlo of neutron matter based on chiral EFT interactions

perfect agreement for soft interactions, first direct validation of calculations within many-body perturbation theory

Gezerlis et. al,
PRL 111, 032501 (2013)

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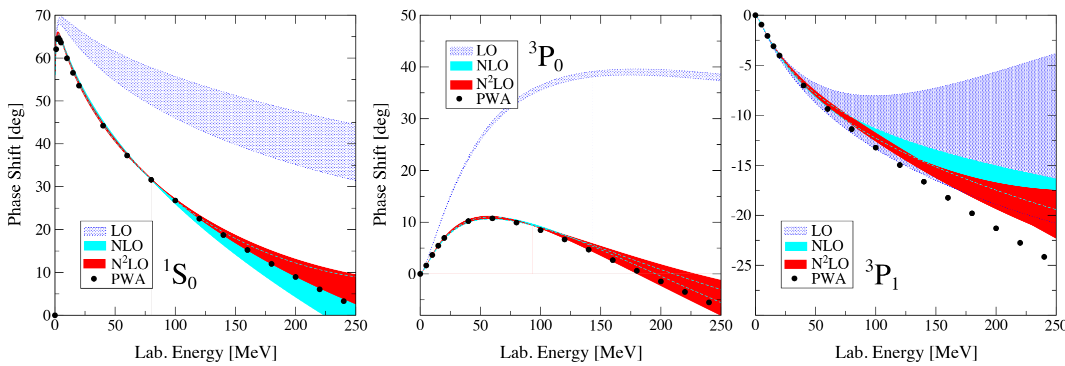

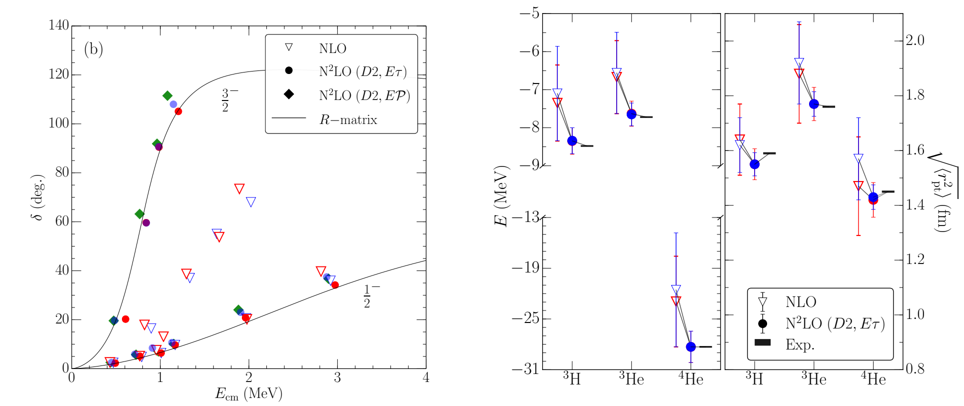

Gezerlis et al.,
PRL 111, 032501 (2013)

Gezerlis et al.,
PRC 90, 054323 (2014)

Lynn et al.,
PRL 116, 062501 (2016)

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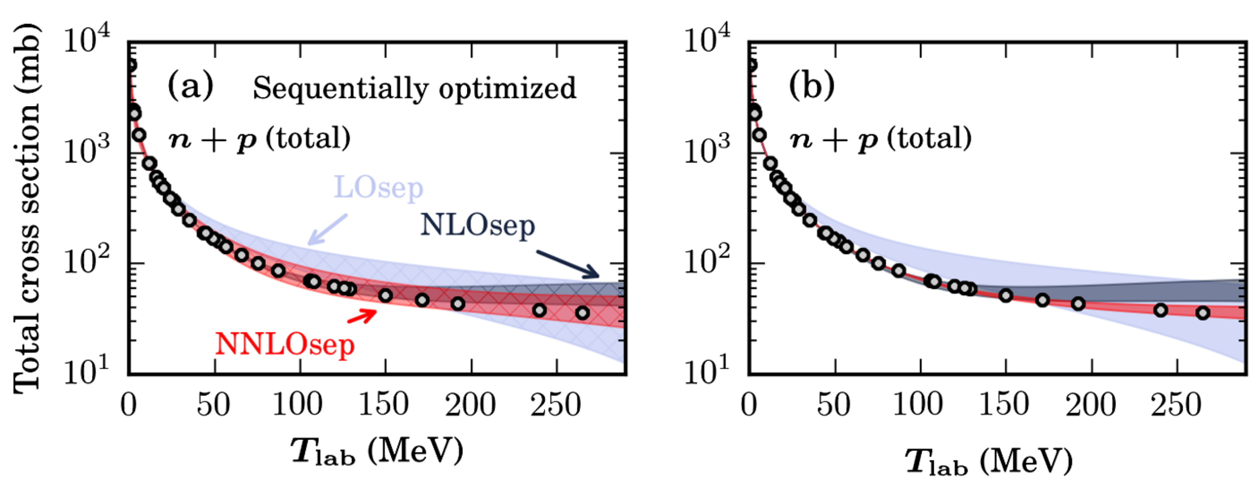
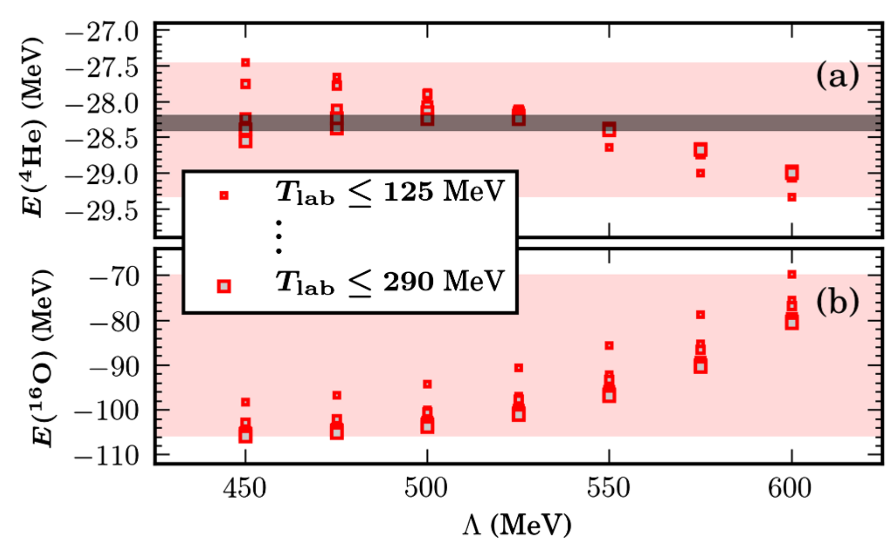
2. simultaneous fit of NN and 3N forces to two- and few-body observables

status: NN plus 3N up to N2LO, N3LO currently in development



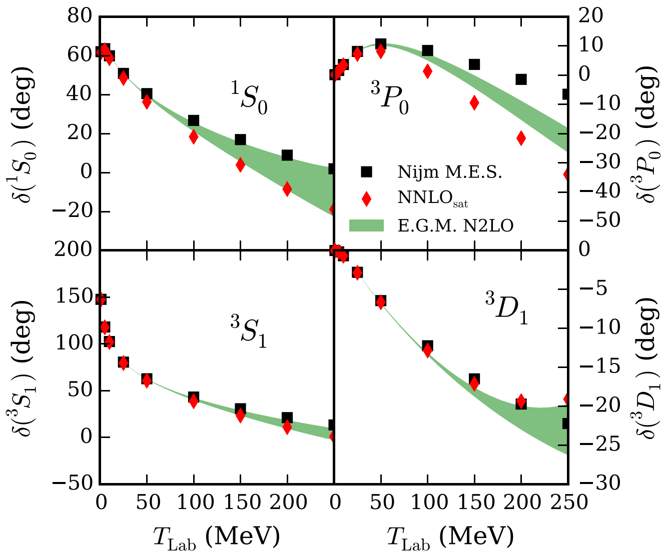


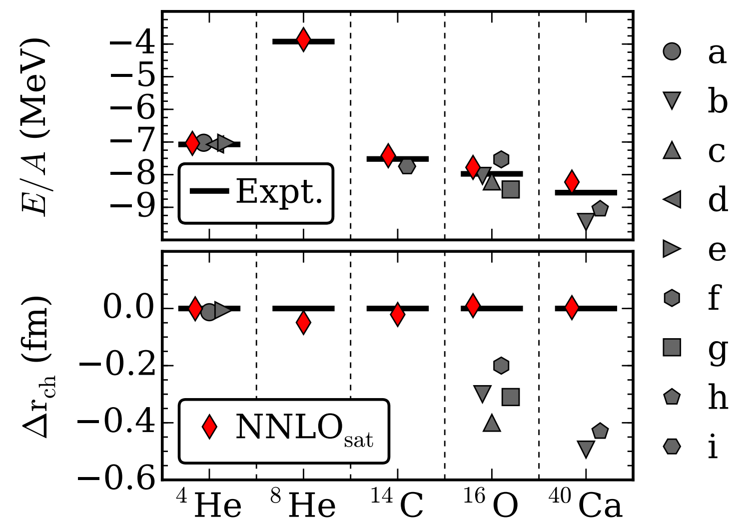
Carlsson et al.,
PRX 6, 011019 (2016)

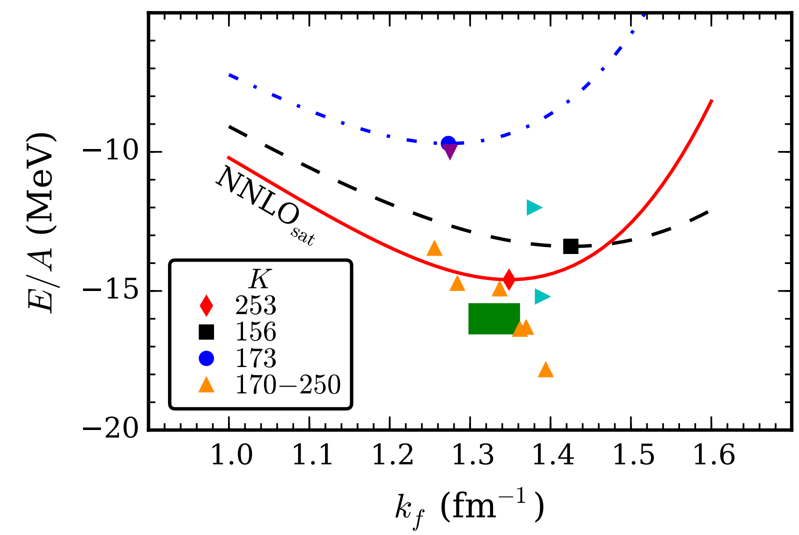
Recent and current developments of novel nuclear interactions

3. fits of NN plus 3N forces to two-, few- and many-body observables

status: NN plus 3N up to N2LO, NN phase shifts fitted up to T_{lab}~35 MeV







Ekström et al., PRC91, 051301 (2015)

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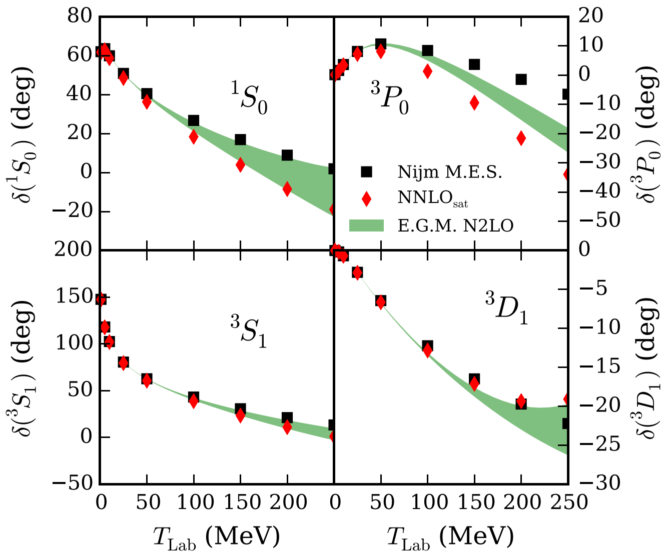
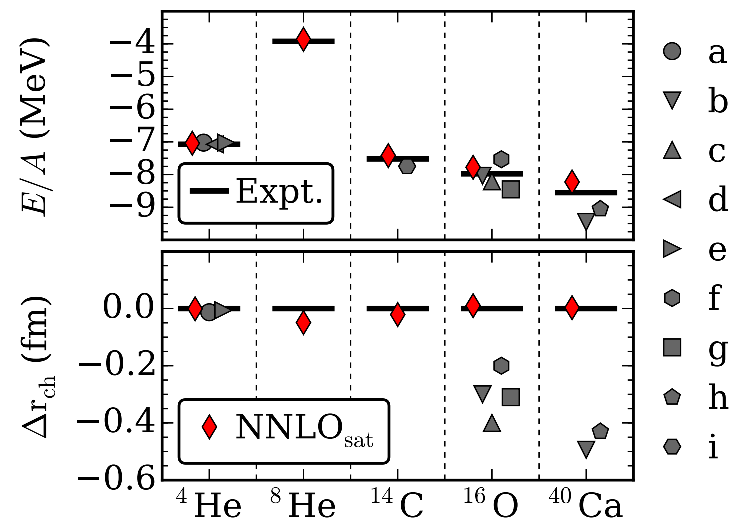
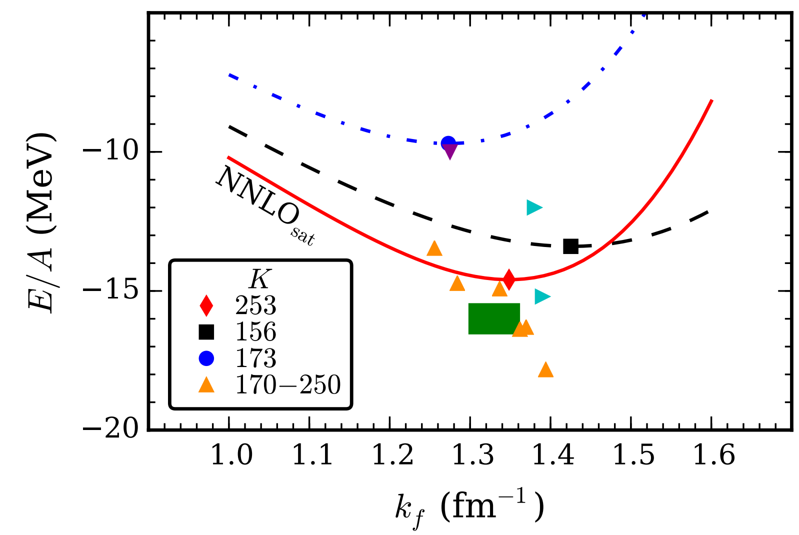


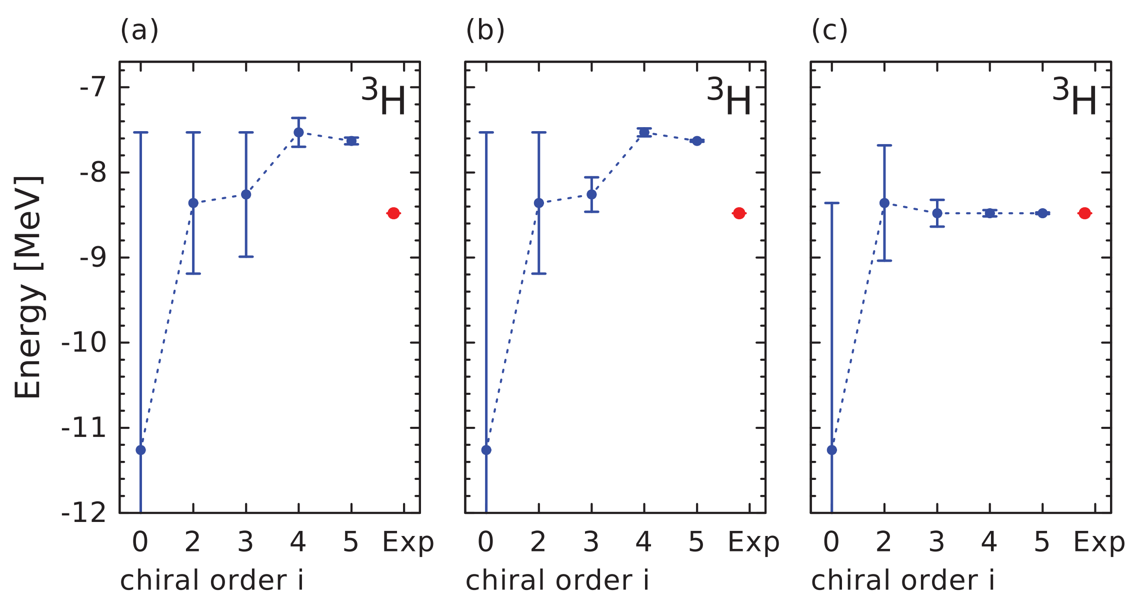




Ekström et al., PRC91, 051301 (2015)

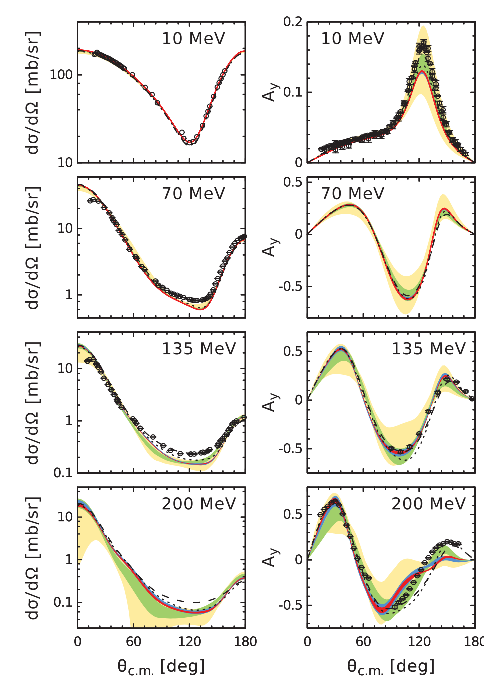
4. semilocal NN forces, development of improved method to estimate uncertainties

status: NN up to N4LO, 3N interactions up to N3LO



Epelbaum, Krebs, Meißner, PRL 115, 122301 (2015)

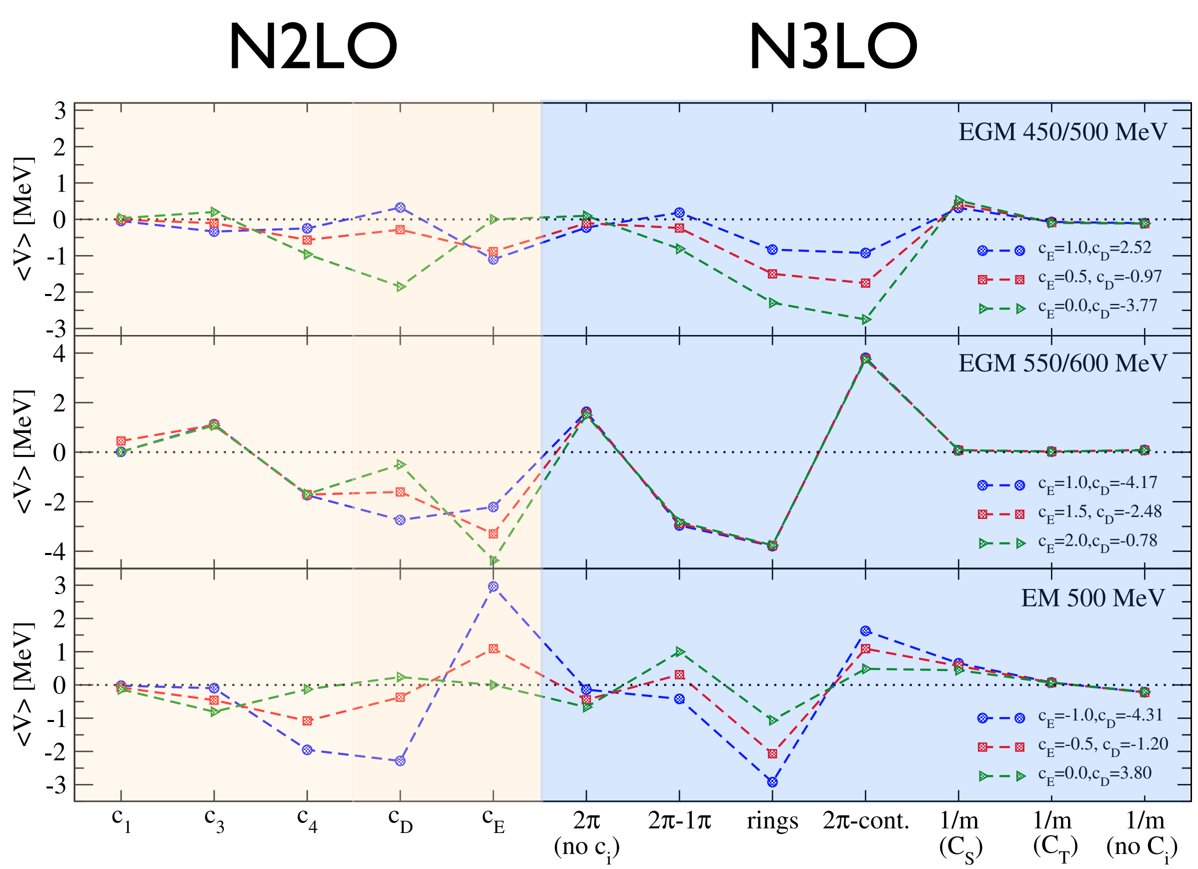
Binder et al., PRC 93, 044002 (2016)



LENPIC

3NF power counting for different regulators

nonlocal



KH et al.,
PRC 91, 044001 (2015)

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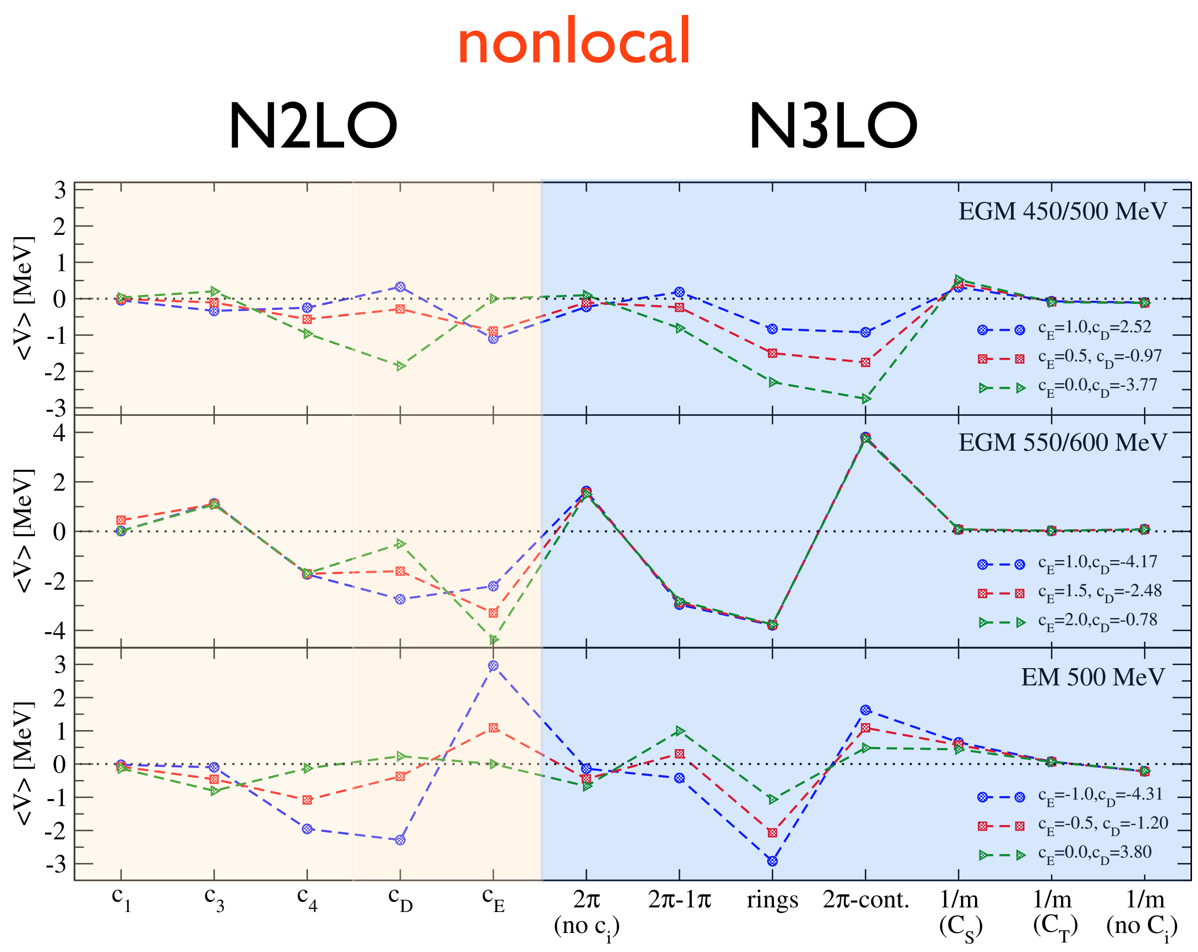

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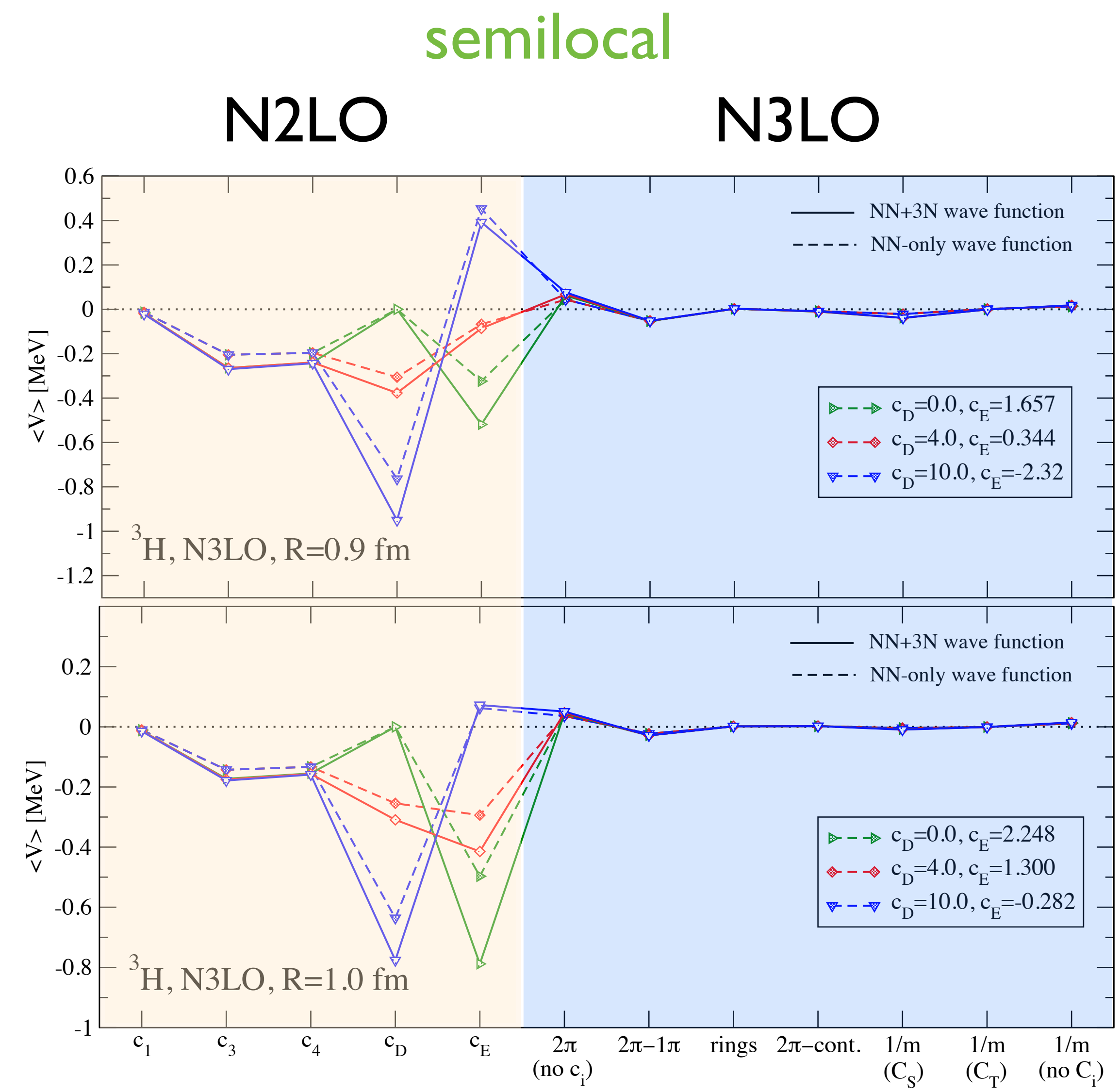
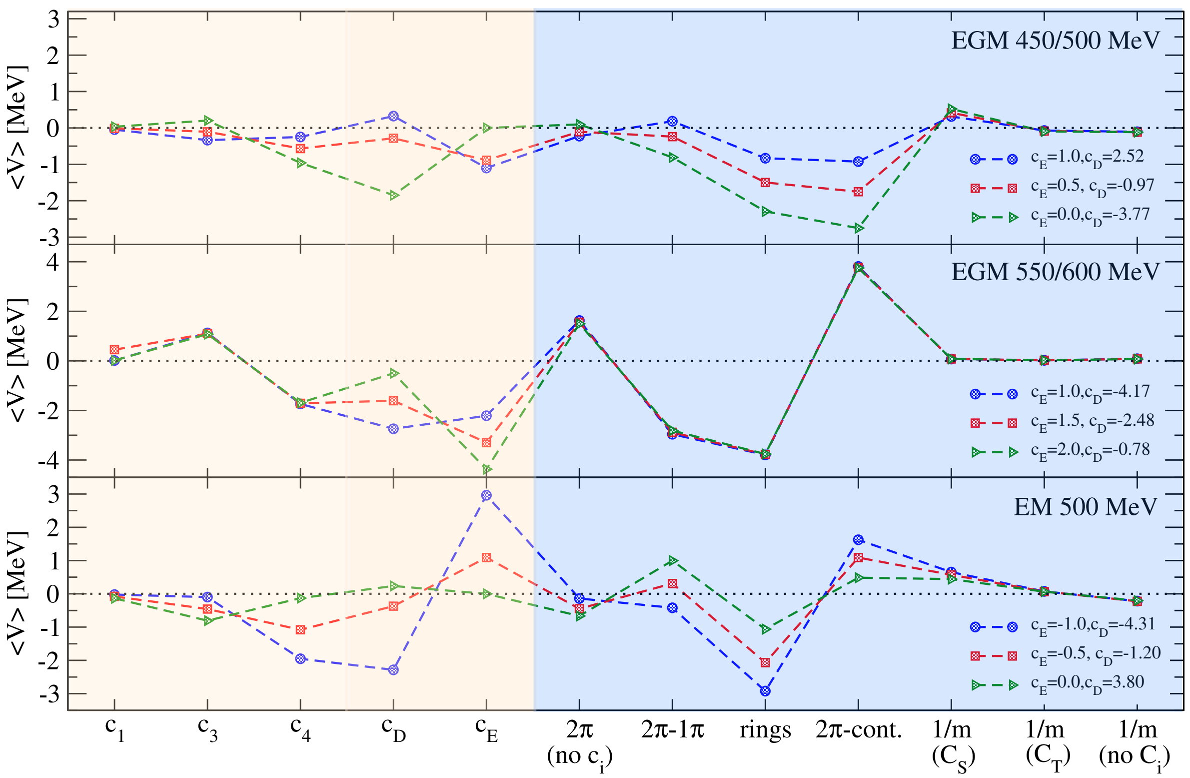


- size of N3LO contribution not suppressed for shown nonlocal interactions
- N3LO contributions suppressed for semilocal interactions
- technical challenges for semilocal interactions:
  - ★ forces non-perturbative, large basis spaces or RG evolution needed
  - ★ implementation of 3N forces hard, stability problems for scattering calculations
  - ★ implementation of nuclear currents hard

3NF power counting for different regulators

nonlocal

N2LO N3LO



KH et al.,
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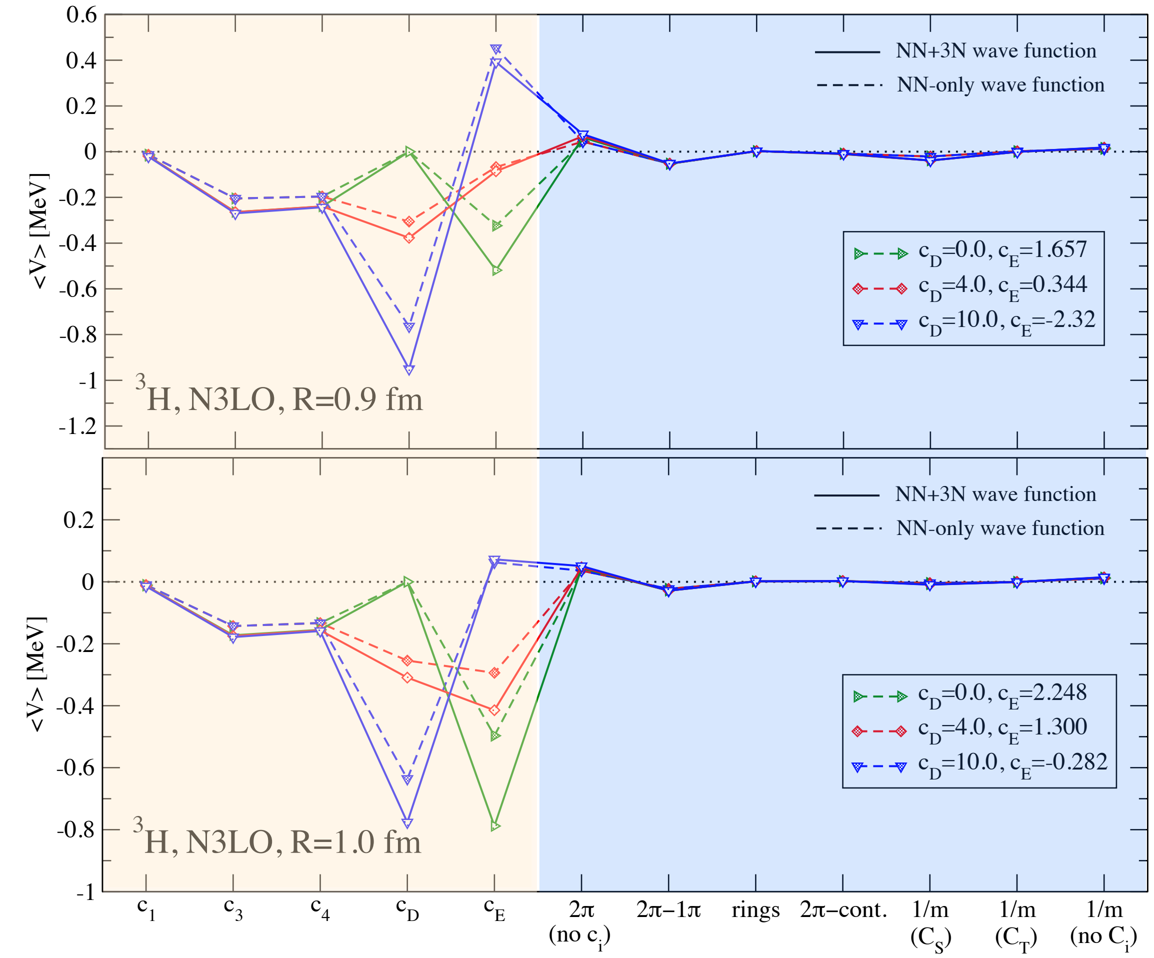
semilocal

N2LO N3LO



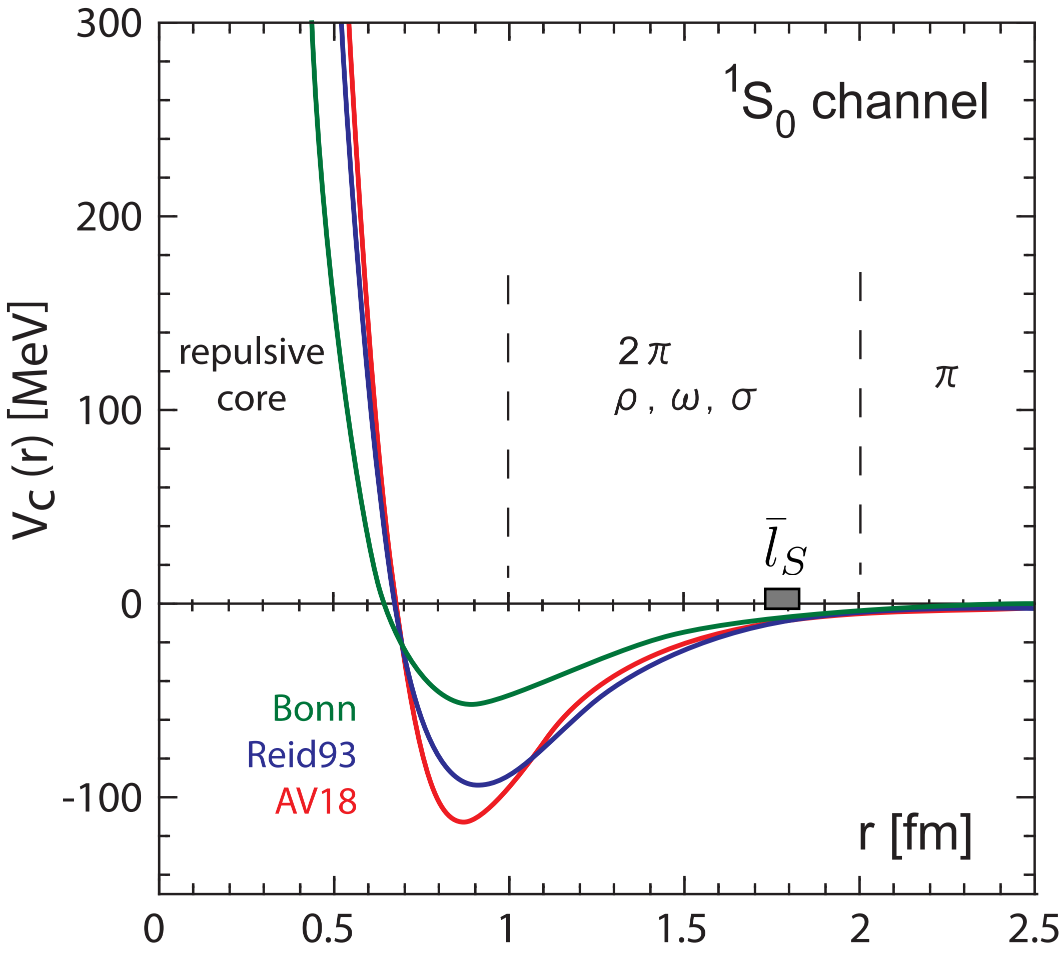
Development of improved novel semilocal NN+3N interactions regularised in momentum space.

$$V_\pi(\mathbf{p},\mathbf{p}') \to V_\pi(\mathbf{p},\mathbf{p}')e^{-(\mathbf{q}^2+m_\pi^2)/\Lambda^2}$$

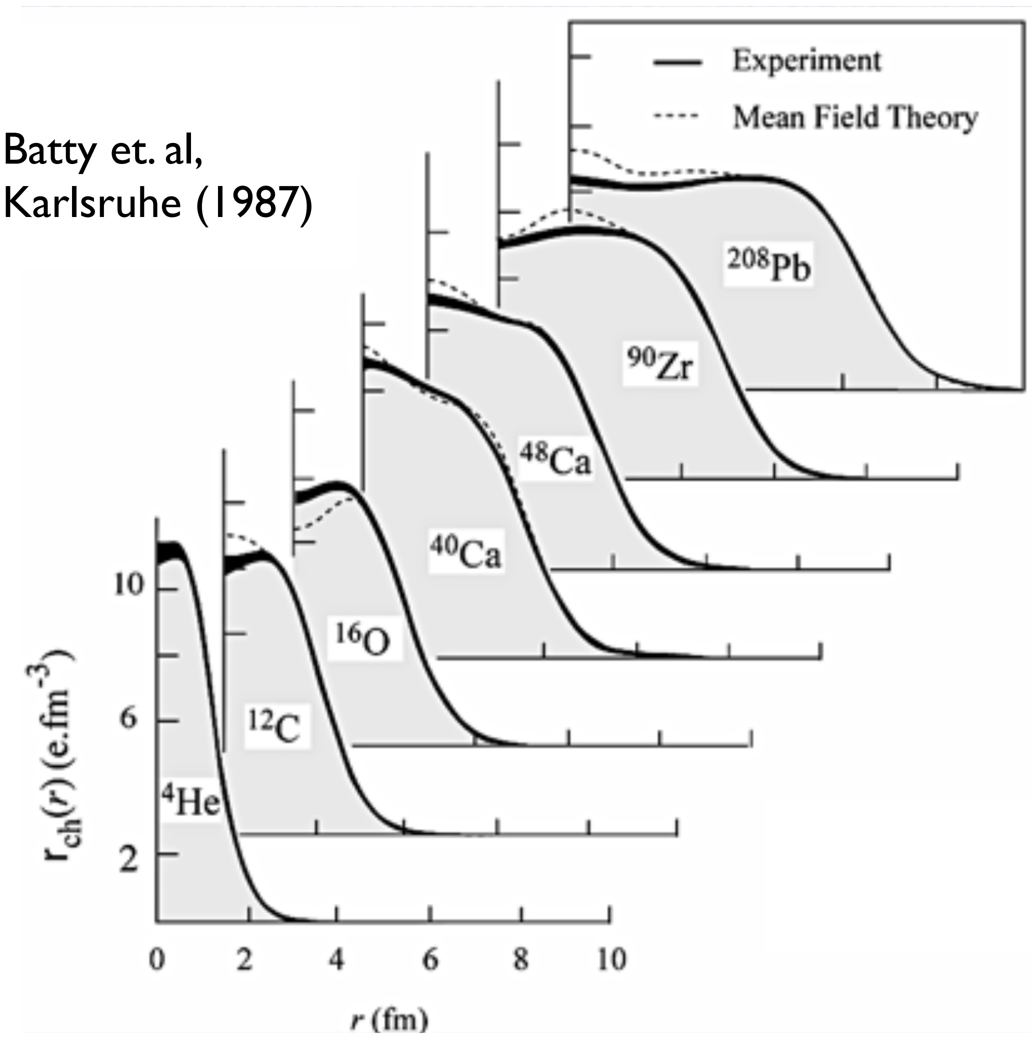
Reinert et al.,
arXiv:1711.08821

Calculation of N2LO 3NFs completed.
Benchmarks and fits in progress!

