Nuclear Structure and Neutron-Rich Matter

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Pictures have been freely borrowed from online sources; I apologize in advance for any omitted citations. Also, inclusion of particular calculations does not imply that they are the "best". No animals were harmed in creating this talk.

Nuclear Structure Discussion Questions

1. What is theoretical uncertainty of the ^{208}Pb neutron skin radius?
2. What is the uncertainty of the neutron skin requested by theory to inform the energy density functional (EDF) in a meaningful way?
3. What part of the above uncertainty comes from the bulk-matter physics and what comes from finite-nuclei physics (e.g., shell effects)?
4. What are additional experiments/calculations that can inform question 3? In particular, are open-shell systems of any interest?
5. There are many correlations between various parameters defining EDF and the neutron skin. What are the independent correlations?
6. What are the complementary quality measurements that can illuminate the question of the neutron skin?
7. Are short-range correlations of any relevance/importance to the question of neutron skin of ^{208}Pb?
8. Are data for light weakly bound nuclei of any relevance/use to the question of the neutron skin of ^{208}Pb?

Aspects of Nuclear Structure in Subsequent Talks

- Basic properties of finite nuclei
  - Semi-empirical mass formula (SEMF) ingredients
  - Charge and matter distributions
- Nuclear/neutron matter features and correlations
  - Density dependence of symmetry energy
  - Pairing
- Many-body methods for nuclear structure
  - Microscopic “ab initio” approaches
  - Density functional theory (DFT) [cf. mean-field models]
  - Virial expansion, . . .
- Inter-nucleon interactions $\Longrightarrow$ Input for structure
  - Boson-exchange (OBE) vs. chiral effective field theory (EFT)
  - Low-momentum potentials: renormalization group $\longrightarrow$ “$V_{\text{low}\,k}$”
  - Three-body forces

Outline

“Just the Facts” About Nuclei

Symmetric and Asymmetric Nuclear Matter

Many-Body Methods

Inter-Nucleon Interactions

Final Thoughts and Prejudices

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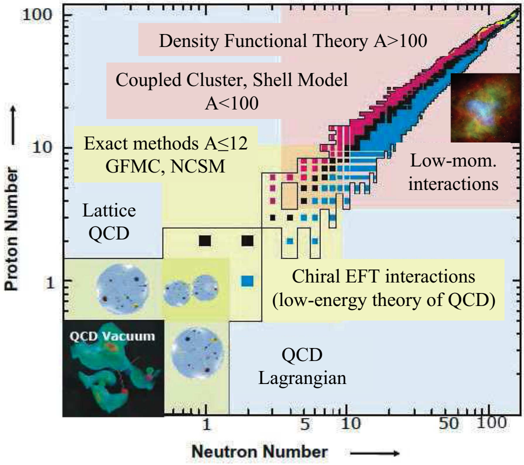
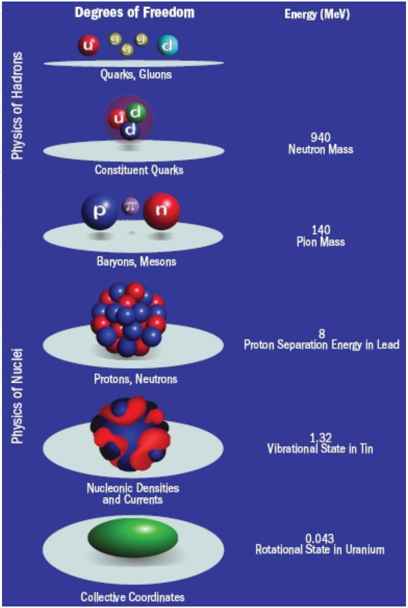
The Big Picture: From QCD to Nuclei

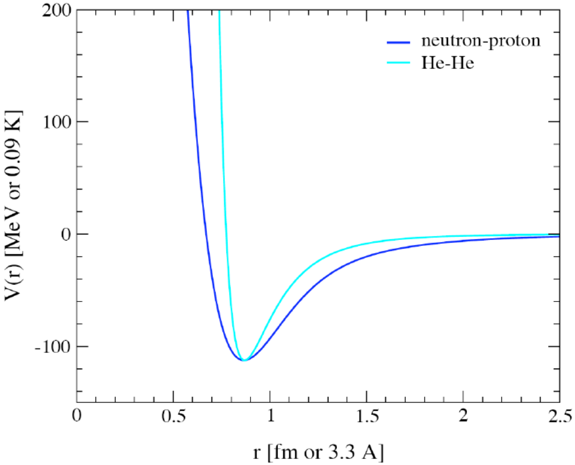




- Note the hierarchy of energy scales!
  - How do we take advantage?
  - Note the (collective) dof’s

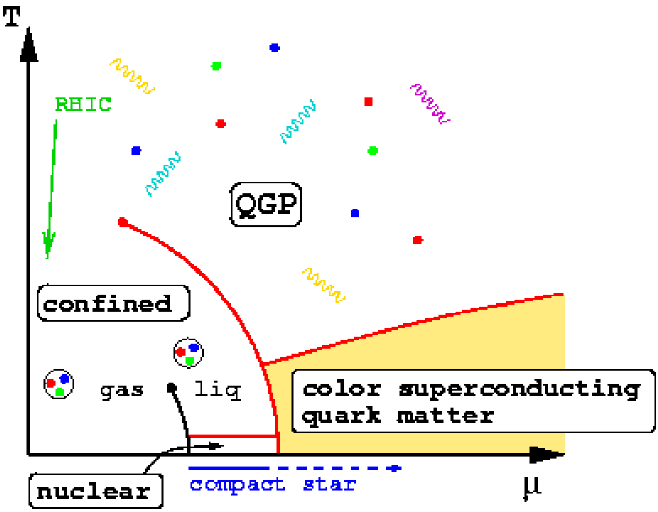
What Does the Nuclear Potential Look Like?

Textbook answer (for ${}^1S_0$) — cf. force between atoms:



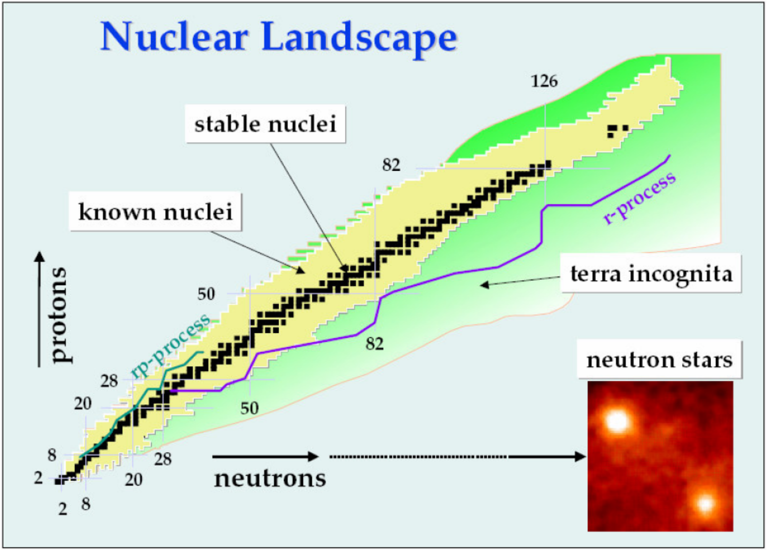
- Momentum units ($\hbar = c = 1$): typical relative momentum in large nucleus $\approx 1\,\text{fm}^{-1} \approx 200\,\text{MeV}$ $[E_{\text{lab}} \approx 83\,\text{MeV–fm}^2 k^2_{\text{rel}}]$

The QCD Phase Diagram [from Mark Alford]



- Nuclei are self-bound “liquid drops” (and superfluid!)
- Isospin axis is critical in our discussion!

Landscape of Finite Nuclei

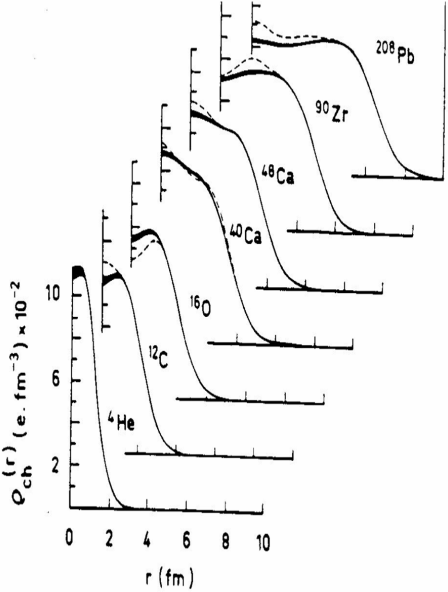


Large extrapolations to neutron stars in density and proton fraction!

What Do (Ordinary) Nuclei Look Like?

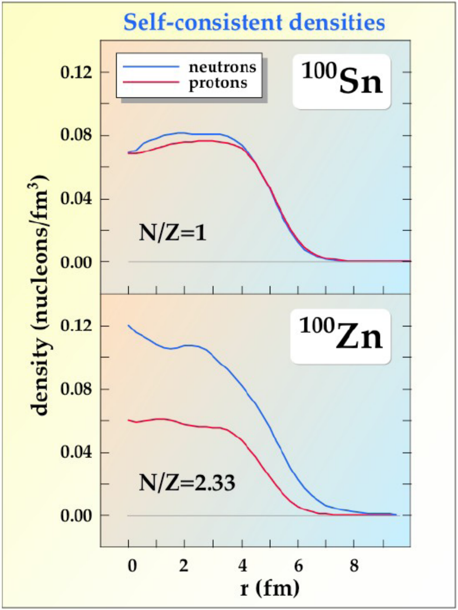
- Charge densities of magic nuclei (mostly) shown
- Proton density has to be "unfolded" from $\rho_{\text{charge}}(r)$, which comes from elastic electron scattering
- Roughly constant interior density with $R \approx (1.1\text{–}1.2\,\text{fm}) \cdot A^{1/3}$
- Roughly constant surface thickness

$\Longrightarrow$ Like a liquid drop!



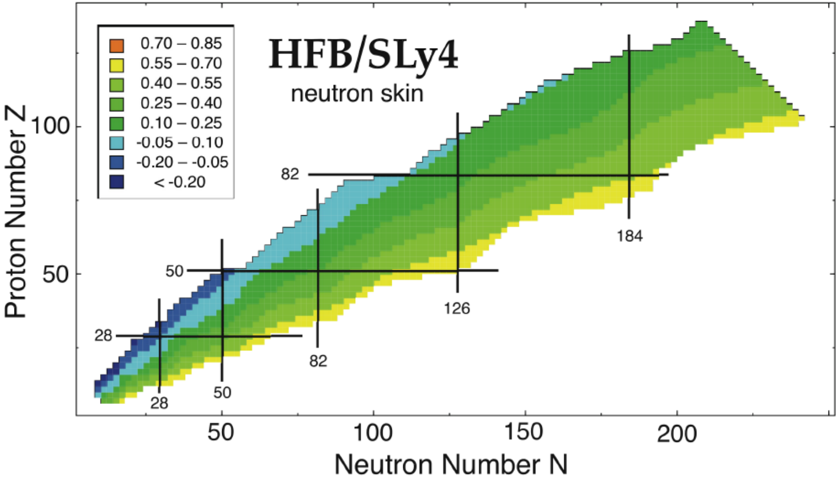
What Do Nuclei Look Like? (figures from Witek)

- Skyrme EDF densities (Energy Density Functional)
- When we have more neutrons than protons, where do the extras go?
- Extreme possibilities:
  - $r_n = r_p$ so $\rho_n > \rho_p$ $\Longrightarrow$ no $(r_n - r_p)$ skin
  - $\rho_n = \rho_p$ so $r_n > r_p$ $\Longrightarrow$ maximal skin
- Reality is in between!
  - What determines the balance?
  - What is it correlated with?



