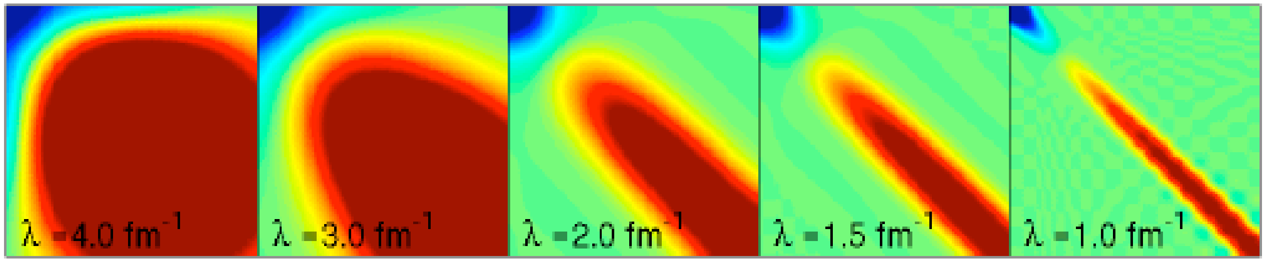


Renormalization group methods in nuclear few- and many-body problems

Lecture 3

S.K. Bogner (NSCL/MSU)

2011 National Nuclear Physics Summer School
University of North Carolina at Chapel Hill

Lecture 2 outline

1) Effective operators

2) Some results for nuclei/nuclear matter

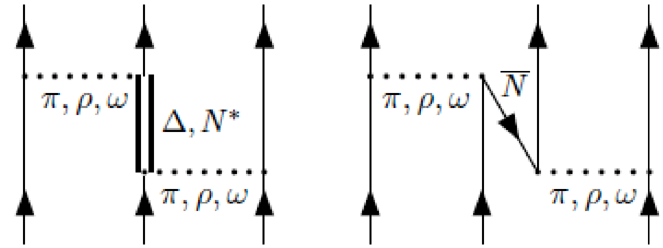
3) Towards a microscopically-based
Density functional theory (DFT) for nuclei

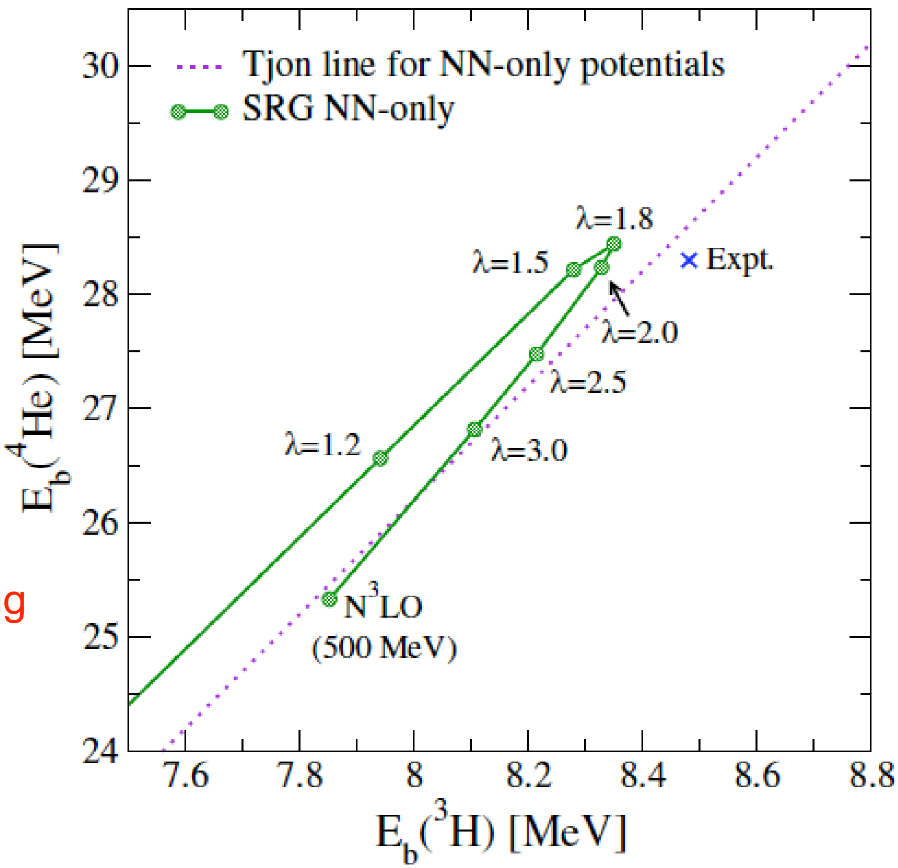
Observations on three-body forces

- Three-body forces arise from eliminating/decoupling dof's
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
  - observables depend on Λ/λ
  - cutoff dependence as tool

1) Tells you if you're missing something

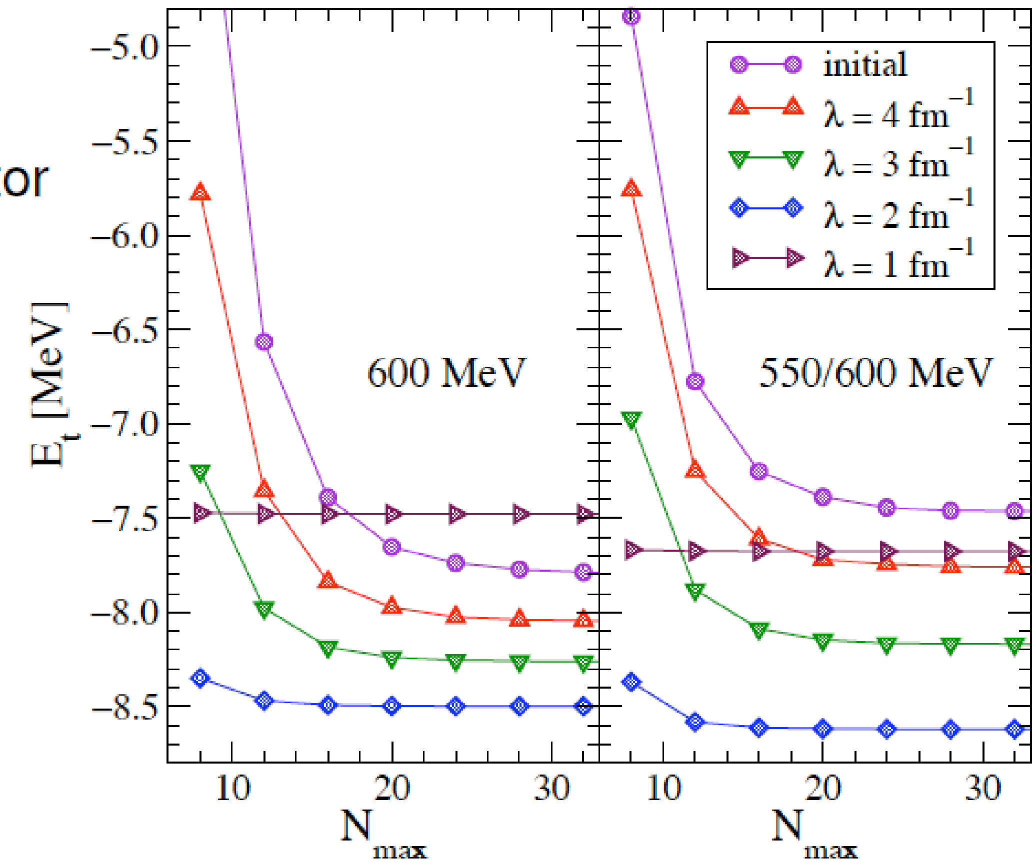
2) Tells you how big it is



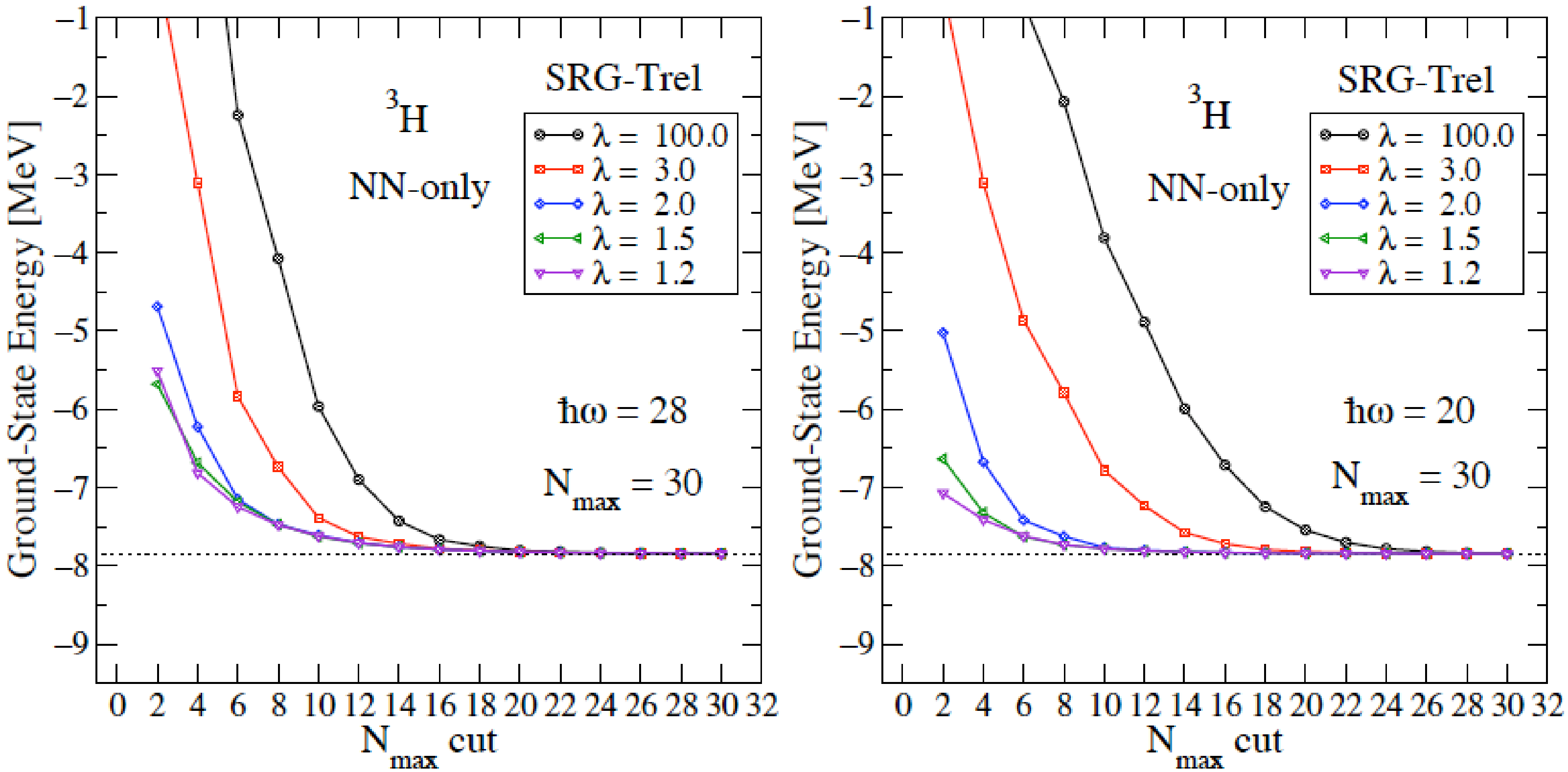


SRG-evolved Hamiltonians at the two-body level

- Triton ground-state energy vs. size of harmonic oscillator basis ($N_{\max}\hbar\omega$ excitations)
- Rapid convergence as λ decreases
- Note softening already at $\lambda = 3\,\mathrm{fm}^{-1}$ with N^3LO EFT $\Lambda = 600\,\mathrm{MeV} = 3\,\mathrm{fm}^{-1}$
- Different binding energies!

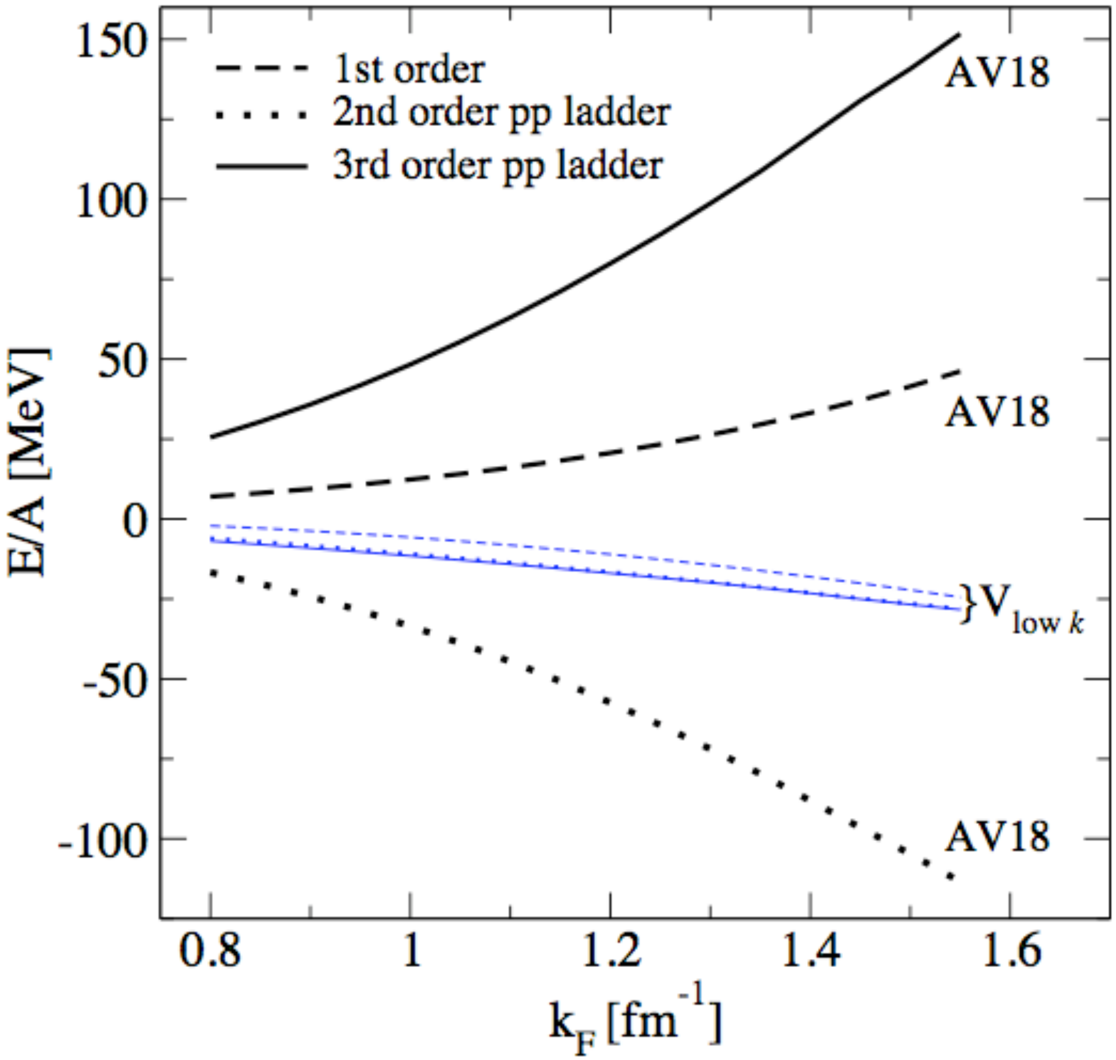


Now with consistent RG evolution of 2+3 body



- same rapid convergence as the NN-only result
- but now the transformation is unitary at the 3-body level
- should also check A>3 to see if induce 4NF's are big

