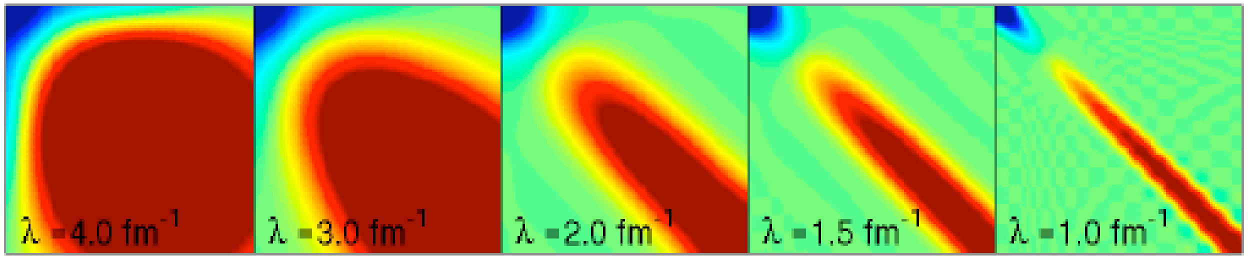

Non-empirical energy density functionals

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SciDAC
Scientific Discovery through Advanced Computing

Outline

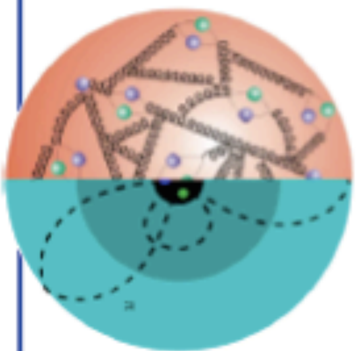
1) Renormalization group methods

2) Microscopically-constrained Skyrme functionals

3) Other efforts towards non-empirical functionals

Λ / Resolution dependence of nuclear forces

with high-energy probes:
quarks+gluons



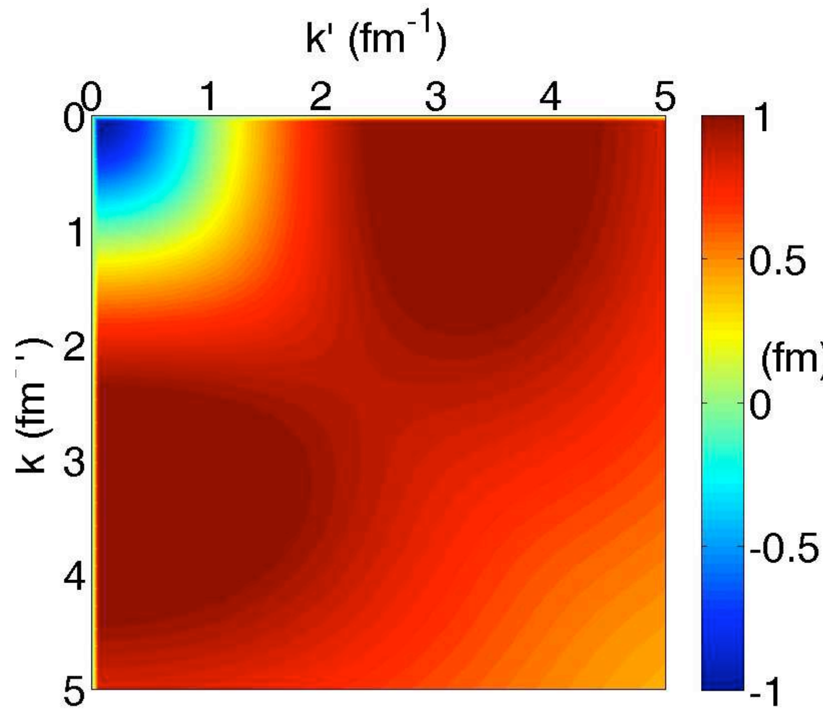
Effective theory for NN, 3N, many-N interactions and electroweak operators: resolution scale/Λ-dependent

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

$\Lambda >> m_\pi, k_F$ in typical interactions

# of sp states for A-body ~ $\Lambda^3 A$

Strong correlations, non-perturbative

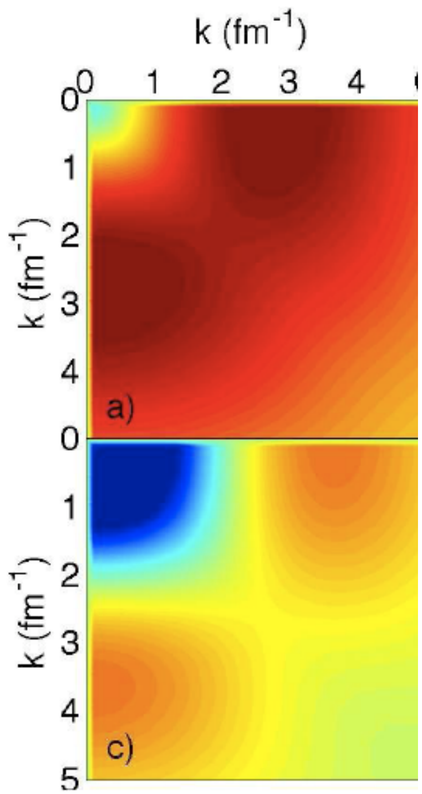


Why large Λ's are complicated: ab initio DFT

Ab initio DFT (OEP/effective action) corresponds to MBPT with

$$
\begin{aligned}
H &= (T+U) + (V-U) \\
  &= H_{KS} + H_1
\end{aligned}
$$

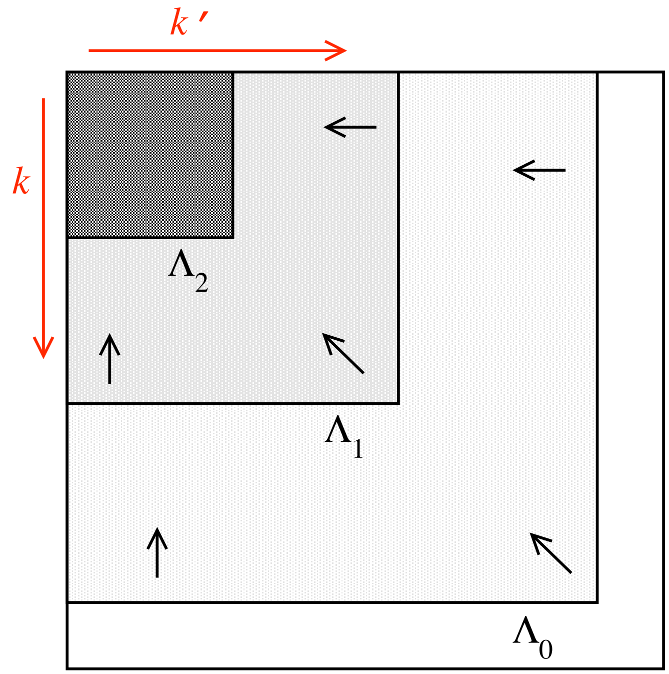
Want freedom to chose U such that corrections to density beyond H_{KS} vanish

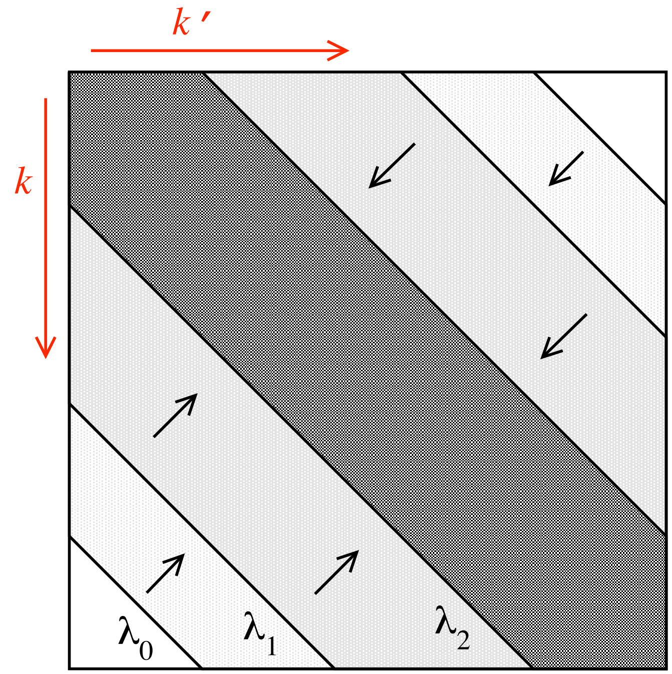


Large Λ V_{NN} strongly couples low/high k

coupling persists even with G matrix resummation ==> non-perturbative in G and convergence of hole-line expansion **strongly depends on U**

2 Types of Renormalization Group Transformations





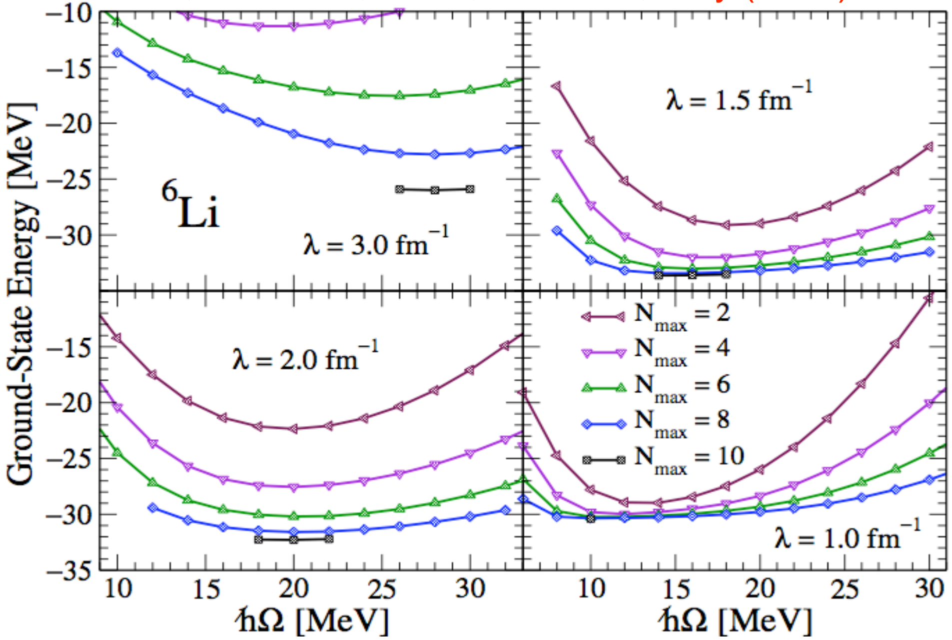
“$V_{\text{low k}}$”
integrate-out high k states
preserves observables for $k < \Lambda$

