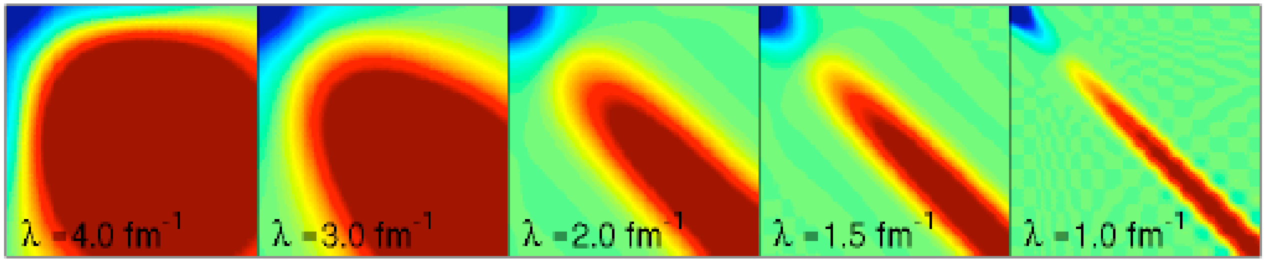


Microscopically Based Energy Functionals

S.K. Bogner (NSCL/MSU)

MICHIGAN STATE UNIVERSITY

NSCL

SciDAC
Scientific Discovery through Advanced Computing

Dream Scenario: From QCD to Nuclei

Microscopic DFT

MB Methods ↑ + DME

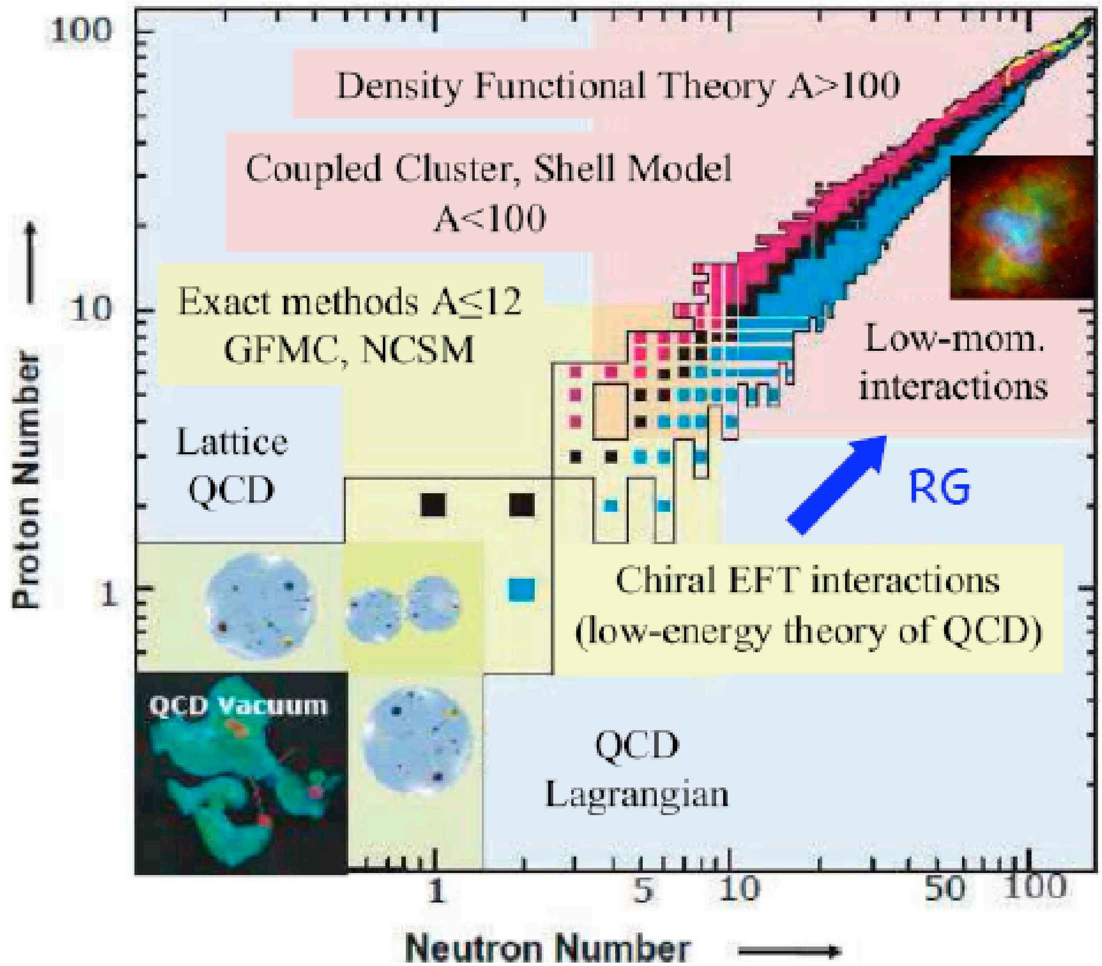
V_{lowk}
(2,3…N interactions)

RG evolution ↑

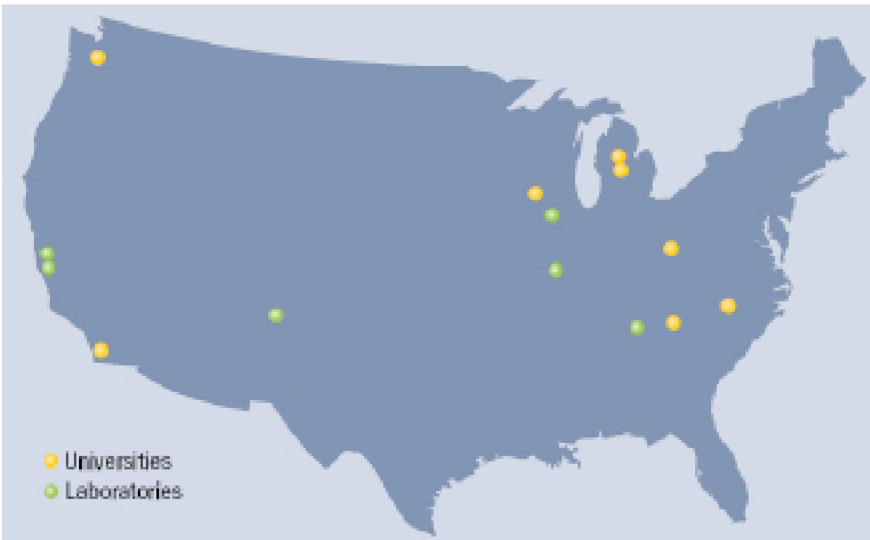
Chiral EFT
(NN…N interactions)

LEC's ↑ for L_{EFT}

Lattice QCD



SciDAC 2 Project *Building a Universal Nuclear Energy Density Functional*

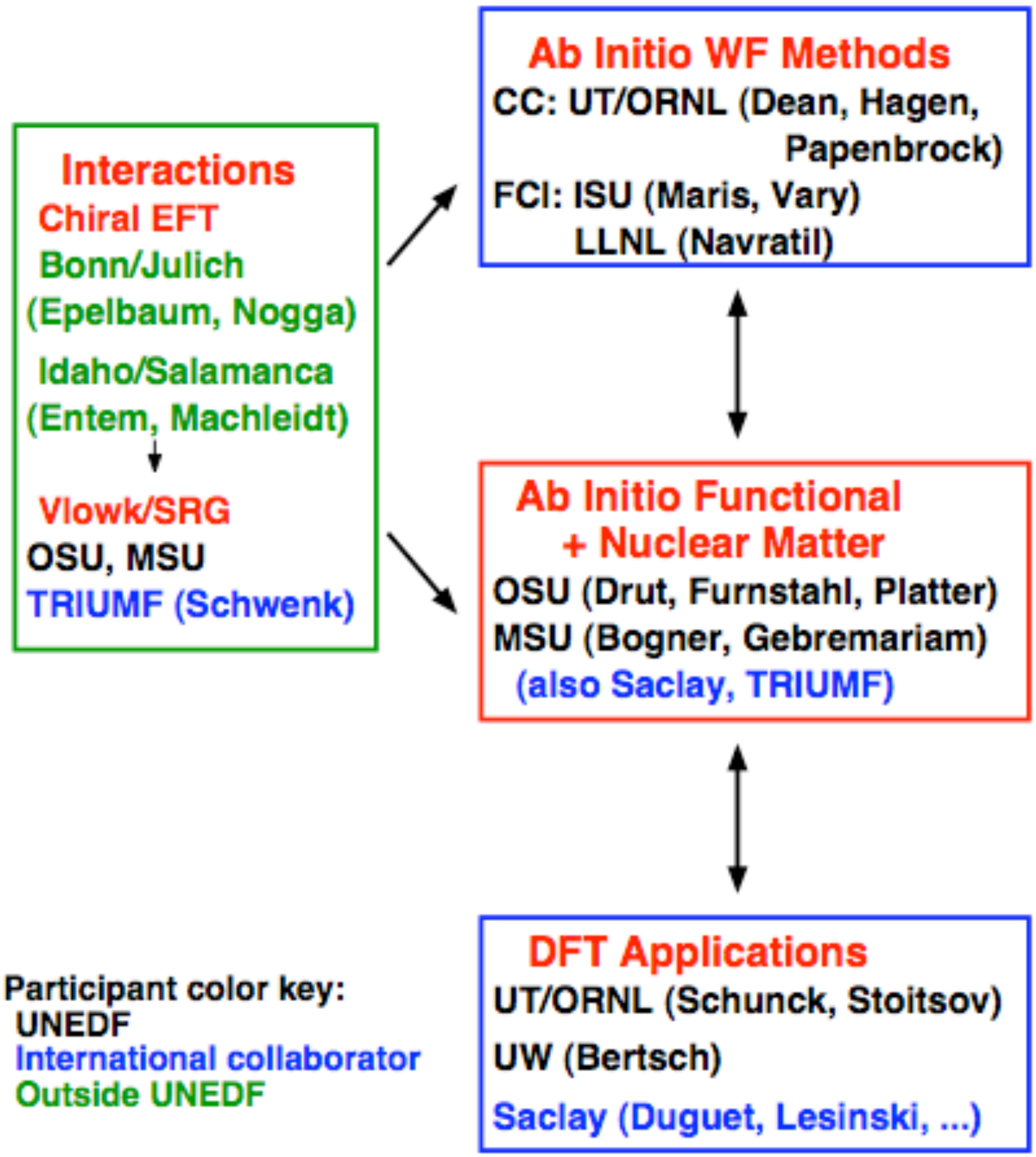


See http://undef.org for details

UNEDF Project Goals

- Understand nuclear properties *"for element formation, for properties of stars, and for present and future energy and defense applications."*
- Scope is *all* nuclei
  ==> DFT the method of choice
- Order of magnitude improvement over present capabilities
  ==> precision calculations of, e.g., masses
- Utilize the ***best available microscopic physics***
  ==> chiral EFT NN and NNN interactions, ab-initio MBT
- Maximize predictive power will *well-quantified theoretical uncertainties*

Years 2 & 3: Personnel, Tasks, and Interconnections



Years 2 & 3: Personnel, Tasks, and Interconnections

Interactions
Chiral EFT
Bonn/Julich
(Epelbaum, Nogga)
Idaho/Salamanca
(Entem, Machleidt)
Vlowk/SRG
OSU, MSU
TRIUMF (Schwenk)

N3LO 3NF
Explicit Delta's

New 3NF fits

SRG 3NF evolution

Participant color key:
UNEDF
International collaborator
Outside UNEDF

Ab Initio WF Methods
CC: UT/ORNL (Dean, Hagen, Papenbrock)
FCI: ISU (Maris, Vary)
LLNL (Navratil)

Wider range of nuclei
Full 3NF
Ab Initio densities
External potentials

Tests of DME: energies, densities with same H
Vary 3NF, external potential parameters
Cutoff dependence as diagnostic

Ab Initio Functional + Nuclear Matter
OSU (Drut, Furnstahl, Platter)
MSU (Bogner, Gebremariam)
(also Saclay, TRIUMF)

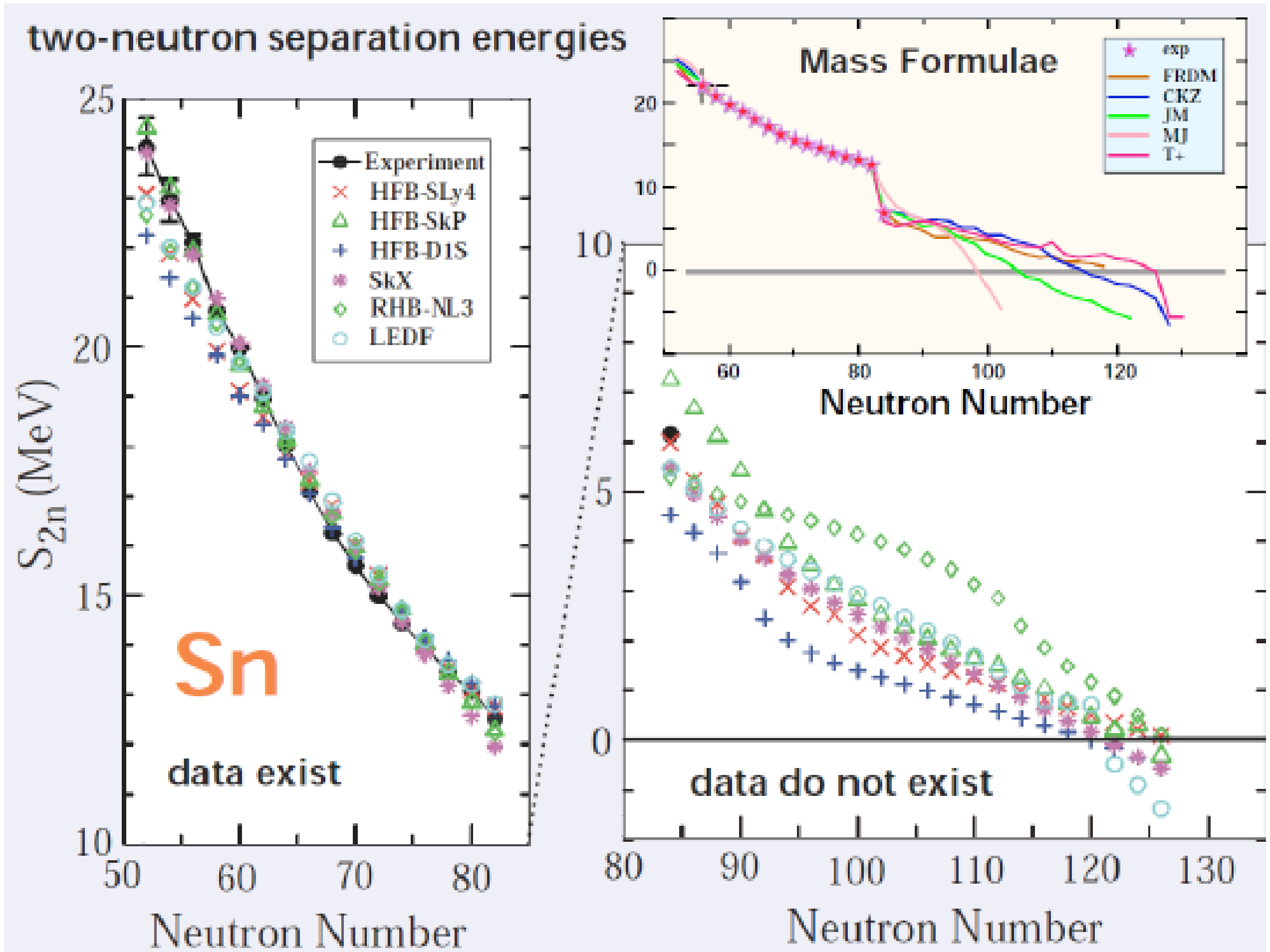
Tests of nuclear matter:
new fits, self–energies, ...
Improved 3NF for DME
Generalized DME
DFT from OPM

Long–range pion contributions
from NN and NNN DME
plus fit residual Skyrme in HFB code

DFT Applications
UT/ORNL (Schunck, Stoitsov)
UW (Bertsch)
Saclay (Duguet, Lesinski, ...)

