

# Effective Field Theory for Density Functional Theory I

Dick Furnstahl

Department of Physics  
Ohio State University



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- I. Overview of EFT, RG, DFT for fermion many-body systems
- II. EFT/DFT for dilute Fermi systems
- III. Refinements: Toward EFT/DFT for nuclei
- IV. Loose ends and challenges, Cold atoms, RG/DFT

# Outline

**Overview of Fermion Many-Body Systems**

**Density Functional Theory for Coulomb Systems**

**DFT for Nuclei?  $\implies$  EFT and RG**

**Summary I**

# Outline

## Overview of Fermion Many-Body Systems

Density Functional Theory for Coulomb Systems

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Summary I

# Examples of Fermion Many-Body Systems

- Collections of “fundamental” fermions (electrons, quarks, ...)
  - or of composites of *odd* number of fermions (e.g., protons)

# Examples of Fermion Many-Body Systems

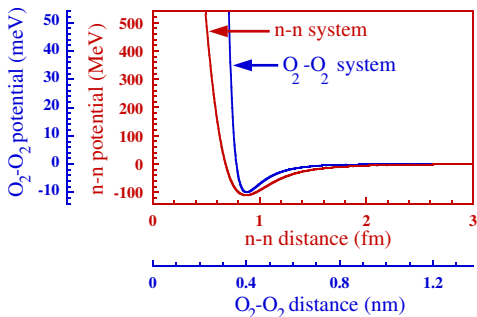
- Collections of “fundamental” fermions (electrons, quarks, ...)
  - or of composites of *odd* number of fermions (e.g., protons)
- Isolated atoms or molecules
  - electrons interacting via long-range (screened) Coulomb
  - find charge distribution, binding energy, bond lengths, ...
- Bulk solid-state materials
  - metals, insulators, semiconductors, superconductors, ...
- Liquid  $^3\text{He}$  (superfluid!)
- Cold fermionic atoms in (optical) traps [ $^6\text{Li}$  or  $^7\text{Li}$ ?]
- Atomic nuclei
- Neutron stars
  - neutron matter
  - color superconducting quark matter

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# Nuclear and Cold Atom Many-Body Problems

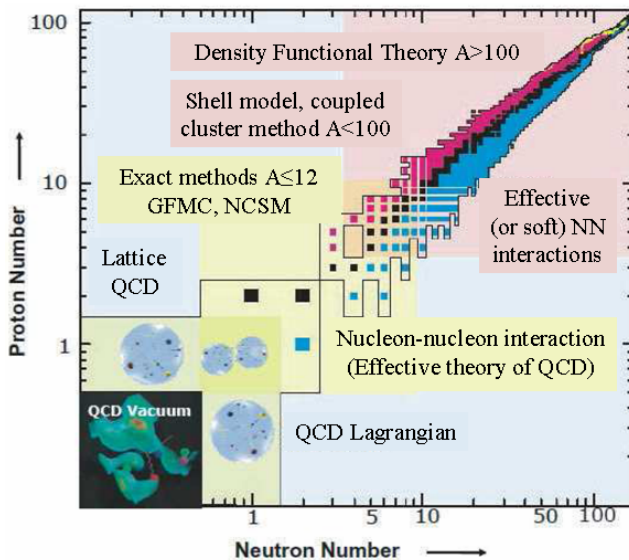
- Lennard-Jones and nucleon-nucleon potentials



[figure borrowed from J. Dobaczewski]

- Are there universal features of such many-body systems?
- How can we deal with “hard cores” in many-body systems?

# The Big Picture (adapted from Richter @INPC2004)





# The Many-Body Schrödinger Wave Function

[adapted from Joe Carlson]

- How to represent the wave function for an  $A$ -body nucleus?
- Consider  ${}^8\text{Be}$  ( $Z = 4$  protons,  $N = 4$  neutrons)

$$|\Psi\rangle = \sum_{\sigma,\tau} \chi_{\sigma} \chi_{\tau} \phi(\mathbf{R}) \quad \text{where } \mathbf{R} \text{ are the } 3A \text{ spatial coordinates}$$

$$\chi_{\sigma} = \downarrow_1 \uparrow_2 \cdots \downarrow_A \quad (2^A \text{ terms}) = 256 \text{ for } A = 8$$

$$\chi_{\tau} = n_1 n_2 \cdots p_A \quad \left(\frac{A!}{N!Z!} \text{ terms}\right) = 70 \text{ for } {}^8\text{Be}$$

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- So for  ${}^8\text{Be}$  there are 17,920 complex functions in  $3A - 3 = 21$  dimensions!
- Suppose you represent this for a nucleus of size 10 fm with a mesh spacing of 0.5 fm. You would need  $10^{27}$  grid points!