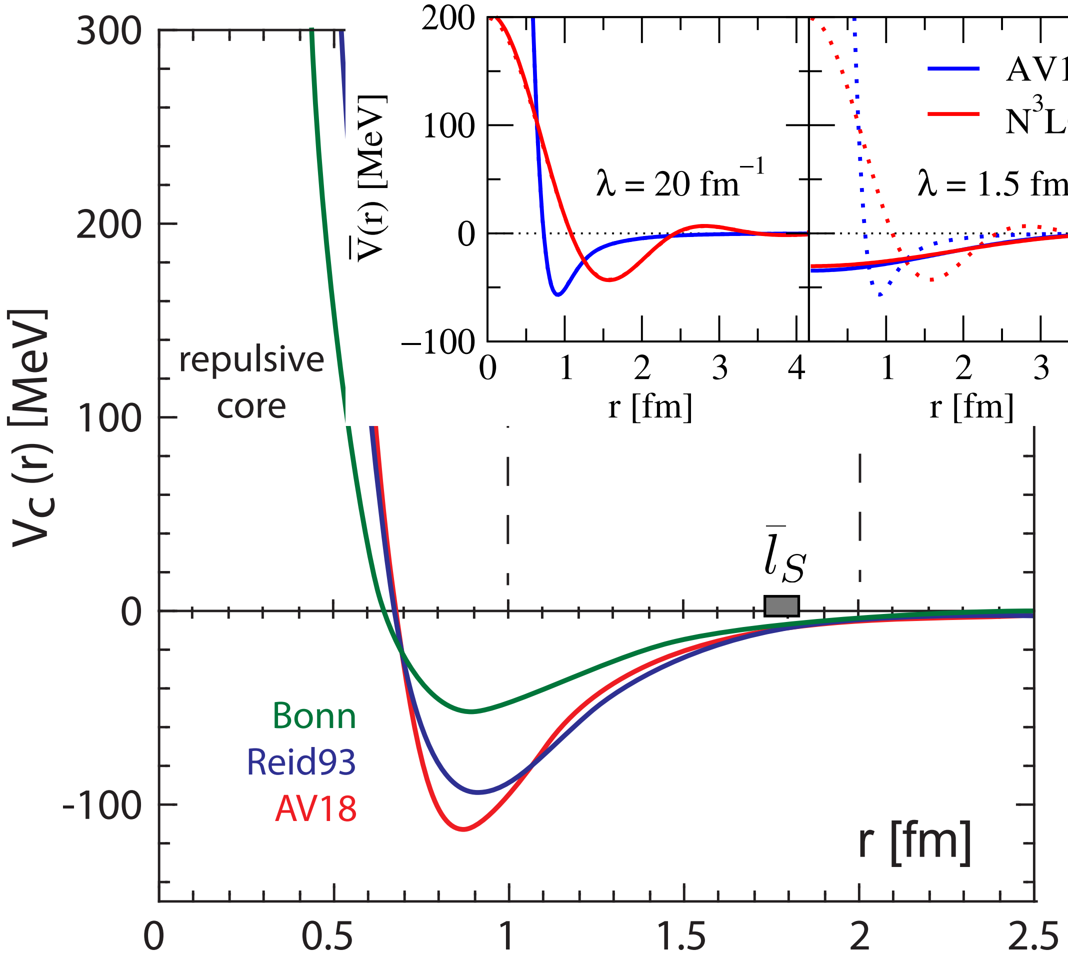
Equation of state of symmetric nuclear matter: nuclear saturation

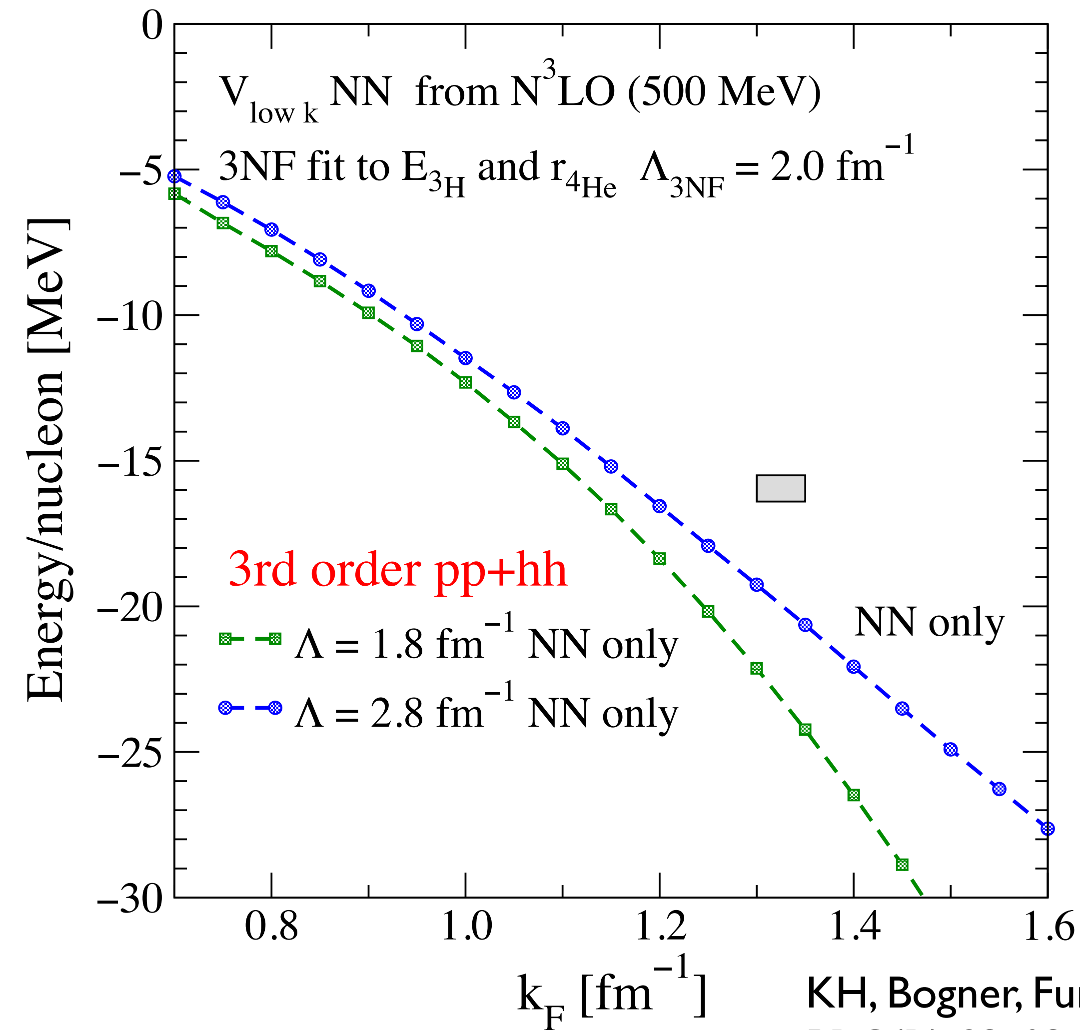


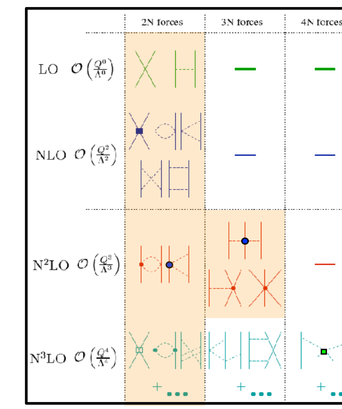
Batty et. al,
Karlsruhe (1987)



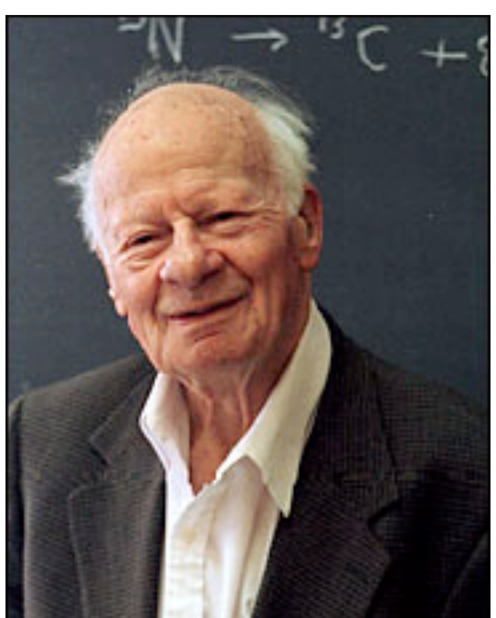
Fitting the 3NF LECs at low resolution scales







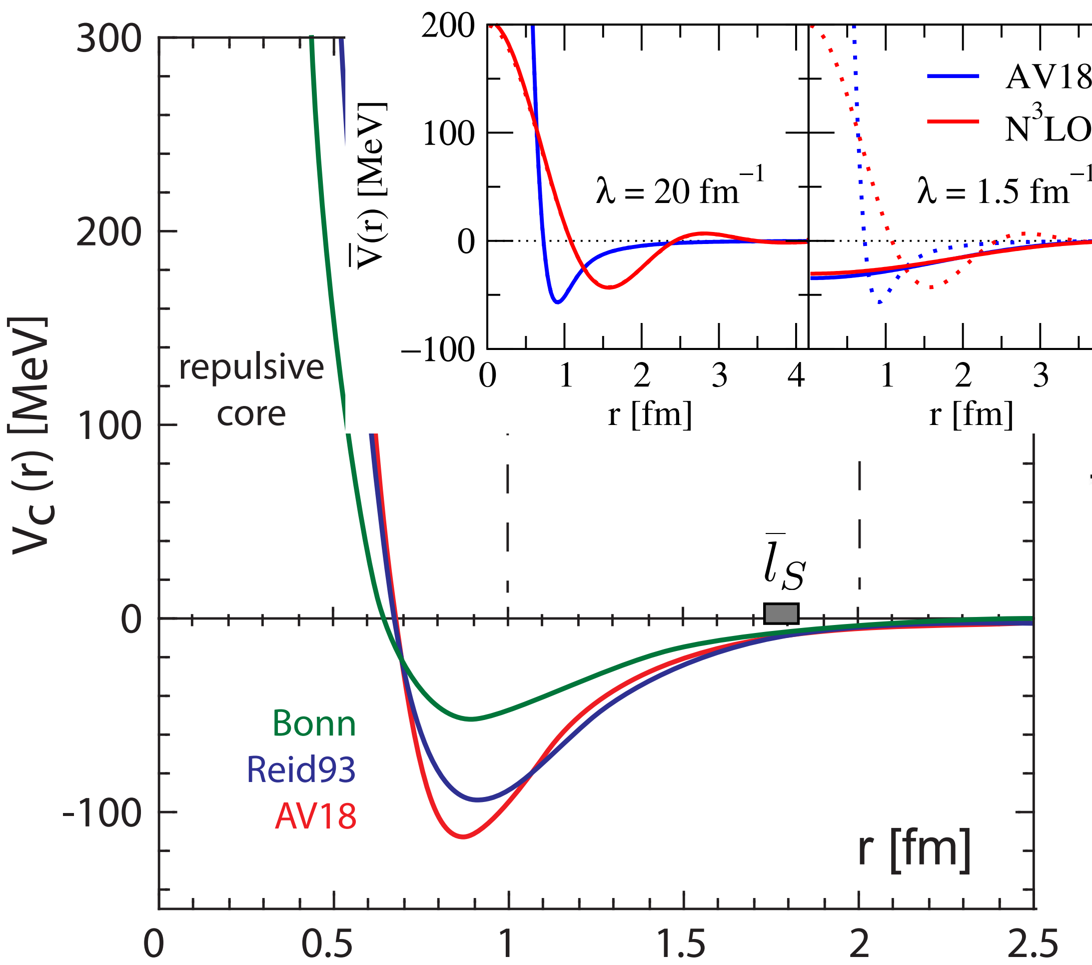
KH, Bogner, Furnstahl, Nogga,
PRC(R) 83, 031301 (2011)

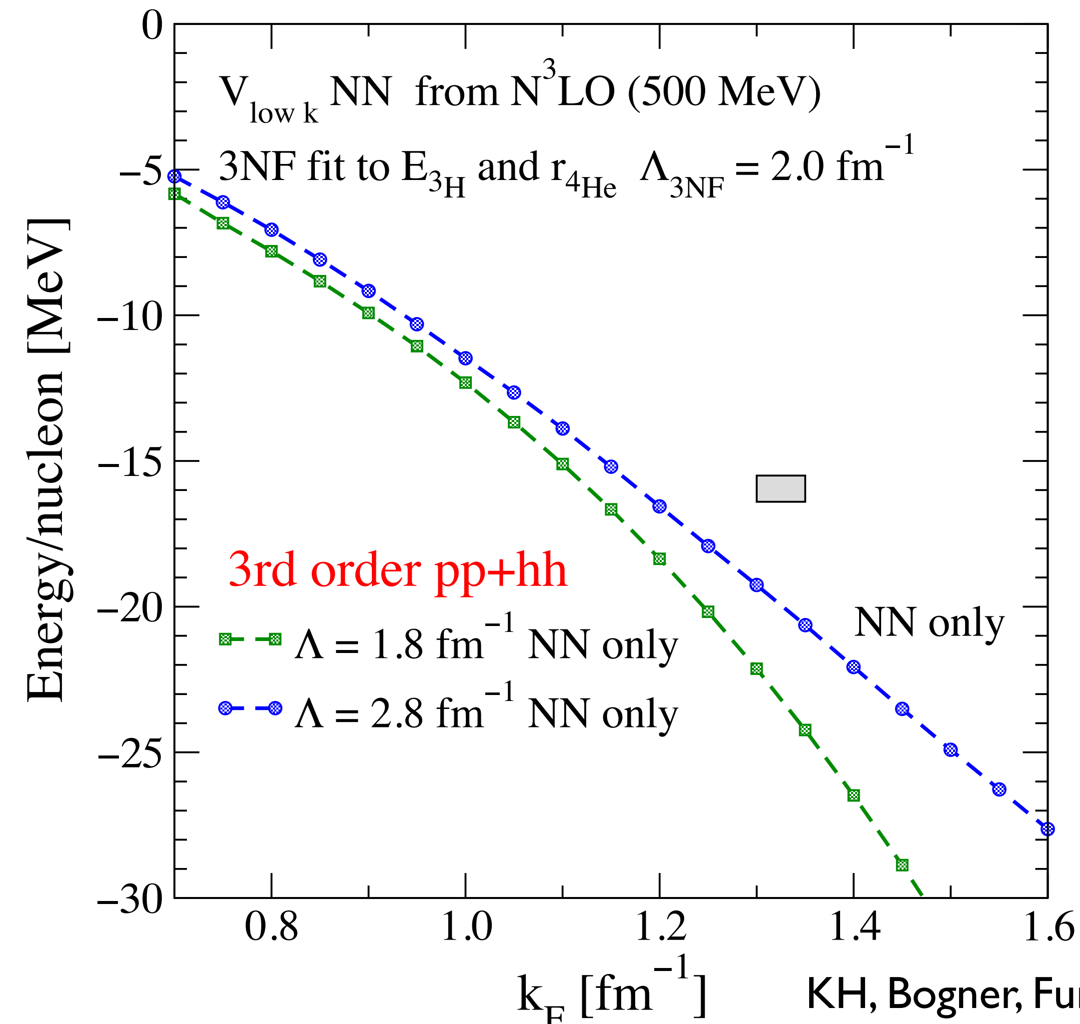


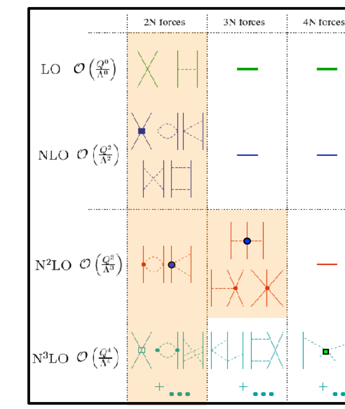
"Very soft potentials must be excluded because they do not give saturation;
they give too much binding and too high density. In particular, a substantial tensor force is required."

Hans Bethe (1971)

Fitting the 3NF LECs at low resolution scales







KH, Bogner, Furnstahl, Nogga,
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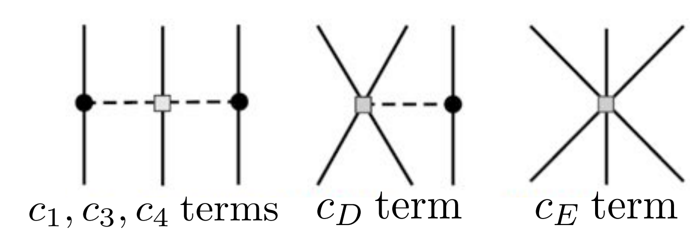
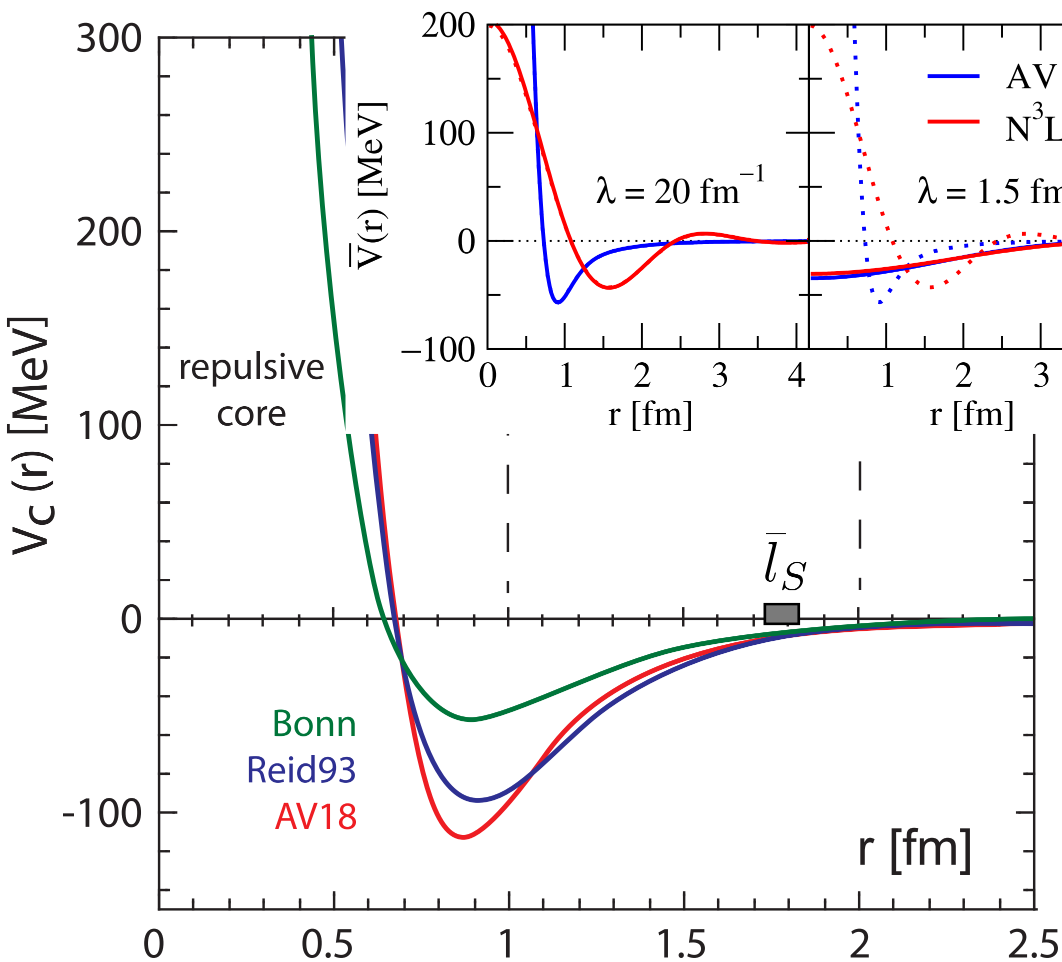
Hans Bethe (1971)

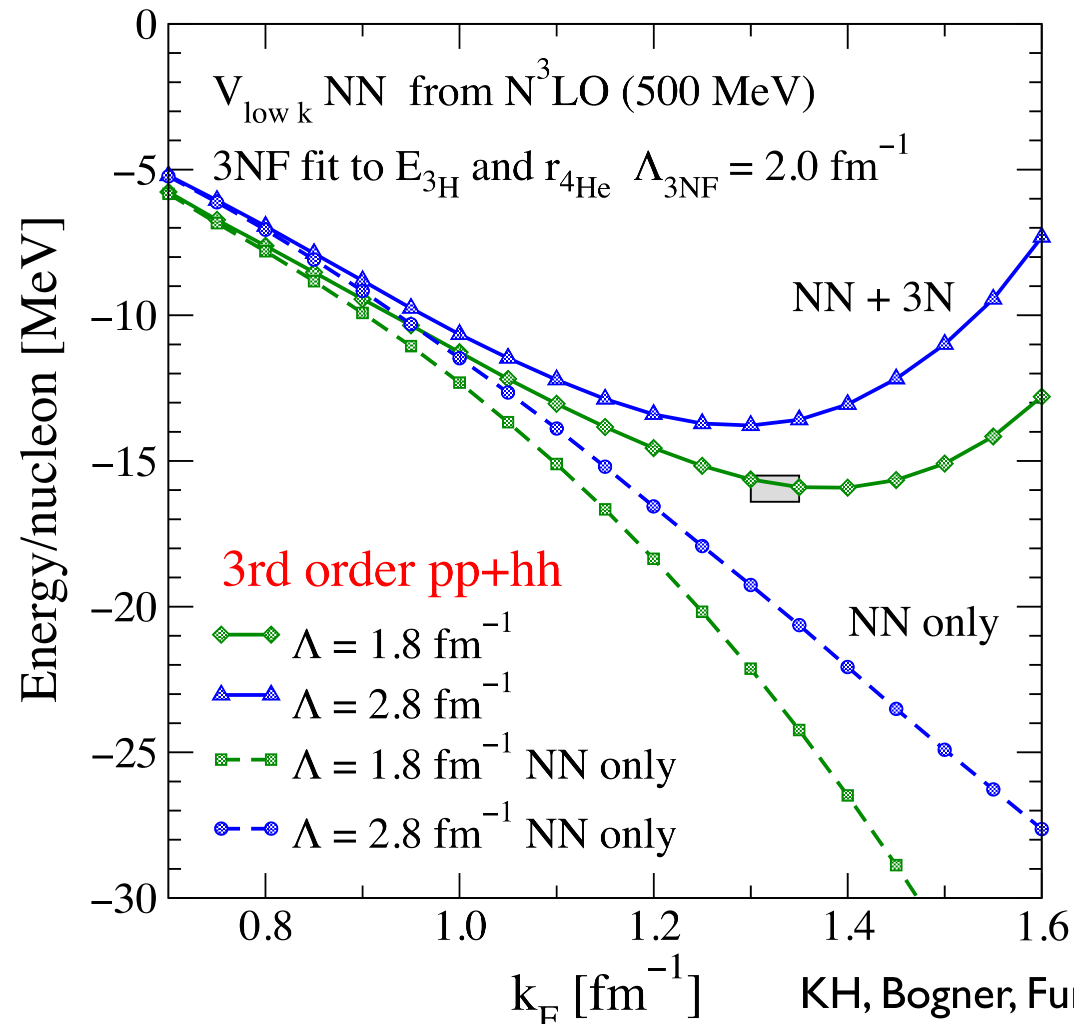
intermediate (c_D) and short-range (c_E) 3NF couplings fitted to few-body systems at different resolution scales:

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

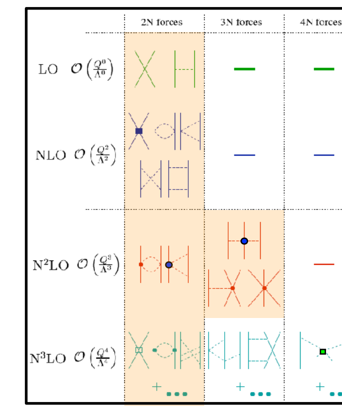


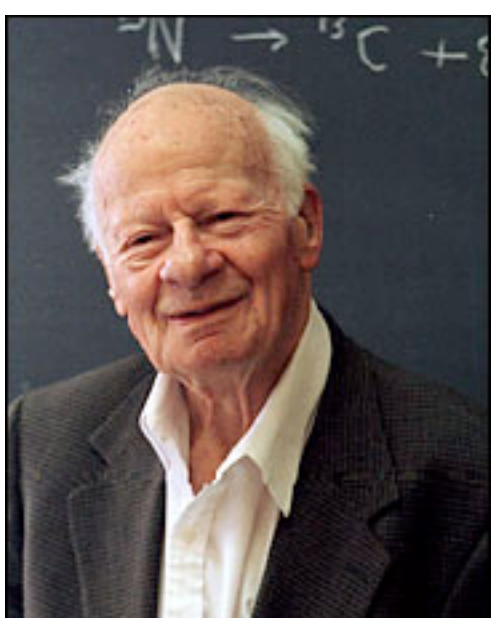
Fitting the 3NF LECs at low resolution scales





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





"Very soft potentials must be excluded because they do not give saturation;
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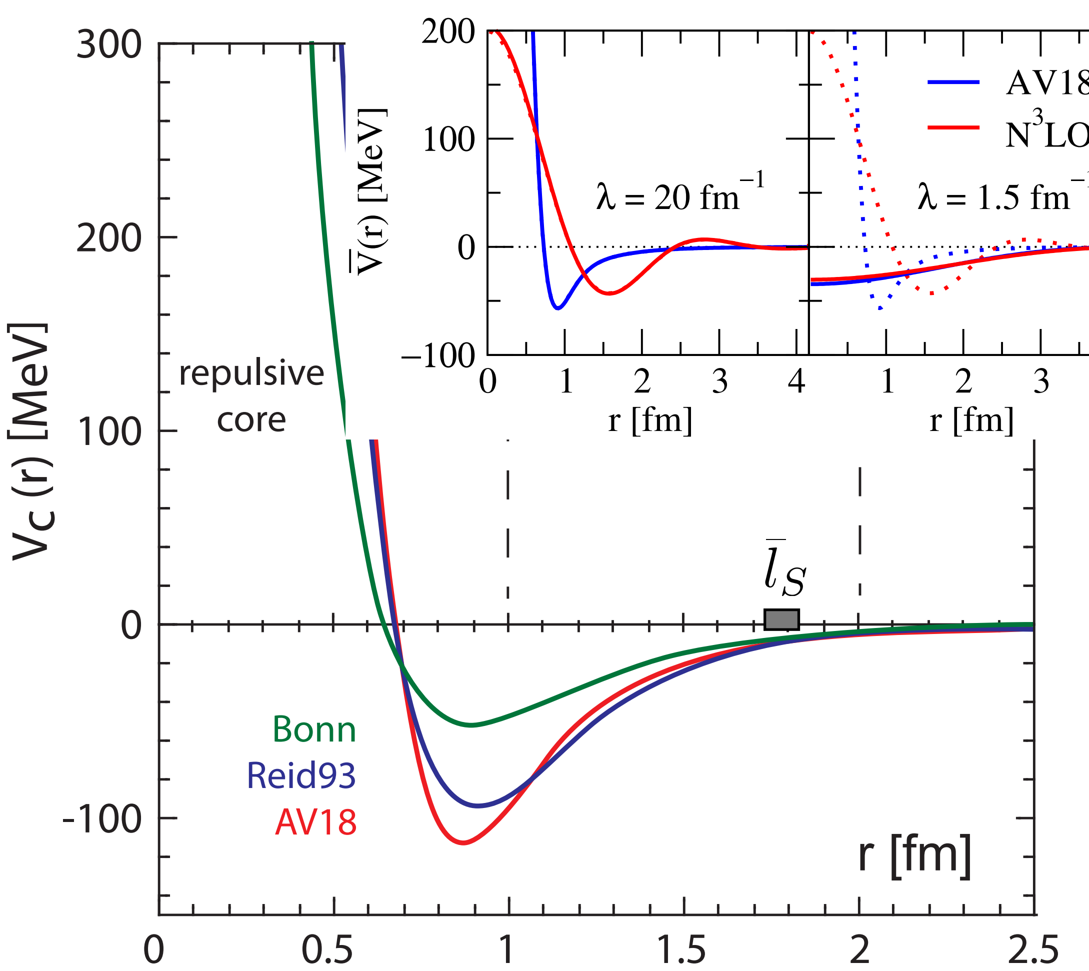
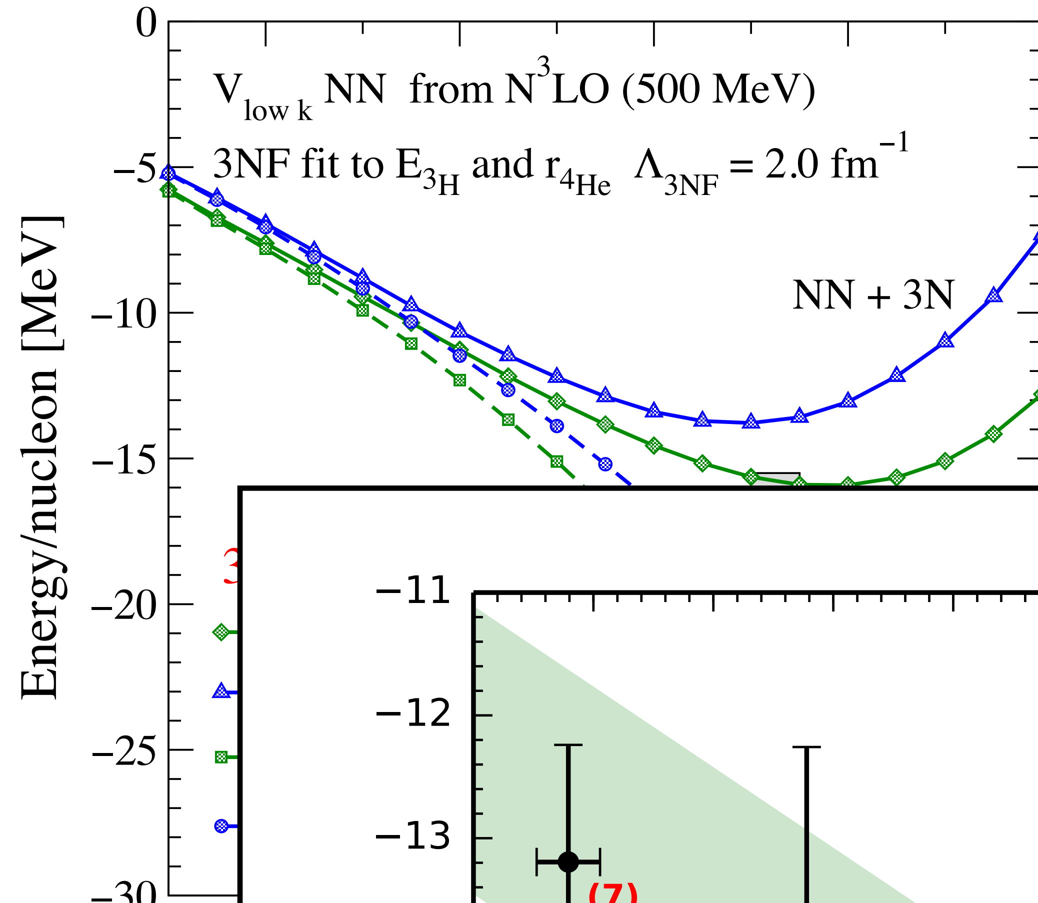
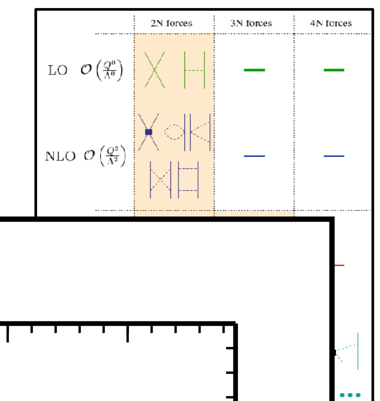
Hans Bethe (1971)

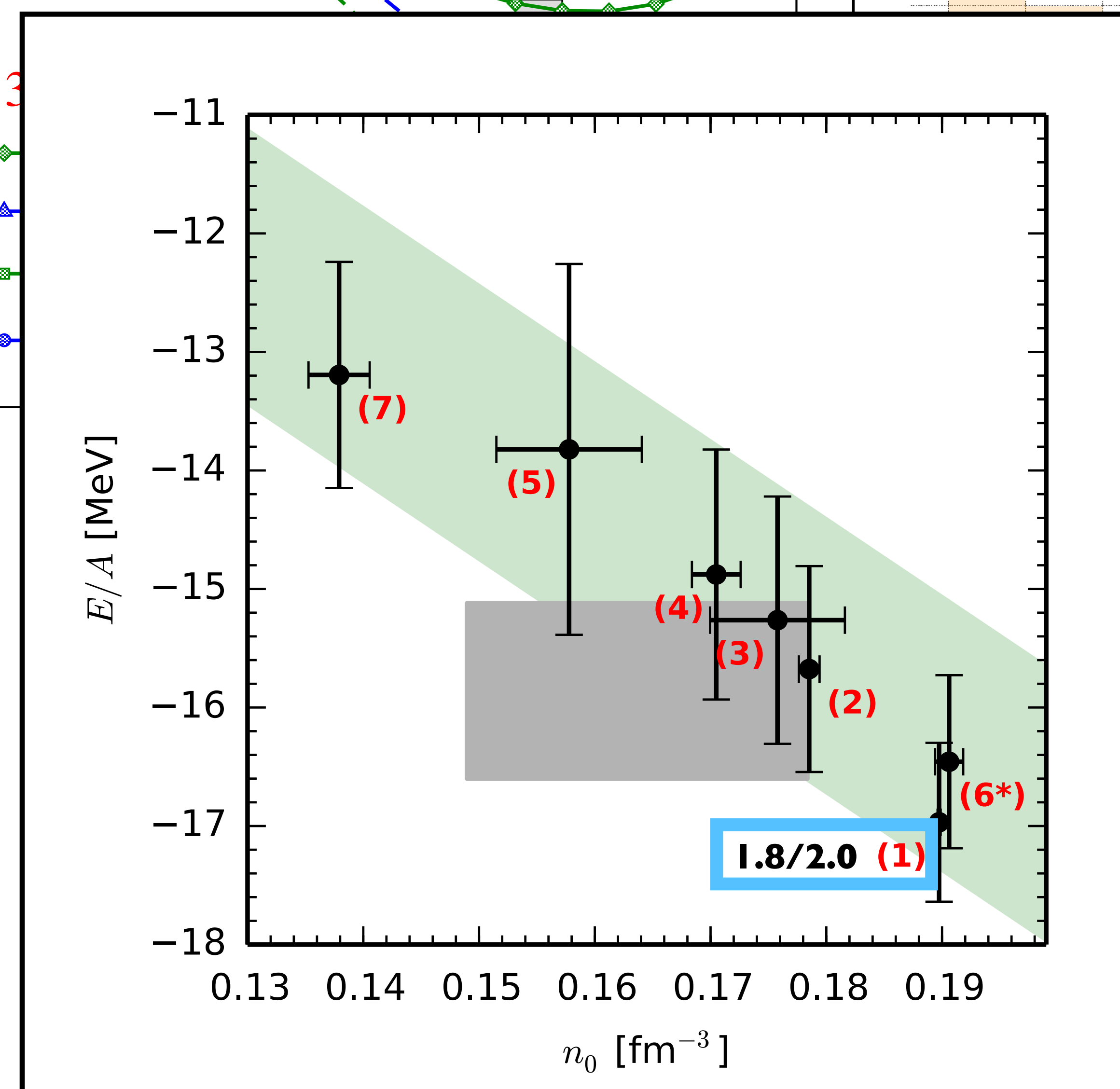
Reproduction of saturation point
without readjusting parameters!