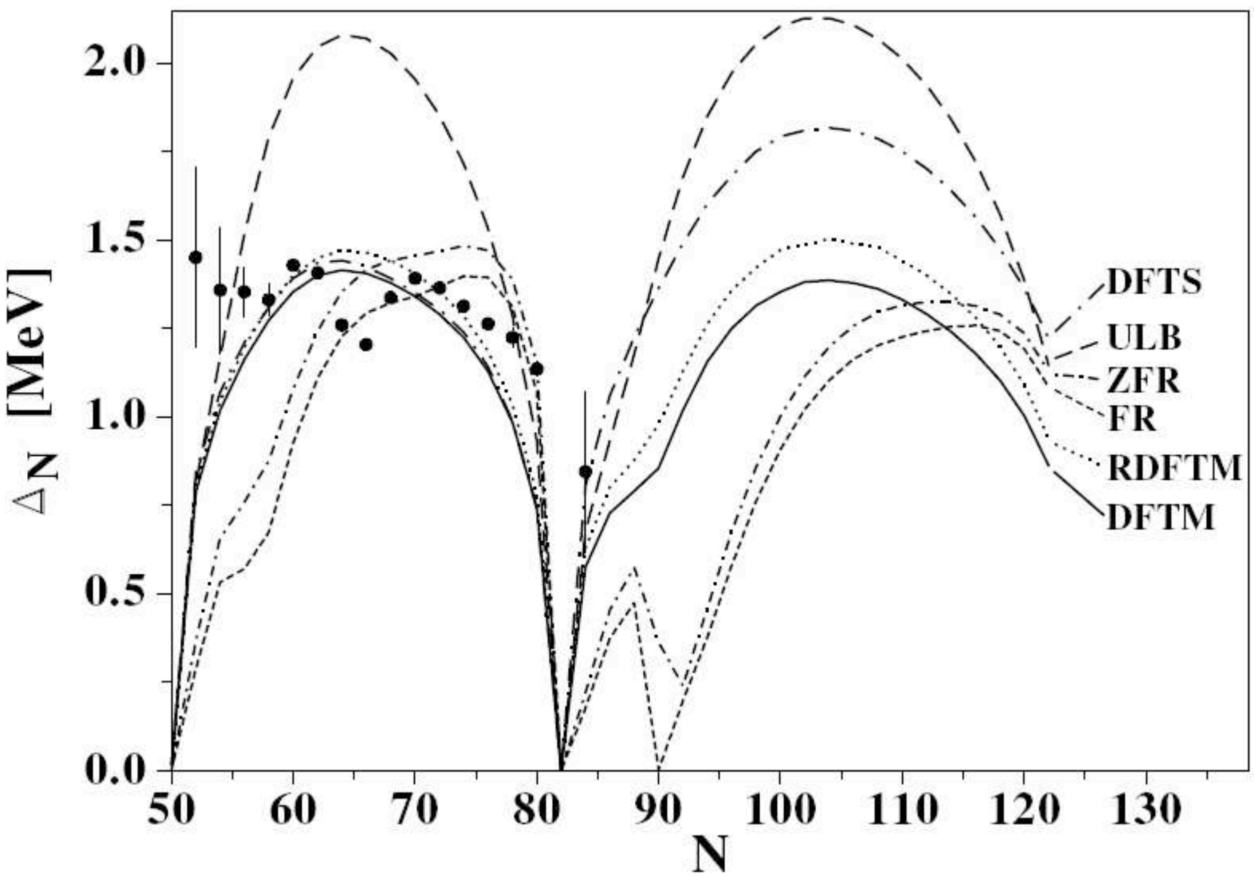
Systematics along
isotope chains
Tests: spin–orbit splittings,
time–odd terms, ...
Non–empirical pairing functional

Limitations of Existing Energy Functionals (Predictability)



- Uncontrolled extrapolations towards the drip-line
- Theoretical error-bars?

Limitations of Existing Energy Functionals (Predictability)



- Pairing gaps not under control for increasing (N-Z)

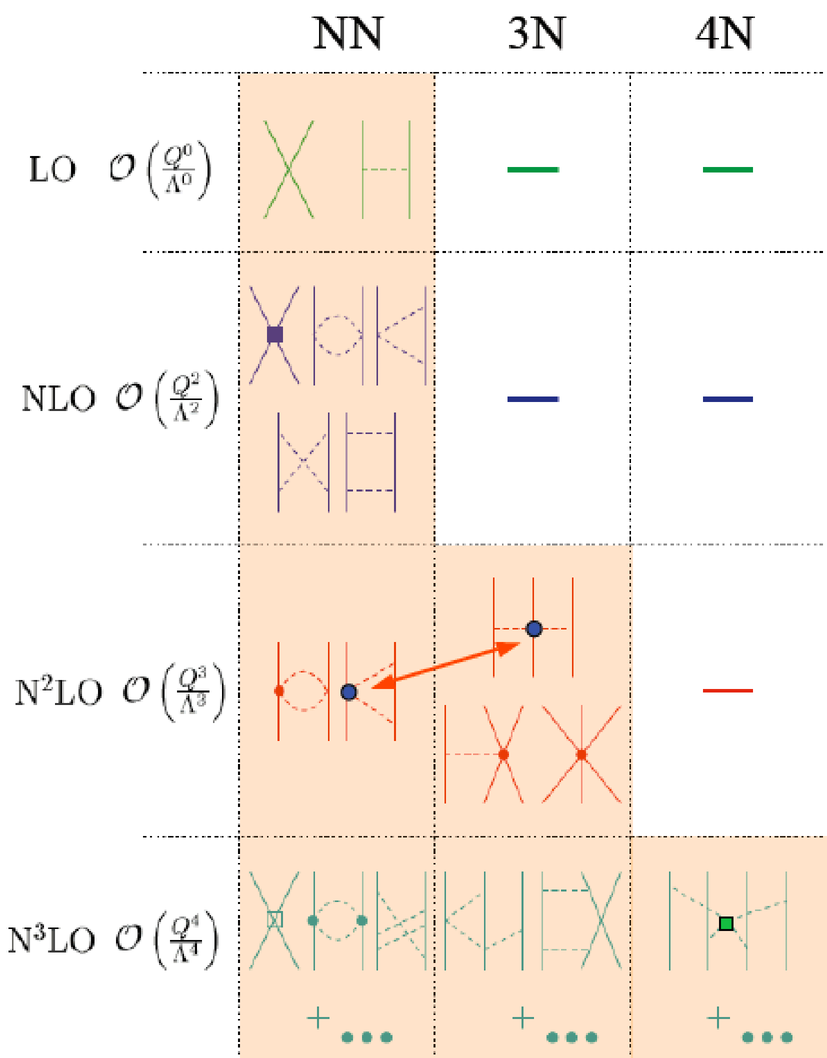
What's missing in phenomenological EDF's

- Density dependencies might be too simplistic
- Isovector components not well constrained
- No systematic organization of terms in the EDF
- No way to estimate theoretical uncertainties
- Over-determined parameters
- What's the connection to many-body forces?
- Pairing part of the EDF not treated on same footing

Turn to microscopic many body theory for guidance

Nuclear forces from Chiral EFT

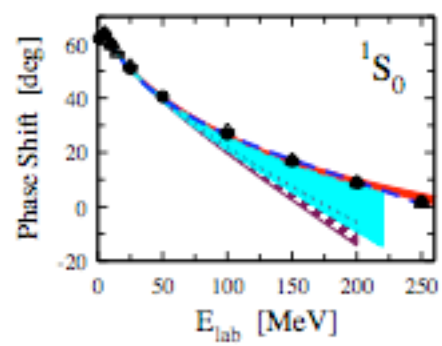
Separation of scales: low momenta Q << Λ_b breakdown scale

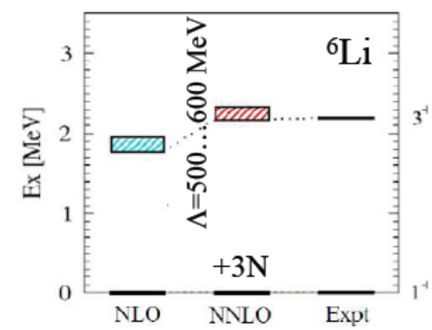


- Explains empirical hierarchy
  NN > 3N > 4N

- Formal Consistency
  NN and NNN forces
  ππ and πN, electroweak operators
  QCD, systematic expansion

- Error estimates from truncation order, lower bound from Λ variation





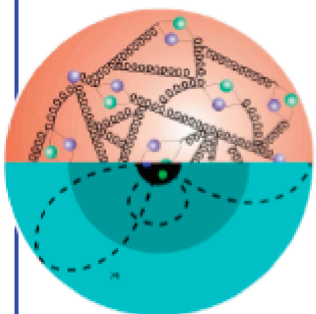
from A. Nogga

Weinberg, van Kolck, Epelbaum, Meissner, Machleidt, …

Λ / Resolution dependence of nuclear interactions

with high-energy probes:
quarks+gluons

cf. scale/scheme dependence
of parton distribution functions

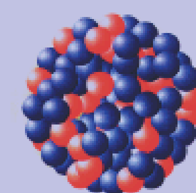


Lattice QCD

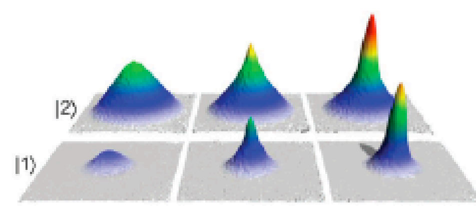
Effective theory for NN, many-N interactions,
operators depend on resolution scale Λ

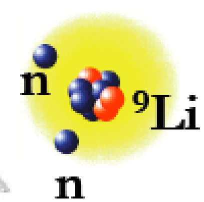
$$H(\Lambda) = T + V_{\rm NN}(\Lambda) + V_{\rm 3N}(\Lambda) + V_{\rm 4N}(\Lambda) + \ldots$$

$\Lambda_{\rm chiral}$
momenta $Q \sim \lambda^{-1} \sim m_\pi$: chiral effective field theory
nucleons interacting via pion exchanges + contact interactions
typical Fermi momenta in nuclei $\sim m_\pi$



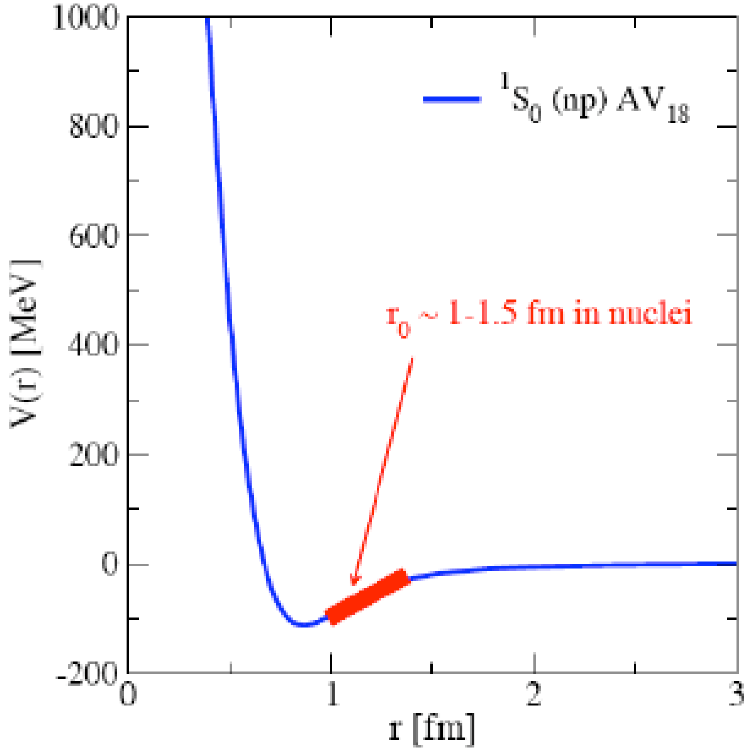
$\Lambda_{\rm pionless}$
$Q \ll m_\pi$=140 MeV: pion not resolved
pionless effective field theory
large scattering lengths + corrections
applicable to loosely-bound, dilute systems, reactions at astro energies

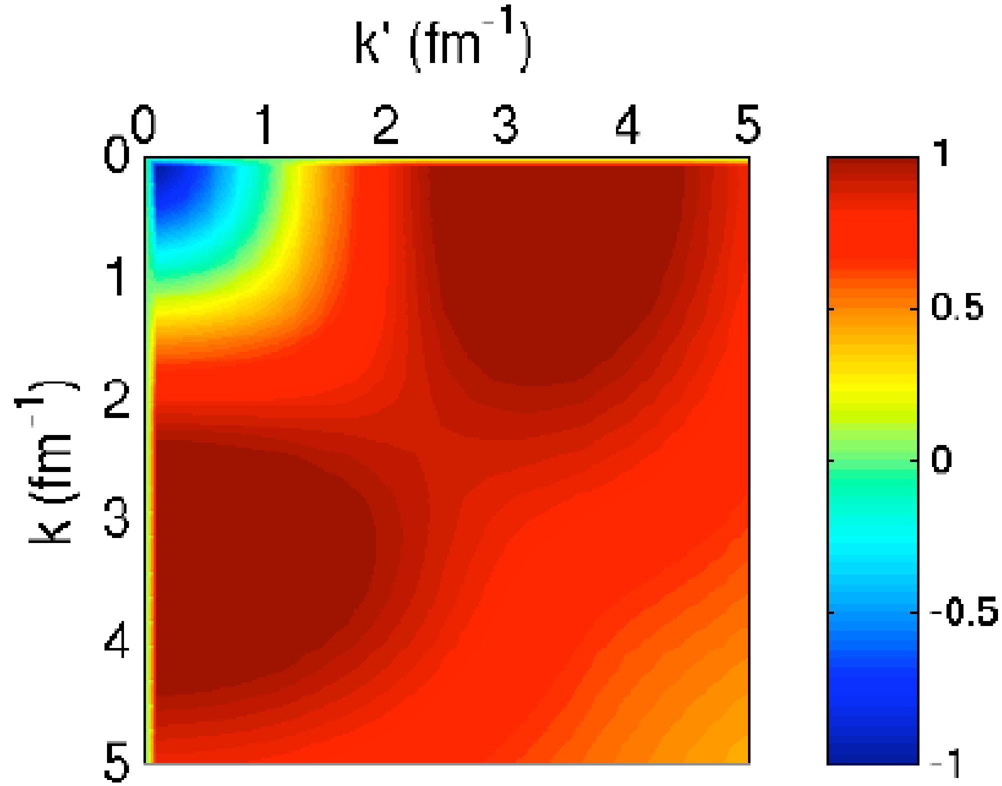




Freedom to vary the resolution via RG to simplify certain features…

"Scheme-Dependent" Sources of Non-perturbative Physics





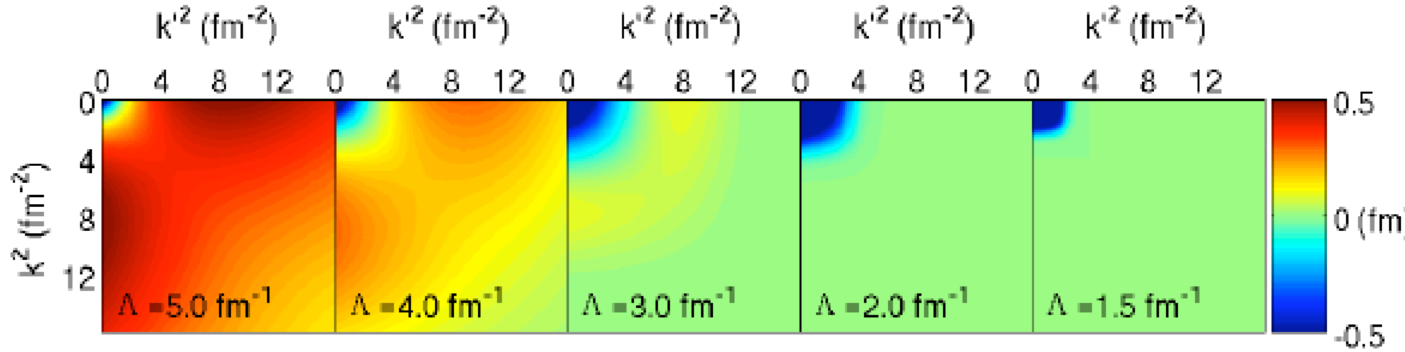
- short-ranged repulsive core
- strong tensor force

→ Strong coupling to high-momentum modes

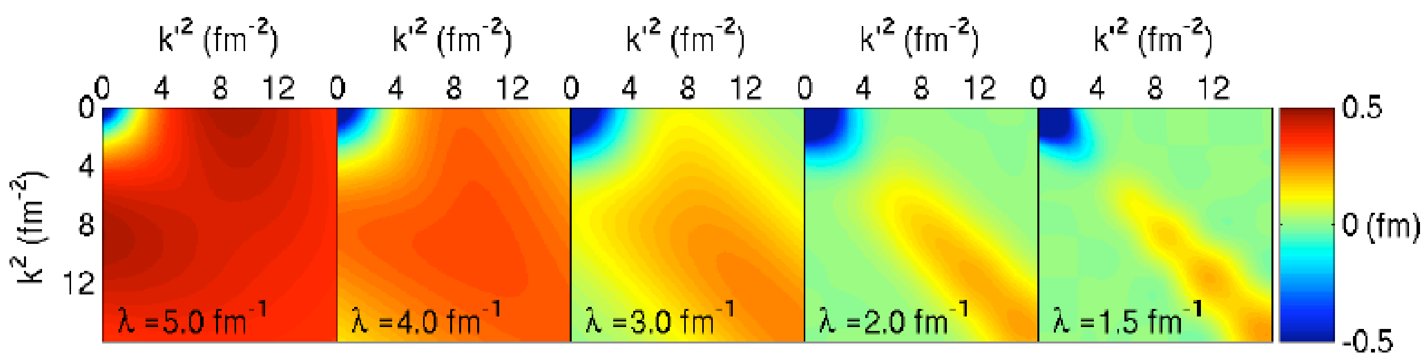
BUT typical momentum in a large nucleus only ≈ 1 fm^{-1} (200 MeV)!