Neutron Skins By One Calculation (from Witek)

S. Mizutori et al., Phys. Rev. C61, 044326 (2000)

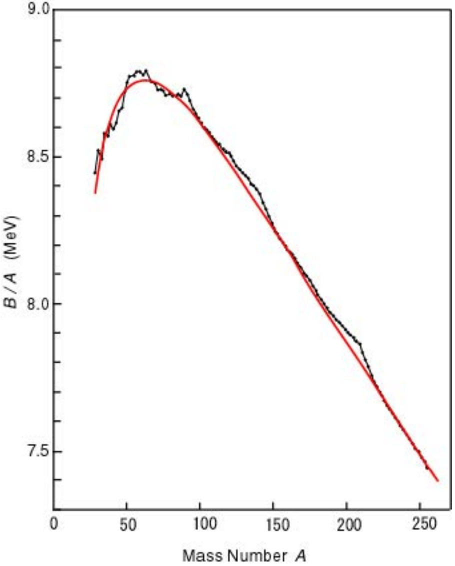


- Skyrme HFB SLy4 (”Hartree-Fock Bogolyubov” $\Longrightarrow$ pairing)
- Other EDF’s (SkX, FSUGold, . . .) give different (?) results
- Skyrme vs. RMF (relativistic mean field) EDF’s

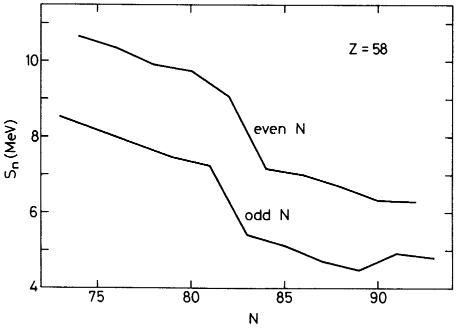
Semi-Empirical Mass Formula $(A = N + Z)$

$$E_B(N, Z) = a_v A - a_s A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_{\mathrm{sym}} \frac{(N-Z)^2}{A} + \Delta$$

- Many predictions!
- Rough numbers:
  $a_v \approx 16\,\mathrm{MeV}$, $a_s \approx 18\,\mathrm{MeV}$,
  $a_C \approx 0.7\,\mathrm{MeV}$, $a_{\mathrm{sym}} \approx 28\,\mathrm{MeV}$
- Pairing $\Delta \approx \pm 12/\sqrt{A}\,\mathrm{MeV}$ (even-even/odd-odd) or 0 [or $43/A^{3/4}$ MeV or …]
- Surface symmetry energy: $a_{\mathrm{surf\ sym}}(N-Z)^2/A^{4/3}$
- Much more sophisticated mass formulas include shell effects, etc.
- Sometimes $a_{\mathrm{sym}} \to a_4$ (or α_i)



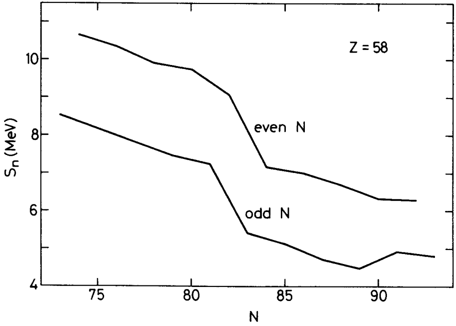
Experimental Evidence for Pairing in Nuclei



$$E_B(N,Z) = (15.6\,\mathrm{MeV})\left[1 - 1.5\left(\frac{N-Z}{A}\right)^2\right]A - (17.2\,\mathrm{MeV})A^{2/3} - (0.70\,\mathrm{MeV})\frac{Z^2}{A^{1/3}} + (6\,\mathrm{MeV})[(-1)^N + (-1)^Z]/A^{1/2}$$

- Odd-even staggering of binding energies (S_n is plotted)

Experimental Evidence for Pairing in Nuclei



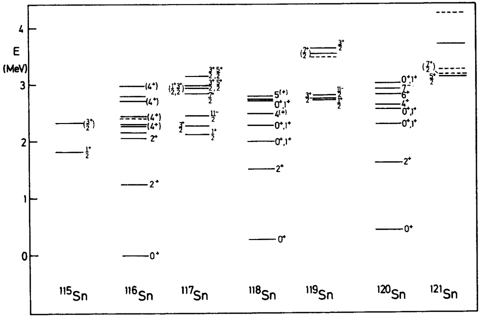


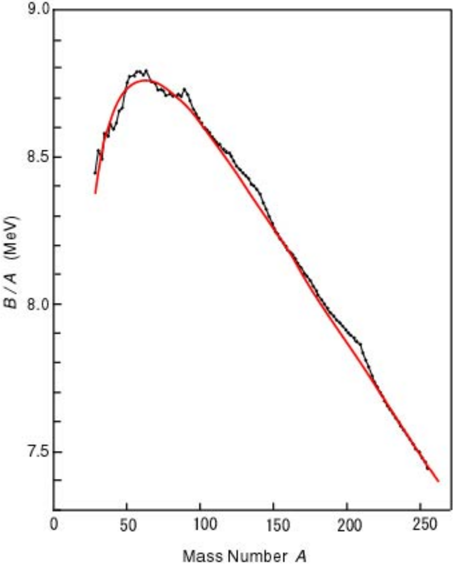
Figure 6.1. Excitation spectra of the $_{50}$Sn isotopes.

- Odd-even staggering of binding energies (S_n is plotted)
- Energy gap in spectra of deformed nuclei
- Low-lying 2^+ states in even nuclei
- Deformations and moments of inertia (theory requires pairing)

Semi-Empirical Mass Formula Per Nucleon

$$\frac{E_B(N,Z)}{A} = a_v - a_s A^{-1/3} - a_C \frac{Z^2}{A^{4/3}} - a_{\text{sym}} \frac{(N-Z)^2}{A^2}$$

- Divide terms by $A = N + Z$
- Rough numbers:
  $a_v \approx 16\,\text{MeV}$, $a_s \approx 18\,\text{MeV}$,
  $a_C \approx 0.7\,\text{MeV}$, $a_{\text{sym}} \approx 28\,\text{MeV}$
- Surface symmetry energy:
  $a_{\text{surf sym}}(N-Z)^2/A^{7/3}$
- Now take $A \to \infty$ with Coulomb $\to 0$ and fixed N/A, Z/A
- Surface terms negligible



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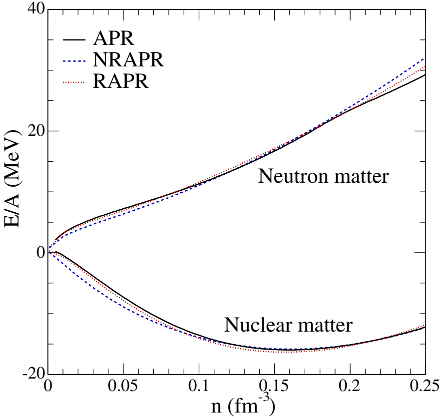
Nuclear and Neutron Matter Energy vs. Density



[Akmal et al. calculations shown]

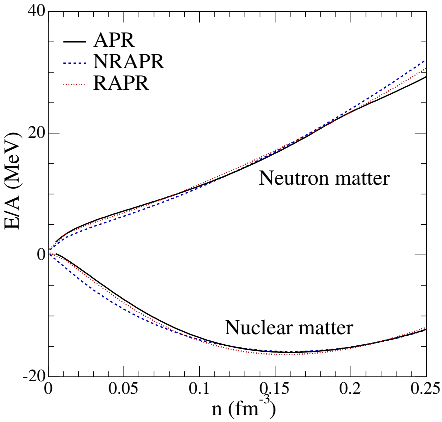
- Uniform with Coulomb turned off
- Density n (or often ρ)
- Fermi momentum $n = (\nu/6\pi^2)k_{\mathrm{F}}^3$
- Neutron matter ($Z = 0$) has positive pressure
- Symmetric nuclear matter ($N = Z = A/2$) saturates

$$E(n, \alpha) = E(n, 0) + S_2(n)\alpha^2 + S_4(n)\alpha^4 + \cdots \qquad \alpha \equiv I = \frac{N - Z}{A}$$

$$E(n, 0) = -a_v + \frac{K_0}{18n_0^2}(n - n_0)^2 + \cdots$$

$$S_2(n) = a_{\mathrm{sym}} + \frac{p_0}{n_0^2}(n - n_0) + \frac{\Delta K_0}{18n_0^2}(n - n_0)^2 + \cdots$$

Density Dependence of Symmetry Energy



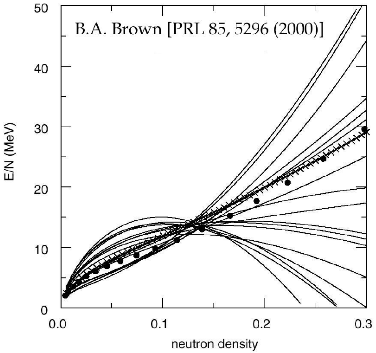


FIG. 2. The neutron EOS for 18 Skyrme parameter sets. The filled circles are the Friedman-Pandharipande (FP) variational calculations and the crosses are SkX. The neutron density is in units of neutron/fm^3.

$$E(n,\alpha) = E(n,\alpha=0) + S_2(n)\alpha^2 + \cdots \qquad \alpha \equiv I = (N-Z)/A$$

- Or proton fraction $x = Z/A$
- Nuclear matter $\Longrightarrow x = 1/2$; Neutron matter $\Longrightarrow x = 0$
- $S_2(n)$ is not pinned down by past fits to nuclei

Neutron Skin in ^{208}Pb vs. Symmetry Energy

$$E(n,\alpha) = E(n,0) + S_2(n)\alpha^2 + S_4(n)\alpha^4 + \cdots \qquad \alpha = I = (N-Z)/A$$

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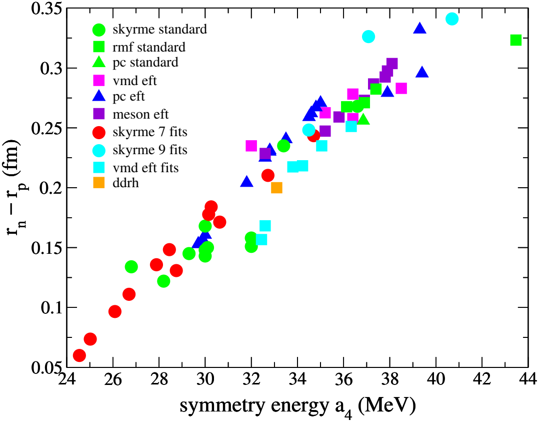

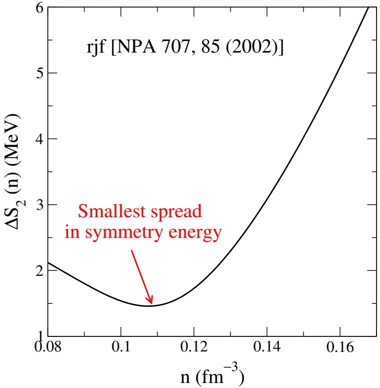

Neutron Skin in ^{208}Pb vs. Symmetry Energy

$$E(n,\alpha) = E(n,0) + S_2(n)\alpha^2 + S_4(n)\alpha^4 + \cdots \qquad \alpha = I = (N-Z)/A$$

$$E(n,0) = -a_v + \frac{K_0}{18n_0^2}(n-n_0)^2 + \cdots$$

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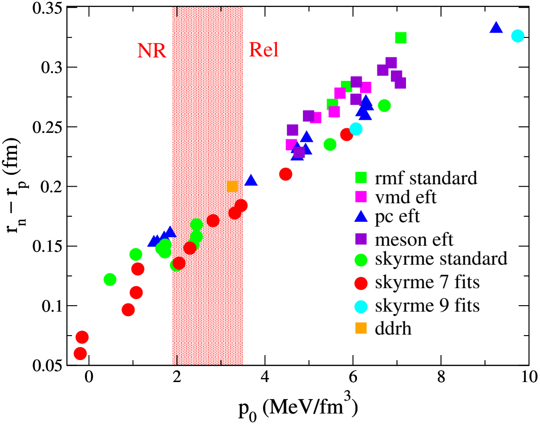
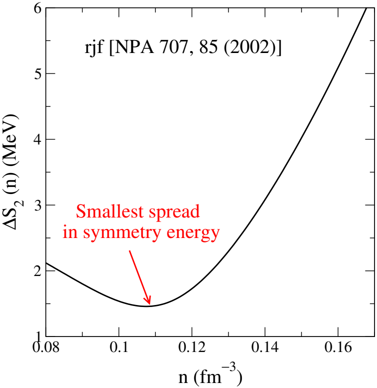
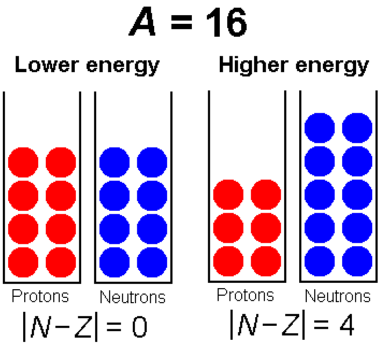




Where Does the Symmetry Energy Come From?