Fitting the 3NF LECs at low resolution scales

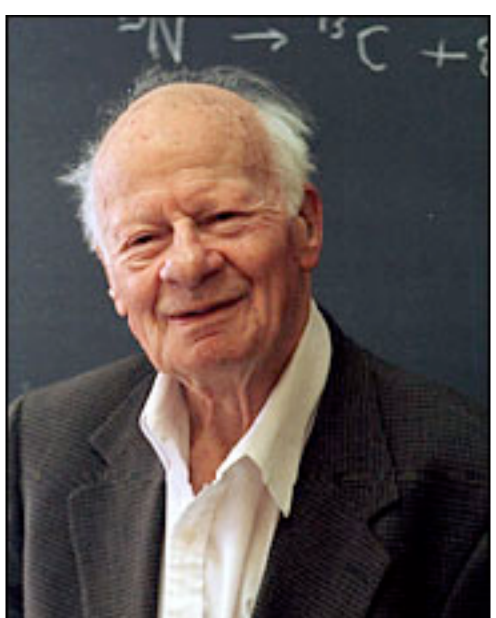








Drischler, KH, Schwenk, PRC93, 054314 (2016)



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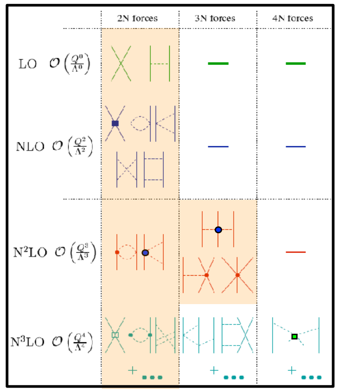
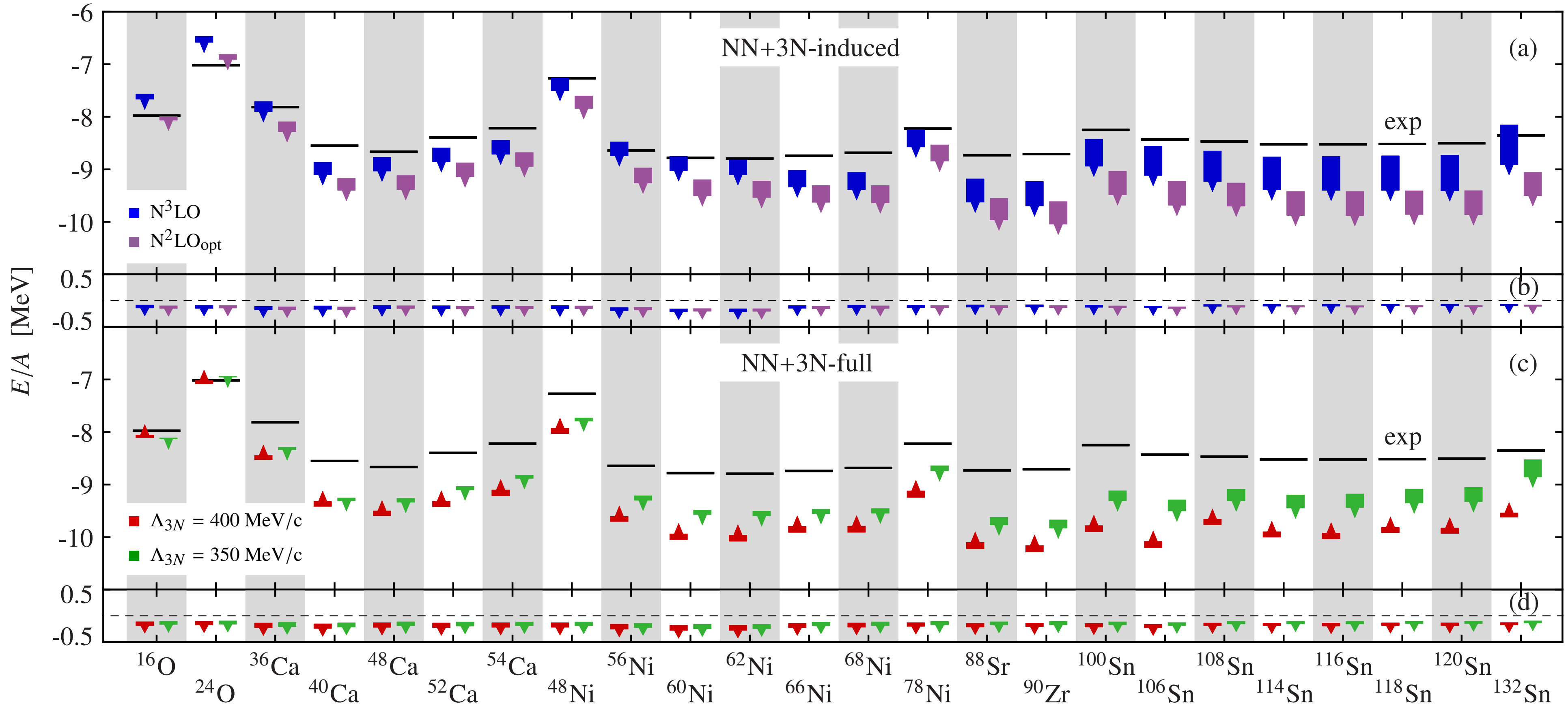
Ab initio calculations of heavier nuclei



coupled cluster (CC) framework



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

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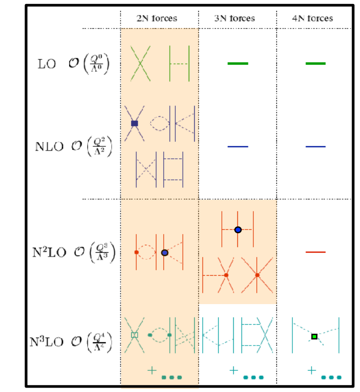

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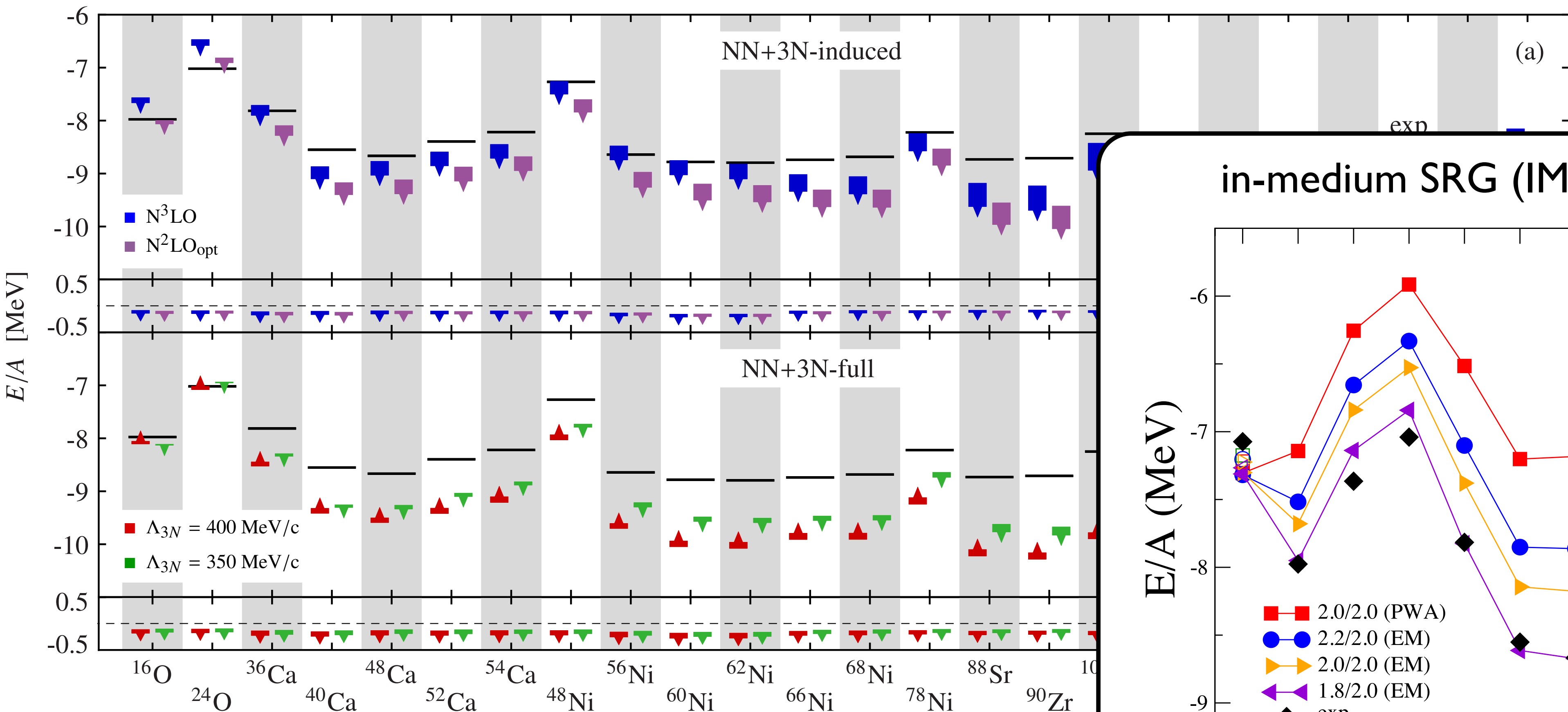
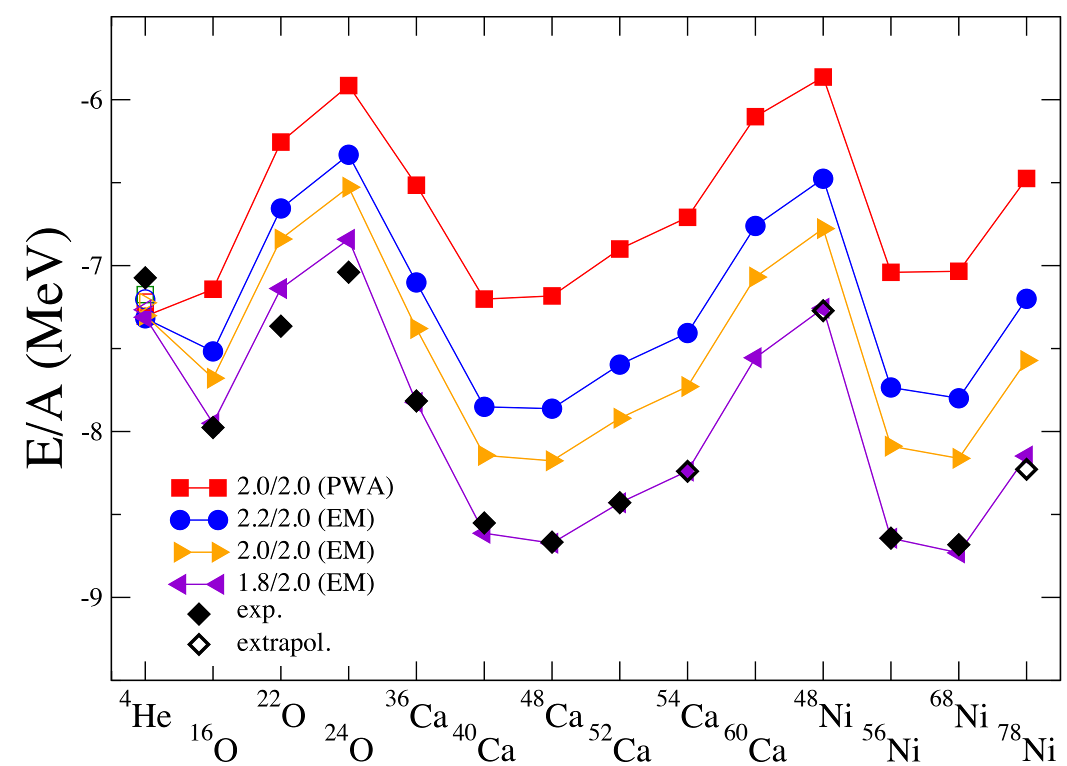


Binder et al., Phys. Lett B 736, 119 (2014)

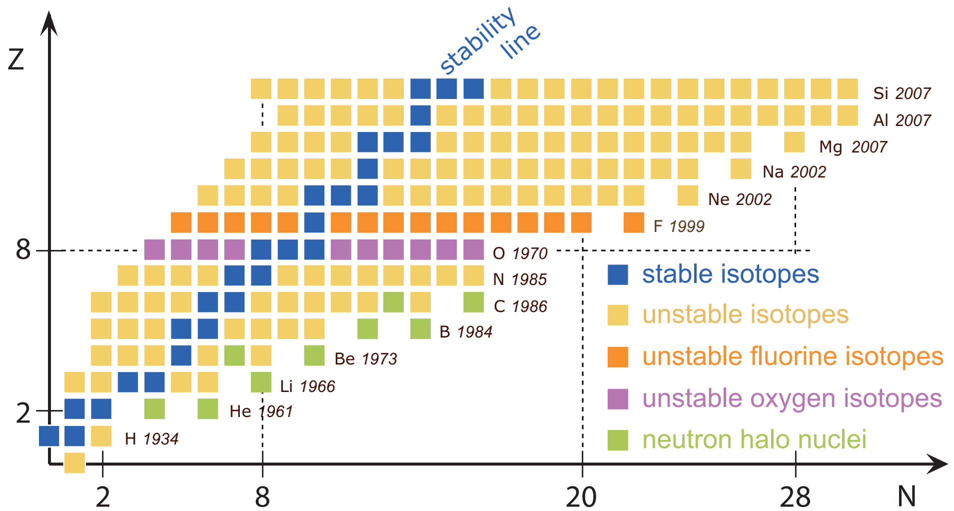
in-medium SRG (IMSRG) framework

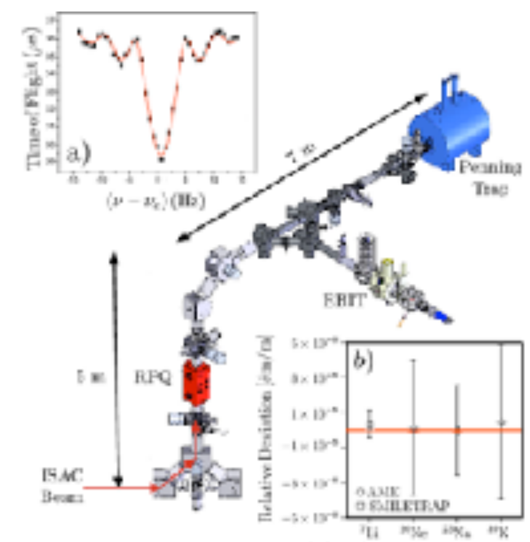


Simonis, Stroberg et al., PRC 96, 014303 (2017)

- spectacular increase in range of applicability of ab initio many body frameworks
- significant discrepancies to experimental data for heavy nuclei for (most of) presently used nuclear interactions
- need to quantify theoretical uncertainties

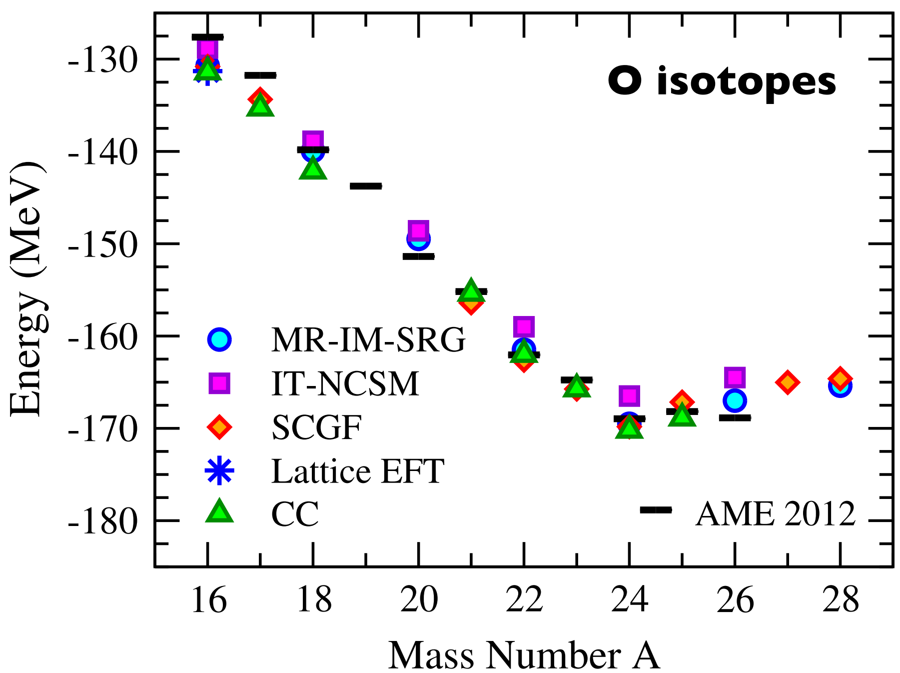
Studies of neutron-rich nuclei

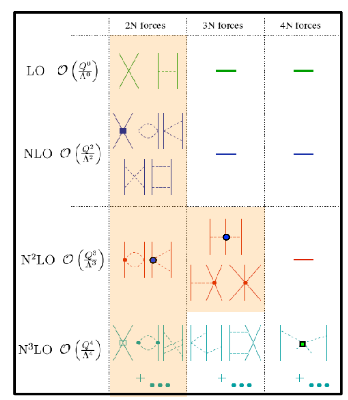


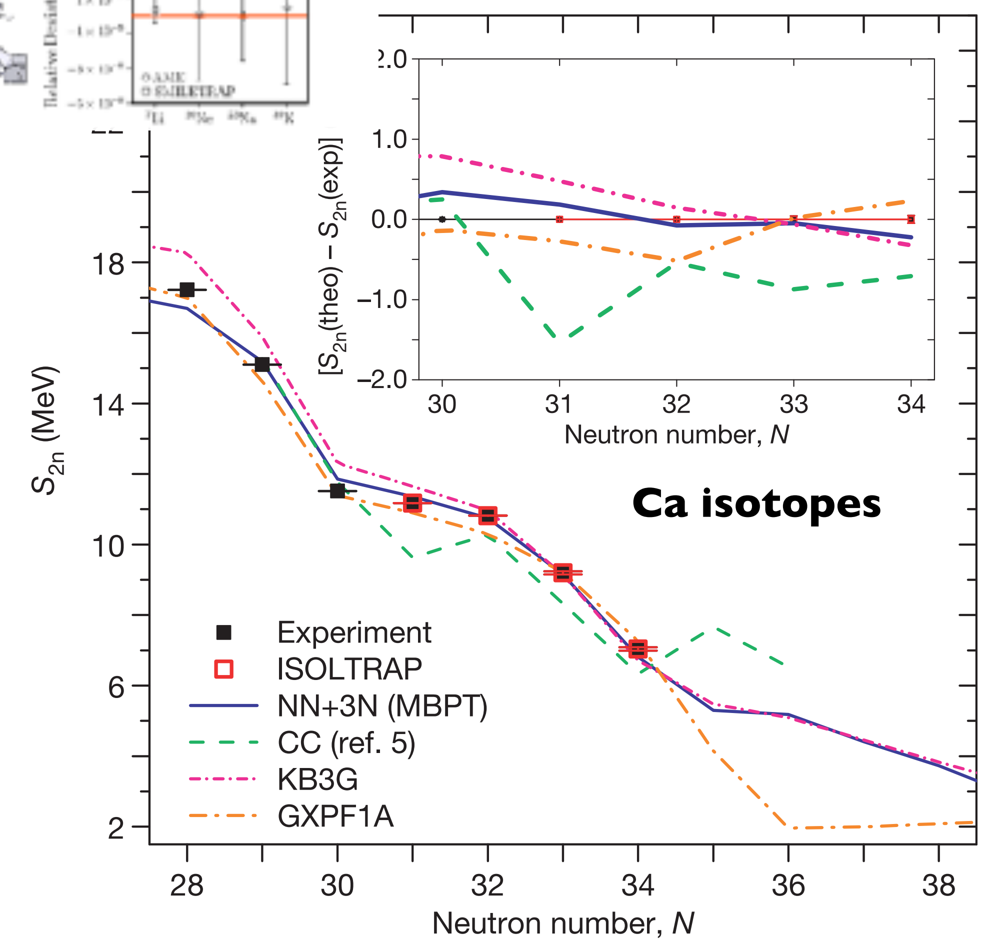


Gallant et al.
PRL 109, 032506 (2012)

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

Novel efficient many-body framework for nuclear matter

Main developer:
Christian Drischler

Problem:

Evaluation of diagrams beyond second order in perturbation theory becomes complicated and tedious in partial wave representation.

Present frameworks too inefficient for including matter properties in force fits.

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Strategy:

Implementation of NN and 3N forces without partial wave decomposition.

Calculate MBPT diagrams in vector basis

$$|12...n\rangle = |\mathbf{k}_1 m_{s_1} m_{t_1}\rangle \otimes |\mathbf{k}_2 m_{s_2} m_{t_2}\rangle \otimes ... \otimes |\mathbf{k}_n m_{s_n} m_{t_n}\rangle$$

using Monte-Carlo techniques. Implementation efficient and very transparent.

Drischler et al. arXiv:1710.08220 (2017)

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Drischler et al. arXiv:1710.08220 (2017)

Status:

Implementation of nonlocal NN plus 3N forces up to N3LO complete.

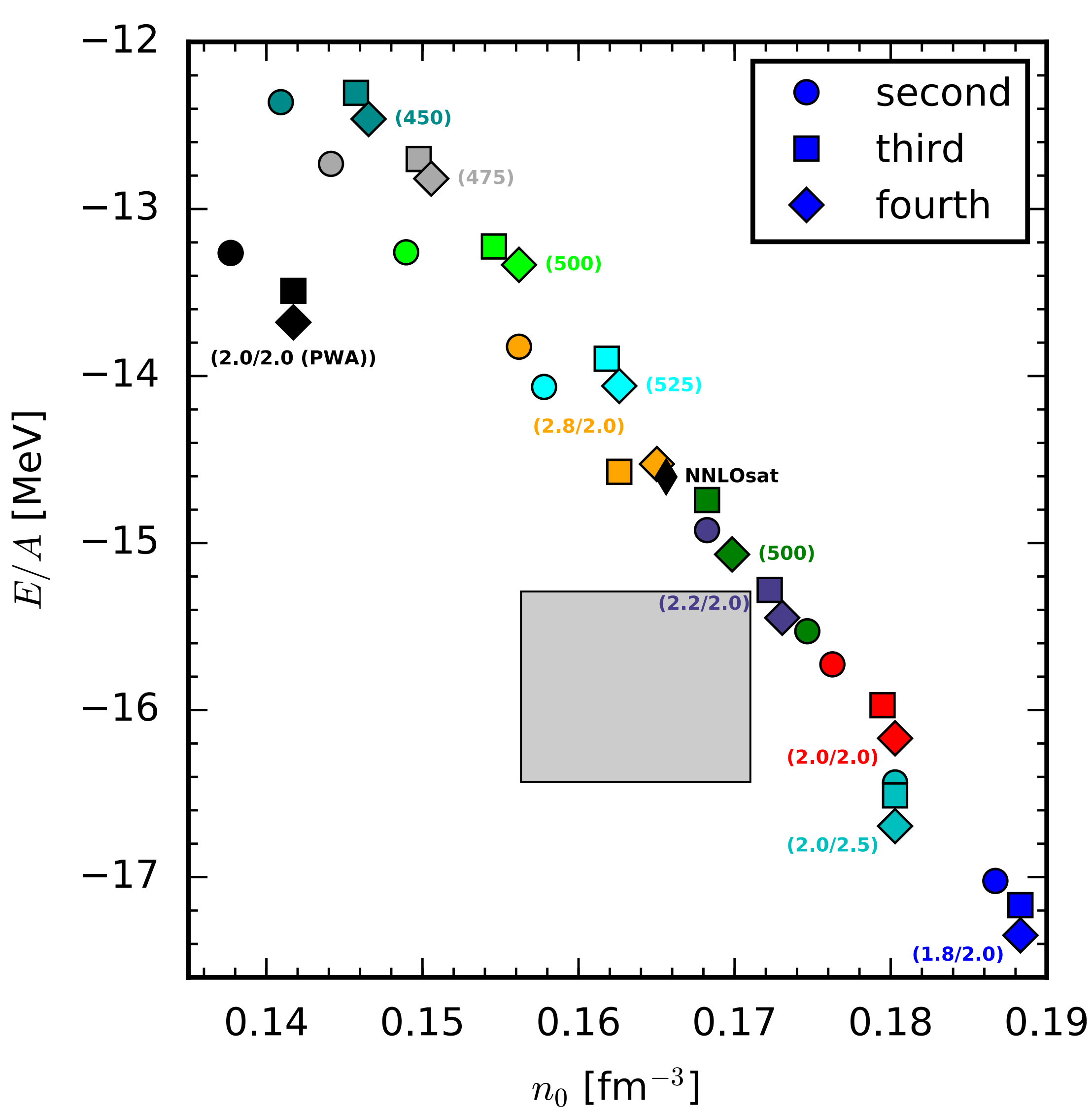
Implemented MBPT diagrams up to 4th order for state-of-the-art interactions.

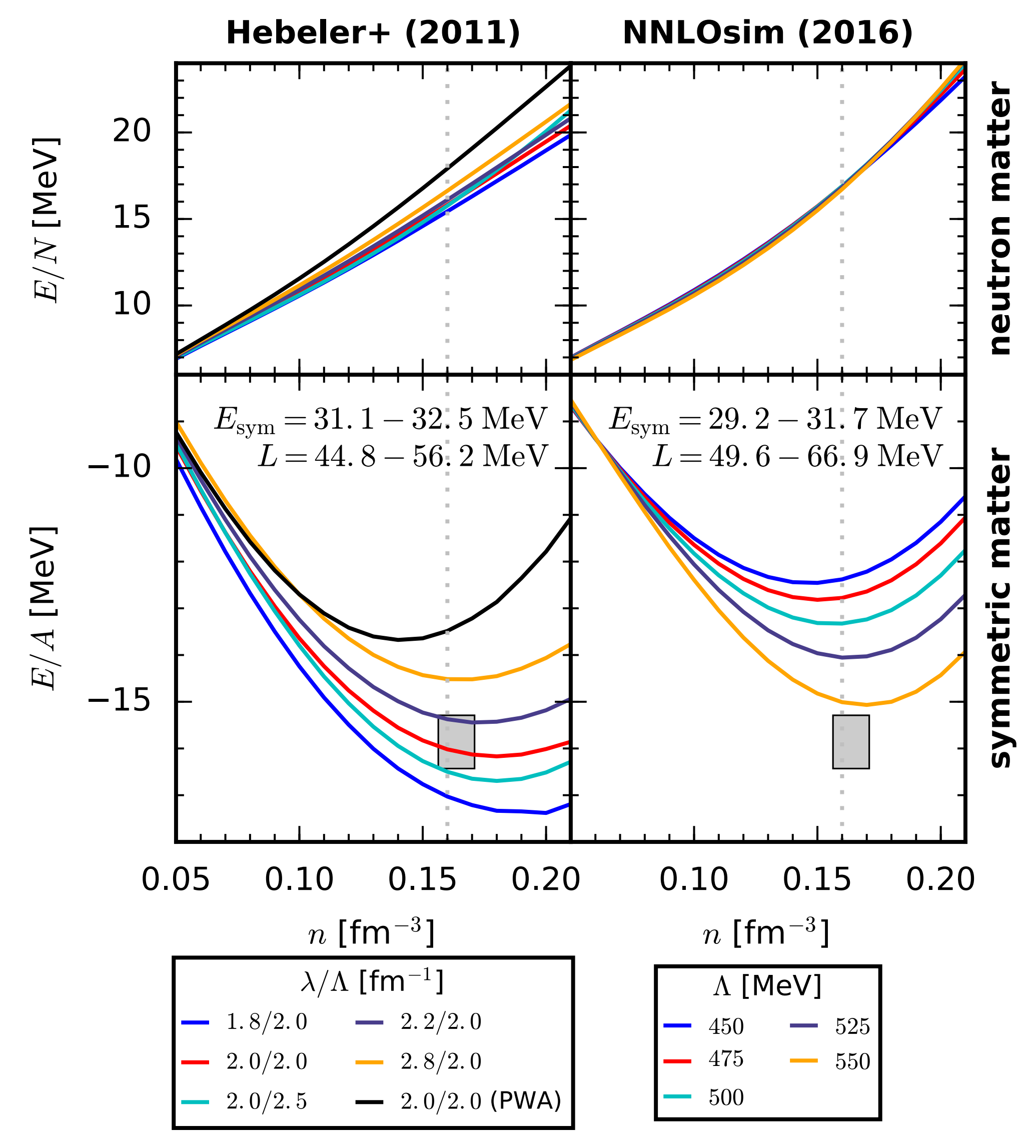
Entem et al. PRC 96, 024004 (2017)

Fits of 3N interactions to saturation properties of nuclear matter

- Incorporation of saturation properties in fits was not possible so far due to insufficient efficiency of many-body calculations
- Performed calculations up to 4th order for set of presently used NN interactions, natural convergence pattern

Drischler et al., arXiv:1710.08220 (2017)





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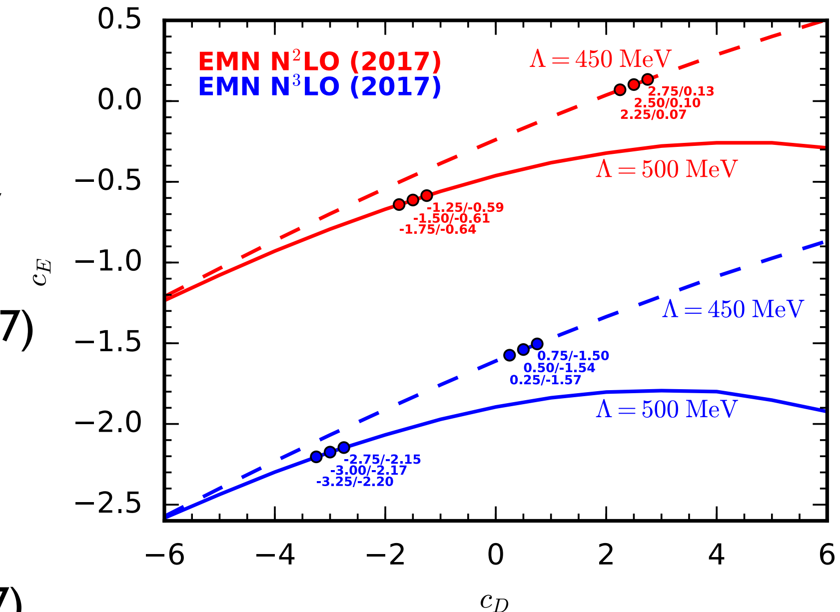
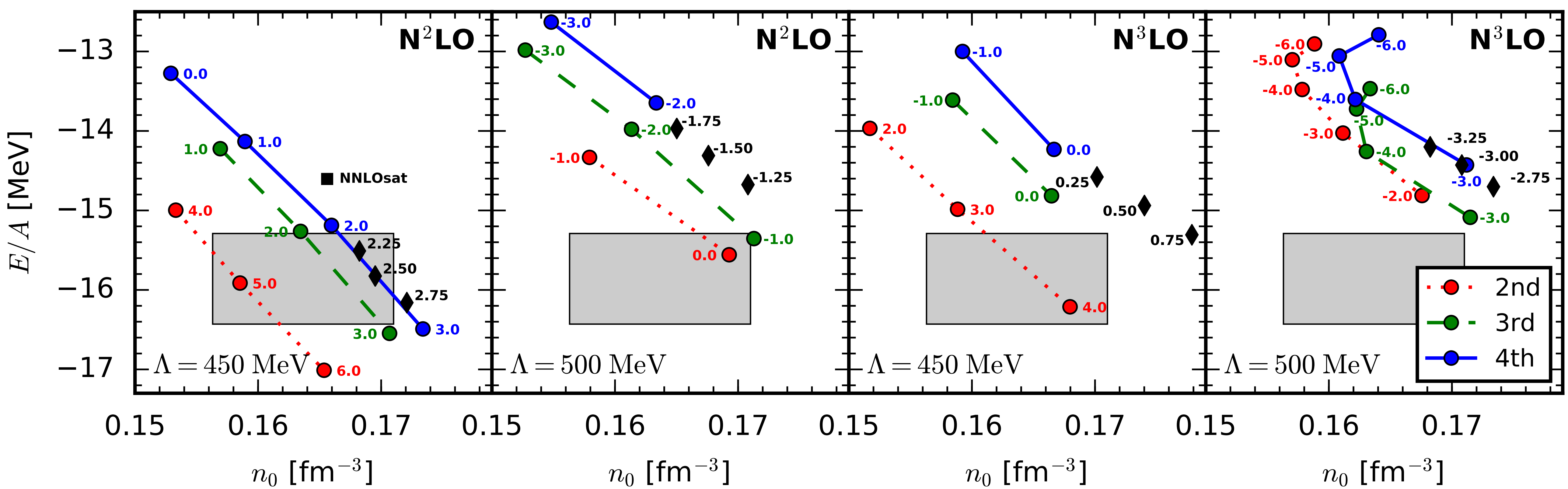


Drischler et al., arXiv:1710.08220 (2017)



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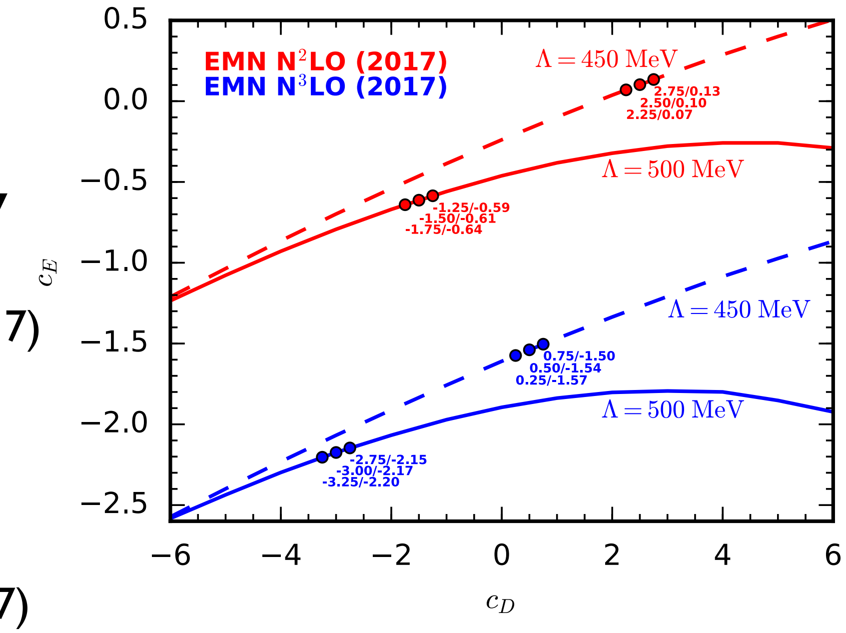
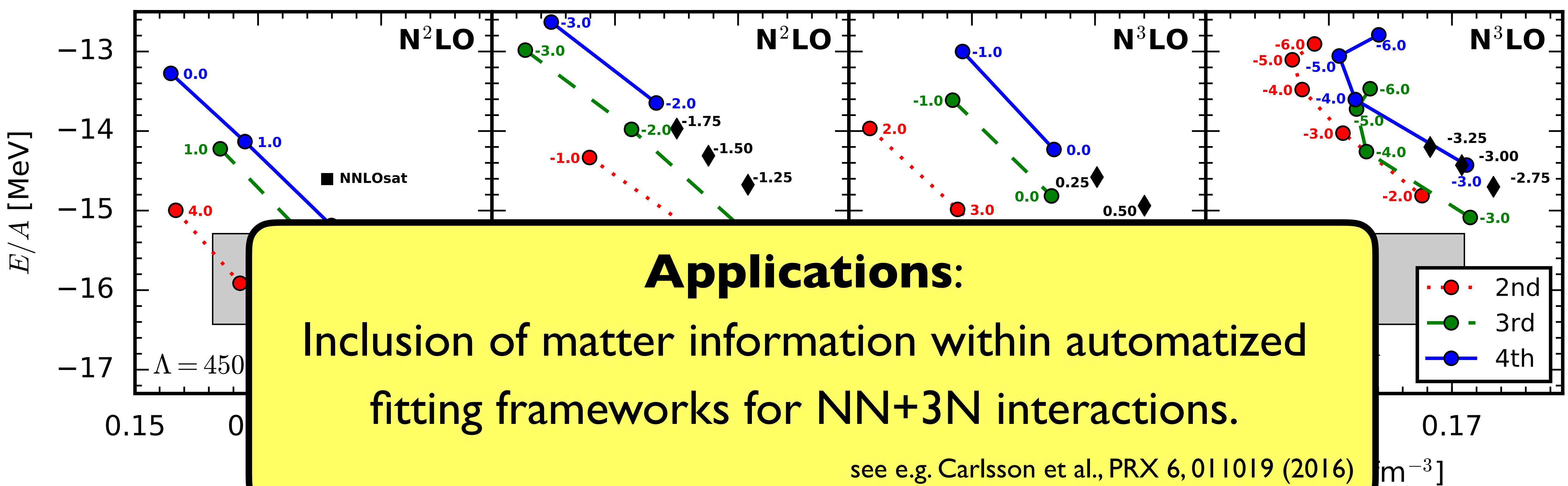


Drischler et al., arXiv:1710.08220 (2017)



Applications:

Inclusion of matter information within automatized fitting frameworks for NN+3N interactions.

see e.g. Carlsson et al., PRX 6, 011019 (2016)

Status and achievements

significant increase in scope of ab initio many-body frameworks

remarkable agreement between different ab intio many-body methods

discrepancies to experiment dominated by deficiencies of present nuclear interactions

Current developments and open questions

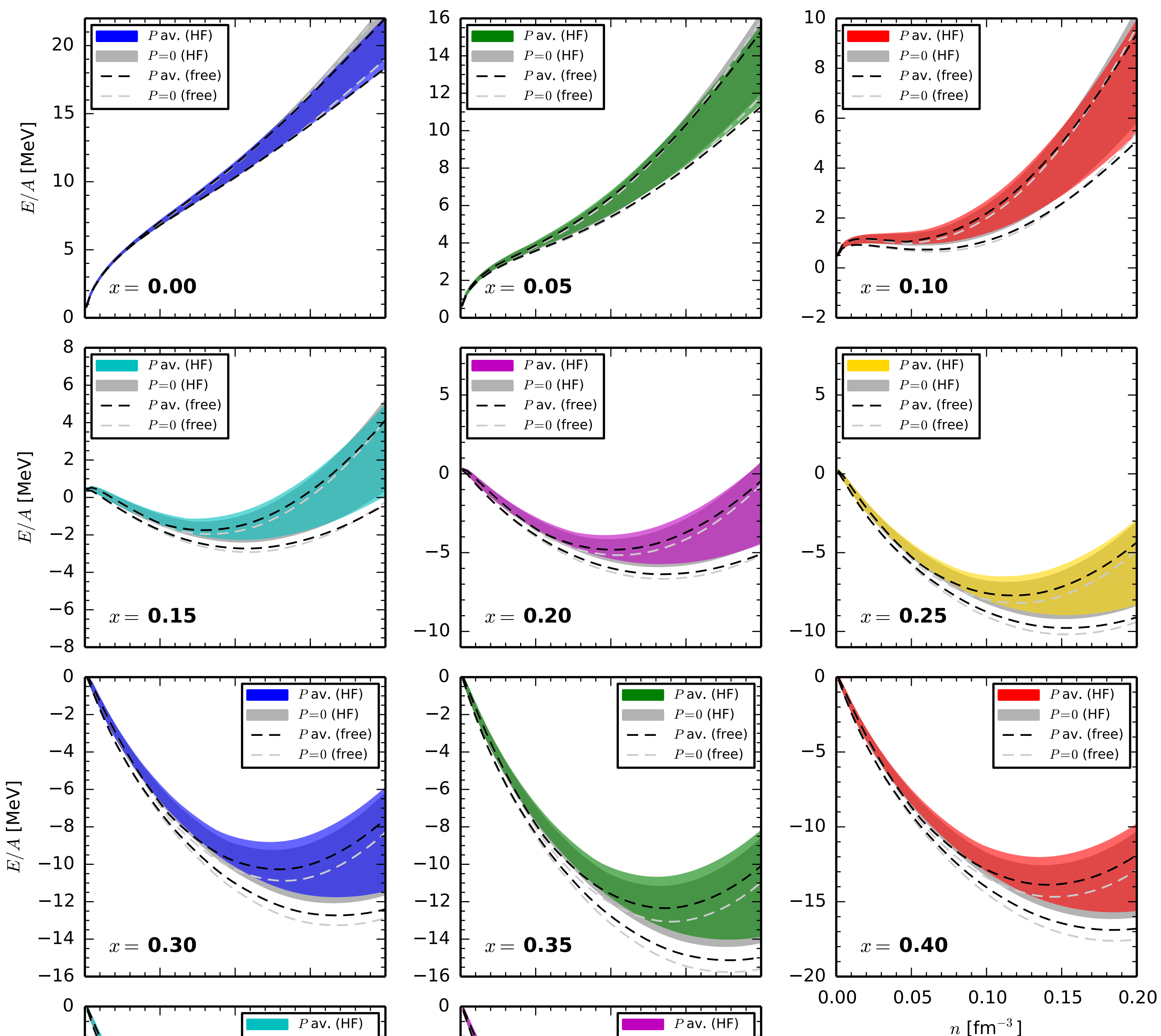
presently active efforts to develop improved nucleon interactions (fitting strategies, power counting, regularization…)

