Density Functional Theory for Nuclei

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Outline

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SciDAC 2 Project: *Building a UNEDF* Goals

- Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications”
- Scope is all nuclei ($A > 12$–16), with particular interest in reliable calculations of unstable nuclei and in reactions
- Order of magnitude improvement over present capabilities $\Longrightarrow$ precision calculations
- Connected to best microscopic physics
- Maximum predictive power with well-quantified uncertainties
- Building the EDF is the heart of the project

[website at http://unedf.org]

Parallel Development Areas

1. Momentum-space Renormalization Group (RG) methods to evolve chiral NN and NNN potentials to more perturbative forms as inputs to nuclear matter and ab initio methods (coupled cluster, NCSM).
2. Controlled nuclear matter calculations based on the RG-improved interactions, as ab initio input to Skyrme EDF benchmarking and microscopic functional.
3. Approximate DFT functional, initially by adapting density matrix expansion (DME) to RG-improved interactions.
4. Adaptation to Skyrme codes and allowance for fine tuning.

Points of emphasis:

- Systematic upgrade path with existing and developing technology
- Theoretical error bars on interaction (vary EFT Λ and order of calculation) and on implementation (vary SRG λ or $V_{\mathrm{low}\,k}$ Λ)

Microscopic Nuclear Structure Methods

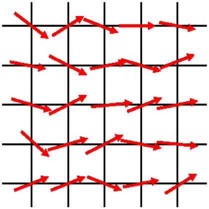
- Wave function methods (GFMC/AFMC, NCSM, CC, ...)
  - many-body wave functions (in approximate form!)
  - $\Psi(x_1, \cdots, x_A) \Longrightarrow$ everything (if operators known)
  - limited to $A < 100$ (??)
- Green's functions (see W. Dickhoff, *Many-Body Theory Exposed*)
  - response of ground state to removing/adding particles
  - single-particle Green's function $\Longrightarrow$ expectation value of one-body operators, Hamiltonian
  - energy, densities, single-particle excitations, ...
- DFT (see C. Fiolhais et al., *A Primer in Density Functional Theory*)
  - response of energy to perturbations of the density
  - energy functional $\Longrightarrow$ plug in candidate density, get out trial energy, minimize (variational)
  - energy and densities (TDFT $\Longrightarrow$ excitations)

DFT and Effective Actions (cf. Negele and Orland)

- External field $\Longleftrightarrow$ Magnetization
- Helmholtz free energy $F[H]$
  $\Longleftrightarrow$ Gibbs free energy $\Gamma[M]$

Legendre transform $\Longrightarrow \Gamma[M] = F[H] + H\,M$

$$H = \frac{\partial \Gamma[M]}{\partial M} \xrightarrow[\text{state}]{\text{ground}} \left.\frac{\partial \Gamma[M]}{\partial M}\right|_{M_{\rm gs}} = 0$$



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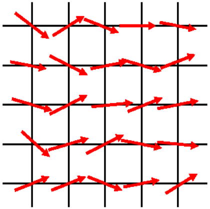

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- Partition function with sources that adjust densities:

$$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H}+J\,\widehat{\rho})} \Longrightarrow \text{path integral for } W[J]$$

- Invert to find $J[\rho]$ and Legendre transform from J to ρ:

$$\rho(\mathbf{x}) = \frac{\delta W[J]}{\delta J(\mathbf{x})} \Longrightarrow \Gamma[\rho] = W[J] - \int J\,\rho \quad \text{and} \quad J(\mathbf{x}) = -\frac{\delta \Gamma[\rho]}{\delta \rho(\mathbf{x})}$$

$\Longrightarrow \Gamma[\rho] \propto$ energy functional $E[\rho]$, stationary at $\rho_{\rm gs}(\mathbf{x})$!

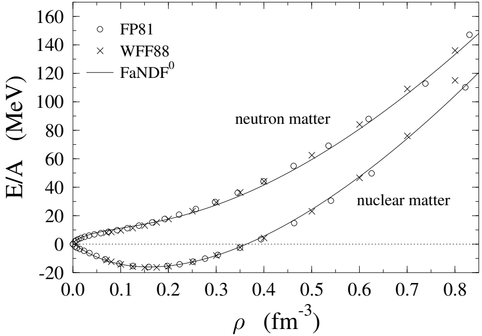
Paths to a Nuclear Energy Functional

- Emulate Coulomb DFT: LDA based on precision calculation of uniform system $E[\rho] = \int d\mathbf{r}\,\mathcal{E}(\rho(\mathbf{r}))$ plus constrained gradient corrections ($\nabla\rho$ factors)

- SLDA (Bulgac et al.)
- Fayans and collaborators (e.g., nucl-th/0009034)

$$\mathcal{E}_v = \frac{2}{3}\epsilon_F\rho_0\left[a_+^v \frac{1-h_{1+}^v x_+^{1/3}}{1-h_{2+}^v x_+^{1/3}} x_+^2 + a_-^v \frac{1-h_{1-}^v x_+^{1/3}}{1-h_{2-}^v x_+^{1/3}} x_-^2\right]$$

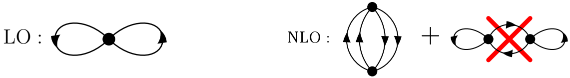
where $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$



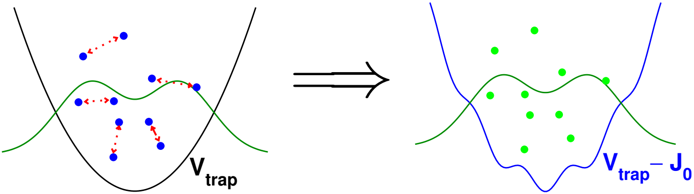
- RG approach (Polonyi and Schwenk, nucl-th/0403011)
- Constructive Kohn-Sham DFT with low-momentum potentials

Construct $W[J]$ and then $\Gamma[\rho]$ order-by-order

- Diagrammatic *expansion* (i.e., use a power counting)



- Inversion method $\Longrightarrow$ Split source $J = J_0 + J_1 + \ldots$
  - cf. $H = (H_0 + U) + (V - U)$ with freedom to choose U
  - J_0 *chosen* to get $\rho(\mathbf{x})$ in noninteracting (Kohn-Sham) system:



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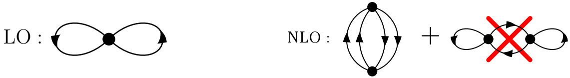

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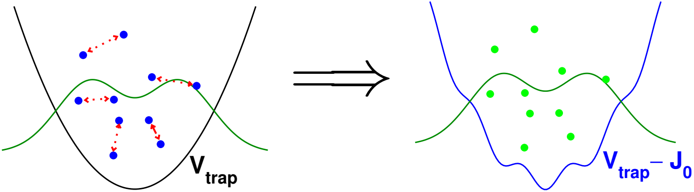

  - Orbitals $\{\psi_\alpha(\mathbf{x})\}$ in local potential $J_0([\rho], \mathbf{x}) \Longrightarrow$ KS propagators

$$[-\nabla^2/2m - J_0(\mathbf{x})]\psi_\alpha = \varepsilon_\alpha \psi_\alpha \Longrightarrow \rho(\mathbf{x}) = \sum_{\alpha=1}^{A} |\psi_\alpha(\mathbf{x})|^2$$

- Self-consistency from $J(\mathbf{x}) = 0 \Longrightarrow J_0(\mathbf{x}) = \delta\Gamma_{\rm int}[\rho]/\delta\rho(\mathbf{x})$

Orbital Dependent DFT (cf. LDA)

- Self-consistency from $J(\mathbf{r}) = 0 \Longrightarrow J_0(\mathbf{r}) = \delta\Gamma_{\text{int}}[\rho]/\delta\rho(\mathbf{r})$
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- Orbital-dependent DFT $\Longrightarrow$ full derivative via chain rule:

$$J_0(\mathbf{r}) = \frac{\delta\Gamma_{\rm int}[\phi_\alpha, \varepsilon_\alpha]}{\delta\rho(\mathbf{r})} = \int d\mathbf{r}' \, \frac{\delta J_0(\mathbf{r}')}{\delta\rho(\mathbf{r})} \sum_\alpha \Bigg\{ \int d\mathbf{r}'' \left[\frac{\delta\phi_\alpha^\dagger(\mathbf{r}'')}{\delta J_0(\mathbf{r}')} \frac{\delta\Gamma_{\rm int}}{\delta\phi_\alpha^\dagger(\mathbf{r}'')} + c.c. \right] + \frac{\delta\varepsilon_\alpha}{\delta J_0(\mathbf{r}')} \frac{\partial\Gamma_{\rm int}}{\partial\varepsilon_\alpha} \Bigg\}$$

  - Solve the OPM equation for J_0 using $\chi_s(\mathbf{r},\mathbf{r}') = \delta\rho(\mathbf{r})/\delta J_0(\mathbf{r}')$

$$\int d^3r' \, \chi_s(\mathbf{r},\mathbf{r}') \, J_0(\mathbf{r}') = \Lambda_{\rm xc}(\mathbf{r})$$

  - $\Lambda_{\rm xc}(\mathbf{r})$ is functional of the orbitals ϕ_α, eigenvalues ε_α, and $G^0_{\rm KS}$

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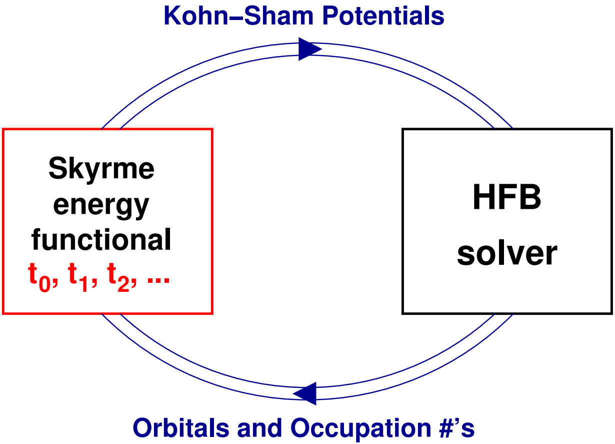
- Approximation with explicit $\rho(\mathbf{R})$, $\tau(\mathbf{R})$, ... dependence?

DFT vs. Solving Skyrme HF



$$J_0(\mathbf{r}) = \frac{\delta E_{\text{int}}[\rho]}{\delta\rho(\mathbf{r})} \quad \Longleftrightarrow \quad [-\frac{\nabla^2}{2m} - J_0(\mathbf{x})]\psi_\alpha = \varepsilon_\alpha \psi_\alpha \Longrightarrow \rho(\mathbf{x}) = \sum_\alpha n_\alpha |\psi_\alpha(\mathbf{x})|^2$$

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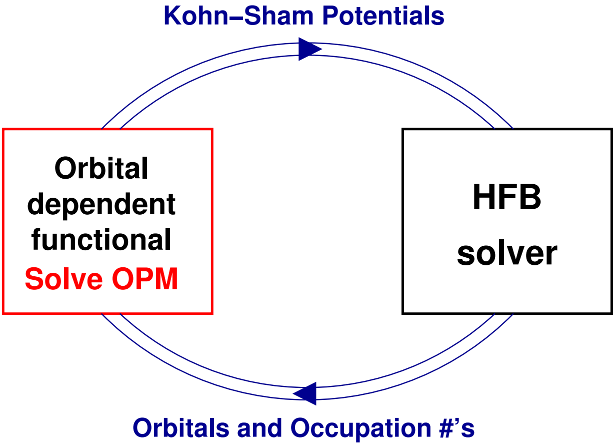

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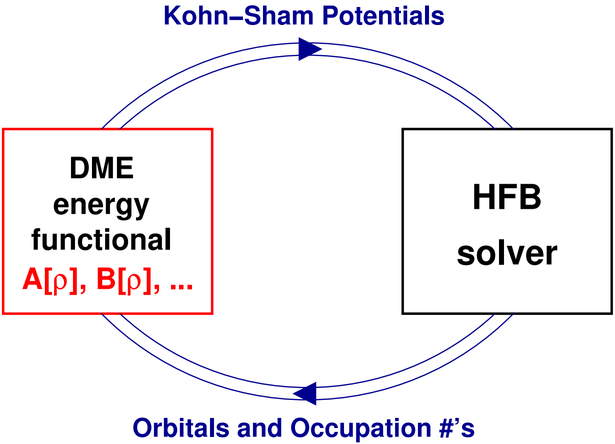

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DFT *Looks* Like Low-Order HF Approximation

- WF: Best single Slater determinant in variational sense:

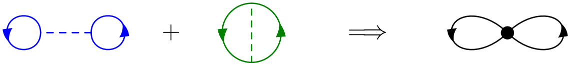
$$|\Psi_{\rm HF}\rangle = \det\{\phi_i(\mathbf{x}), i = 1\cdots A\}\,, \quad \mathbf{x} = (\mathbf{r}, \sigma, \tau)$$

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

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

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

- Self-consistent Green's function: same result from just



- Kohn-Sham DFT equations *always* look like Hartree or zero-range Hartree-Fock ("multiplicative potential")

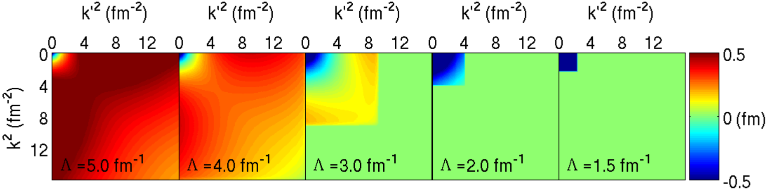
Outline

DFT Issues

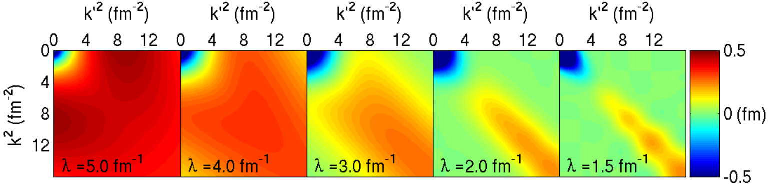
- Organization about mean field: need convergent expansion
  - like loop expansion: only mean field is nonperturbative
  - can DFT deal with nuclear short-range correlations?
  - claim: need low-momentum interactions
- DFT for self-bound systems
  - does DFT even exist? (HK theorem for intrinic states?)
  - symmetry breaking and zero modes
  - game plans proposed:
    - J. Engel, find intrinsic functional (one-d boson system)
    - Giraud et al., use harmonic oscillator tricks
    - methods to deal with soliton zero modes
- How to deal with long-range correlations?
- Effectiveness of approximations (e.g., DME)

Low-Momentum Interactions from RG [AV18 $^3S_1$]

- "$V_{\mathrm{low}\,k}$" $\Longrightarrow$ Lower a cutoff Λ in relative k, k' [sharp]



- SRG $\Longrightarrow$ Drive the Hamiltonian toward diagonal [$\lambda \equiv 1/s^{1/4}$]



- Other transformations also decouple (e.g., UCOM)
- Isn't chiral EFT already soft?