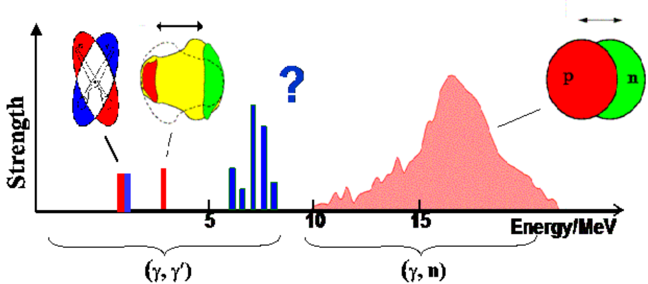
Textbook discussion:

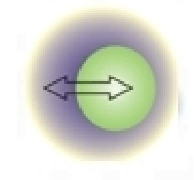
- Take $\alpha \equiv (N - Z)/A$ small
- Kinetic energy difference.
  Use $k_F^{n,p} = k_F(1 \pm \alpha)^{1/3}$
  and expand: $\langle T_{sym}/A \rangle = \frac{1}{3}\frac{\hbar^2 k_F^2}{2M}\alpha^2$
- Average one-body potential $U(k)$ is most attractive for $k = 0$
  $\Longrightarrow \frac{1}{6}k_F\left(\frac{\partial U}{\partial k}\right)_{k_F}\alpha^2$
- More attraction for $T = 0$ n-p (singlet) than $T = 1$ n-p, p-p, n-n (triplet) and more n-p pairs when $N = Z \Longrightarrow \frac{1}{4}\rho(\widetilde{V}_1 - \widetilde{V}_0)\alpha^2$
- All cost energy like α^2



Symmetry Energy Restoring Force in Nuclei

- Giant dipole resonance: bulk neutrons against protons



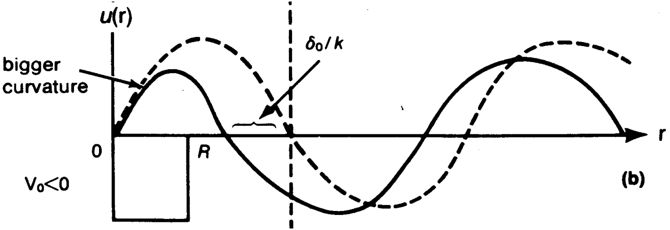


- Pygmy resonances: skin against symmetric $N = Z$ core
- See Witek's talk for assessment of correlations

What About at Very Low Densities?

- We can use scattering data directly!
  - If we want model independence, what could be better than using only data?
- EOS for a dilute gas based on virial expansion to 2nd order does this!
  - Controlled expansion in small parameter (fugacity $e^{\mu/T}$) with well-defined range of validity
  - For neutron matter, applies for $n \leq 4 \cdot 10^{11} (T/\mathrm{MeV})^{3/2}$ g/cm^3
  - Virial EOS provides benchmark for *all* nuclear EOS's at low density and temperature
  - See A. Schwenk's talk for details (and assumptions)

At Low Energies: Effective Range Expansion



Total cross section: $\sigma_{\text{total}} = \dfrac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l(k)$

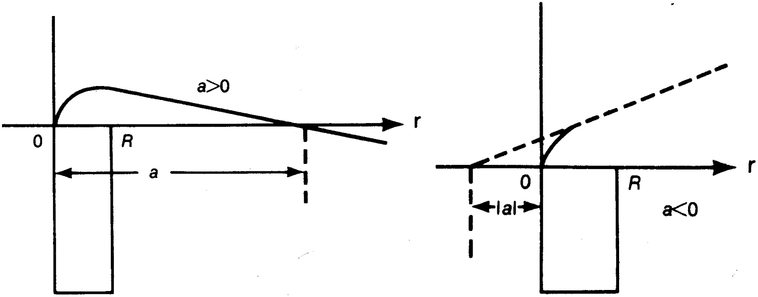
- What happens at low energy ($\lambda = 2\pi/k \gg 1/R$)?

$$k \cot \delta_0(k) \xrightarrow{k \to 0} -\frac{1}{a_0} + \frac{1}{2} r_0 k^2 + \ldots$$

  - a_0 (or a_s) = "scattering length" and r_0 = "effective range"
- While $r_0 \sim R$, the range of the potential, a_0 can be anything
  - if $a_0 \sim R$, it is called "natural"
  - $|a_0| \gg R$ (unnatural) is particularly interesting
    $\Longrightarrow$ cold atoms and neutrons

Near-Zero-Energy Bound States

- Bound-state or near-bound state at zero energy
  $\Longrightarrow$ large scattering lengths ($a_0 \to \pm\infty$)

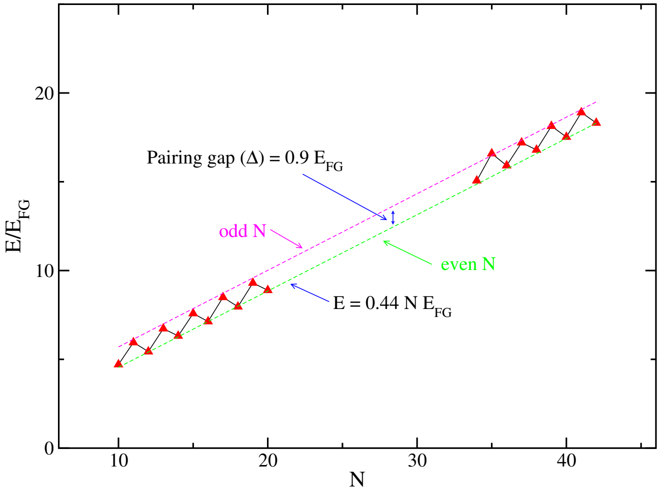


- For $kR \to 0$, the total cross section is

$$\sigma_{\text{total}} = \sigma_{I=0} = \frac{4\pi a_0^2}{1+(ka_0)^2} = \begin{cases} 4\pi a_0^2 & \text{for } ka_0 \ll 1 \\ \dfrac{4\pi}{k^2} & \text{for } ka_0 \gg 1 \text{ (unitarity limit)} \end{cases}$$

GFMC Results for Unitary Gas [J. Carlson et al.]

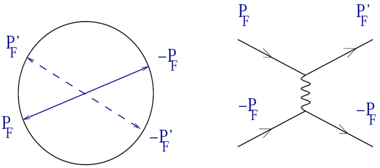
- Extrapolate to large numbers of fermions



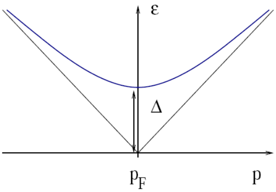
- Energy per particle: $E/N = 0.44(1)E_{\mathrm{FG}}$ for $a_0 \to \infty$ and $r_0 \to 0$
- See Joe's talk for latest neutron matter (finite a_0, r_0)

When Does Cooper Pairing Occur?

- If there is an attractive interaction at the Fermi surface, back-to-back fermions condense as Cooper pairs



- The excitation spectrum (energy vs. momentum relation) develops a *gap* Δ



$$\epsilon(p) = \sqrt{(p - p_F)^2 + \Delta^2}$$

- For very dilute fermions, $\Delta \propto e^{-\pi/2k_\mathrm{F}|a_0|}$

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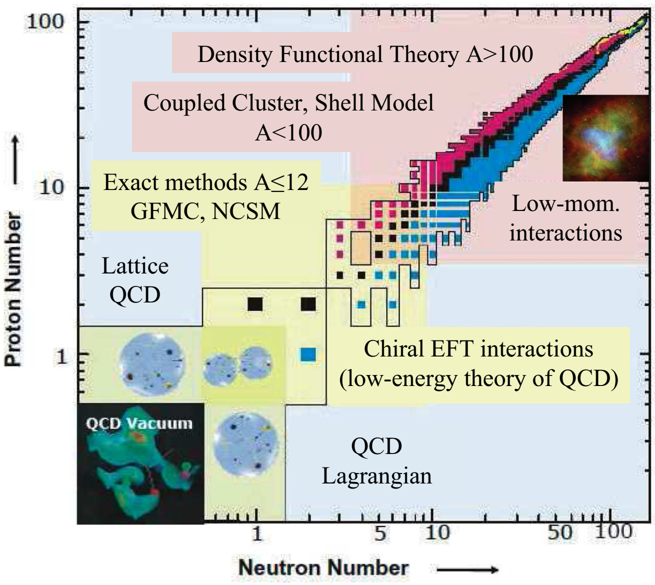
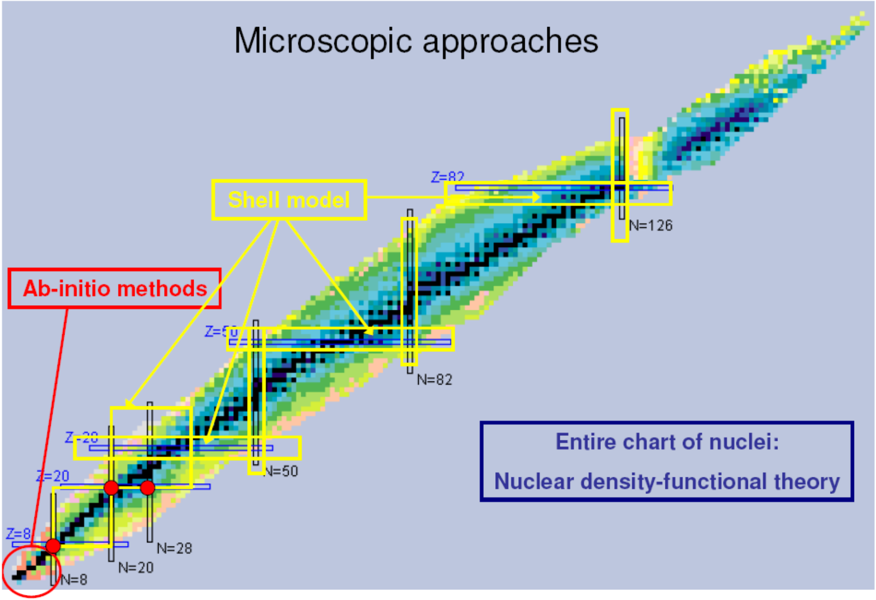
Given an Interaction, Why Not Just Solve?



Reach of Microscopic Approaches (from T. Papenbrock)



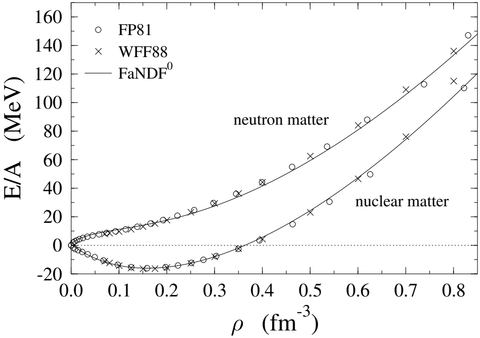
Paths to a Nuclear Energy Functional (EDF)

- Empirical energy functional (Skyrme or RMF)
- 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 (J. Braun, from Polonyi and Schwenk, nucl-th/0403011)
- EDF from perturbative chiral interactions + DME (Kaiser et al.)
- Constructive Kohn-Sham DFT with RG-softened $V_{\chi\mathrm{EFT}}$'s

Hartree-Fock Wave Function

- Best single Slater determinant in variational sense

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

- Hartree-Fock energy:

$$\langle\Psi_{\mathrm{HF}}|\widehat{H}|\Psi_{\mathrm{HF}}\rangle = \sum_{i=1}^{A} \frac{\hbar^2}{2M} \int d\mathbf{x}\, \nabla\phi_i^* \cdot \nabla\phi_i + \frac{1}{2}\sum_{i,j=1}^{A} \int d\mathbf{x} \int d\mathbf{y}\, |\phi_i(\mathbf{x})|^2 v(\mathbf{x},\mathbf{y}) |\phi_j(\mathbf{y})|^2$$

$$-\frac{1}{2}\sum_{i,j=1}^{A} \int d\mathbf{x} \int d\mathbf{y}\, \phi_i^*(\mathbf{x})\phi_i(\mathbf{y}) v(\mathbf{x},\mathbf{y}) \phi_j^*(\mathbf{y})\phi_j(\mathbf{x}) + \sum_{i=1}^{A} \int d\mathbf{y}\, v_{\mathrm{ext}}(\mathbf{y}) |\phi_j(\mathbf{y})|^2$$

- Determine the ϕ_i by varying with fixed normalization:

$$\frac{\delta}{\delta\phi_i^*(\mathbf{x})}\left(\langle\Psi_{\mathrm{HF}}|\widehat{H}|\Psi_{\mathrm{HF}}\rangle - \sum_{j=1}^{A} \epsilon_j \int d\mathbf{y}\, |\phi_j(\mathbf{y})|^2\right) = 0$$

Hartree-Fock Wave Function

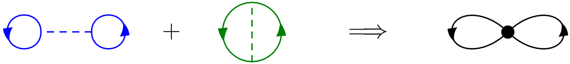
- Best single Slater determinant in variational sense

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

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

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

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



- Solve self-consistently; non-local unless zero range
- Skyrme HF or RMF have local potentials $\Longrightarrow$ look like DFT

Skyrme Hartree-Fock Energy Functionals

- Skyrme energy density functional (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 $\mathbf{J}$)

- Minimize $E = \int d\mathbf{x}\,\mathcal{E}[\rho,\tau,\mathbf{J}]$ by varying the (normalized) ϕ_i's

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

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

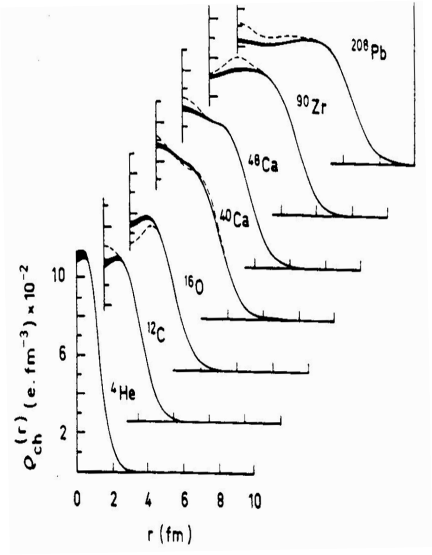
- Iterate until ϕ_i's and ϵ_i's are self-consistent
- In practice: other densities, pairing is very important (HFB), projection needed, ... $\Longrightarrow$ see Witek's talk for modern status