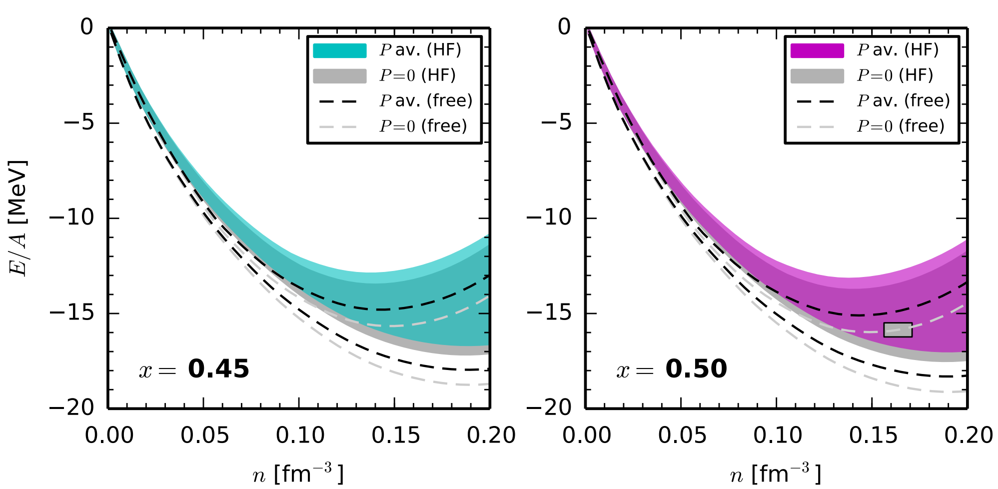
Key goals

unified study of atomic nuclei, nuclear matter and reactions based on novel interactions

systematic estimates of theoretical uncertainties

Microscopic calculations of the equation of state

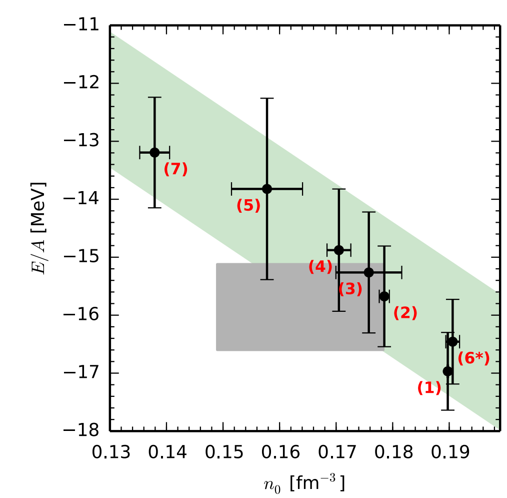




$$x = \frac{n_p}{n_p + n_n}$$

- microscopic framework to calculate equation of state for general proton fractions

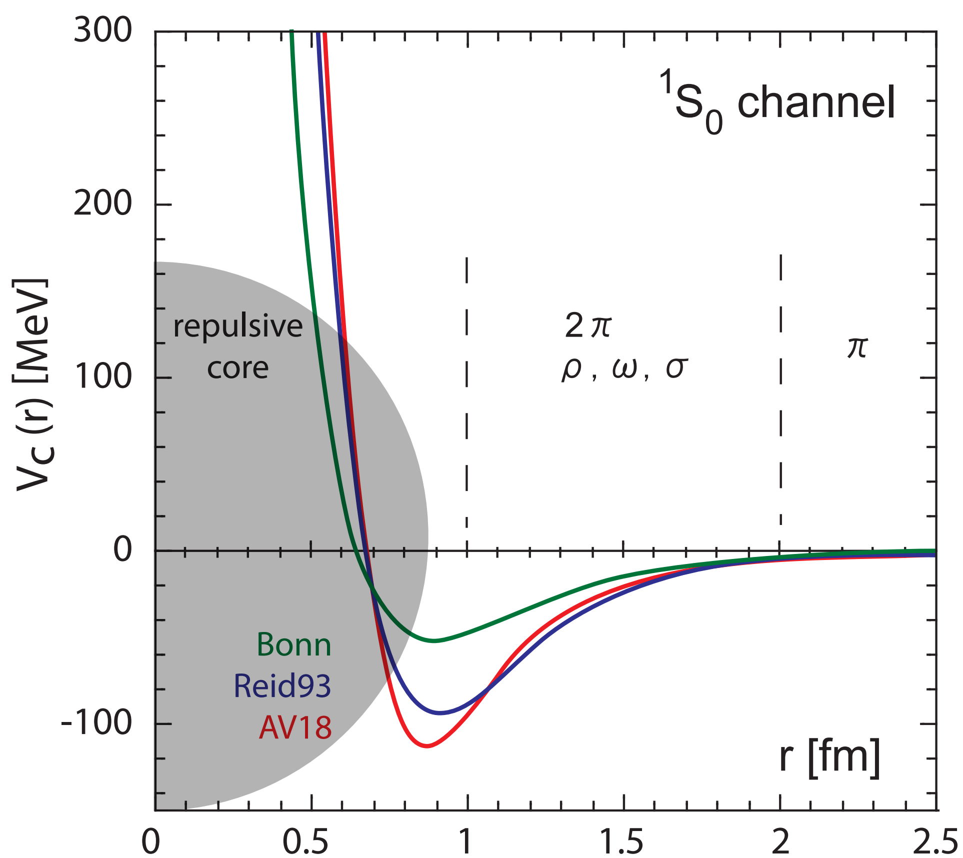
- uncertainty bands determined by set of 7 Hamiltonians

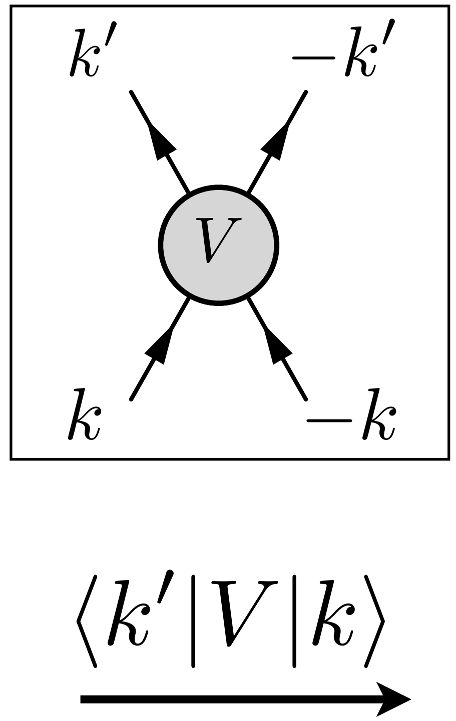


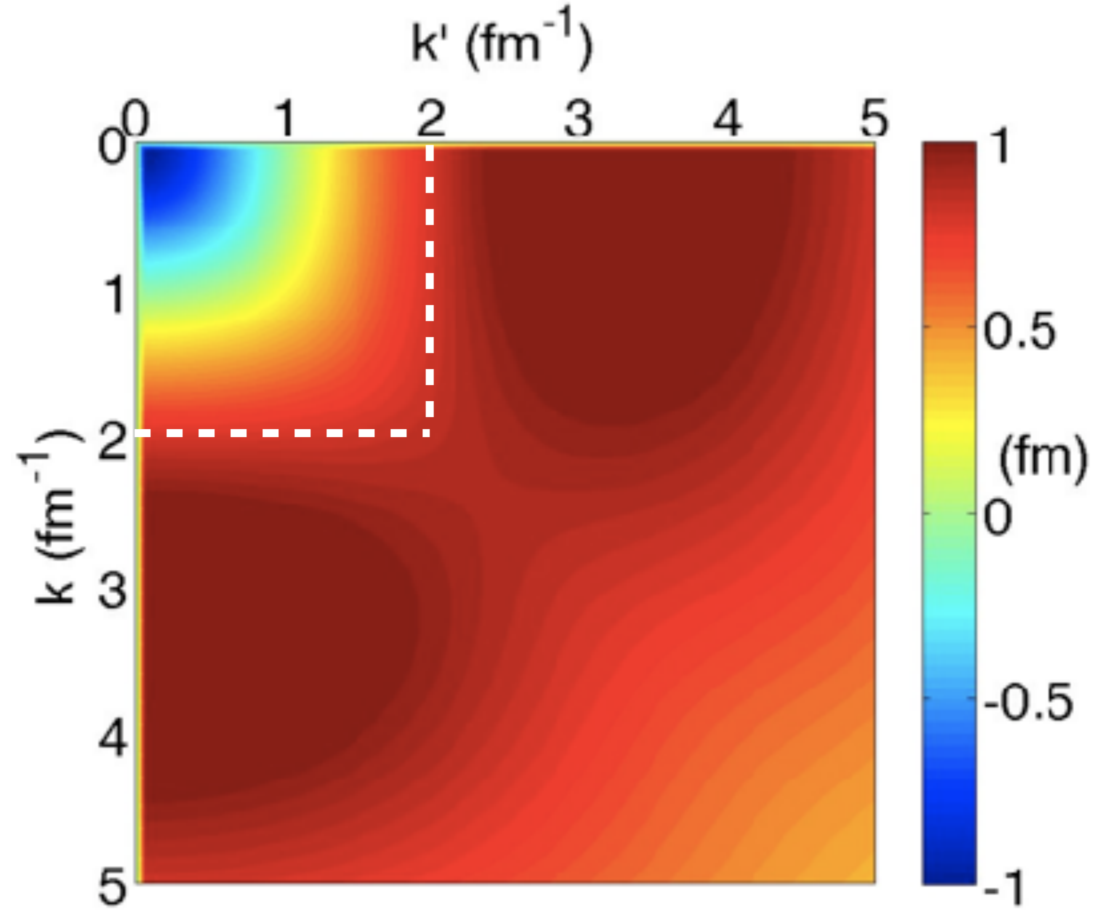
- many-body framework allows treatment of general 3N interaction

Drischler, KH, Schwenk,
PRC 054314 (2016)

"Traditional" NN interactions

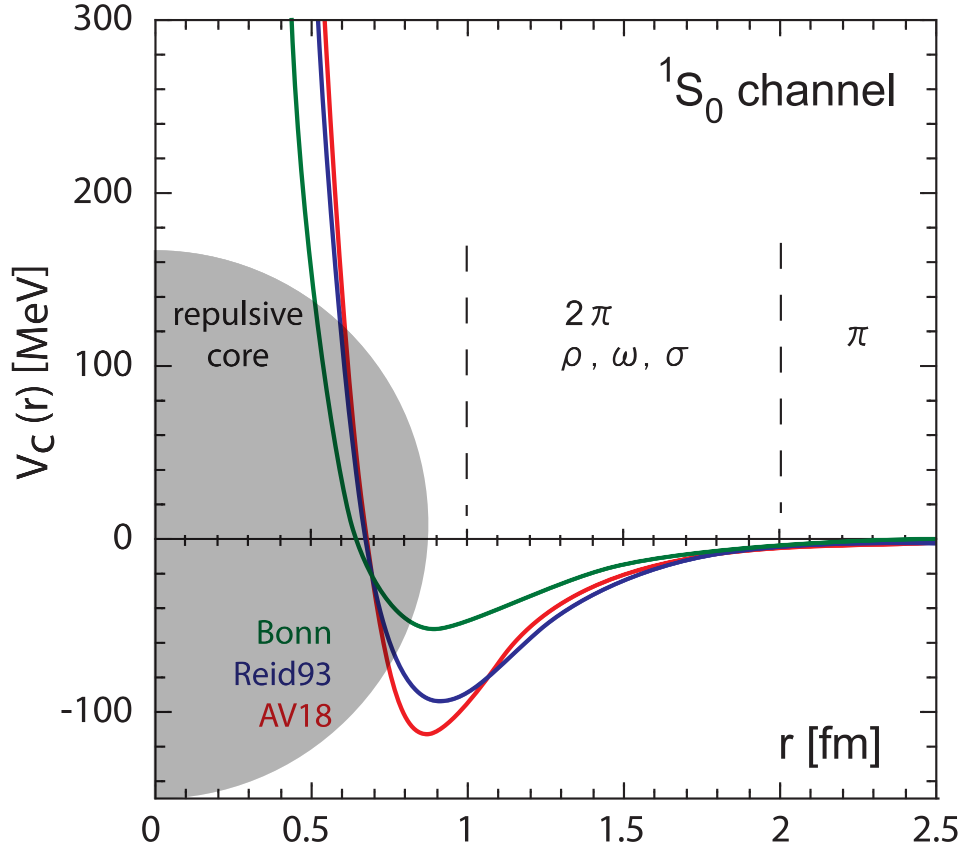


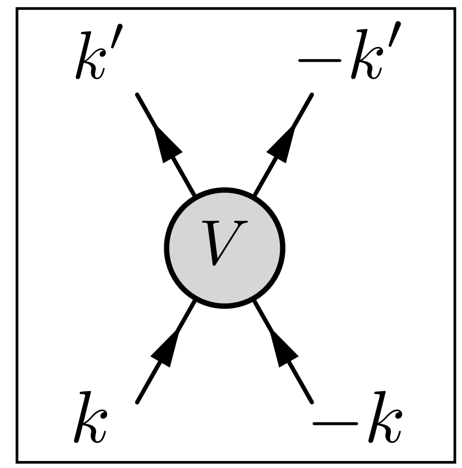




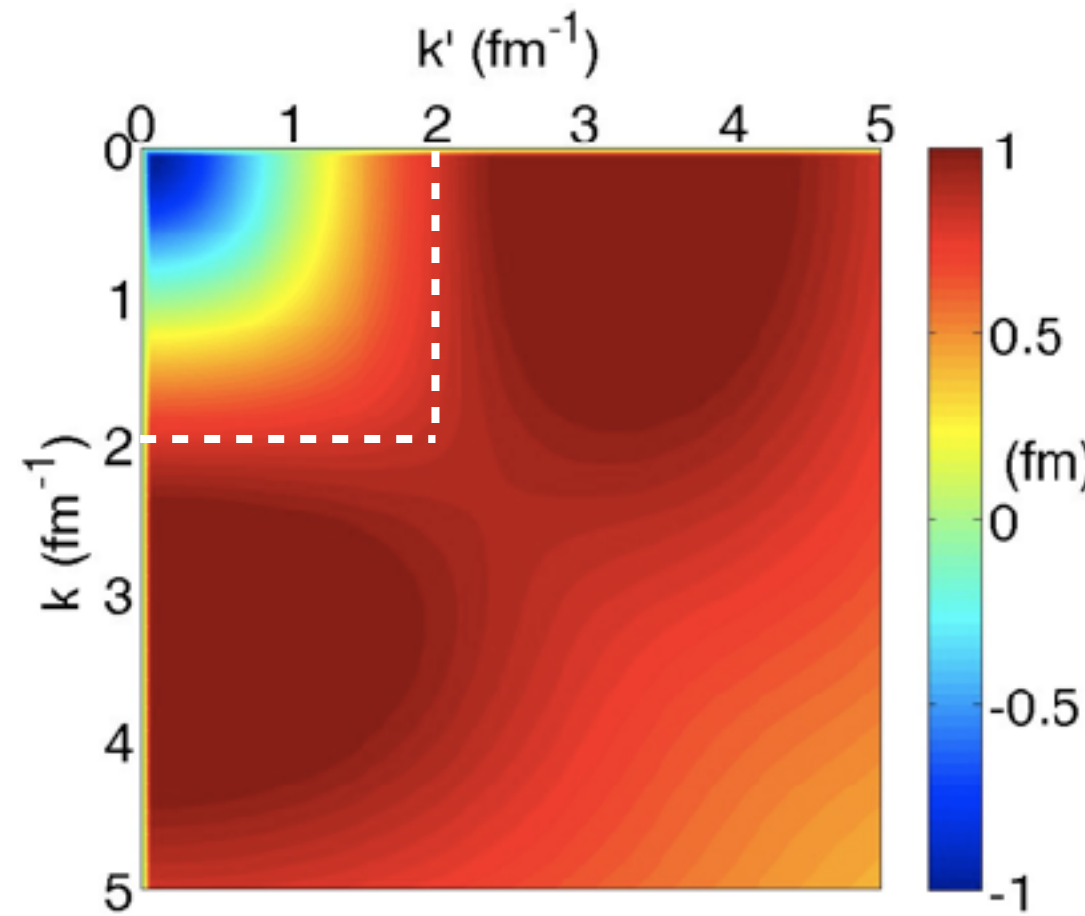
- constructed to fit NN-scattering data (long-wavelength information)
- long-range part dominated by one pion exchange interaction
- short range part strongly model dependent!
- traditional NN interactions contain strongly repulsive core at small distance
  - strong coupling between low and high-momenta
  - many-body problem hard to solve!

“Traditional” NN interactions





$$\langle k' | V | k \rangle$$

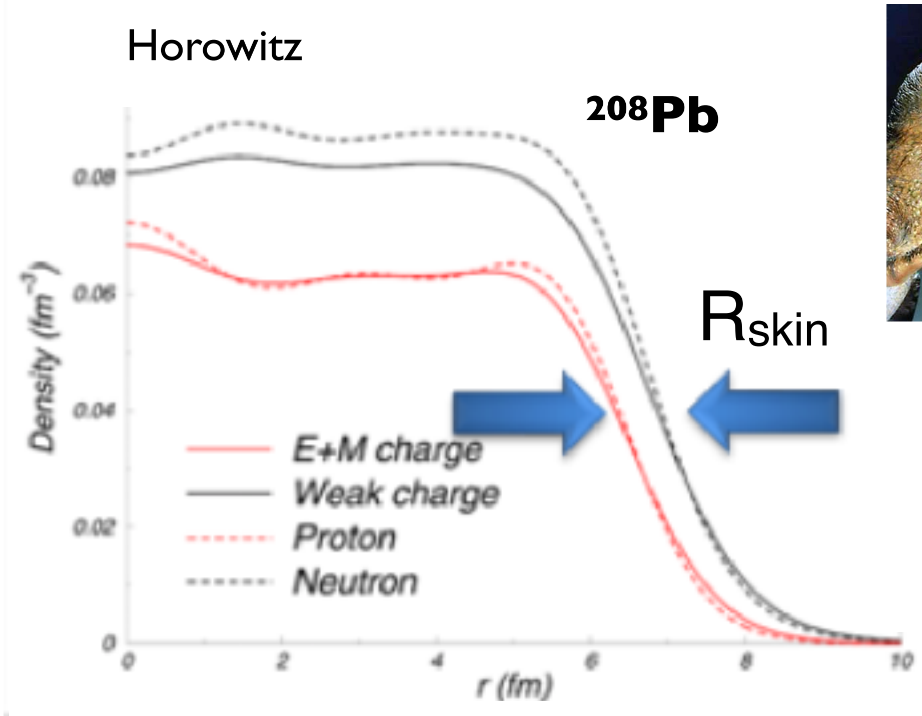


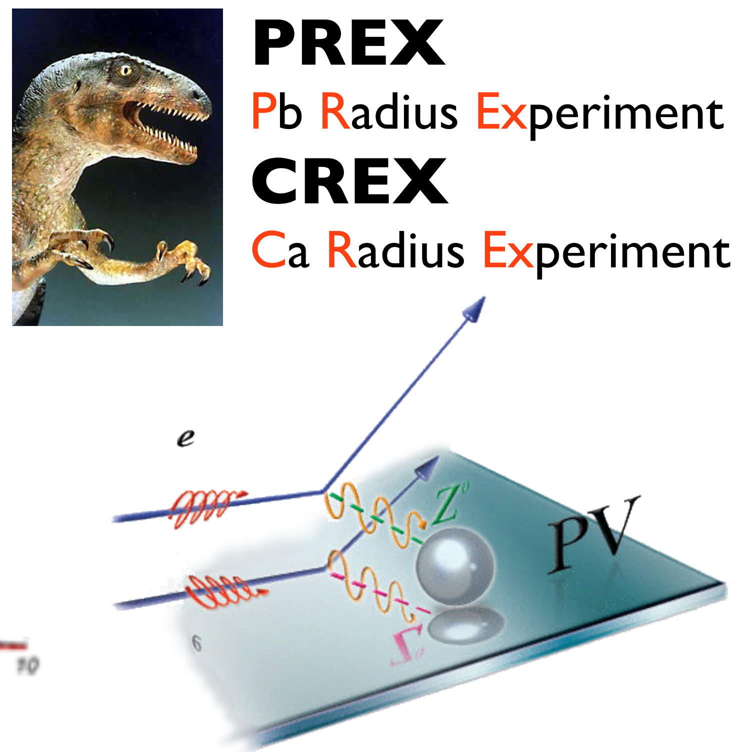
- constructed to fit NN-scattering data (long-wavelength information)
- long-range part dominated by one pion exchange interaction
- short range part strongly model dependent!
- tr… …ance

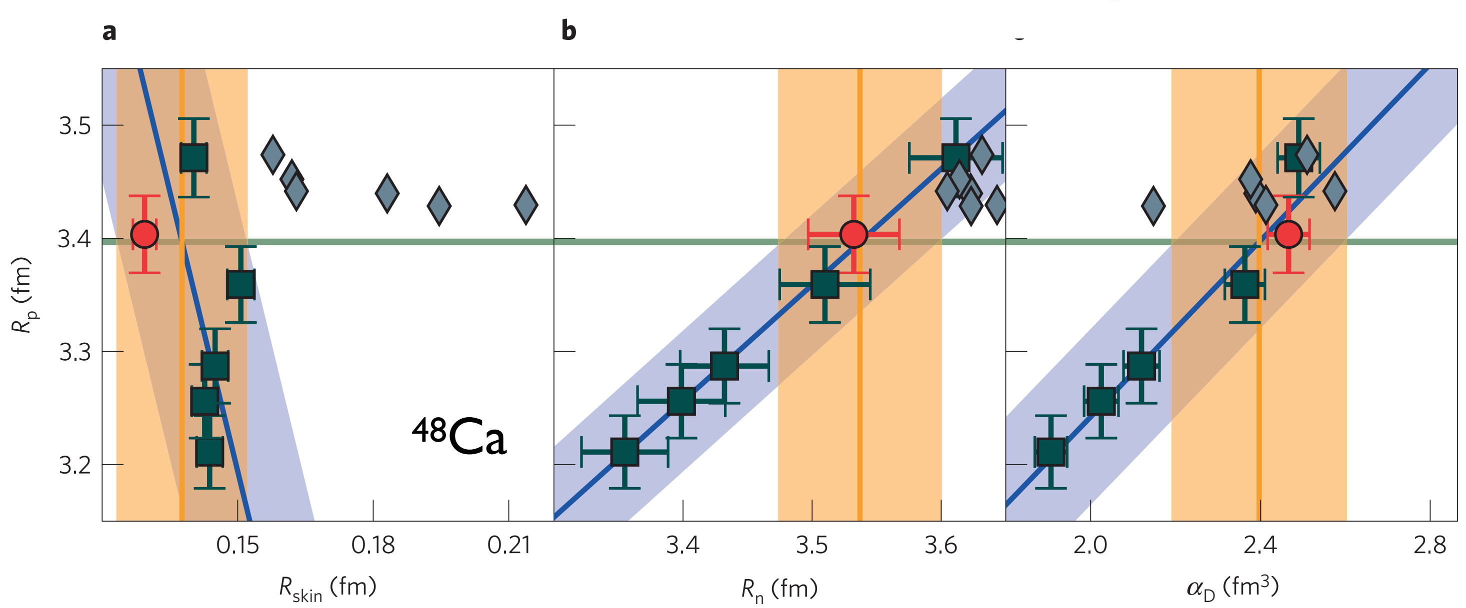
  How do we estimate uncertainties for many-body observables?

  - strong coupling between low and high-momenta
  - many-body problem hard to solve!

The size of the atomic nucleus: challenges from novel high-precision measurements



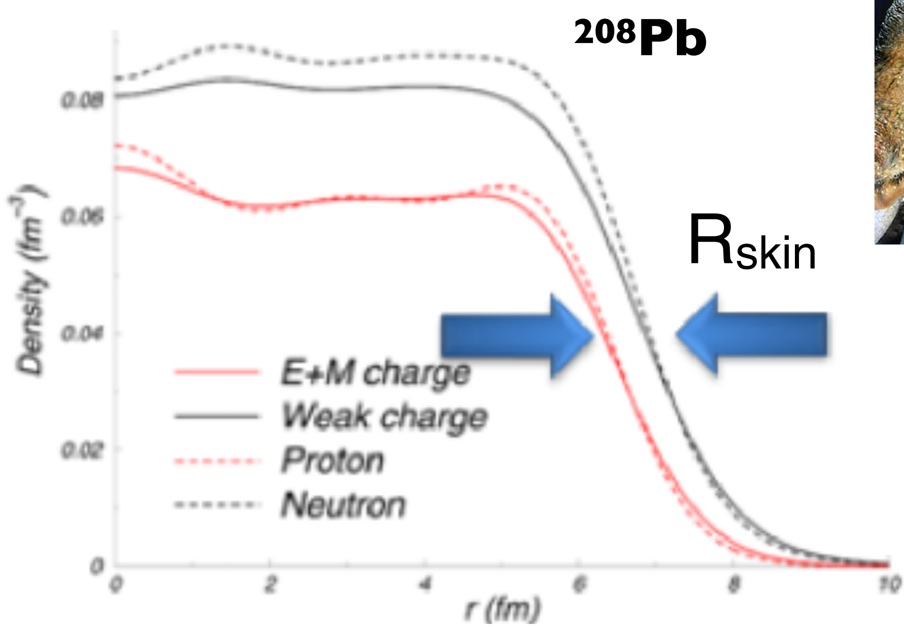




Hagen. et al.. Nature Phys. 12, 186 (2015)

The size of the atomic nucleus: challenges from novel high-precision measurements

Horowitz

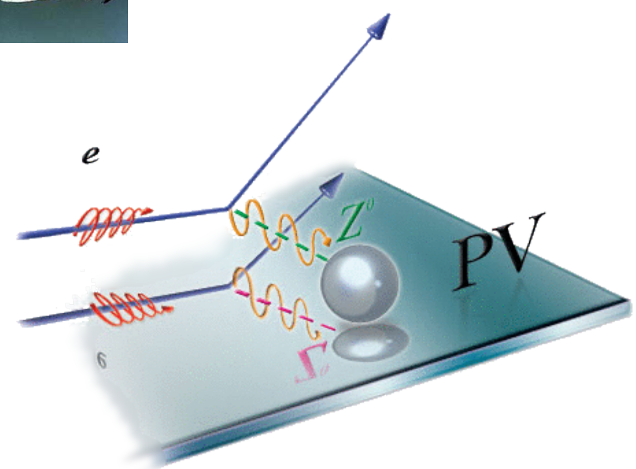


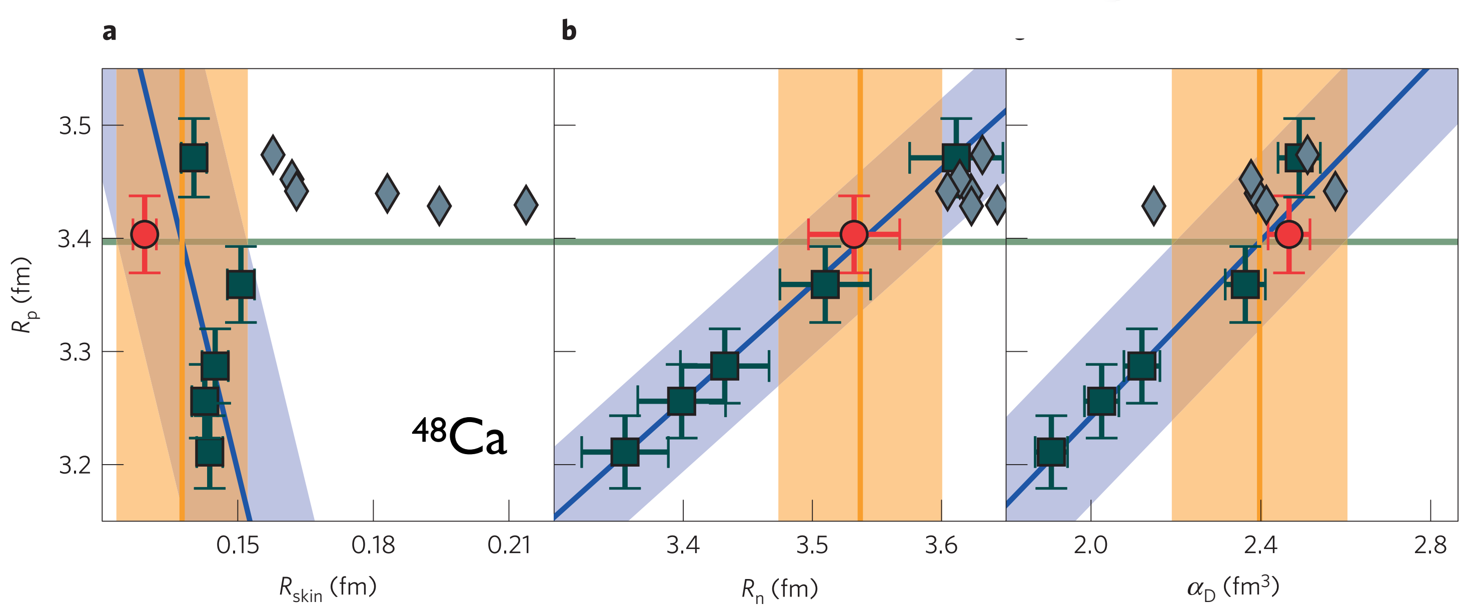
PREX

Pb Radius Experiment

CREX

Ca Radius Experiment





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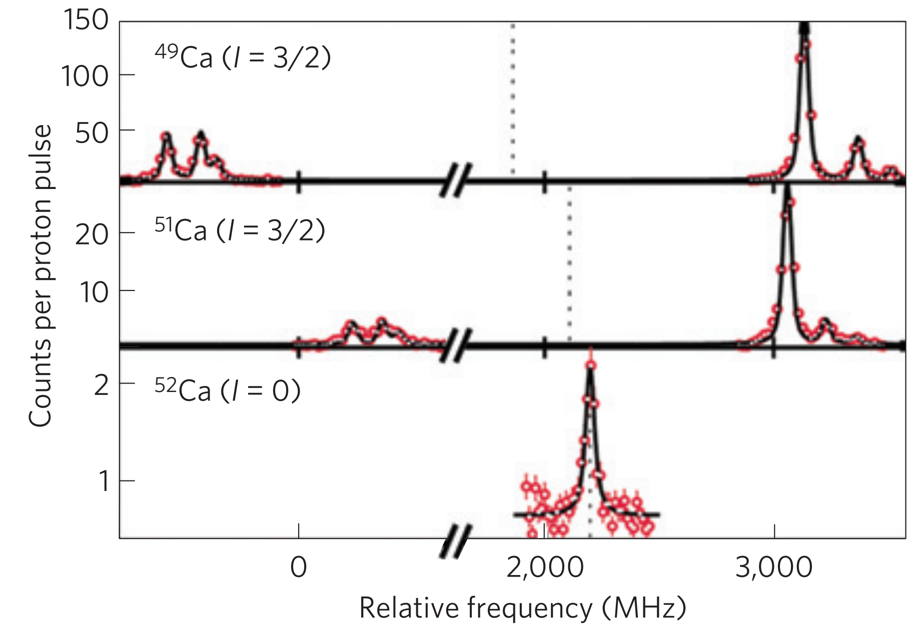
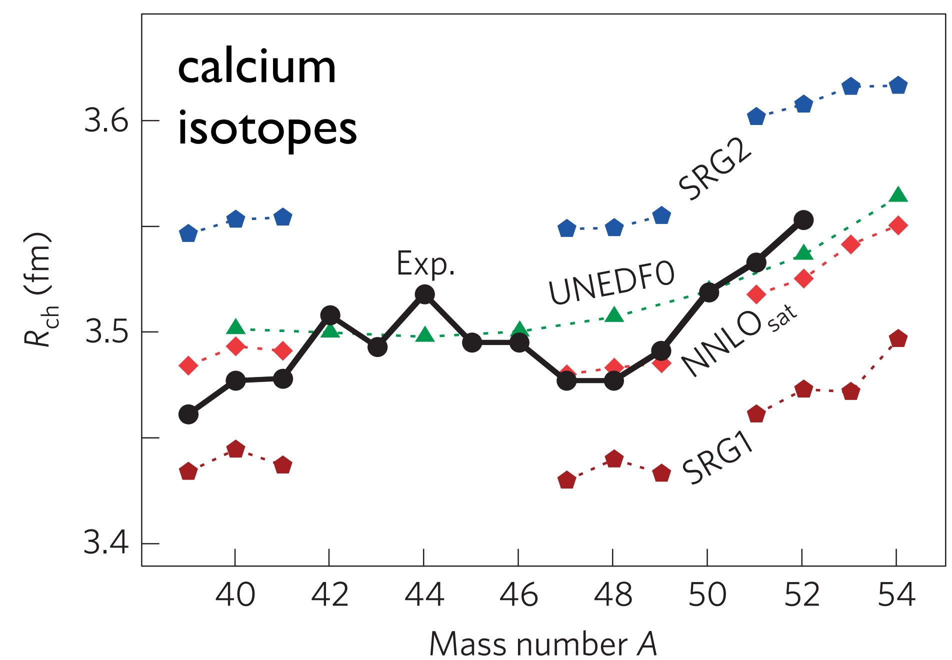
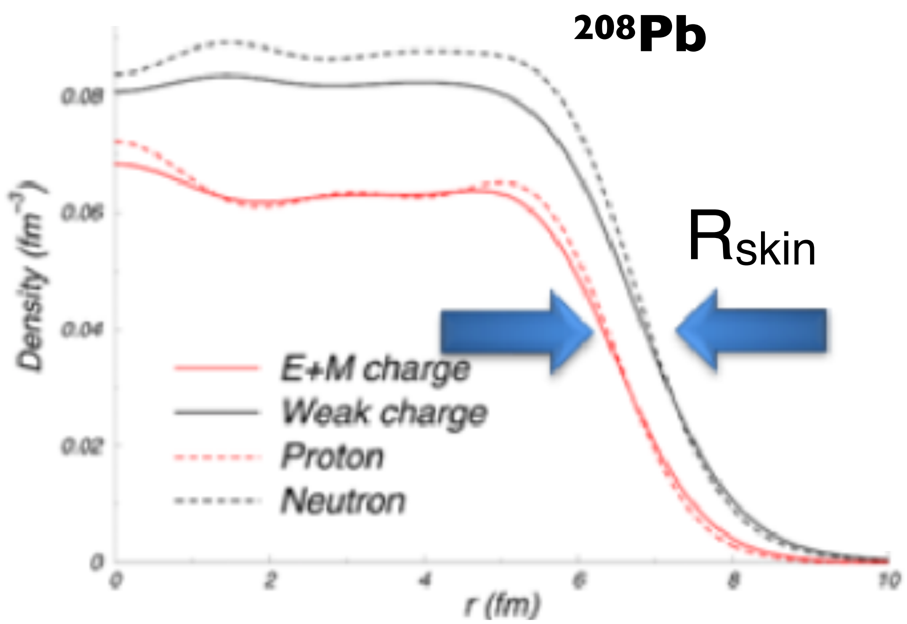


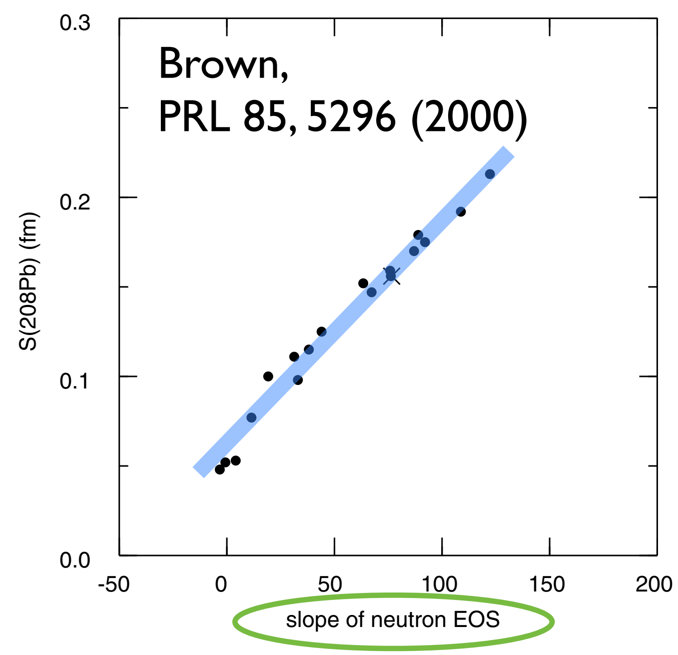


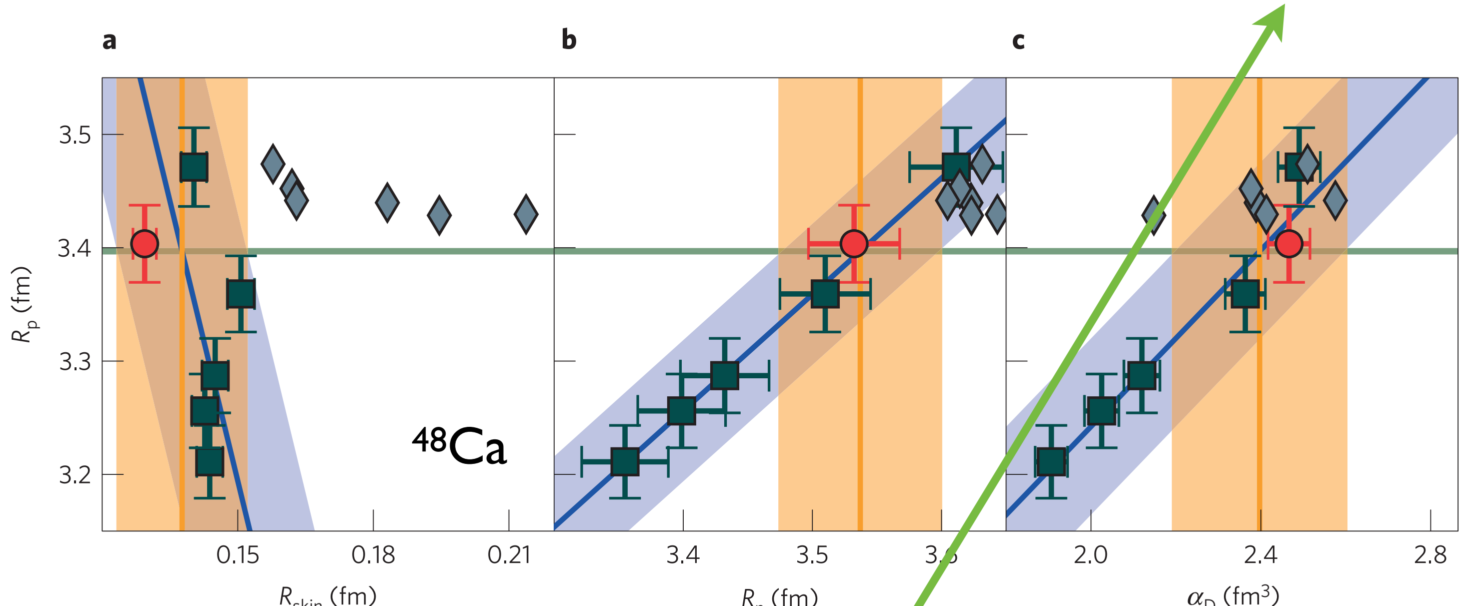
Garcia Ruiz. et al.,
Nature Phys. 12, 594 (2016)