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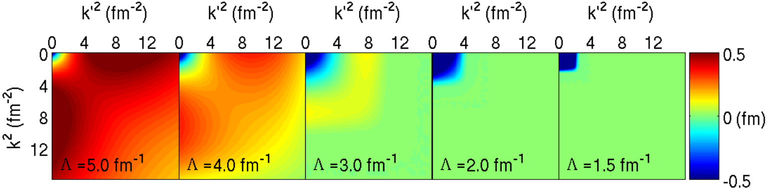

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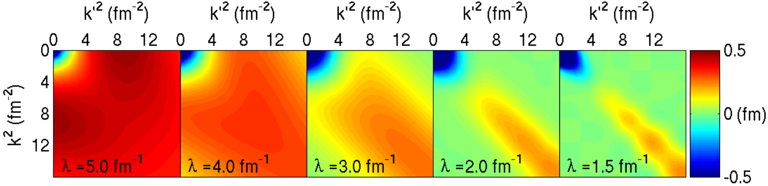

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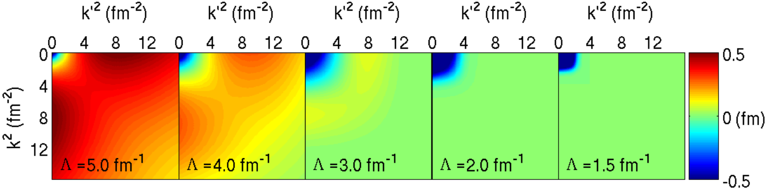

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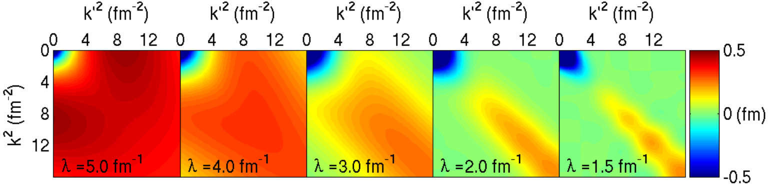

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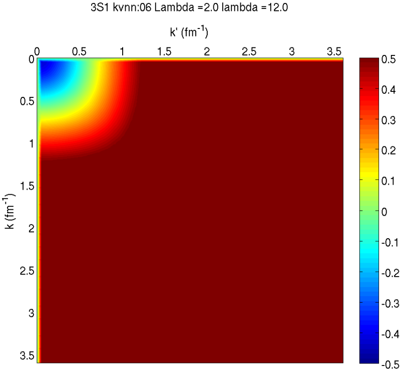
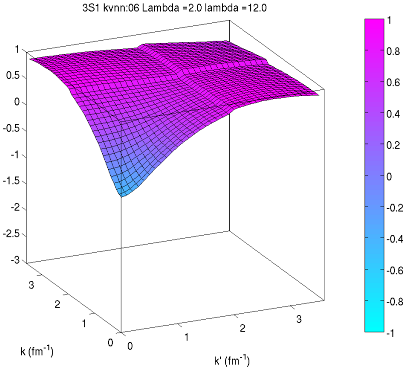
Block Diagonalization Via SRG

- Can we get a $\Lambda = 2\,\text{fm}^{-1}$ $V_{\text{low}\,k}$-like potential with SRG?
- Yes! Use $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$ with $G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$





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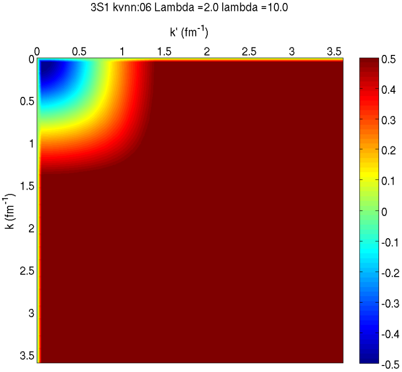

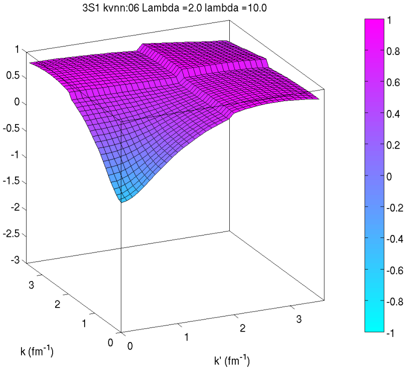

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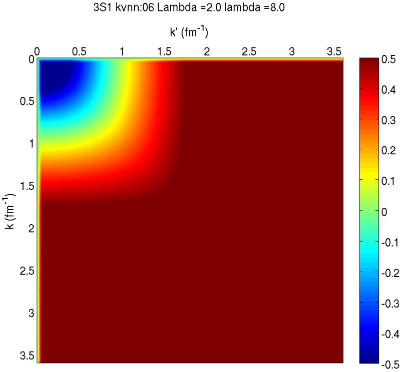

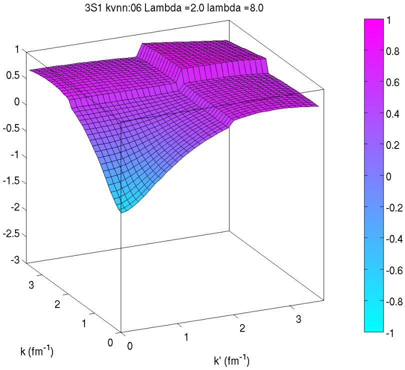

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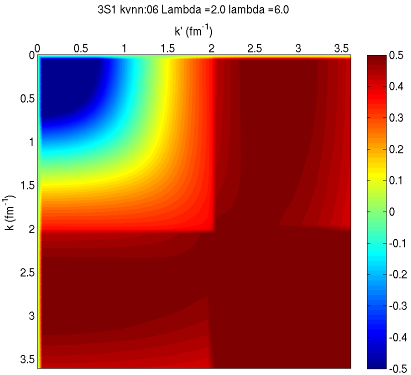

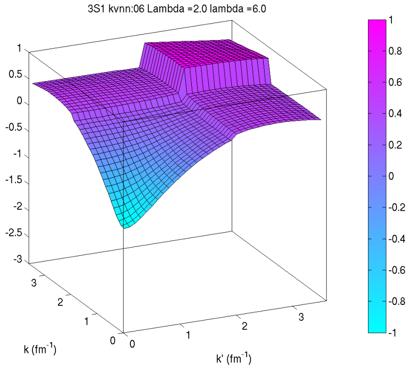

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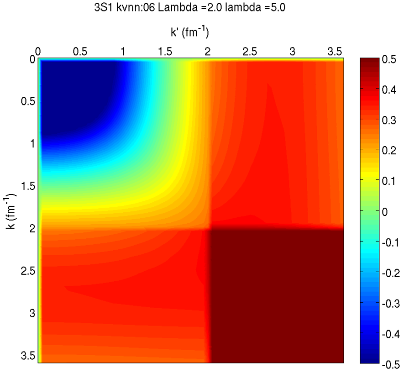

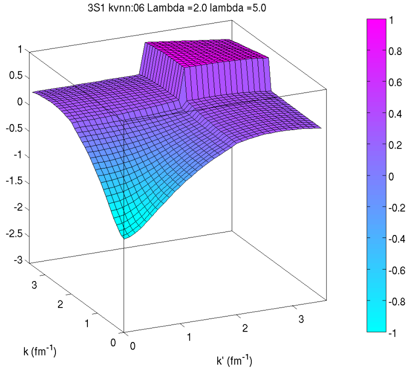

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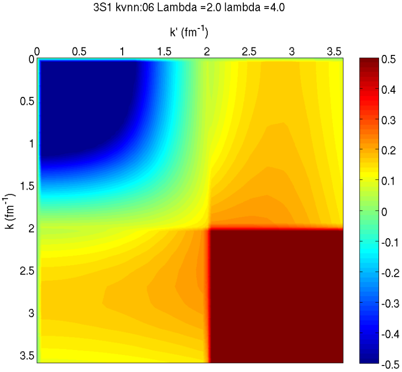

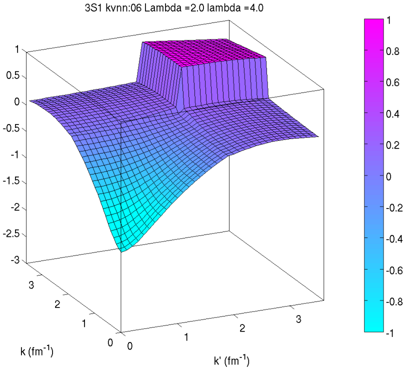

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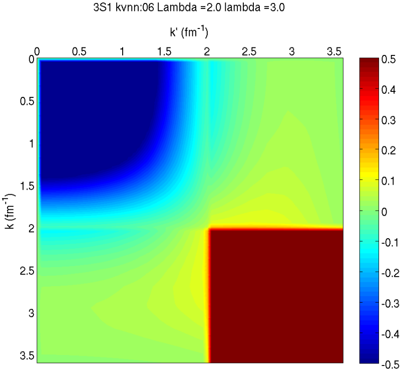

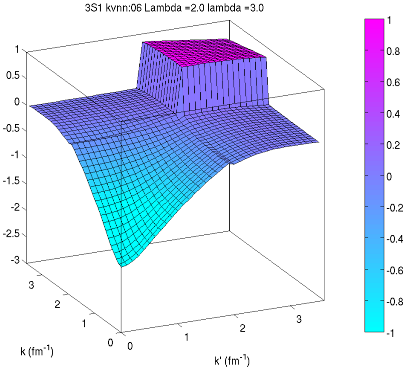

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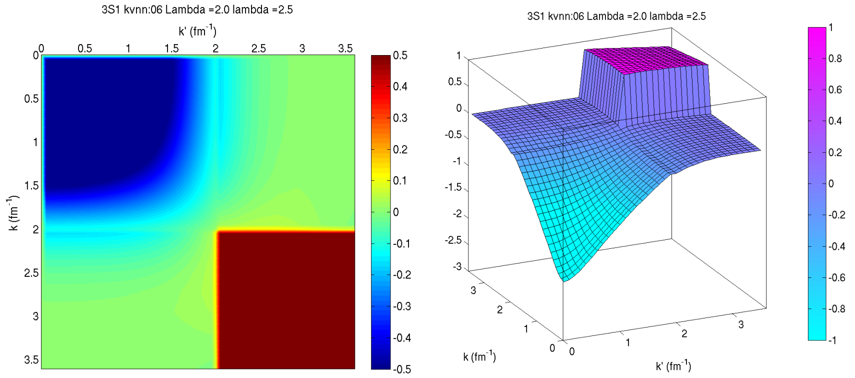

Block Diagonalization Via SRG

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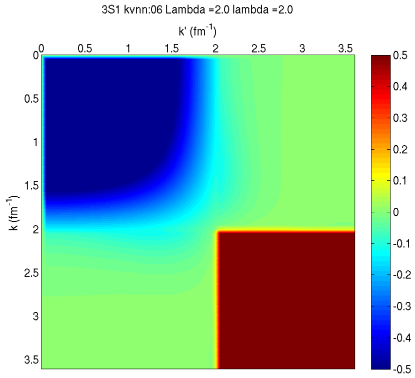

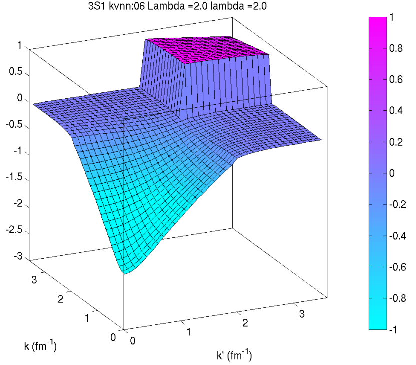

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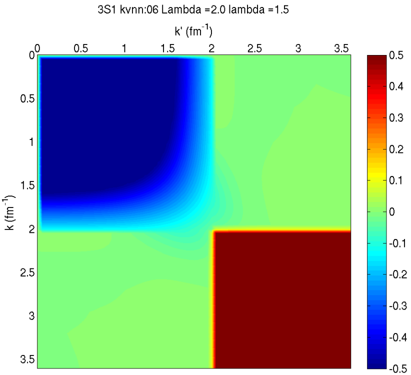

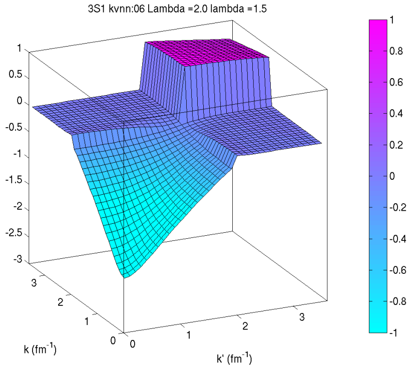

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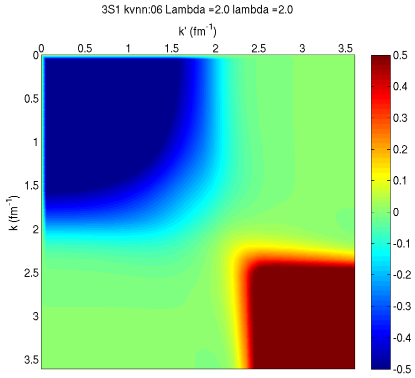

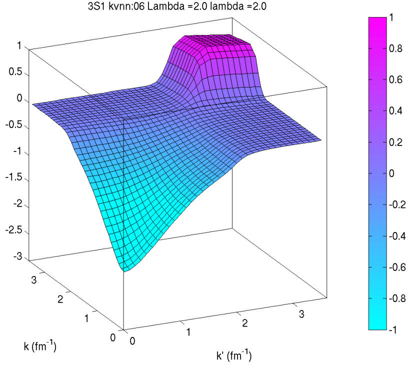

Decoupling of N^{3}LO Potentials ($^1S_0$)

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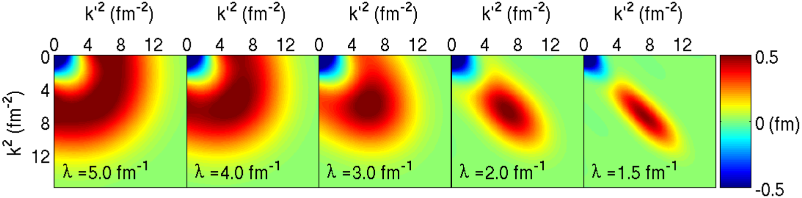
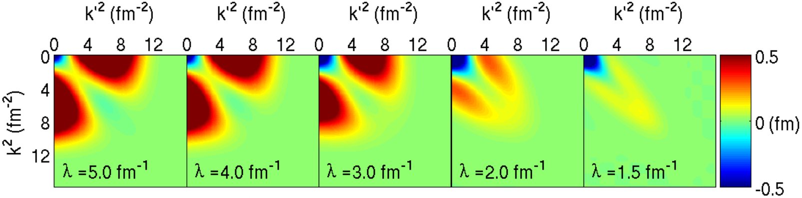


- $^1S_0$ from N^{3}LO (550/600 MeV) of Epelbaum et al.



- See http://www.physics.ohio-state.edu/∼srg/ for more!