2 Types of Renormalization Group Transformations

- "$V_{low\ k}$" => lowers a cutoff Λ in k',k

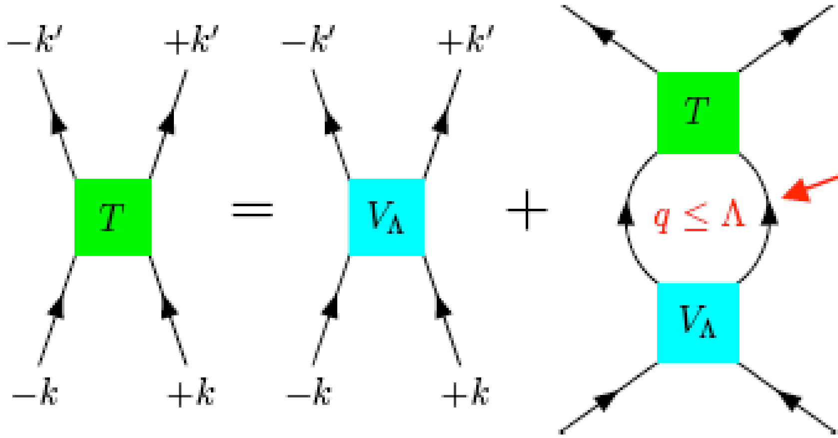


- SRG => drives H towards the diagonal (λ = width about diagonal)



Both decouple the high momentum modes ***leaving low E NN observables unchanged***.

Integrating out high-momentum modes ("$V_{\text{low k}}$")



UV cutoff Λ

- Demand $\frac{d}{d\Lambda} T = 0$

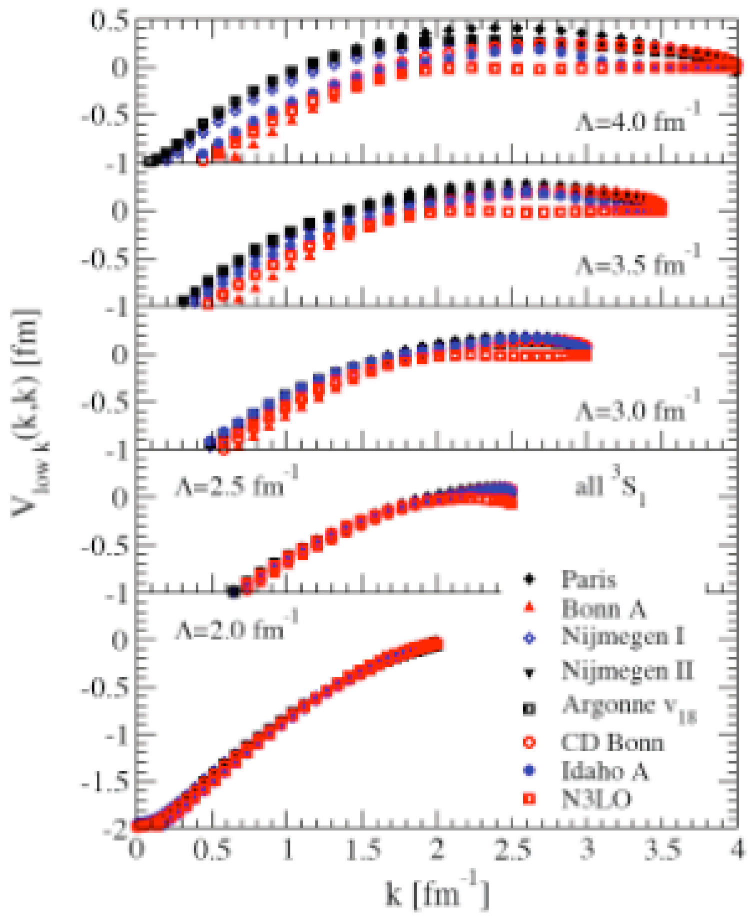
  => RGE's for "running" of V_Λ w/Λ

- Integrate RGE's to smaller Λ

  => decouples high k modes

- **Low momentum universality**

  => evolved interactions ("$V_{\text{low k}}$") coalesce to ≈ universal curve



The Similarity Renormalization Group

[Wegner, Glazek and Wilson]

- Unitary transformation on an initial H = T + V

$$H_s = U(s) H U^\dagger(s) \equiv T + V_s$$

s = continuous flow parameter

- Differentiating with respect to s:

$$\frac{dH_s}{ds} = [\eta(s), H_s] \qquad \text{with} \qquad \eta(s) \equiv \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s)$$

- Engineer η(s) to do different things as s -> ∞

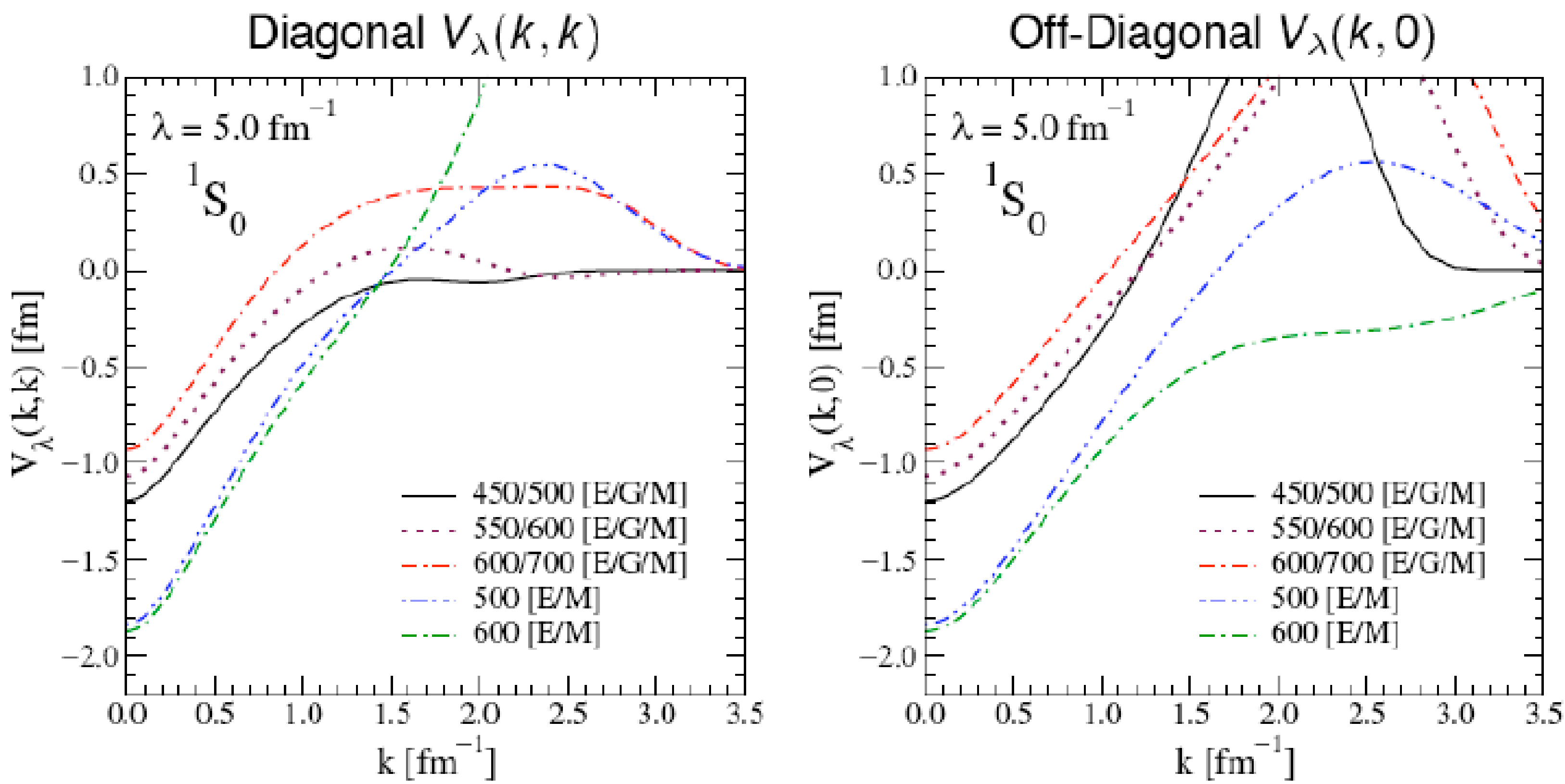
$$\eta(s) = [\mathcal{G}_s, H_s]$$

$$\mathcal{G}_s = T \;\Rightarrow\; H_s \text{ driven towards the diagonal in k} - \text{space}$$

$$\mathcal{G}_s = PH_sP + QH_sQ \;\Rightarrow\; H_s \text{ driven towards block diagonal form}$$

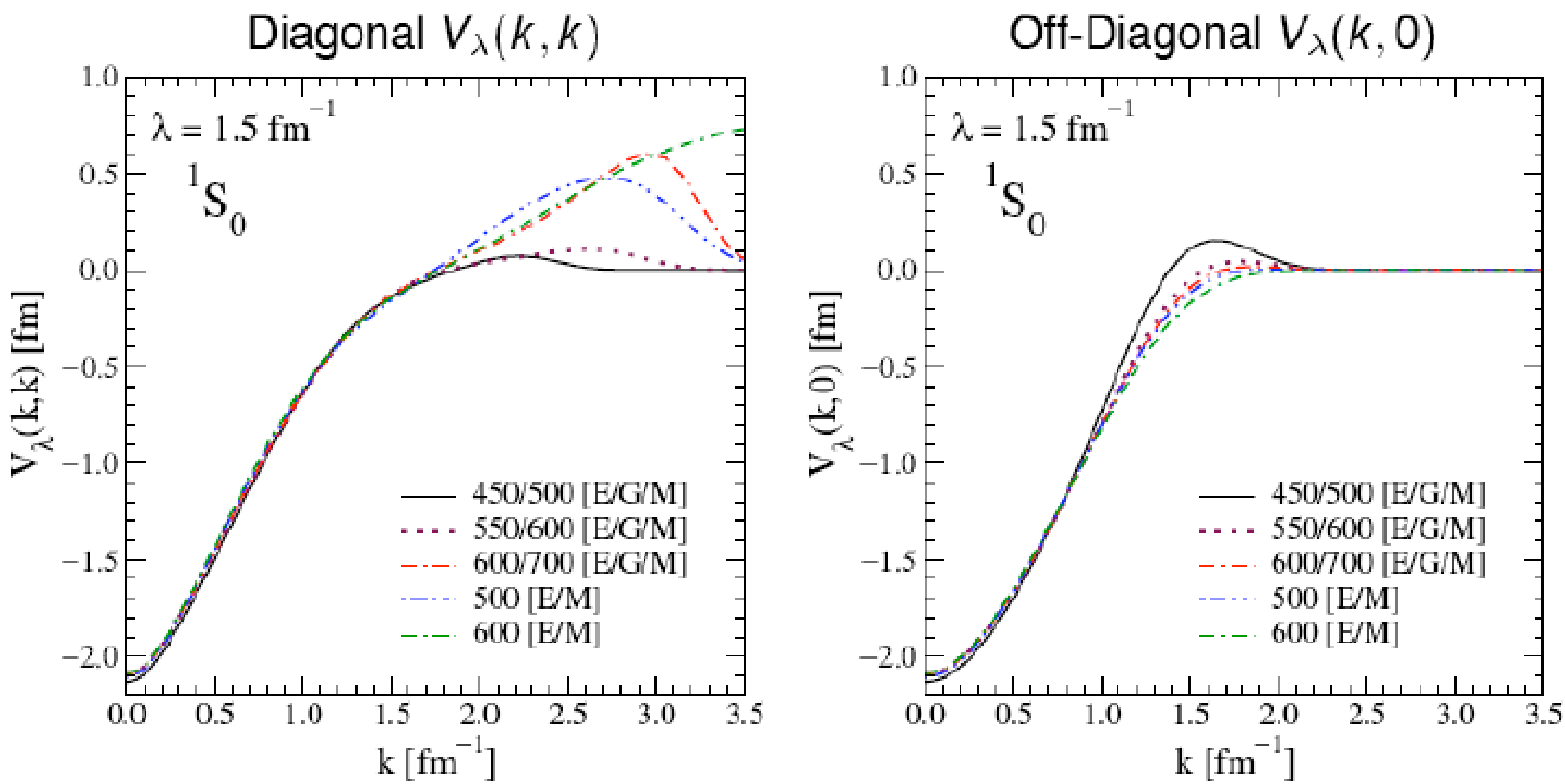
$\vdots$

Run to Lower λ via SRG $\Longrightarrow$ $\approx$Universality



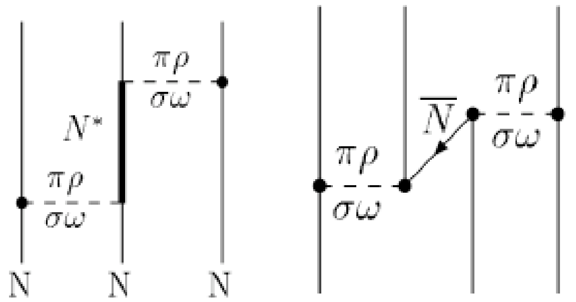
Note: $\lambda = s^{-1/4}$

Run to Lower λ via SRG $\Longrightarrow$ ≈Universality

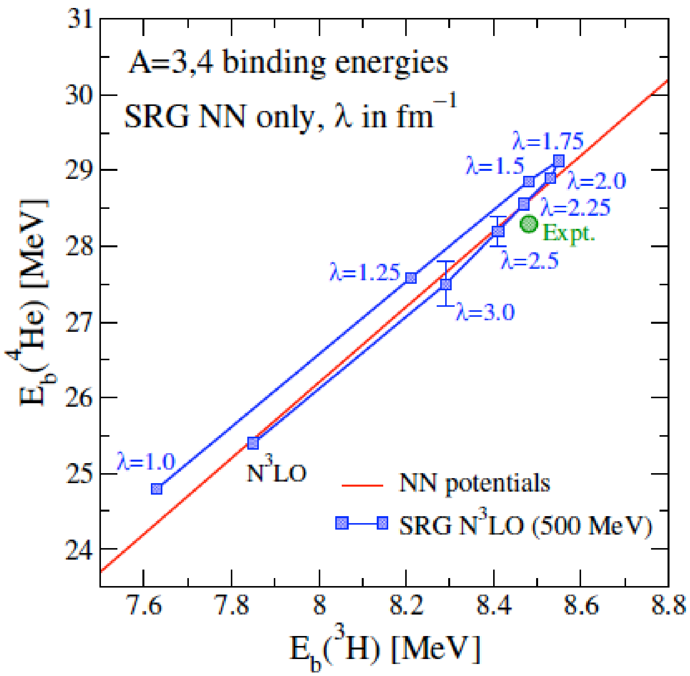


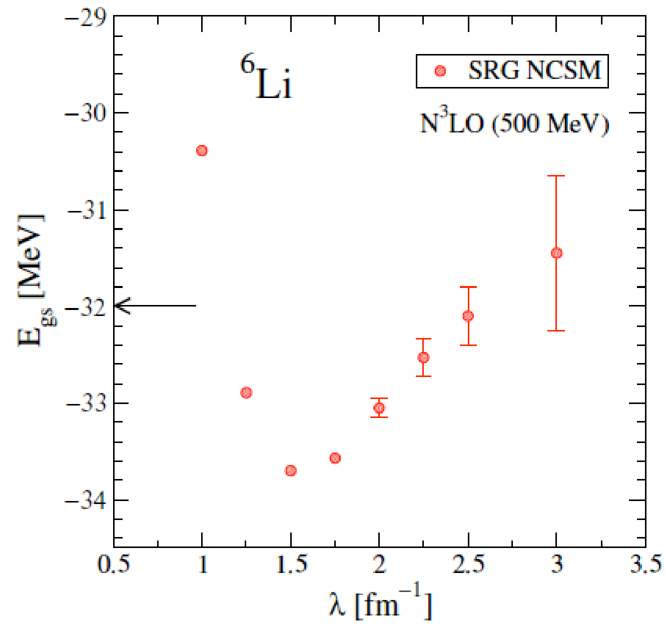
Note: $\lambda = s^{-1/4}$

Observations on 3N forces



Arise whenever eliminate DOF
(relativity, nucleon excitations, high momentum intermediate states)