Density Functional Theory (DFT)

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

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

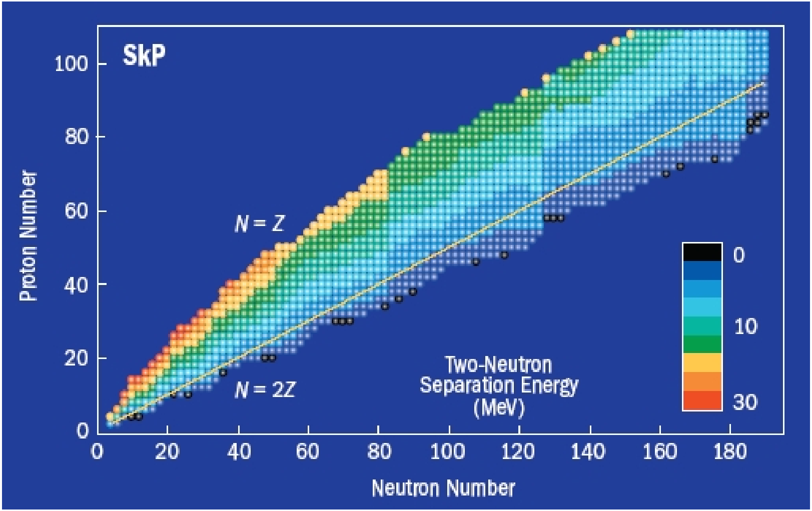
- F_{HK} is *universal* (same for any external v_{ext}) $\Longrightarrow$ H_2 to DNA!
- Introduce orbitals and minimize energy functional $\Longrightarrow E_{gs}, \rho_{gs}$
- Useful if you can approximate the energy functional
- Construct microscopically or fit a "general" form



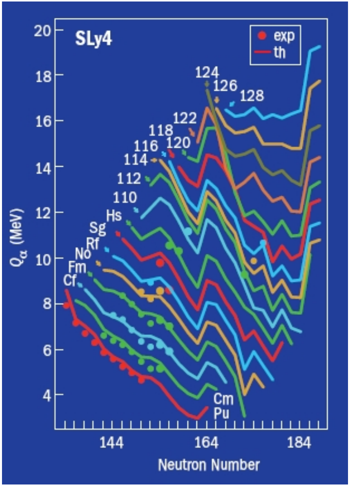
Microscopic Nuclear Structure Methods

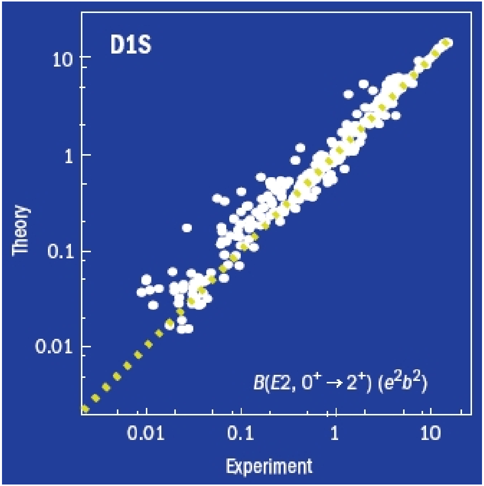
- Wave function methods (GFMC/AFMC, NCSM/FCI, CC, ...)
  - many-body wave functions (in approximate form!)
  - $\Psi(x_1, \cdots, x_A) \Longrightarrow$ everything (if operators known)
  - limited to $A < 100$? or < 200? or ???
- Green's functions (see W. Dickhoff and D. Van Neck text)
  - response of 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 $J(\mathbf{x})\psi^\dagger\psi$
  - natural framework is effective actions for composite operators $\Gamma[\rho] = \Gamma_0[\rho] + \Gamma_{\rm int}[\rho]$ (e.g., for EFT/DFT) but also consider quantum chemistry MBPT+ approach (Bartlett et al.)
  - energy functional $\Longrightarrow$ plug in candidate density, get out trial energy, minimize (variational?)
  - energy and densities (TDFT $\Longrightarrow$ excitations)

Two-Neutron Separation Energies

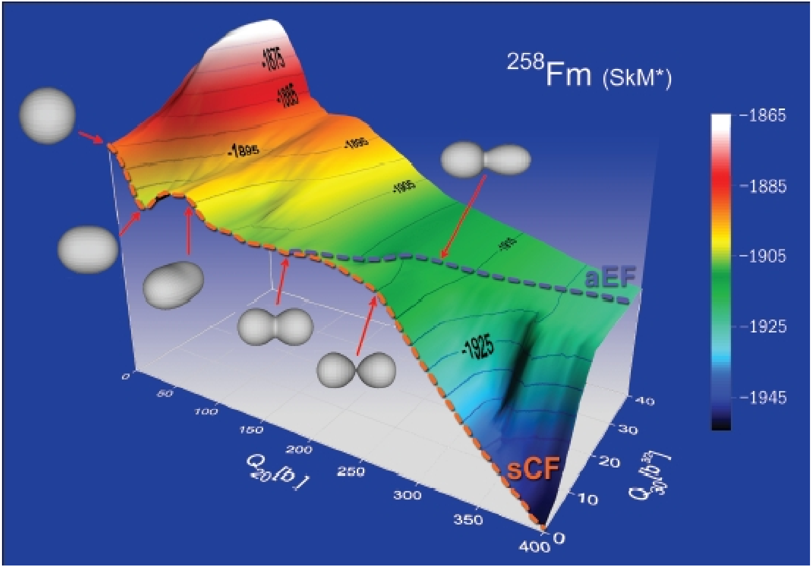


Quadrupole Deformations and B(E2)



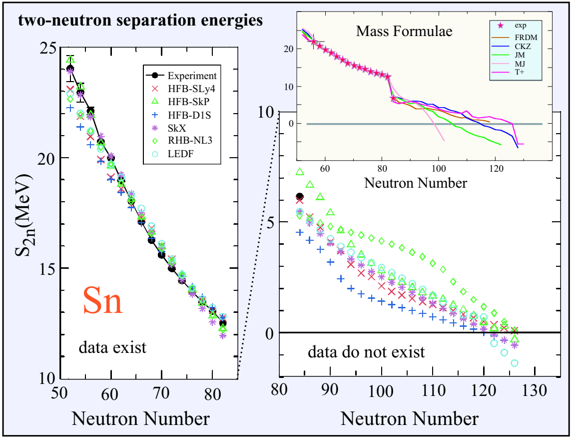


Fission: Energy Surface from DFT

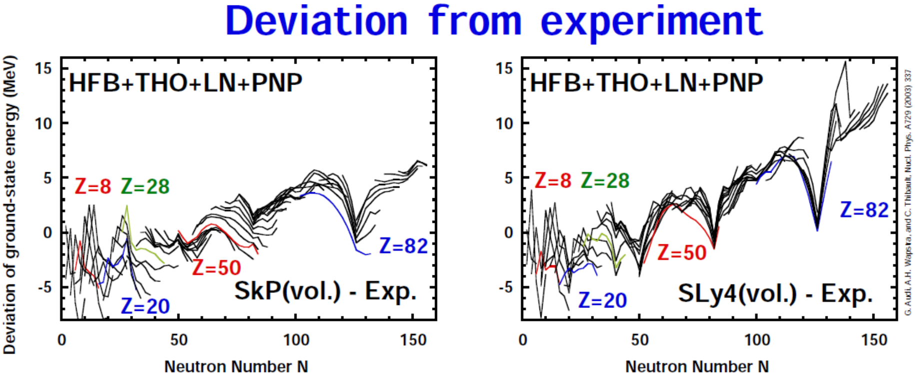


Problems with Extrapolations

- Mass formulas and energy functionals do well where there is data, but elsewhere . . .



HFB Mass Formula: $\Delta m \sim 1\text{–}2\,\mathrm{MeV}$



- Current empirical functionals hit wall at $\sim 1\,\mathrm{MeV}$ (!)
- (cf., expected accuracy of an ab initio functional fit to few-body data)

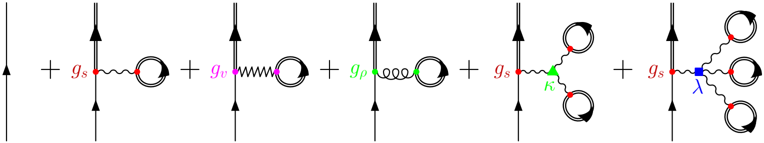
Issues with Empirical EDF's

- Density dependencies might be too simplistic
- Isovector components not well constrained
- No (fully) systematic organization of terms in the EDF
- Difficult to estimate theoretical uncertainties
- What's the connection to many-body forces?
- Pairing part of the EDF not treated on same footing
- and so on . . .

$\Longrightarrow$ Turn to microscopic many-body theory for guidance (UNEDF project!)

"Old" View of Relativistic Mean-Field Models

- QHD Lagrangian with one-boson-exchange meson fields
  - Covariant Walecka model + ϕ^3 and ϕ^4 terms to get K_0



  - Mean meson fields $\langle\phi\rangle = \phi_0$, $\langle V_\mu\rangle = \delta_{\mu 0} V_0$
  - Parameters: $g_s, g_v \approx 10$, $\kappa \approx 5000\,\text{MeV}$, $\lambda \approx -200$
- Unexplained features:
  - justification of mean-field, "no-sea" approximation
  - how to deal with large couplings and loop corrections
  - truncation at ϕ^4; why not V_0^4?
  - minimal isovector physics (chiral symmetry?)
- Reinterpret as *natural* covariant density functional

New Terms for Covariant Energy Functionals

- Mueller/Serot $\Longrightarrow$ isoscalar (V_0) and isovector (b_0) vector
  - add $\frac{\zeta}{4!} g_v^4 V_0^4 + \frac{\xi}{4!} g_\rho^4 b_0^4$
  - explore natural size ζ and ξ impact on EOS $\Longrightarrow$ MSn EOS's
- Horowitz/Piekarewicz et al. $\Longrightarrow$ FSUGold
  - add $\frac{\zeta}{4!} g_v V_0^4 + g_\rho^2 b_0^2 [\Lambda_4 g_s^2 \phi^2 + \Lambda_v g_v^2 V_0^2]$
  - knobs for symmetry energy and high-density EOS
- See also Ring et al., DDRMF (density dependent) and G-matrix based covariant EDF's
- Similar questions
  - Is the energy functional general enough? (E.g., are nonanalytic or nonlocal terms needed?)
  - Can we derive/constrain the functional more microscopically?
  - How can we better constrain parameters?

Outline

"Just the Facts" About Nuclei

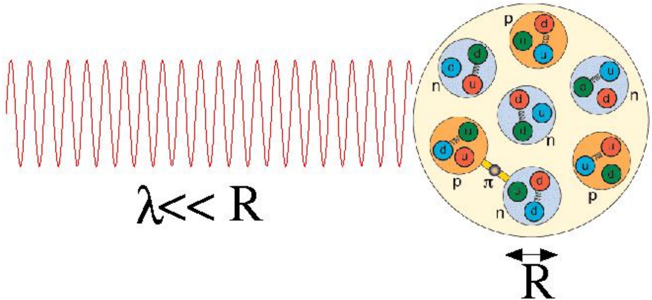
Symmetric and Asymmetric Nuclear Matter

Many-Body Methods

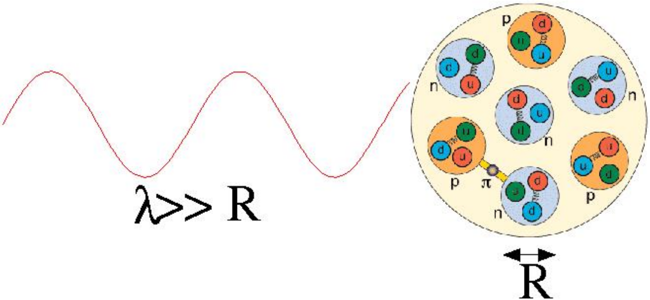
Inter-Nucleon Interactions

Final Thoughts and Prejudices

Principle of *Any* Effective Low-Energy Description



Principle of *Any* Effective Low-Energy Description



- If system is probed at low energies, fine details not resolved

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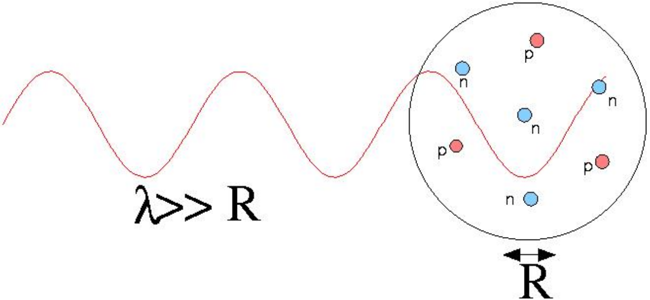
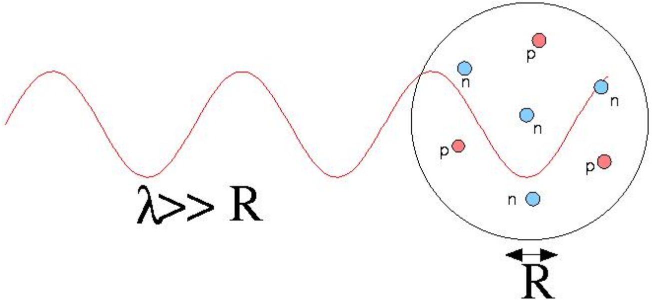