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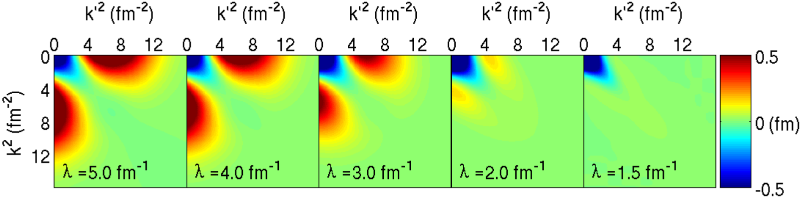

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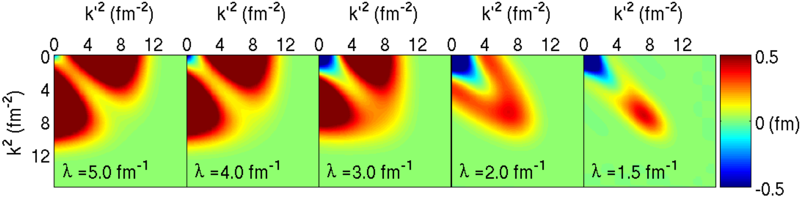

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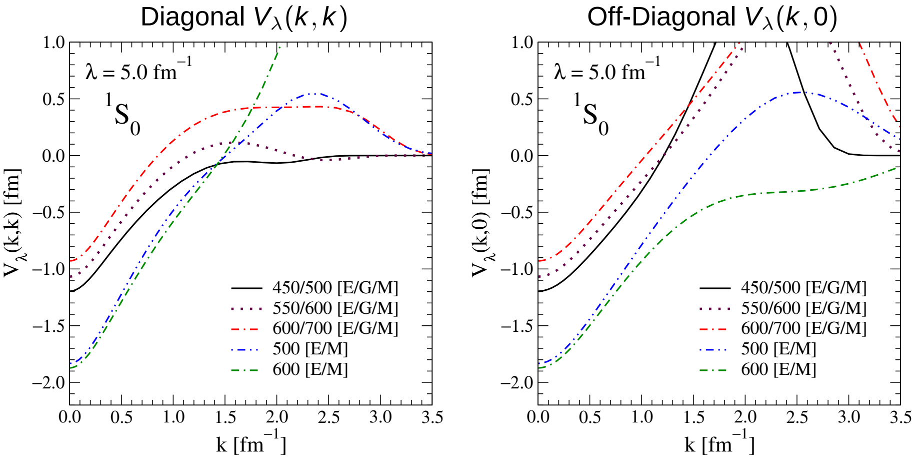
Run to Lower λ via SRG $\Longrightarrow$ $\approx$Universality



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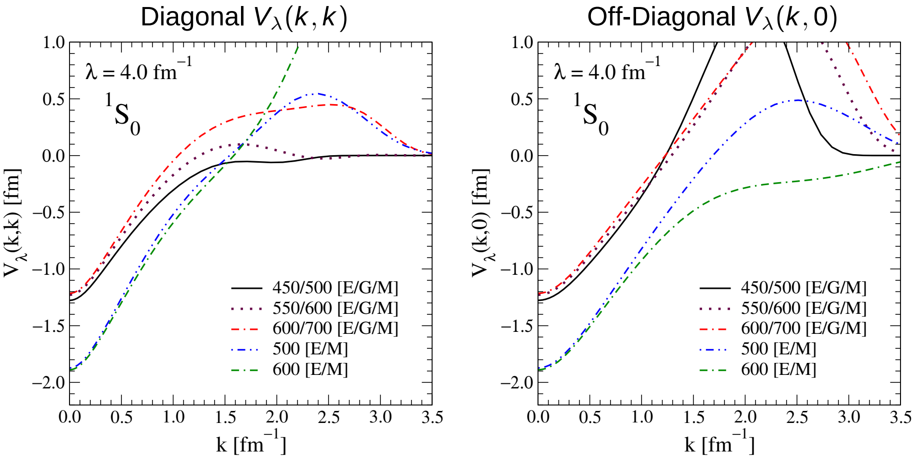

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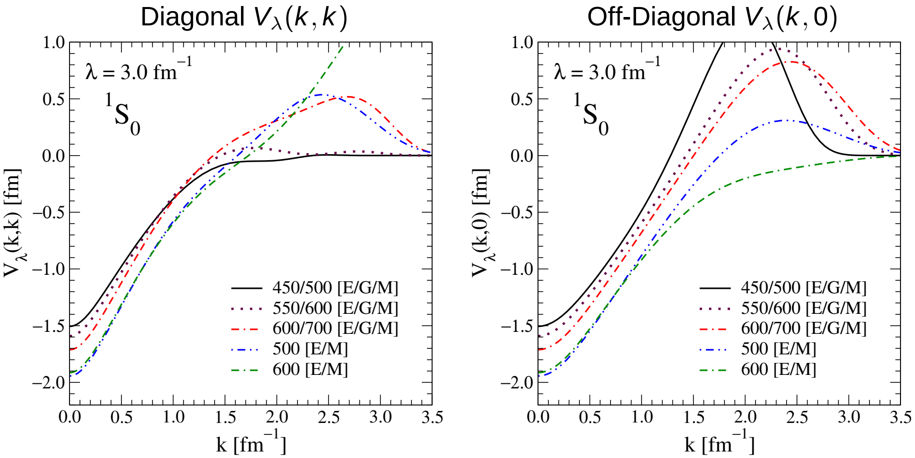

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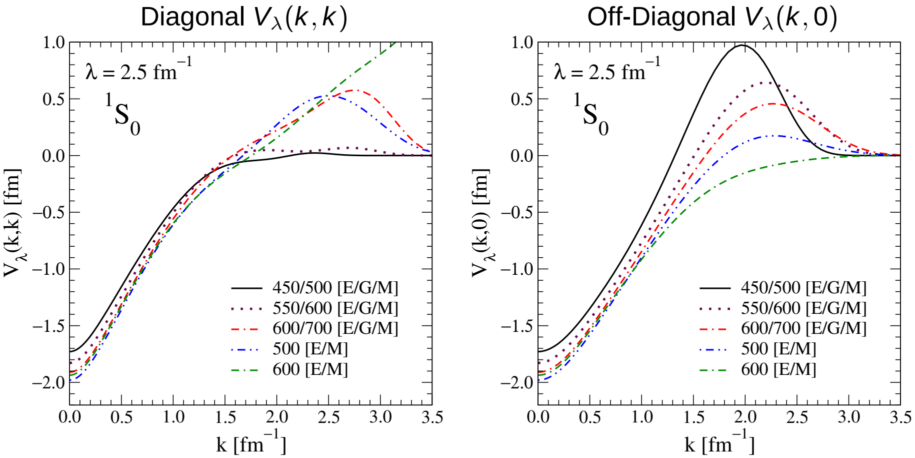

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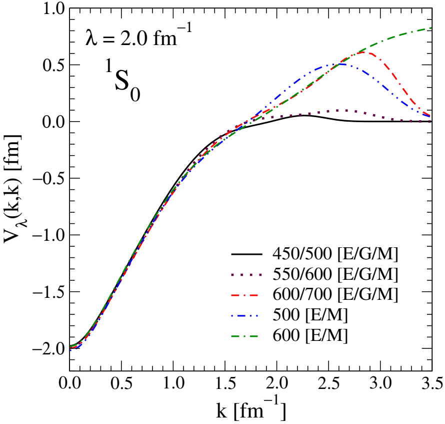
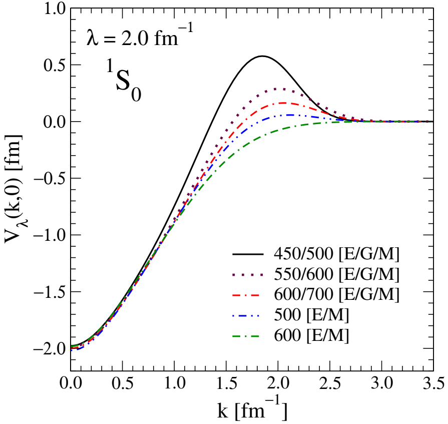
Diagonal $V_\lambda(k,k)$



Off-Diagonal $V_\lambda(k,0)$



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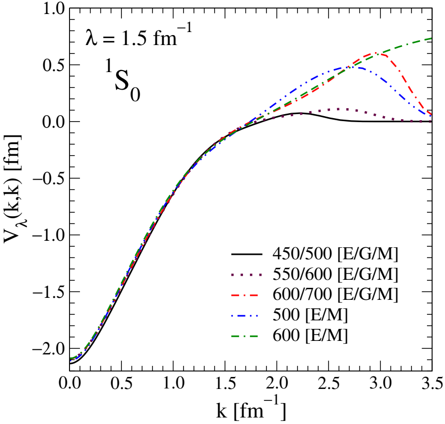

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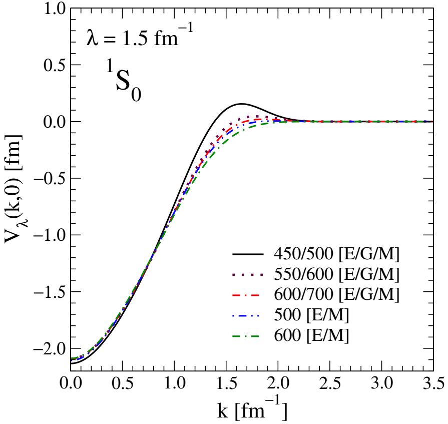
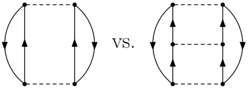
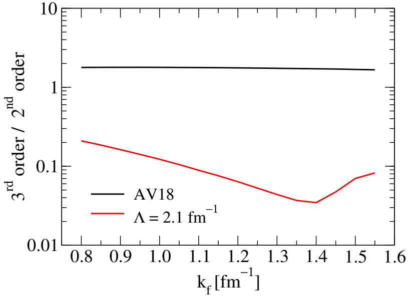


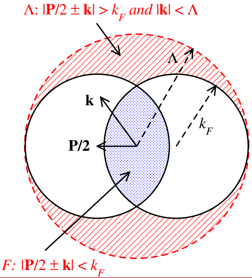
Bethe-Brueckner-Goldstone Power Counting

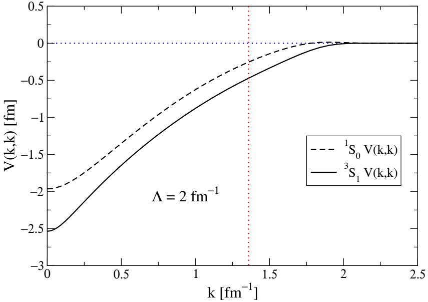
Strong short-range repulsion
$\Longrightarrow$ Sum V ladders $\Longrightarrow$ G





$V_{\mathrm{low}\,k}$ momentum dependence + phase space
$\Longrightarrow$ perturbative





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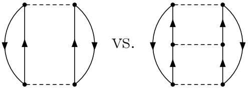

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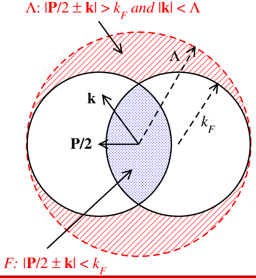
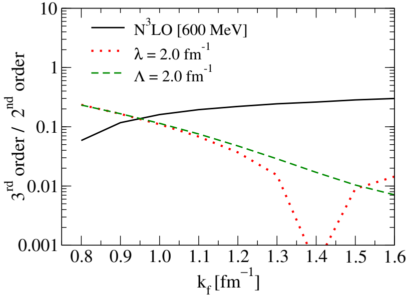
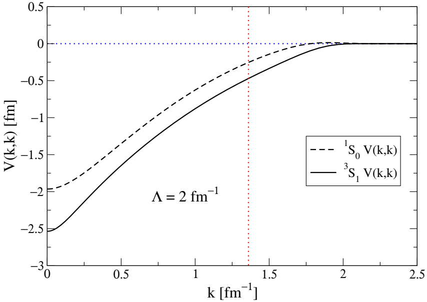
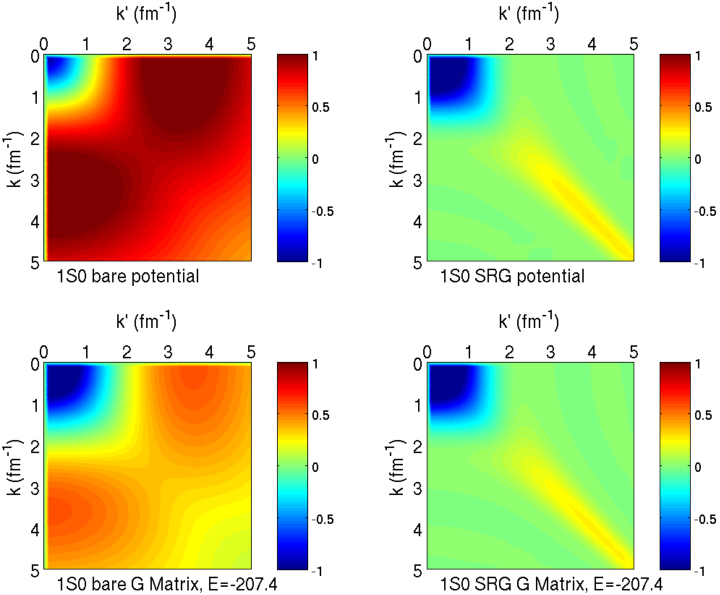






Compare Potential and G Matrix: AV18



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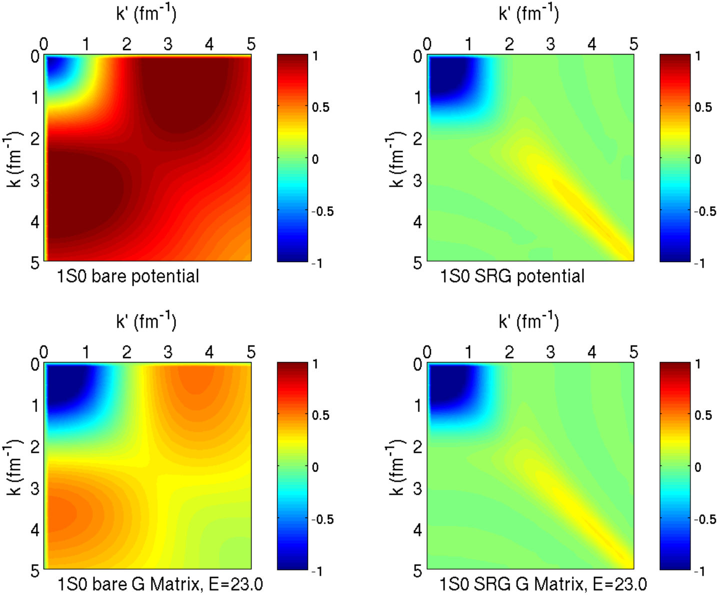

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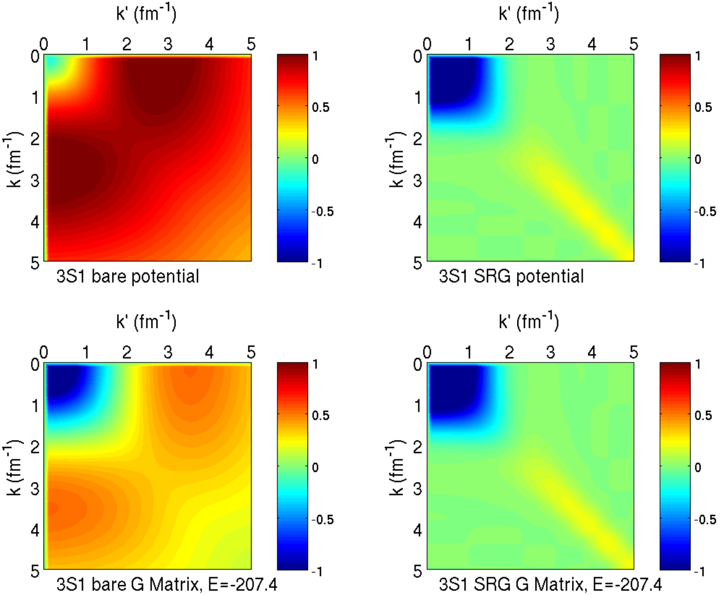