The size of the atomic nucleus: challenges from novel high-precision measurements

Horowitz







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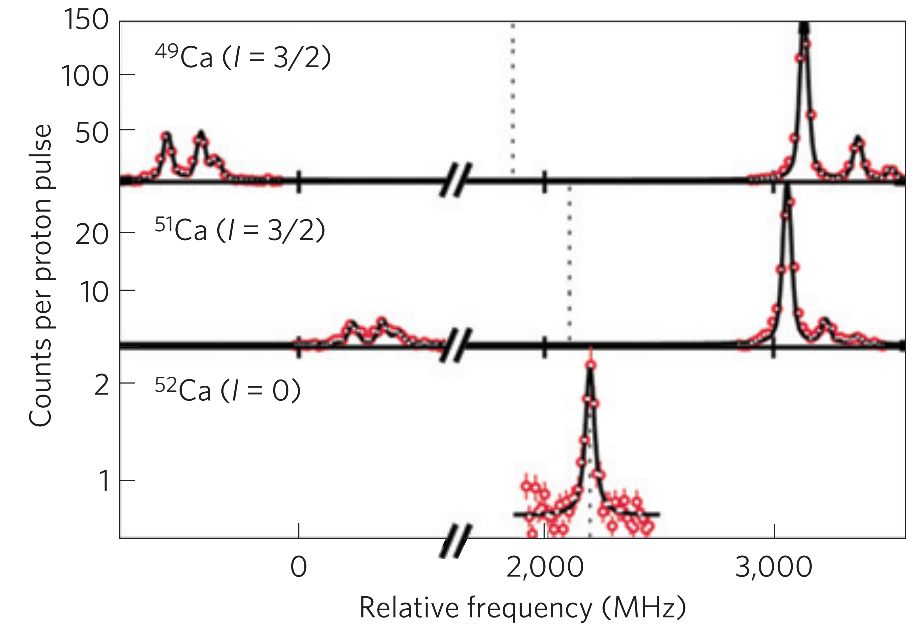

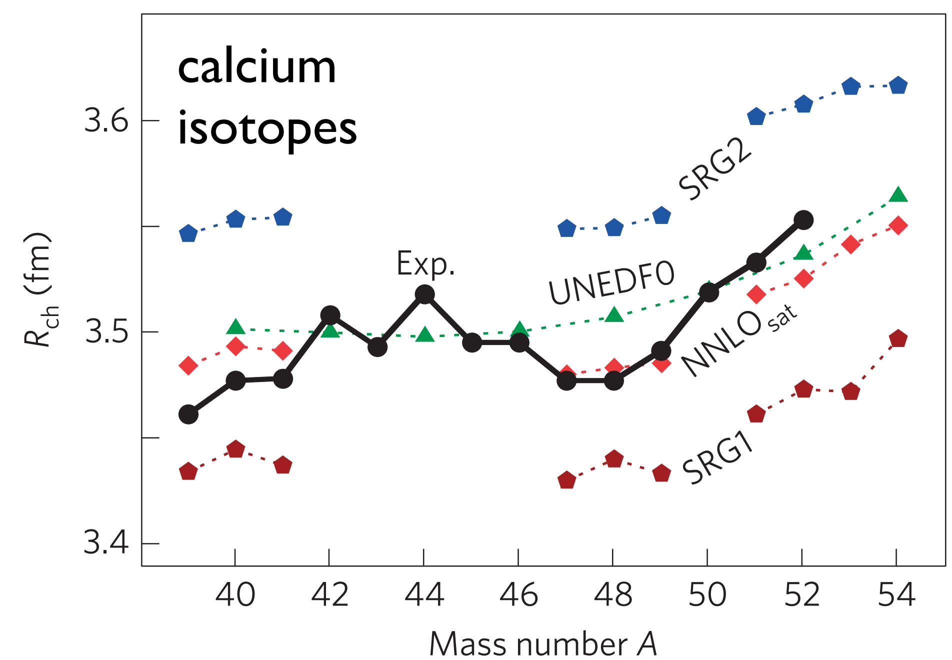

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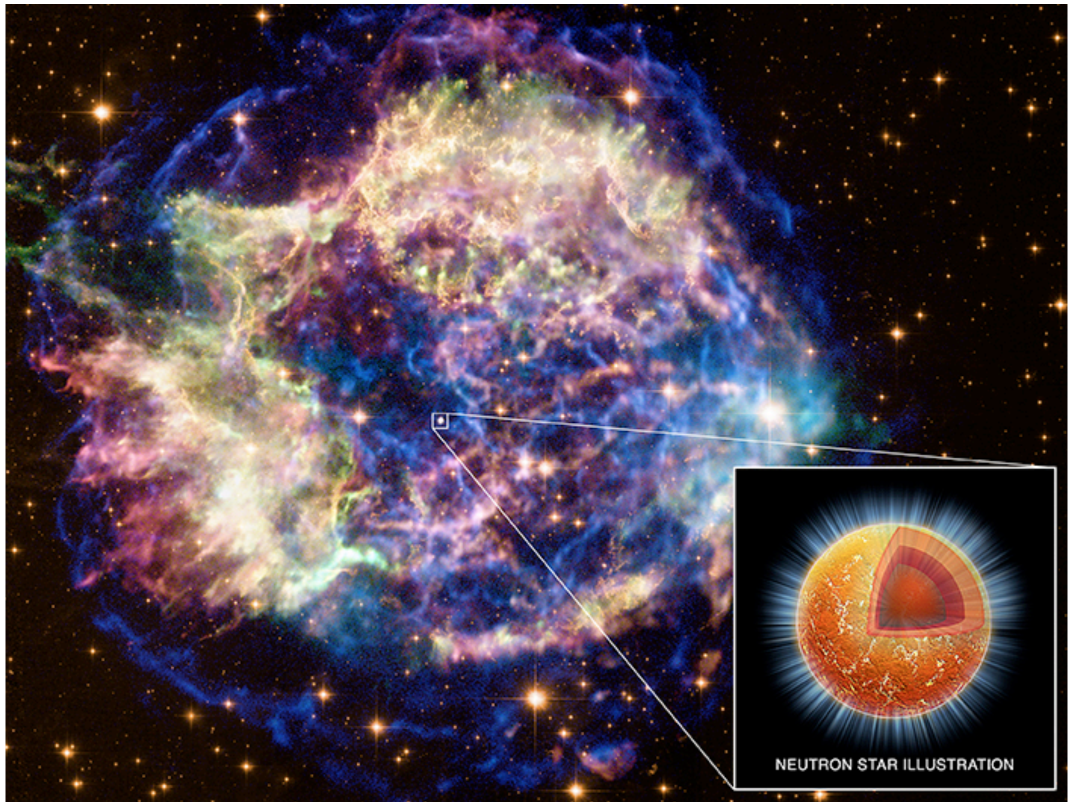
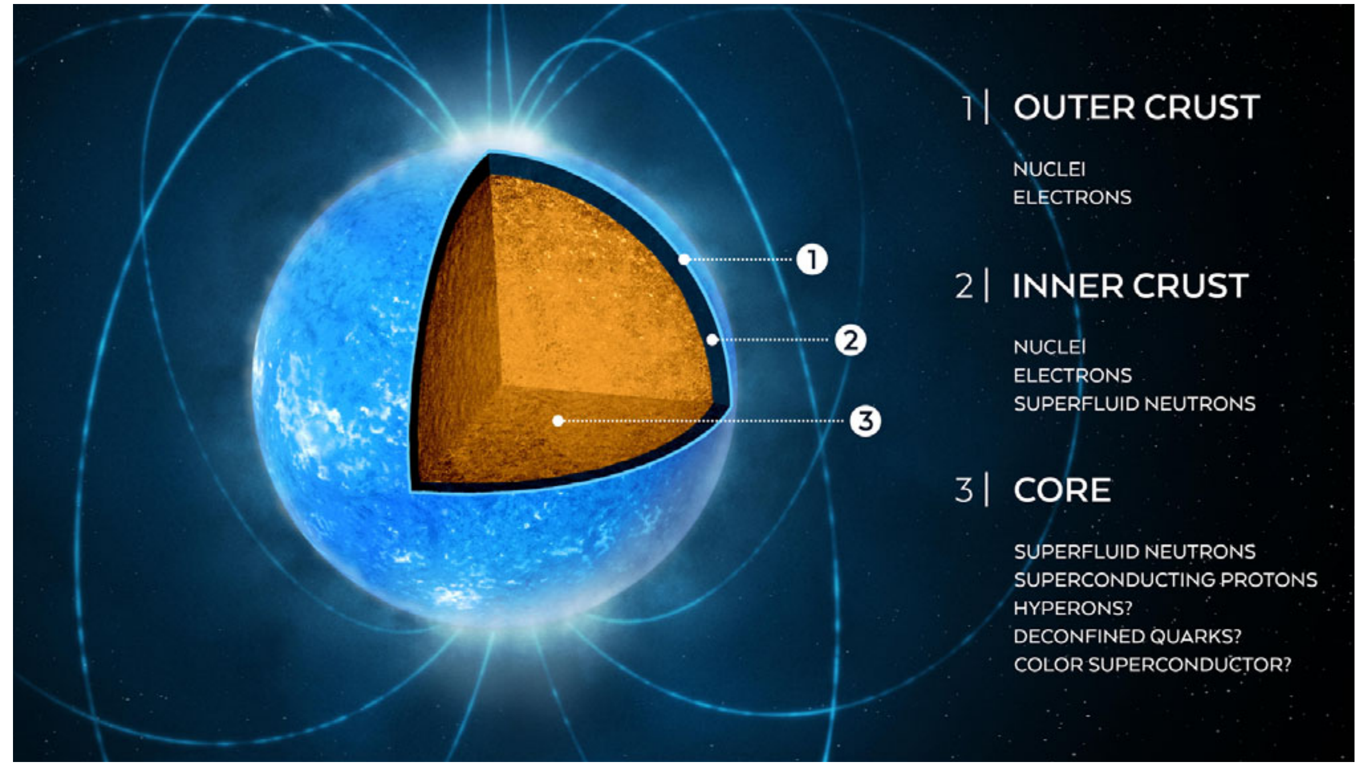
direct connections to astrophysics!

The equation of state of high-density matter: constraints for neutron stars from nuclear physics





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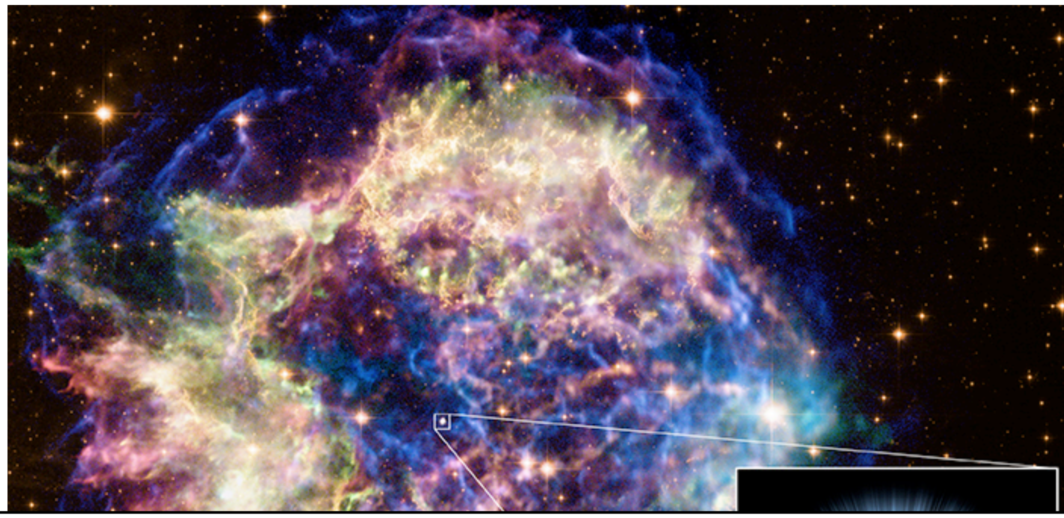

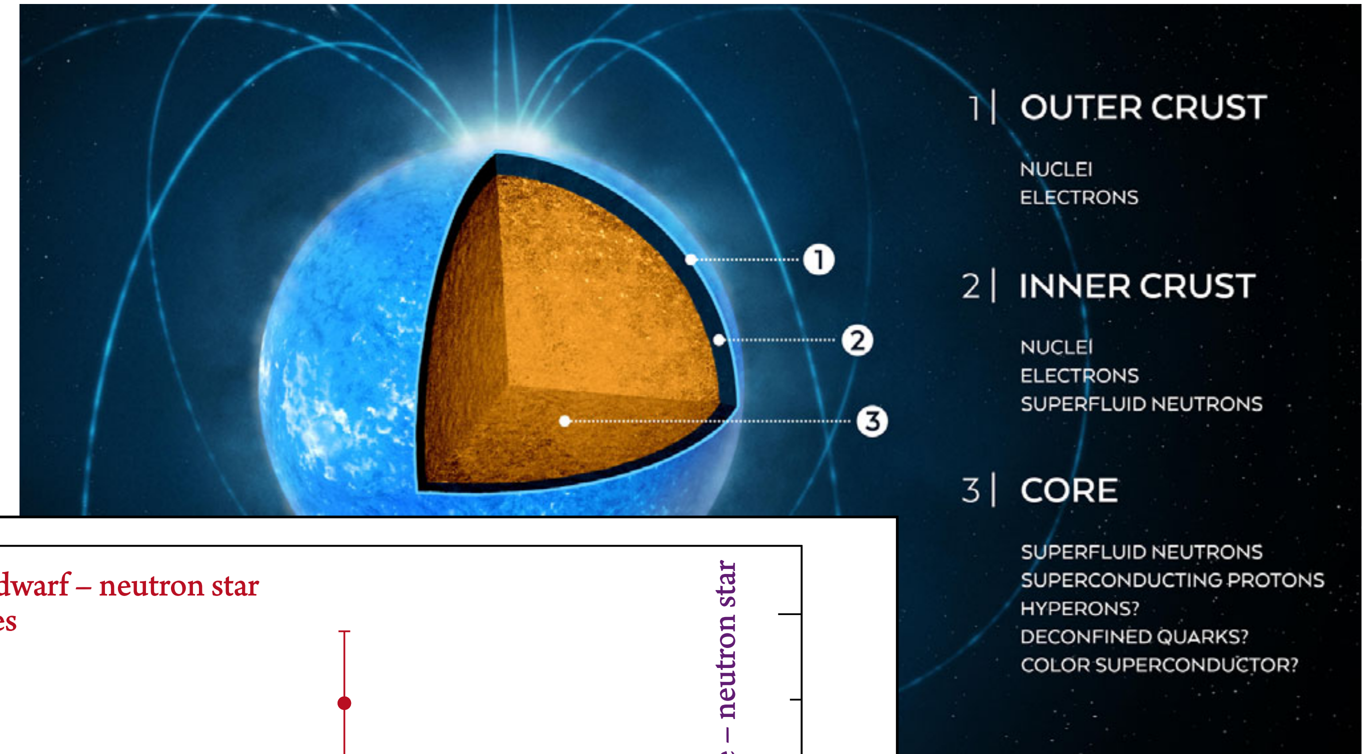

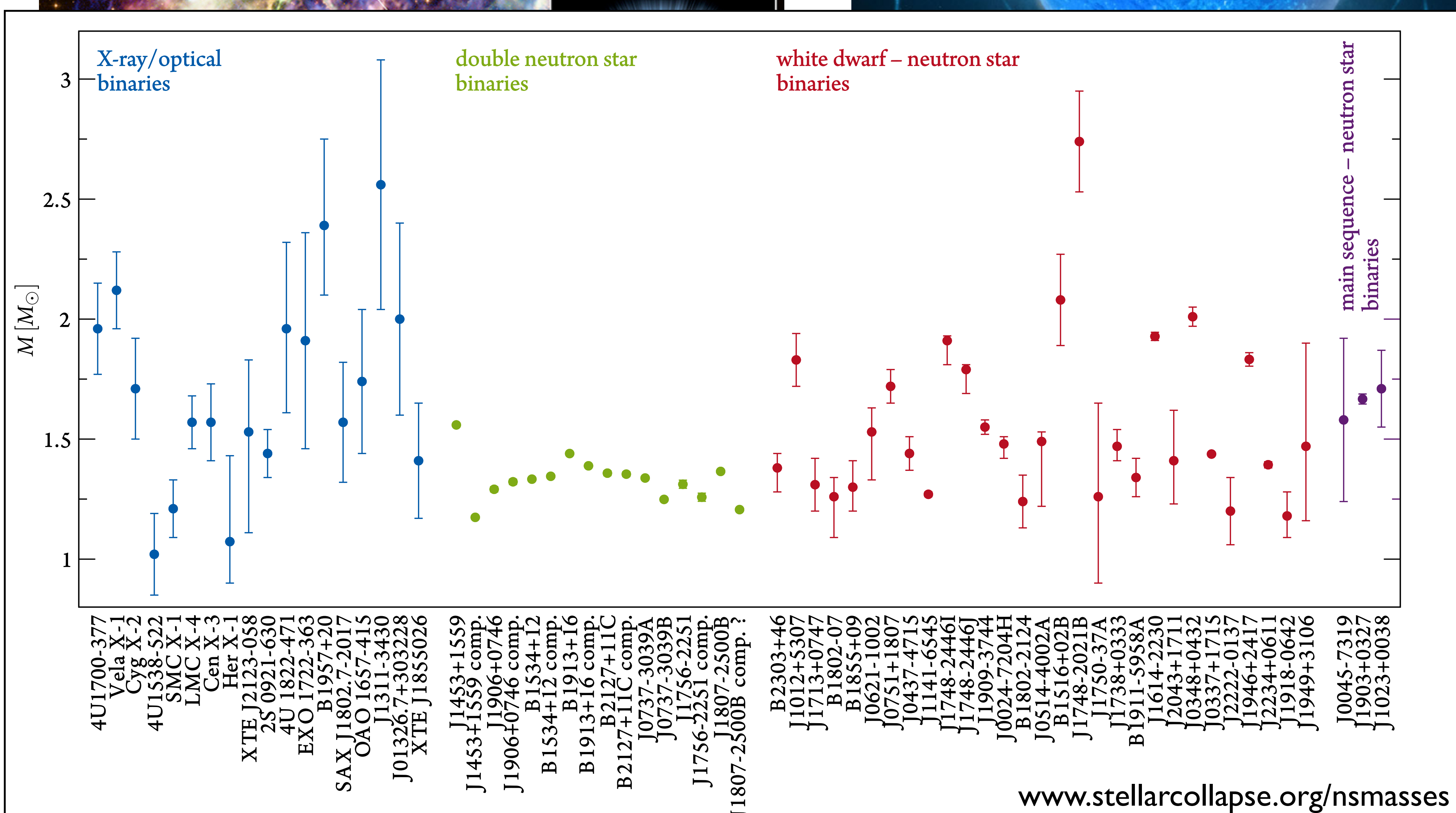

figure taken from Krüger, doctoral thesis (2016)

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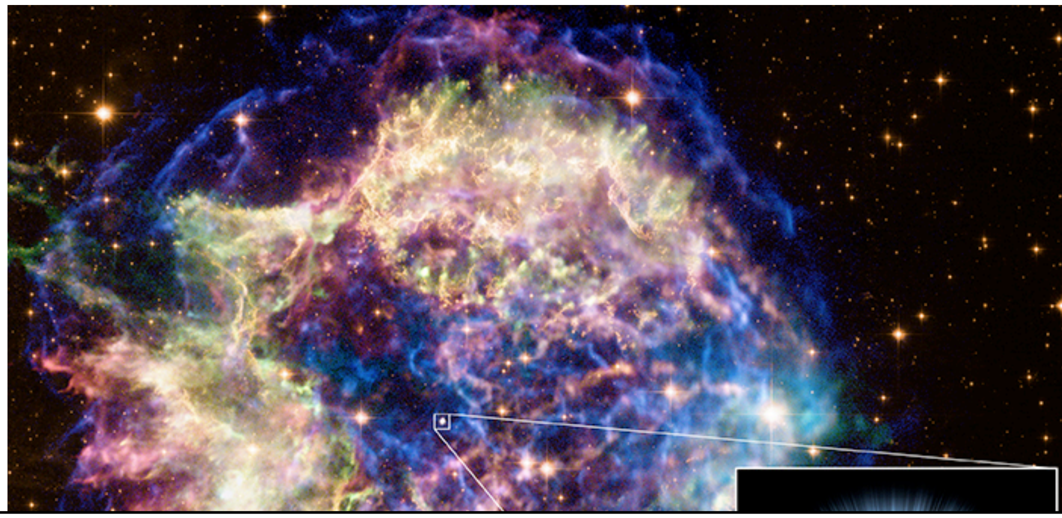

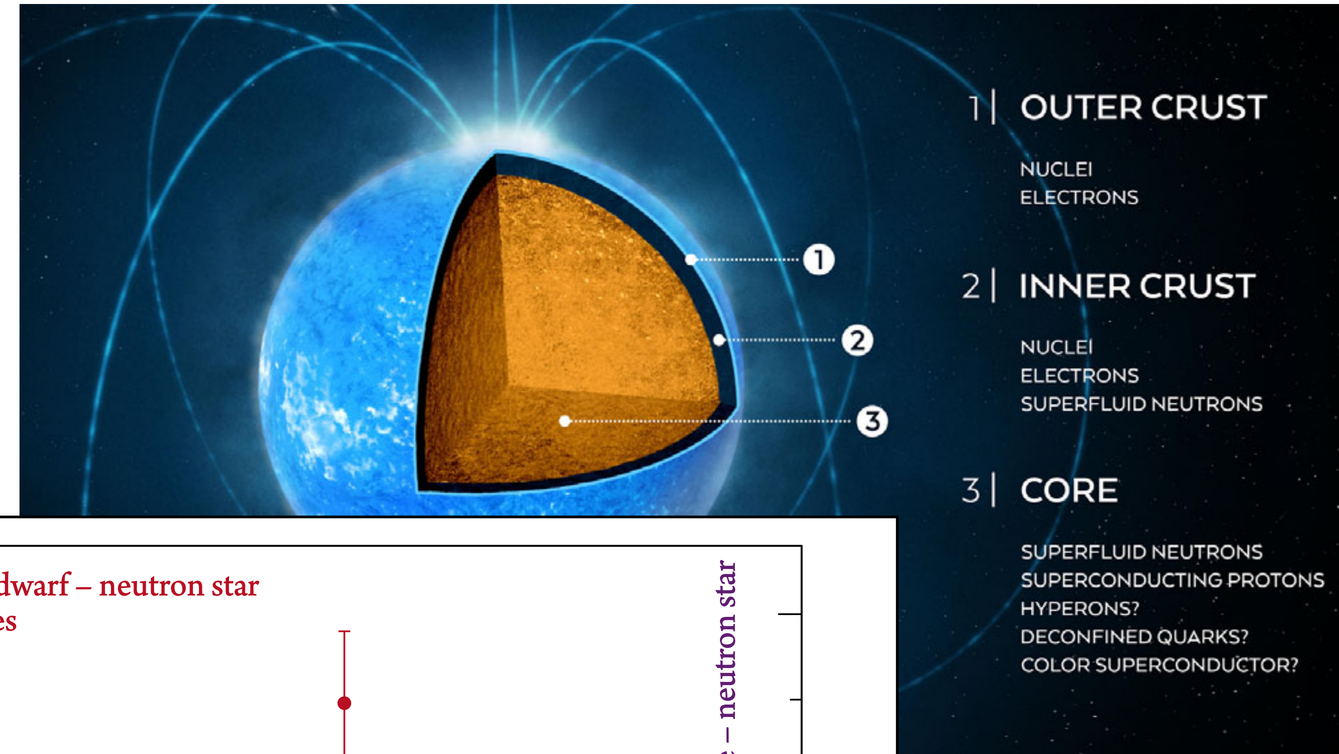

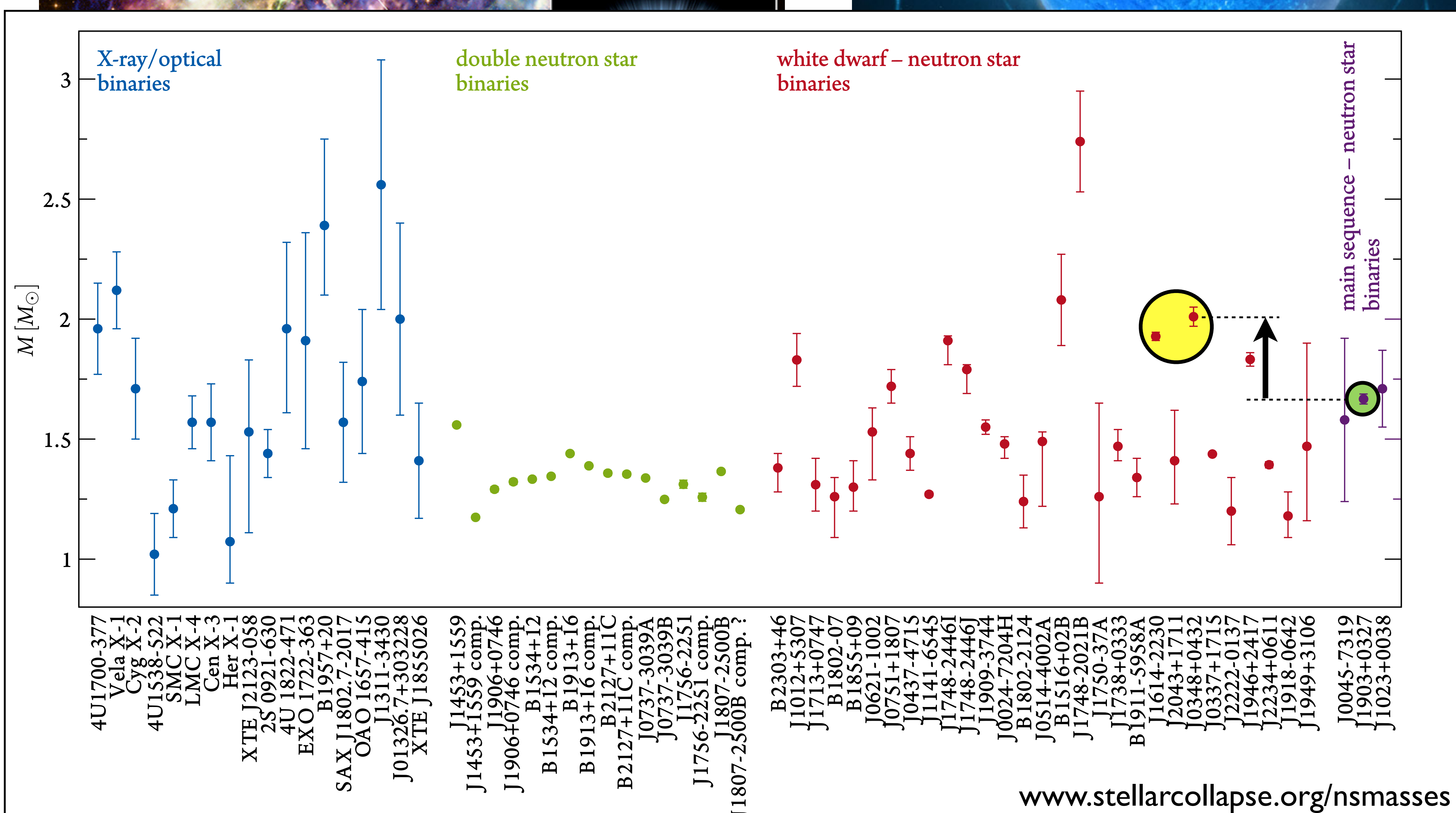

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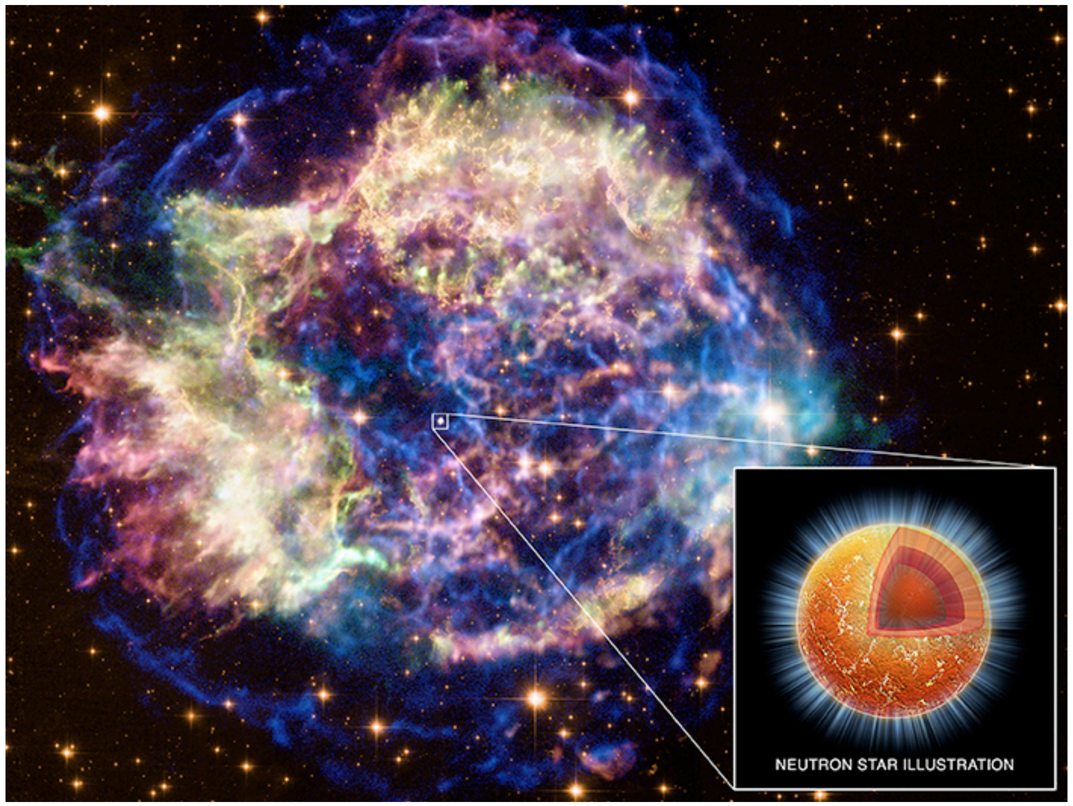
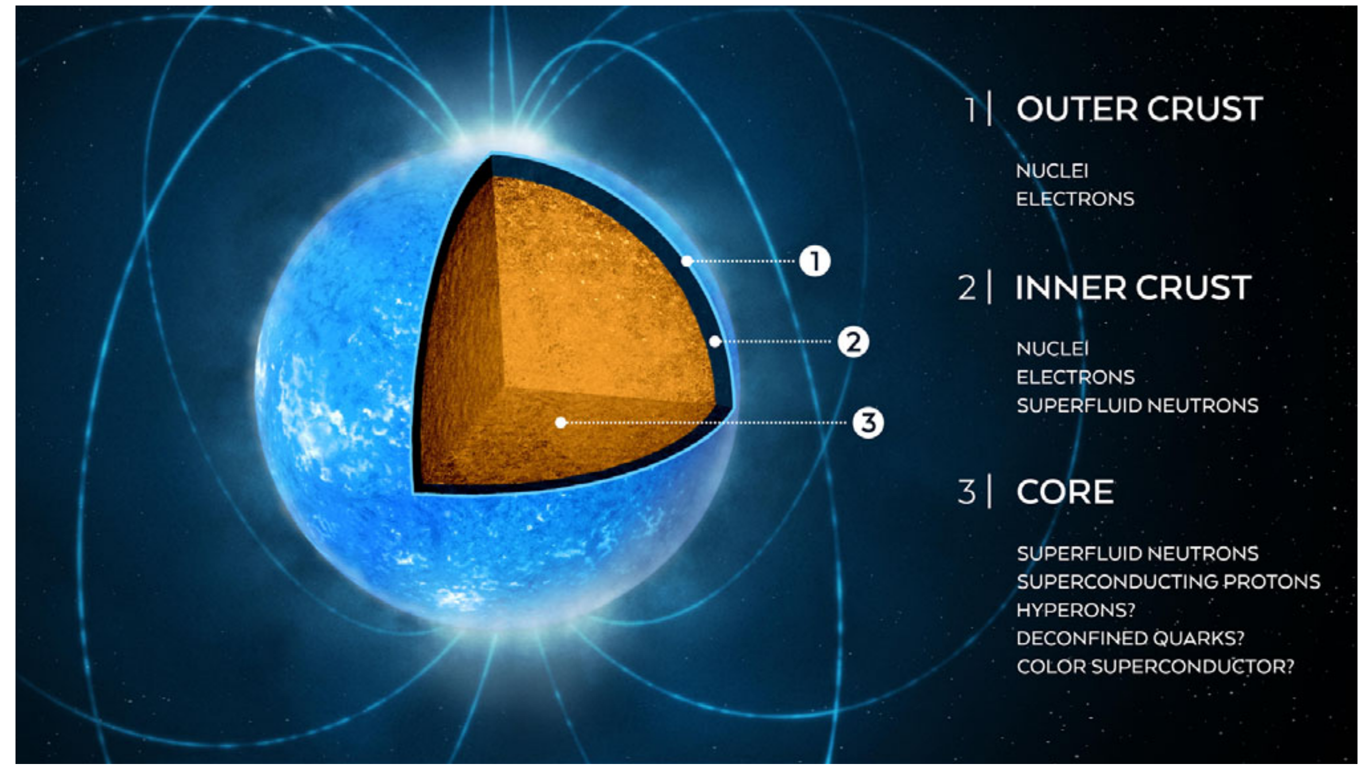
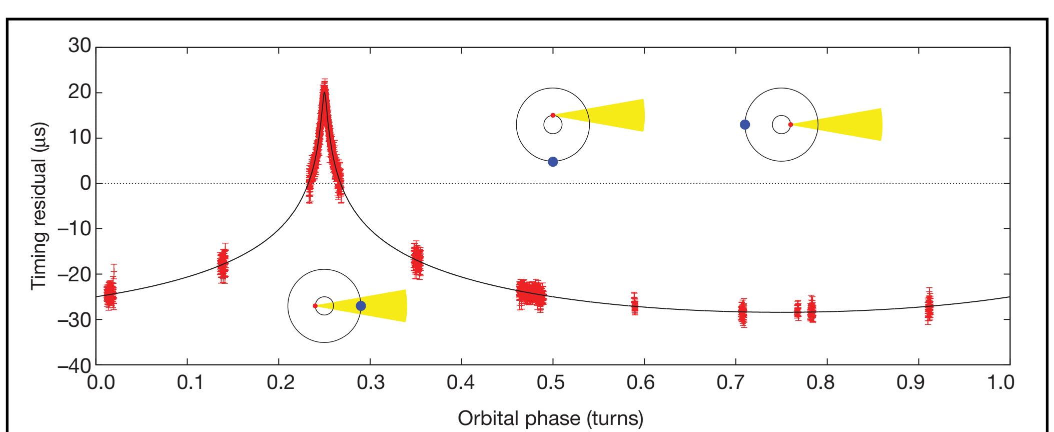
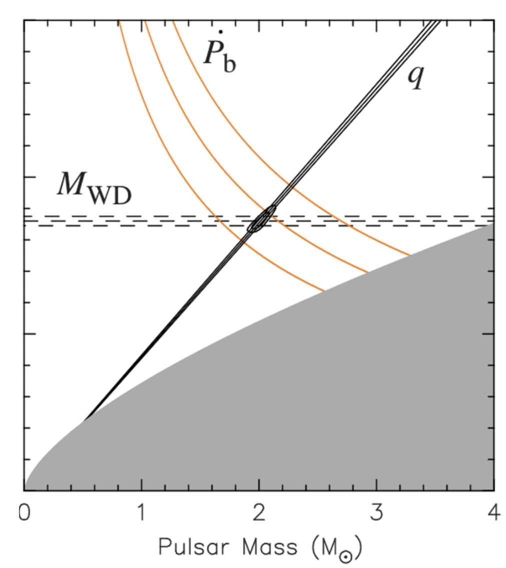




nature — **A two-solar-mass neutron star measured using Shapiro delay** — Demorest et al., Nature 467, 1081 (2010)

Science — **A Massive Pulsar in a Compact Relativistic Binary** — Antoniadis et al., Science 340, 448 (2013)