“Similarity RG”
eliminate far off-diagonal coupling
preserves “all” observables

Very similar consequences despite differences in appearance
(low and high momentum decoupled)

RG-Improved Convergence in ab-initio calculations

SKB, Furnstahl, Maris, Schwenk, Vary (2008)



Li-6 diagonalization in HO basis

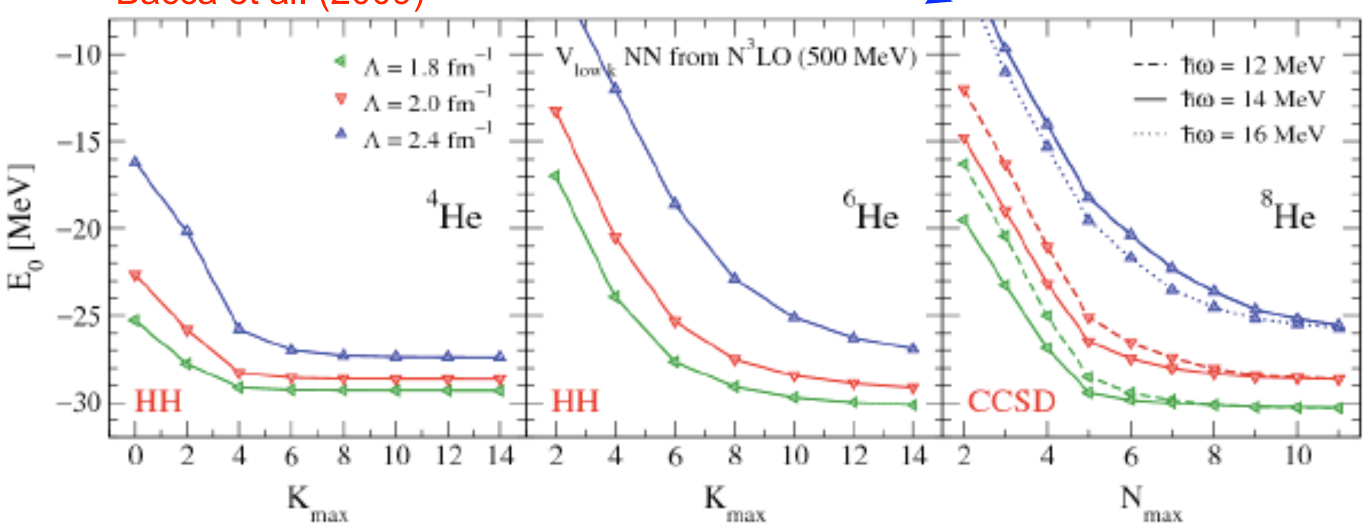
10^3 states for N_{max} = 2

versus

10^7 states for N_{max} = 10

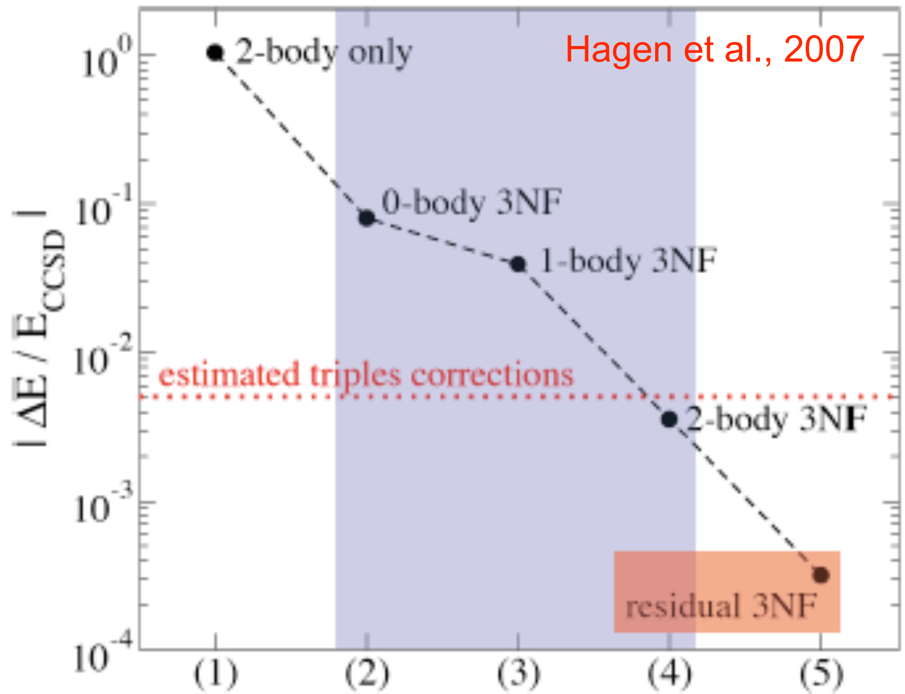
Helium Halo Nuclei

Bacca et al. (2009)



Ab-initio calculations of heavier nuclei accessible…

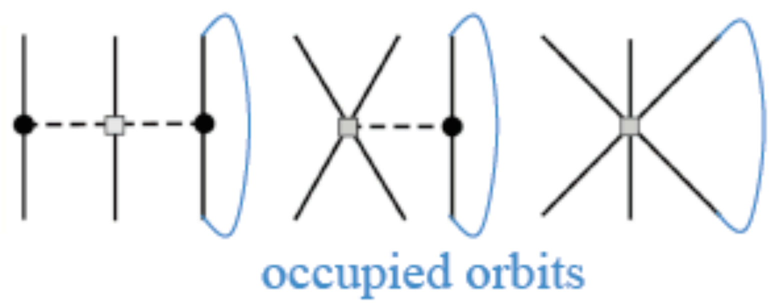
Towards including 3N interactions in medium mass nuclei



coupled-cluster calculations of closed-shell nuclei

normal-ordered 0-, 1- and 2-body parts of 3N interaction dominate

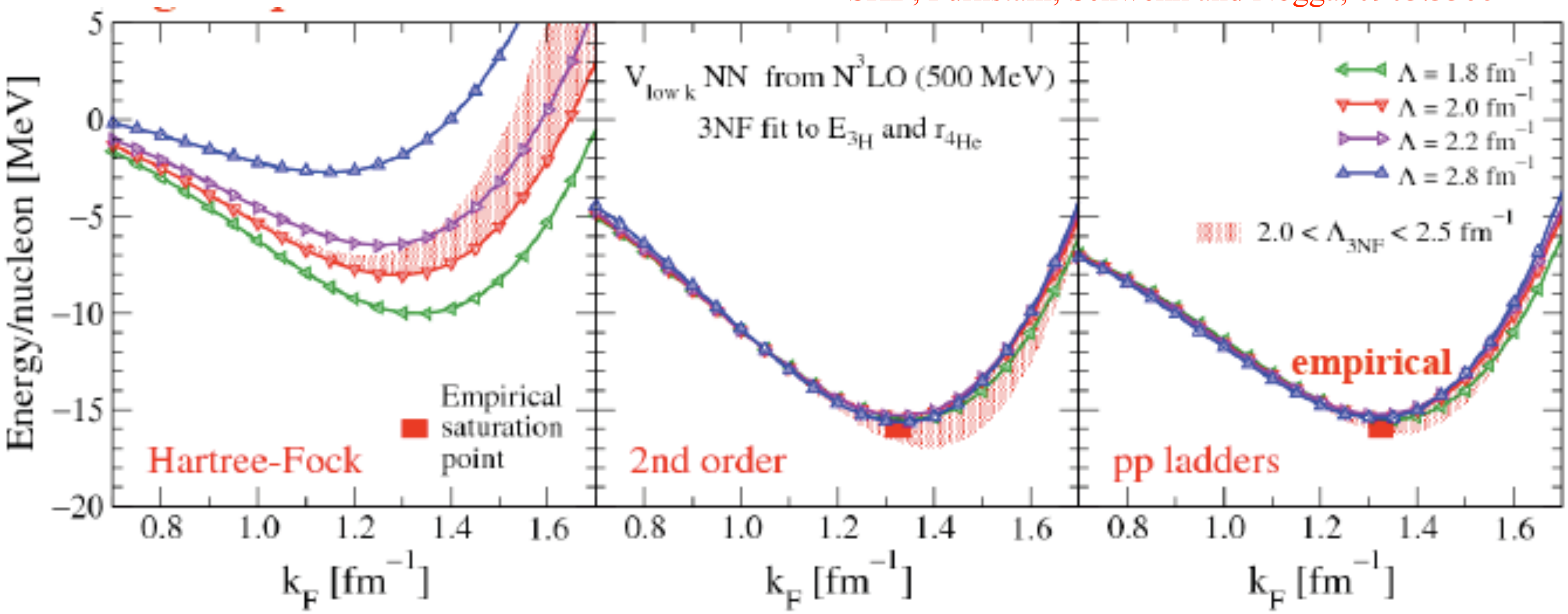
2-body part



residual 3N interaction can be neglected: very promising

Perturbative Nuclear Matter with chiral EFT + RG?

SKB, Furnstahl, Schwenk and Nogga, 0903.3366



HF bound and saturates, converged at ≈ 2nd order MBPT

3N drives saturation, theoretical error bands

Empirical saturation lies in theoretical error bands w/out fine-tuning

Is a solution to a 50 year old problem in reach?

Promising for a microscopic nuclear Density Functional Theory (DFT)?