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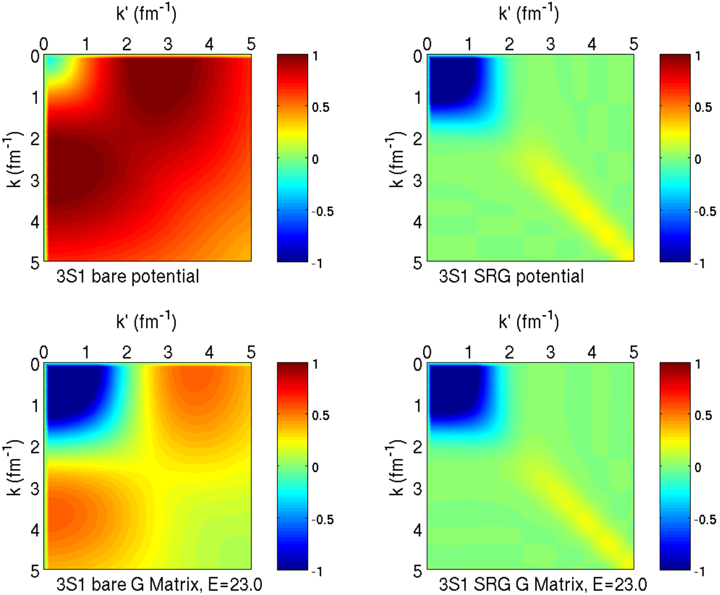

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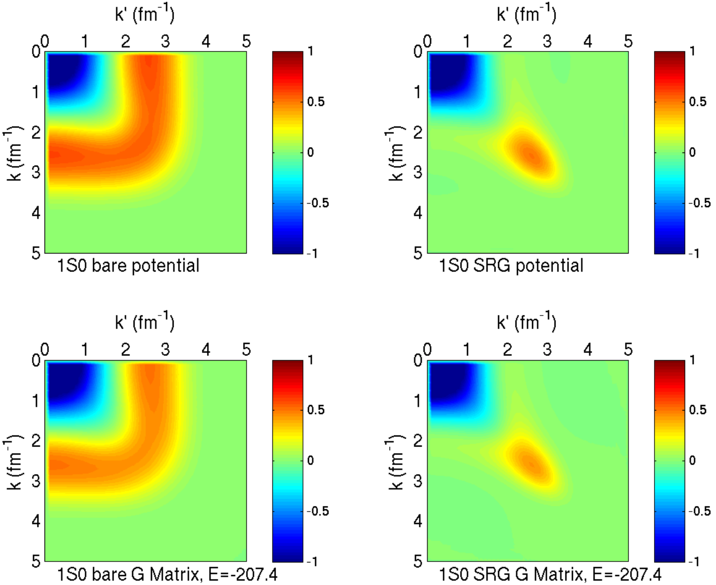

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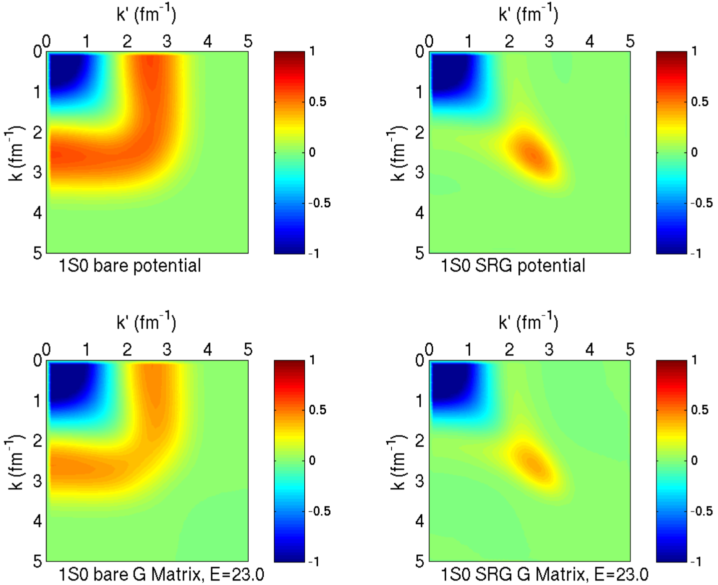

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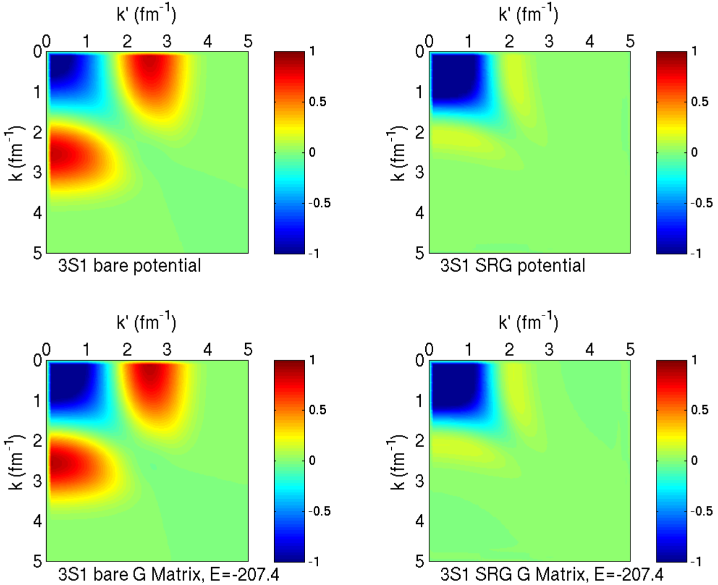

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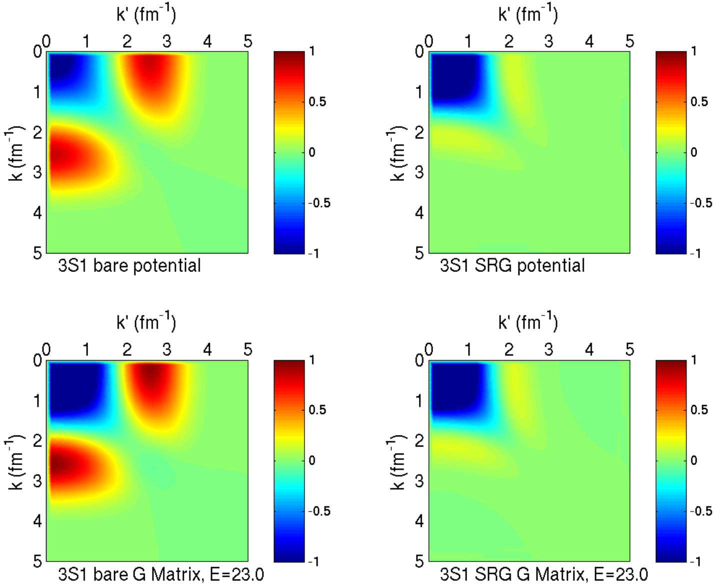
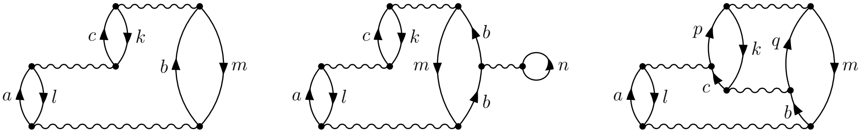


Hole-Line Expansion Revisited (Bethe, Day, . . .)

- Consider ratio of fourth-order diagrams to third-order:

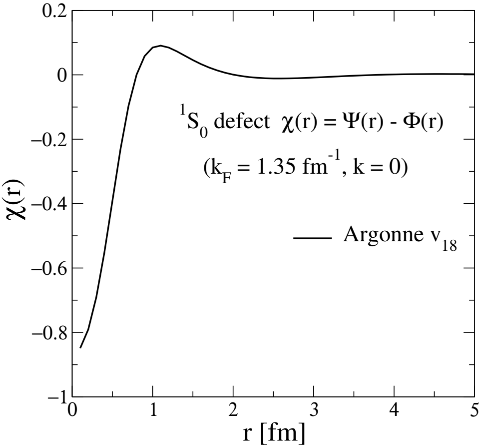


- “Conventional” G matrix still couples low-k and high-k
  - add a hole line $\Longrightarrow$ ratio $\approx \sum_{n\leq k_\mathrm{F}} \langle bn|(1/e)G|bn\rangle \approx \kappa \approx 0.15$
  - no new hole line $\Longrightarrow$ ratio $\approx -\chi(\mathbf{r}=0) \approx -1 \Longrightarrow$ sum all orders
- Low-momentum potentials decouple low-k and high-k
  - add a hole line $\Longrightarrow$ still suppressed
  - no new hole line $\Longrightarrow$ also suppressed (limited phase space)
  - freedom to choose single-particle U $\Longrightarrow$ use for Kohn-Sham

$\Longrightarrow$ Density functional theory (DFT) should work!

Two-Body Correlations at Nuclear Matter Density

- Defect wf $\chi(r)$ for particular kinematics ($k = 0$, $P_{\rm cm} = 0$)
- AV18: "Wound integral" provides expansion parameter



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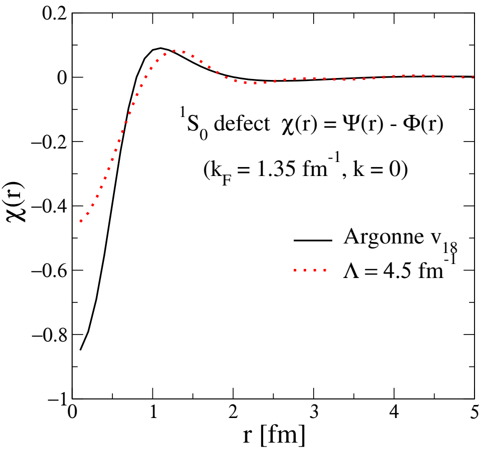

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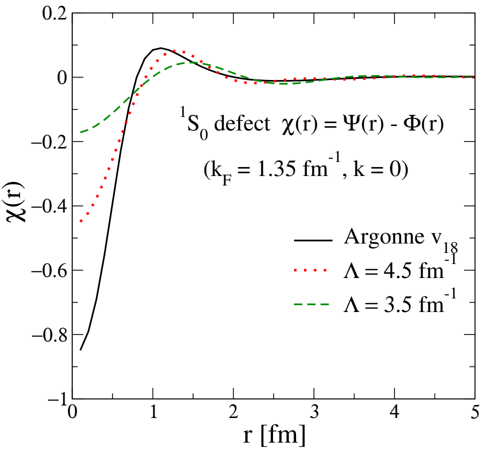

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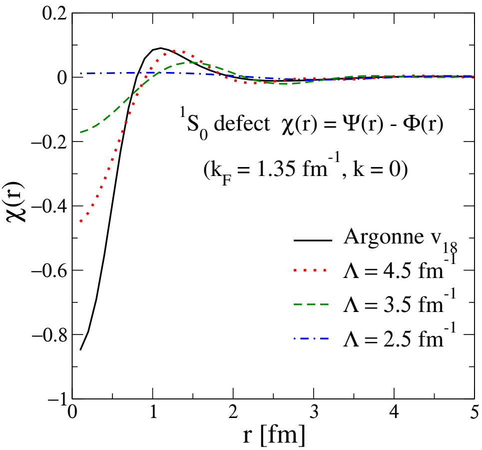

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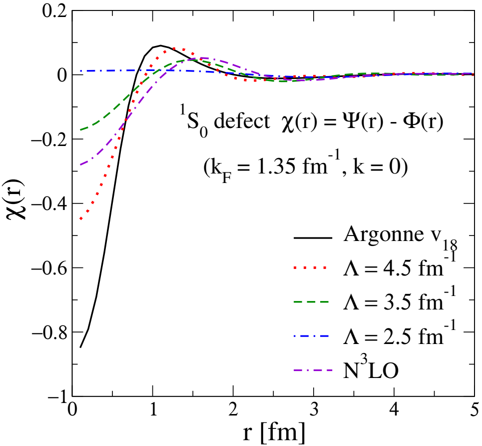
- Still a sizable wound for N^3LO



Nuclear Matter with NN Ladders Only [nucl-th/0504043]

- Brueckner ladders order-by-order
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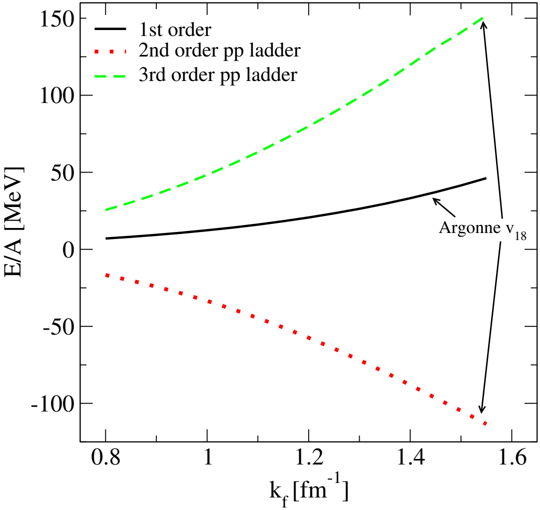

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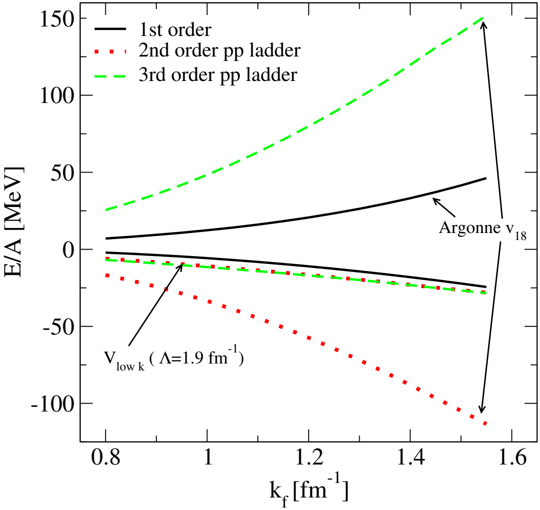
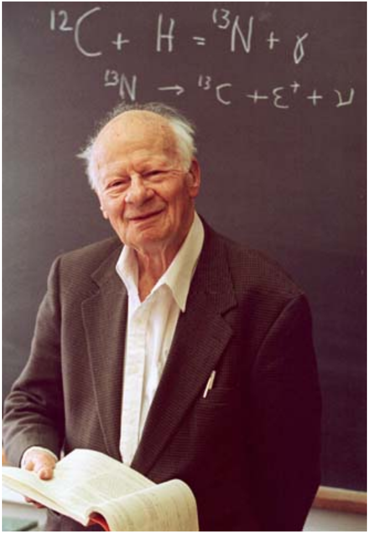
- Brueckner ladders order-by-order
- Repulsive core $\Longrightarrow$ series diverges
- $V_{\text{low}\,k}$ converges
- No saturation in sight!



Deja Vu All Over Again?