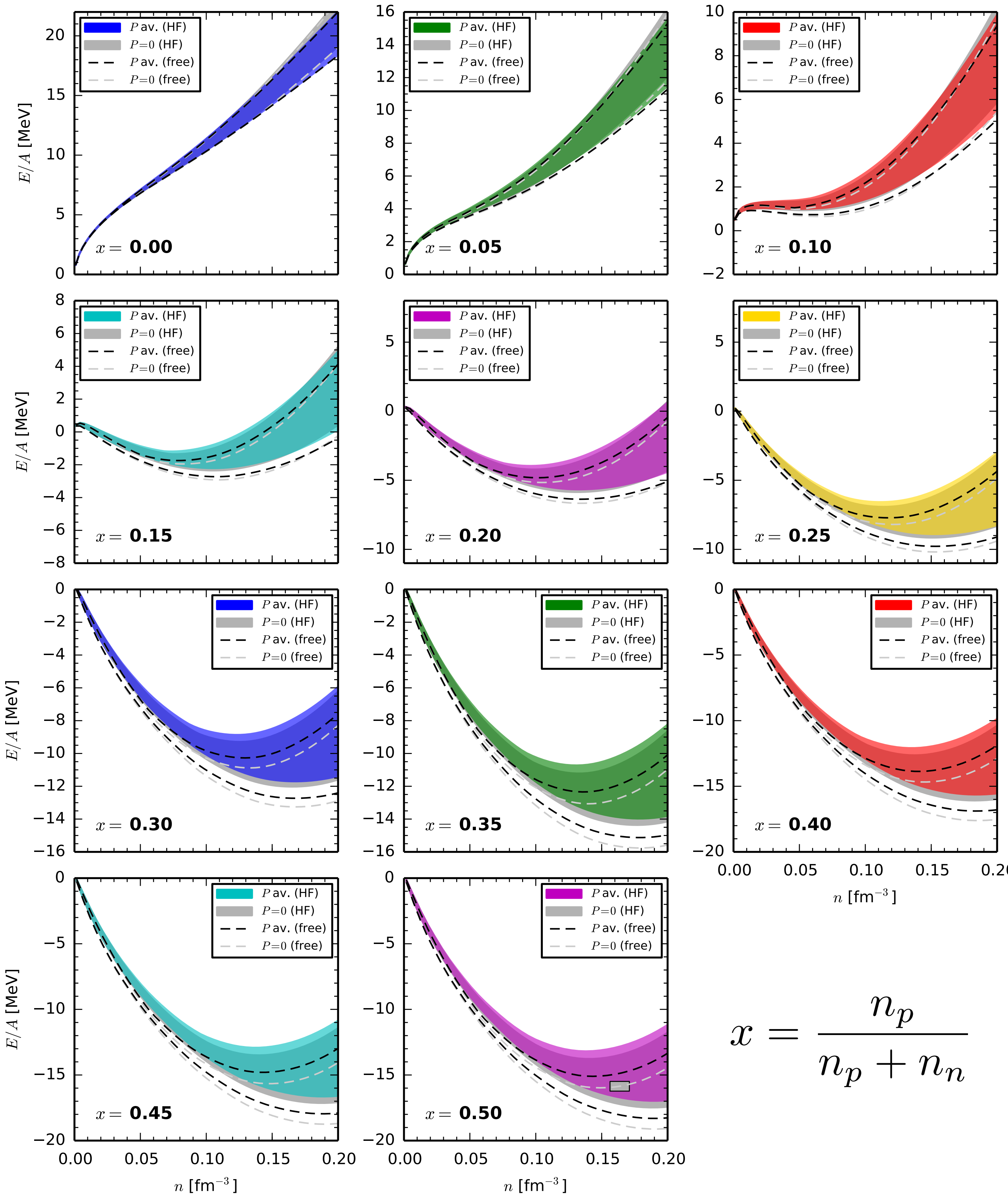




$$M_{\max} = 2.0 \pm 0.04\, M_\odot$$

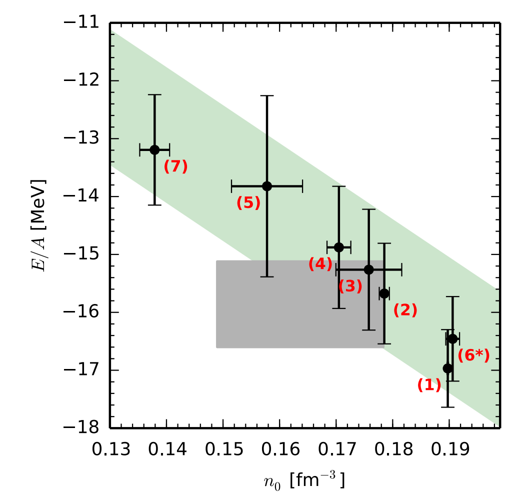
$$R \sim 10\ \mathrm{km}$$

Microscopic calculations of the equation of state



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

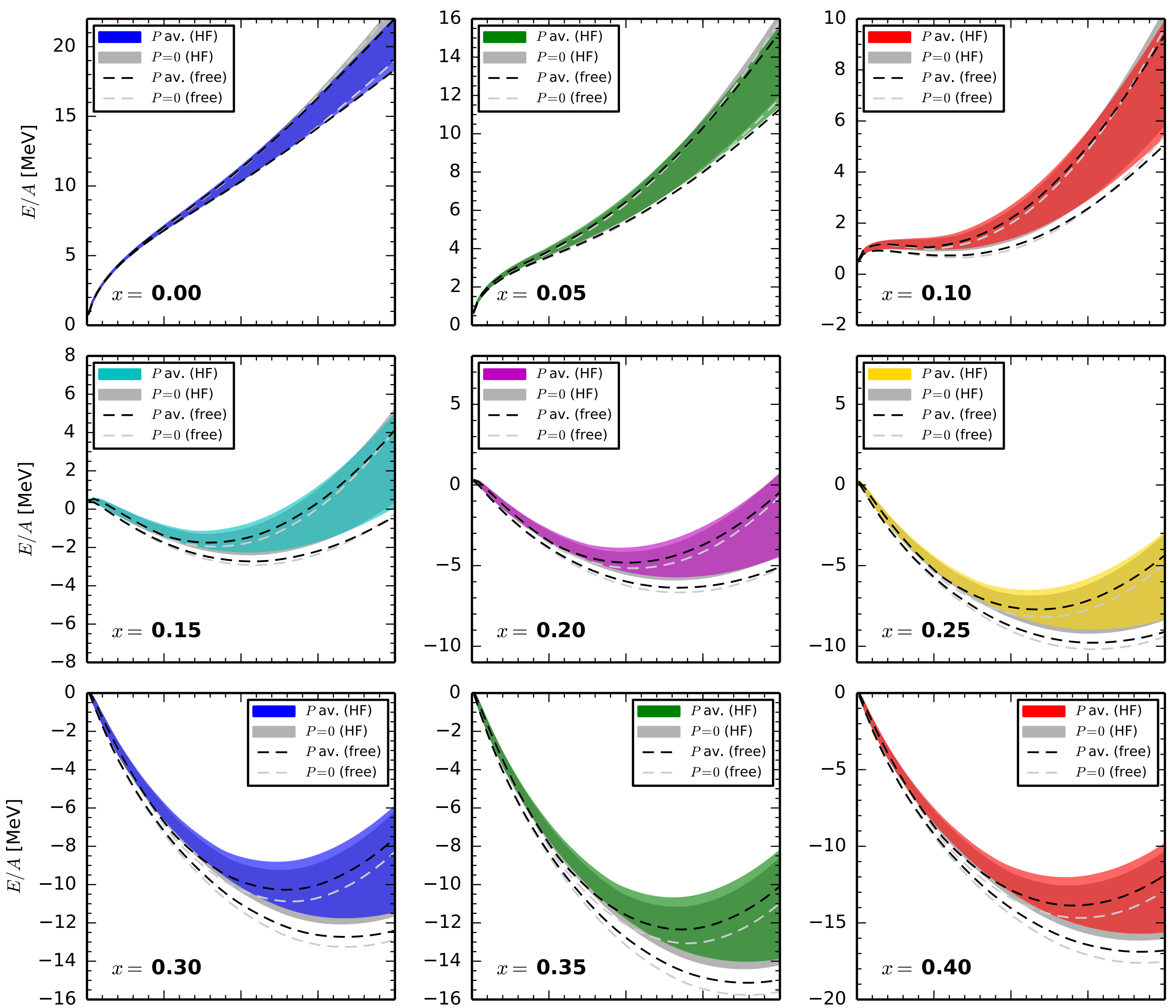
- microscopic framework to calculate equation of state for general proton fractions
- uncertainty bands determined by set of 7 Hamiltonians



- many-body framework allows treatment of general 3N interaction

Drischler, KH, Schwenk,
PRC 054314 (2016)

Microscopic calculations of the equation of state



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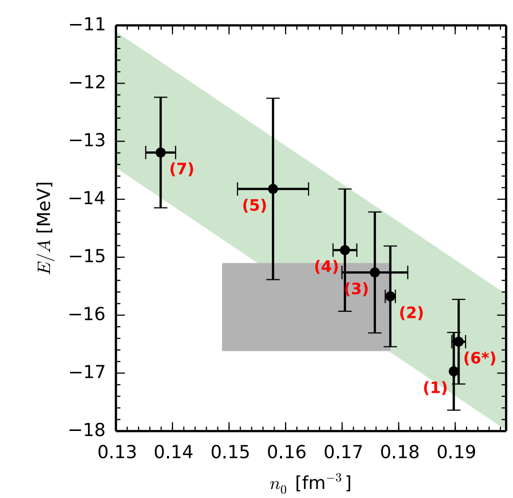


- many body framework allows

Problem:

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

Strategy:

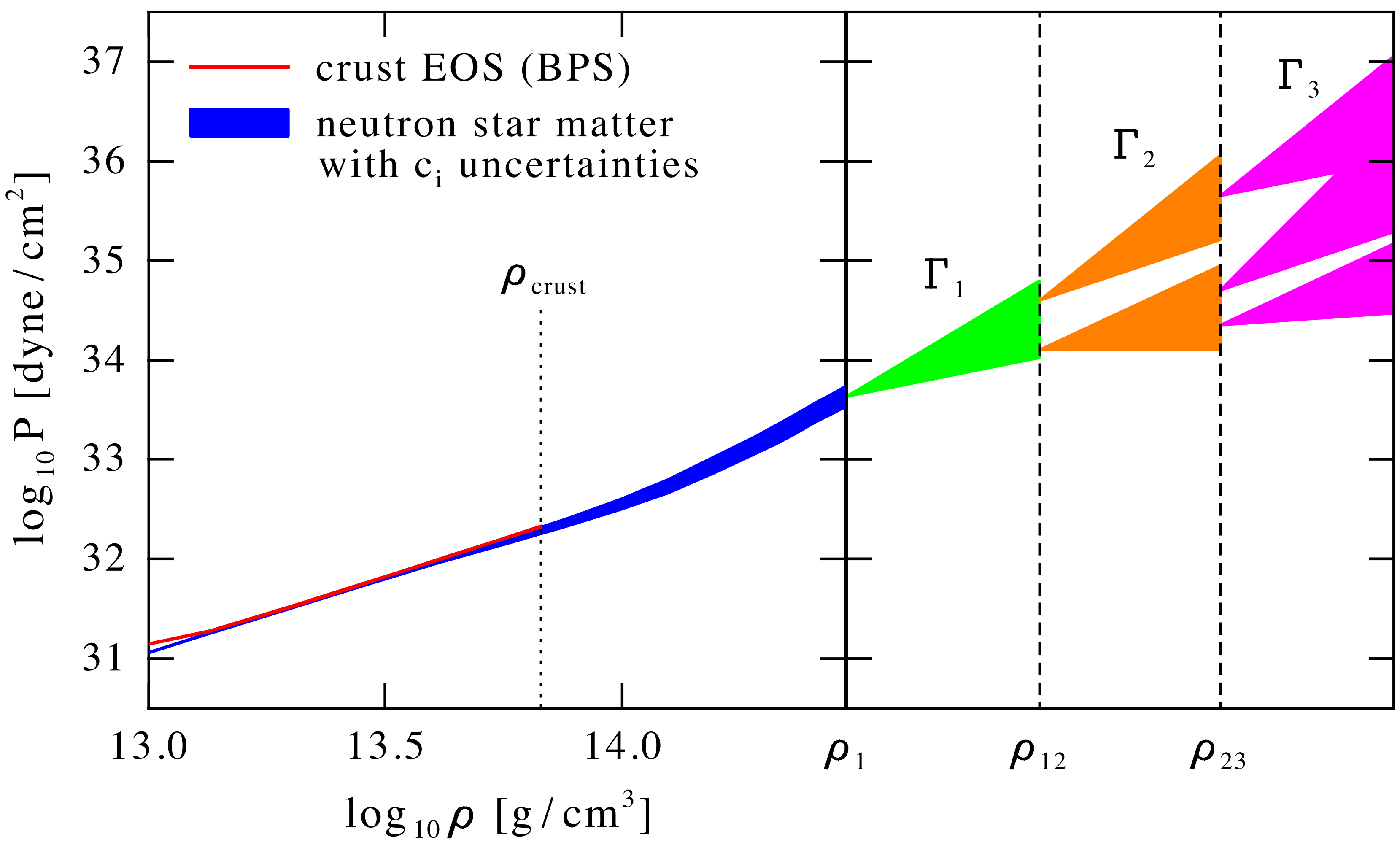
Use observations to constrain the high-density part of the nuclear EOS.

Neutron star radius constraints

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

parametrize our ignorance via piecewise high-density extensions of EOS:

- use polytropic ansatz $p \sim \rho^{\Gamma}$ (results insensitive to particular form)
- 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:

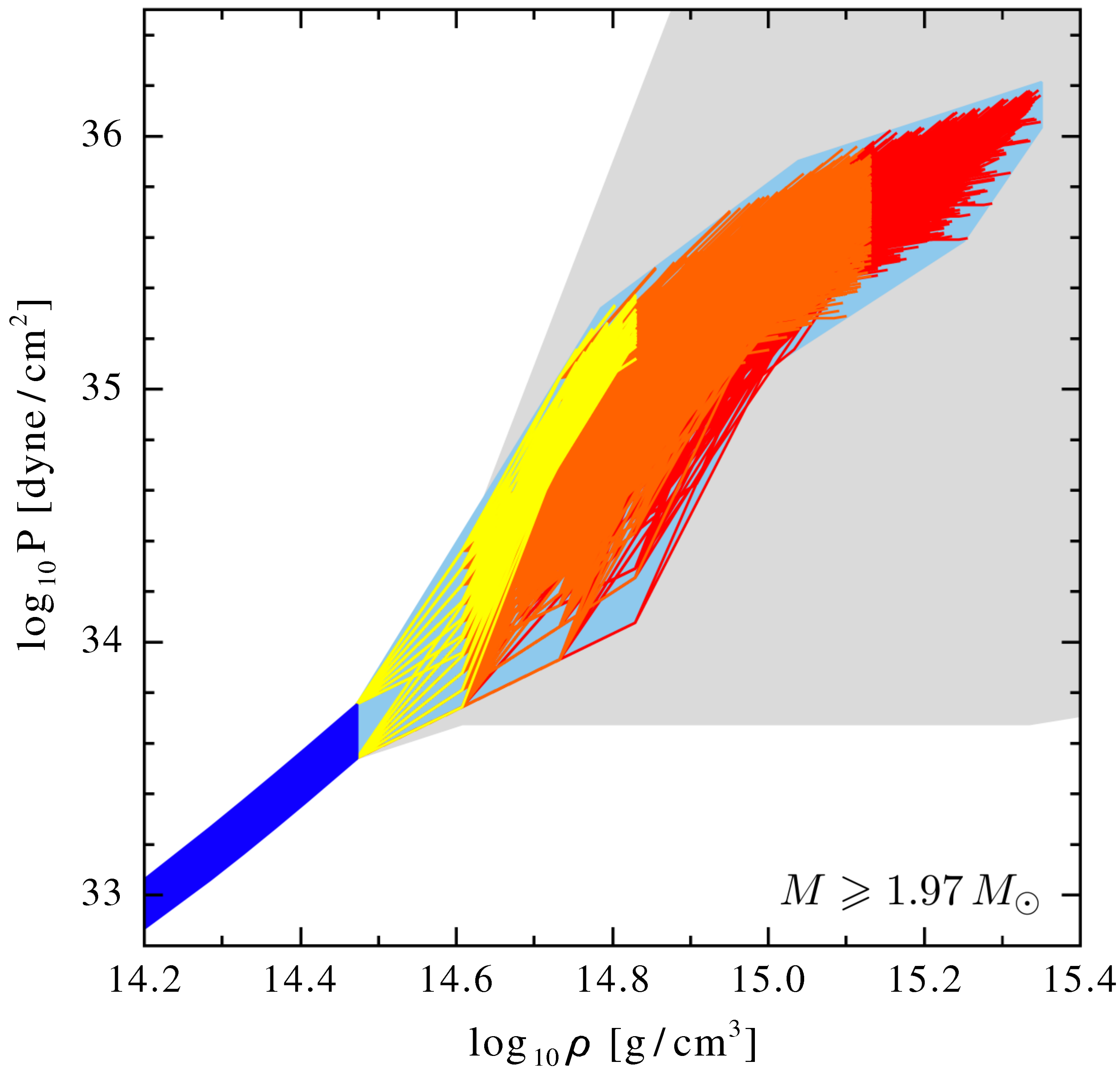
recent NS observations

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

causality

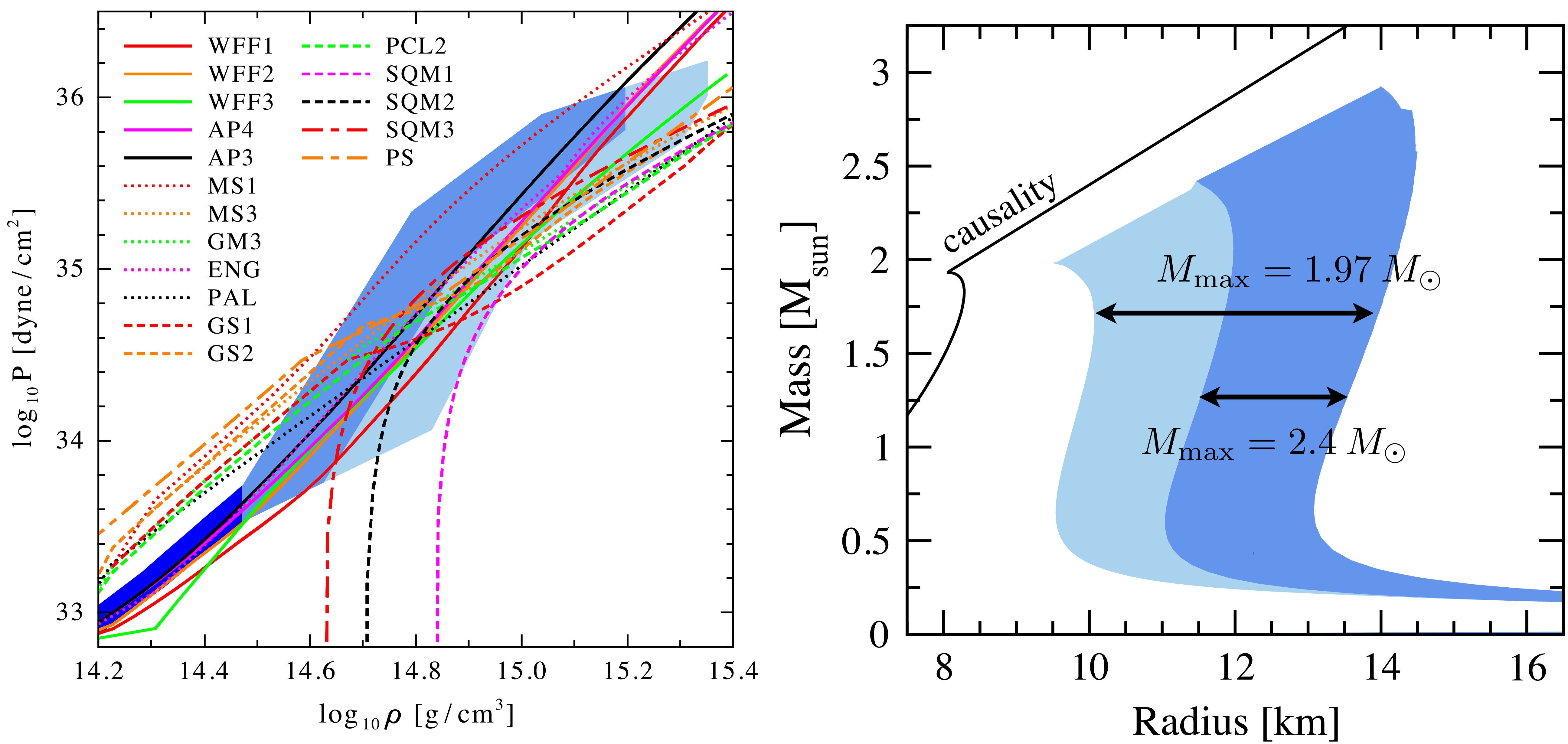
$$v_s(\rho) = \sqrt{dP/d\varepsilon} < c$$

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



constraints lead to significant reduction of EOS uncertainty band

Constraints on neutron star radii



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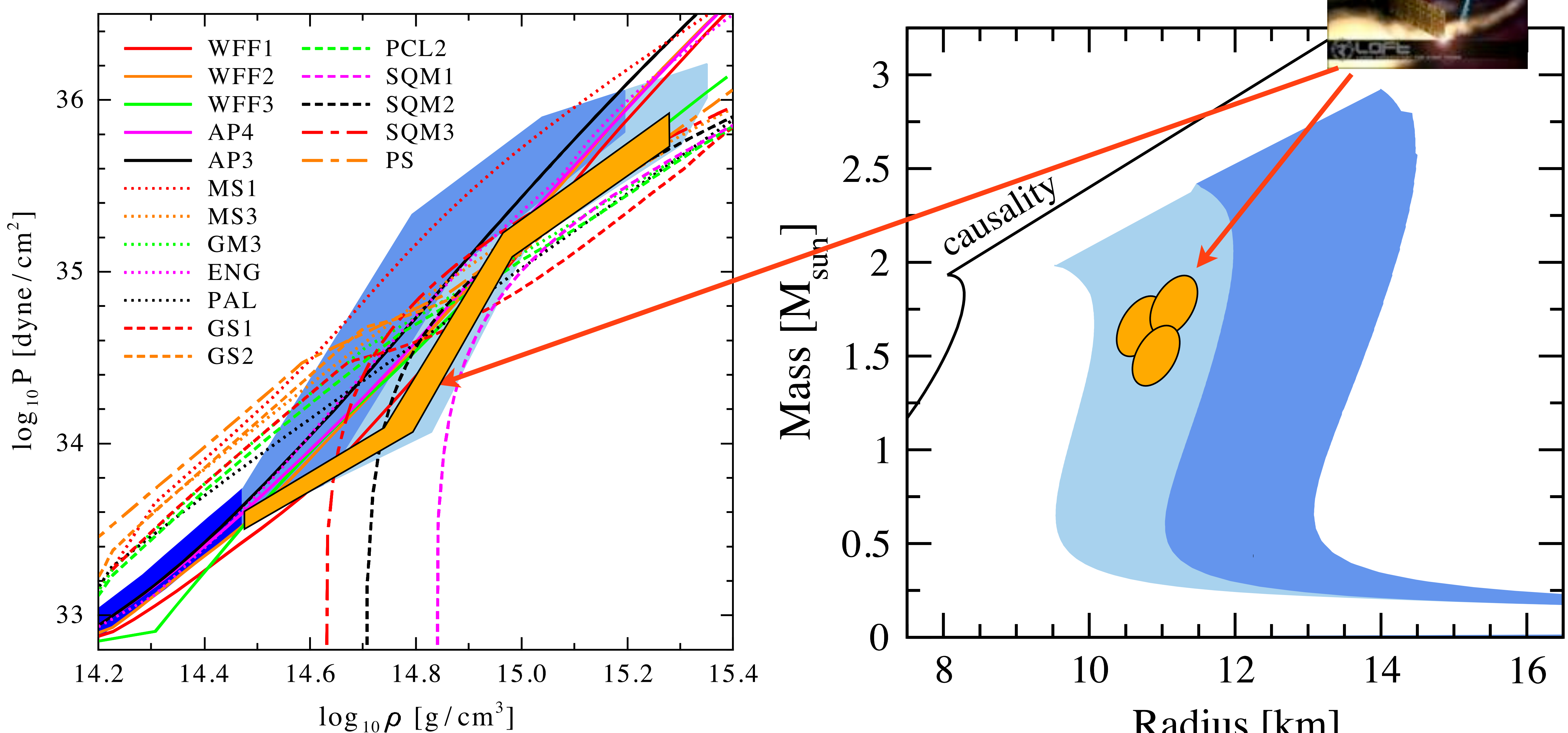

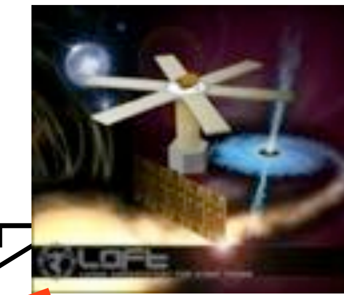

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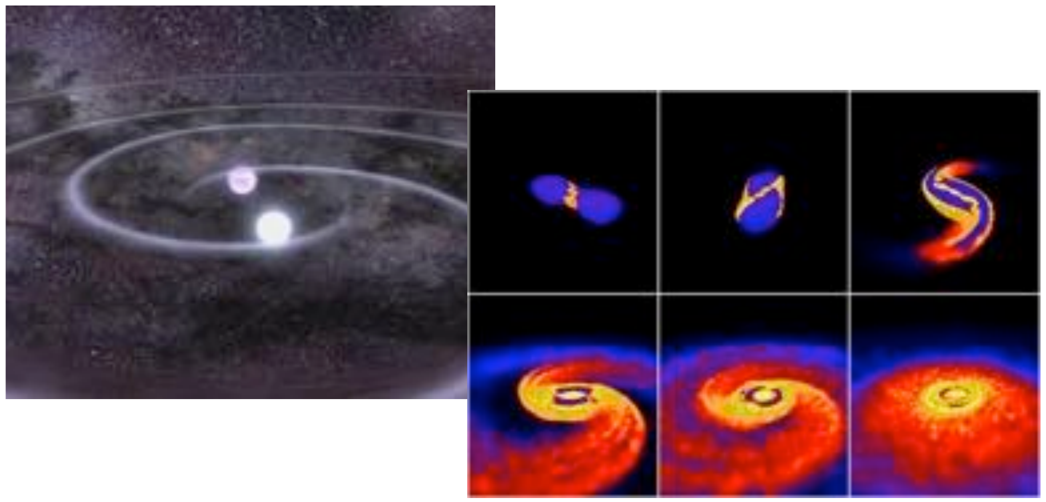
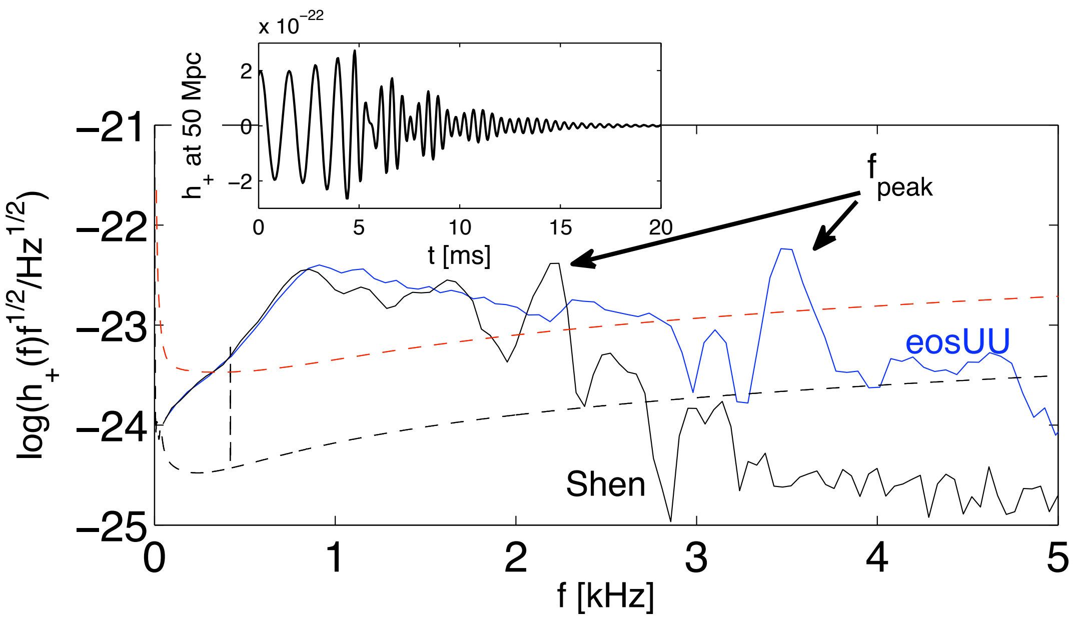
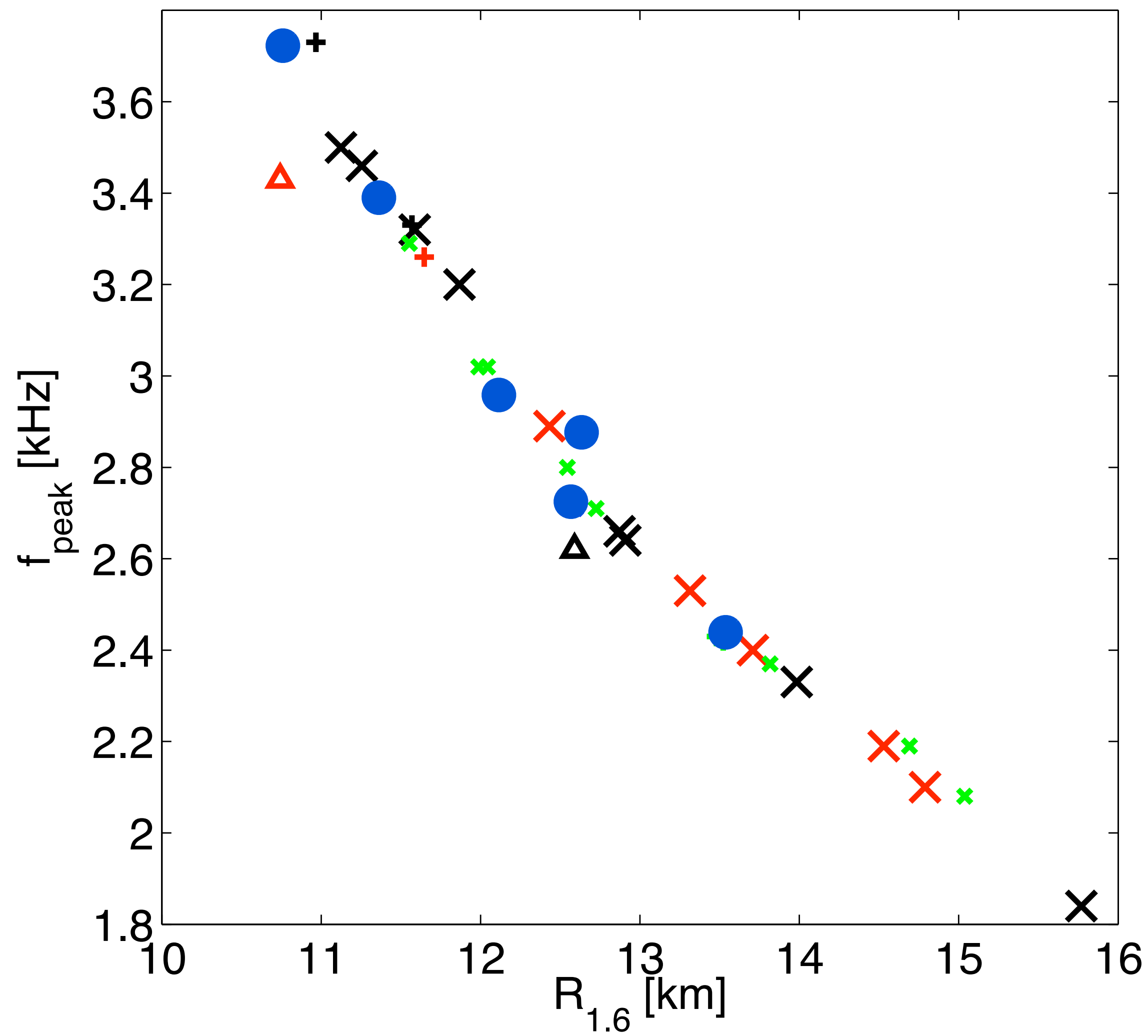
- low-density part of EOS sets scale for allowed high-density extensions
- current radius prediction for typical $1.4\,M_\odot$ neutron star: $9.7 - 13.9\,\mathrm{km}$
- proposed missions (LOFT, NICER...) could significantly improve constraints

Gravitational wave signals from neutron star binary mergers







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

- 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

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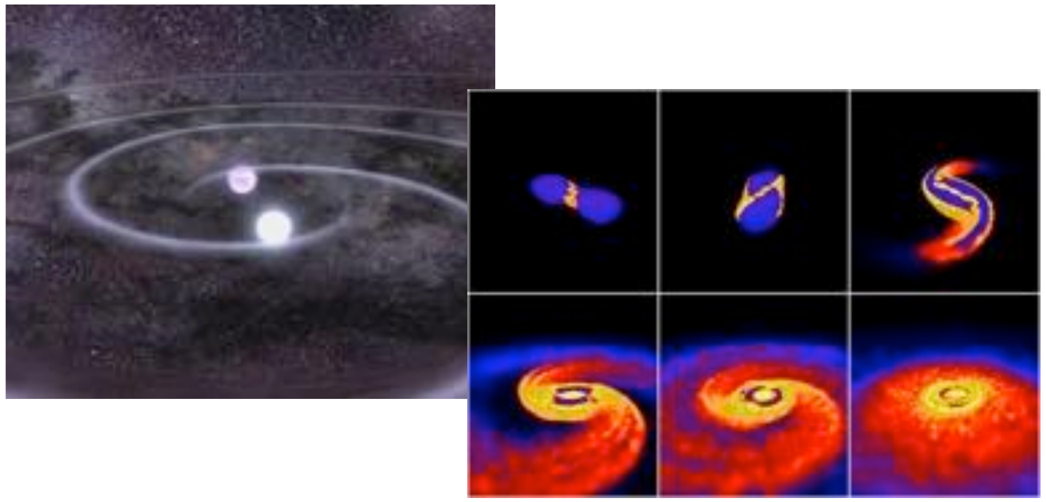

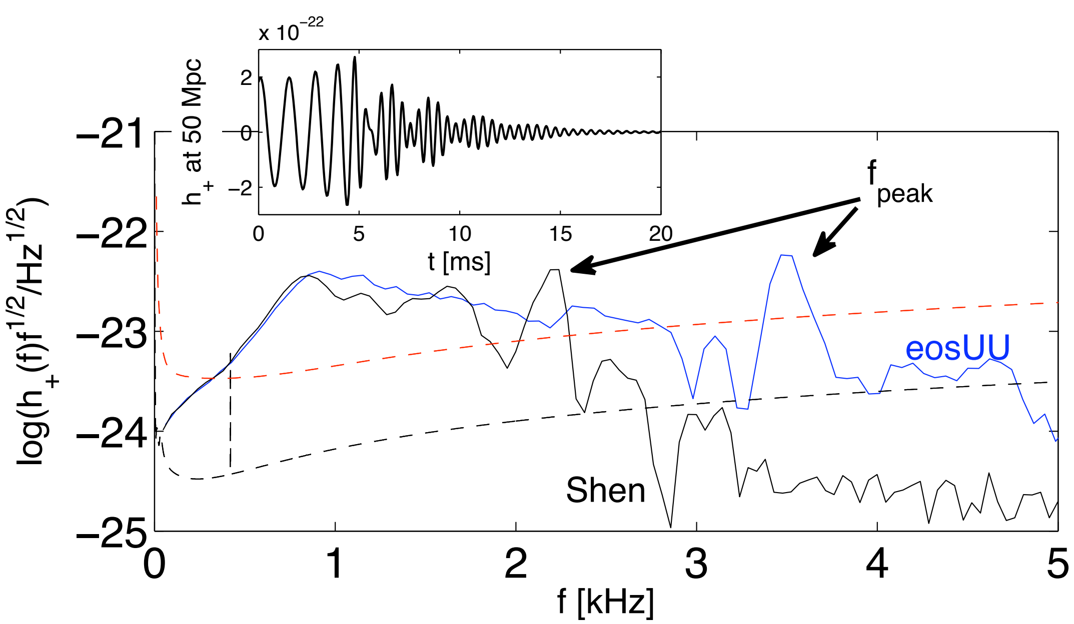

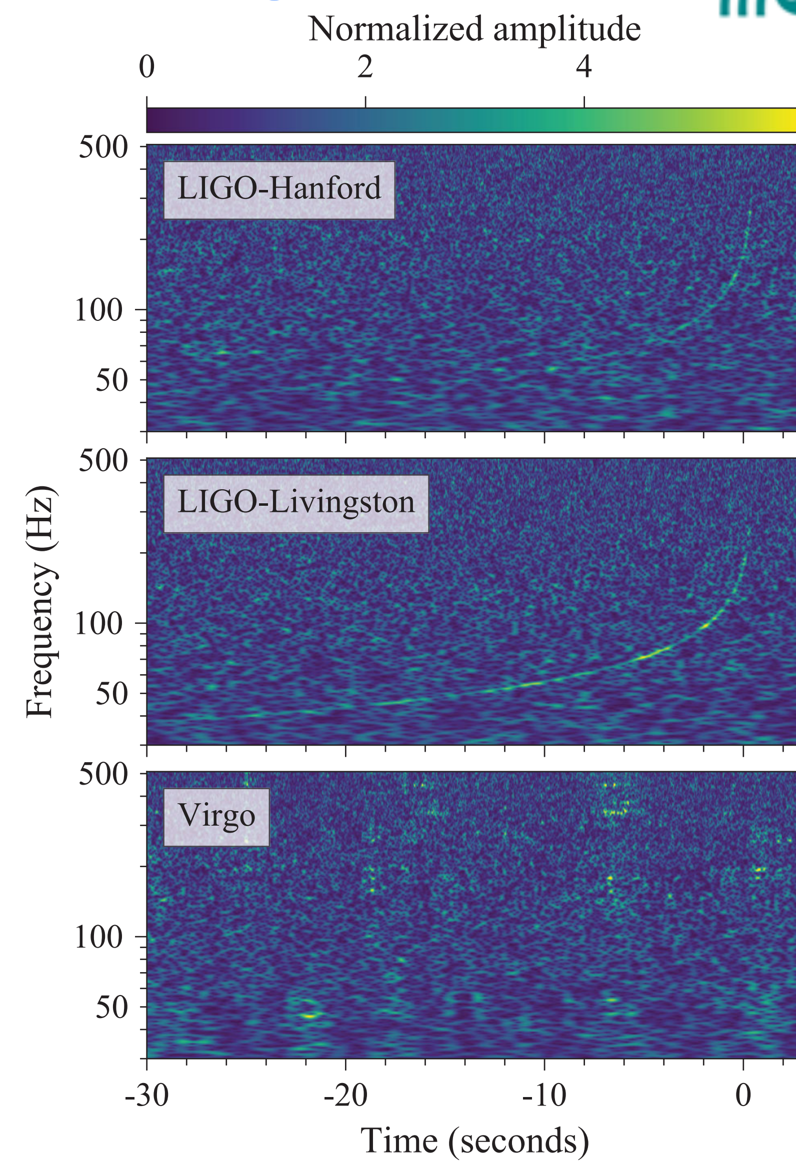

LIGO and VIRGO collaboration, PRL 119, 161101 (2017)

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Softening of nuclear interactions: the Similarity Renormalization Group

- generate unitary transformation which decouples low- and high momenta:

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

- change resolution systematically in small steps: $$\boxed{\frac{dH_\lambda}{d\lambda} = [\eta_\lambda, H_\lambda]}$$

- generator η_λ can be chosen and tailored to different applications

- observables are preserved due to unitarity of transformation

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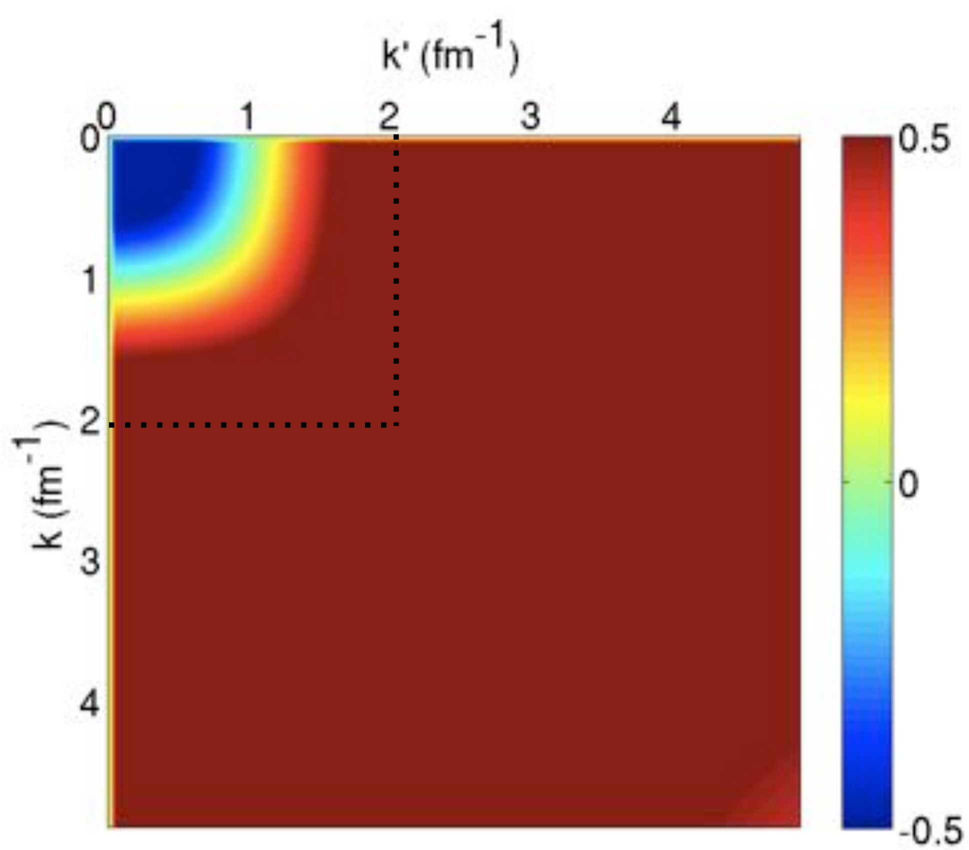
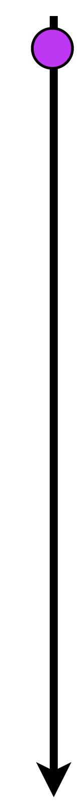