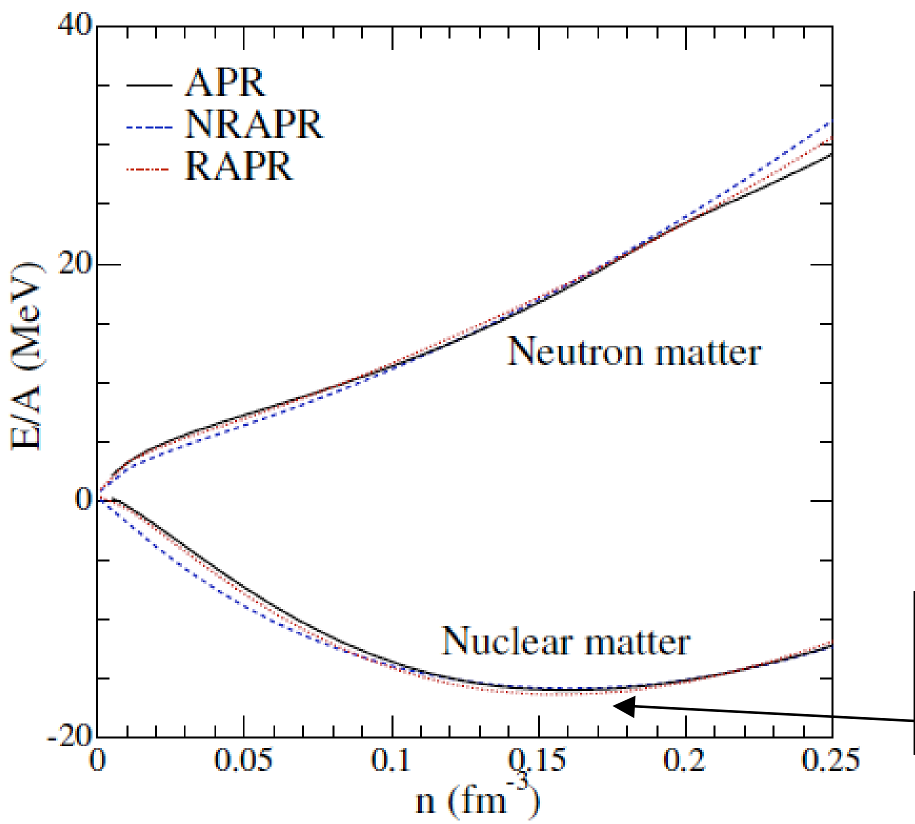
Nuclear matter with NN-only RG-evolved interactions



Perturbative….but
No saturation in sight

What infinite nuclear matter should look like

V18 + 3N (hard potentials)



[Akmal et al. calculations shown]

- Uniform with Coulomb turned off
- Density n (or often ρ)
- Fermi momentum $n = (\nu/6\pi^2)k_F^3$
- Neutron matter ($Z = 0$) has positive pressure
- Symmetric nuclear matter ($N = Z = A/2$) saturates

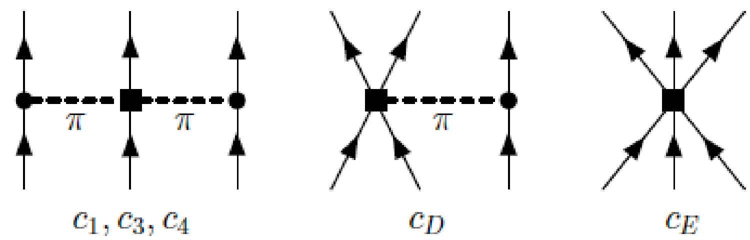
Q: How do we know it saturates?

NOTE: still saturates with V18 NN-only (but at too high density and overbound)

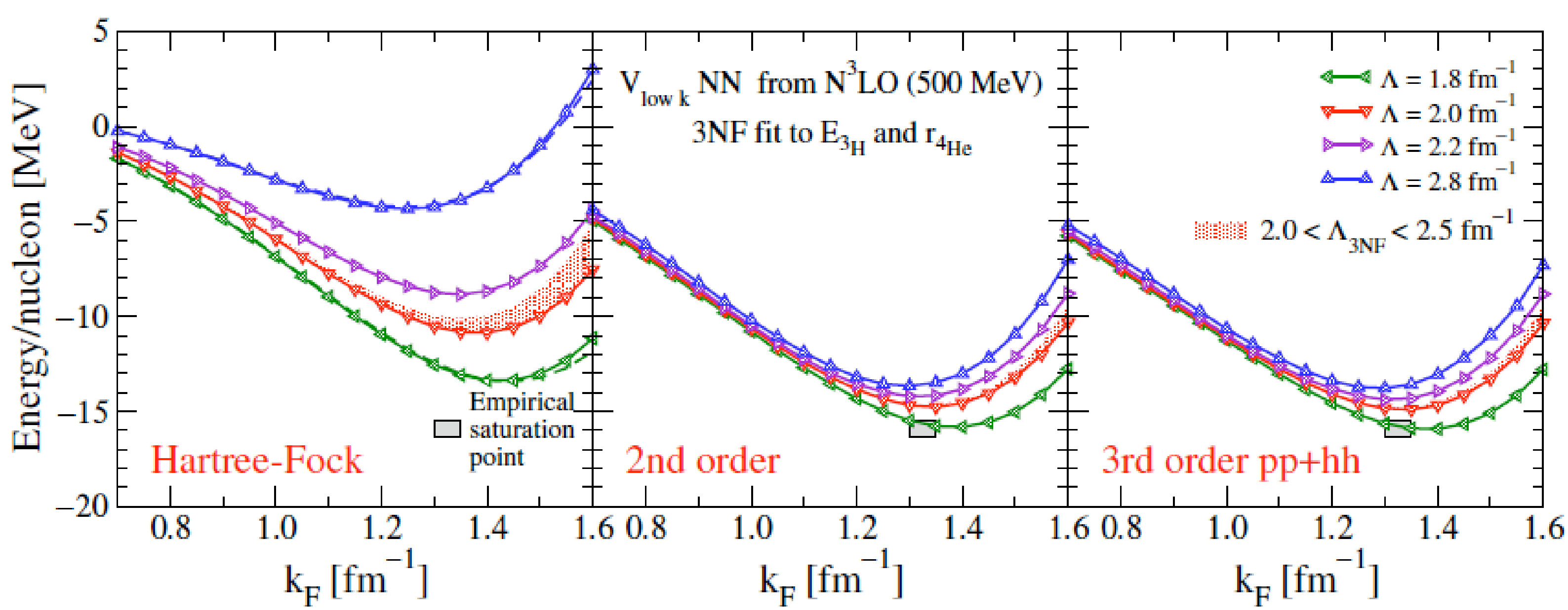
"Improved nuclear matter calculations from chiral low-momentum interactions"

K. Hebeler, S.K. Bogner, R.J. Furnstahl, A. Nogga, and A. Schwenk, Phys. Rev. C 83, 031301 (2011)

- Evolve Λ down with RG (to $\Lambda \approx 2\,\mathrm{fm}^{-1}$ for ordinary nuclei)
  - NN interactions fully, NNN interactions approximately
- Fit two 3NF constants to triton binding and ^{4}He radius
  $\Longrightarrow$ predict nuclear matter



Use effective $\overline{V}_{3N}$ in MBPT



"Improved nuclear matter calculations from chiral low-momentum interactions"

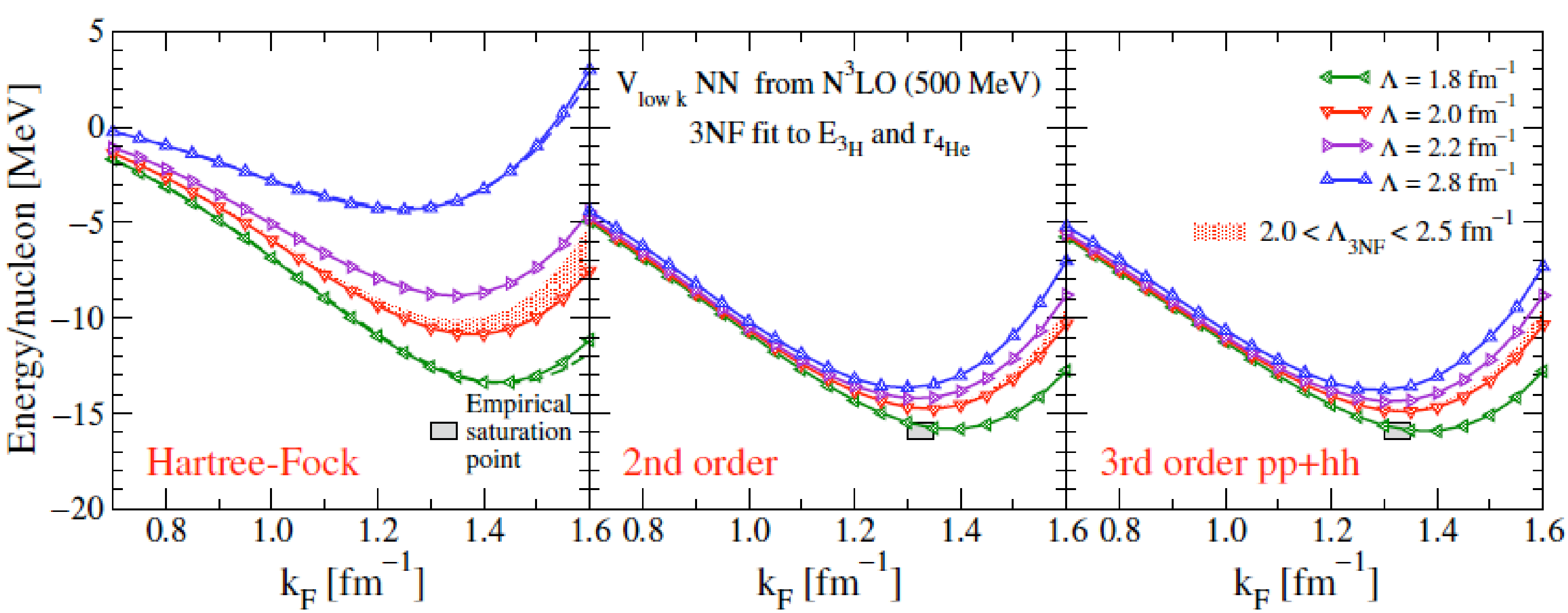
K. Hebeler, S.K. Bogner, R.J. Furnstahl, A. Nogga, and A. Schwenk, Phys. Rev. C 83, 031301 (2011)

- Reduced cutoff dependence
  (renormalization is working!)

- Hartree-Fock (mean-field theory) bound and saturates

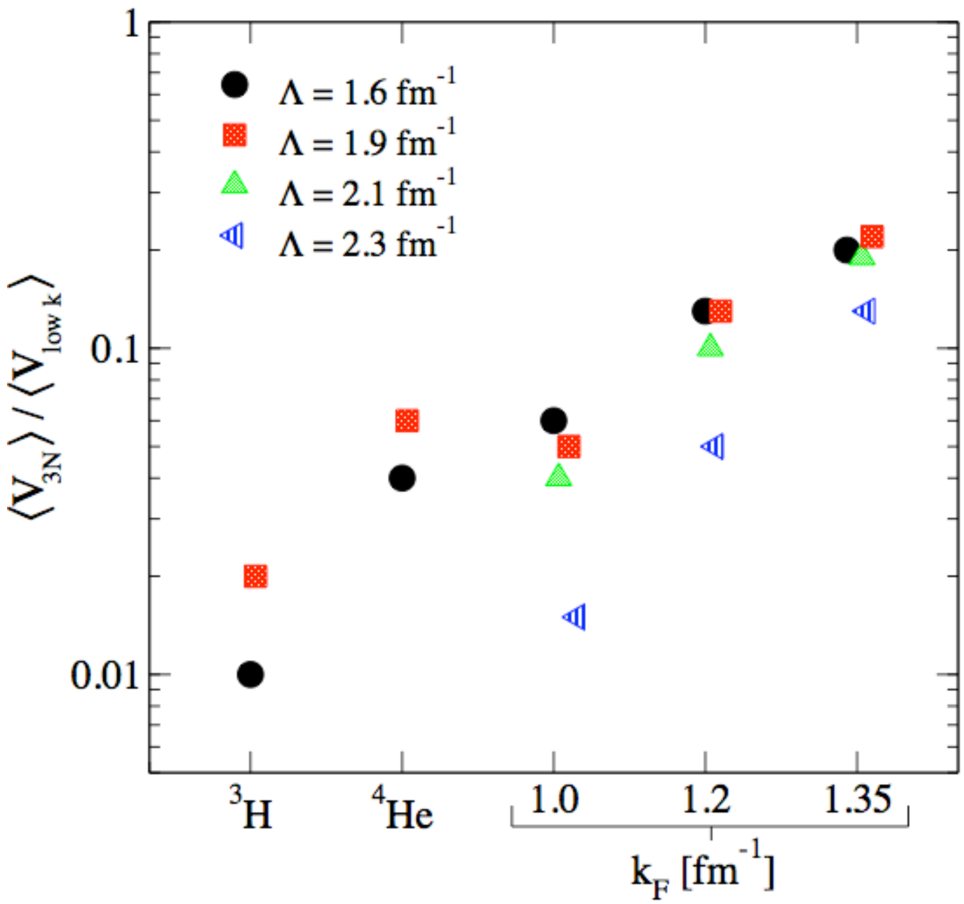
- Perturbation theory under control

Like quantum chemistry
Promising for DFT?



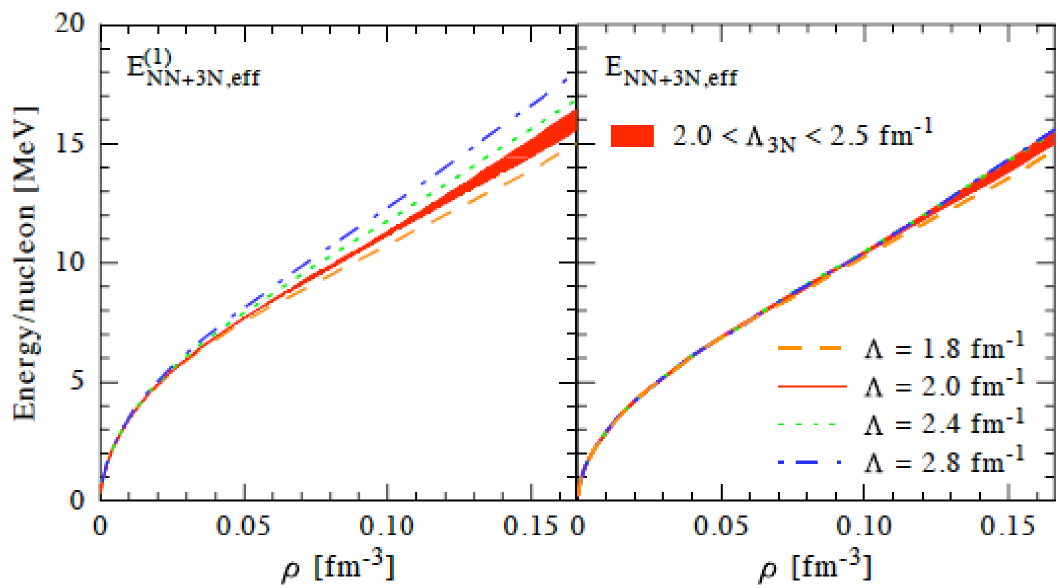
Q: If 3NF's play such a crucial role in giving saturation for low-k effective theories, does that mean it is unnaturally large

i.e., do we lose the nice hierarchy of terms (powercounting) in the input chiral EFT?