The Similarity Renormalization Group

Wegner, Glazek and Wilson

Unitary transformation on an initial H = T + V

$$H_\lambda = U(\lambda) H U^\dagger(\lambda) \equiv T + V_\lambda$$

λ = continuous flow parameter

Differentiating with respect to λ:

$$\frac{dH_\lambda}{d\lambda} = [\eta(\lambda), H_\lambda] \qquad \text{with} \qquad \eta(\lambda) \equiv \frac{dU(\lambda)}{d\lambda} U^\dagger(\lambda)$$

Engineer η to do different things as λ => 0

$$\eta(\lambda) = [\mathcal{G}_\lambda, H_\lambda]$$

$$\mathcal{G}_\lambda = T \;\Rightarrow\; H_\lambda \text{ driven towards diagonal in k} - \text{space}$$

$$\mathcal{G}_\lambda = PH_\lambda P + QH_\lambda Q \;\Rightarrow\; H_\lambda \text{ driven to block} - \text{diagonal}$$

$$\vdots$$

Normal Ordered Hamiltonians

$$H = \sum t_i a_i^\dagger a_i + \frac{1}{4}\sum V^{(2)}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{36}\sum V^{(3)}_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l$$

Normal-order w.r.t. some reference state Φ (e.g., HF) :

$$H = E_{vac} + \sum f_i N(a_i^\dagger a_i) + \frac{1}{4}\sum \Gamma_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k) + \frac{1}{36}\sum W_{ijklmn} N(a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l)$$

$$\begin{aligned} E_{vac} &= \langle\Phi|H|\Phi\rangle \\ f_i &= t_{ii} + \sum_h \langle ih|V_2|ih\rangle\, n_h + \frac{1}{2}\sum_{hh'} \langle ihh'|V_3|ihh'\rangle\, n_h n_{h'} \\ \Gamma_{ijkl} &= \langle ij|V_2|kl\rangle + \sum_h \langle ijh|V_3|klh\rangle\, n_h \\ W_{ijklmn} &= \langle ijk|V_3|lmn\rangle \end{aligned}$$

$$\langle\Phi|N(\cdots)|\Phi\rangle = 0$$

0-, 1-, 2-body terms contain some 3NF effects thru density dependence => Efficient truncation scheme for evolution of 3N?

In-medium SRG for Infinite NM and closed-shell nuclei

- Normal order H w.r.t. fermi sea
- Choose SRG generator to eliminate "energy off-diagonal" pieces

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

$$\eta = [\hat{f}, \hat{\Gamma}]$$

⇨

$$\lim_{s\to\infty} \Gamma_{od}(s) = 0$$

$$\lambda \equiv s^{-1/4}$$

$$\langle 12|\Gamma_{od}|34\rangle = 0 \text{ if } f_{12} = f_{34}$$

- Truncate flow equations to 2-body normal-ordered operators
  - dominant parts of induced many-body forces included implicitly

$$H(\infty) = E_{vac}(\infty) + \sum f_i(\infty) N(a_i^\dagger a_i) + \frac{1}{4}\sum [\Gamma_d(\infty)]_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k)$$

$$\begin{aligned} E_{vac}(\infty) &\rightarrow E_{gs} \\ f_k(\infty) &\rightarrow \epsilon_k \text{ (fully dressed s.p.e.)} \\ \Gamma_d(\infty) &\rightarrow f(k', k) \text{ (Landau q.p. interaction)} \end{aligned}$$

Microscopic realization of SM ideas: dominant MF + weak A-dependent NN_{eff}

Some observations

1) $\frac{d}{ds}\langle H\rangle_0 \leq 0$ for monotonic f_k correlations weakened, HF picks up more binding with increasing s.

2) pp channel + 2 ph channels treated on equal footing

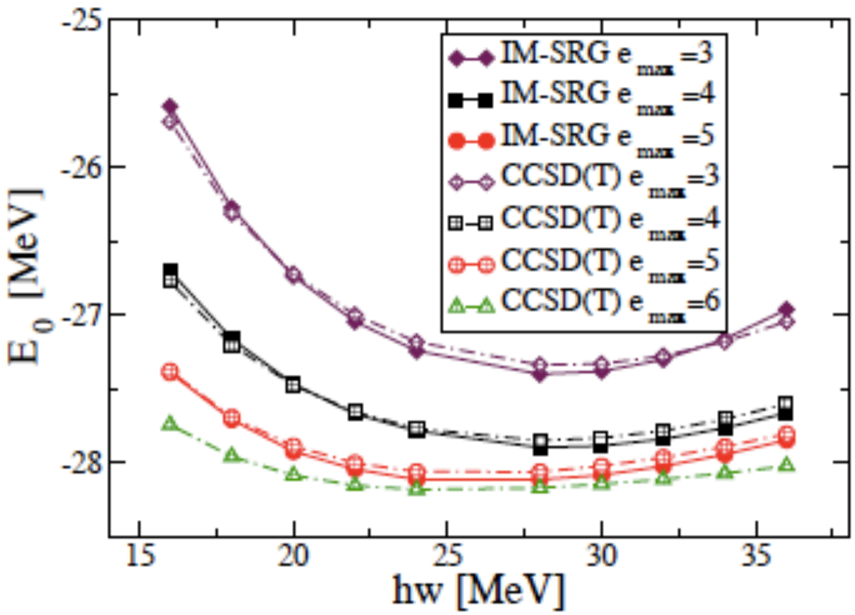
3) Intrinsically non-perturbative

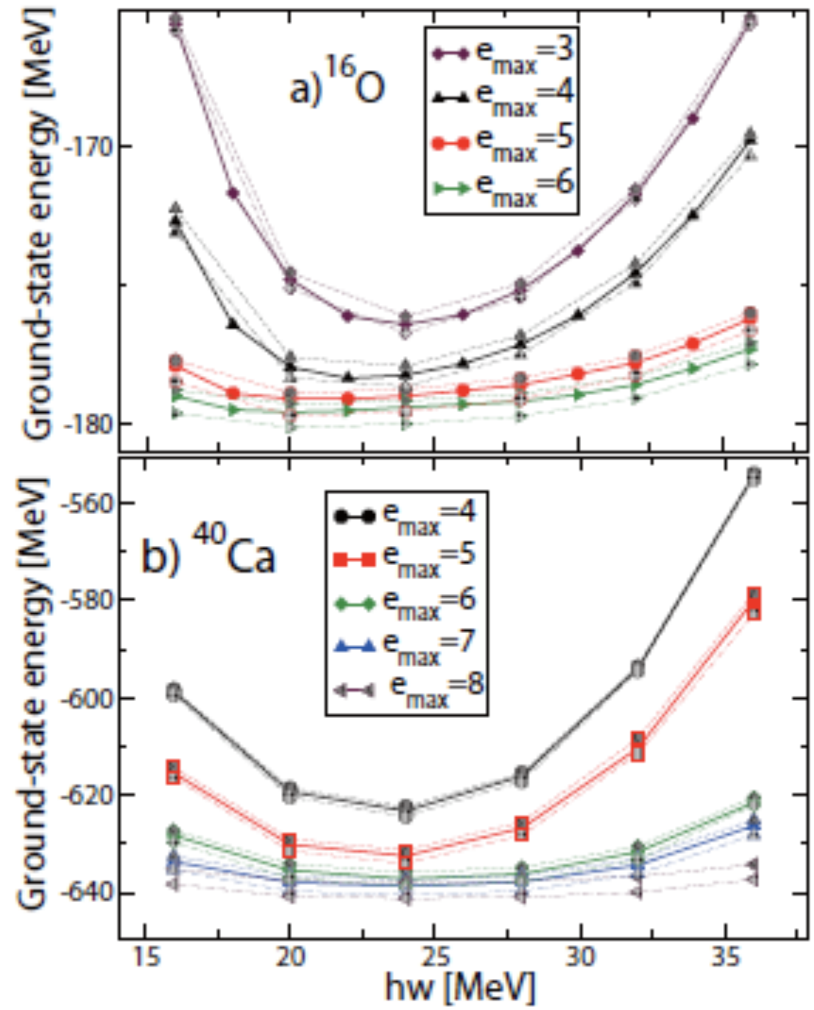
4) no unlinked diagrams (size extensive, etc.)