Resolution λ



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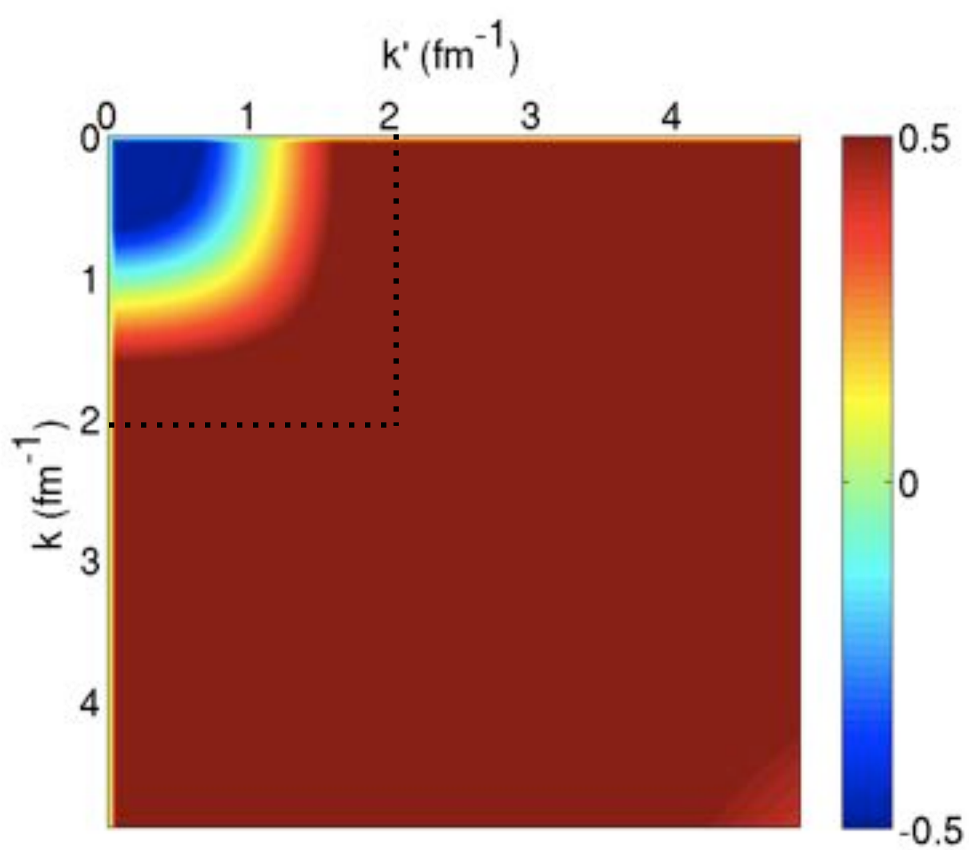

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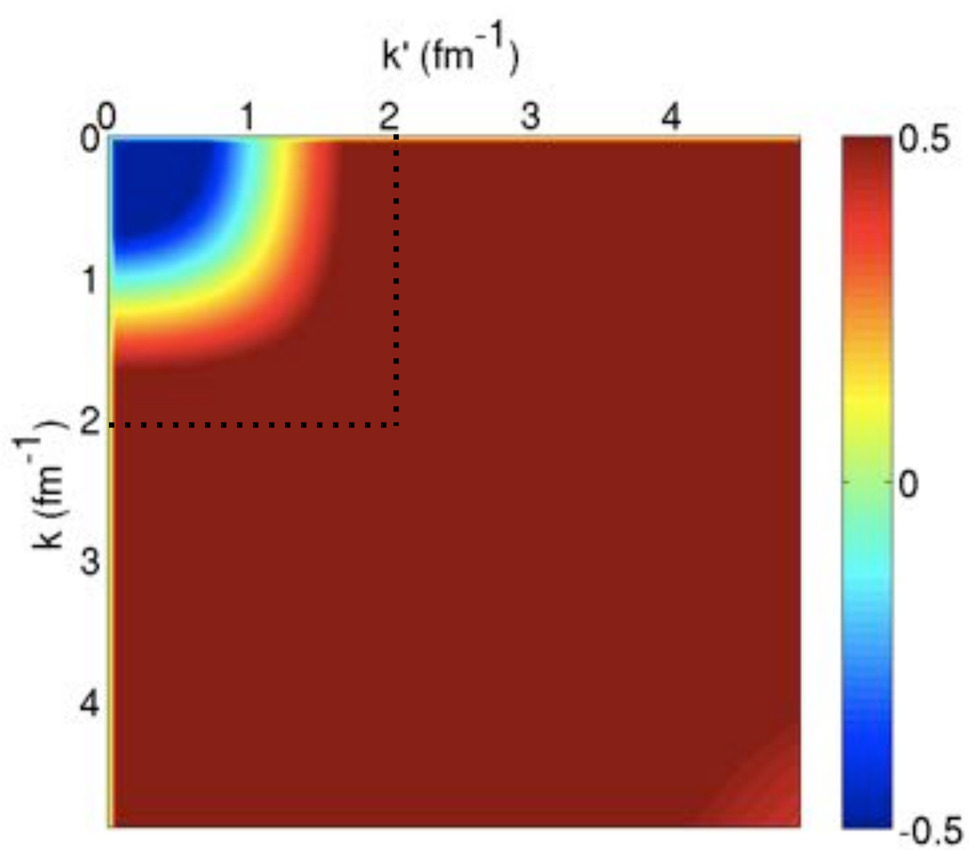

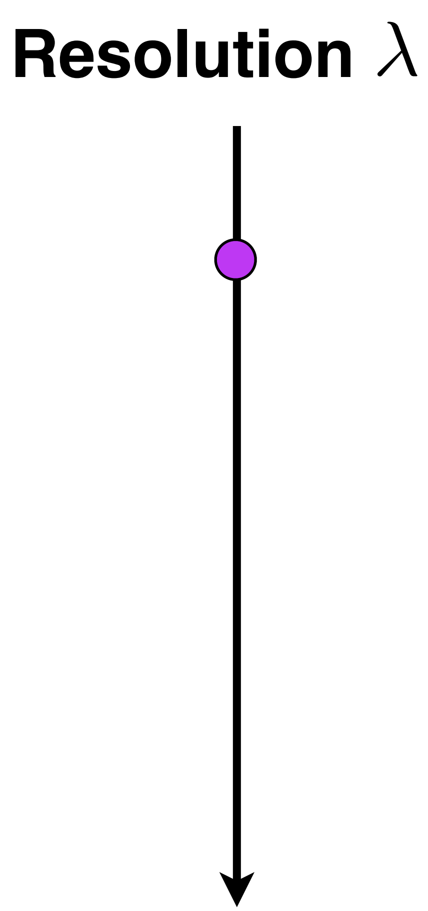

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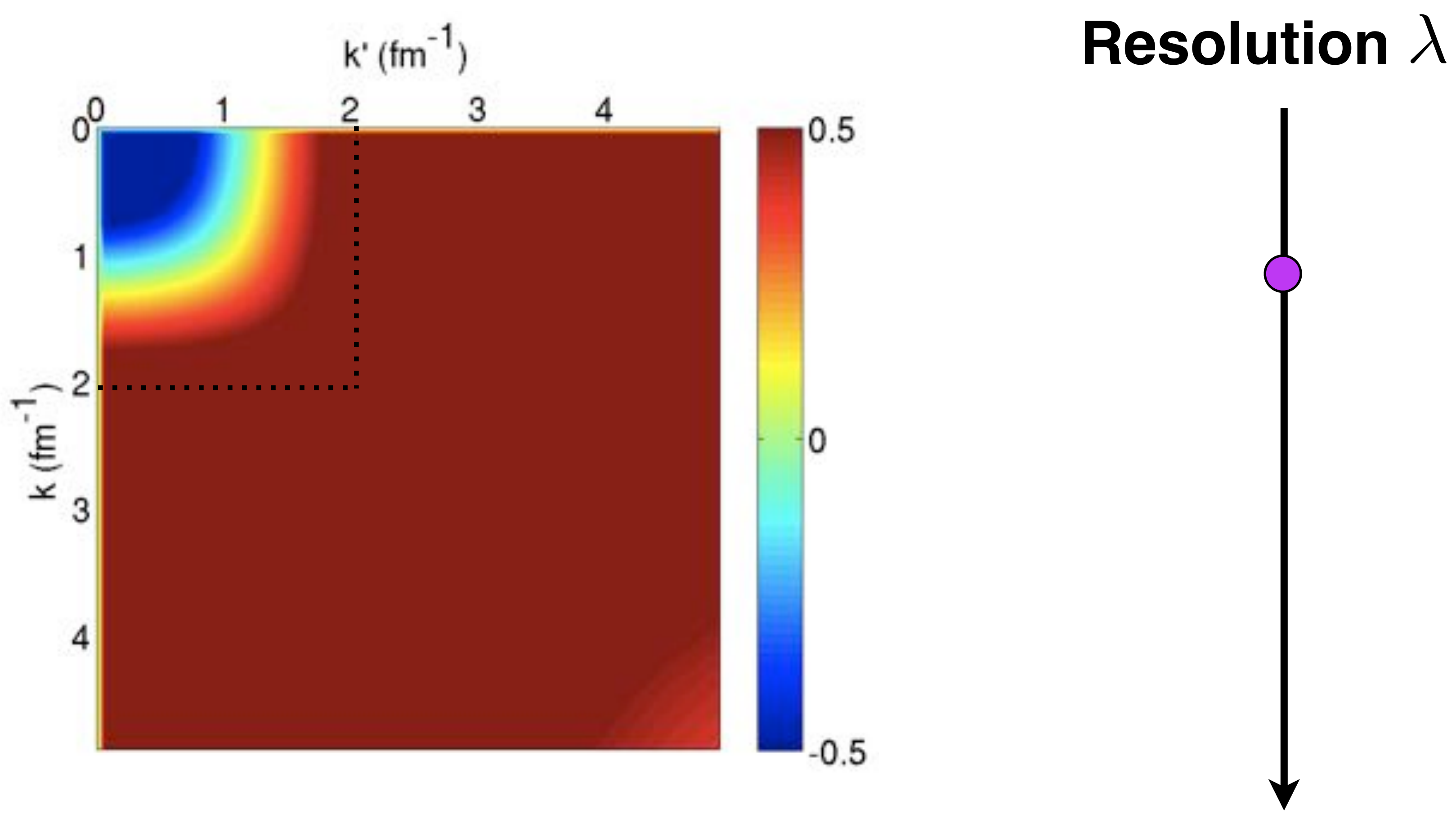

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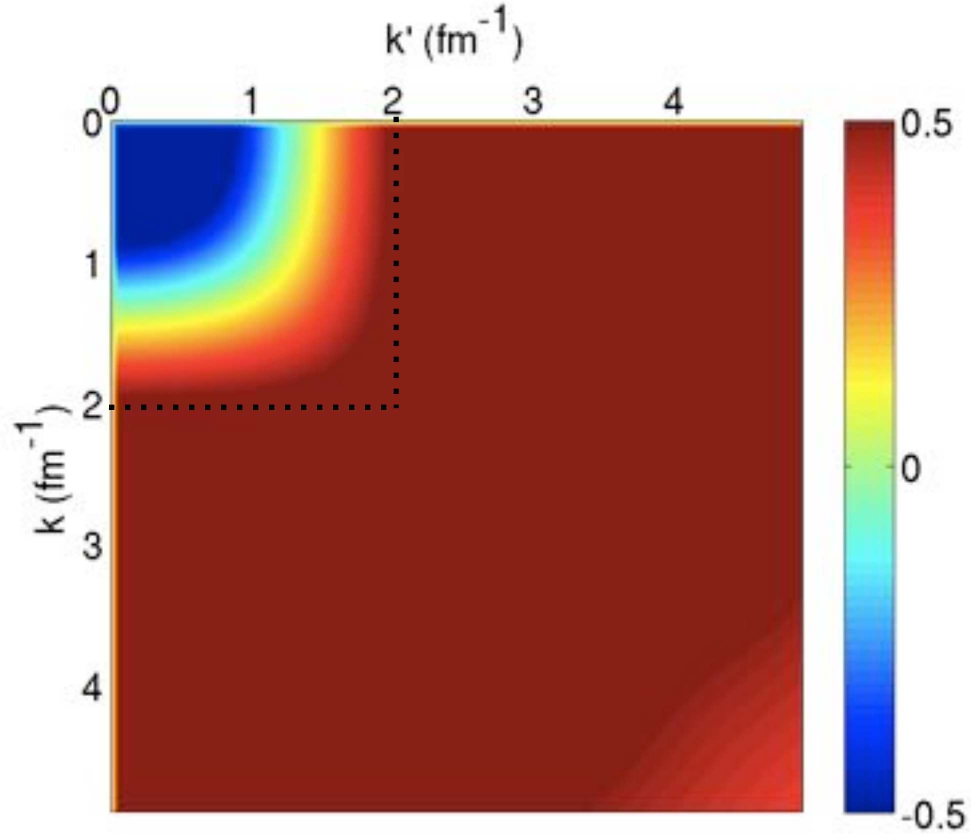

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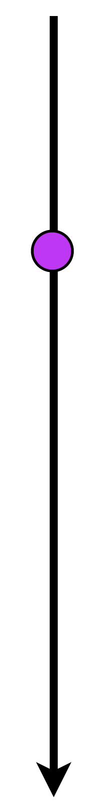

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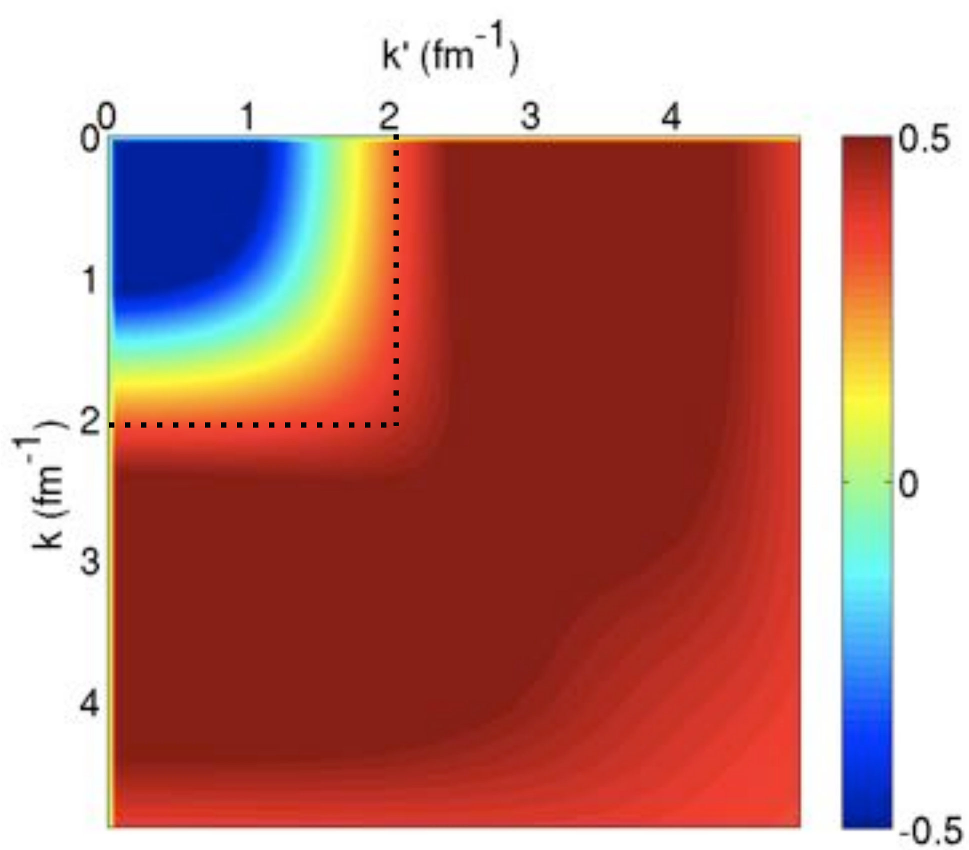

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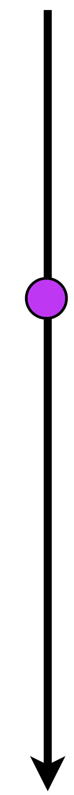

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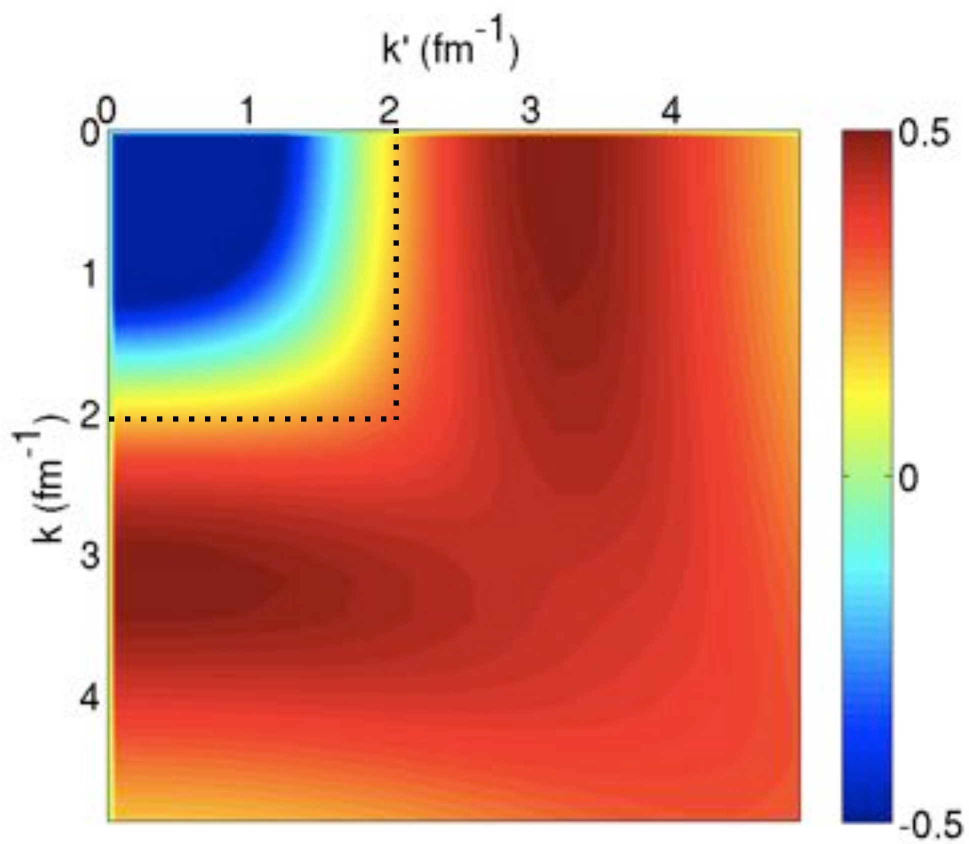

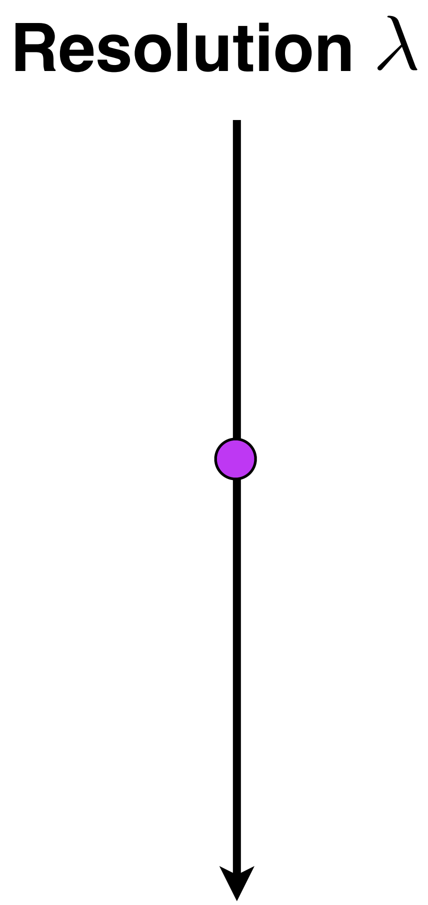

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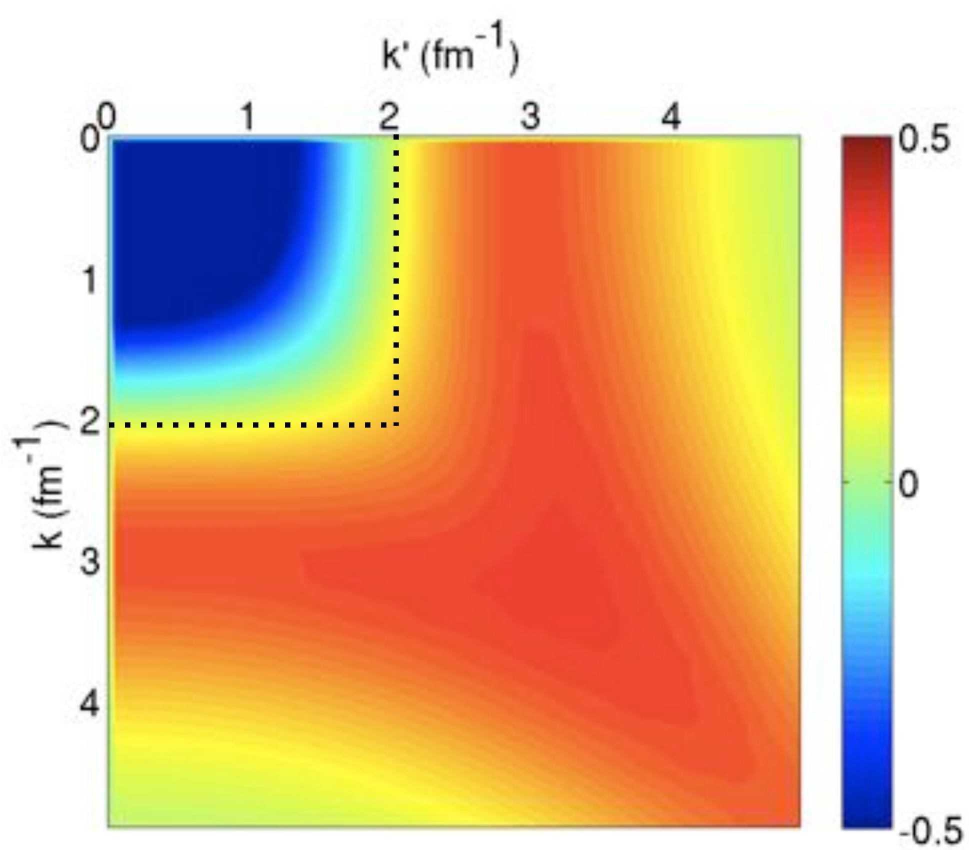

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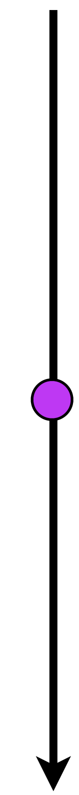

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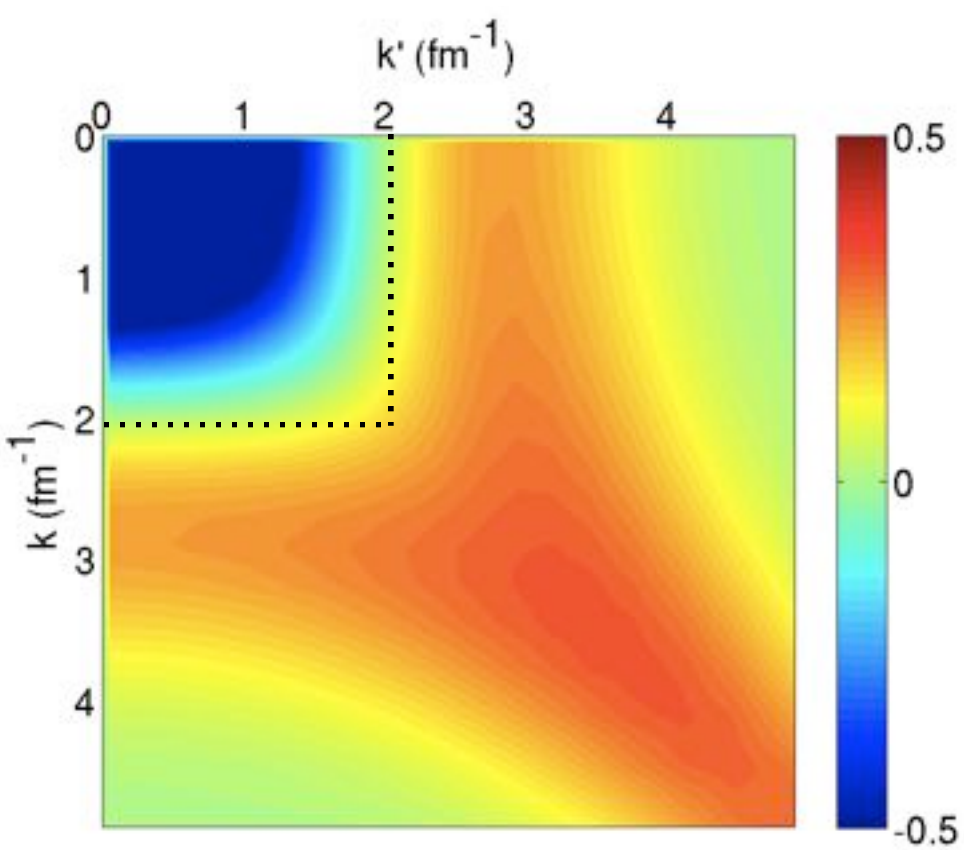

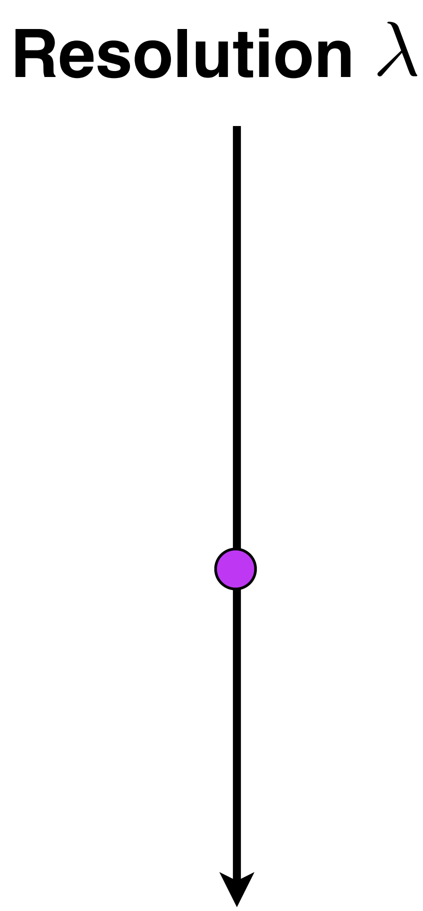

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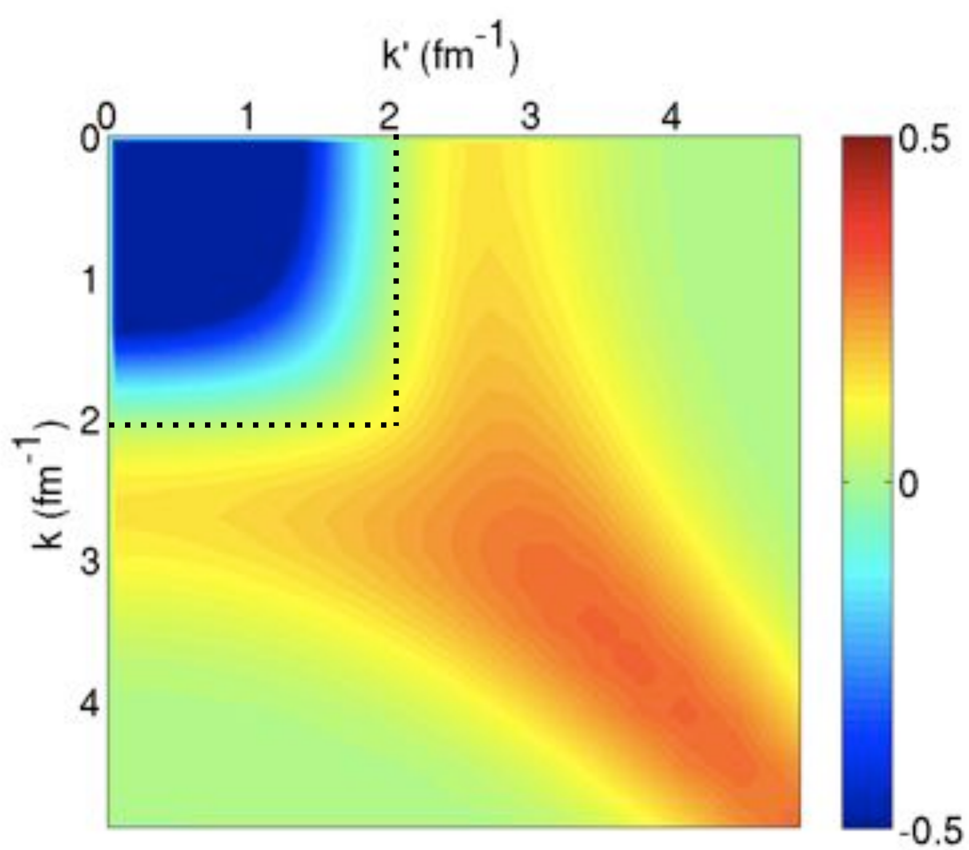

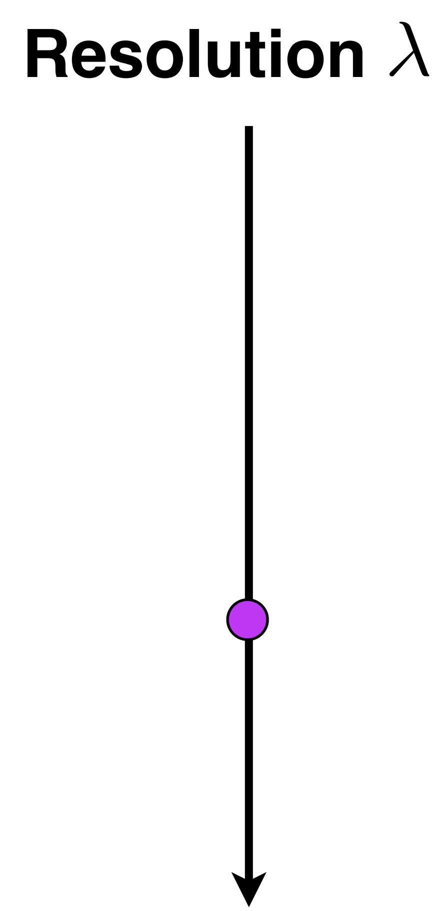

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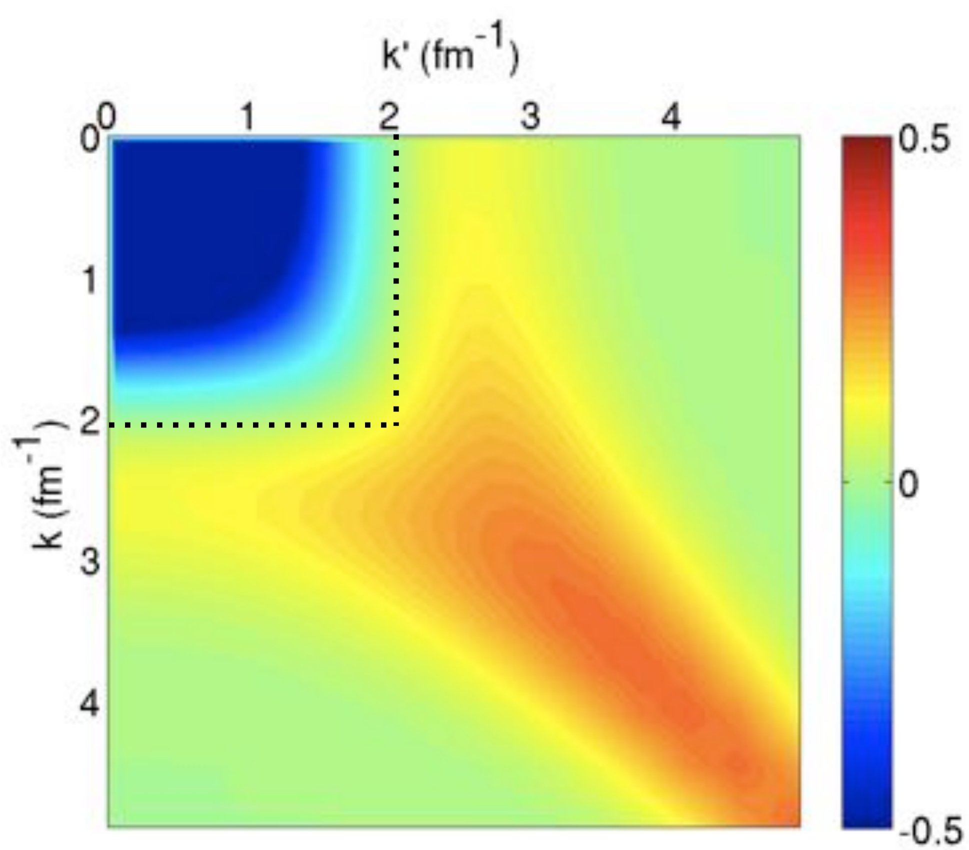

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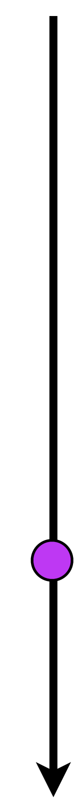

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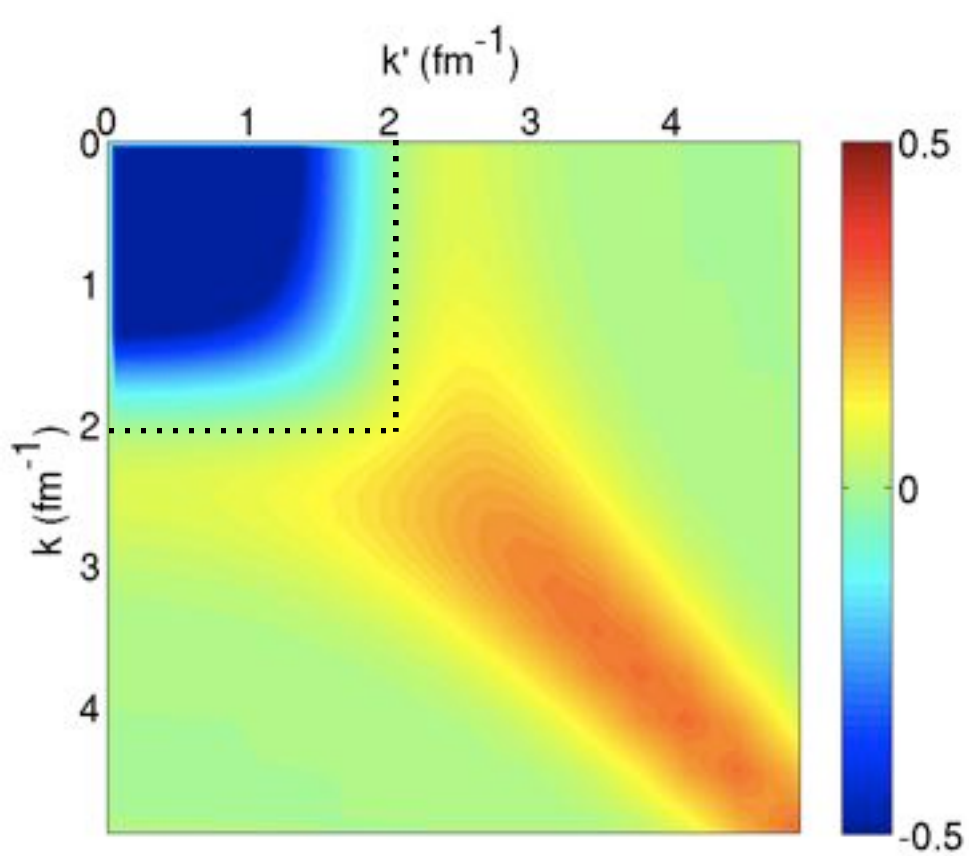