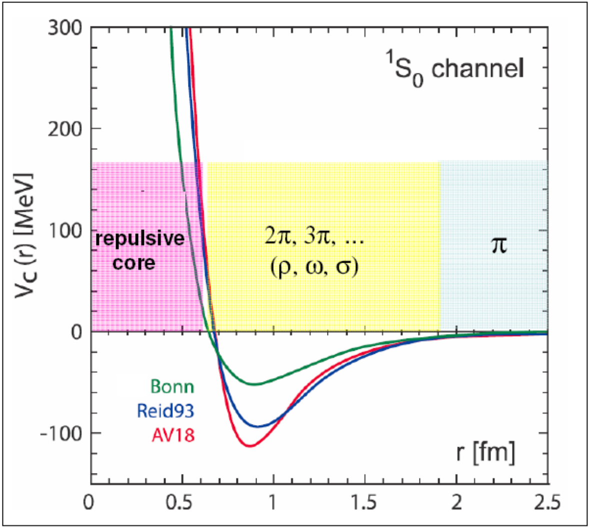
- If system is probed at low energies, fine details not resolved
  - use low-energy variables for low-energy processes
  - short-distance structure can be replaced by something simpler without distorting low-energy observables

Principle of *Any* Effective Low-Energy Description



- If system is probed at low energies, fine details not resolved
  - use low-energy variables for low-energy processes
  - short-distance structure can be replaced by something simpler without distorting low-energy observables
- Could be a model or systematic (e.g., effective field theory)
  - *physics intepretation can change with resolution!*
- Low density ⇔ low interaction energy ⇔ low resolution

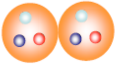
Nucleon-Nucleon Interaction (from T. Papenbrock)



From T. Hatsuda (Oslo 2008)

One-pion exchange by Yukawa (1935)

Multi-pions by Taketani (1951)



Repulsive core by Jastrow (1951)

Nucleon-Nucleon Interaction

- Potential for nonrelativistic many-body Schrödinger equation
- Depends on spins *and* isospins of nucleons; non-central
  - longest-range part is one-pion-exchange potential

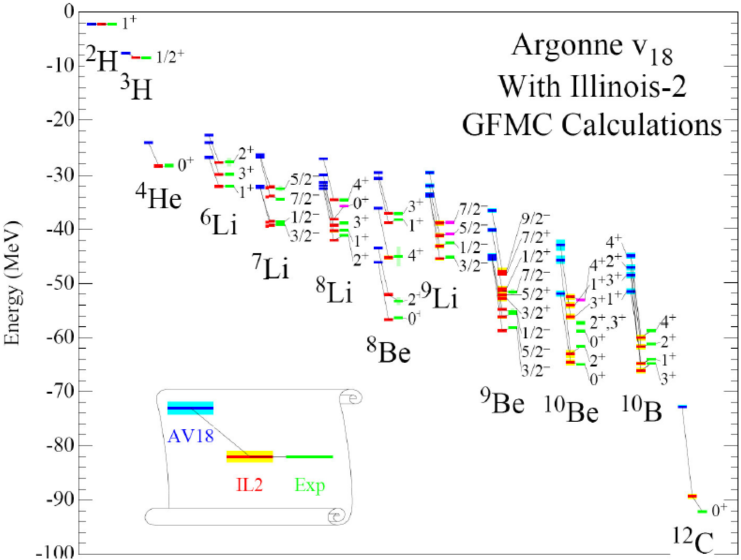
$$V_\pi(\mathbf{r}) \propto (\boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}) \left[(3\boldsymbol{\sigma_1}\cdot\hat{\mathbf{r}}\,\boldsymbol{\sigma_2}\cdot\hat{\mathbf{r}} - \boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2})(1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2}) + \boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2} \right] \frac{e^{-m_\pi r}}{r}$$

- Characterize operator structure of shorter-range potential
  - central, spin-spin, non-central tensor and spin-orbit

$$\{1, \boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}, S_{12}, \mathbf{L}\cdot\mathbf{S}, \mathbf{L}^2, \mathbf{L}^2\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}, (\mathbf{L}\cdot\mathbf{S})^2\} \otimes \{1, \boldsymbol{\tau_1}\cdot\boldsymbol{\tau_2}\}$$

  - Argonne v_{18} is $V_{\rm EM} + V_\pi + V_{\rm short\ range}$ (all cut off at small r)
- Fit to NN scattering data up to 350 MeV (or $k_{\rm rel} \leq 2.05\,\mathrm{fm}^{-1}$)
- Alternative characterization is one-boson-exchange
- Systematic treatment: chiral effective field theory (EFT)

Green’s Function Monte Carlo for Light Nuclei

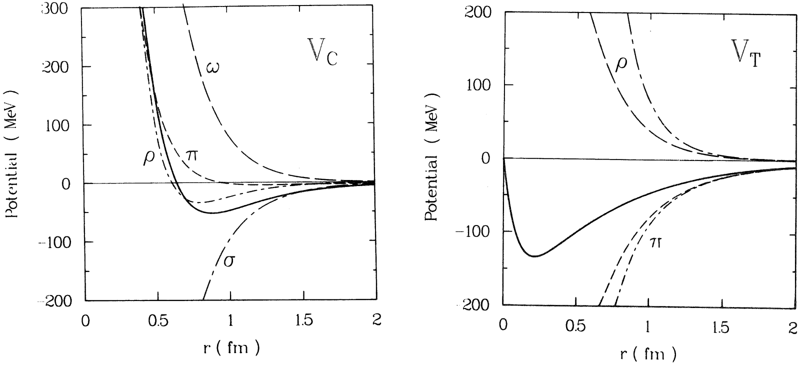


S. C. Pieper and R. B. Wiringa, Ann.Rev.Nucl.Part.Sci. 51 (2001) 53

- Note the essential role of 3-body forces!

One-Boson-Exchange Model Scorecard (Machleidt)

coupling	$T=0$ $[1]$	$T=1$ $[\tau_1 \cdot \tau_2]$	Central $[1]$	Spin-Spin $[\sigma_1 \cdot \sigma_2]$	Tensor $[S_{12}]$	Spin-Orbit $[\mathbf{L} \cdot \mathbf{S}]$
pseudoscalar	η	π	—	weak	strong	—
scalar	σ	δ	strong attractive	—	—	adds to vector
vector	ω	ρ	strong repulsive	weak	opposes ps	strong adds to s
tensor	ω	ρ	—	weak	opposes ps	—



Effective Field Theory Ingredients

See, e.g., “Crossing the Border” [nucl-th/0008064]

1. Use most general $\mathcal{L}$ with low-energy dof’s consistent with the global and local symmetries of the underlying theory

2. Declaration of regularization and renormalization scheme

3. Well-defined power counting $\Longrightarrow$ expansion parameters

Effective Field Theory Ingredients: Chiral NN

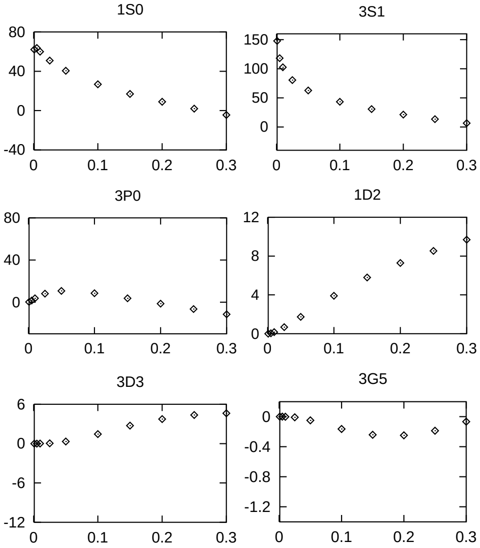
See, e.g., "Crossing the Border" [nucl-th/0008064]

1. Use most general $\mathcal{L}$ with low-energy dof's consistent with the global and local symmetries of the underlying theory
   - $\mathcal{L}_{\text{eft}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN}$
   - chiral symmetry $\Longrightarrow$ systematic long-distance pion physics
2. Declaration of regularization and renormalization scheme
   - momentum cutoff and "Weinberg counting" (still open!) $\Longrightarrow$ define irreducible potential and sum with LS eqn
   - use cutoff sensitivity as measure of uncertainties
3. Well-defined power counting $\Longrightarrow$ expansion parameters
   - use the separation of scales $\Longrightarrow \dfrac{\{\mathbf{p}, m_\pi\}}{\Lambda_\chi}$ with $\Lambda_\chi \sim 1\,\text{GeV}$
   - chiral symmetry $\Longrightarrow V_{NN} = \sum_{\nu=\nu_{\min}}^{\infty} c_\nu Q^\nu$ with $\nu \geq 0$
     $(\nu = 4 - A + 2(L - C) + \sum_i V_i(d_i + f_i/2 - 2))$
   - naturalness: LEC's are $\mathcal{O}(1)$ in appropriate units

Chiral Effective Field Theory for Two Nucleons

- Epelbaum, Meißner, et al.
- Also Entem, Machleidt
- $\mathcal{L}_{\pi N}$ + match at low energy

Q^ν	1π	2π	$4N$



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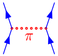
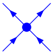
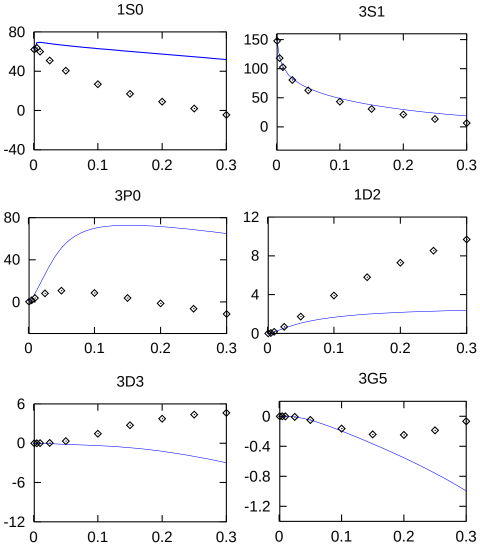
Q^0		—	 (2)



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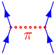
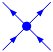
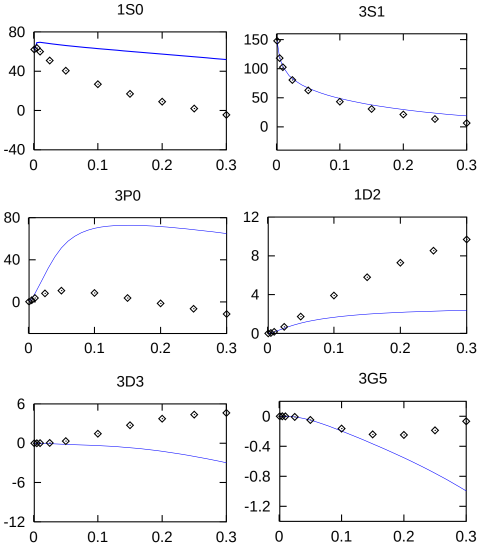
Q^0		—	 (2)
Q^1			



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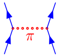
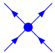
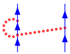
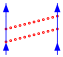
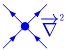
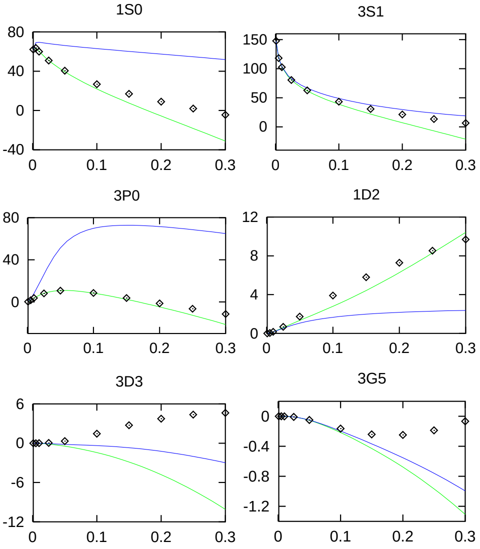
Q^0		—	 (2)
Q^1			
Q^2			 (7)