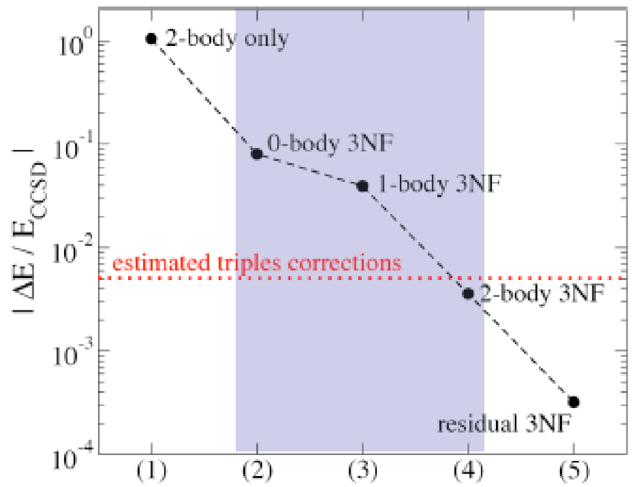


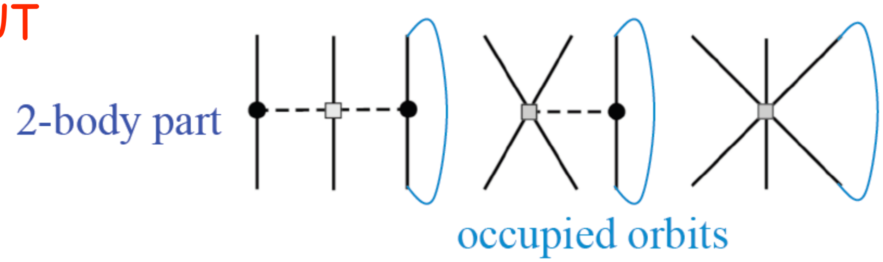


Omitting 3NF's => observables depend on Λ.

Why Bother lowering Λ if 3NF's grow ?

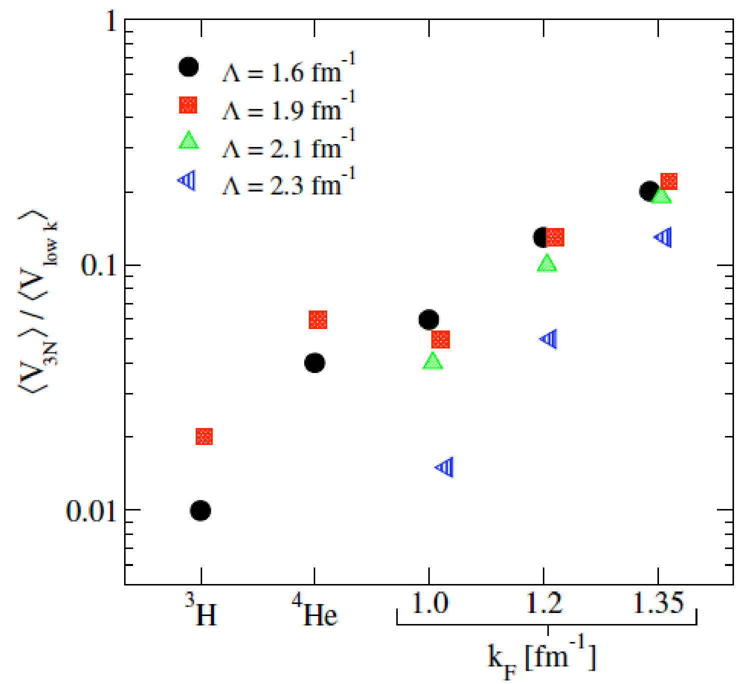
<3N> gets bigger for low Λ BUT





- Approximate treatments of 3NF "work" better
  - e.g., normal ordering (D. Dean's talk)
  - perturbative, HF dominates

Ratio <3N>/<2N> not unnaturally large

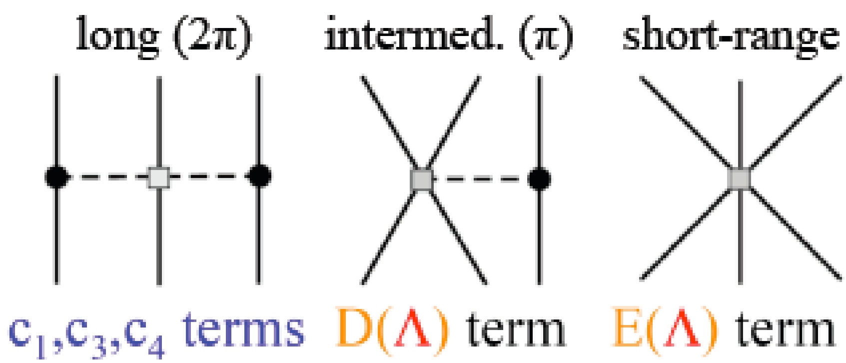


Chiral: $\langle V_{3N} \rangle \sim (Q/\Lambda)^3 \langle V_{NN} \rangle$

Hard work for a small contribution (large Λ) versus less work for a larger contribution (small Λ)?

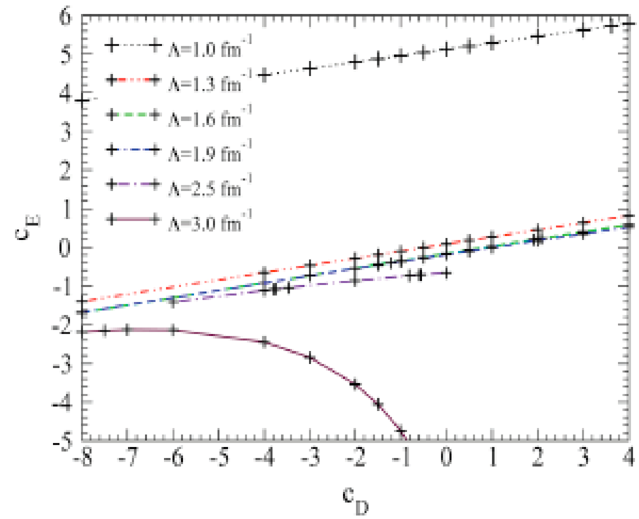
Approximate RG Evolution of 3NF

Leading chiral EFT 3NF appears in N^{2}LO



$c_1 = -0.9^{+0.2}_{-0.5}$, $c_3 = -4.7^{+1.2}_{-1.0}$, $c_4 = 3.5^{+0.5}_{-0.2}$

Note: significant decrease of c_3 and c_4 in N^{3}LO



LECs D and E fit to A=3,4 BE

- Chiral EFT is a complete operator basis
- **Approximate** RG running by refitting D and E at each Λ
- Equivalent to truncating RGE to leading operators

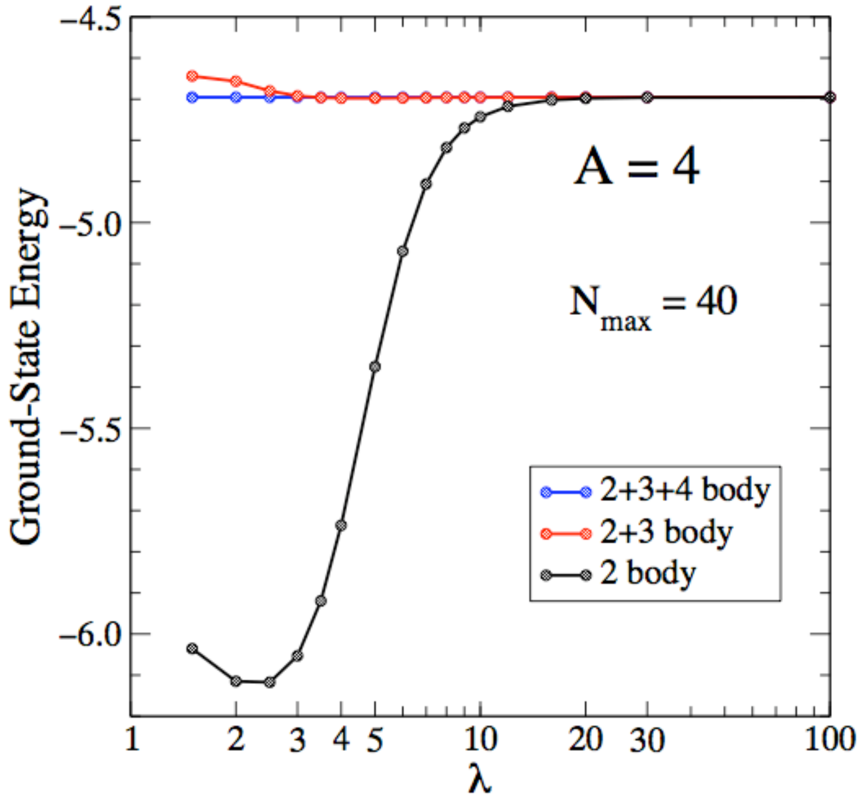
Consistency checks of the approximation:

weak Λ-dependence in NM (renormalization is working)

<3N>/<2N> agrees w/power counting estimates

Progress on “honest” 3NF RG evolutions

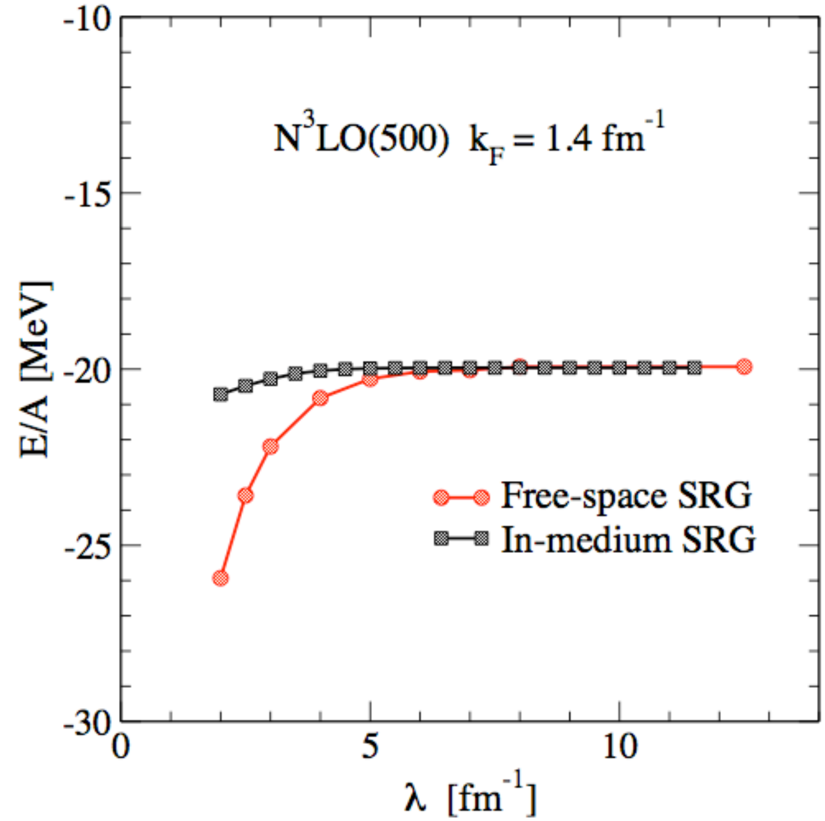
4-boson model problem



Anderson and Furnstahl 2008

SRG in H.O. basis

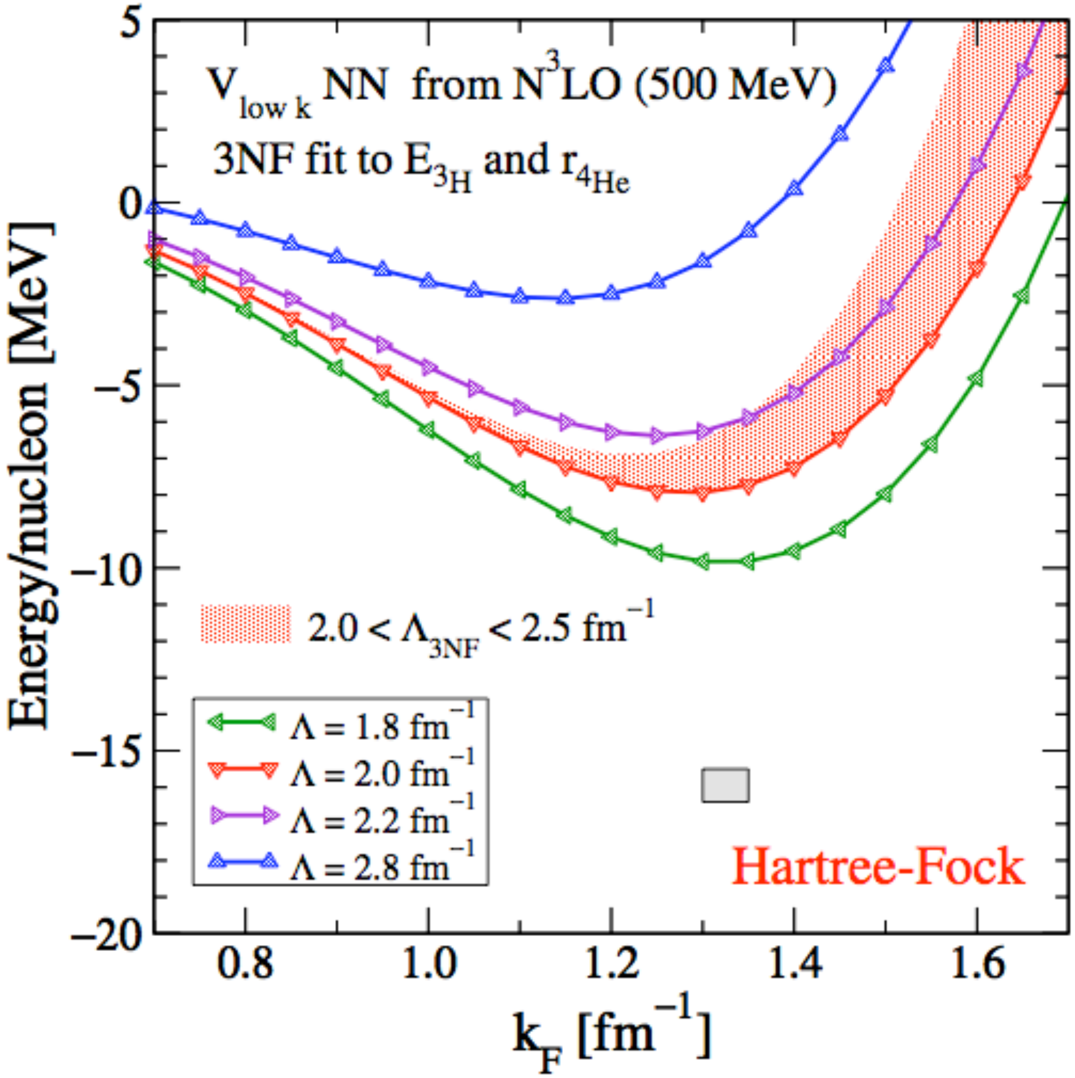
NM using in-medium SRG



S.K. Bogner, in prep

In-medium SRG w/normal-ordering

New low-momentum NNN fits and Nuclear Matter

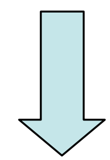


Smooth cutoff $V_{low\,k}$ from $N^3LO(500)$

N^2LO 3NF fit to A =3,4 B.E. and ^4He radii

[A. Nogga]