- There were active attempts to transform away hard cores and soften the tensor interaction in the late sixties and early seventies.
- But the requiem for soft potentials was given by Bethe (1971):
  "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."
- Next 35+ years struggling to solve accurately with "hard" potential



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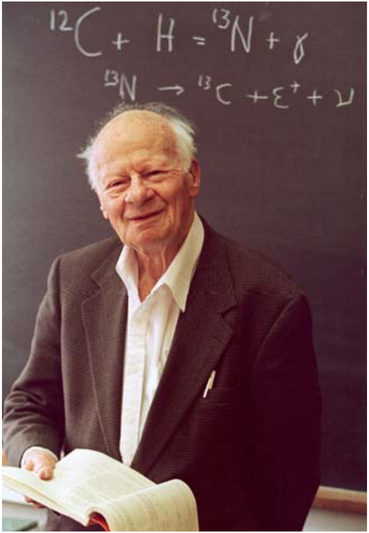
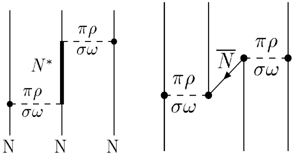
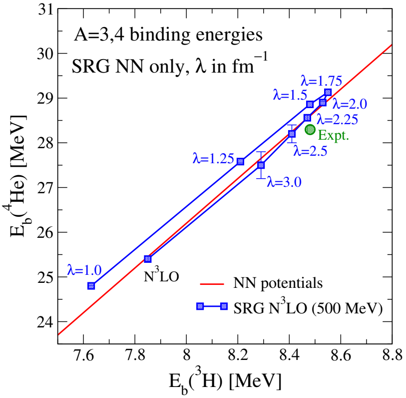
- But the story is not complete: three-nucleon forces (3NF)!



Observations on Three-Body Forces

- Three-body forces arise from eliminating dof's
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
  - observables depend on λ
  - e.g., Tjon line
- 3-body contributions increase with density
  - saturates nuclear matter
  - how large is 4-body?





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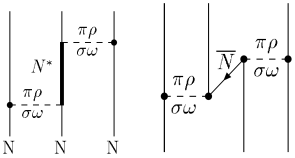
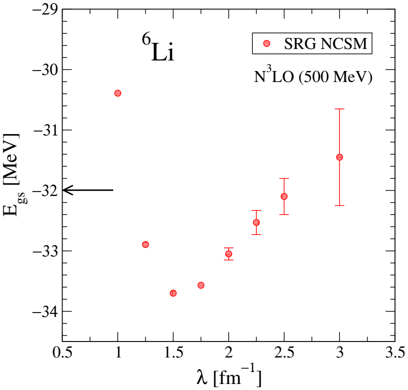
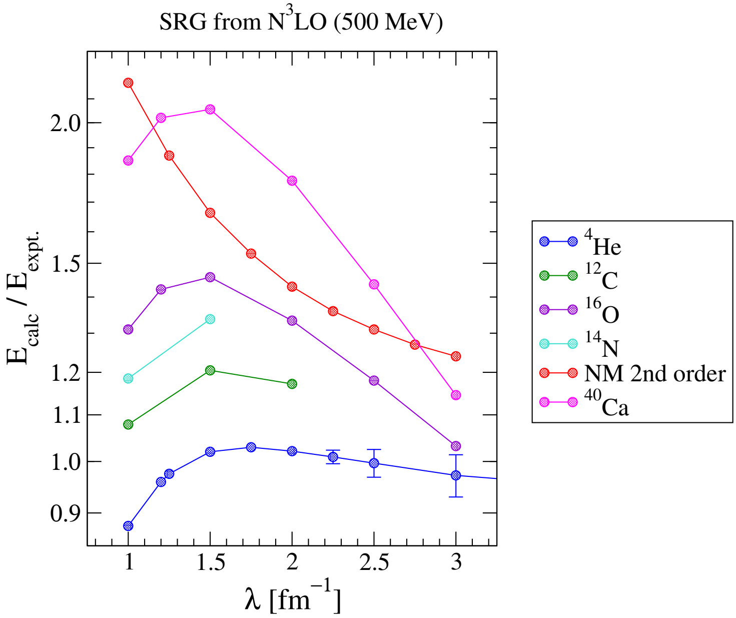
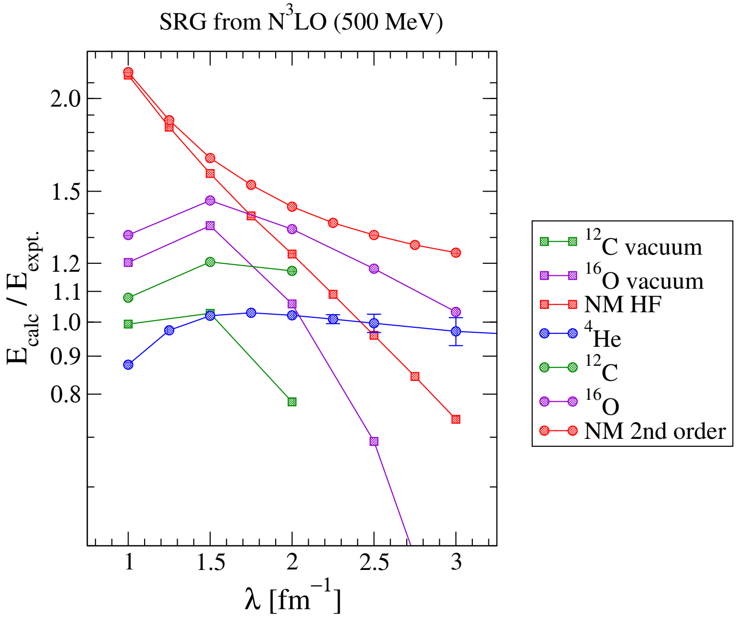




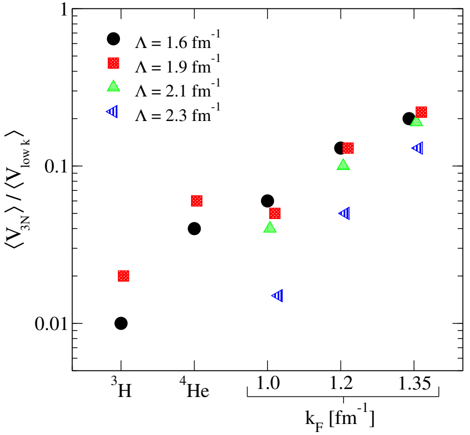

SRG from N3LO (500 MeV)
E_calc / E_expt.
2.0
1.5
1.2
1.1
1.0
0.9
1
1.5
2
2.5
3
λ [fm^-1]
4He
12C
16O
14N
NM 2nd order
40Ca


SRG from N^{3}LO (500 MeV)
$E_{calc} / E_{expt.}$
2.0
1.5
1.2
1.1
1.0
0.9
0.8
1
1.5
2
2.5
3
λ [fm^{-1}]
^{12}C vacuum
^{16}O vacuum
NM HF
^{4}He
^{12}C
^{16}O
NM 2nd order

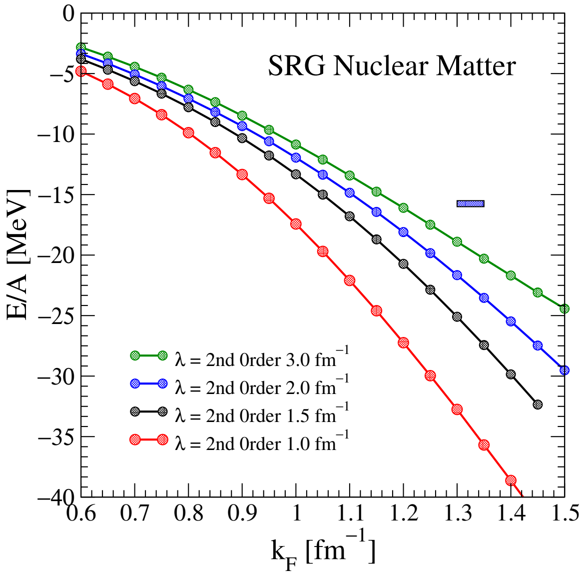
How Does The 3N Contribution Scale?

- Saturation driven by 3NF
- 3N force perturbative
  for $\Lambda \lesssim 2.5\,\text{fm}^{-1}$
- Coupled cluster results very promising
- Unnaturally large?
  Chiral: $\langle V_{3N} \rangle \sim (Q/\Lambda)^3 \langle V_{NN} \rangle$
- Four-body contributions?
- Power counting with
  NN + 3N HF at LO?

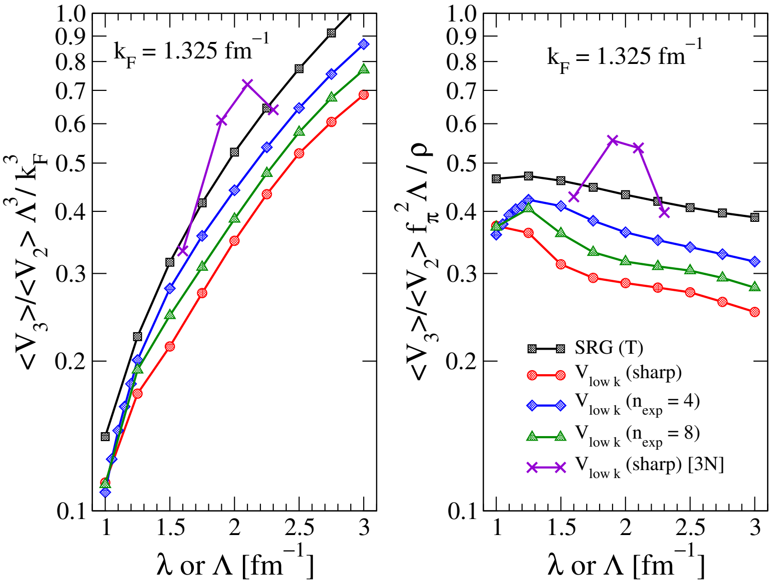
Check ratios:



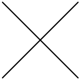
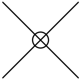
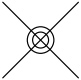
Compare 2nd-Order NN-Only to Empirical Point

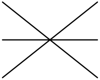
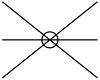
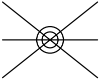


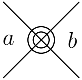
Does 3N/2N Ratio Scale Like $1/\Lambda^3$ or $1/\Lambda$?

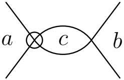


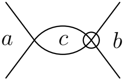
Diagrams for SRG $\Longrightarrow$ Disconnected Cancels

$V_s^{(2)} =$  $[T, V_s^{(2)}] =$  $[[T, V_s^{(2)}], T] =$ 

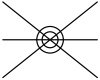
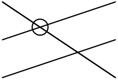
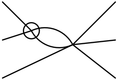
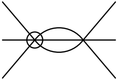
$V_s^{(3)} =$  $[T, V_s^{(3)}] =$  $[[T, V_s^{(3)}], T] =$ 

$\frac{dV_s^{(2)}(a,b)}{ds} =$ 

$+$ 

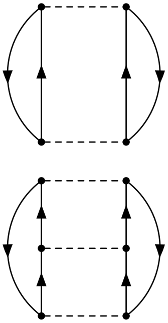
$-$ 

$-(\epsilon_a - \epsilon_b)^2 V_s^{(2)}(a,b)$ $\quad$ $\sum_c [(\epsilon_a - \epsilon_c) - (\epsilon_c - \epsilon_b)] V_s^{(2)}(a,c) V_s^{(2)}(c,b)$

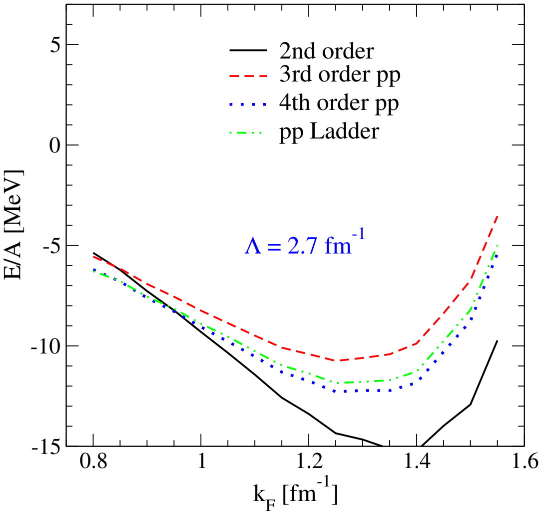
$\frac{dV_s^{(3)}}{ds} =$  $+$  $+$  $+$  $+ \cdots$

Nuclear Matter Ladders [nucl-th/0504043]

- Brueckner ladders order-by-order



- 3-body approximated



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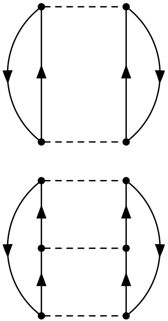

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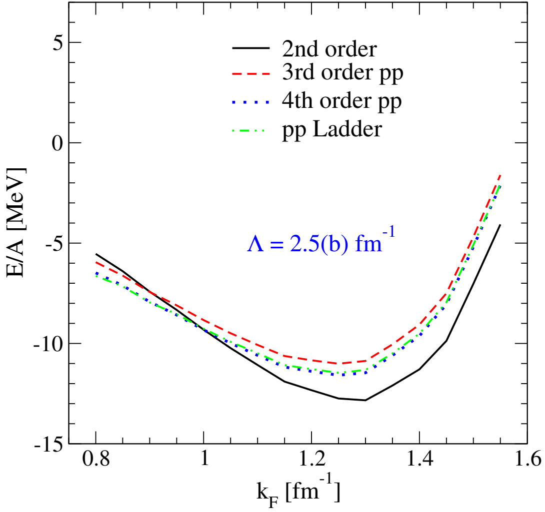

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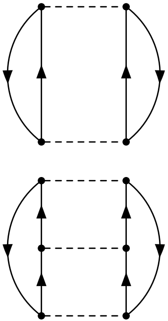

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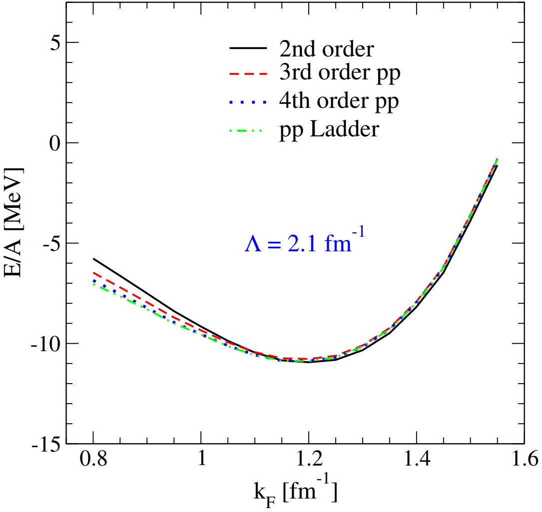

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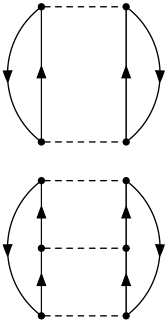