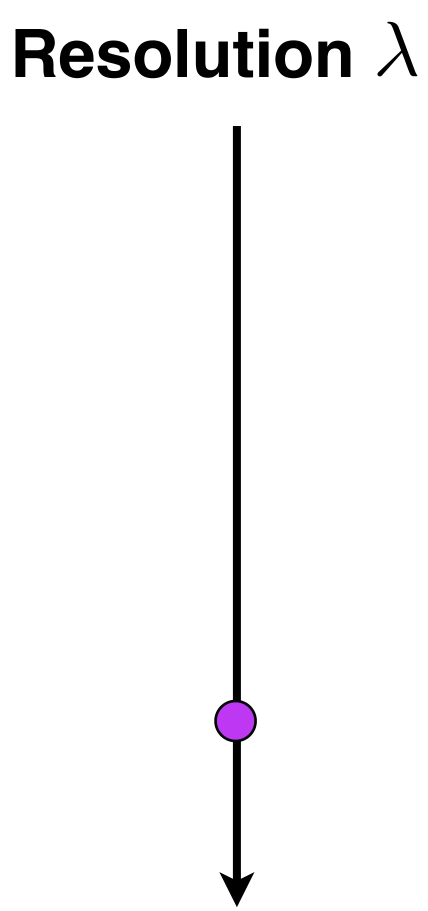

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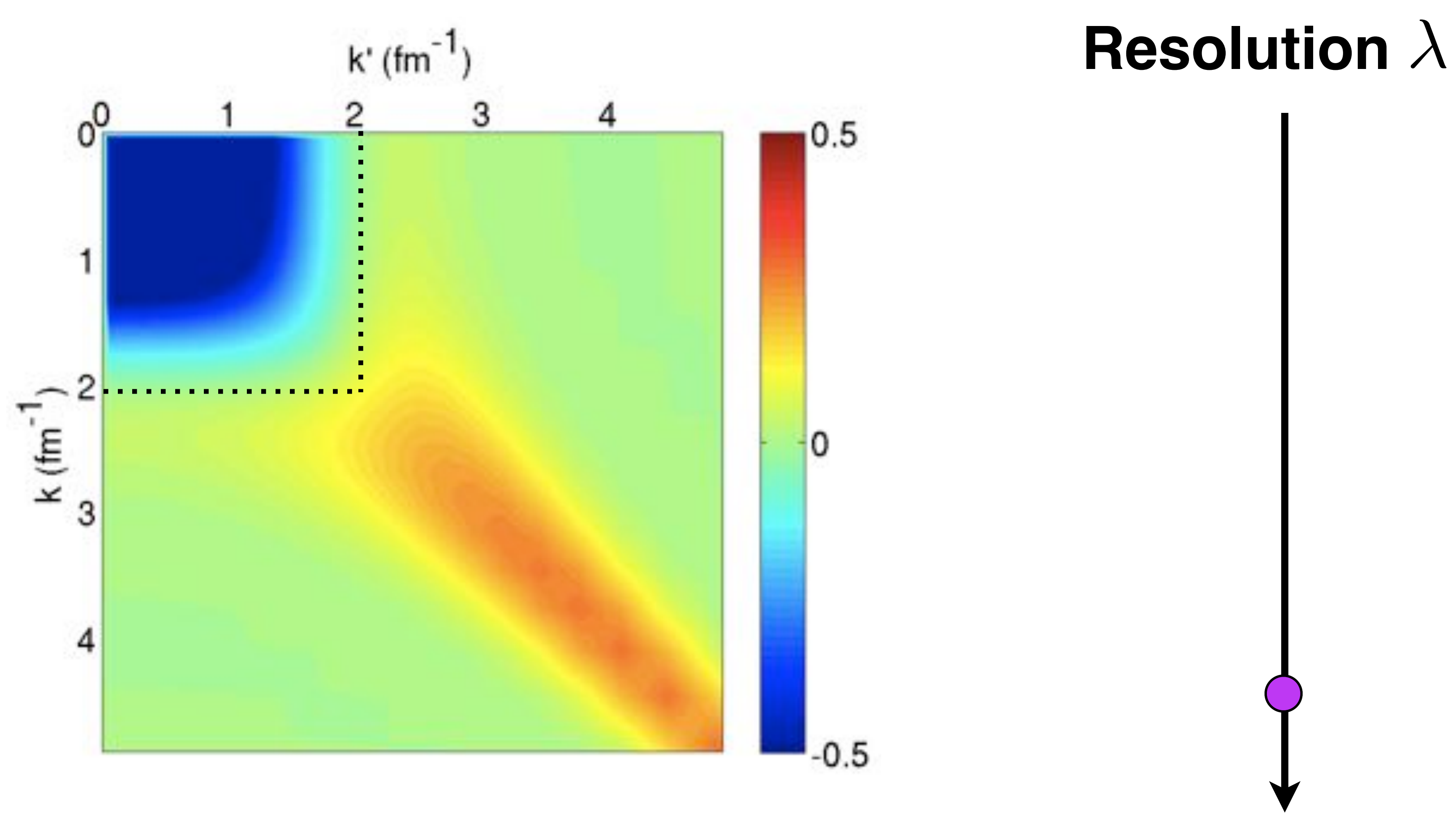

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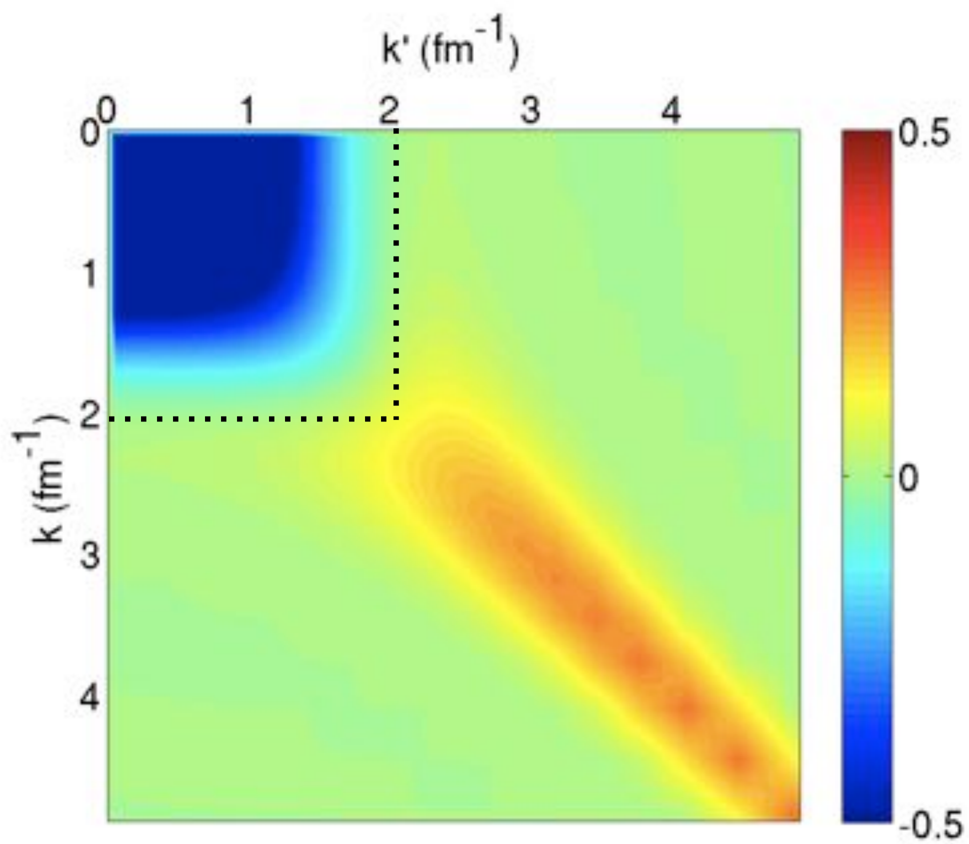
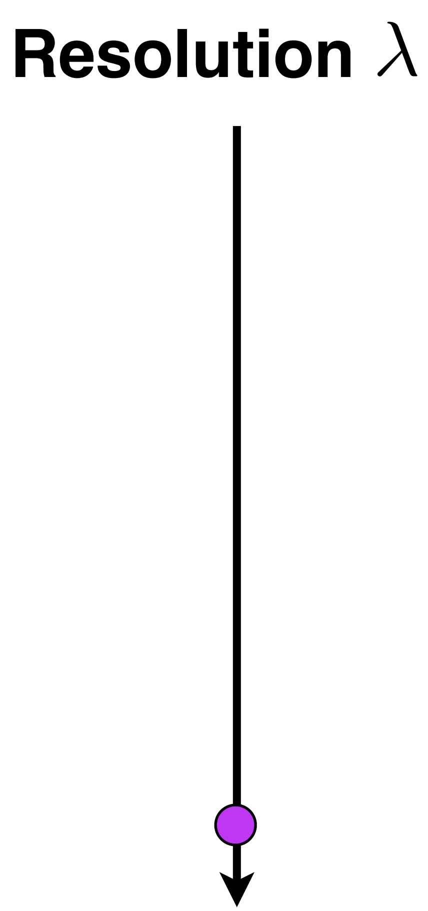
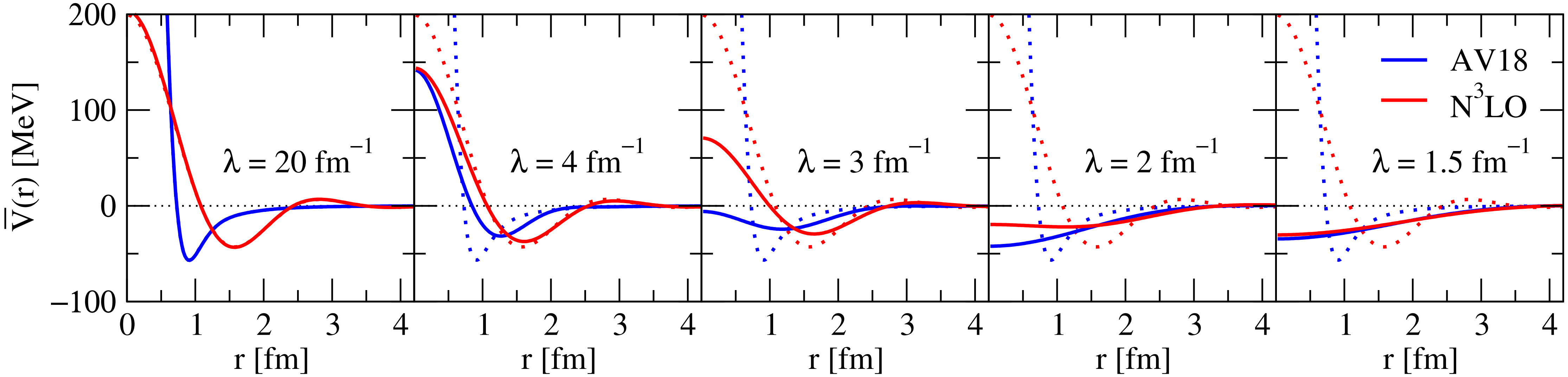
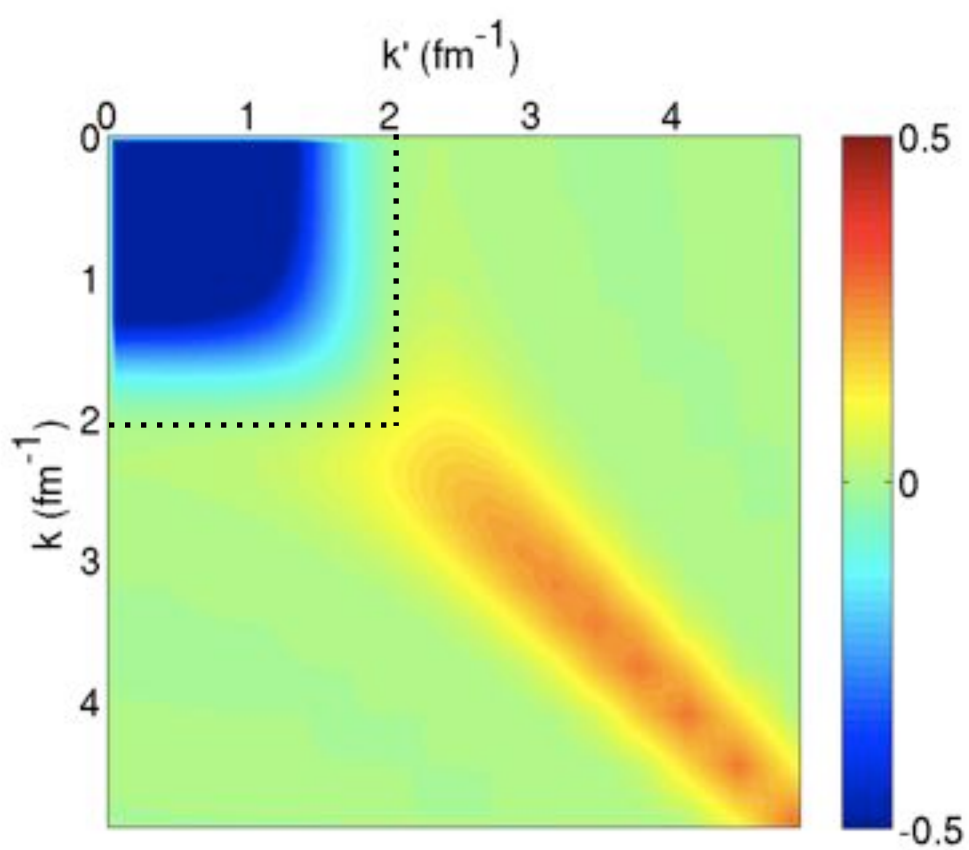


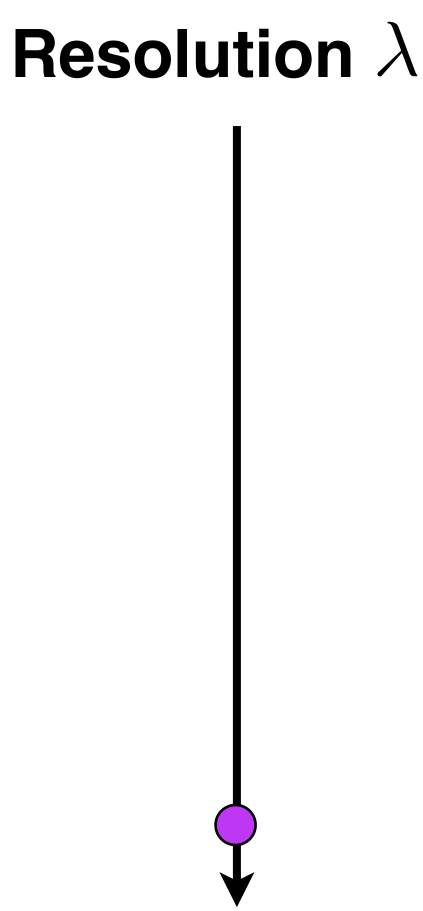


Softening of nuclear interactions: the Similarity Renormalization Group

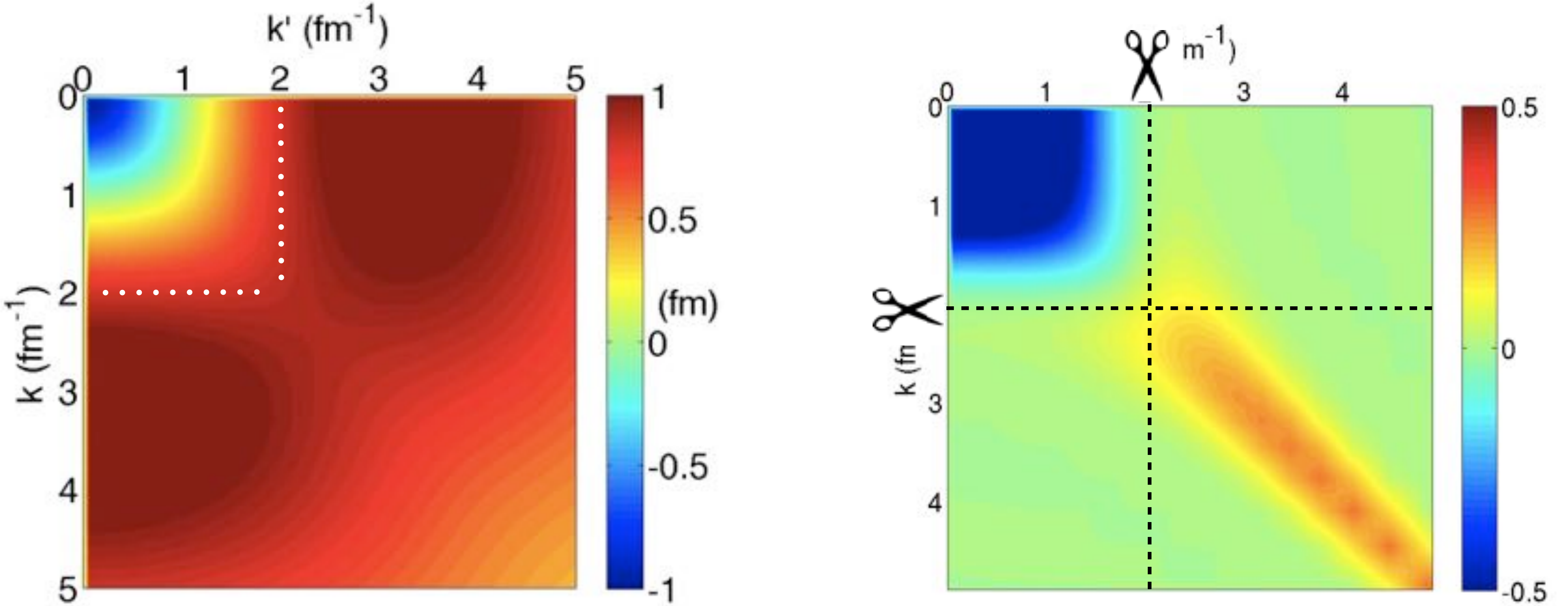


$$\overline{V}_\lambda(r) = \int dr' r'^2 V_\lambda(r, r')$$





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

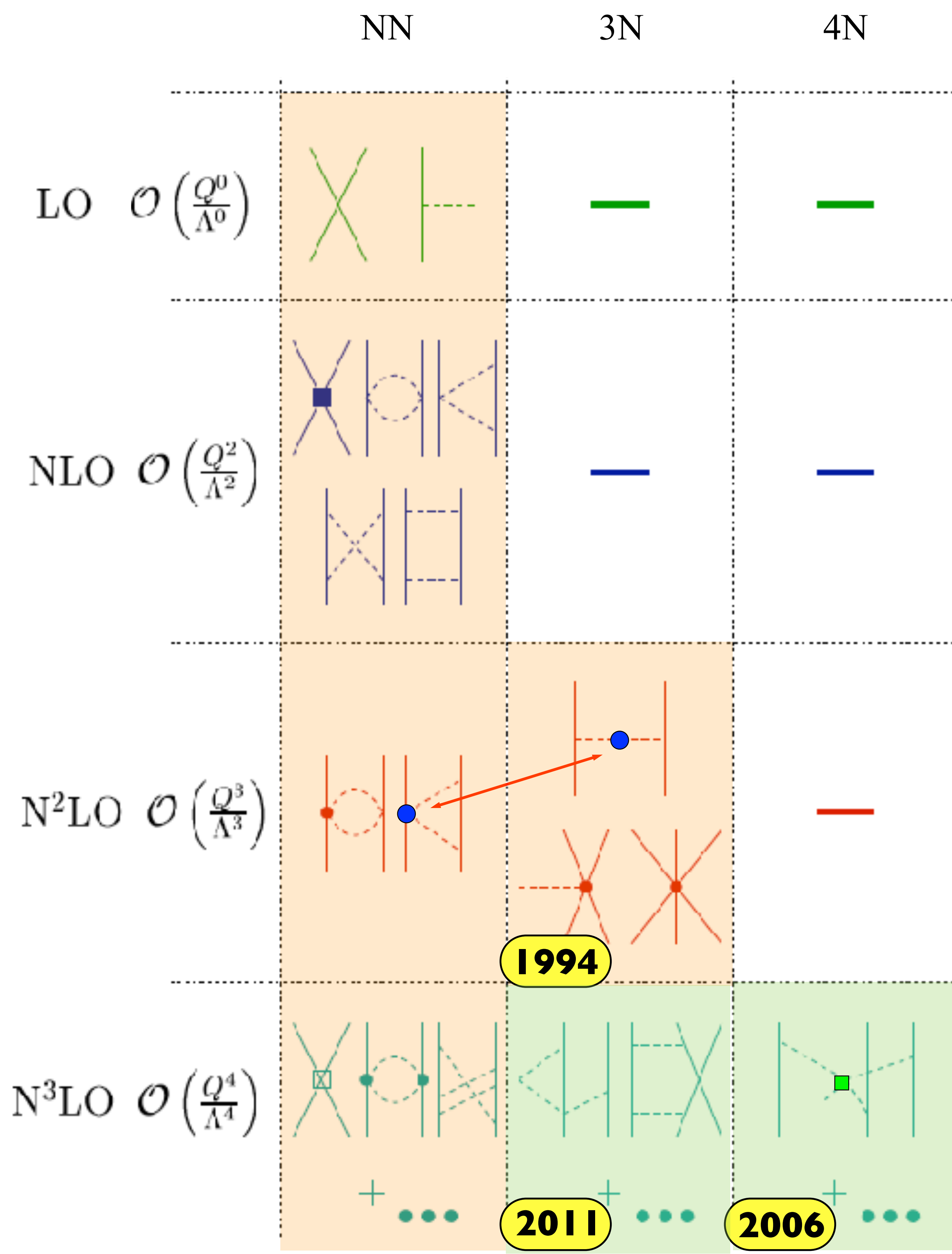


- elimination of coupling between low- and high momentum components,
  $\longrightarrow$ simplified many-body calculations!
- observables unaffected by resolution change (for exact calculations)
- residual resolution dependences can be used as tool to test calculations

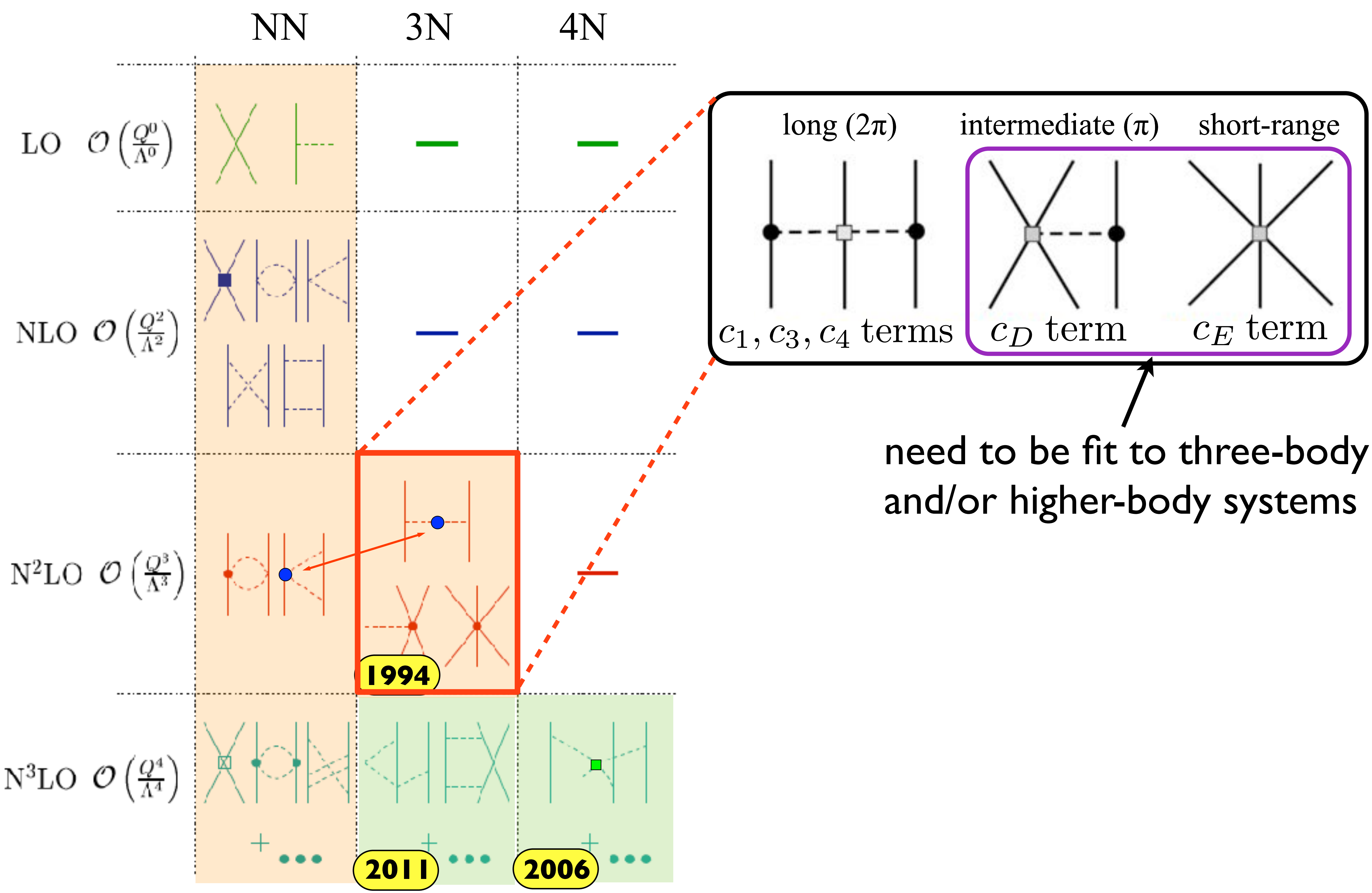
Not the full story:
RG transformations also change three-body (and higher-body) interactions!

Chiral effective field theory for nuclear forces

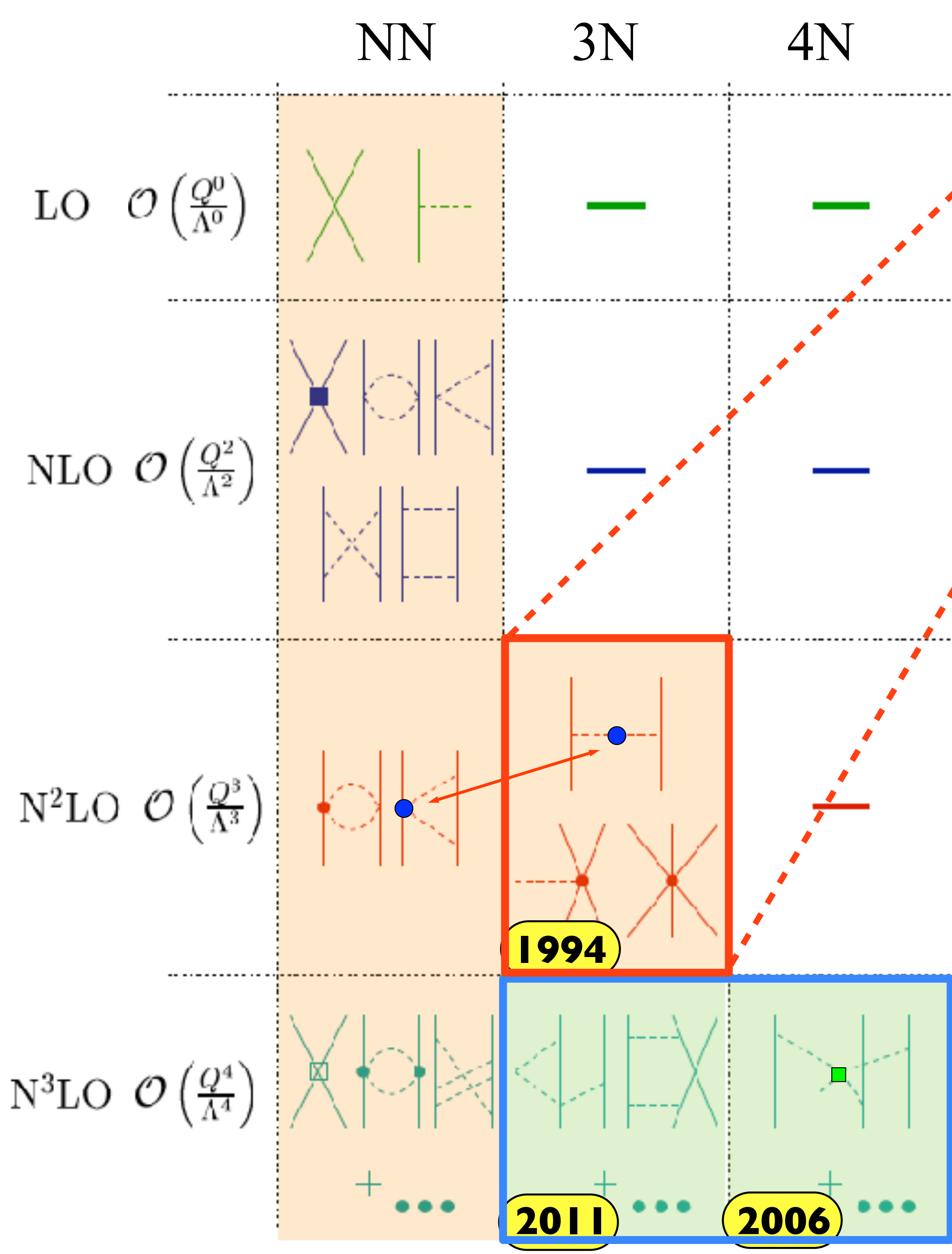
- choose relevant degrees of freedom: here nucleons and pions
- operators constrained by symmetries of QCD
- short-range physics captured in short-range couplings
- separation of scales: $Q << \Lambda_b$, breakdown scale Λ_b~500 MeV
- power-counting: expand in Q/Λ_b
- systematic, obtain error estimates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

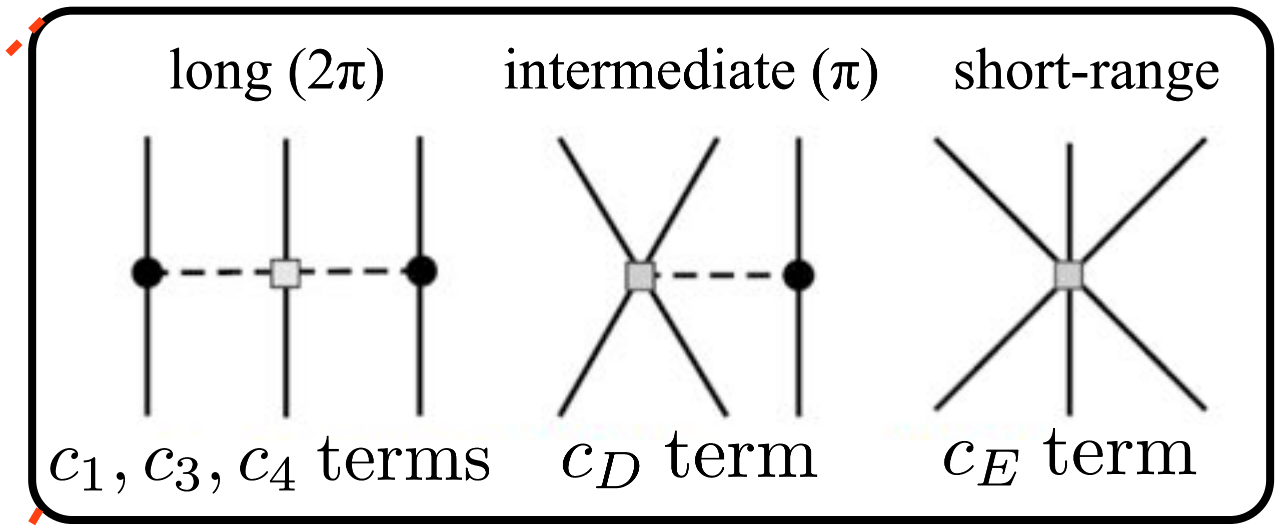


Many-body forces in chiral EFT



Many-body forces in chiral EFT



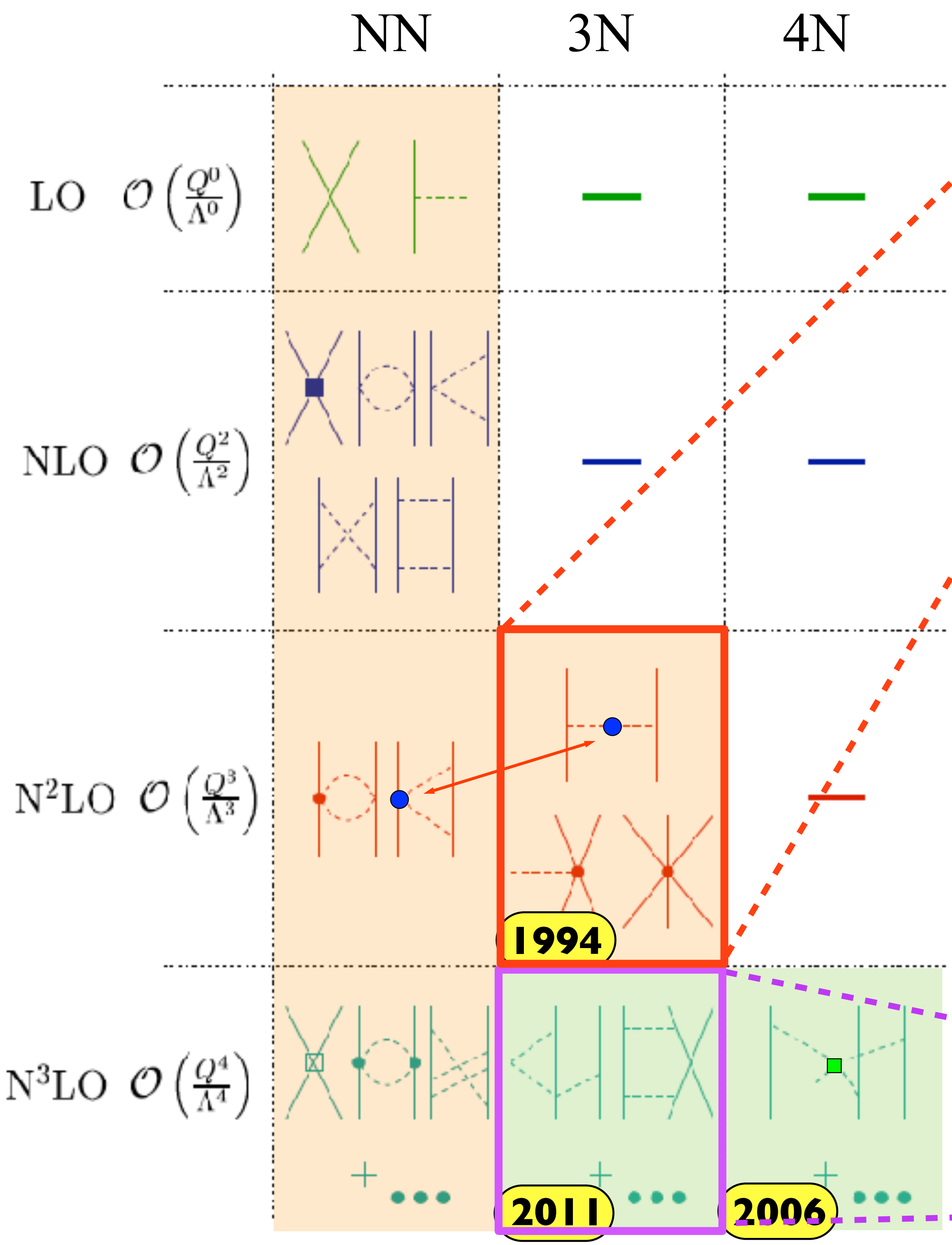


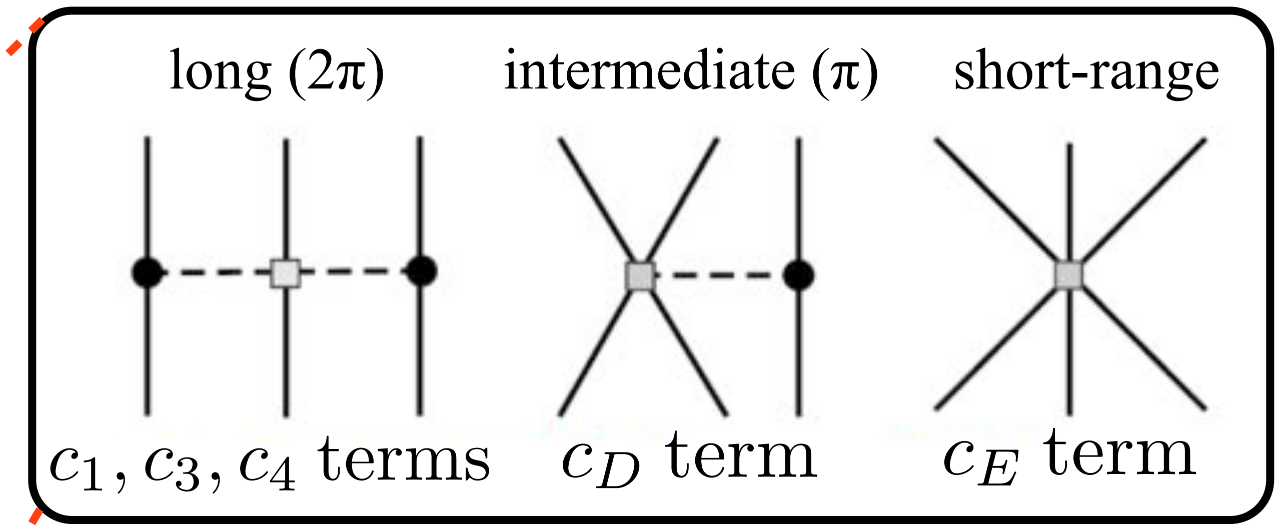
first incorporation in calculations of neutron and nuclear matter

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

all terms predicted
(no new low-energy couplings)

Many-body forces in chiral EFT





first incorporation in calculations of neutron and nuclear matter

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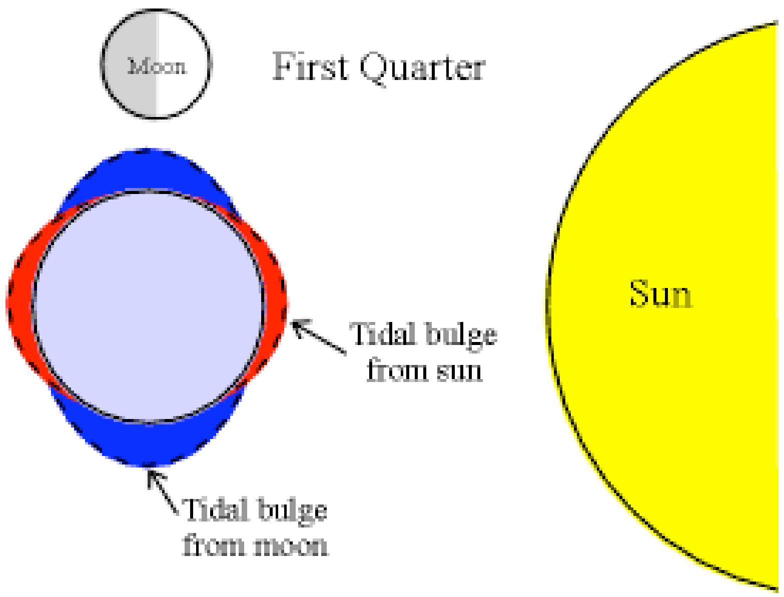
Krüger, Tews, KH, Schwenk, PRC 88, 025802 (2013)

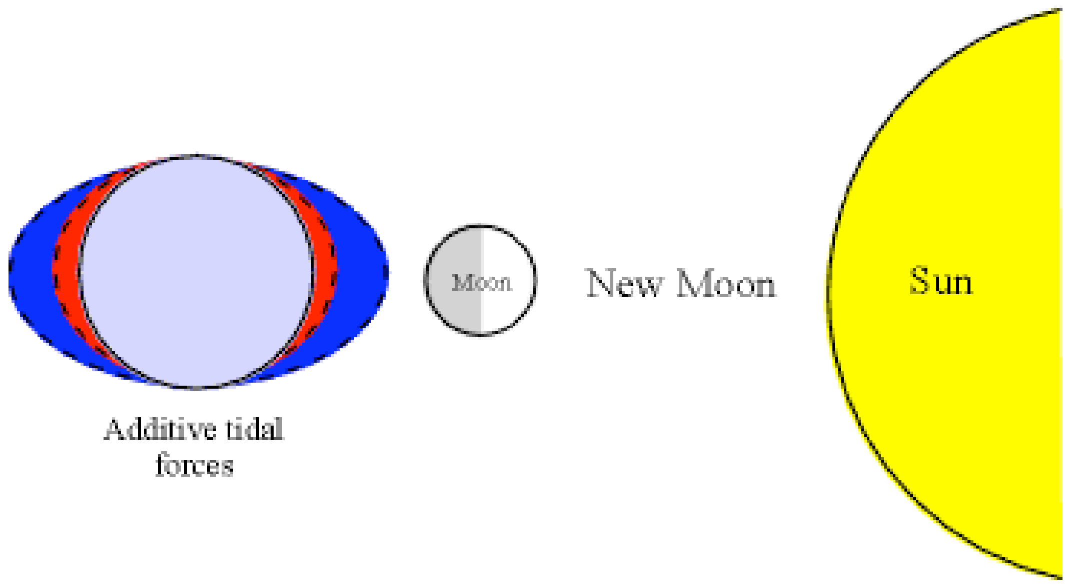
first calculation of matrix elements for ab initio studies of matter and nuclei

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

Aren't 3N forces unnatural? Do we really need them?

Consider classical analog: tidal effects in earth-sun-moon system





- force between earth and moon depends on the position of sun
- tidal deformations represent internal excitations
- describe system using point particles $\longrightarrow$ 3N forces inevitable!

- nucleons are composite particles, can also be excited
- change of resolution change excitations that can be described explicitly
  - existence of three-nucleon forces natural
  - crucial question: how important are their contributions?

Development of nuclear interactions