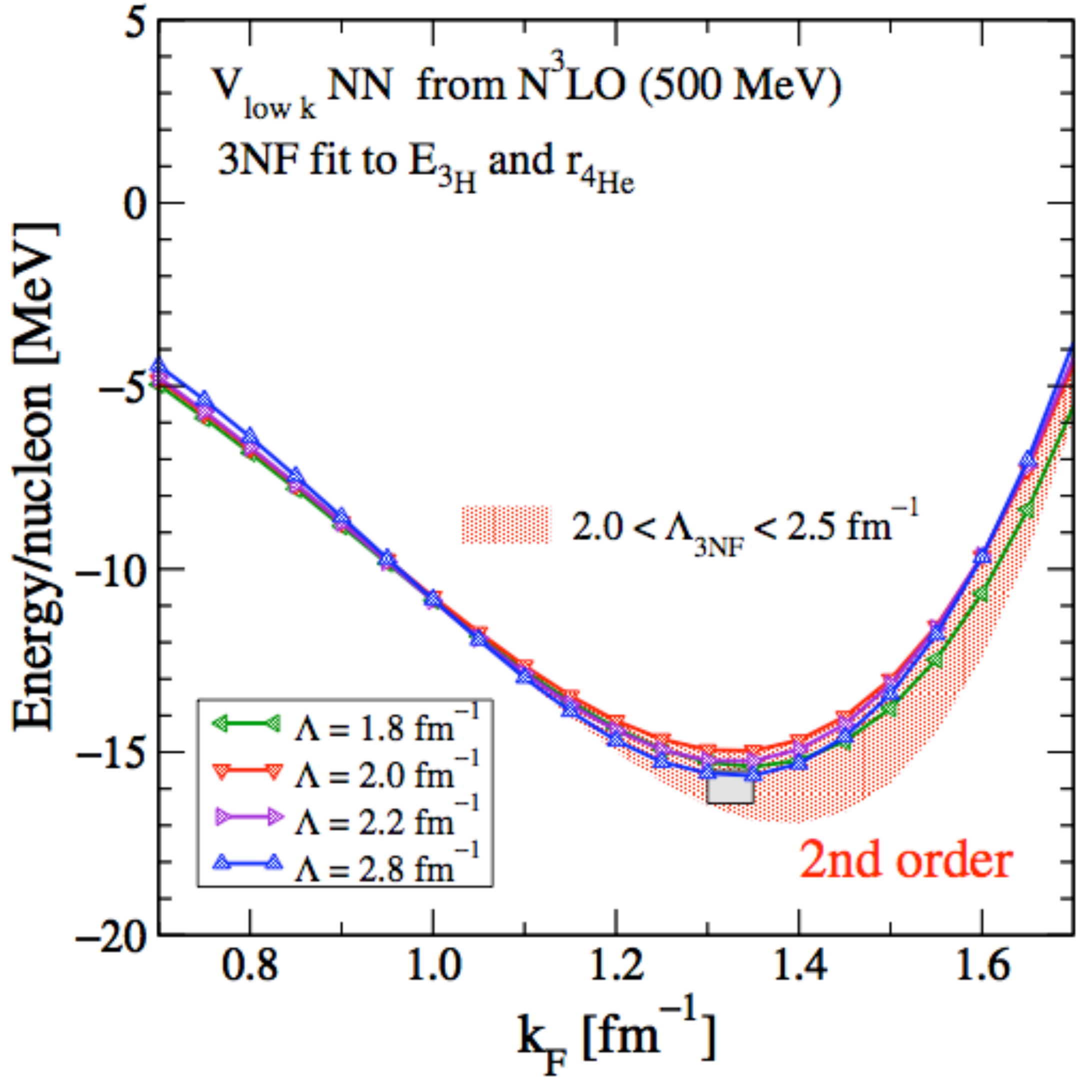
self-bound w/ saturation



Perturbative expansion about HF becomes sensible

NOTE: 3NF drives saturation NOT the tensor force

New low-momentum NNN fits and Nuclear Matter



Knobs to estimate
Theoretical error bars:

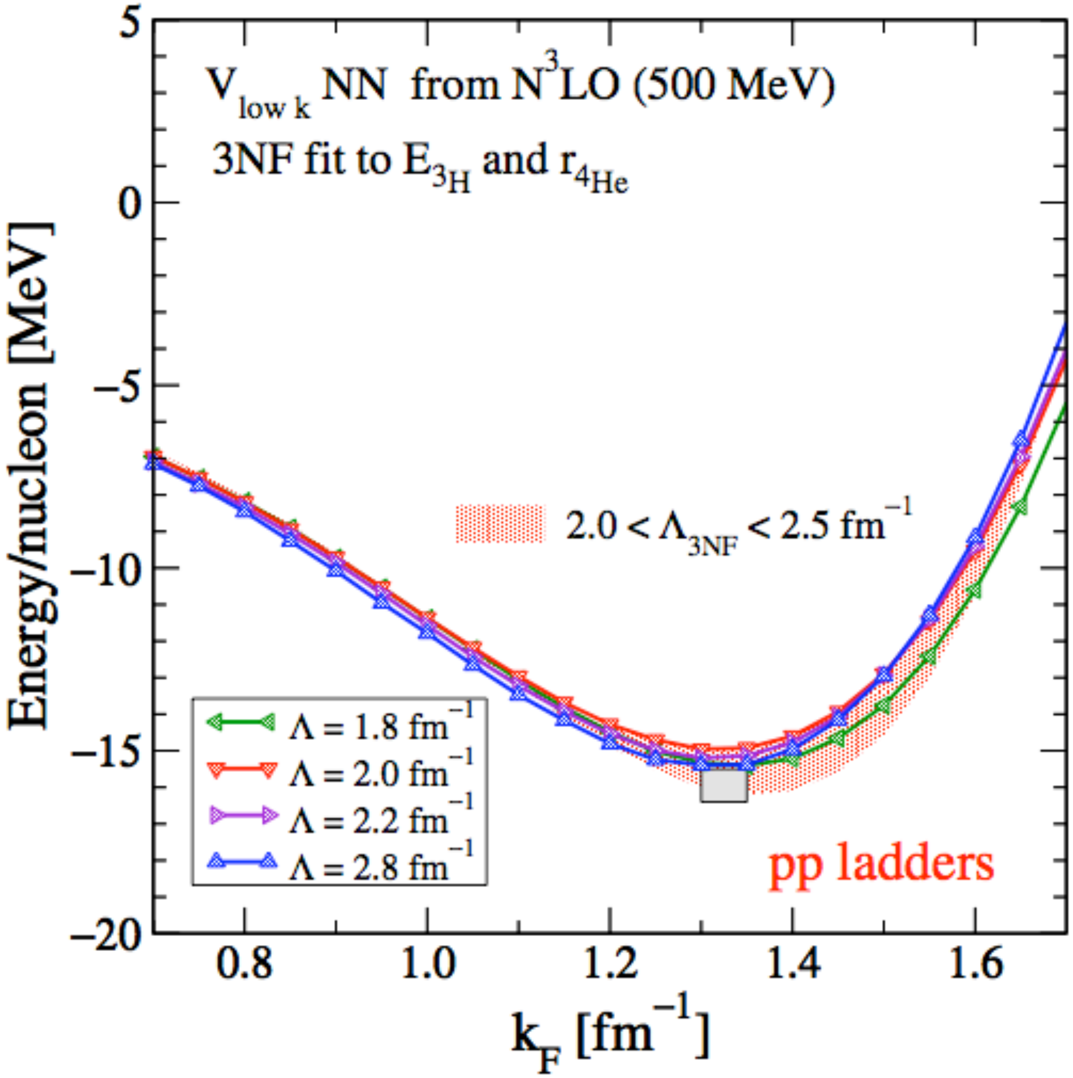
Λ-dependence => theoretical error bands (lower limit)

Assess the impact of large uncertainties in the c_i's appearing in 2- and 3-body TPEP (to do)

Vary the order of the underlying EFT (to do)

Sensitivity to many-body approximations

New low-momentum NNN fits and Nuclear Matter



Ladder sum ≈ 2nd-order

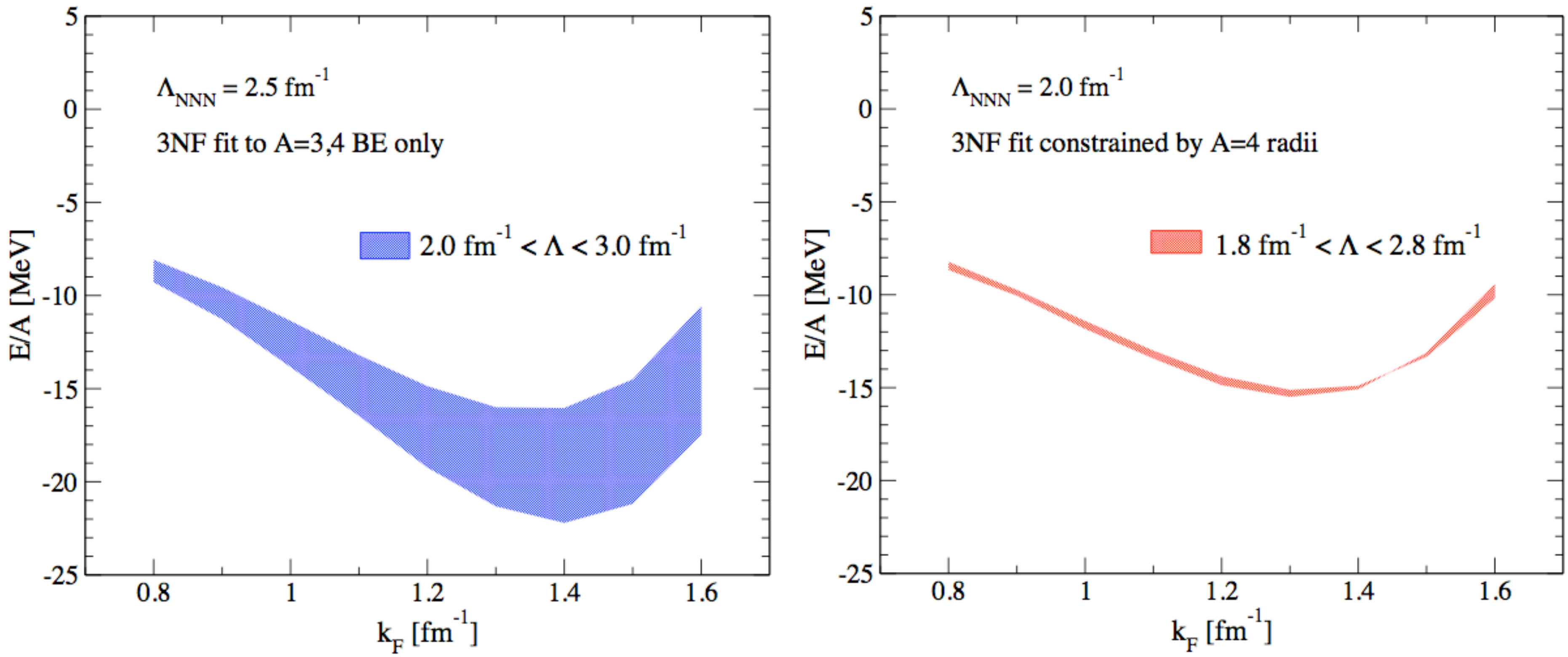
Excellent saturation, NO fine-tuning to nuclear matter

But…

1) V_{NNN} => $V_{2N}(r)$
2) HF propagators
3) Beyond 2-hole lines?
4) Angle-averaging
5) Particle-hole channel
6) …

Coupled-cluster calculations of nuclear matter, ^{16}O and ^{40}Ca would be a huge help!

Guidance from NM for fixing EFT couplings



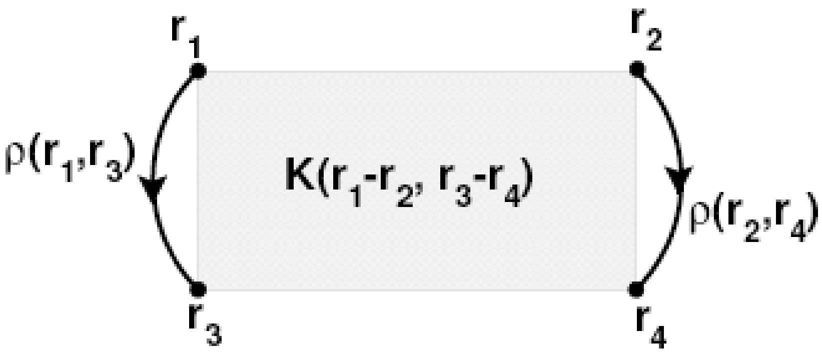
Supports suggestion of Navratil et al. to use ^{4}He radii to constrain fits of 3NF couplings (c_E and c_D)

NM to constrain c_3 and c_4 ?

Local Functionals from Many-Body Theory

- Dominant MBPT contributions to bulk properties take the form

$$\langle V \rangle \sim \mathrm{Tr}_1 \mathrm{Tr}_2 \int d\mathbf{R}\, d\mathbf{r}_{12}\, d\mathbf{r}_{34}\, \rho(\mathbf{r_1}, \mathbf{r_3})\, K(\mathbf{r}_{12}, \mathbf{r}_{34})\, \rho(\mathbf{r_2}, \mathbf{r_4}) \;+\; \mathrm{NNN} \cdots$$



K is either free-space interaction (HF) or resummed in-medium vertex (BHF)

- Written in terms on non-local quantities
  - density matrices and s.p. propagators
  - finite range and non-local resummed vertices K

Connection to E = E[ρ] is not obvious!

Density Matrix Expansion Revisited (Negele and Vautherin)

- Expand of DM in local operators w/factorized non-locality

$$\langle\Phi|\psi^\dagger(\mathbf{R}-\frac{1}{2}\mathbf{r})\psi(\mathbf{R}+\frac{1}{2}\mathbf{r}|\Phi\rangle = \sum_n \Pi_n(k_F r)\langle\mathcal{O}_n(\mathbf{R})\rangle$$

$$\langle\mathcal{O}_n(\mathbf{R})\rangle = [\rho(\mathbf{R}), \nabla^2\rho(\mathbf{R}), \tau(\mathbf{R}), \mathbf{J}(\mathbf{R}), \ldots]$$

- Fall off in r controlled by local k_F

  => expand and resum so LO term exact in uniform limit

  => NOT a simple short-distance expansion in r

$$\rho(\mathbf{R}+\frac{1}{2}\mathbf{r}, \mathbf{R}-\frac{1}{2}\mathbf{r}) = \frac{3j_1(k_F r)}{k_F r}\rho(R) + \frac{35 j_3(k_F r)}{2k_F^3 r}\left(\frac{1}{4}\nabla^2\rho(R) - \tau(R) + \frac{3}{5}k_F^2\rho(R)\right) + \cdots$$

- Dependence on *local* densities now manifest

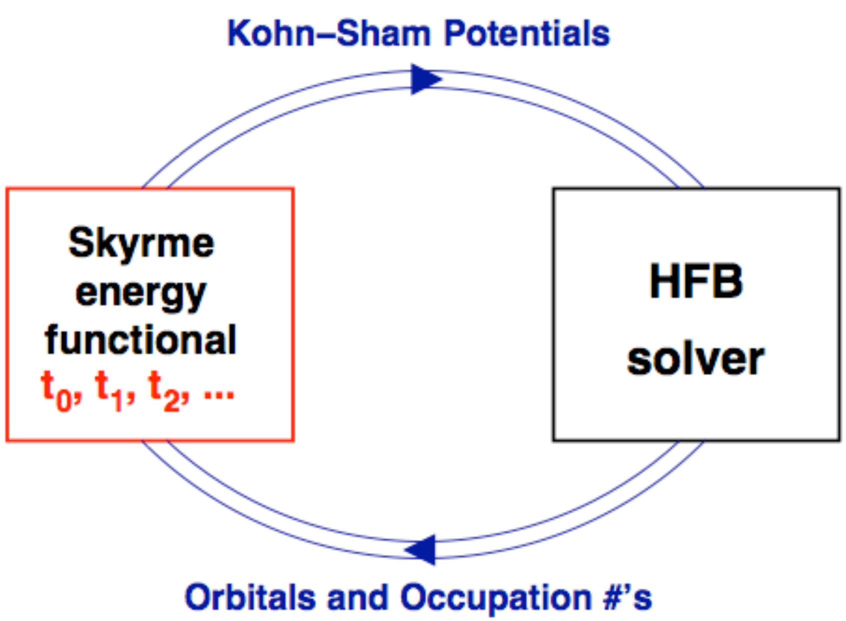
Skyrme-like EDF's from the DME

$$\mathcal{E} = \frac{\tau}{2M} + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)|\nabla\rho|^2 + \cdots \quad \text{Skyrme}$$

$$\mathcal{E} = \frac{\tau}{2M} + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \cdots \quad \text{DME}$$

- coupling *constants* --> coupling *functions*

  - finite range effects encoded as ρ-dependence in ABC
  - microscopic isovector, spin-orbit terms
  - well-suited for existing SkyHF codes