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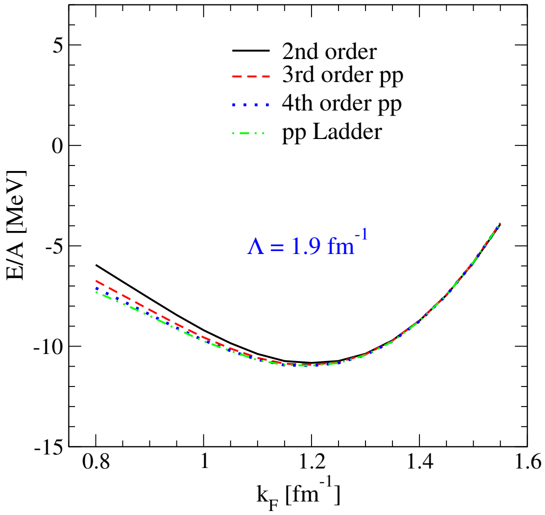
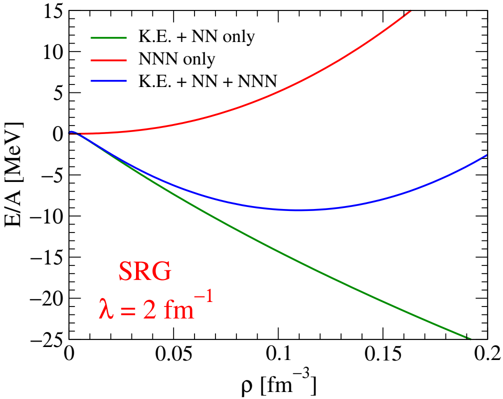
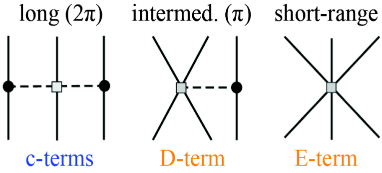


Nuclear matter: Connecting to DFT

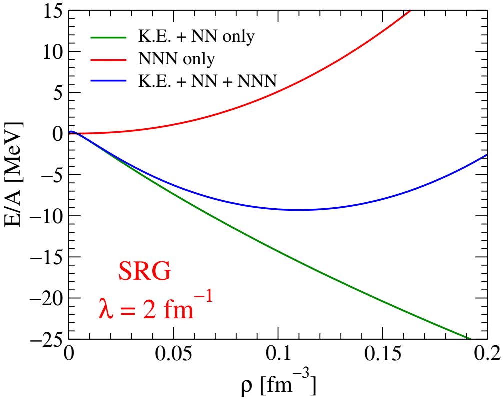
- HF + 2nd order
- NN-only $V_{\mathrm{low}\,k}$ or SRG with $\Lambda, \lambda \leq 2\,\mathrm{fm}^{-1}$ doesn't saturate nuclear matter $\Longrightarrow$ as $A \uparrow$, nuclei collapse
- Typical fit to NNN from chiral EFT at N^{2}LO from $A = 3, 4 \Longrightarrow c_D, c_E$ (but not fit to SRG yet)
- Large uncertainty for c-terms from πN or NN
- Only symmetric nuclear matter so far

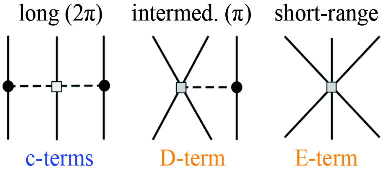




Nuclear matter: Connecting to DFT

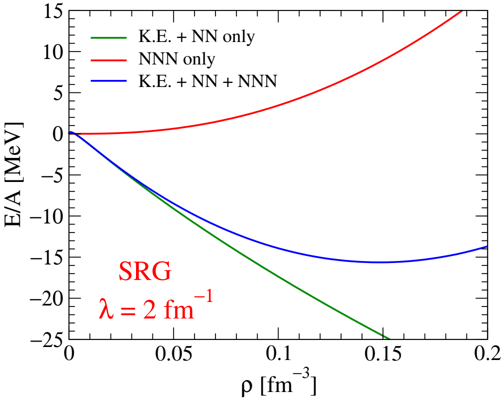
- Coefficients of NNN force can be used to fine-tune nuclear matter within error bands
- "Naturalness" implies $\mathcal{O}(1)$ factors
- Should also be consistent with small $A \Longrightarrow$ need NNN fits (and eventually SRG running)
- In the short term: add short-distance counterterms for adjustments

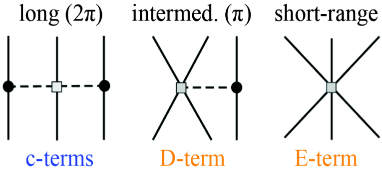




Nuclear matter: Connecting to DFT

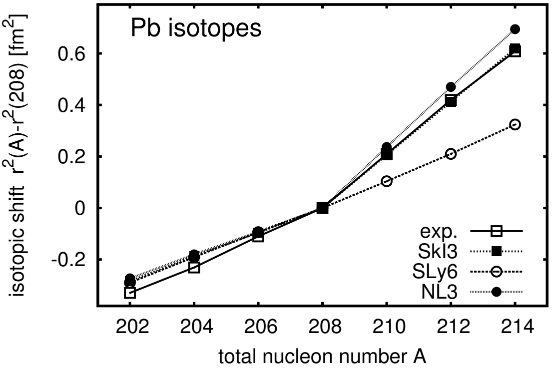
- Preliminary: may need more binding from NN to get naturalness and reasonable K_{sat}
- What is missing in NN part at MeV/particle level? Need accurate nuclear matter calculation to assess (coupled cluster!)





Observables Sensitive to 3N Interactions?

- Study systematics along isotopic chains
- Example: kink in radius shift $\langle r^2 \rangle(A) - \langle r^2 \rangle(208)$ [Reinhard/Flocard, NPA 584]



- Can we constrain 3N forces from nuclear structure?
  - Already practiced for light nuclei (GFMC, NCSM)

Misconceptions vs. Correct Interpretations

- DFT is a Hartree-(Fock) approximation to an effective interaction
  - DFT can accomodate *all* correlations in principle,
    but they are included perturbatively (which can fail for some V)
- Nuclear matter is strongly nonperturbative in the potential
  - "perturbativeness" is highly resolution dependent
- (fill in the blank) causes nuclear saturation
  - another resolution-dependent inference
- Generating low-momentum interactions loses important information
  - long-range physics is preserved
  - relevant short-range physics encoded in potential
- Low-momentum NN potentials are just like G-matrices
  - important distinction: conventional G-matrix still
    has high-momentum, off-diagonal matrix elements

Outline

DFT in Context

Necessary Conditions for Constructive DFT to Work

Near-Term Gameplan for Microscopic Nuclear DFT

Summary

SciDAC 2 Project: *Building a UNEDF* Goals

- Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications”
- Scope is all nuclei ($A > 12$–16), with particular interest in reliable calculations of unstable nuclei and in reactions
- Order of magnitude improvement over present capabilities
  $\Longrightarrow$ precision calculations
- Connected to best microscopic physics
- Maximum predictive power with well-quantified uncertainties
- Building the EDF is the heart of the project

[website at http://unedf.org]

Parallel Development Areas

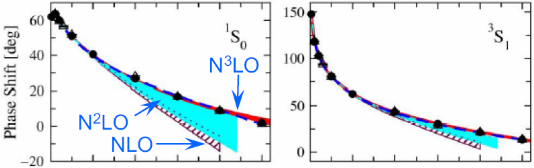
1. Momentum-space Renormalization Group (RG) methods to evolve chiral NN and NNN potentials to more perturbative forms as inputs to nuclear matter and ab initio methods (coupled cluster, NCSM).
2. Controlled nuclear matter calculations based on the RG-improved interactions, as ab initio input to Skyrme EDF benchmarking and microscopic functional.
3. Approximate DFT functional, initially by adapting density matrix expansion (DME) to RG-improved interactions.
4. Adaptation to Skyrme codes and allowance for fine tuning.

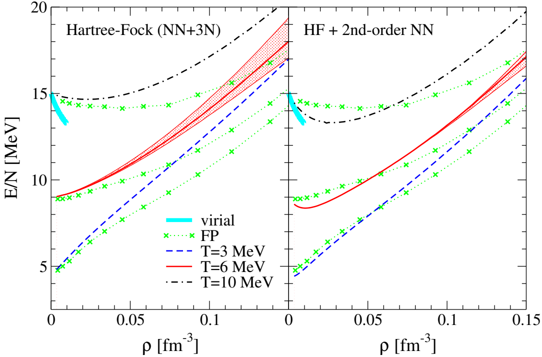
Points of emphasis:

- Systematic upgrade path with existing and developing technology
- Theoretical error bars on interaction (vary EFT Λ and order of calculation) and on implementation (vary SRG λ or $V_{\mathrm{low}\,k}$ Λ)

Sources of Theoretical Error Bars

1. EFT Hamiltonian
   - estimate from order of EFT power counting
   - lower bound from varying Λ_{EFT}
2. RG ($V_{\mathrm{low}\,k}$, V_{SRG}) truncation: NN$\cdots$N contributions
   - vary λ_{SRG} or $\Lambda_{V_{\mathrm{low}\,k}}$
3. Many-body approximations
   - vary λ_{SRG} or $\Lambda_{V_{\mathrm{low}\,k}}$
4. Numerical approximations
   - vary basis size, etc.

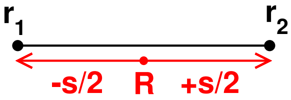




Density Matrix Expansion Revisited [Negele/Vautherin]

- DME: Write one-particle density matrix in Kohn-Sham basis

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\epsilon_\alpha \leq \epsilon_F} \psi^\dagger_\alpha(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2)$$



- $\rho(\mathbf{r}_1, \mathbf{r}_2)$ falls off with $|\mathbf{r}_1 - \mathbf{r}_2| \Longrightarrow$ expand in s (and resum)
- Fall off well approximated by nuclear matter
  $\Longrightarrow$ expand so that first term exact in uniform system

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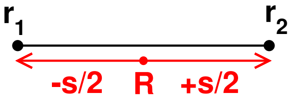

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- Fall off well approximated by nuclear matter
  $\Longrightarrow$ expand so that first term exact in uniform system
- Change to $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ and $\mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2$ and resum in $\mathbf{s}$

$$\rho(\mathbf{R} + \mathbf{s}/2, \mathbf{R} - \mathbf{s}/2) = e^{\mathbf{s}\cdot(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)/2}\, \rho(\mathbf{r}_1, \mathbf{r}_2)|_{\mathbf{s}=0}$$

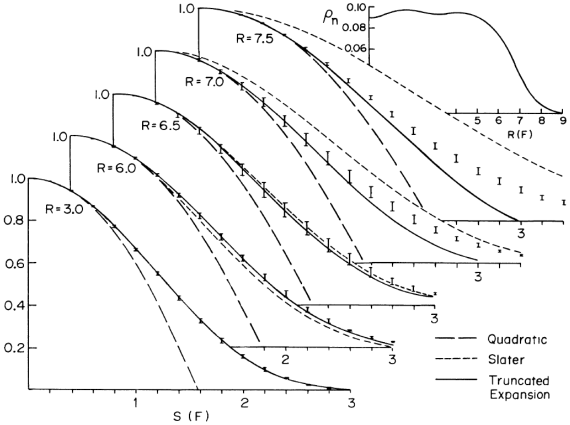
$$\Longrightarrow \frac{3j_1(sk_{\mathrm{F}})}{sk_{\mathrm{F}}}\rho(\mathbf{R}) + \frac{35j_3(sk_{\mathrm{F}})}{2sk_{\mathrm{F}}^3}\left(\frac{1}{4}\nabla^2\rho(\mathbf{R}) - \tau(\mathbf{R}) + \frac{3}{5}k_{\mathrm{F}}^2\rho(\mathbf{R}) + \cdots\right)$$

- In terms of local densities $\rho(\mathbf{R})$, $\tau(\mathbf{R})$, $\ldots \Longrightarrow$ DFT with these

Physics of the DME [Negele et al.]

- Local rather than global properties of density matrix
- *Not* a short-distance expansion; preserve long-range effects
  - Expanding the difference between exact and nuclear matter results in powers of s (nuclear matter k_F)

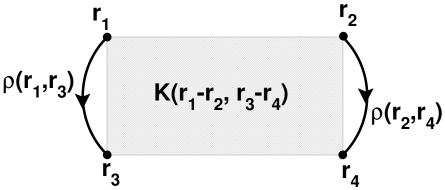
- Exact neutron density matrix squared in ^{208}Pb compared with DME



DME With a Nonlocal Interaction

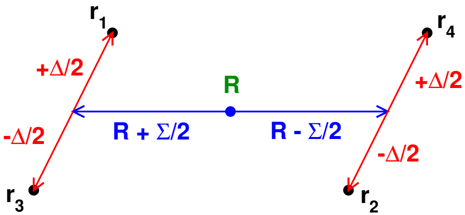
- HF+ functional for two-body V is (spin/isospin implicit):

$$W[J_0] = \frac{1}{2}\int d^3\mathbf{R}\, d^3(\mathbf{r}_1-\mathbf{r}_2)\, d^3(\mathbf{r}_3-\mathbf{r}_4)\, \rho(\mathbf{r}_1,\mathbf{r}_3) K(\mathbf{r}_1-\mathbf{r}_2,\mathbf{r}_3-\mathbf{r}_4)\rho(\mathbf{r}_2,\mathbf{r}_4)$$



where K is the anti-symmetrized interaction

- Expand about **R**:



- Analogous expansion of 3N contributions
- Treat frequency in K using factorization (V. Rotival et al.)

New Aspects of the DME for UNEDF

1. EFT, $V_{\mathrm{low}\,k}$, V_{srg} are strongly non-local
   - DME for nonlocal V never tested in original papers (not to mention many typos! :)
   - 2 expansions required
2. Treat 3N force contributions (N^2LO NNN for now)
   - 3 expansions needed now
3. Momentum space formulation
   - not tied to a 3d, operator representation of V

DME Compared to Skyrme Hartree-Fock

- $E[\rho, \tau, \ldots] = \int d^3\mathbf{R}\, \mathcal{E}(\rho, \tau, \ldots)|_{\rho=\rho(\mathbf{R}),\tau=\tau(\mathbf{R}),\ldots}$
- Phenomenological Skyrme energy functional (here for $N = Z$, even-even, spin-saturated nuclei)

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

- DME energy functional

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

- $A, B, C, \ldots$ are functions of ρ vs. Skyrme constants t_i $\Longrightarrow$ replace as inputs to codes
- Beyond a short-range expansion: long-range pion in n.m.
- Qualitative insight first. Fine-tuning needed for quantitative?