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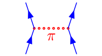
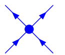
Q^0		—	 (2)
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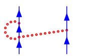
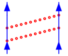
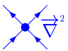
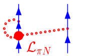
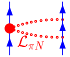
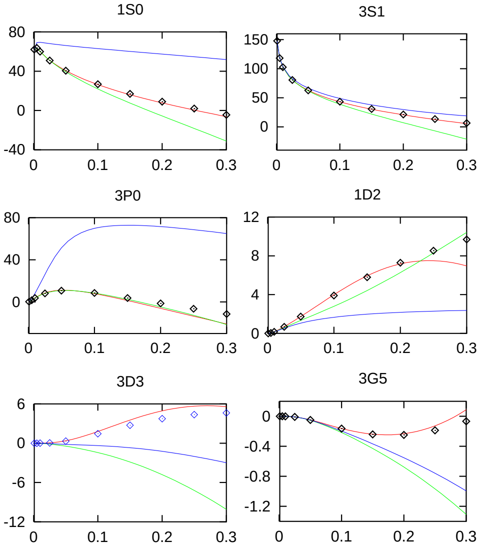
Q^2			 (7)
Q^3			



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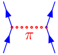
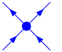
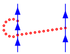
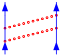
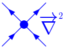
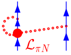
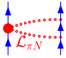
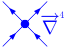
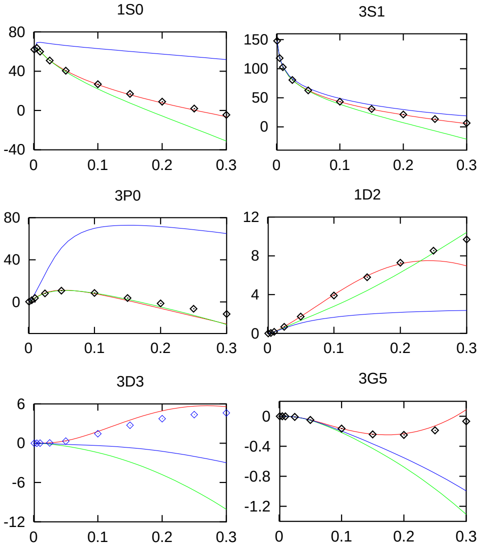
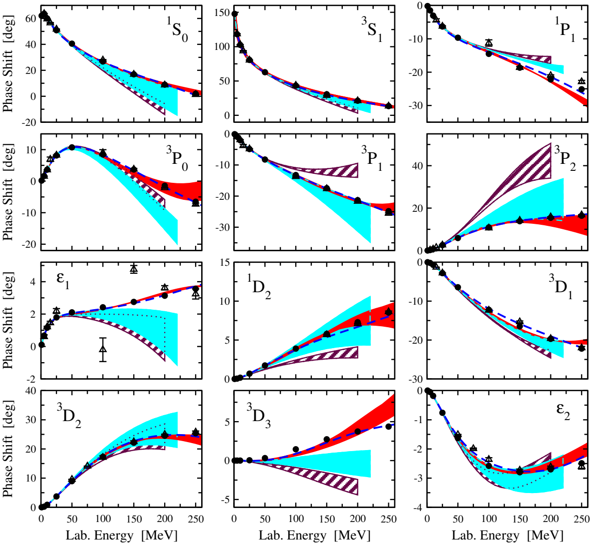
Q^0		—	 (2)
Q^1			
Q^2			 (7)
Q^3			
Q^4	many	many	 (15)



State of the Art: N^3LO (Epelbaum, nucl-th/0509032)



- Theoretical error estimates from varying cutoff

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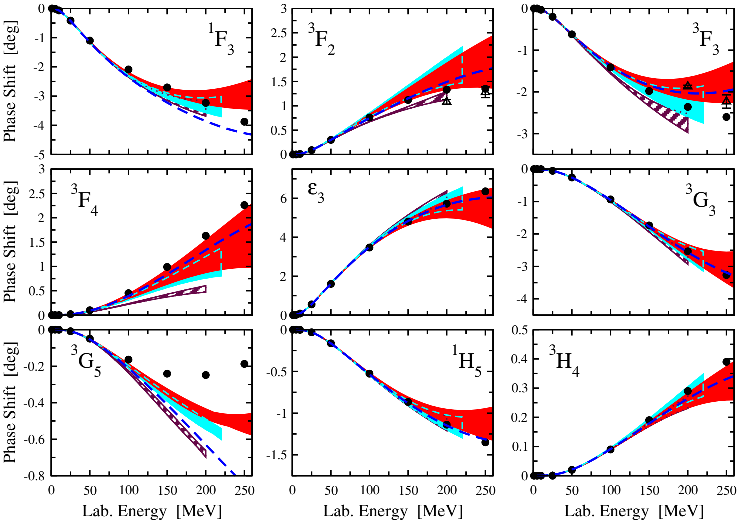
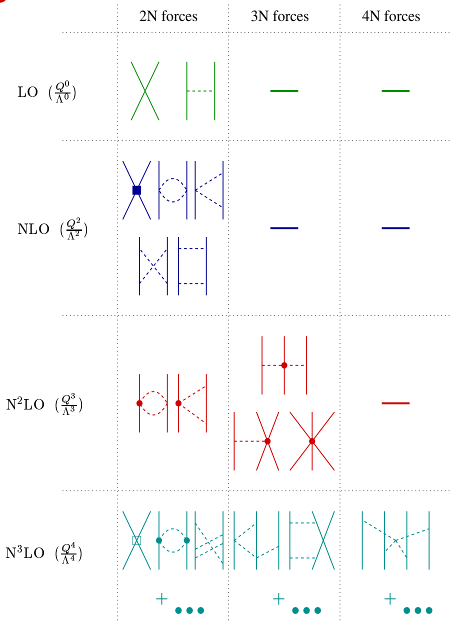


- Theoretical error estimates from varying cutoff

Few-Body Chiral Forces

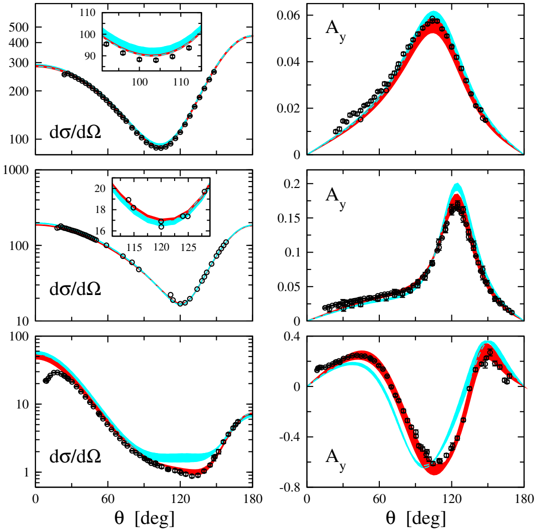
- At what orders? $\nu = -4 + 2N + 2L + \sum_i (d_i + n_i/2 - 2)$, so adding a nucleon ($N$++) suppresses by Q^2/Λ^2.
- Power counting confirms $2N \gg 3N > 4N$
- $\mathrm{N^2LO}$ diagrams cancel
- 3NF vertices may appear in NN and other processes
- Fits to the c_i's have sizable error bars



Sample Results with N^{2}LO 3NF

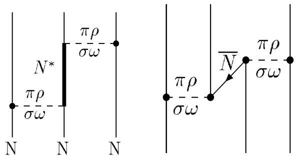
(Epelbaum, nucl-th/0509032)

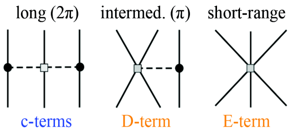
- *nd* scattering at 3, 10, 65 MeV
- *D* and *E* fixed from triton BE and *nd* doublet scattering length
- These are predictions!
- NLO vs. N2LO
- See review for more!

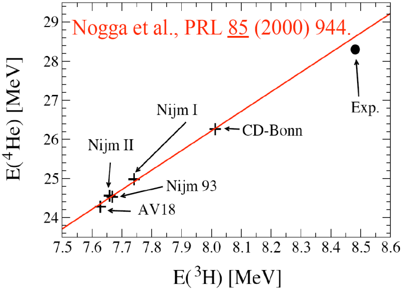


Observations on Three-Body Forces

- 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
  - but different for each Hamiltonian
- 3-body contributions increase with density
  - uncertain extrapolation if not constrained







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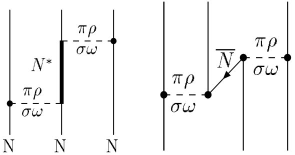
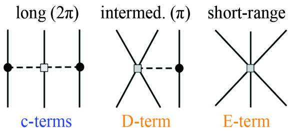
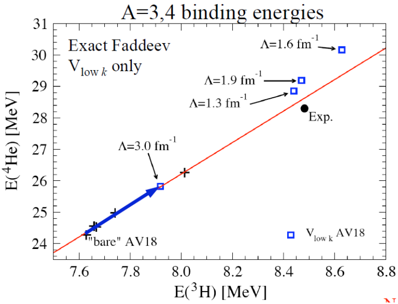


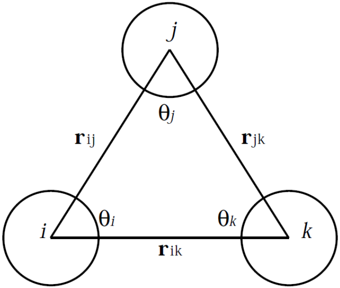




Atomic 3-Body Forces: Axilrod-Teller Term (1943)

- Three-body potential for atoms/molecules from triple-dipole mutual polarization (3rd-order perturbation correction)

$$V(i,j,k) = \frac{\nu(1 + 3\cos\theta_i \cos\theta_j \cos\theta_k)}{(r_{ij} r_{ik} r_{jk})^3}$$

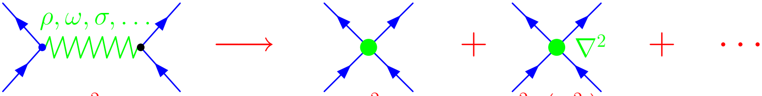


- Usually negligible in metals and semiconductors
- Can be important for ground-state energy of solids bound by van der Waals potentials
- Bell and Zuker (1976): 10% of energy in solid xenon

Chiral EFT: Resonance Saturation

[Epelbaum et al. (2002)]

- How is chiral EFT potential related to phenomenological NN potentials based on one-boson exchange?
- Boson exchange $\Longrightarrow$ model of short-distance physics
  $\Longrightarrow$ unresolved in chiral EFT (except for pion)
  $\Longrightarrow$ encoded in coefficients of contact terms

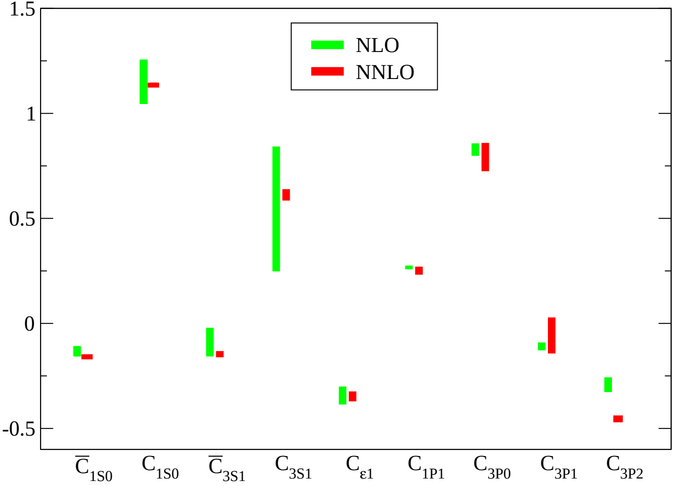


$$\frac{g^2}{\mathbf{q^2} + m^2} \qquad \frac{g^2}{m^2} \qquad - \frac{g^2}{m^2}\left(\frac{q^2}{m^2}\right)$$

- treat multiple pion exchanges systematically
- breakdown when $\mathbf{q} \approx m$ (how high in density?)

Chiral EFT: Resonance Saturation (cont.)

- Compare coefficients from phenomenological models to low-energy constants of chiral EFT:



Chiral EFT: Resonance Saturation (cont.)

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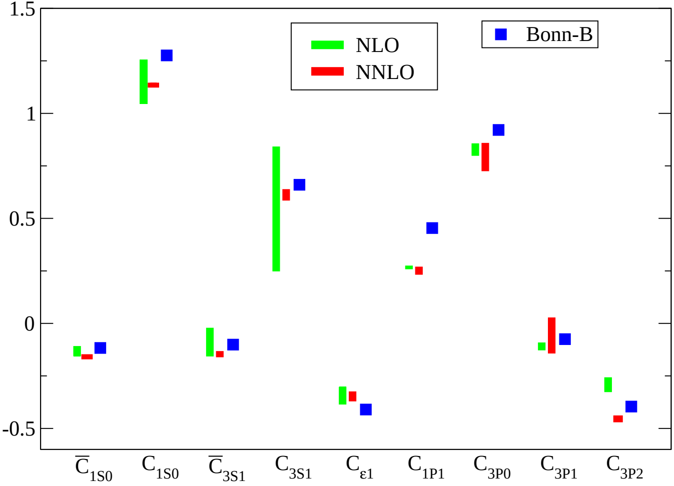

Chiral EFT: Resonance Saturation (cont.)