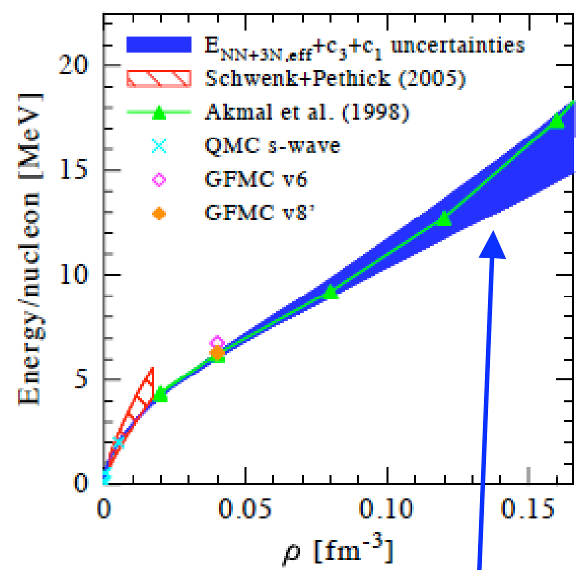


A: No. We still see the k_F/Λ suppression as predicted by the EFT powercounting

Application to neutron matter and neutron stars



K.Hebeler and A. Schwenk

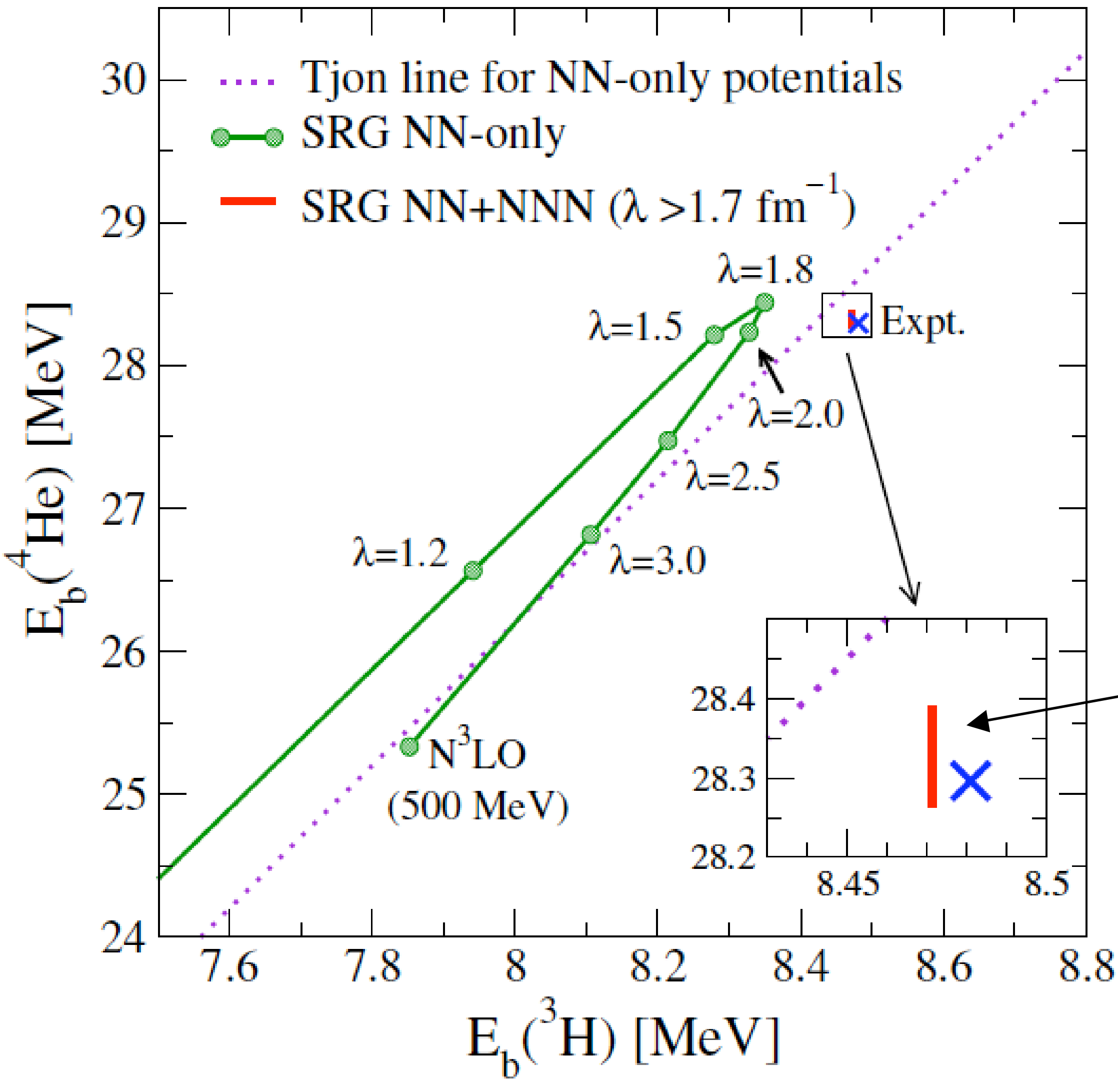


KH and A. Schwenk PRC 82, 014314 (2010)

- Significantly reduced cutoff dependence at 2nd order
- Energy sensitive to long-range 3NF c_3 variations
- Good agreement with other approaches (different NN)

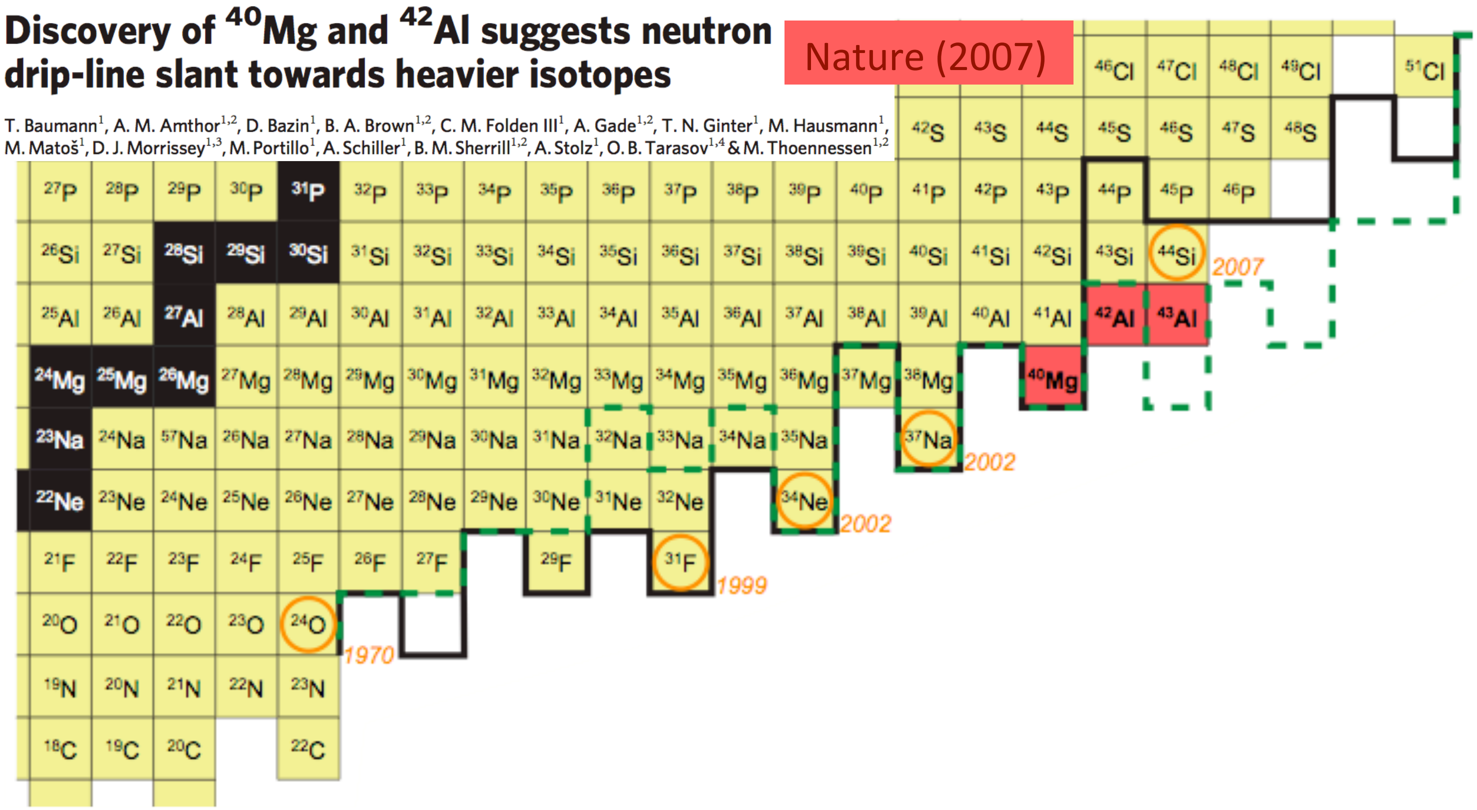
Theoretical error bands!

Tjon line revisited (cutoff dependence as a tool)



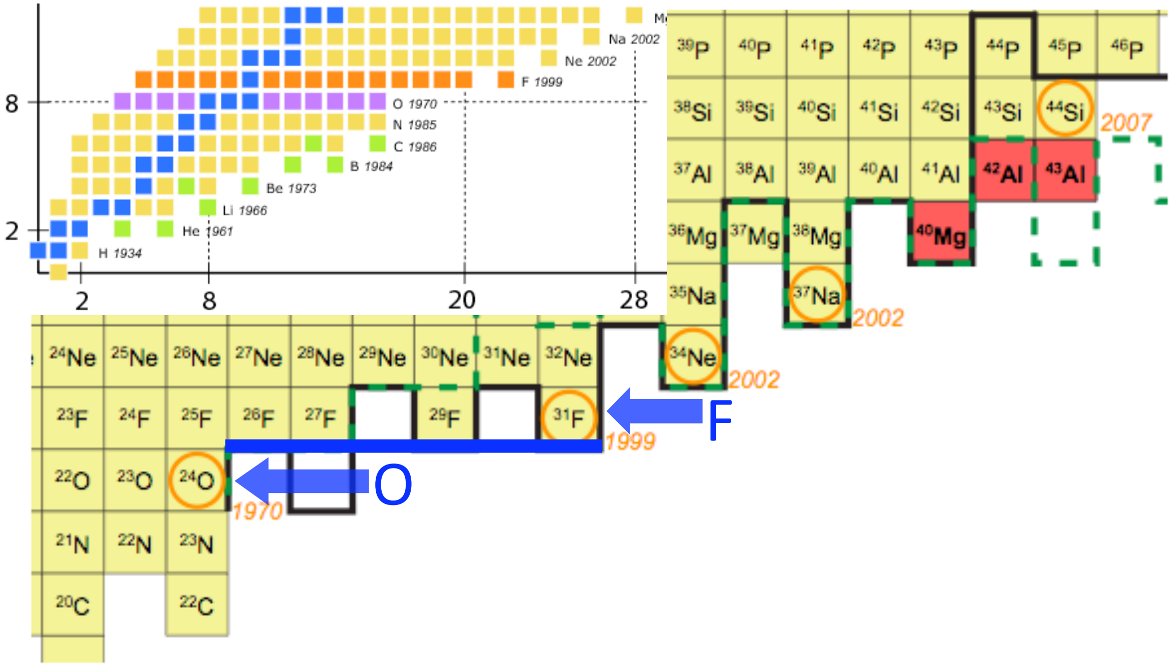
Negligible 4N forces are Induced!

3N forces and neutron-rich nuclei

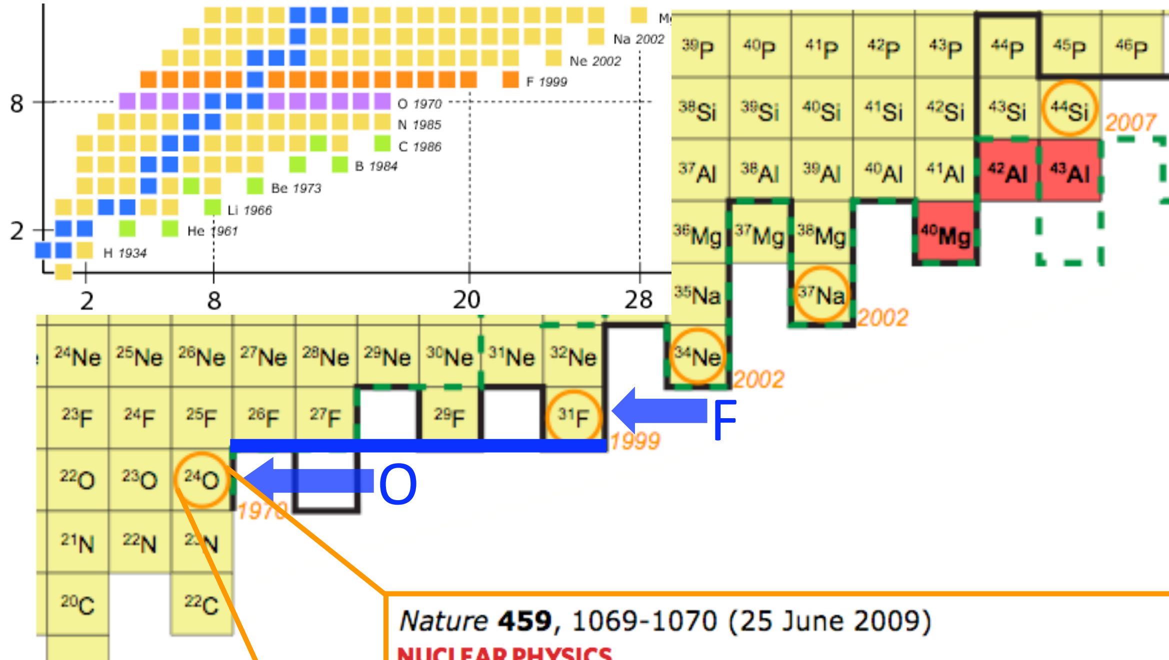


(Holt, Schwenk, Otsuka)

The oxygen anomaly



The oxygen anomaly



Nature **459**, 1069-1070 (25 June 2009)