DME Meets Low-Momentum V [Bogner, Platter, rjf]

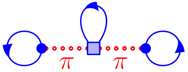
- $\mathcal{E} = \frac{1}{2M}\tau + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \cdots$ in momentum space $\Longrightarrow$ A and B functions determine bulk nuclear matter:

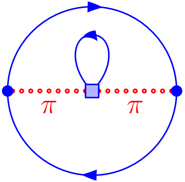
$$A[\rho] \sim k_{\rm F}^3 \sum_{lsj} \widehat{j}\,\widehat{t} \int_0^{k_{\rm F}} k^2\,dk\; V_{lsjt}(k,k)\,P_A(k/k_{\rm F}) \;+\; \{V_{3N}\} \;+\; \cdots$$

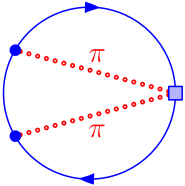
$$B[\rho] \sim k_{\rm F}^{-3} \sum_{lsj} \widehat{j}\,\widehat{t} \int_0^{k_{\rm F}} k^2\,dk\; V_{lsjt}(k,k)\,P_B(k/k_{\rm F}) \;+\; \{V_{3N}\} \;+\; \cdots$$

  - P_A, P_B are simple polynomials in $k/k_{\rm F}$
- $C[\rho]$ has two-dimensional integral over off-diagonal V
- Also spin-orbit, tensor, ...
- 3-body contributions have density matrices that are expanded in Jacobi coordinates; double-exchange is hardest

Chiral Three-Body Interactions in DME

- Direct 

- Single exchange 

- Double exchange 

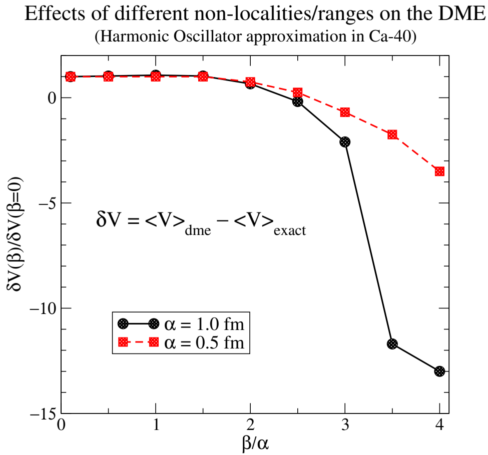
- c_i's from πN or NN + short-range LEC's

Non-Local Interactions and the DME

- Two expansions now!
- Consider HO approximation to fully self-consistent HF $\langle V \rangle$ (NN only)
- Schematic model to study effect of non-locality on DME

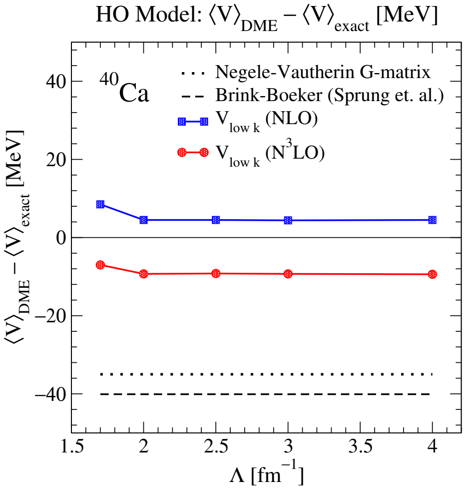
$$V(\mathbf{r},\mathbf{r}') = v\left(\frac{\mathbf{r}+\mathbf{r}'}{2\alpha}\right) \times \frac{e^{-\left(\frac{\mathbf{r}-\mathbf{r}'}{\beta}\right)^2}}{(\pi\beta^2)^{3/2}}$$

- No problem increasing non-locality β until $\approx$ 3 times range α



DME for Low-momentum Interactions (HF/NN only)

- Test with HO model
- errors $\approx +5$ MeV (NLO), ≈ -10 MeV (N^{3}LO)
- Λ–independent errors
- cf. schematic *V*'s (1970's) (finite-range direct terms)



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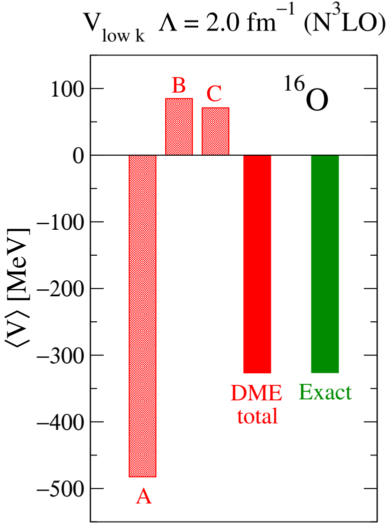
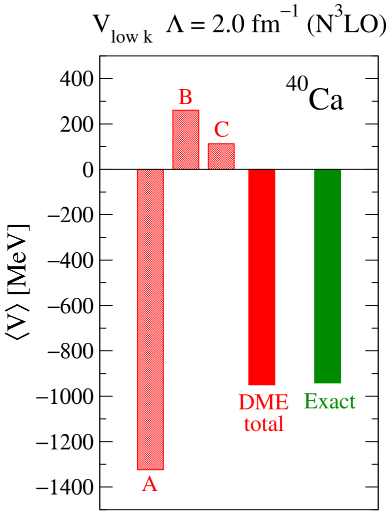
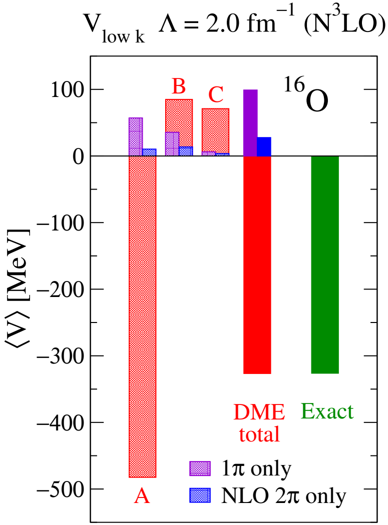
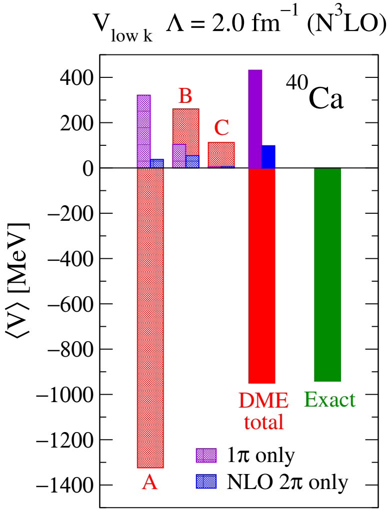




$$\mathcal{E} = \frac{\tau}{2M} + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \cdots$$

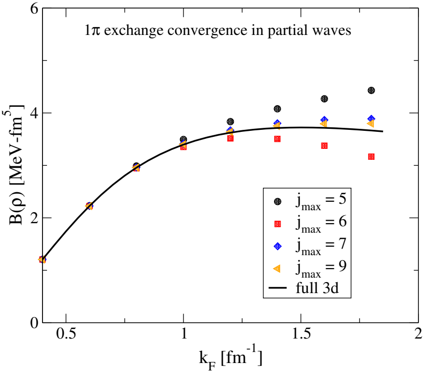
HF Long-Range Contributions (1π, leading 2π)

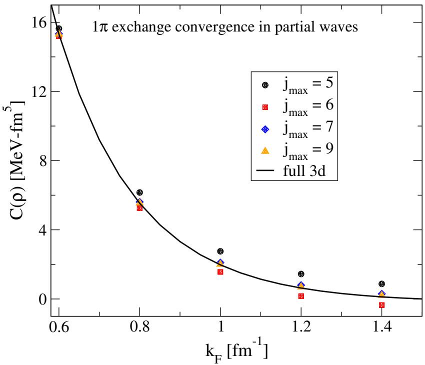




DME error in 1π exchange $\approx$ 4 MeV (out of 431 MeV) in ^{40}Ca

Subtleties With One-Pion Exchange





- Poor convergence of 1π exchange DME in partial wave expansion
- Is this a fundamental limitation of the momentum-space, non-local formulation of the DME that we employ?

Separating Out Finite Range Pion Physics

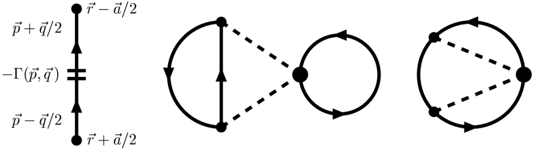
- RG evolution only affects short-distance structure

$$V_{\Lambda_0}(k,k') - V_\Lambda(k,k') = \widetilde{C}_0 + \widetilde{C}_2(k^2 + k'^2) + \cdots$$ [nucl-th/0308036]

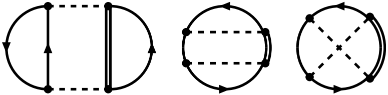
  - Long-range (low-k) pion-physics (e.g., from χ-EFT) unchanged
  - short-range $C_n(\Lambda)k^{2n}$ generated to give Λ-independent observables
- Apply partial-wave DME to $(V_{\mathrm{low}\,k} - V_\pi)$
- Treat V_π analytically (3D) and add it back in at the end
- DME EDF splits into 2 types of terms:
  1. Λ-independent finite range pion contributions that have non-trivial density dependencies (a lot can be done analytically)
  2. Λ-dependent $C_n(\Lambda)k^{2n}$ terms (Skyrme-like) with simple density-dependencies (Λ-dependence $\Longrightarrow$ theoretical guidance for fine-tuning to data!)

DME from Perturbative Chiral Interactions

- N. Kaiser et al. in ongoing series of papers (nucl-th/0212049, 0312058, 0312059, 0406038, 0407116, 0509040, 0601100, . . .)
- Fourier transform of expanded density matrix defines a momentum-space medium insertion, leading to DME:

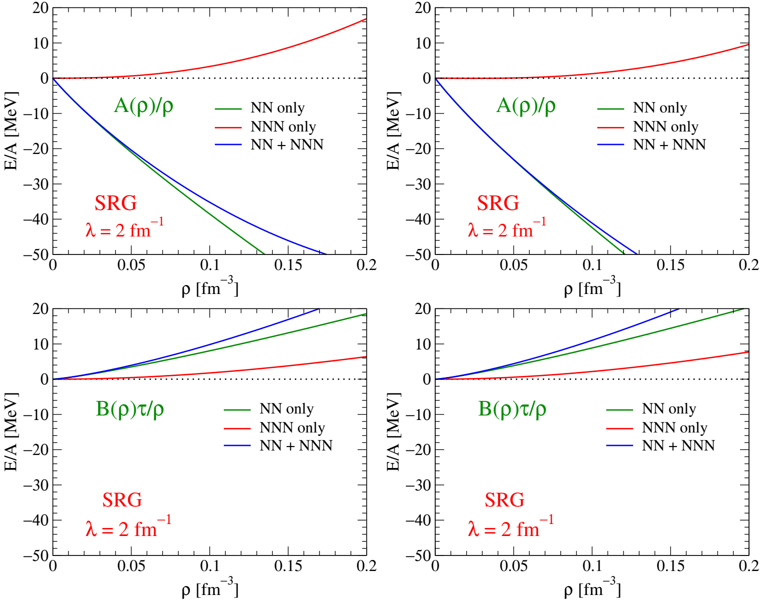


- Three-body forces from explicit Δ, e.g.,

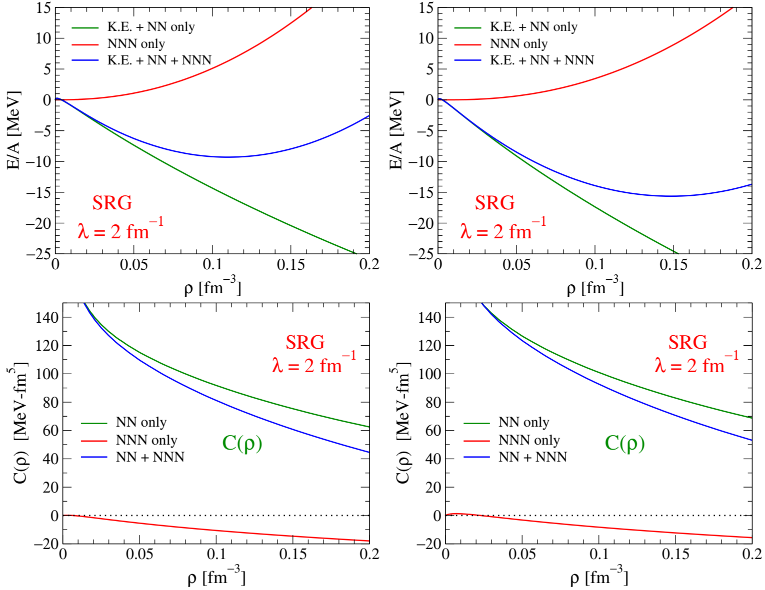


- Perturbative expansion for energy tuned to nuclear matter
- Many analytic results $\Longrightarrow$ qualitative insight, checks for quantitative calculations with low-momentum interactions

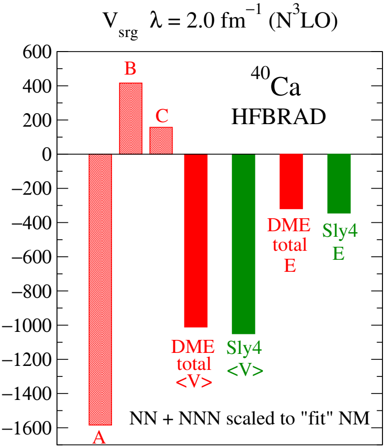
DME ABC Functions: Original and Fine-Tuned

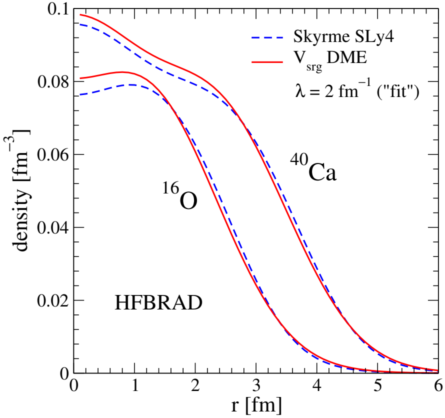


DME ABC Functions: Original and Fine-Tuned



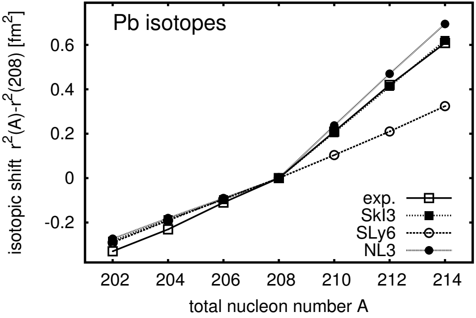
Proof of Principle Calculation with HFBRAD





Observables Sensitive to 3N Interactions?

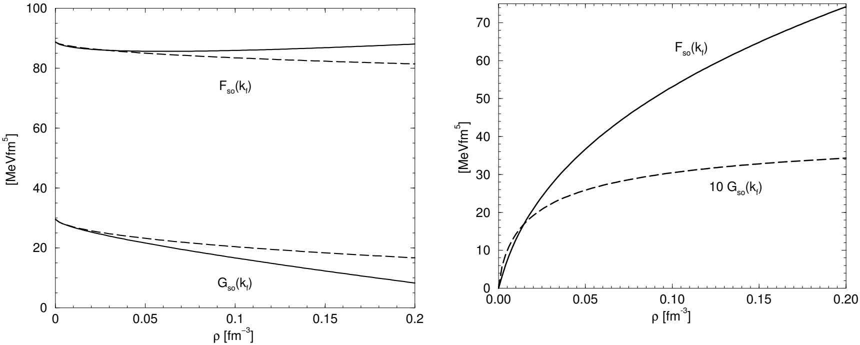
- Study systematics along isotopic chains
- Example: kink in radius shift $\langle r^2 \rangle(A) - \langle r^2 \rangle(208)$



- 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

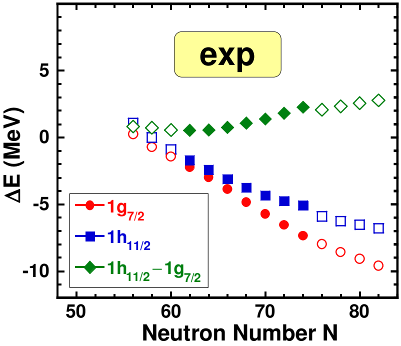
- Ratio fixed at 3:1 for short-range spin-orbit (usual Skyrme)
- Kaiser: DME spin-orbit from chiral two-body (left) and three-body (right)

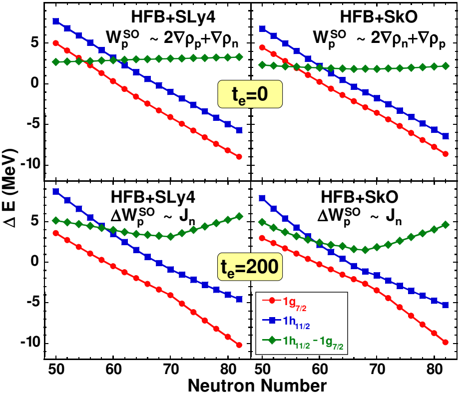


- Systematic investigation needed

Observables Sensitive to 3N Interactions?