5) "3rd-order exact" a-la CCSD

6) Extension to effective operators/Shell model possible

In-medium SRG for nuclei Tsukiyama, SKB, Schwenk, in prep

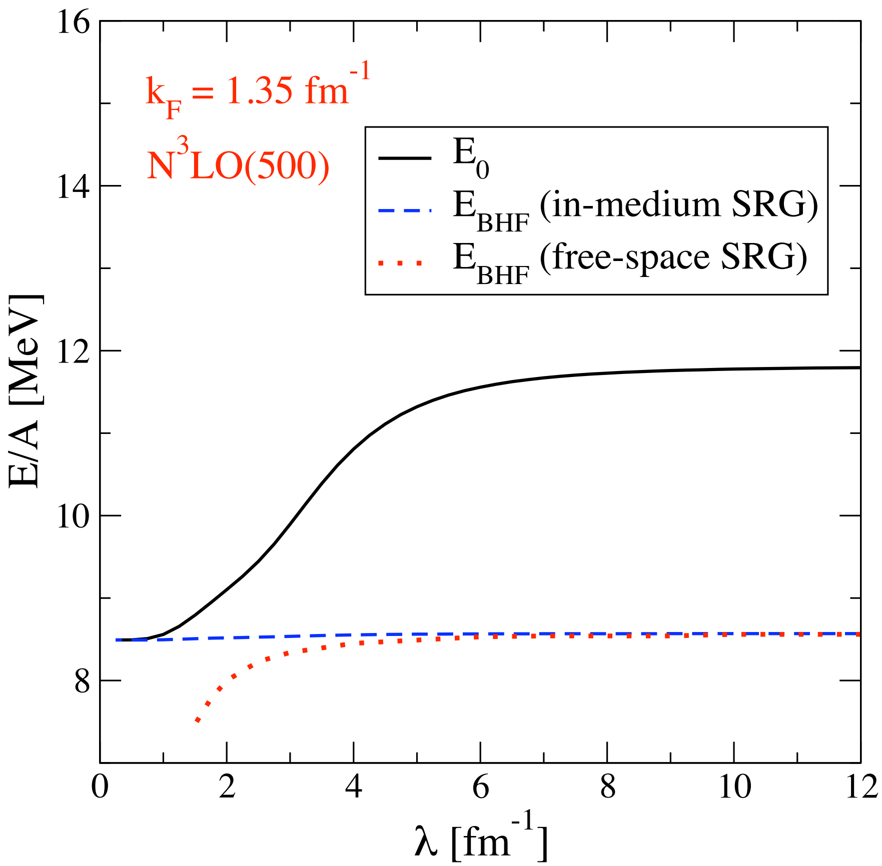




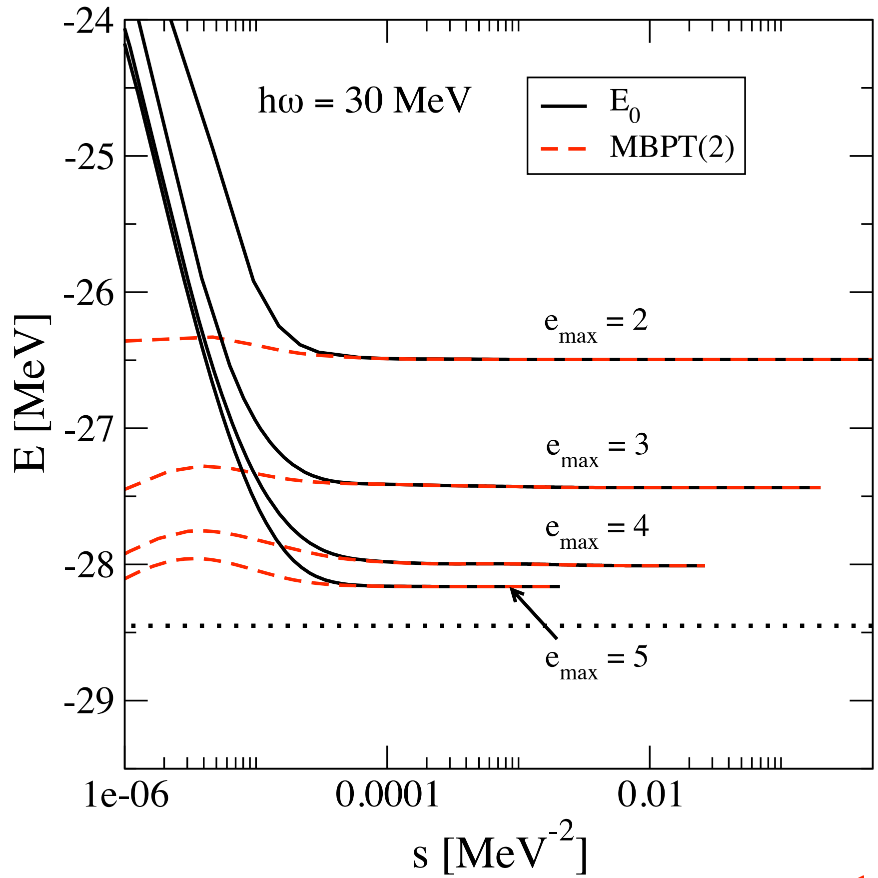
Comparable to CCSD(T) in closed shell nuclei

Promising method to calculate shell model valence H_{eff}/O_{eff}

Correlations “adiabatically” summed into H(λ)



INM

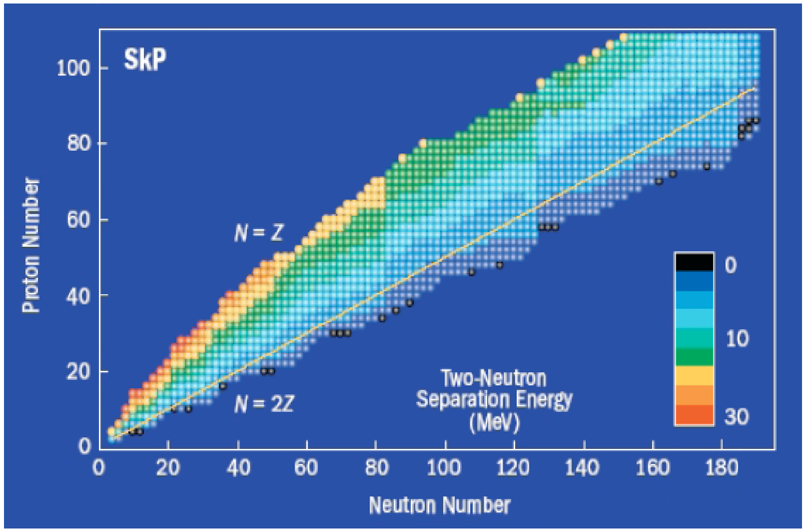


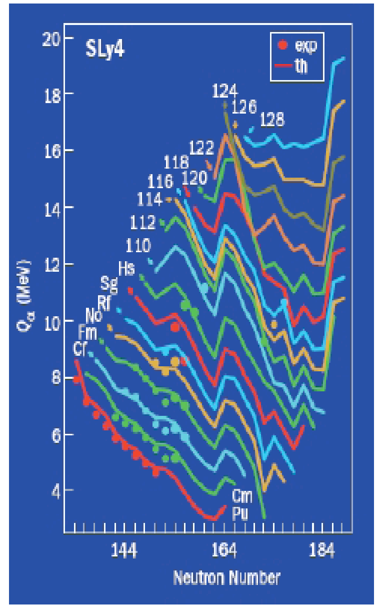
$s = 1/\lambda^4$

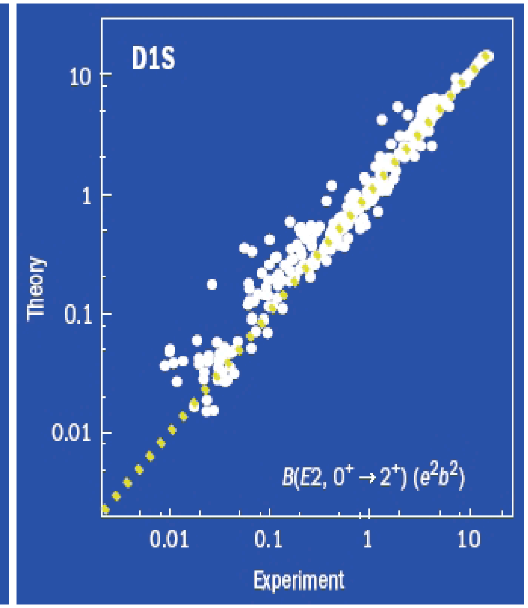
^{4}He

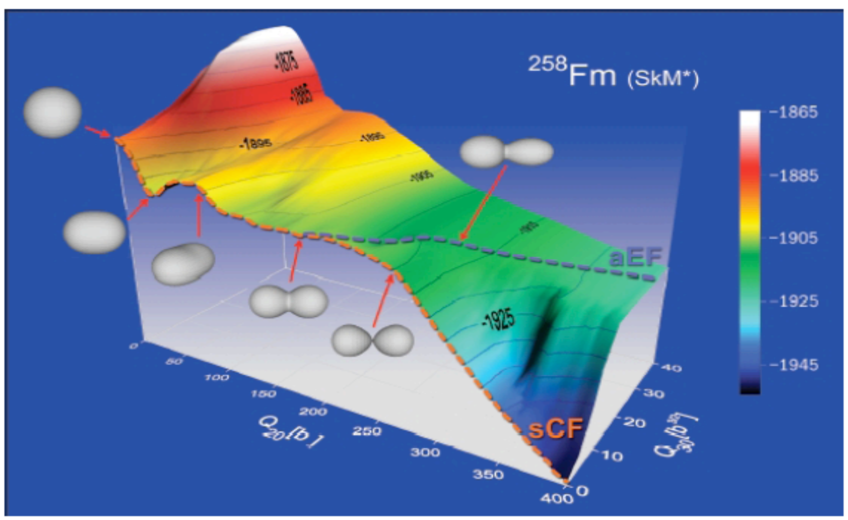
Useful for ab initio DFT? Shell model?

Accomplishments of Phenomenological Energy Functionals





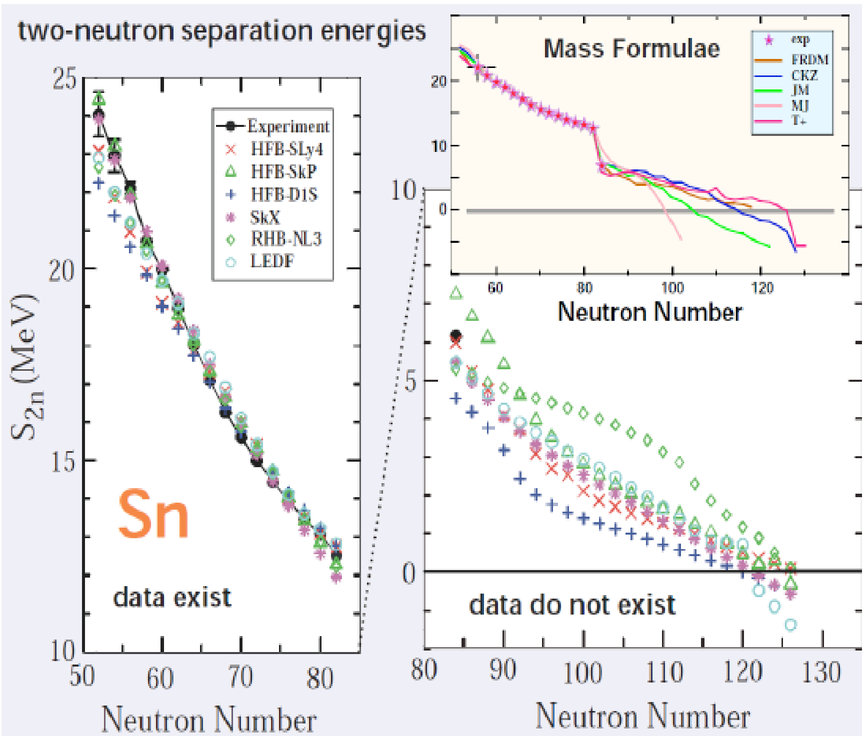


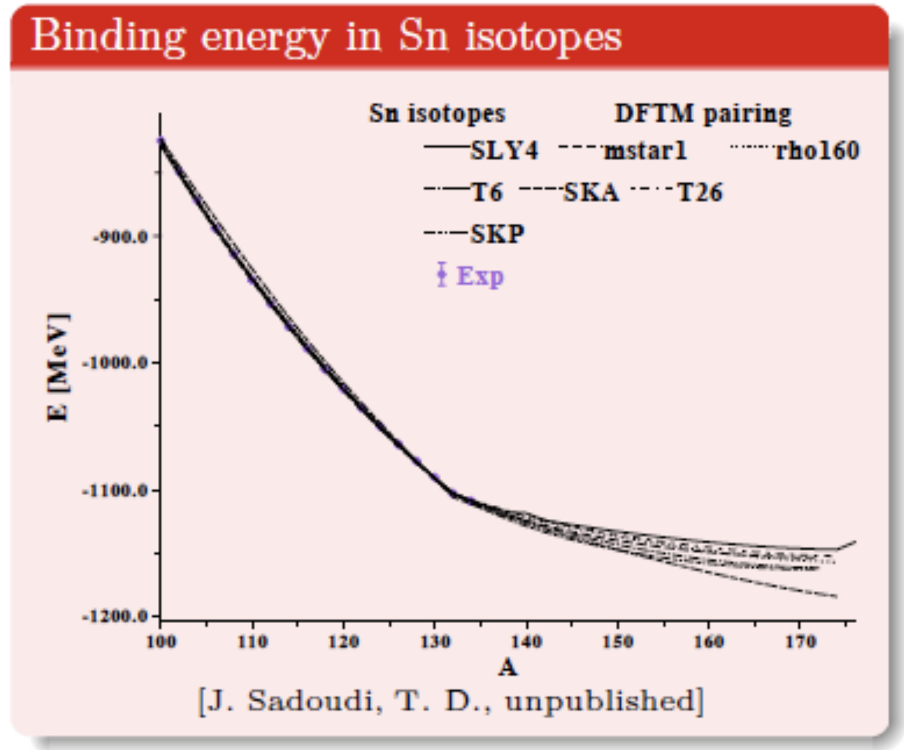


2N separation energies, Quadrupole and BE2 values, Fission energy surfaces, mass tables in a day, plus many other impressive feats

BUT...