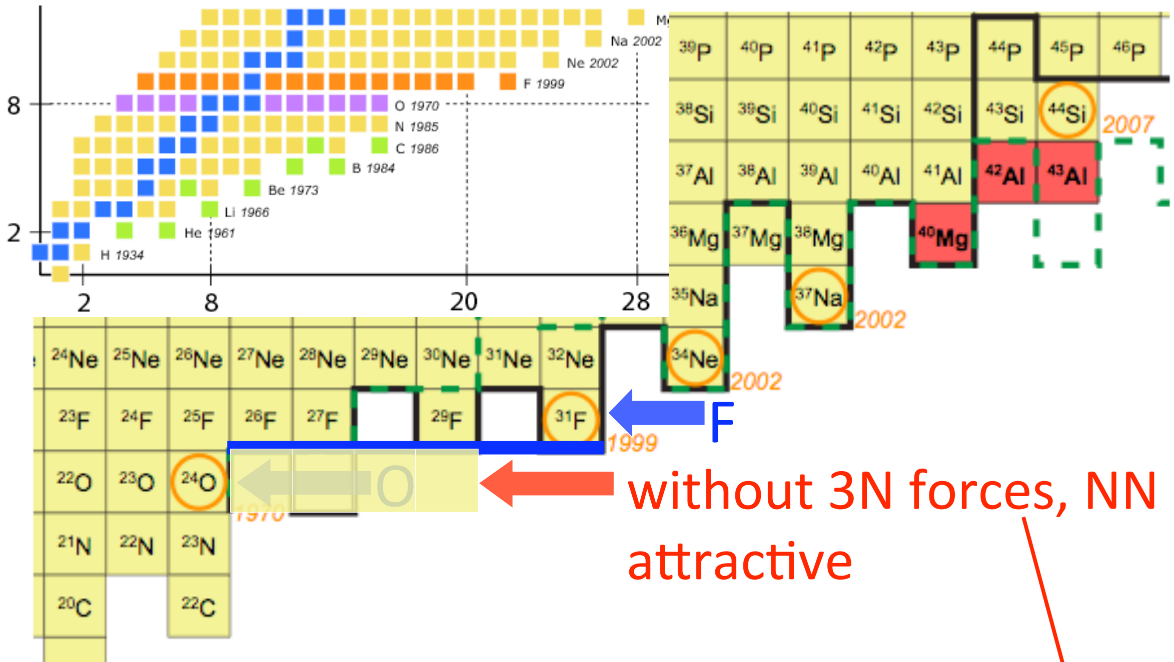
NUCLEAR PHYSICS

Unexpected doubly magic nucleus

Robert V. F. Janssens

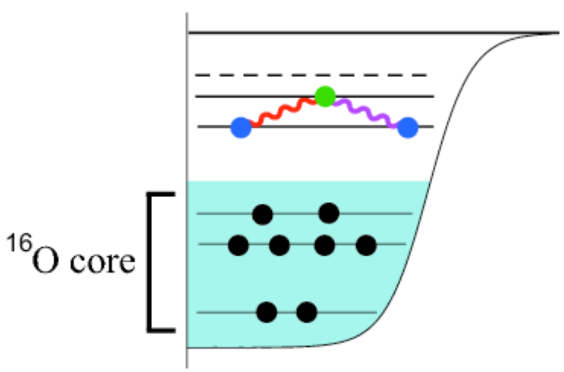
Nuclei with a 'magic' number of both protons and neutrons, dubbed doubly magic, are particularly stable. The oxygen isotope ^{24}O has been found to be one such nucleus — yet it lies just at the limit of stability.

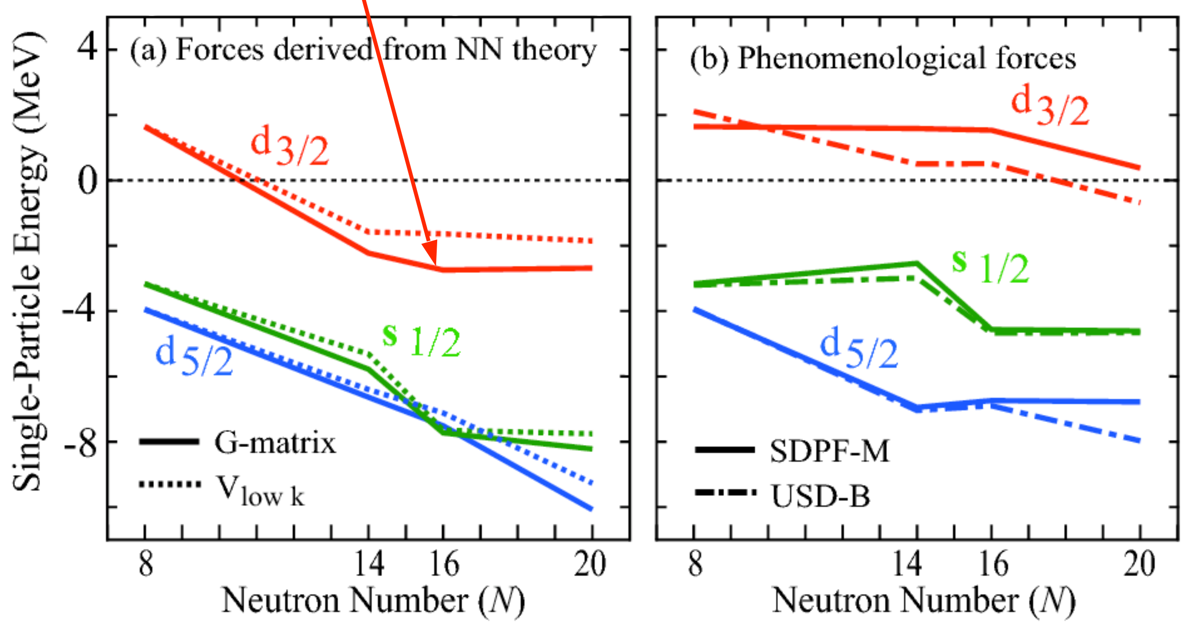
The oxygen anomaly - not reproduced without 3N forces



without 3N forces, NN interactions too attractive

drip-line incorrect at ^{28}O

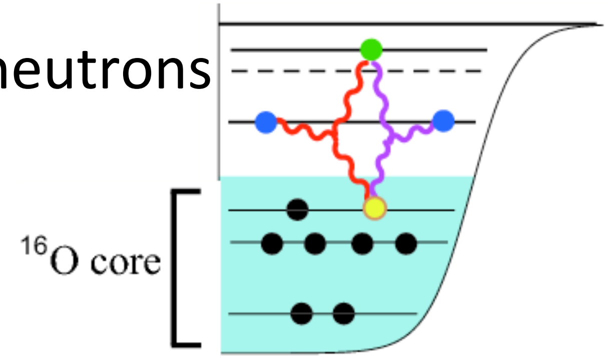




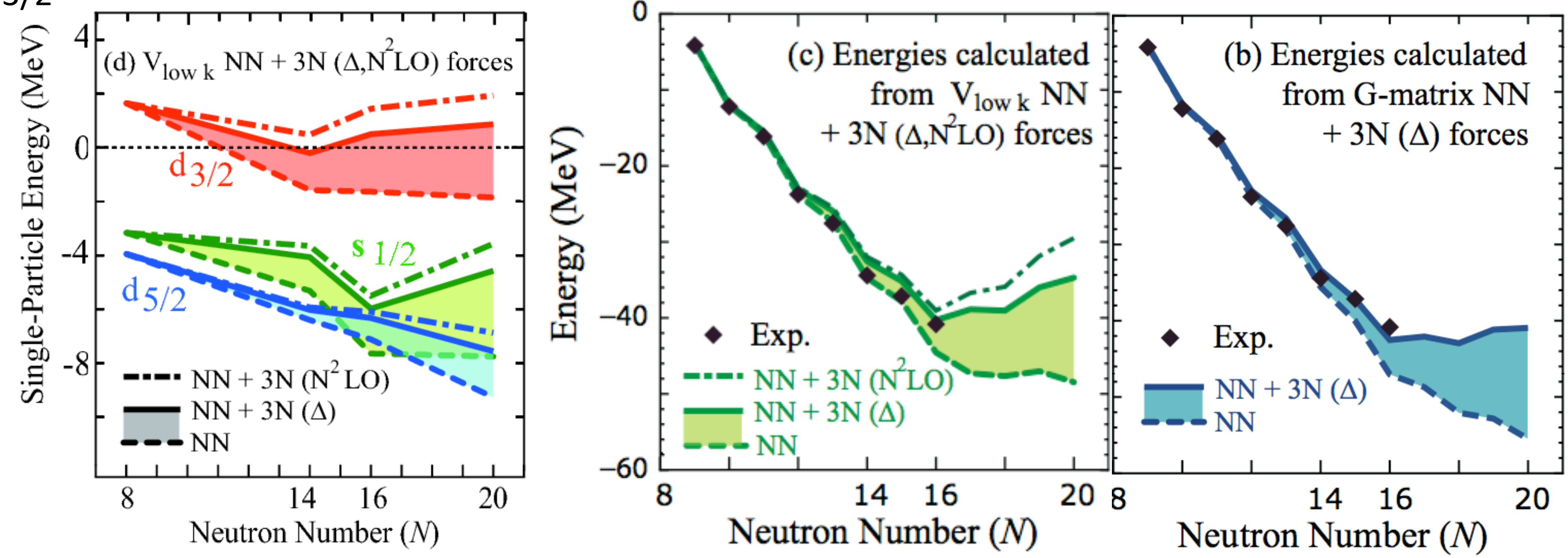
The oxygen anomaly - impact of 3N forces

include "normal-ordered" 2-body part of 3N forces (enhanced by core A)

leads to repulsive interactions between valence neutrons
(can understand partly based on Pauli principle)



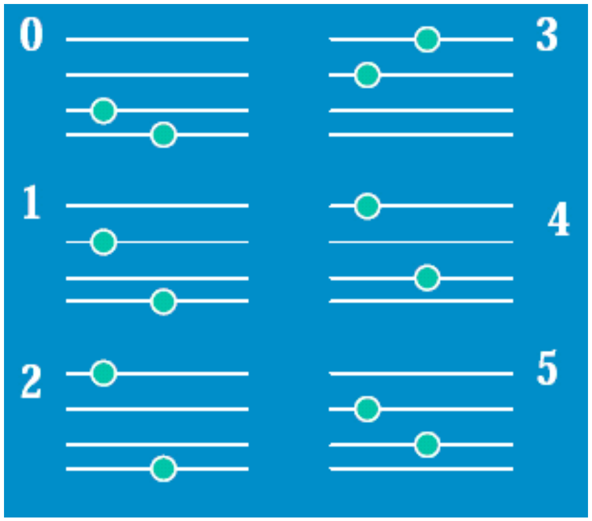
$d_{3/2}$ orbital remains unbound from ^{16}O to ^{28}O



first microscopic explanation of the oxygen anomaly

Otsuka et al., PRL (2010)

The N! catastrophe.
Specific example: 2 particles in 4 states



$$I=0 \quad a_2^+ a_1^+|--\rangle = |1100\rangle = |\Phi_0\rangle$$
$$I=1 \quad a_3^+ a_1^+|--\rangle = |1010\rangle = |\Phi_1\rangle$$
$$I=2 \quad a_4^+ a_1^+|--\rangle = |1001\rangle = |\Phi_2\rangle$$
$$I=3 \quad a_3^+ a_2^+|--\rangle = |0110\rangle = |\Phi_3\rangle$$
$$I=4 \quad a_4^+ a_2^+|--\rangle = |0101\rangle = |\Phi_4\rangle$$
$$I=5 \quad a_4^+ a_3^+|--\rangle = |0011\rangle = |\Phi_5\rangle$$

Scaling: Number of basis states

Ooops.. These are huge numbers

Problem : How to deal with such large dimensions

$n =$ number of particles;