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



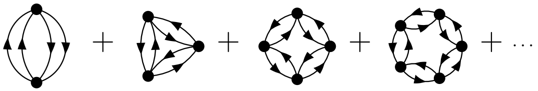


- See also Brown et al., PRC **74** (2006)

Outline

Summary: DFT from EFT and RG

- Plan: Chiral EFT $\longrightarrow$ low k $V_{NN}, V_{NNN}, \ldots \longrightarrow$ DFT for nuclei
  - Effective action formalism provides framework
  - DME provides testable, improvable path to functional
  - Three-body contributions are critical for low-momentum interactions
- DFT Issues to resolve (partial list!)
  - Quantitative power counting with low-momentum V
  - Symmetry breaking and restoration in DFT
    (self-bound systems)
  - Non-localities from near-on-shell particle-hole excitations



Skyrme Energy Functionals (cf. Coulomb meta-GGA)

- 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 $\mathbf{J}$)

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  - 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:

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

$U = \frac{3}{4}t_0\rho + (\frac{3}{16}t_1 + \frac{5}{16}t_2)\tau + \cdots$ 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, ...

Skyrme Energy Functionals (cf. Coulomb meta-GGA)

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

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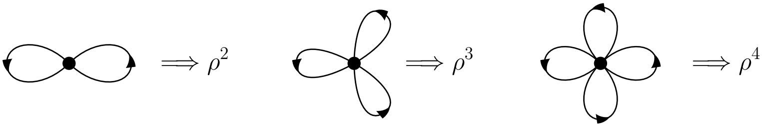
  - where $\rho(x) = \sum_i |\phi_i(x)|^2$ and $\tau(x) = \sum_i |\nabla\phi_i(x)|^2$ (and **J**)

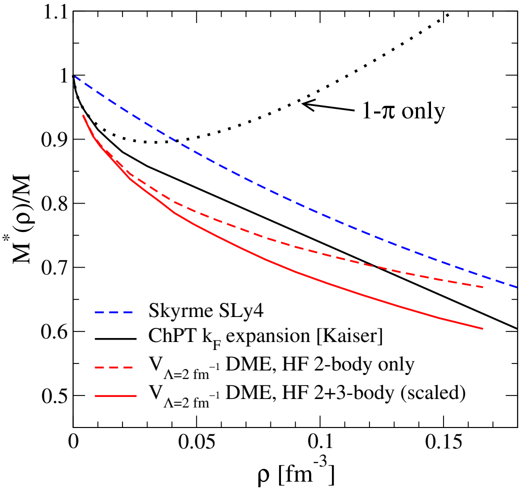
- First Skyrme interaction had short-range 3N force ($\alpha = 1$)



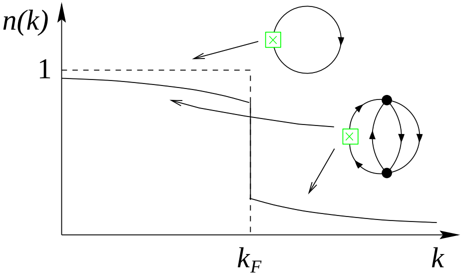
- $\alpha = 1/6, 1/3, 1/2$ in modern Skyrme parameterizations.
  Connection to microscopic many-body forces?

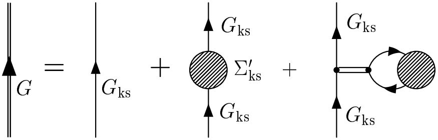
Skyrme Effective Mass $M^\star$

- τ dependence $\Longrightarrow \frac{M^*(\rho)}{M}$
- Negele: comes from off-diagonal range of density matrix and long-range part of G-matrix $\Longrightarrow$ long-range part of potential
- $\frac{M^*(\rho)}{M} = 1/(1 + 2MB[\rho])$
- Skyrme at ρ_{sat}: 0.6–1.0
- Kaiser et al., NP **A750** (2005) 259: perturbative k_F expansion in ChPT



Kohn-Sham DFT and "Mean-Field" Models





- KS propagators (lines) *always* have "mean-field" structure

$$G^0_{\mathrm{KS}}(\mathbf{x},\mathbf{x}';\omega) = \sum_\alpha \psi_\alpha(\mathbf{x})\psi^*_\alpha(\mathbf{x}') \left[\frac{\theta(\epsilon_\alpha-\epsilon_{\mathrm{F}})}{\omega-\epsilon_\alpha+i\eta} + \frac{\theta(\epsilon_{\mathrm{F}}-\epsilon_\alpha)}{\omega-\epsilon_\alpha-i\eta}\right]$$

where $\psi_\alpha(\mathbf{x})$ satisfies: $\left[-\frac{\nabla^2}{2M} - J_0(\mathbf{x})\right]\psi_\alpha(\mathbf{x}) = \epsilon_\alpha\psi_\alpha(\mathbf{x})$

- We can use the Kohn-Sham basis to calculate $n(\mathbf{k}) = \langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}}\rangle$, but this is beyond standard DFT [see nucl-th/0410105]

Many-Body Forces in Skyrme HF?

- Old NDA analysis:

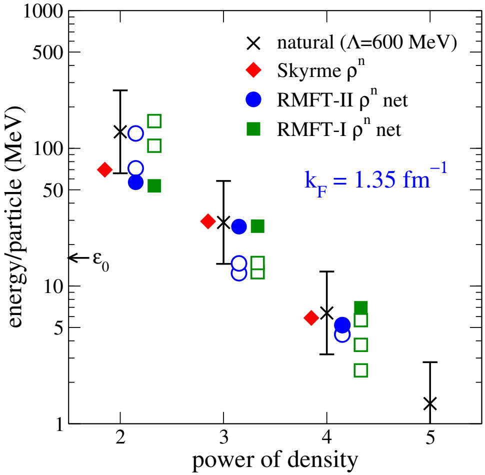
$$c\left[\frac{\psi^\dagger\psi}{f_\pi^2\Lambda}\right]^l\left[\frac{\nabla}{\Lambda}\right]^n f_\pi^2\Lambda^2$$

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

- Density expansion?

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

for $1000 \geq \Lambda \geq 500$



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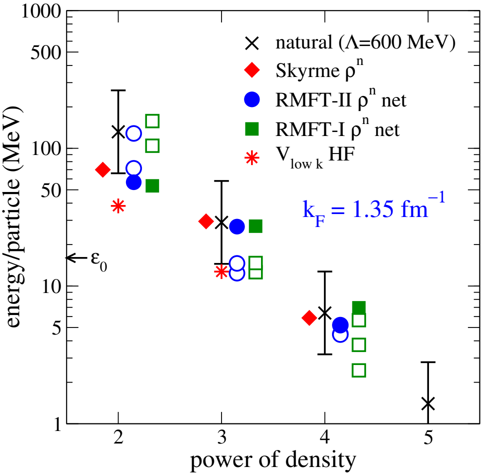

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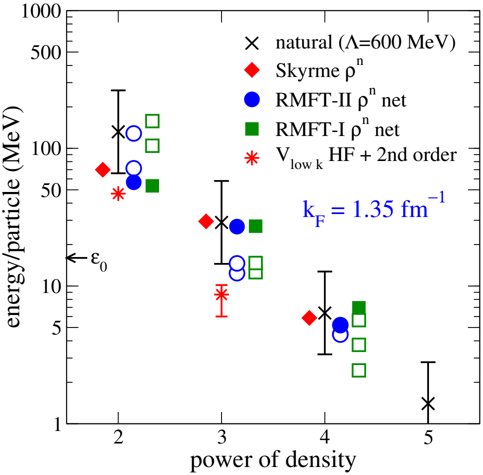
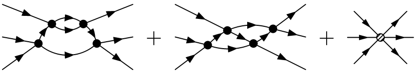
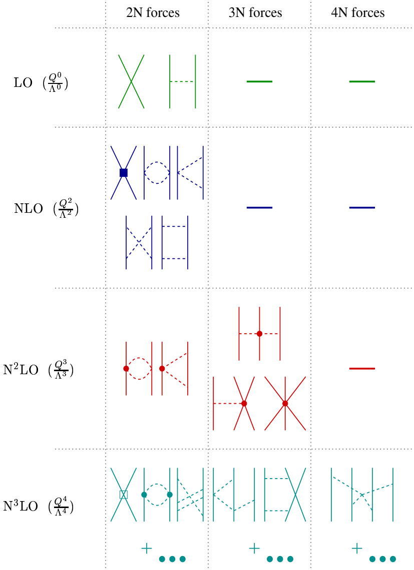


Many-Body Forces are Inevitable in EFT!

- What if we have three nucleons interacting?
- Successive two-body scatterings with short-lived high-energy intermediate states unresolved $\Longrightarrow$ must be absorbed into three-body force



- A feature, not a bug!
- How do we organize $(3, 4, \cdots)$–body forces? EFT! [nucl-th/0312063]



(Nuclear) Many-Body Physics: “Old” vs. “New”

One Hamiltonian for all problems and energy/length scales	Infinite # of low-energy potentials; different resolutions $\Longrightarrow$ different dof’s and Hamiltonians
Find the “best” potential	There is no best potential $\Longrightarrow$ use a convenient one!
Two-body data may be sufficient; many-body forces as last resort	Many-body data needed and many-body forces inevitable
Avoid (hide) divergences	Exploit divergences (cutoff dependence as tool)
Choose diagrams by “art”	Power counting determines diagrams and truncation error

Beyond Kohn-Sham LDA [Bhattacharyya, rjf, nucl-th/0408014]

- Add additional sources to Lagrangian, e.g., $\eta(\mathbf{x})\,\boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\nabla}\psi$

$$\Gamma[\rho,\tau] = W[J,\eta] - \int J(x)\rho(x) - \int \eta(x)\tau(x)$$

- Two Kohn-Sham potentials: $[\rho\equiv\langle\psi^\dagger\psi\rangle,\quad \tau\equiv\langle\boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\nabla}\psi\rangle]$

$$J_0(\mathbf{x}) = \frac{\delta\Gamma_{\rm int}[\rho,\tau]}{\delta\rho(\mathbf{x})} \quad \text{and} \quad \eta_0(\mathbf{x}) = \frac{\delta\Gamma_{\rm int}[\rho,\tau]}{\delta\tau(\mathbf{x})}$$

- Kohn-Sham equation $\Longrightarrow$ defines $\frac{1}{2M^*(\mathbf{x})}\equiv\frac{1}{2M}-\eta_0(\mathbf{x})$:

$$\left(-\nabla\cdot\frac{1}{2M^*(\mathbf{x})}\nabla - J_0(\mathbf{x})\right)\phi_\alpha(\mathbf{x}) = \epsilon_\alpha\,\phi_\alpha(\mathbf{x})$$

- HF dilute energy density with ρ only vs. ρ and τ (for $\nu=2$) :

$$\frac{C_2}{8}\left[\frac{3}{5}\left(\frac{6\pi^2}{\nu}\right)^{2/3}\rho^{8/3}\right]+\ldots \quad\Longrightarrow\quad \frac{C_2}{8}\left[\rho\tau+\frac{3}{4}(\boldsymbol{\nabla}\rho)^2\right]+\ldots$$

Pairing in DFT [Hammer, rjf, Puglia nucl-th/0612086]

- Add source j coupled to anomalous density:

$$Z[J,j] = e^{-W[J,j]} = \int D(\psi^\dagger\psi)\, \exp\left\{-\int d^4x\, [\mathcal{L} + J(x)\, \psi_\alpha^\dagger\psi_\alpha + j(x)(\psi_\uparrow^\dagger\psi_\downarrow^\dagger + \psi_\downarrow\psi_\uparrow)]\right\}$$

- Densities found by functional derivatives wrt J, j:

$$\rho(x) = \left.\frac{\delta W[J,j]}{\delta J(x)}\right|_j, \quad \phi(x) \equiv \langle\psi_\uparrow^\dagger(x)\psi_\downarrow^\dagger(x) + \psi_\downarrow(x)\psi_\uparrow(x)\rangle_{J,j} = \left.\frac{\delta W[J,j]}{\delta j(x)}\right|_J$$

- Find $\Gamma[\rho,\phi]$ from $W[J_0, j_0]$ by inversion method
- Kohn-Sham system looks like short-range HFB with j_0 as gap

$$\begin{pmatrix} h_0(\mathbf{x}) - \mu_0 & j_0(\mathbf{x}) \\ j_0(\mathbf{x}) & -h_0(\mathbf{x}) + \mu_0 \end{pmatrix} \begin{pmatrix} u_i(\mathbf{x}) \\ v_i(\mathbf{x}) \end{pmatrix} = E_i \begin{pmatrix} u_i(\mathbf{x}) \\ v_i(\mathbf{x}) \end{pmatrix}$$

where $$h_0(\mathbf{x}) \equiv -\frac{\boldsymbol{\nabla}^2}{2M} - J_0(\mathbf{x})$$

Constructive DFT via Effective Action [nucl-th/0212071]

- Partition function with sources that adjust densities:

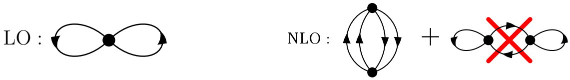
$$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H}+J\,\widehat{\rho})} \implies \text{path integral for } W[J]$$

- Invert to find $J[\rho]$ and Legendre transform from J to ρ:

$$\rho(\mathbf{x}) = \frac{\delta W[J]}{\delta J(\mathbf{x})} \implies \Gamma[\rho] = W[J] - \int J\,\rho \quad \text{and} \quad J(\mathbf{x}) = -\frac{\delta \Gamma[\rho]}{\delta \rho(\mathbf{x})}$$

$\implies \Gamma[\rho] \propto$ ground-state energy, stationary at $\rho_{\mathrm{gs}}(\mathbf{x})$!

- Diagrammatic *expansion* (e.g., use BBG power counting)



- Orbitals $\{\psi_i(\mathbf{x})\}$ in local Kohn-Sham (KS) potential $J_0([\rho],\mathbf{x})$

$$[-\nabla^2/2m + J_0(\mathbf{x})]\psi_\alpha = \varepsilon_\alpha \psi_\alpha \implies \rho(\mathbf{x}) = \sum_{i=1}^{A} |\psi_\alpha(\mathbf{x})|^2$$

- KS propagators (lines):

$$G^0_{\mathrm{KS}}(\mathbf{x},\mathbf{x}';\omega) = \sum_\alpha \psi_\alpha(\mathbf{x})\psi^*_\alpha(\mathbf{x}')\left[\frac{\theta(\varepsilon_\alpha - \varepsilon_{\mathrm{F}})}{\omega - \varepsilon_\alpha + i\eta} + \frac{\theta(\varepsilon_{\mathrm{F}} - \varepsilon_\alpha)}{\omega - \varepsilon_\alpha - i\eta}\right]$$