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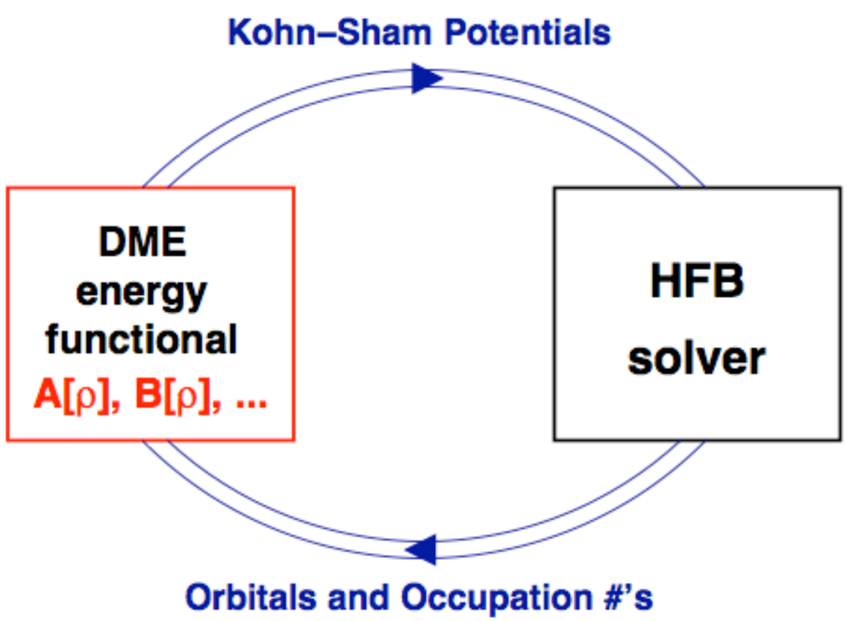


- Don't touch the HFB solver
- Trivial to upgrade as each new coupling becomes available
- Implemented in HFBRAD

Including Long Range Chiral EFT in Skyrme-like EDFs

Derived the most general (N≠Z, spin-unsaturated) EDF from chiral EFT thru N²LO at HF level [SKB and B. Gebremariam]

$$
\begin{aligned}
\mathcal{E}^{\rho\rho} \equiv \sum_q \int d\mathbf{r} \Big[& A^{\rho\rho}\,\rho_q\rho_q + A^{\rho\Delta\rho}\,\rho_q\Delta\rho_q + A^{\nabla\rho\cdot\nabla\rho}\,\nabla\rho_q\cdot\nabla\rho_q + A^{\rho\tau}\left(\rho_q\tau_q - \mathbf{j}_q\cdot\mathbf{j}_q\right) \\
& + A^{ss}\,\mathbf{s}_q\cdot\mathbf{s}_q + A^{s\Delta s}\,\mathbf{s}_q\cdot\Delta\mathbf{s}_q + A^{\nabla s\circ\nabla s}\,\nabla\mathbf{s}_q\circ\nabla\mathbf{s}_q \\
& + A^{\rho\nabla J}\left(\rho_q\nabla\cdot\mathbf{J}_q + \mathbf{j}_q\cdot\nabla\times\mathbf{s}_q\right) + A^{\nabla\cdot s\nabla\cdot s}\left(\nabla\cdot\mathbf{s}_q\right)\left(\nabla\cdot\mathbf{s}_q\right) \\
& + A^{JJ}\Big(\sum_{\mu\nu} J_{q,\mu\nu}J_{q,\mu\nu} - \mathbf{s}_q\cdot\mathbf{T}_q\Big) + A^{JJ}\Big[\Big(\sum_{\mu} J_{q,\mu\mu}\Big)\Big(\sum_{\mu} J_{q,\mu\mu}\Big) + \sum_{\mu\nu} J_{q,\mu\nu}J_{q,\nu\mu} - 2\,\mathbf{s}_q\cdot\mathbf{F}_q\Big]\Big]
\end{aligned}
$$

Each coupling function splits into 2 terms

1) Λ-**dependent** Skyrme-like coupling **constants**
2) Λ-**independent** coupling **functions** from pion physics with non-trivial density dependence

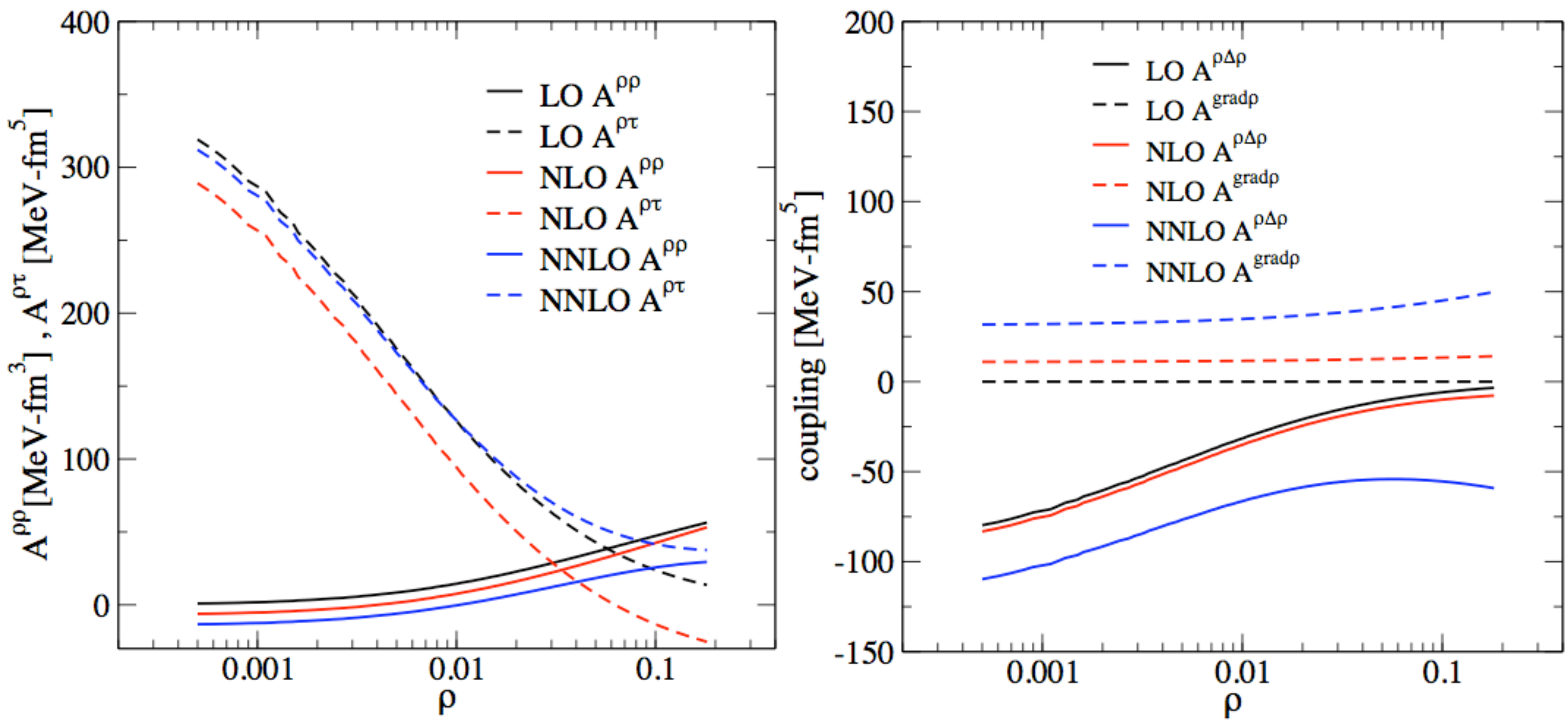
$$A^{\rho\Delta\rho} \Rightarrow A^{\rho\Delta\rho}(\Lambda) + A^{\rho\Delta\rho}[\rho]$$

Etc…

From contact terms in EFT/RG V's

From pion exchanges

Long-range pion exchange contributions to the EDF



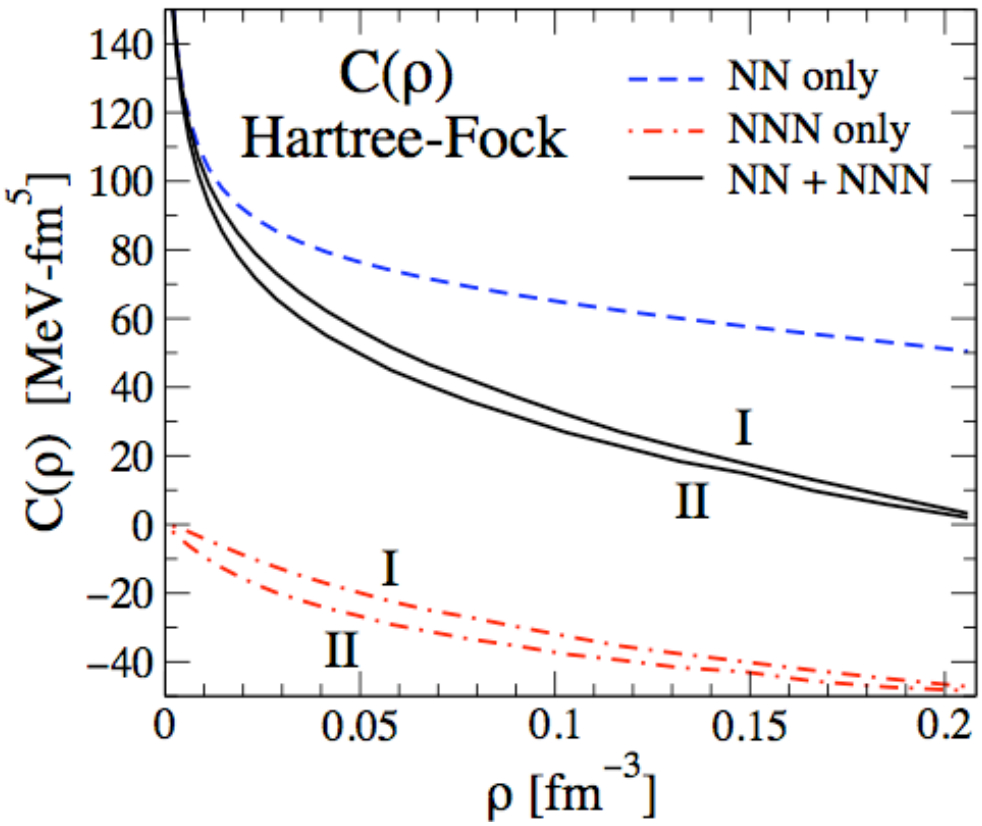
Longest range V <==> Strongest density dependence in EDF

Novel density-dependencies in EDF from 1π and 2π exchanges:

$$\rho^{7/3}, \quad \rho^{4/3}, \quad \rho^{2/3}, \quad \frac{1}{\rho^{2/3}} log(1 + c\rho^{2/3}), \quad \ldots$$

Effects of NNN on Couplings

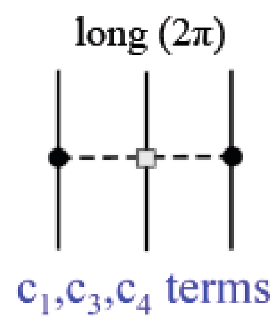
Gradient term $(\nabla\rho)^2$



SKB, Furnstahl and Platter, in prep.

- Only scalar-isoscalar terms worked out so far
- Consistent with Kaiser et al. results with explicit Δ's

In Progress:



Spin-orbit couplings from 2π 3NF

Should find interesting density dependencies compared to NN spin-orbit, which is a short-range effect!

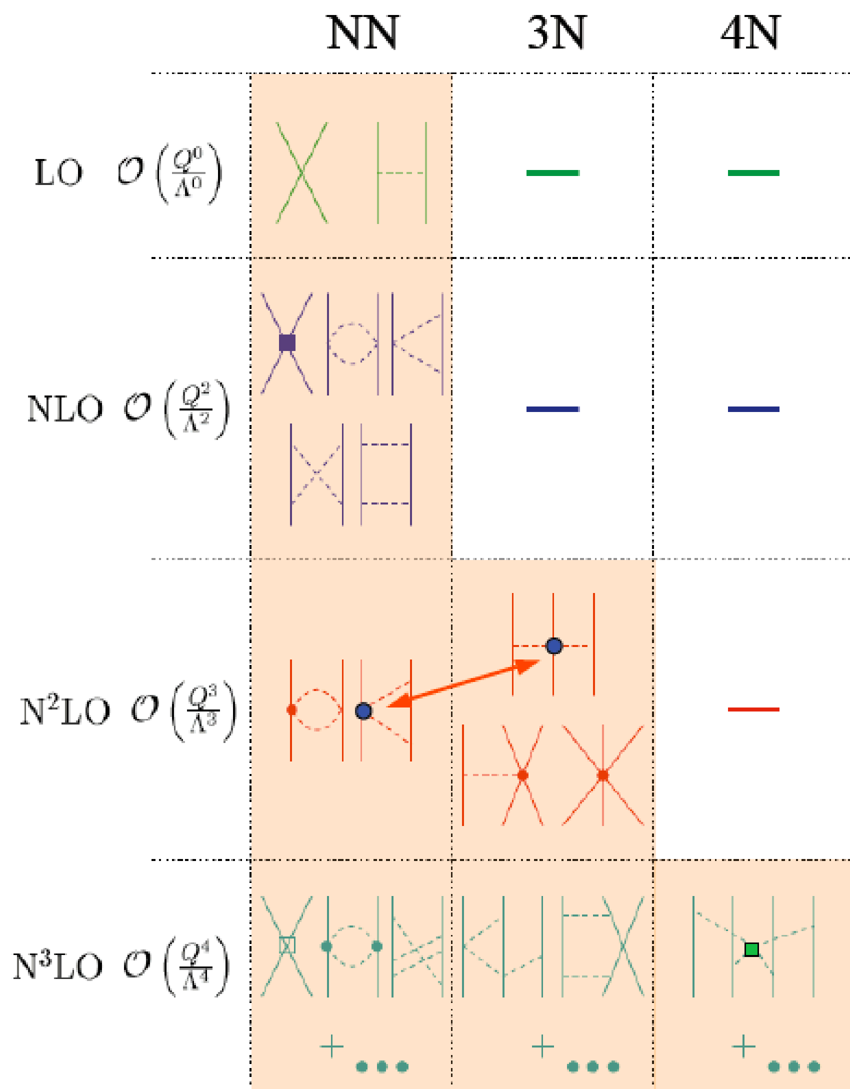
Including Long Range Chiral EFT in Skyrme-like EDFs

- Derive coupling *functions* from χ-EFT pion exchange NN and NNN interactions via the DME

- Refit the Skyrme coupling *constants* (EFT constraints => naturalness, Λ-dependence, etc.)

- Look for improved observables and for sensitivities

- Can we "see" the pion as in NN phase shift analyses



Comparison to ab-initio calculations

Start from *the same* Hamiltonian and compare ab initio solution to the Microscopic DFT calculation based on the DME functional

CC or FCI calculations of nuclei and
nuclei in external fields

⇓

How important is non-locality and how accurate is the DME?

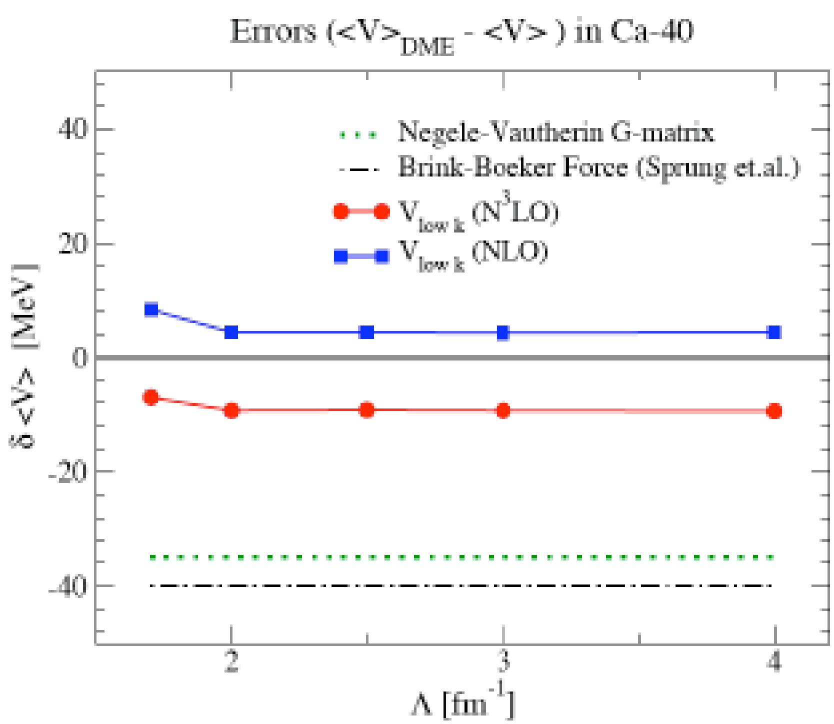
Are systematics reproduced by DME as we vary parameters (e.g., 3NF couplings, RG cutoff Λ, order of input EFT, ...) in H?