Limitations of Existing Energy Functionals (Predictability)





- Uncontrolled extrapolations away from known data
- Theoretical error-bars?

What's missing in phenomenological EDFs ?

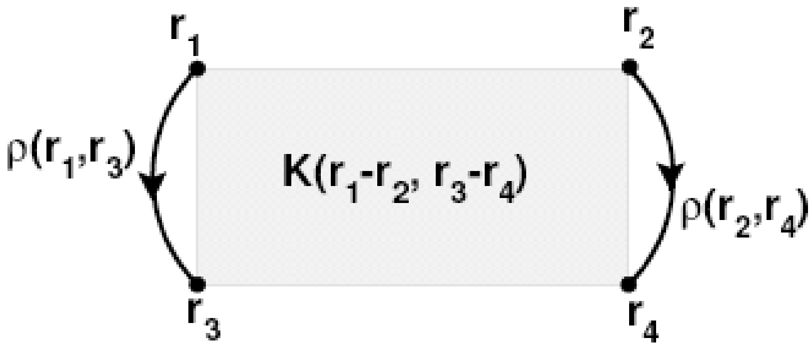
- Density dependencies too simplistic
- Isovector components not well constrained
- No way to estimate theoretical uncertainties
- What's the connection to many-body forces?

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 on non-local quantities

density matrices and s.p. propagators
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

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

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

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 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)

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

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

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

Easy to build in physics associated with surface effects in finite fermi systems

Crucial to accurately describe spin-vector part of OBDM

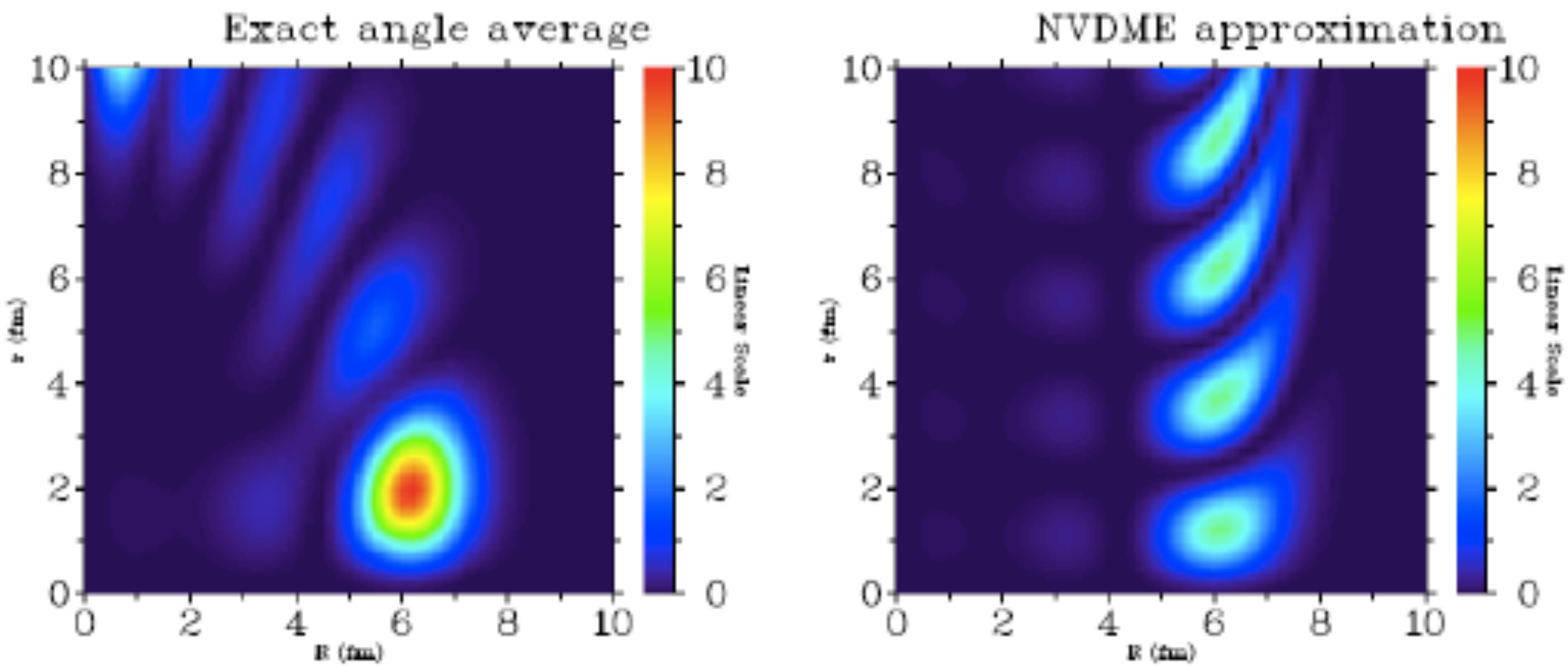
Prescriptions for Π_n-functions

<u>Negele and Vautherin (NV-DME)</u>

Truncated Bessel expansion of non-locality operator

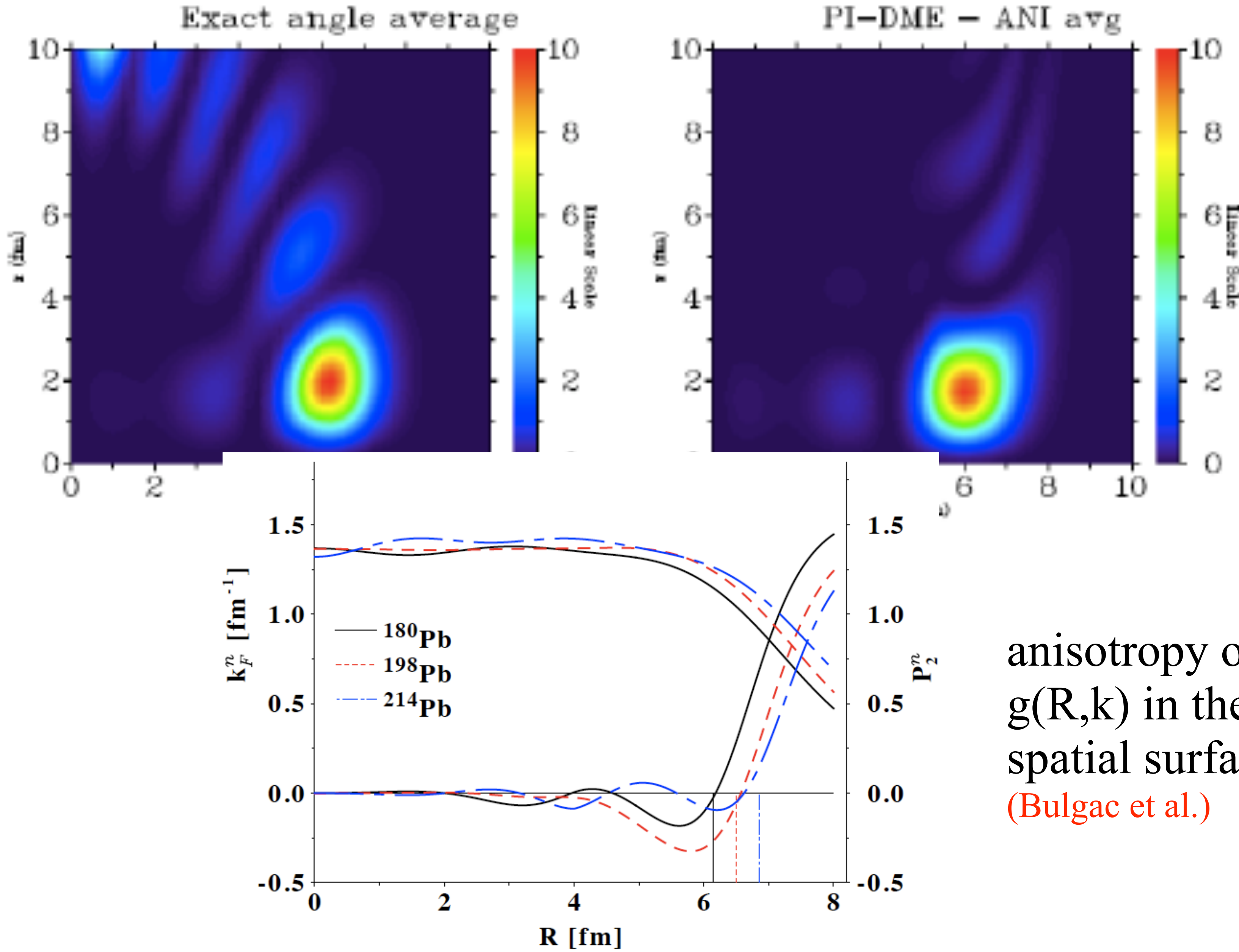
Sufficient for spin-unsaturated nuclei only

$$\int d\Omega_r \, \mathbf{s}_n(\mathbf{r}_1, \mathbf{r}_2) \cdot \mathbf{s}_n(\mathbf{r}_2, \mathbf{r}_1)$$