$N =$ number of single - particle states

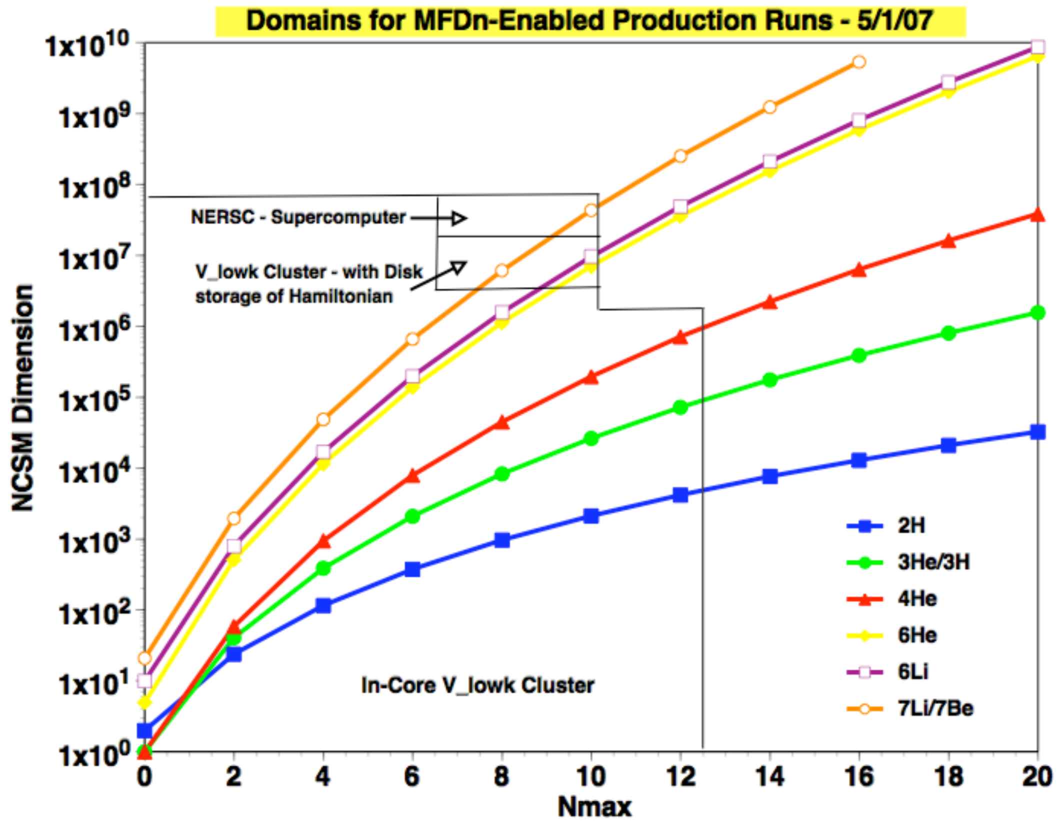
$$C(N,n) = \frac{N!}{(N-n)!\,n!}$$

$$C(10,100) = 1.7x10^{13}$$

$$C(1000,100) = 6x10^{139}$$

18

Limitations of Wave function Methods

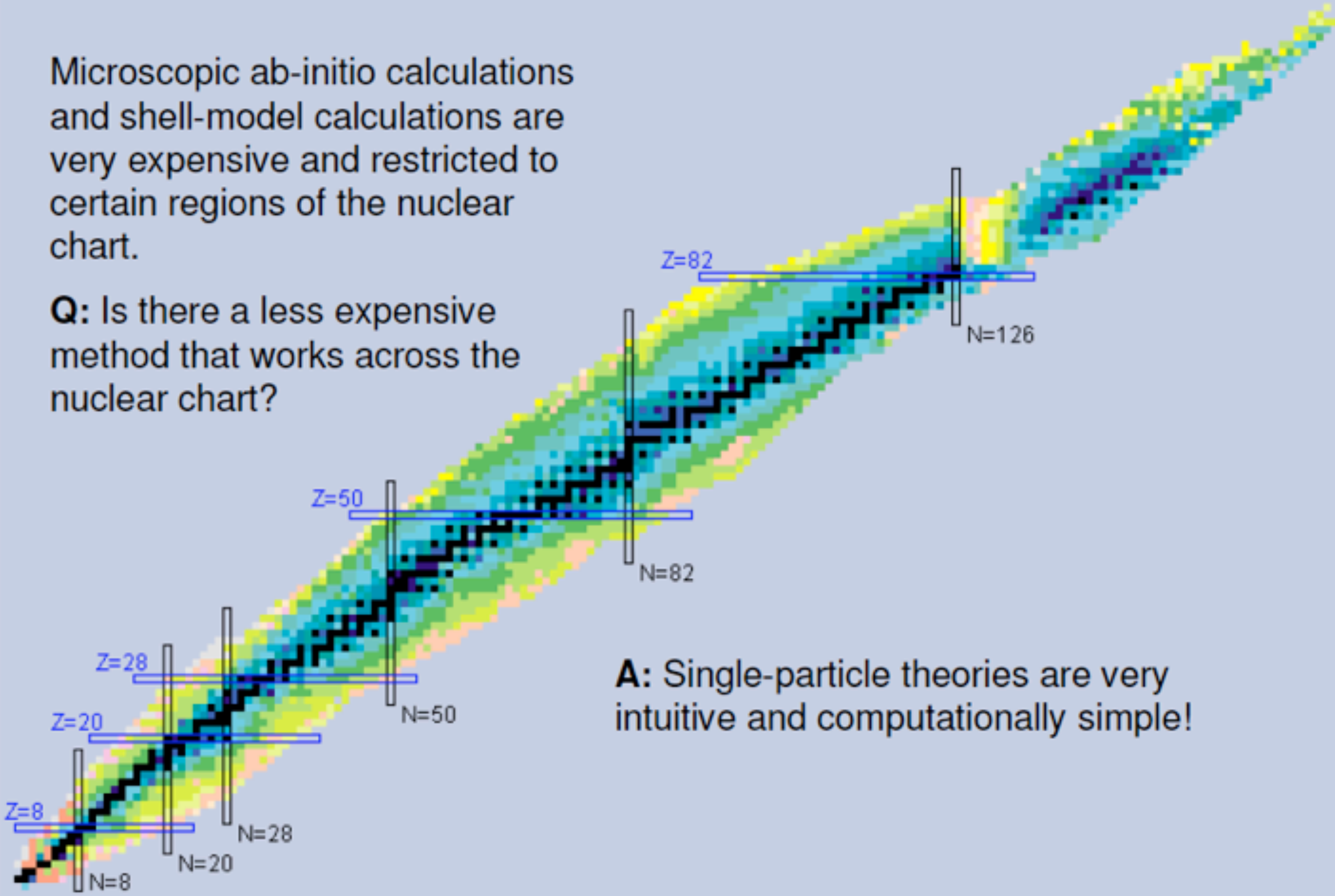


- Factorial/exponential growth with increasing A
- Conventional NN…N interactions => A_{max} ≈ 12
- RG softened NN….N interactions => A_{max} ≈ 40
- A_{max} ≈ 100 (??) w/coupled cluster + RG ?

Theoretical method for the entire nuclear chart ?

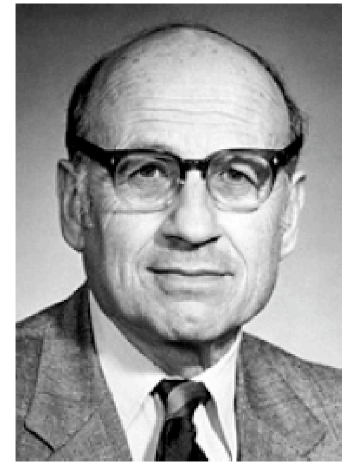
Microscopic ab-initio calculations and shell-model calculations are very expensive and restricted to certain regions of the nuclear chart.

Q: Is there a less expensive method that works across the nuclear chart?



A: Single-particle theories are very intuitive and computationally simple!

Nobel Prize in chemistry 1998



Walter Kohn

"for his development of the density-functional theory"

Two quotes from Kohn's Nobel lecture:

I begin with a provocative statement. *In general the many-electron wavefunction* $\Psi(r_1,...,r_N)$ *for a system of N electrons is not a legitimate scientific concept, when* $N \geq N_0$*, where* $N_0 \approx 10^3$.

I will use two criteria for defining "legitimacy": a) That Ψ can be calculated with sufficient accuracy and b) can be recorded with sufficient accuracy.

In concluding this section I remark that DFT, while *derived* from the N-particle Schroedinger equation, is finally expressed entirely in terms of the density $n(r)$, in the Hohenberg-Kohn formulation,[1] and in terms of $n(r)$ and *single*-particle wavefunctions $\psi_j(r)$, in the Kohn-Sham formulation[2]. This is why it has been most useful for systems of very many electrons where wavefunction methods encounter and are stopped by the "exponential wall".

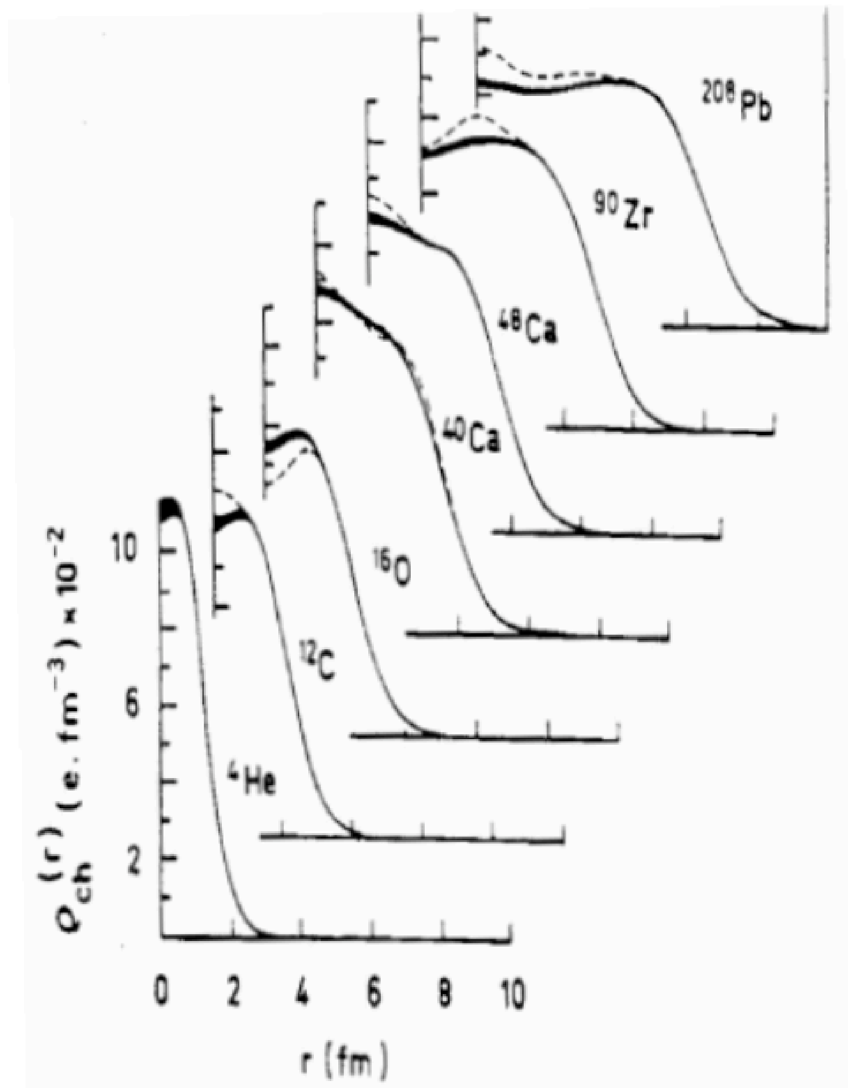
Density functional theory in a nutshell

- Hohenberg-Kohn: There exists an energy functional $E_{v_{\rm ext}}[\rho]$ ...

$$E_{v_{\rm ext}}[\rho] = F_{\rm HK}[\rho] + \int d^3x \, v_{\rm ext}(\mathbf{x})\rho(\mathbf{x})$$

- $F_{\rm HK}$ is *universal* (same for any external $v_{\rm ext}$) $\Longrightarrow$ H_2 to DNA!
- Useful if you can approximate the energy functional
- Introduce orbitals and minimize energy functional $\Longrightarrow E_{gs}, \rho_{gs}$

Solve a single particle equation (Kohn-Sham DFT)



Thermodynamic analogy

Alternative view: Energy functional is a Legendre transform (Lieb, 1983)

Find ground-state energy for all external potentials (this is a functional)

$$v(r) \to E[v(r)]$$

Perform functional Legendre transform

1. Compute density as functional derivative

$$\rho(r) = \frac{\delta E[v(r)]}{\delta v(r)}$$

2. Inversion: Find potential in terms of density
3. Construct Legendre transform

$$F[\rho(r)] \;=\; E[v(r)] - \int \mathrm{d}r v(r)\rho(r)$$

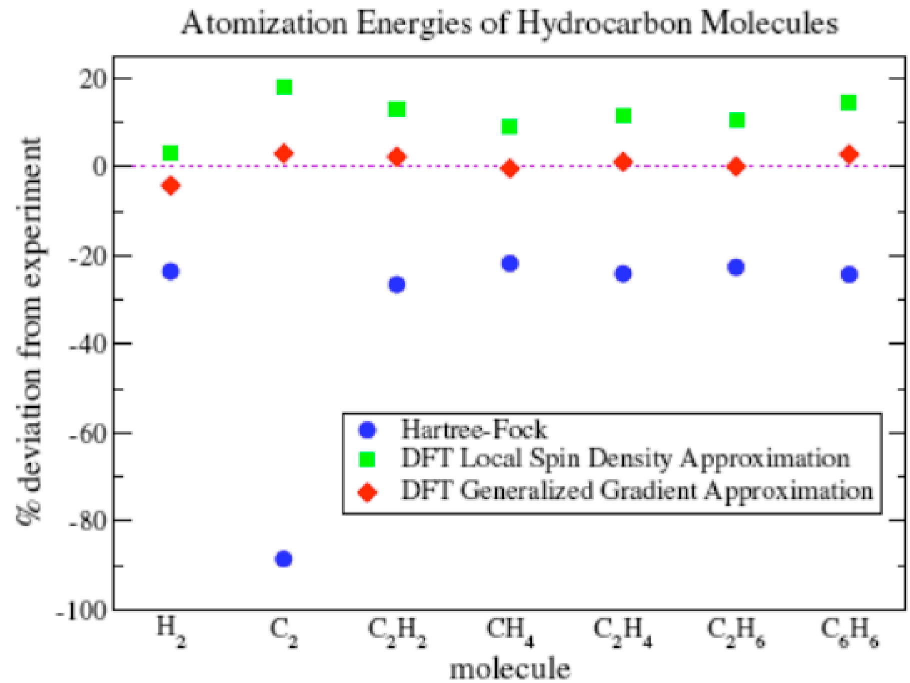
This path of construction can actually be followed for dilute Fermi gases!

Density Functional Theory (DFT) with Coulomb

- Dominant application: inhomogeneous electron gas
- Interacting point electrons in static potential of atomic nuclei
- “Ab initio” calculations of atoms, molecules, crystals, surfaces, . . .
- HF is good starting point, DFT/LDA is better, DFT/GGA is best

?!?

need accurate calculation of infinite e- gas



With RG-evolved interactions these are in reach for the nuclear case!

Hartree-Fock Wave Function

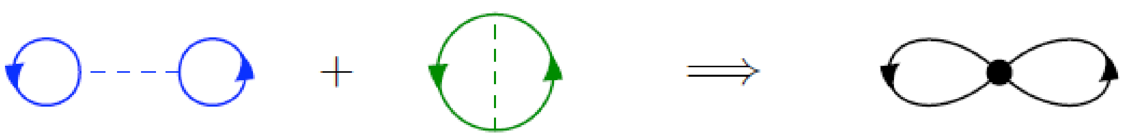
- Best single Slater determinant in variational sense

$$|\Psi_{\rm HF}\rangle = \det\{\phi_i(\mathbf{x}), i = 1\cdots A\}\,, \quad \mathbf{x} = (\mathbf{r}, \sigma, \tau)$$

- The $\phi_i(\mathbf{x})$ satisfy *non-local* Schrödinger equations:

$$-\frac{\nabla^2}{2M}\phi_i(\mathbf{x}) + V_{\rm H}(\mathbf{x})\phi_i(\mathbf{x}) + \int d\mathbf{y}\, V_{\rm E}(\mathbf{x},\mathbf{y})\phi_i(\mathbf{y}) = \epsilon_i\phi_i(\mathbf{x})$$

with $V_{\rm H}(\mathbf{x}) = \int d\mathbf{y} \sum_{j=1}^{A} |\phi_j(\mathbf{y})|^2 \mathbf{v}(\mathbf{x},\mathbf{y})\,, \quad V_{\rm E}(\mathbf{x},\mathbf{y}) = -v(\mathbf{x},\mathbf{y}) \sum_{j=1}^{A} \phi_j(\mathbf{x})\phi_j^*(\mathbf{y})$



- Solve self-consistently using occupied orbitals for V_H and V_E
- Slater determinants from *all* orbitals forms an A-body basis

Phenomenological Skyrme Functionals

- Minimize $E = \int d\mathbf{x}\, \mathcal{E}[\rho(x), \tau(x), \mathbf{J}(\mathbf{x}), \ldots]$ (for $N = Z$):

$$
\begin{aligned}
\mathcal{E}[\rho, \tau, \mathbf{J}] \;=\; & \frac{1}{2M}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau \\
& + \frac{1}{64}(9t_1 - 5t_2)(\nabla\rho)^2 - \frac{3}{4}W_0\rho\nabla\cdot\mathbf{J} + \frac{1}{32}(t_1 - t_2)\mathbf{J}^2
\end{aligned}
$$

- where $\rho(x) = \sum_i |\phi_i(x)|^2$ and $\tau(x) = \sum_i |\nabla\phi_i(x)|^2$ (and $\mathbf{J}$)

t_0, t_1, W_0, α, etc. are fit to infinite nuclear matter properties and to
Some set of finite nuclei data

Phenomenological Skyrme Functionals

- Minimize $E = \int d\mathbf{x}\, \mathcal{E}[\rho(x), \tau(x), \mathbf{J}(\mathbf{x}), \ldots]$ (for $N = Z$):

$$\mathcal{E}[\rho,\tau,\mathbf{J}] = \frac{1}{2M}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)(\nabla\rho)^2 - \frac{3}{4}W_0\rho\nabla\cdot\mathbf{J} + \frac{1}{32}(t_1 - t_2)\mathbf{J}^2$$

  - where $\rho(x) = \sum_i |\phi_i(x)|^2$ and $\tau(x) = \sum_i |\nabla\phi_i(x)|^2$ (and $\mathbf{J}$)

- Varying the (normalized) ϕ_i's yields "Kohn-Sham" equation:

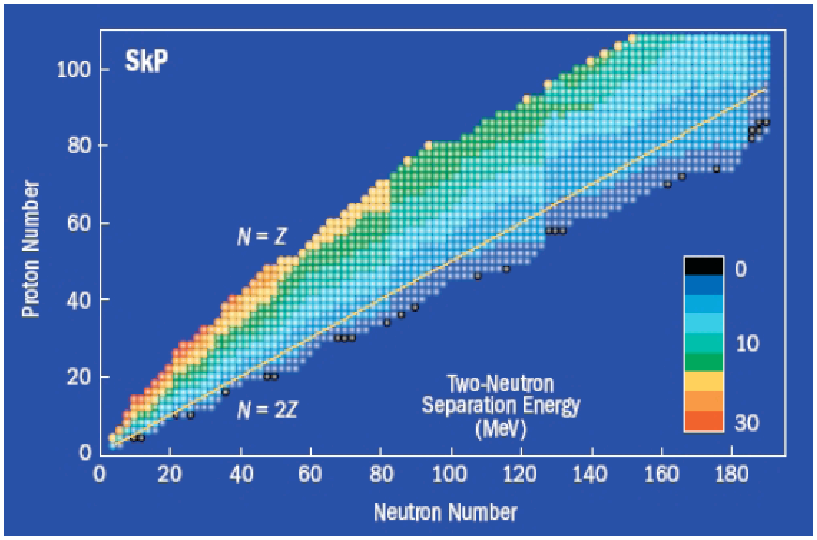
$$\left(-\nabla\frac{1}{2M^*(\mathbf{x})}\nabla + U(\mathbf{x}) + \frac{3}{4}W_0\nabla\rho\cdot\frac{1}{i}\nabla\times\sigma\right)\phi_\mathrm{I}(\mathbf{x}) = \epsilon_\mathrm{I}\,\phi_\mathrm{I}(\mathbf{x}) ,$$

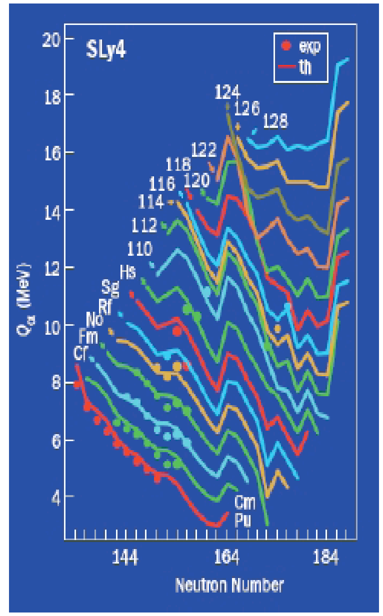
$U = \frac{3}{4}t_0\rho + (\frac{3}{16}t_1 + \frac{5}{16}t_2)\tau + \cdots$ and $\frac{1}{2M^*(\mathbf{x})} = \frac{1}{2M} + (\frac{3}{16}t_1 + \frac{5}{16}t_2)\rho$

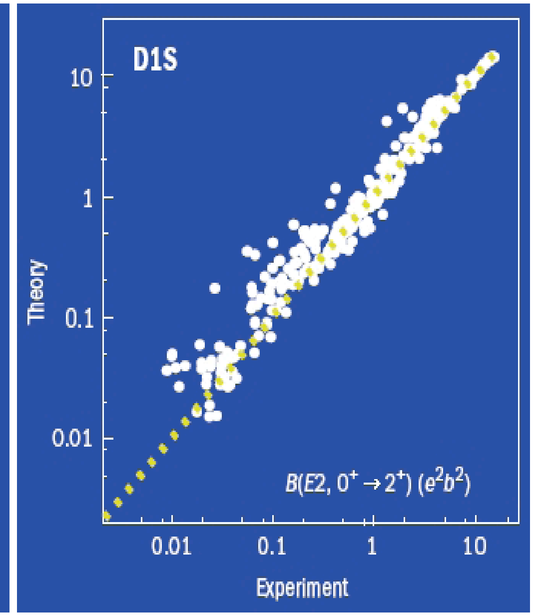
- Iterate until ϕ_i's and ϵ_i's are self-consistent
- In practice: other densities, pairing is very important (HFB), projection needed, . . .

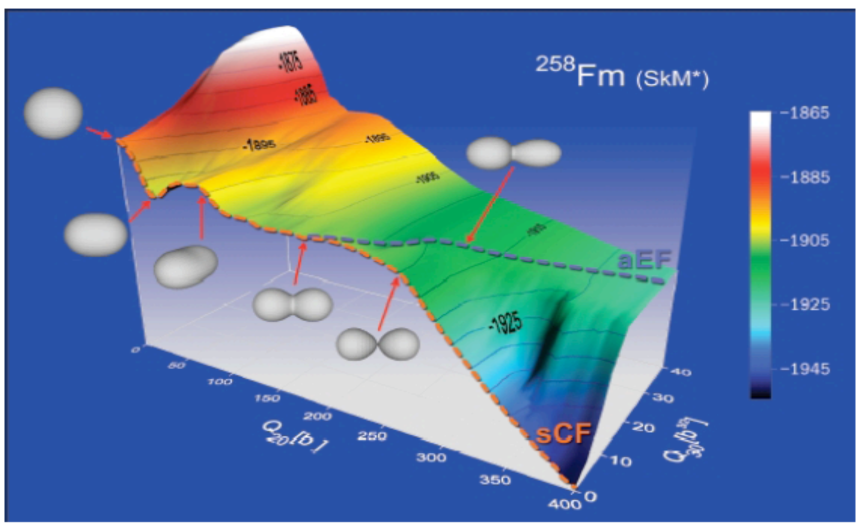
> • Solve simple Hartree-like equations
> • DFT is exact if the "true" E[ρ]

Accomplishments of Phenomenological Energy Functionals





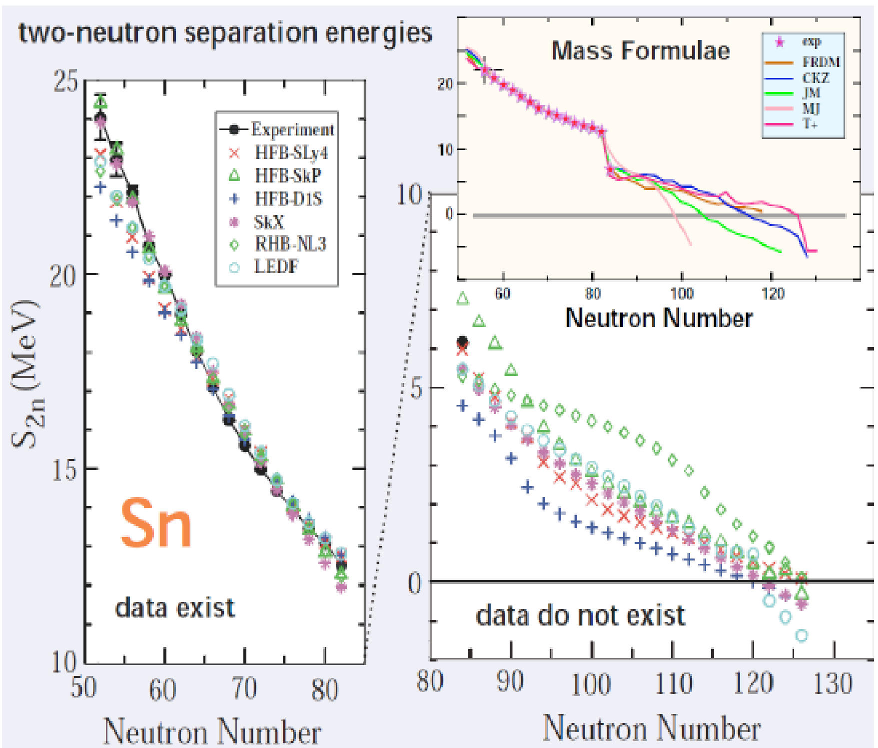


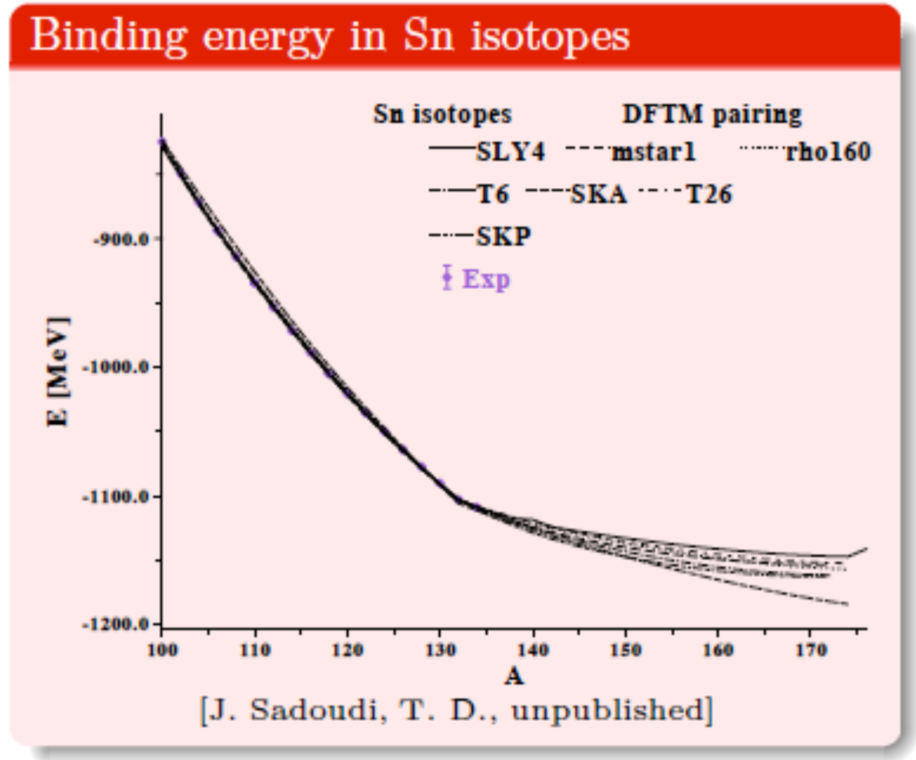


2N separation energies, Quadrupole and BE2 values, Fission energy surfaces, mass tables in a day, plus many other impressive feats

BUT...

Limitations of Existing Energy Functionals (Predictability)





- Uncontrolled extrapolations away from known data!
- Loss of predictive power
- Theoretical error-bars?

What's missing in phenomenological EDFs ?

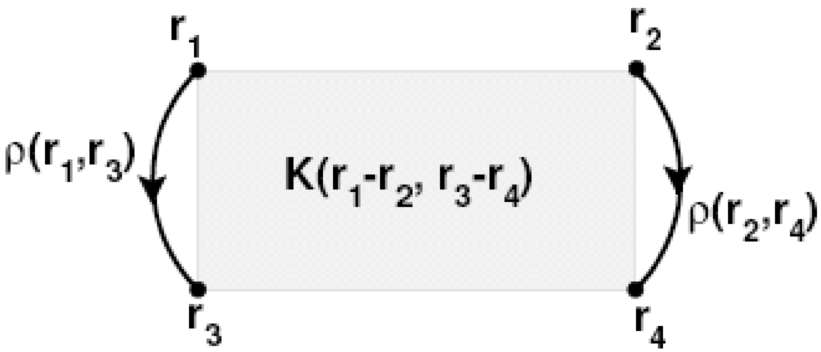
- Density dependencies too simplistic (integer powers)
- Isovector components not well constrained (pions!)
- No way to estimate theoretical uncertainties
- What's the connection to many-body forces?

Turn to microscopic many body theory for guidance, aided by the simplifications enabled by RG-evolved interactions

Local Skyrme-like Functionals from RG-evolved Interactions

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 of non-local quantities

density matrices
finite range interaction vertex 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

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

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

Dependence on local densities/currents now manifest

$$\langle V_2 \rangle \sim \sum_{n,m} \int d\mathbf{R}\, \mathcal{O}_n(\mathbf{R}) \mathcal{O}_m(\mathbf{R}) \int d\mathbf{r}\, \Pi_n(k_F r) \Pi_m(k_F r) V_2(r)$$

$$\sim \sum_t \int d\mathbf{R} \left\{ C_t^{\rho\rho} \rho_t^2 + C_t^{\rho\tau} \rho_t \tau_t + C_t^{\rho\Delta\rho} \rho_t \Delta\rho_t + C_t^{JJ} \mathbf{J}_t^2 + C_t^{J\nabla\rho} \mathbf{J}_t \nabla\rho_t \cdots \right\}$$

Skyrme-like EDF but with **density-dependent** couplings
dominated by long-range pion-physics

Prescriptions for Π_n-functions

Phase space averaging (PSA-DME) (Gebremariam et al. arXiv:0910.4979)

$$\rho(\vec{r}_1, \vec{r}_2) = e^{i\vec{r}\cdot\vec{k}}\, e^{\frac{\vec{r}}{2}\cdot(\nabla_1 - \nabla_2) - i\vec{r}\cdot\vec{k}} \rho(\vec{r}_1, \vec{r}_2)\Big|_{\vec{r}_1 = \vec{r}_2 = \vec{R}}$$

Average the non-locality operator over local momentum distribution g(**R**,**k**) and expand exponentiated gradients

$$\rho(\vec{r}_1, \vec{r}_2) \approx \int d^3\vec{k}\; g(\vec{R}, \vec{k})\, e^{i\vec{k}\cdot\vec{r}} \sum_{n=0}^{2} \frac{1}{n!} \left\{ \vec{r}\cdot\left(\frac{\nabla_1 - \nabla_2}{2} - i\vec{k} \right) \right\}^n \rho(\vec{r}_1, \vec{r}_2)\Big|_{\vec{r}_1 = \vec{r}_2 = \vec{R}}$$

Easy to build in physics associated with surface effects in finite fermi systems (spin-orbit physics)

Exact in homogenous infinite matter limit

Including Long Range Chiral EFT in Skyrme-like EDFs

$$V_{EFT} = V_{ct}(\Lambda) + V_{1\pi} + V_{2\pi} + \cdots$$

Each EDF coupling function at HF-level splits into 2 terms

1) Λ-**dependent** Skyrme-like coupling **constants (short-distance)**
2) Λ-**independent** coupling **functions** from "universal" pion physics

$$C_t^{\rho\tau} \Rightarrow C_t^{\rho\tau}(\Lambda; V_{ct}) + C_t^{\rho\tau}[k_F(\mathbf{R}); V_\pi]$$ Etc…

From contact terms in EFT/RG V's

From pion exchanges

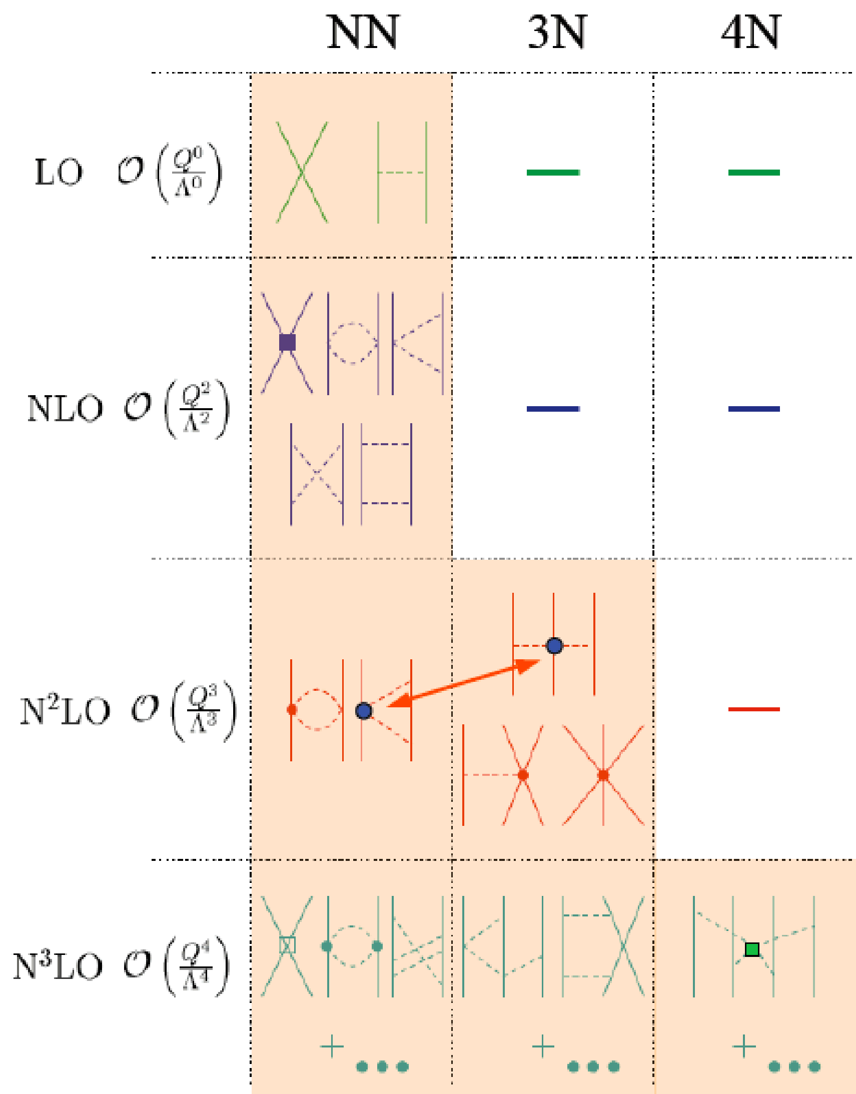
Suggests a microscopically-improved Skyrme phenomenology

Add pion-exchange couplings to existing Skyrmes and refit constants using guidance from EFT (naturalness, etc.)