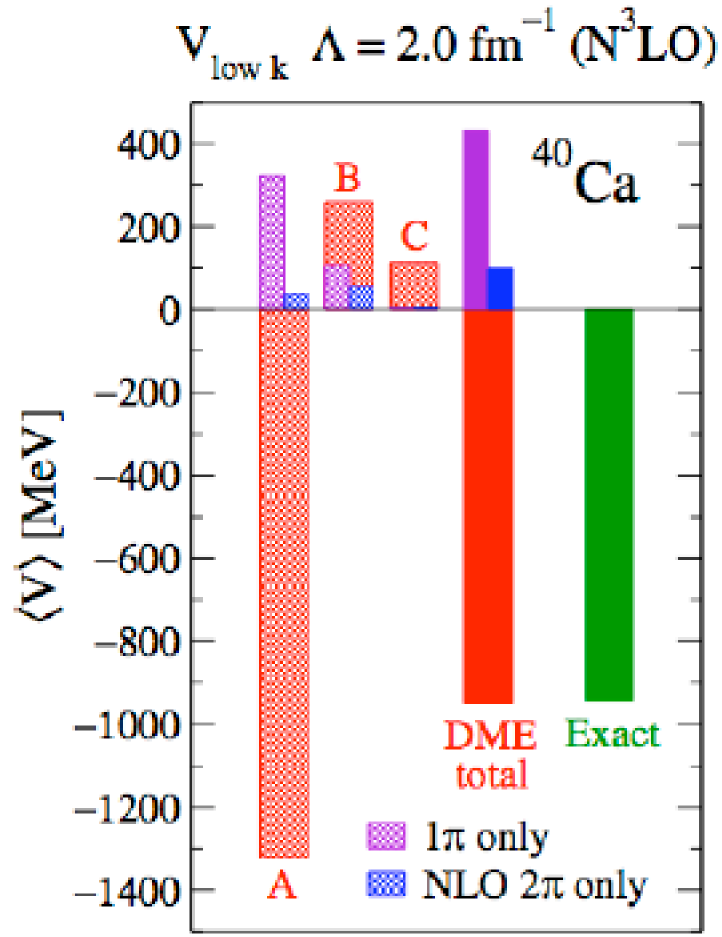
Is the many-body treatment of nuclear matter sufficient?

Early indications are that non-trivial extensions of the DME are needed

DME for Low-Momentum Interactions

- HO model
- errors ≈ +5 MeV (NLO), −10 MeV (N^3LO),
- Λ-independent errors
- Schematic V's (1970's) much worse
  (larger finite-range direct terms)





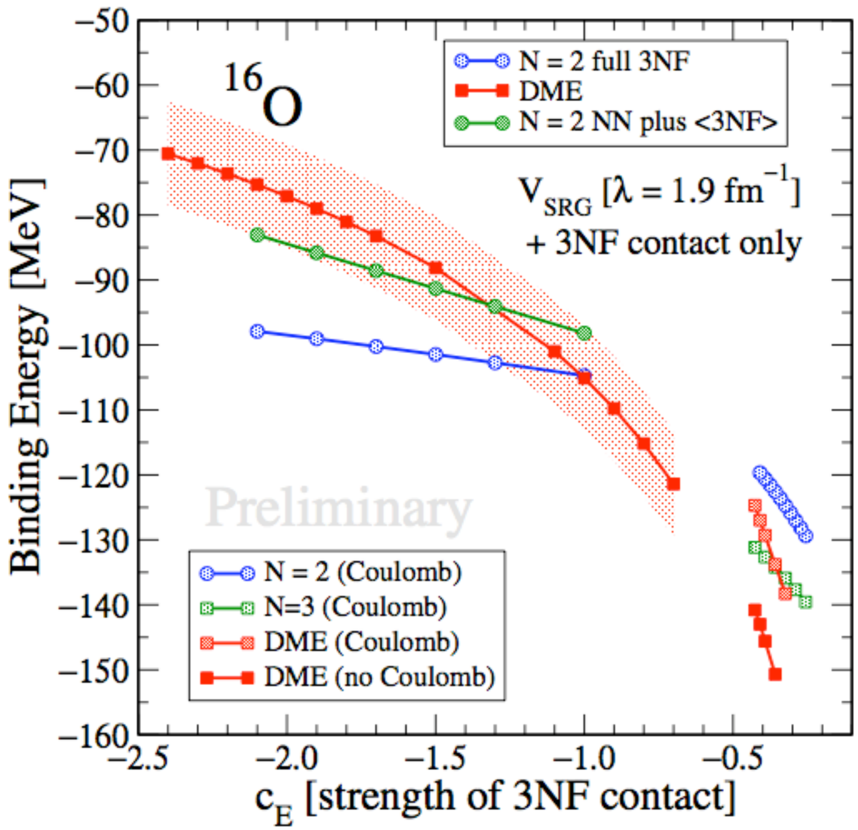
Long-range contributions (1π, leading 2π)

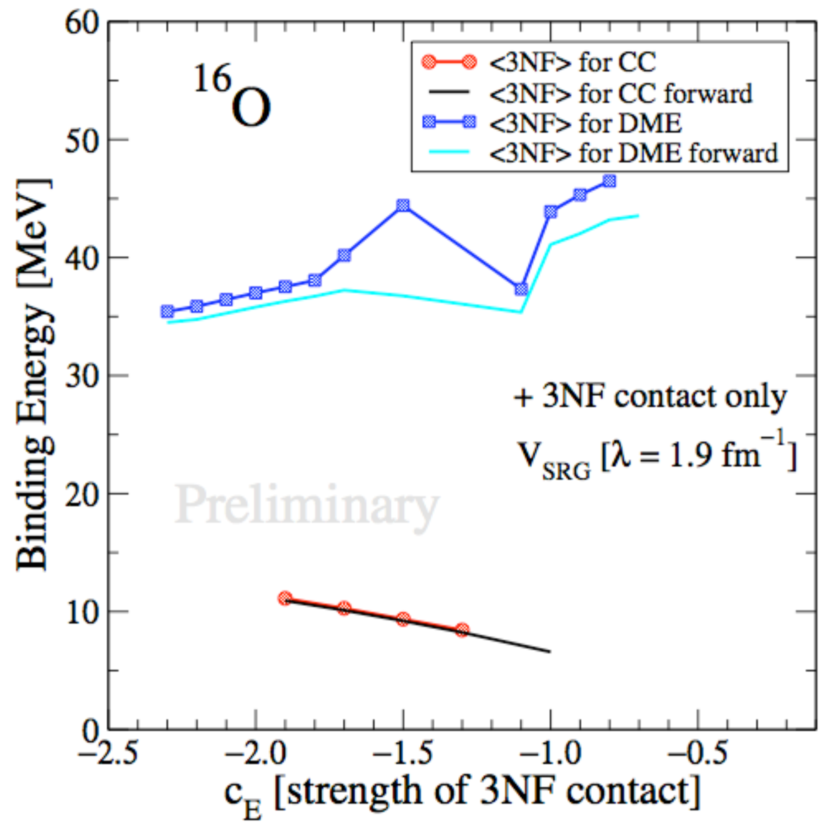
DME error in 1π exchange ≈ 4 MeV (out of 431 MeV)

...But the "success" of this test of the DME is misleading...

Comparison to ab-initio calculations

CC and DFT calculations of ^{16}O (w/3N contact of varying strength)



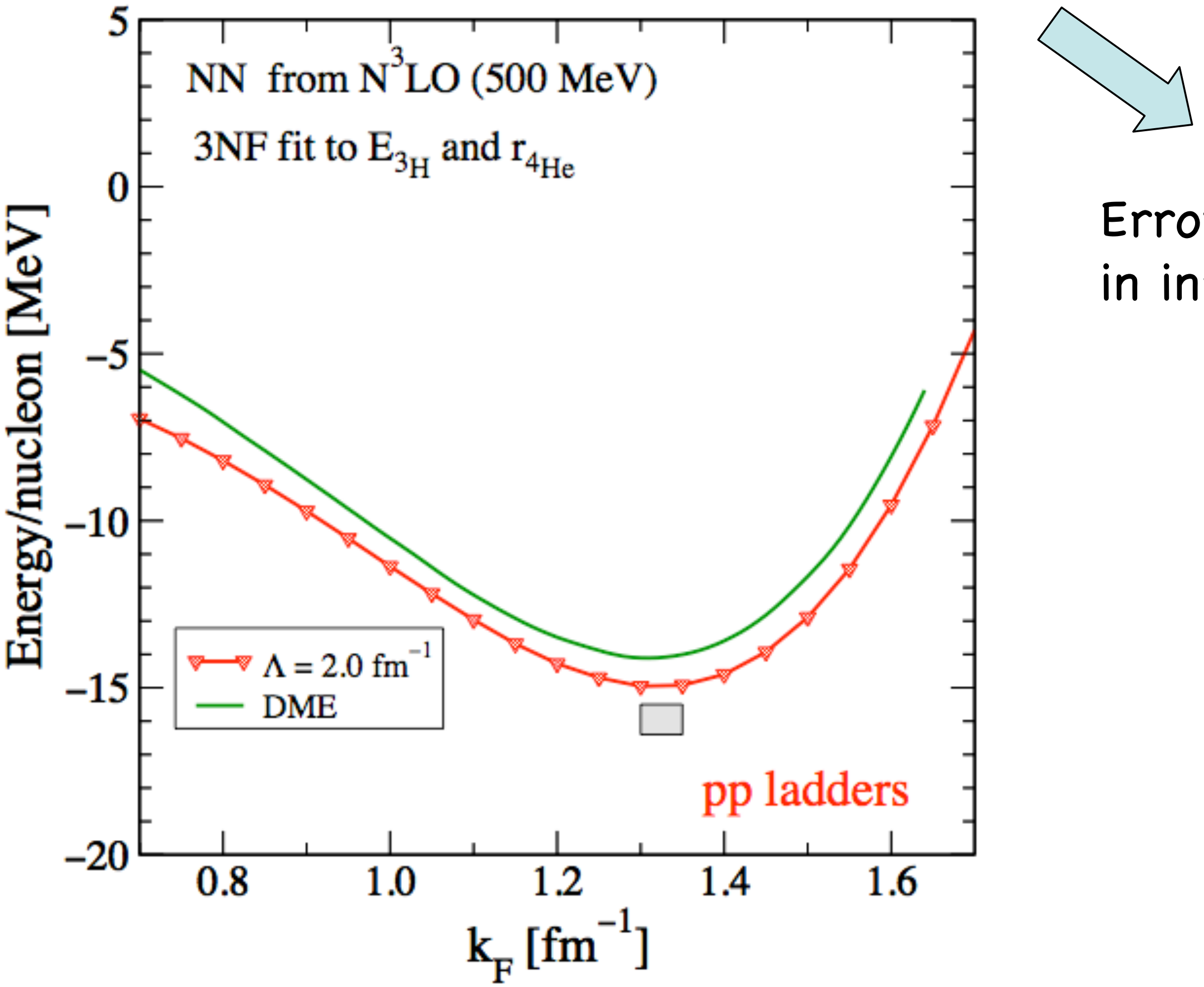


Quantitative and qualitative disagreement btw. coupled-cluster and DFT calculation. What is going on?

Possible Reasons for the Poor Agreement

1) DME averages out too much information

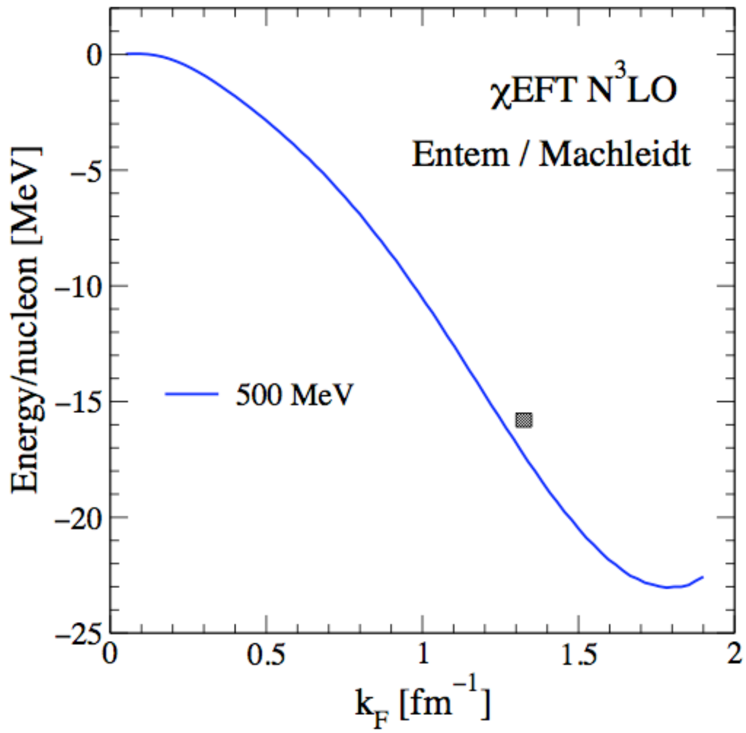
- COM P-dependence (spatial non-locality)
- energy-dependence



Errors of 1 MeV/nucleon in infinite NM

Possible Reasons for the Poor Agreement

2) Gradient expansion breaks down when saturation not good



e.g., N3LO NM looks reasonable at lower densities despite poor saturation

Ab-initio results for O16 and Ca40 pretty decent, but DME is poor

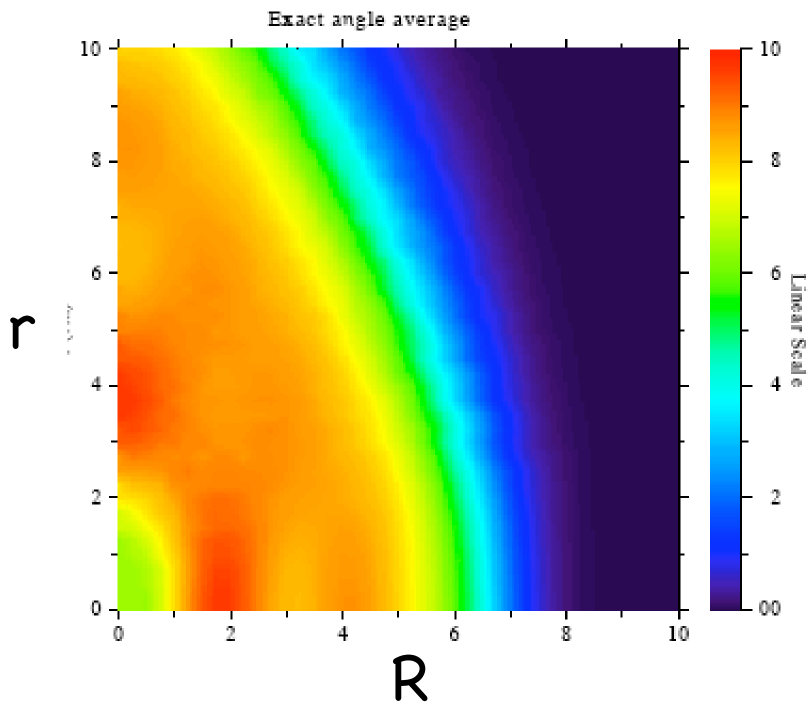
Gradients no longer "small" since DME = expansion about NM?