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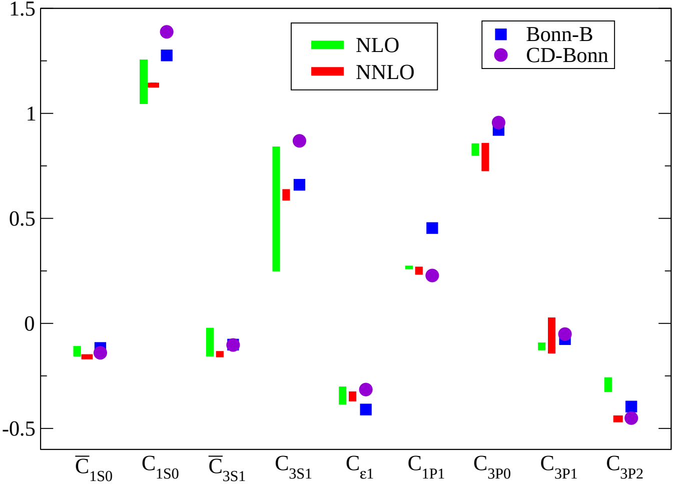

Chiral EFT: Resonance Saturation (cont.)

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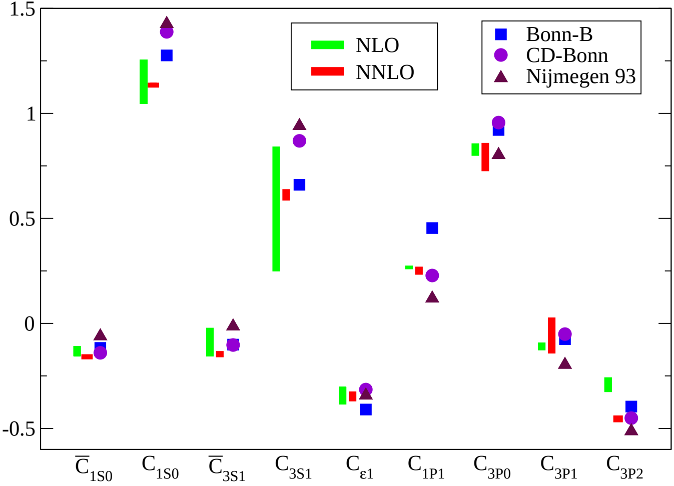


Naturalness of Coefficients (Epelbaum et al.)

- Georgi-Manohar naive dimensional analysis (NDA):

$$\mathcal{L}_{\chi\,\mathrm{eft}} = c_{lmn} \left(\frac{N^\dagger(\cdots)N}{f_\pi^2 \Lambda_\chi}\right)^l \left(\frac{\pi}{f_\pi}\right)^m \left(\frac{\partial^\mu, m_\pi}{\Lambda_\chi}\right)^n f_\pi^2 \Lambda_\chi^2$$

  - $f_\pi \sim 100\,\mathrm{MeV}$ and $\Lambda_\chi \sim 1000\,\mathrm{MeV}$
  - check NLO, NNLO constants from $\mathcal{L}_{NN}$ (vary cutoff from 500...600 MeV):

$f_\pi^2 C_S$	$-1.079 \ldots -0.953$	$f_\pi^2 C_T$	$0.002 \ldots 0.040$
$f_\pi^2 \Lambda_\chi^2 C_1$	$3.143 \ldots 2.665$	$4 f_\pi^2 \Lambda_\chi^2 C_2$	$2.029 \ldots 2.251$
$f_\pi^2 \Lambda_\chi^2 C_3$	$0.403 \ldots 0.281$	$4 f_\pi^2 \Lambda_\chi^2 C_4$	$-0.364 \ldots -0.428$
$2 f_\pi^2 \Lambda_\chi^2 C_5$	$2.846 \ldots 3.410$	$f_\pi^2 \Lambda_\chi^2 C_6$	$-0.728 \ldots -0.668$
$4 f_\pi^2 \Lambda_\chi^2 C_7$	$-1.929 \ldots -1.681$		

- $1/3 \lesssim c_{lmn} \lesssim 3 \Longrightarrow$ natural! $\Longrightarrow$ truncation error estimates
- $f_\pi^2 C_T$ *unnaturally small* $\Longrightarrow SU(4)$ spin-isospin symmetry

Power Counting in Skyrme and RMF Functionals?

- NDA analysis:
  [Friar et al., rjf et al.]

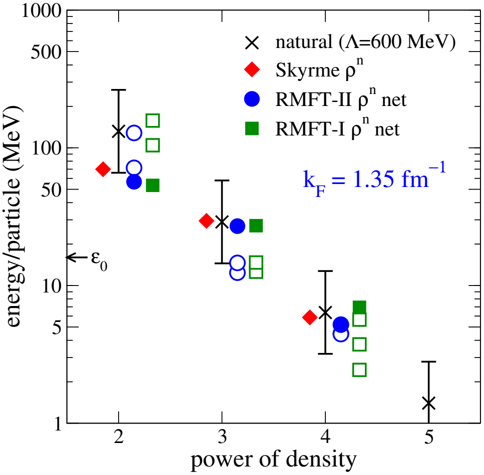
$$c \left[\frac{\psi^\dagger\psi}{f_\pi^2\Lambda}\right]^l \left[\frac{\nabla}{\Lambda}\right]^n f_\pi^2\Lambda^2$$

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

- Density expansion?

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

for $1000 \ge \Lambda \ge 500$



Naive Dimensional Analysis for RMF

- Mass scales in low-energy QCD: [Georgi & Manohar, 1984]

$$f_\pi \approx 93\,\mathrm{MeV}\ , \qquad \Lambda \approx 500 \text{ to } 800\,\mathrm{MeV}$$

- NDA rules for a generic term in energy functional:

$$c\,[f_\pi^2\Lambda^2]\left[\left(\frac{\overline{N}N}{f_\pi^2\Lambda}\right)^{\ell}\frac{1}{m!}\left(\frac{g\phi}{\Lambda}\right)^{m}\frac{1}{n!}\left(\frac{gV_0}{\Lambda}\right)^{n}\left(\frac{\nabla}{\Lambda}\right)^{p}\right]$$

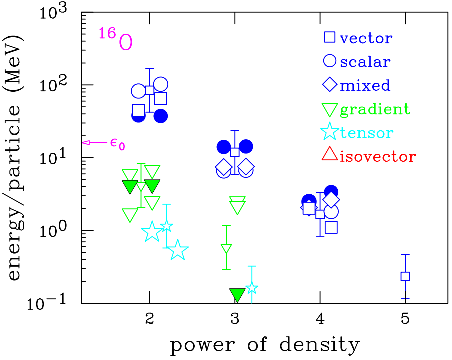
  - "Naturalness" $\Longrightarrow$ dimensionless c is of order unity
  - ratio $\Lambda/f_\pi \rightarrow g \approx$ 5–10 is origin of strong couplings
    $$\Longrightarrow \quad g_s, g_v \sim g \qquad \kappa \sim g\Lambda \qquad \lambda \sim g^2$$

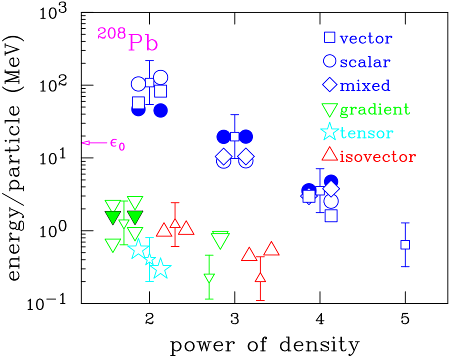
- Provides expansion parameters at finite density:

$$\frac{g_s\phi}{\Lambda} \approx \frac{g_v V_0}{\Lambda} \approx 1/2\ , \qquad \frac{\rho_{\mathrm{S}}}{f_\pi^2\Lambda} \approx \frac{\rho_{\mathrm{B}}}{f_\pi^2\Lambda} \approx 1/5 \quad \text{at } \rho_{\mathrm{B}}^0$$

RMF Estimates in Finite Nuclei

$$\widetilde{\rho}_{\mathrm{S}}, \widetilde{\rho}_{\mathrm{B}} \to \frac{\langle \rho_{\mathrm{B}} \rangle}{f_\pi^2 \Lambda} \qquad \widetilde{\nabla} \rho_{\mathrm{B}} \to \frac{\langle \nabla \rho_{\mathrm{B}} \rangle}{f_\pi^2 \Lambda^2} \qquad \widetilde{s} \to \frac{\langle \widetilde{s} \rangle}{f_\pi^2 \Lambda} \qquad \widetilde{\rho}_3 \to \frac{Z-N}{2A} \frac{\langle \rho_{\mathrm{B}} \rangle}{f_\pi^2 \Lambda}$$

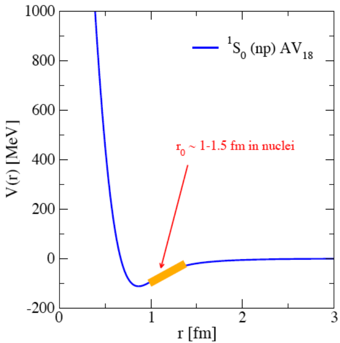




- $\approx$ 1 isovector parameter constrained by energy fit

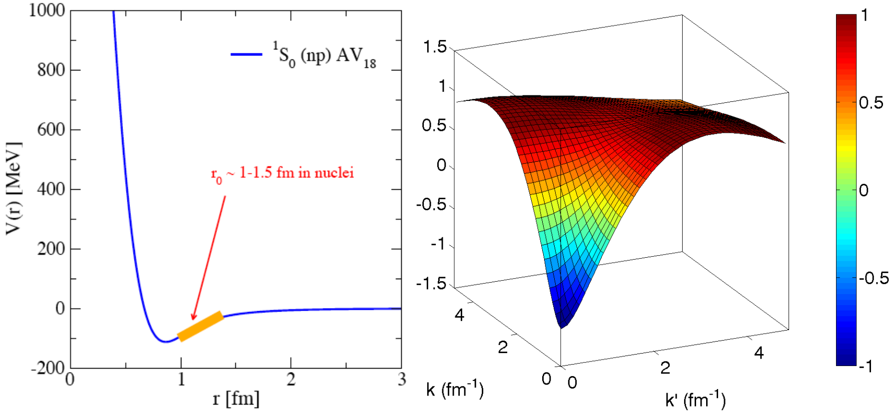
Sources of Nonperturbative Physics for NN

1. Strong short-range repulsion ("hard core" or singular $V_{2\pi}$)
2. Iterated tensor (S_{12}) interaction
3. Near zero-energy bound states



- Consequences:
  - In Coulomb DFT, Hartree-Fock gives dominate contribution $\Longrightarrow$ correlations are small corrections $\Longrightarrow$ DFT works!
  - cf. NN interactions $\Longrightarrow$ correlations $\gg$ HF $\Longrightarrow$ DFT fails??
- However ...
  - the first two depend on the *resolution* $\Longrightarrow$ changed by RG
  - all three are affected by Pauli blocking

S-Wave ($L = 0$) NN Potential in Momentum Space



- Fourier transform in partial waves (Bessel transform)

$$V_{L=0}(k,k') = \int d^3r\, j_0(kr)\, V(r)\, j_0(k'r) = \langle k|V_{L=0}|k'\rangle$$

- Repulsive core $\Longrightarrow$ big high-k ($\gtrsim 2\,\mathrm{fm}^{-1}$) components

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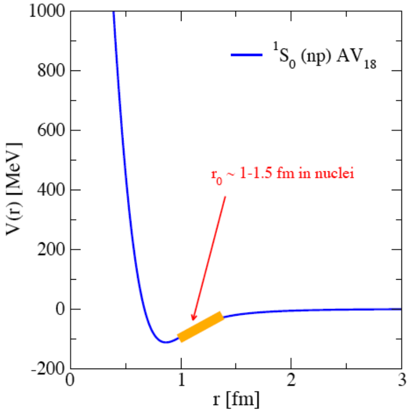

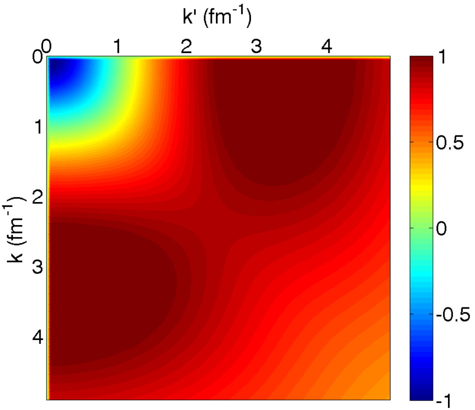

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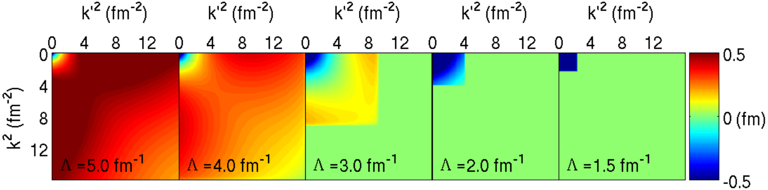
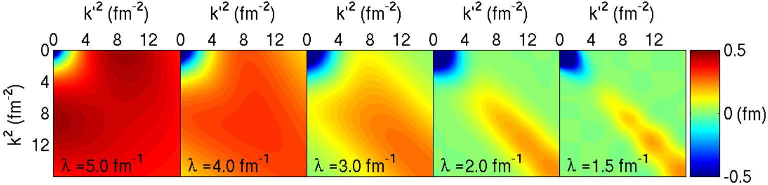
Low-Momentum Interactions from RG [AV18 $^3S_1$]