Gameplan - Include pion physics in Skyrme EDFs and refit

- Include DME coupling functions from finite-range NN and NNN chiral EFT thru N2LO
- Refit the contact coupling constants (EFT constraints => naturalness)
- Look for improved observables and for sensitivities
- Can we "see" the pion as in NN phase shift analyses ?

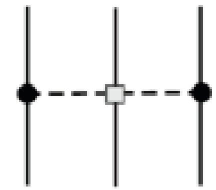
Expect interesting spin-orbit consequences (NN vs NNN)



in progress w/ORNL group (Stoitsov et al.)

New development: DME for chiral NNN force (N2LO)

- Expect interesting spin-orbit/tensor couplings from TPE



$$V_c(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) \sim \frac{\sigma_1 \cdot \mathbf{q_1} \sigma_2 \cdot \mathbf{q_2}}{(q_1^2 + m_\pi^2)(q_2^2 + m_\pi^2)} F_{123}^{\alpha\beta} \tau_1^\alpha \tau_2^\beta + perms$$

$$F_{123}^{\alpha\beta} \equiv \delta_{\alpha\beta}\left[-4\frac{c_1 m_\pi^2}{f_\pi^2} + 2\frac{c_3}{f_\pi^2}\mathbf{q}_1 \cdot \mathbf{q}_2\right] + \frac{c_4}{f_\pi^2}\epsilon^{\alpha\beta\gamma}\tau_3^\gamma \sigma_3 \cdot (\mathbf{q}_1 \times \mathbf{q}_2)$$

Empirical EDFs (Skyrme, Gogny,...) spin-orbit coupling is density independent => appropriate for NN spin-orbit forces (short range)

This is a mismatch since microscopic NNN interactions are long-range (DME ==> strong density dependent J·∇ρ couplings)

$$
\begin{aligned}
\mathcal{E}^{CR4,2x} = \int d\vec{r}\Big\{ & C_7^{\rho_0^3}\,\rho_0^3(\vec{r}) + C_7^{\rho_0\rho_1^2}\,\rho_0(\vec{r})\,\rho_1^2(\vec{r}) + C_7^{\rho_0\rho_1\varsigma_1^1}\,\rho_0(\vec{r})\,\rho_1(\vec{r})\,\varsigma_1^1(\vec{r}) \\
& + C_7^{\rho_0^2\Delta\rho_0}\,\rho_0^2(\vec{r})\,\Delta\rho_0(\vec{r}) + C_7^{\rho_0\rho_1\Delta\rho_1}\,\rho_0(\vec{r})\,\rho_1(\vec{r})\,\Delta\rho_1(\vec{r}) + C_7^{\rho_0^2\varsigma_0^2}\,\rho_0^2(\vec{r})\,\varsigma_0^2(\vec{r}) \\
& + C_7^{\rho_1^2\varsigma_0^2}\,\rho_1^2(\vec{r})\,\varsigma_0^2(\vec{r}) + C_7^{\rho_0\rho_1\varsigma_1^2}\,\rho_0(\vec{r})\,\rho_1(\vec{r})\,\varsigma_1^2(\vec{r}) + C_7^{\rho_0^2\varsigma_0^1}\,\rho_0^2(\vec{r})\,\varsigma_0^1(\vec{r}) \\
& + C_7^{\rho_0 J_0^2}\,\rho_0(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r}) + C_7^{\rho_1 J_0 J_1}\,\rho_1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_1(\vec{r}) + C_7^{\rho_0 J_1^2}\,\rho_0(\vec{r})\,\vec{J}_1(\vec{r})\cdot\vec{J}_1(\vec{r}) \\
& + C_7^{J_0^2\nabla J_0}\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r}) + C_7^{J_1^2\nabla J_0}\,\vec{J}_1(\vec{r})\cdot\vec{J}_1(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r}) + C_7^{J_0 J_1\nabla J_1}\,\vec{J}_0(\vec{r})\,\vec{J}_1(\vec{r})\,\vec{\nabla}\cdot\vec{J}_1(\vec{r}) \\
& + C_7^{\Delta\rho_0 J_0^2}\,\Delta\rho_0(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r}) + C_7^{\varsigma_0^2 J_0^2}\,\varsigma_0^2(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r}) + C_7^{\varsigma_0^1 J_0^2}\,\varsigma_0^1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r}) \\
& + C_7^{\nabla\rho_0 J_0\nabla J_0}\,\vec{\nabla}\rho_0(\vec{r})\,\vec{J}_0(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r}) + C_7^{\rho_0\nabla J_0\nabla J_0}\,\rho_0(\vec{r})\,[\vec{\nabla}\cdot\vec{J}_0(\vec{r})]^2 + C_7^{\rho_0 J_0\Delta J_0}\,\rho_0(\vec{r})\,\vec{J}_0(\vec{r})\cdot\Delta\vec{J}_0(\vec{r}) \\
& + C_7^{\varsigma_1^1 J_0 J_1}\,\varsigma_1^1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_1(\vec{r}) + C_7^{\Delta\rho_1 J_0 J_1}\,\Delta\rho_1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_1(\vec{r}) + C_7^{\varsigma_1^2 J_0 J_1}\,\varsigma_1^2(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_1(\vec{r}) \\
& + C_7^{\nabla\rho_1 J_1\nabla J_0}\,\vec{\nabla}\rho_1(\vec{r})\cdot\vec{J}_1(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r}) + C_7^{\rho_1 J_1\Delta J_0}\,\rho_1(\vec{r})\,\vec{J}_1(\vec{r})\cdot\Delta\vec{J}_0(\vec{r}) + C_7^{\varsigma_0^2 J_1^2}\,\varsigma_0^2(\vec{r})\,\vec{J}_1(\vec{r})\cdot\vec{J}_1(\vec{r}) \\
& + C_7^{\nabla\rho_1 J_0\nabla J_1}\,\vec{\nabla}\rho_1(\vec{r})\cdot\vec{J}_0(\vec{r})\,\vec{\nabla}\cdot\vec{J}_1(\vec{r}) + C_7^{\rho_1\nabla J_0\nabla J_1}\,\rho_1(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r})\,\vec{\nabla}\cdot\vec{J}_1(\vec{r}) + C_7^{\rho_0\nabla J_1\nabla J_1}\,\rho_0(\vec{r})\,[\vec{\nabla}\cdot\vec{J}_1(\vec{r})]^2 \\
& + C_7^{\rho_1 J_0\Delta J_1}\,\rho_1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\Delta\vec{J}_1(\vec{r}) + C_7^{\rho_0 J_1\Delta J_1}\,\rho_0(\vec{r})\,\vec{J}_1(\vec{r})\cdot\Delta\vec{J}_1(\vec{r})\Big\}. \qquad (91)
\end{aligned}
$$

+ 4 other classes of similar terms

Looks ugly (or beautiful, depending on your view), but a regular structure emerges:

$$C^{ijk}[u]\xi_i\xi_j\xi_k\ , \quad u \equiv \frac{k_F(R)}{m_\pi}$$

(note: u is NOT small)

$$C^{ijk}[u] = C_1^{ijk}[u] + C_2^{ijk}[u]\ \ln(1+4u^2) + C_3^{ijk}[u]\arctan(2u),$$

$$C_\alpha^{ijk}[u] = \text{rational polynomial}$$

Including NN and NNN pion-exchanges in Skyrme EDFs

Pre-optimization (test if we can calculate with the new EDF)

Parameters	SLY4	SLY4′	LO	NLO	N2LO
		Volume Parameters			
$C_{00}^{\rho^2}$		-933.342	-727.093	-757.689	-607.108
$C_{10}^{\rho^2}$		830.052	474.871	477.931	316.939
$C_{0D}^{\rho^2}$		861.062	612.104	628.504	-1082.854
$C_{1D}^{\rho^2}$		-1064.273	-705.739	-694.665	-4369.425
$C_0^{\rho\tau}$		57.129	33.885	18.471	322.4
$C_1^{\rho\tau}$		24.657	32.405	92.233	-156.901
γ		0.16667	0.30622	0.287419	1.06429
		Surface Parameters			
$C_0^{\rho\Delta\rho}$	-76.287	-76.180	-67.437	-63.996	-197.132
$C_1^{\rho\Delta\rho}$	15.951	24.823	21.551	-9.276	-12.503
$C_0^{\rho\nabla J}$	-92.250	-92.959	-95.451	-95.463	-193.188
$C_1^{\rho\nabla J}$	-30.75	-82.356	-65.906	-60.800	37.790
		Pairing Parameters			
V_n	-258.992	-232.135	-241.203	-241.484	-272.164
V_p	-258.992	-244.050	-252.818	-252.222	-286.965
		SVD Optimization Results			
χ^2	12.5002	2.1235	1.837	1.7662	1.7884
$RMSD(E)$	7.008	2.6931	2.5539	2.5143	2.590
$RMSD(\Delta_n)$	0.1297	0.0828	0.0587	0.0554	0.0476
$RMSD(\Delta_p)$	0.094	0.0988	0.0902	0.0866	0.0706

- non-derivative contacts fixed to infinite nuclear matter saturation
- gradient contacts fixed to finite nuclei data
- SLY4 and SLY'4 are Conventional Skyrme results
- Small but robust reduction In RMS errors when include pion physics via DME

Including NN and NNN pion-exchanges in Skyrme EDFs

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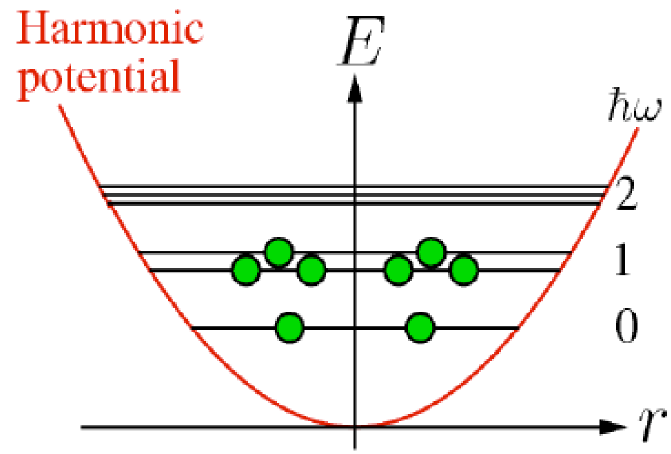
Didn't expect to improve Bulk properties, but **we did**

Hope to see big improvements for single particle spectra (spectroscopy)

next step: Large scale optimization and calculations across the mass table

Neutron drops and DFT

- inhomogeneous neutron matter can be studied theoretically in some trapping potential



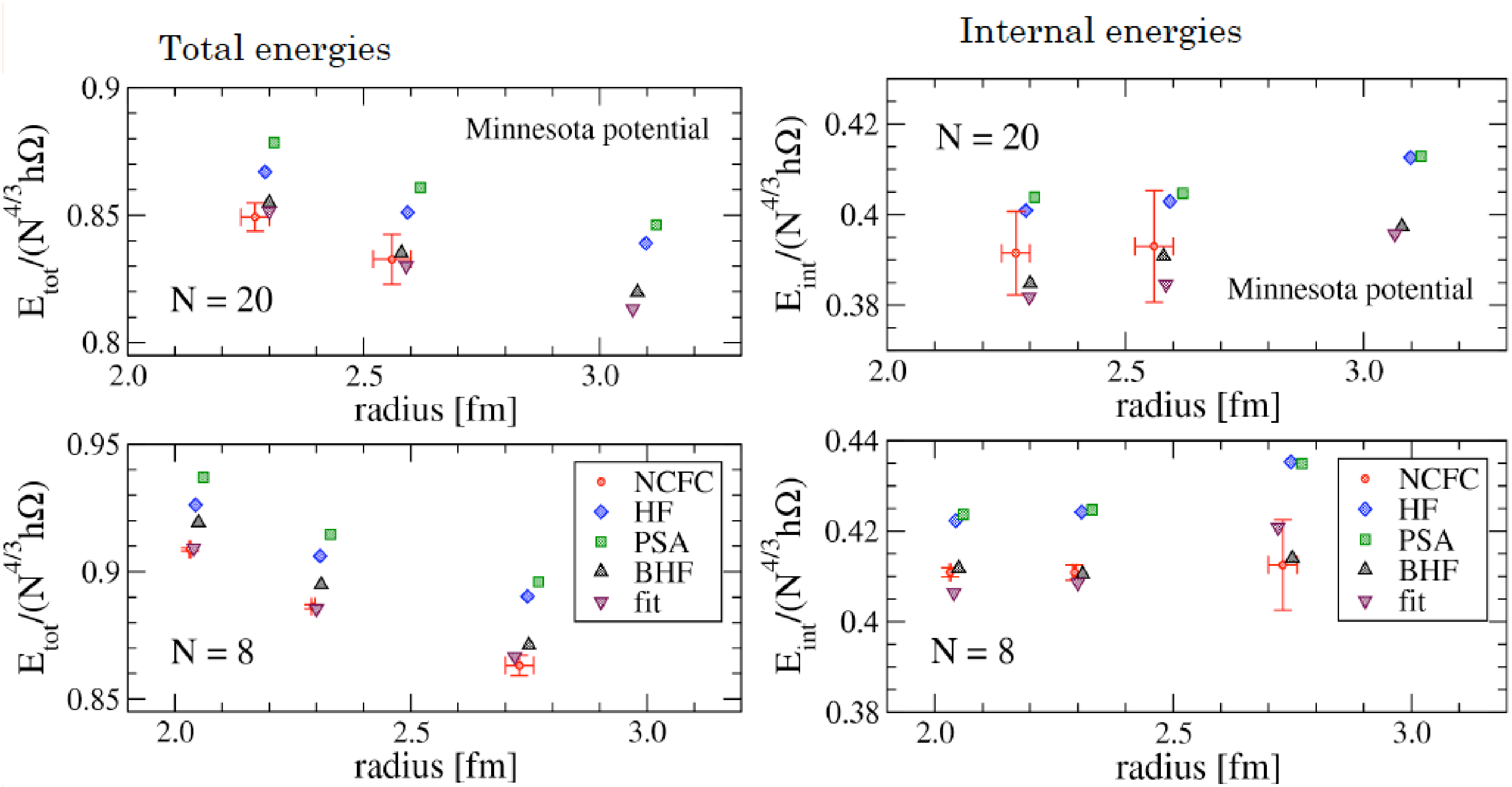
Use as "pseudodata" for poorly constrained
Isovector (n >> p) part of nuclear functionals

Challenge:

Given some microscopic NN potential, can one microscopically construct the energy functional (EDF)?