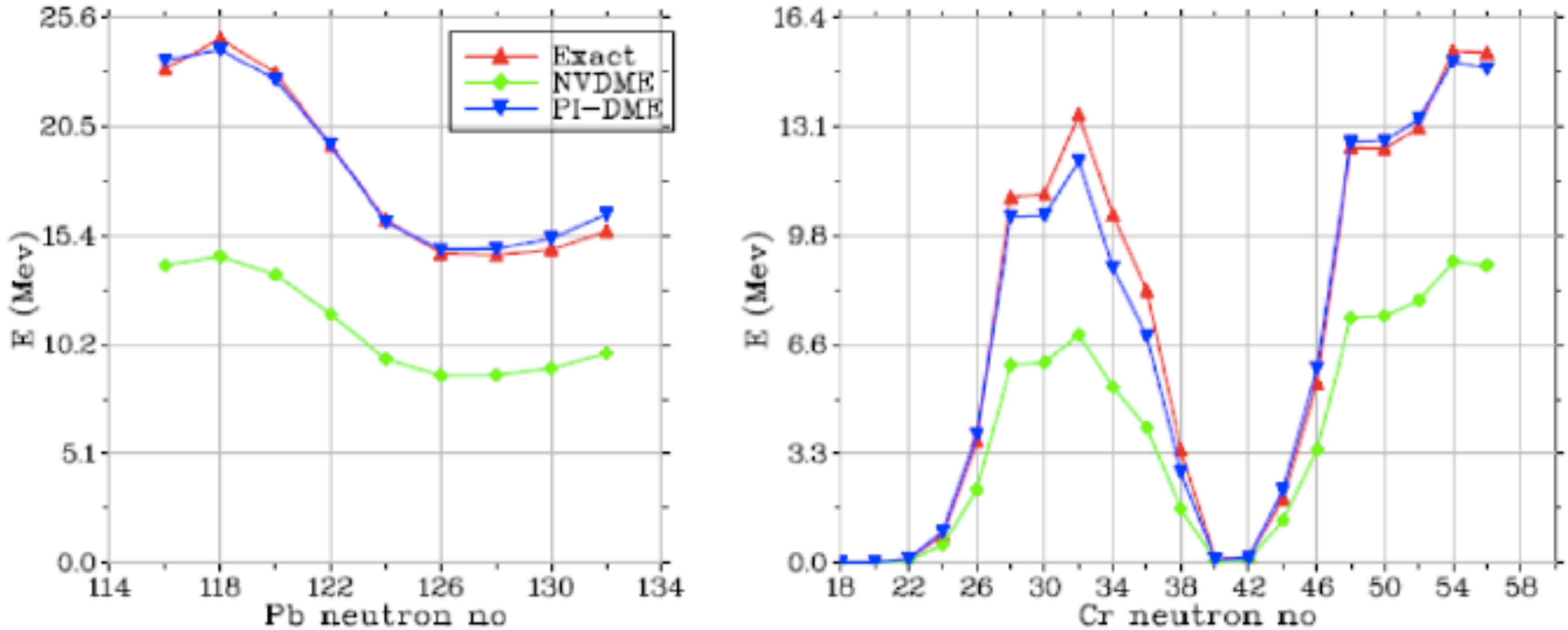
Why it fails: no phase space averaging done for spin-vector part

Improved Vector PSA-DME



anisotropy of g(R,k) in the spatial surface
(Bulgac et al.)

Look at $\int d\mathbf{r}\, d\mathbf{R}\, V_{1\pi}(r)\, \mathbf{s}_n(\mathbf{r}_1, \mathbf{r}_2) \cdot \mathbf{s}_n(\mathbf{r}_2, \mathbf{r}_1)$:



- Inclusion of finite fermi phase space effects crucial for **quantitative** agreement
- completely parameter-free

Can now apply modified DME with confidence
to spin-unsaturated systems

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 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

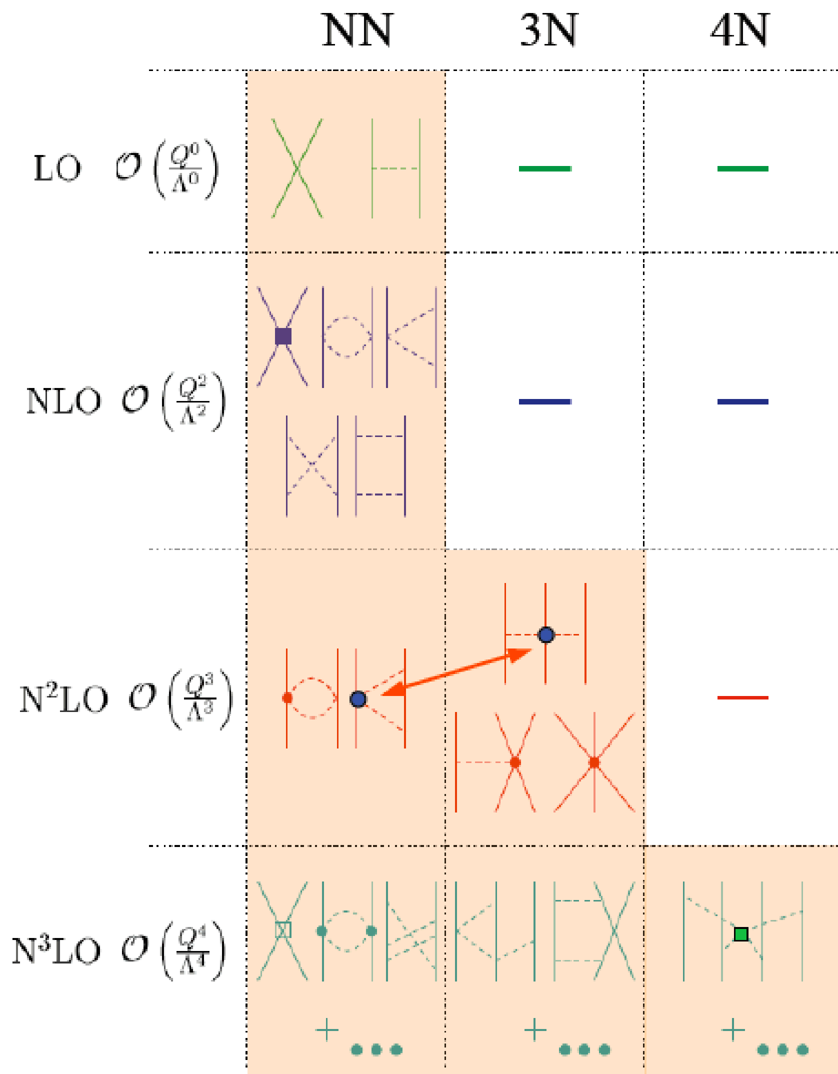
Suggests a microscopically-improved Skyrme phenomenology

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 Skyrme coupling constants (EFT constraints => naturalness)
- Look for improved observables and for sensitivities
- Can we “see” the pion as in NN phase shift analyses

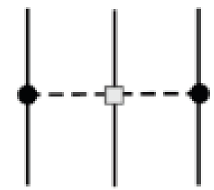
Expect interesting spin-orbit consequences (NN vs NNN)



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)

Complexity explodes ==> Automated symbolic tools developed (Gebremariam et al) will be available at www.unedf.org

$$
\begin{aligned}
\mathcal{E}^{CR4,2x} \;=\; \int d\vec{r} \Big\{ & \mathcal{C}_7^{\rho_0^3}\, \rho_0^3(\vec{r}) + \mathcal{C}_7^{\rho_0\rho_1^2}\, \rho_0(\vec{r})\, \rho_1^2(\vec{r}) + \mathcal{C}_7^{\rho_0\rho_1\varsigma_1^1}\, \rho_0(\vec{r})\, \rho_1(\vec{r})\, \varsigma_1^1(\vec{r}) \\
& + \mathcal{C}_7^{\rho_0^2\Delta\rho_0}\, \rho_0^2(\vec{r})\, \Delta\rho_0(\vec{r}) + \mathcal{C}_7^{\rho_0\rho_1\Delta\rho_1}\, \rho_0(\vec{r})\, \rho_1(\vec{r})\, \Delta\rho_1(\vec{r}) + \mathcal{C}_7^{\rho_0^2\varsigma_0^2}\, \rho_0^2(\vec{r})\, \varsigma_0^2(\vec{r}) \\
& + \mathcal{C}_7^{\rho_1^2\varsigma_0^2}\, \rho_1^2(\vec{r})\, \varsigma_0^2(\vec{r}) + \mathcal{C}_7^{\rho_0\rho_1\varsigma_1^2}\, \rho_0(\vec{r})\, \rho_1(\vec{r})\, \varsigma_1^2(\vec{r}) + \mathcal{C}_7^{\rho_0^2\varsigma_0^1}\, \rho_0^2(\vec{r})\, \varsigma_0^1(\vec{r}) \\
& + \mathcal{C}_7^{\rho_0 J_0^2}\, \rho_0(\vec{r})\, \vec{J}_0(\vec{r}) \cdot \vec{J}_0(\vec{r}) + \mathcal{C}_7^{\rho_1 J_0 J_1}\, \rho_1(\vec{r})\, \vec{J}_0(\vec{r}) \cdot \vec{J}_1(\vec{r}) + \mathcal{C}_7^{\rho_0 J_1^2}\, \rho_0(\vec{r})\, \vec{J}_1(\vec{r}) \cdot \vec{J}_1(\vec{r}) \\
& + \mathcal{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}) + \mathcal{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}) + \mathcal{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}) \\
& + \mathcal{C}_7^{\Delta\rho_0 J_0^2}\, \Delta\rho_0(\vec{r})\, \vec{J}_0(\vec{r}) \cdot \vec{J}_0(\vec{r}) + \mathcal{C}_7^{\varsigma_0^2 J_0^2}\, \varsigma_0^2(\vec{r})\, \vec{J}_0(\vec{r}) \cdot \vec{J}_0(\vec{r}) + \mathcal{C}_7^{\varsigma_0^1 J_0^2}\, \varsigma_0^1(\vec{r})\, \vec{J}_0(\vec{r}) \cdot \vec{J}_0(\vec{r}) \\
& + \mathcal{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}) + \mathcal{C}_7^{\rho_0\nabla J_0\nabla J_0}\, \rho_0(\vec{r})\, \big[\vec{\nabla} \cdot \vec{J}_0(\vec{r})\big]^2 + \mathcal{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}) \\
& + \mathcal{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}) + \mathcal{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}) + \mathcal{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}) \\
& + \mathcal{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}) + \mathcal{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}) + \mathcal{C}_7^{\varsigma_0^2 J_1^2}\, \varsigma_0^2(\vec{r})\, \vec{J}_1(\vec{r}) \cdot \vec{J}_1(\vec{r}) \\
& + \mathcal{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}) + \mathcal{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}) + \mathcal{C}_7^{\rho_0\nabla J_1\nabla J_1}\, \rho_0(\vec{r})\, \big[\vec{\nabla} \cdot \vec{J}_1(\vec{r})\big]^2 \\
& + \mathcal{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}) + \mathcal{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:

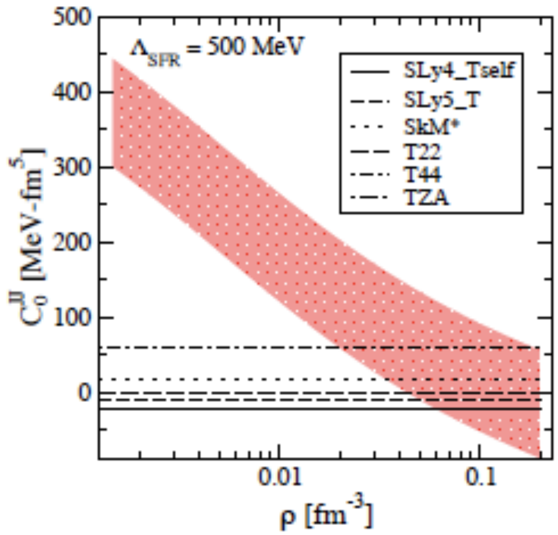
$$C^{ijk}[u]\xi_i\xi_j\xi_k \;, \quad u \equiv \frac{k_F(R)}{m_\pi}$$

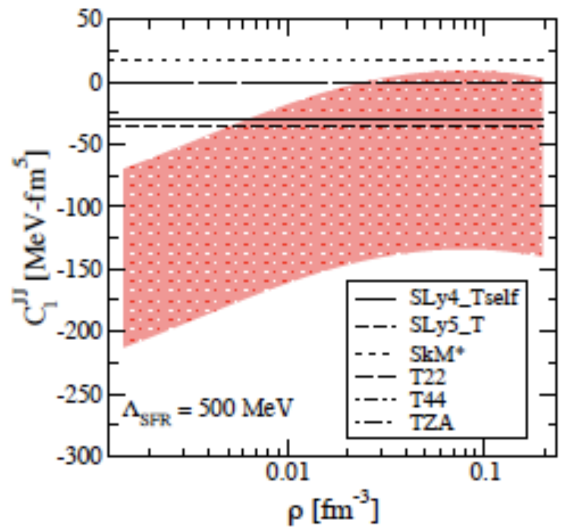
(note: u is NOT small)

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

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

Some examples (Gebremariam, SKB, Duguet 2010)

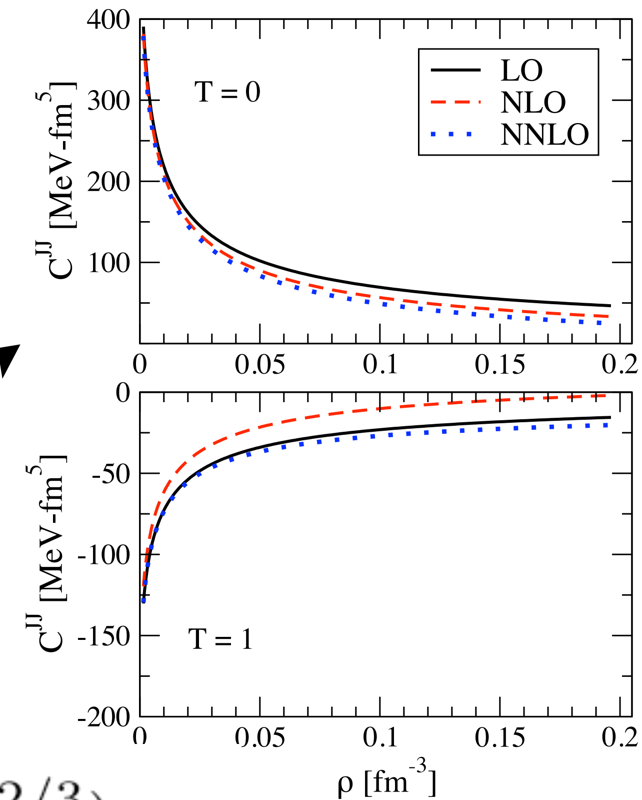




red "error bands" from EFT naturalness

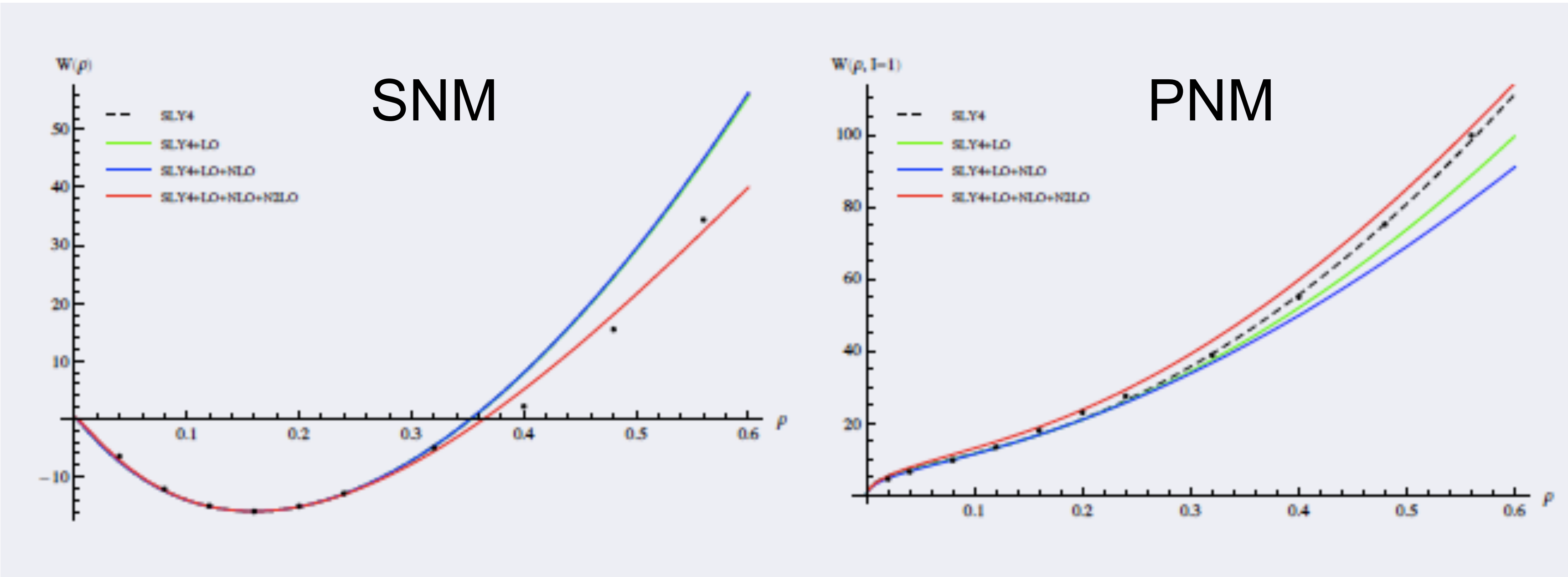
Comparison of EDF w/pions to Skyrme couplings w/tensor force

density dependence controlled by longest range component



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

Moral: Simple many-body theory + current understanding of underlying NN + NNN interactions tells us Skyrme is way too simple.



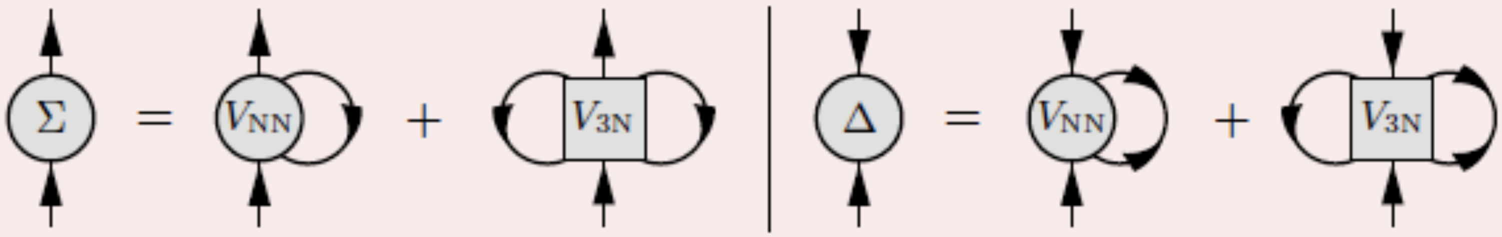
First exploratory calculations in progress w/M.Stoitsov et al. using the extended EDF (implemented in HFBRAD and HFBTHO)

Mathematica nb's with 2N/3N DME couplings available at <u>www.unedf.org</u>

Other efforts developing non-empirical EDFs

<u>Non-empirical pairing functional</u> (Duguet, Lesinski, Hebeler, Schwenk)

Build first Σ^q and Δ^q at lowest-order in $V_{\rm NN}$ and $V_{\rm NNN}$ (RG-evolved)

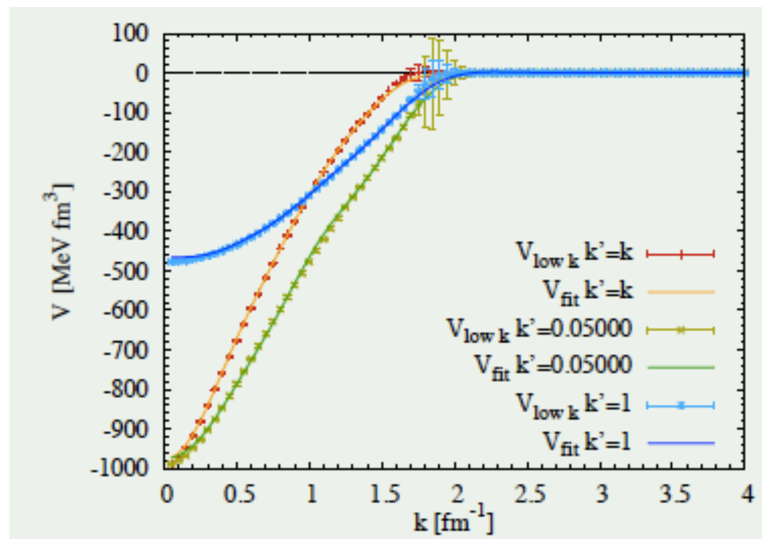


- v^{pp}: microscopically built from $V_{\rm NN}$ and $V_{\rm NNN}$
- v^{ph}: semi-empirical from constrained Skyrme EDF ($m^* \approx 0.7\, m$)

$$V_{qq}^{{}^1S_0}(k,k') = \sum_{\alpha,\beta=1}^{n} g_\alpha(k)\, \lambda_{\alpha\beta}\, g_\beta(k')$$