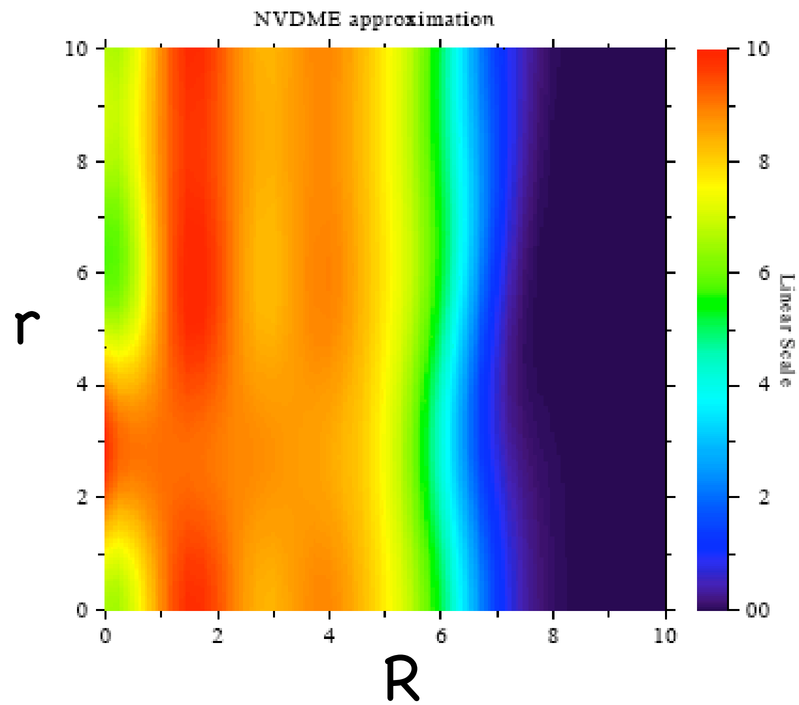
	O16		Ca40		Ca48	
	Coupled Cluster	DME	Coupled Cluster	DME	Coupled Cluster	DME
E/A	-6.72	-7.89	-7.72	-9.66	-7.40	-10.1
r_{ch}	2.73	2.47	3.35	2.95	3.24	2.84

Possible Reasons for the Poor Agreement

3) Errors in the Hartree contribution => **feedback via self-consistency!**

Exact $\rho(\mathbf{R}+\mathbf{r}/2)\rho(\mathbf{R}-\mathbf{r}/2)$ DME





Treat Hartree exactly a-la Coulomb? [Negele and Vautherin, Sprung et al.]

- "Ab-initio DFT" should be taken with a grain of salt!
- However, microscopic MBT still useful to build in missing physics (density dependencies) to Skyrme

Work in the near-term

- spin-orbit couplings from N^2LO 3NF

- Extension of DME beyond even-even nuclei (time-odd couplings)

- Refits of Skyrme + Long-range coupling functions (ORNL group)

- Extension of DME to pairing channel (B. Gebremariam)

- Generalization of DME to handle non-localities in time (I.e., energy-dependence from beyond HF)

- Refinements of original DME (B. Gebremariam)

Conclusions

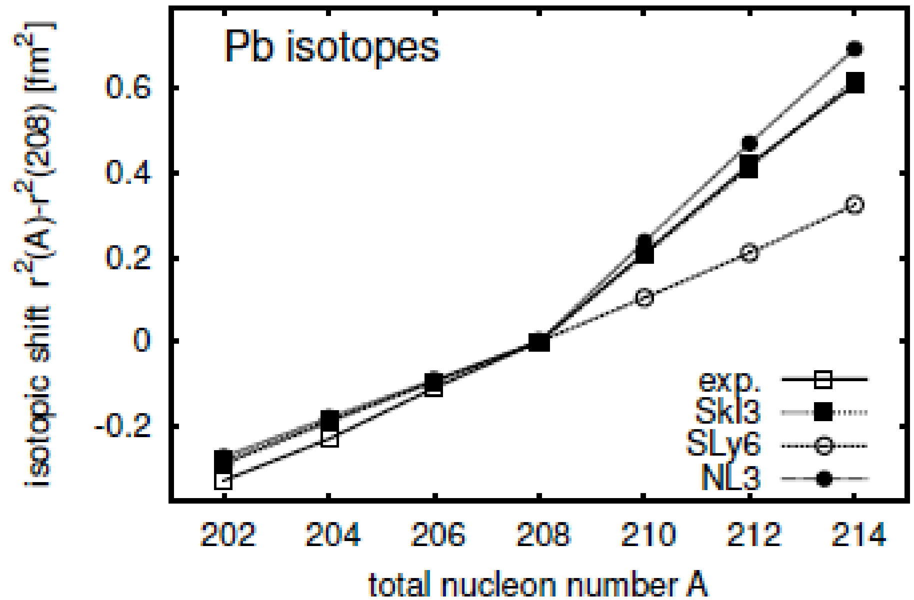
- Lowering Λ via RG greatly simplifies nuclear few and many-body problems
  - Comparison of DFT to ab initio (same H) now possible
  - use Λ-dependence as a tool for estimating errors
  - V_{3N} can be treated as perturbation/simple approximations
  - perturbative nuclear matter?
  - Correlations "blurred out" => HF is decent starting point
  - Extension of Skyrme EDF's via DME (novel density dep.)
  - Theoretical guidance for future fits possible using "error bars" generated from Λ-dependence

Collaborators

- MSU/NSCL: B. Gebremariam
- Ohio State: R. Furnstahl, L. Platter
- Iowa State: J. Vary, P. Maris
- ORNL: G. Hagen, T. Papenbrock
- TRIUMF: A. Schwenk
- Orsay/France: T. Duguet, V. Rotival

Observables Sensitive to 3N Interactions?

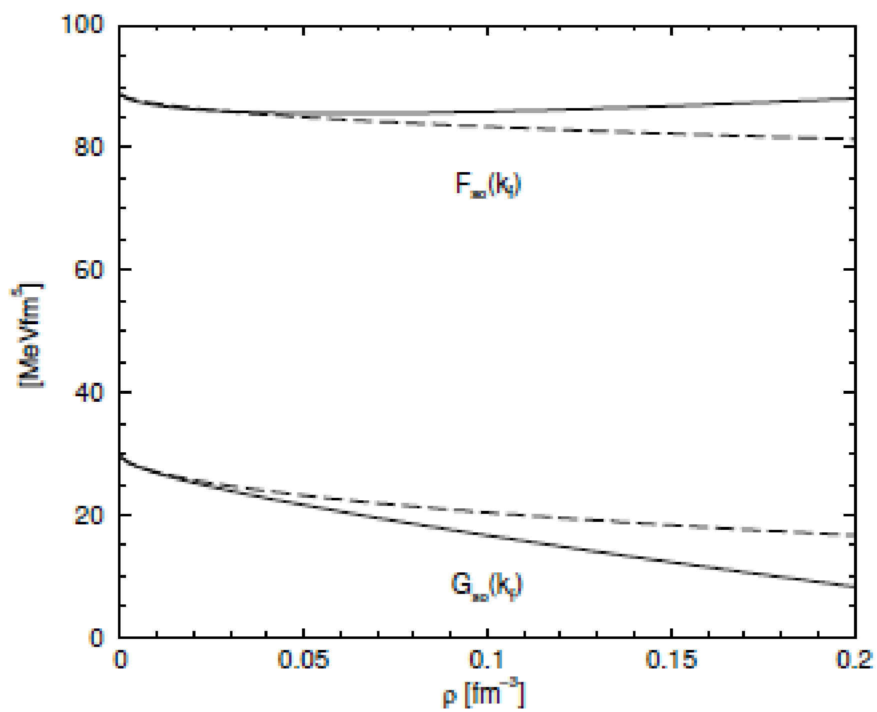
- Study systematics along isotopic chains
- Example: kink in radius shift $\langle r^2 \rangle(A) - \langle r^2 \rangle(208)$

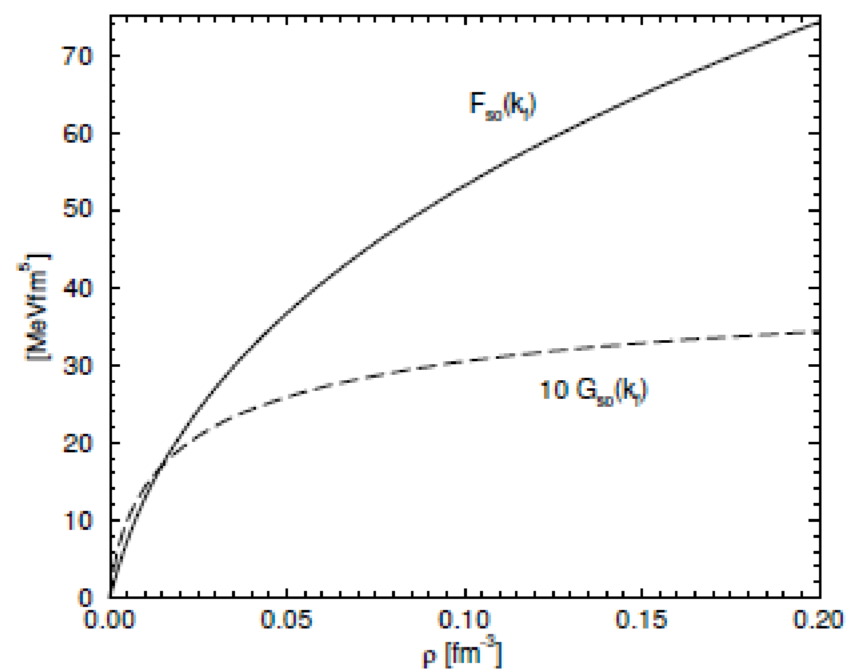


- Associated phenomenologically with behavior of spin-orbit
  - isoscalar to isovector ratio fixed in original Skyrme
- Clues from chiral EFT contributions? (Kaiser et al.)

Ratio of Isoscalar to Isovector Spin-Orbit

- Ratio fixed at 3:1 for short-range spin-orbit (usual Skyrme)
- Kaiser: DME spin-orbit from chiral two-body (left) and three-body (right)

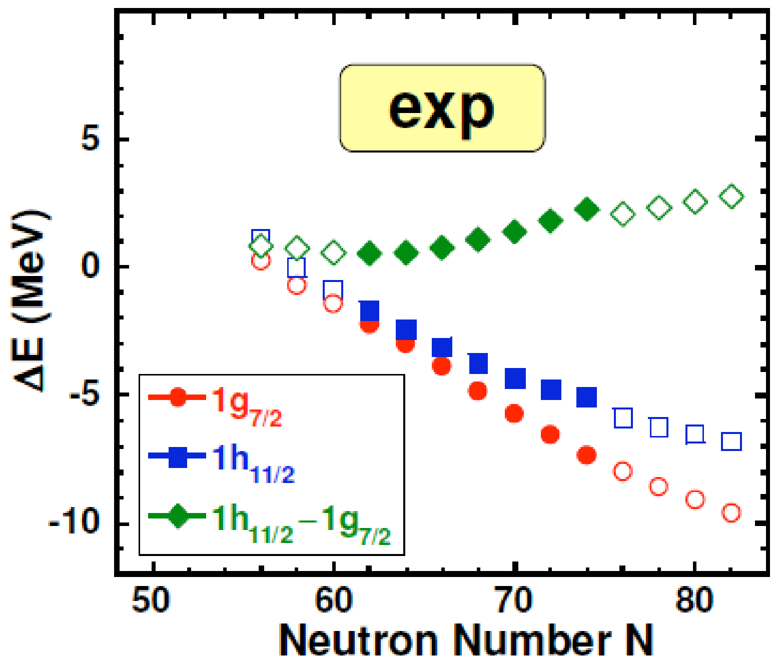


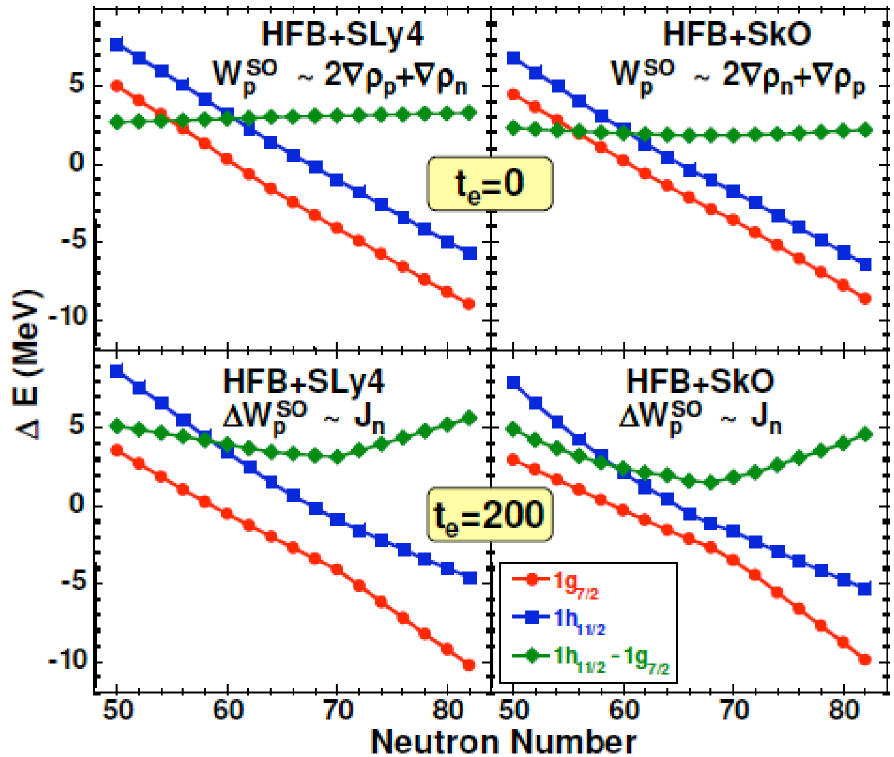


- Systematic investigation needed

Observables Sensitive to 3N Interactions?

- Recent studies of tensor contributions [e.g., nucl-th/0701047]





- See also Brown et al., PRC **74** (2006)

Naturalness to Constrain Skyrme Couplings

- Old NDA analysis:

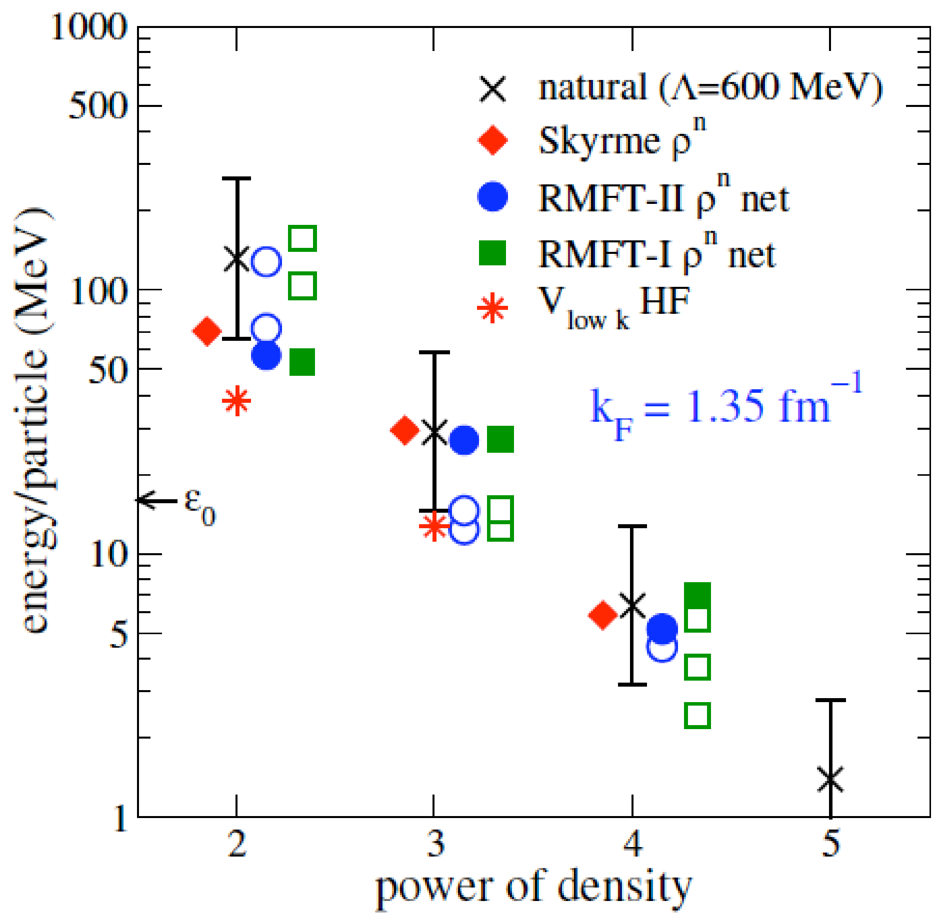
$$c \left[\frac{\psi^\dagger \psi}{f_\pi^2 \Lambda}\right]^l \left[\frac{\nabla}{\Lambda}\right]^n f_\pi^2 \Lambda^2$$

$$\Longrightarrow \quad \begin{array}{l} \rho \longleftrightarrow \psi^\dagger \psi \\ \tau \longleftrightarrow \nabla\psi^\dagger \cdot \nabla\psi \\ \mathbf{J} \longleftrightarrow \psi^\dagger \nabla \psi \end{array}$$

- Density expansion?

$$\frac{1}{7} \leq \frac{\rho_0}{f_\pi^2 \Lambda} \leq \frac{1}{4}$$

for $1000 \geq \Lambda \geq 500$



Furnstahl and Hackworth 1997

3NF's for N^3LO not necessarily small