How close can the microscopic DFT calculation come to the exact result from many-body diagonalization ?

1st proof-of-principle results in 1106.3557 [nucl-th]

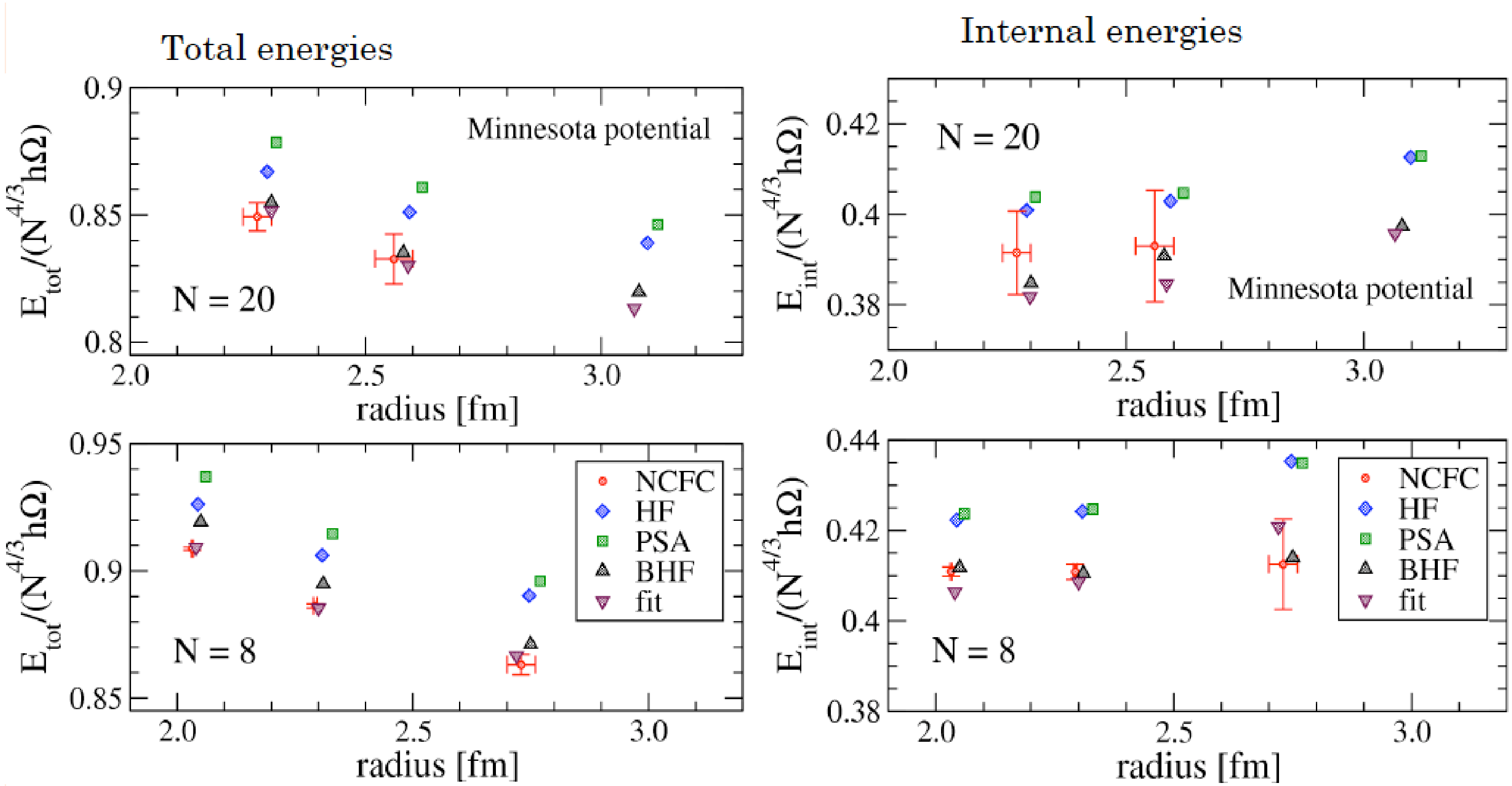


1106.3557 [nucl-th]

Harmonic oscillator hΩ = 20, 15, 5 MeV (left-to-right)

N = 20 (top row) , N = 8 (bottom row)

(energies scaled by Thomas-Fermi to remove “fast” hΩ and N dependence)



NCFC = exact diagonalization of H

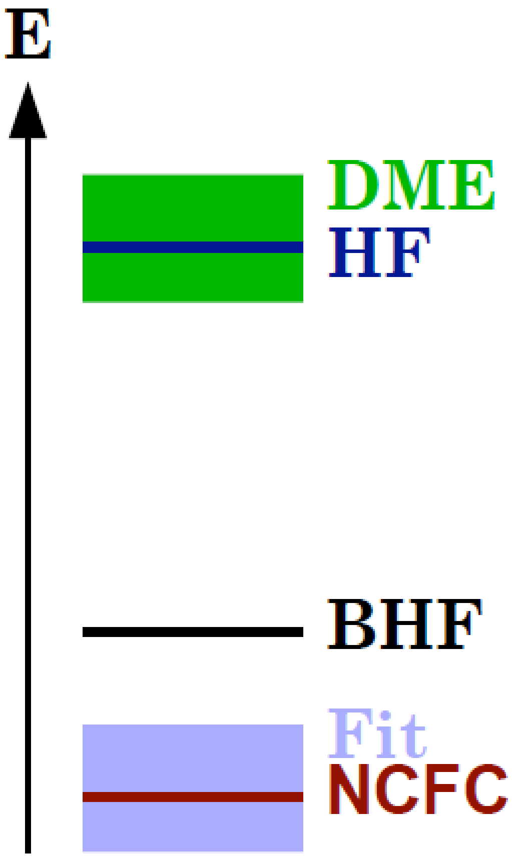
HF = Hartree-Fock using the finite-range V_{NN} ("non-local EDF")

PSA = DME functional calculated at the level of HF in perturbation theory

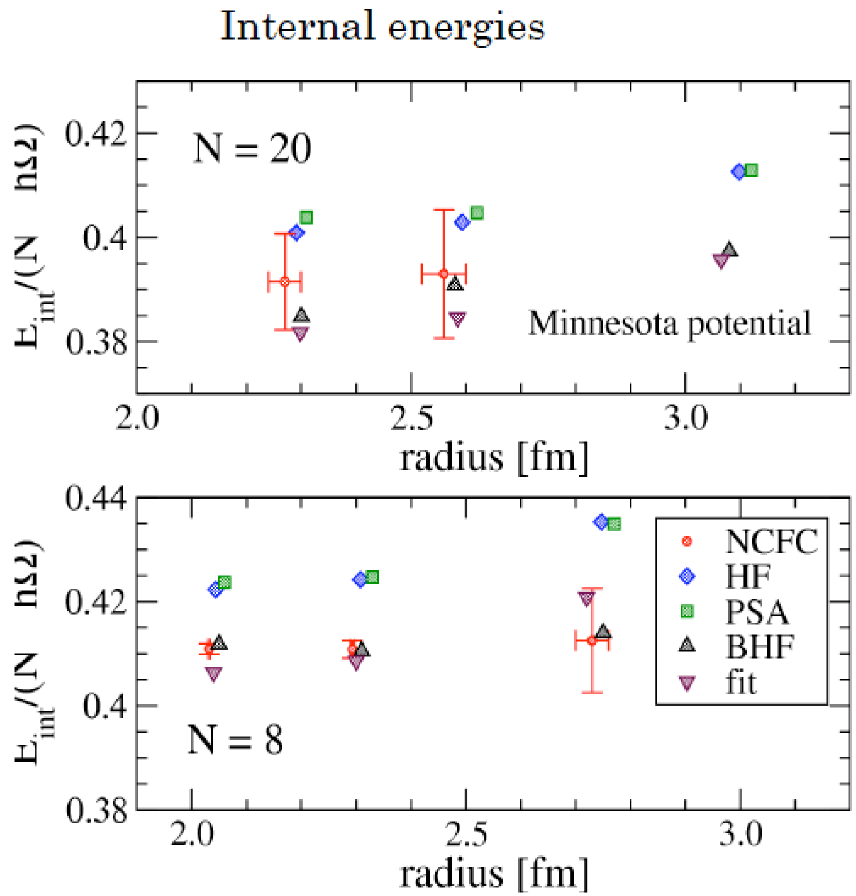
BHF = DME functional at the level of Brueckner-HF in perturbation theory

FIT = DME functional at HF level + fitted contact terms

(energies scaled by Thomas-Fermi to remove "fast" hΩ and N dependence)

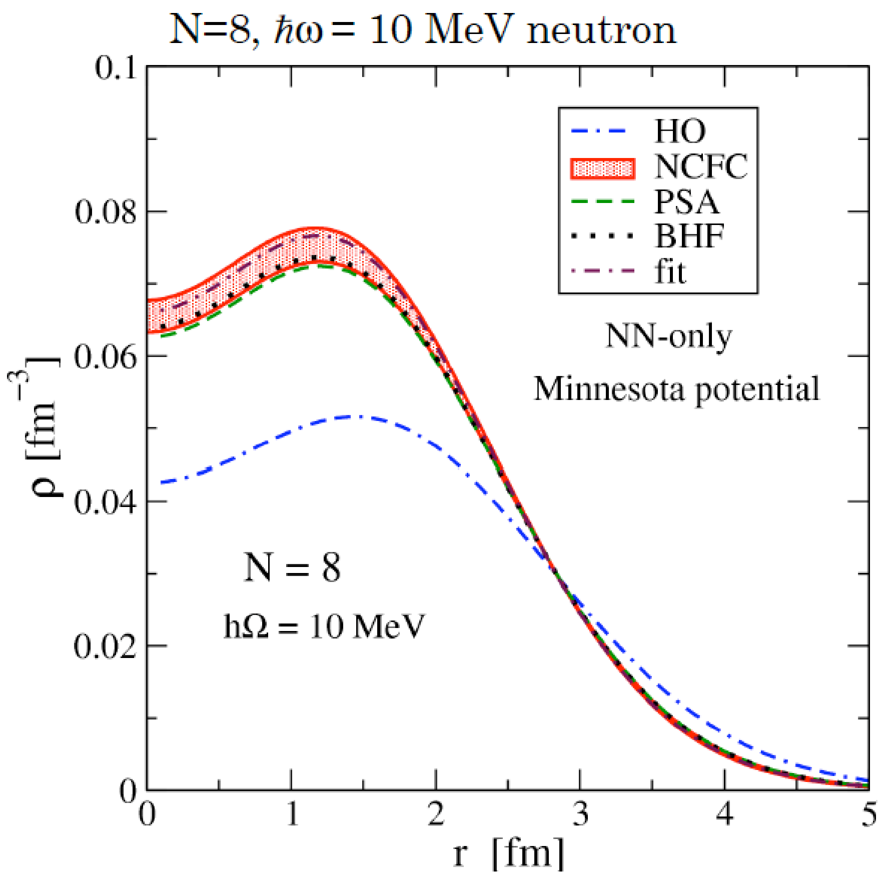


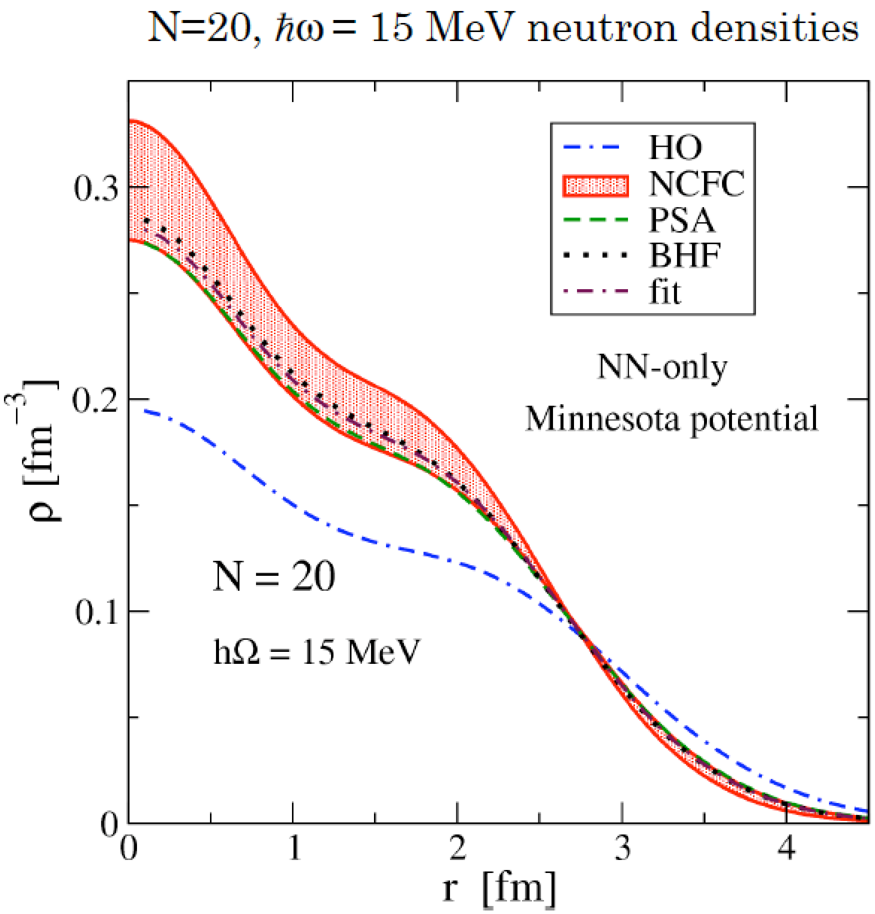
Expected pattern



- Good agreement with exact results
- Systematic improvement at different levels of building the EDF

Densities agree within error bars of exact result





- external trap allows exploration of wide range of density regimes
- next steps
    - chiral EFT interactions, larger N (no problem for DFT)
    - open shell systems (probe pairing correlations)
    - see if "real" neutron-rich nuclei can be improved

Lecture 3 take-away points

- Cutoff-dependence is a tool
    - tells you when something is missing (e.g., 3N)
    - tells you how important it is
    - theoretical errors

- RG generates 3N forces…is this a bad thing?
    - They're there to begin with, even with "hard" interactions
    - Might as well make them soft and easy to use in MB calcs.

- Density functional theory evades the N! wall of wave function methods
    - can in principle cover the entire mass table
    - suffers from empirical nature (model dependent extrapolations,etc.)
    - easiest to draw a microscopic connection to DFT with soft RG-evolved interactions
    - 1st steps in nuclei and neutron drops look very promising