Low-rank separable expansion good at low Λ

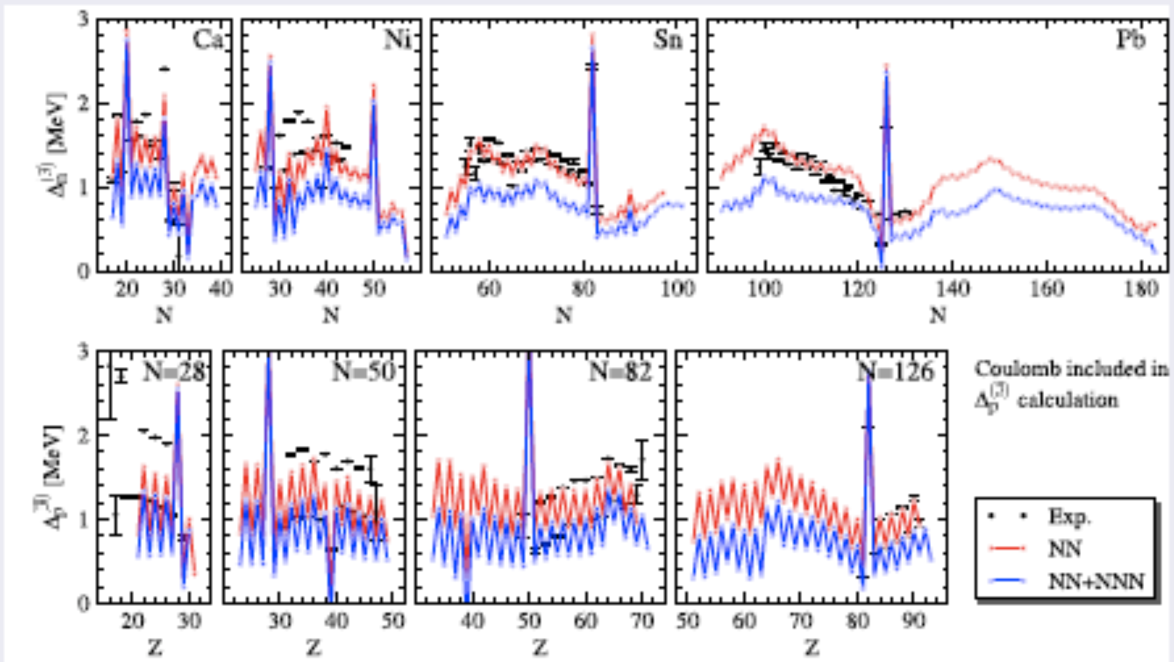
Almost as cheap as local pairing EDF calculations



With $V_{\text{low k}}$ + V_{coulomb} + approximate NNN

[T. Lesinski, T. D., K. Bennaceur, J. Meyer, in preparation]

$\Delta^{(3)}_{q,\text{exp}}$ versus $\Delta^{(3)}_{q,\text{th}}$



- $\Delta^{(3)}_q$ decreased by 20% with slight isovector trend ($|V^{^1S_0}_{qq\langle\bar{q}\rangle}| > |V^{^1S_0}_{qq\langle q\rangle}|$)
- Leave $\sim 20-30\%$ for coupling to (collective) fluctuations

Next: Beyond 1st order (Gorkov 2nd-order, In-medium SRG), local approx's

Other efforts developing non-empirical EDFs

DME functional vs. ab initio (SKB, Furnstahl, Platter)

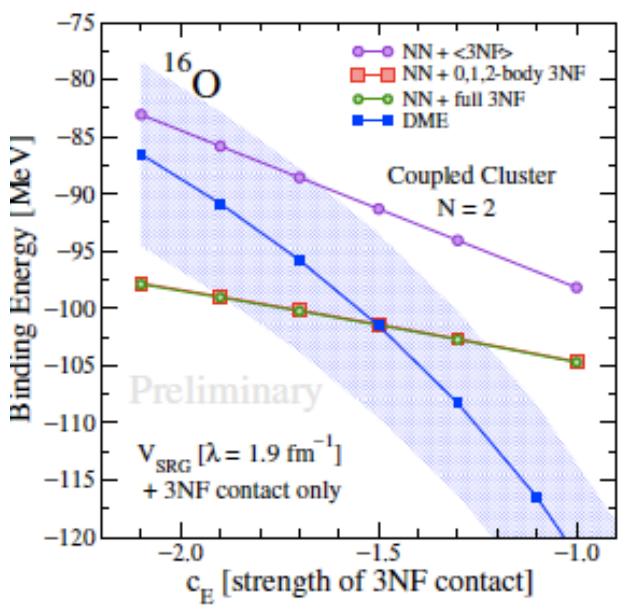
Start from the **same** H and compare with no adjustments

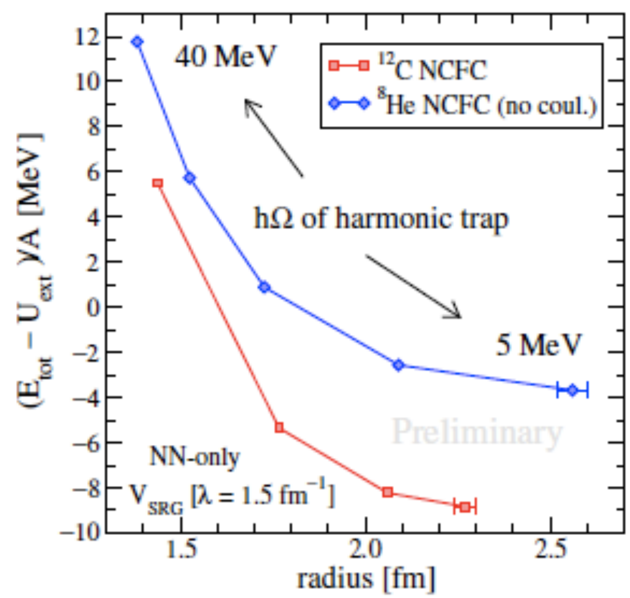
"Coester Lines"

- Compare systematics, e.g., by varying 3NF coupling in Hamiltonian

External Potentials

- DFT from response of energy to perturbation of densities
  $\Longrightarrow$ Apply external fields

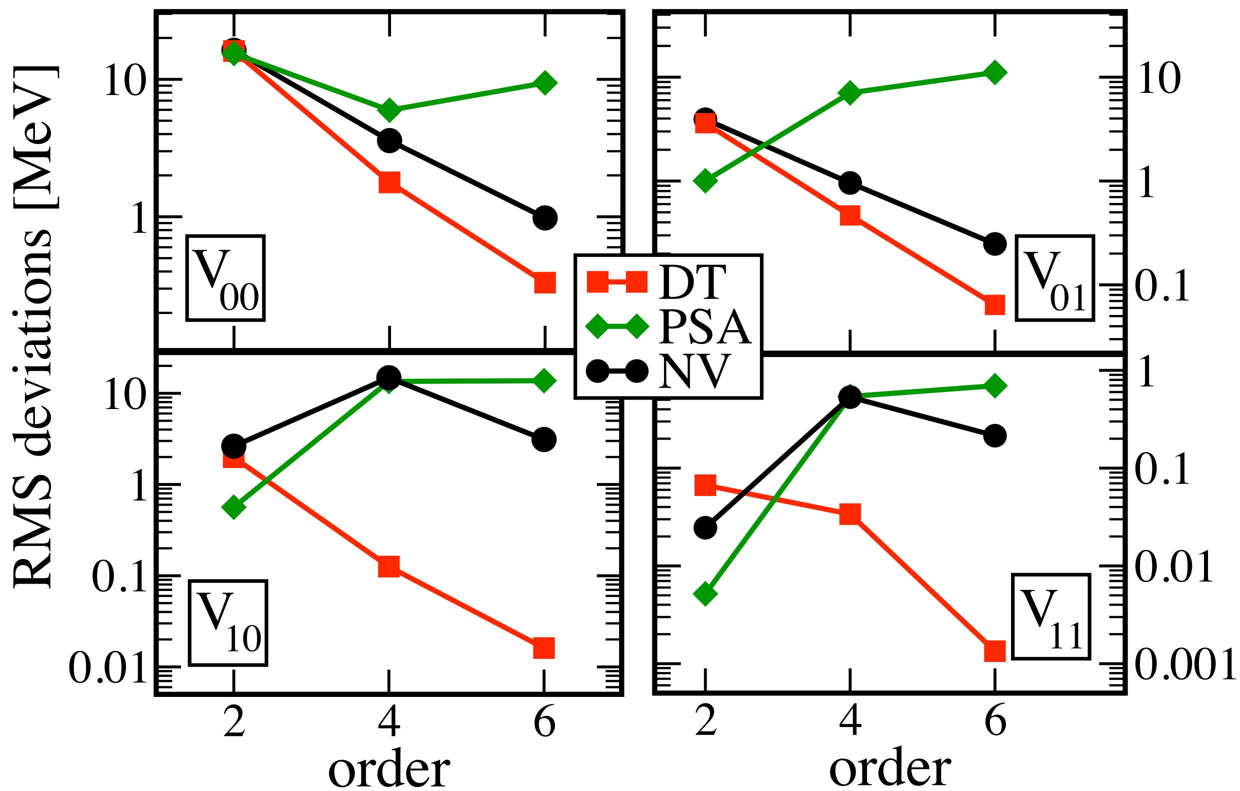




This was pre- PSADME improvements and implementation of exact Hartree. Worth revisiting!

Other efforts developing non-empirical EDFs

DME beyond ∇^2 (Carlsson, Dobaczewski, arXiv:1003.2543)



New “Damped Taylor” DME gives dramatic improvements with higher order gradients

Solves the problem of exploding # of parameters with higher ∇

Summary

- RG methods simplify nuclear many-body calculations
  - faster convergence, more perturbative, low k "universality"
  - empirical NM saturation within theoretical errors
- In-medium SRG
  - Normal-ordering => simple way to evolve many-body operators
  - analogous to CC; diagonalize many-body problems
  - non-perturbative path for shell model and possible ab-initio DFT
- Microscopic connections to DFT now possible
  - explicit inclusion of long-distance chiral EFT physics via the density matrix expansion (microscopic guidance for density dependence, isovector and spin-orbit properties, etc.)