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

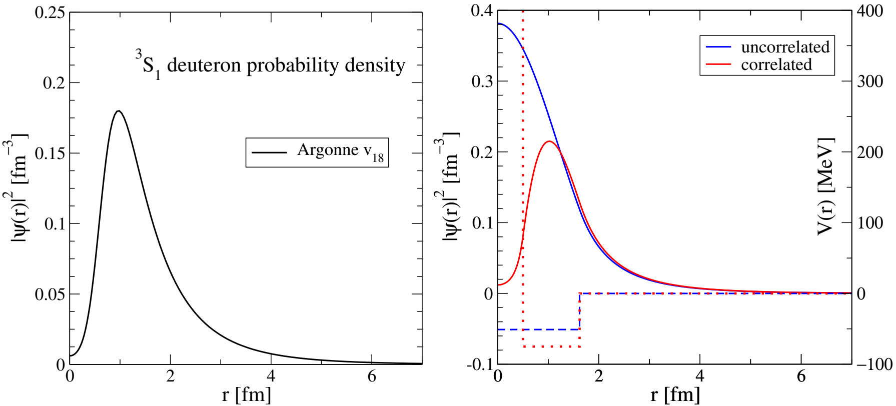


- SRG $\Longrightarrow$ Drive the Hamiltonian toward diagonal [$\lambda \equiv 1/s^{1/4}$]



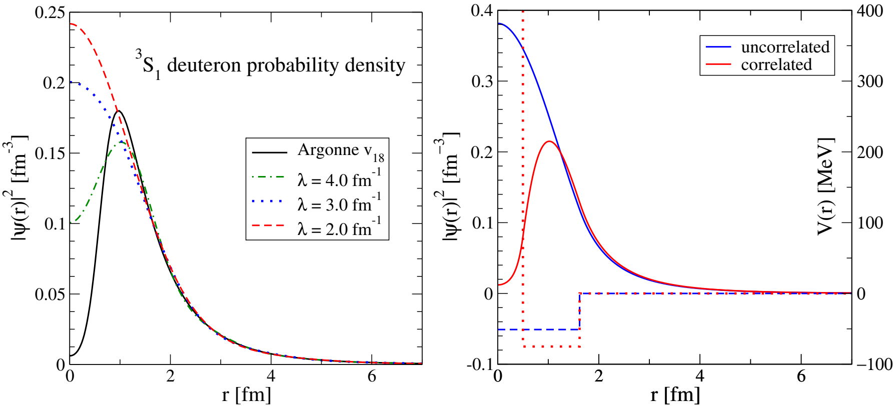
- Other transformations also decouple (e.g., UCOM)
- Isn't chiral EFT already soft? Or why not use a lower cutoff?
  [e.g., E/G/M: 450 MeV, E/M: N3LOW (400 MeV)]

Repulsive Core Before and After



- Probability at short separations suppressed $\Longrightarrow$ "correlations"
- Greatly complicates expansion of many-body wave functions
- Short-distance structure $\Leftrightarrow$ high-momentum components

Repulsive Core Before and After



- Transformed potential $\Longrightarrow$ no short-range correlations in wf
- Potential is now non-local: $V(\mathbf{r})\psi(\mathbf{r}) \longrightarrow \int d^3\mathbf{r}'\, V(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')$
  - Also few-body forces. Problems for many-body methods?
    $\Longrightarrow$ For some yes, for others no!

What are the measurable quantities?

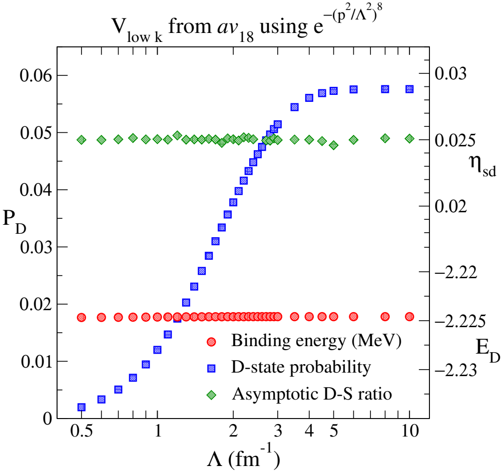
- True observables do not change under field redefinitions or unitary transformations in low-energy effective theories
  - Examples: cross sections, conserved quantities like charge
- Many useful quantities are extracted from measurements via a convolution (e.g., using some type of factorization)
  - But these will vary with the convention used
  - E.g., parton distributions
- Conventions are renormalization prescriptions, cutoffs, ...
  - Different potentials reflect different conventions
  - Unitary transformation ($U^\dagger U = 1$) of H and other operators $\Longrightarrow$ choose U to decouple!

$$
\begin{aligned}
E_n &= \langle\Psi_n|H|\Psi_n\rangle = (\langle\Psi_n|U^\dagger)UHU^\dagger(U|\Psi_n\rangle) \\
&= \langle\widetilde{\Psi}_n|\widetilde{H}|\widetilde{\Psi}_n\rangle
\end{aligned}
$$

  - The convention for the long-range part of NN$\cdots$N potentials is agreed to be (local) pion exchange, but differs widely for the short-range part. (Note: $V_{\text{low}\,k}$ preserves long-distance part.)

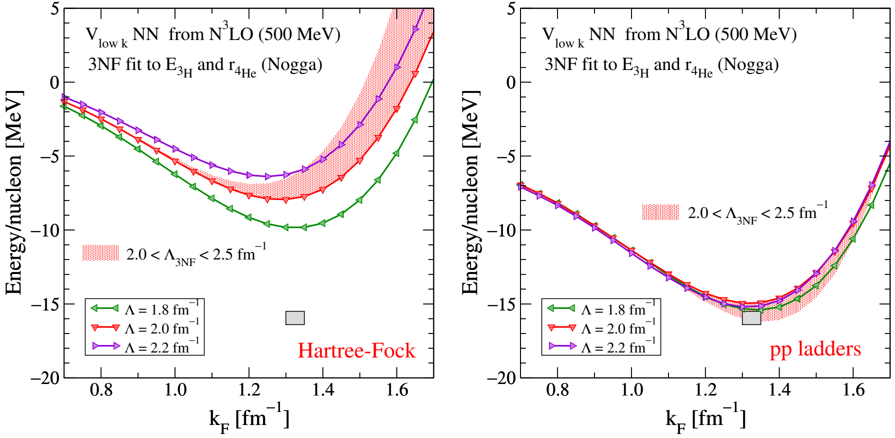
Quantities that vary with convention $\Longrightarrow$ *not* observables

- deuteron D-state probability [Friar, PRC **20** (1979)]
- off-shell effects [Fearing/Scherer]
- occupation numbers [Hammer/Furnstahl]
- wound integrals
- short-range part of wave functions
- short-range potentials; e.g., contribution of short-range 3-body forces



Short-Term Roadmap for Microscopic Nuclear DFT

- Use a chiral EFT to a given order (e.g., E/M N^3LO below)
- Soften with RG (evolve to $\Lambda \approx 2\,\mathrm{fm}^{-1}$ for ordinary nuclei)
  - NN interactions fully, NNN interactions (3NF) approximately
- Generate density functional using DME in k-space



Outline

“Just the Facts” About Nuclei

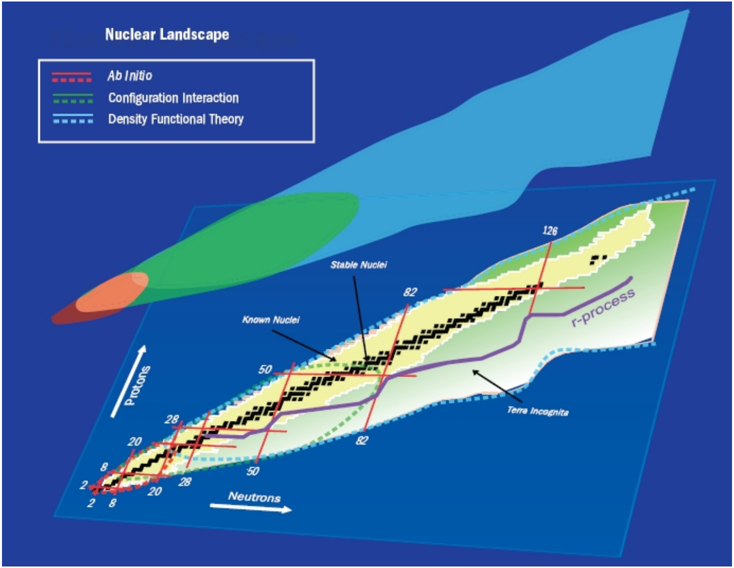
Symmetric and Asymmetric Nuclear Matter

Many-Body Methods

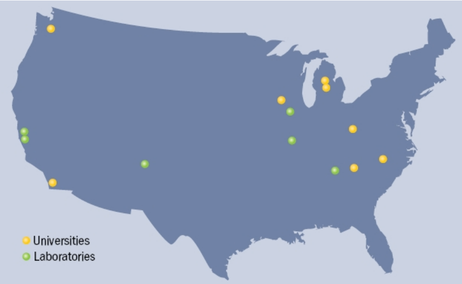
Inter-Nucleon Interactions

Final Thoughts and Prejudices

Universal Nuclear Energy Density Functional



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



- Collaboration of physicists, applied mathematicians, and computer scientists
- Funding in US but international collaborators also

Goals of SciDAC 2 Project: *Building a Universal Nuclear Energy Density Functional*

- Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications”
- Scope is all nuclei (there are more than 5000!),
  with particular interest in reliable calculations of unstable nuclei and in reactions
  $\Longrightarrow$ Density functional theory (DFT) is method of choice
- Order of magnitude improvement over present capabilities
  $\Longrightarrow$ precision calculations of masses, . . .
- Connected to the best microscopic physics
- Maximum predictive power with well-quantified uncertainties

[See http://www.scidacreview.org/0704/html/unedf.html
by Bertsch, Dean, and Nazarewicz]

Major UNEDF Research Areas

- Ab initio structure — Nuclear wf's from microscopic NN$\cdots$N
  - NCSM/NCFC, CC, GFMC/AFMC
  - AV18/ILx, chiral EFT $\longrightarrow V_{\mathrm{low}\,k}$
- Ab initio energy functionals — DFT from microscopic N$\cdots$N
  - Cold atoms — superfluid LDA+ as prototype for nuclear DFT
  - χEFT $\longrightarrow$ $V_{\mathrm{low}\,k}$ $\longrightarrow$ MBPT $\longrightarrow$ DME
- DFT applications — Technology to calculate observables
  - Skyrme HFB+ for all nuclei (solvers)
  - Fitting the functional to data (e.g., correlation analysis)
- DFT extensions — Long-range correlations, excited states
  - LACM, GCM, TDDFT, QRPA, CI
- Reactions – Low-energy reactions, fission, . . .

(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 (e.g., with form factors)	Exploit divergences (cutoff dependence as diagnostic)
Choose diagrams by "art"	Power counting determines diagrams and truncation error
Test models only by comparison to experiment	Theory itself predicts limits, errors, improvements

Plan: Use DOF's to Simplify and Make Efficient

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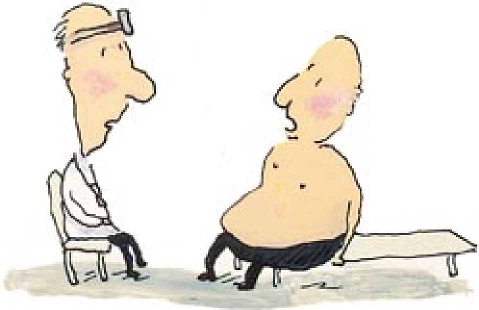

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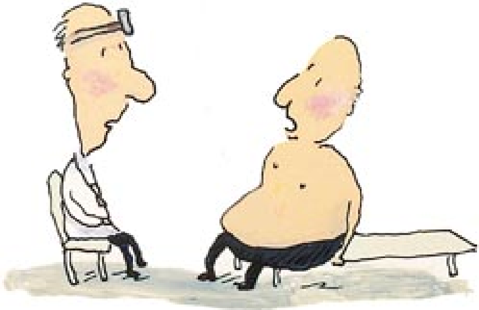

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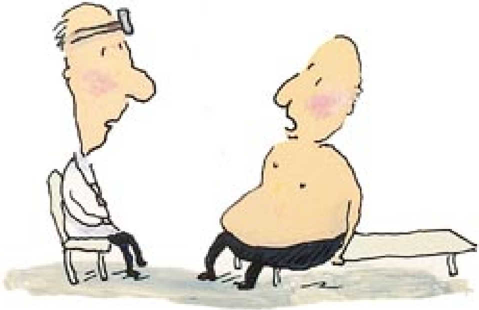

Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don't do that.