# Hartree-Fock Wave Function

- Best single **Slater determinant** in variational sense

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

- Hartree-Fock energy:



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

- Determine the  $\phi_i$  by varying with fixed normalization:

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

# Hartree-Fock Wave Function

- Best single **Slater determinant** in variational sense

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

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

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

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



- Solve self-consistently; non-trivial because **non-local**

# Outline

Overview of Fermion Many-Body Systems

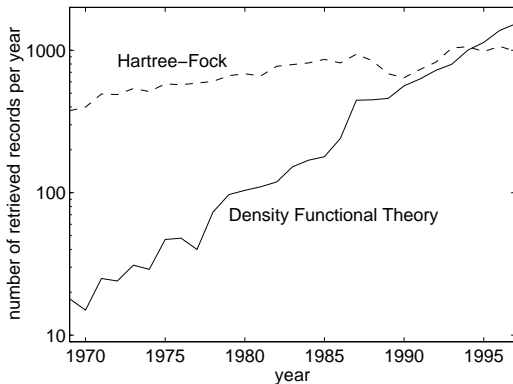
## **Density Functional Theory for Coulomb Systems**

DFT for Nuclei?  $\implies$  EFT and RG

Summary I

# Density Functional Theory (DFT)

- Dominant application: inhomogeneous electron gas
- Interacting point electrons in static potential of atomic nuclei
- “Ab initio” calculations of atoms, molecules, crystals, surfaces, ...

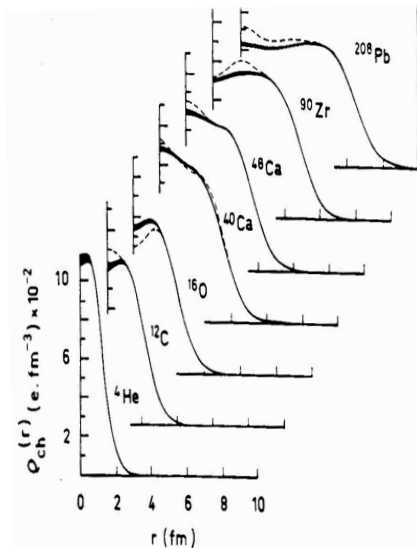


# Density Functional Theory (DFT)

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

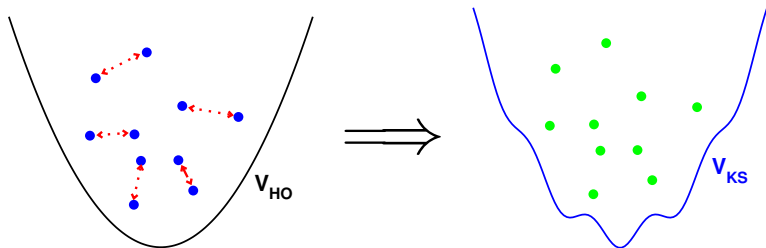
$$E_{v_{\text{ext}}}[\rho] = F_{\text{HK}}[\rho] + \int d^3x v_{\text{ext}}(\mathbf{x})\rho(\mathbf{x})$$

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

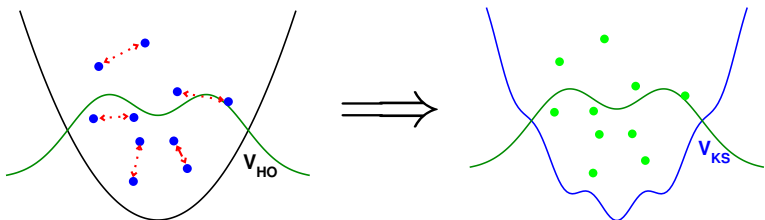




# Kohn-Sham DFT for $v_{\text{ext}} = V_{\text{HO}}$ Harmonic Trap



# Kohn-Sham DFT for $V_{\text{ext}} = V_{\text{HO}}$ Harmonic Trap



- Interacting **density** in  $V_{\text{HO}} \equiv$  **Non-interacting density** in  $V_{\text{KS}}$
- Orbitals  $\{\psi_i(\mathbf{x})\}$  in **local** potential  $V_{\text{KS}}([\rho], \mathbf{x})$

$$[-\nabla^2/2m + V_{\text{KS}}(\mathbf{x})]\psi_i = \varepsilon_i\psi_i \implies \rho(\mathbf{x}) = \sum_{i=1}^A |\psi_i(\mathbf{x})|^2$$

- Find Kohn-Sham potential  $V_{\text{KS}}([\rho], \mathbf{x})$  from  $\delta E_{v_{\text{ext}}}[\rho]/\delta\rho(\mathbf{x})$
- Solve **self-consistently**

# DFT for Solid-State or Molecular Systems

- HK free energy for an inhomogeneous electron gas

$$F_{\text{HK}}[\rho(\mathbf{x})] = T_{\text{KS}}[\rho(\mathbf{x})] + \frac{e^2}{2} \int d^3x d^3x' \frac{\rho(\mathbf{x})\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} + E_{\text{xc}}[\rho(\mathbf{x})]$$

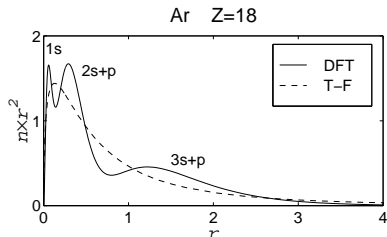
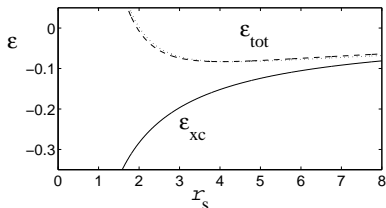
- Then  $V_{\text{KS}} = v_{\text{ext}} - e\phi + v_{\text{xc}}$  with  $v_{\text{xc}}(\mathbf{x}) = \delta E_{\text{xc}}/\delta\rho(\mathbf{x})$
- Kohn-Sham  $T_{\text{KS}}[\rho(\mathbf{x})]$ : find normalized  $\{\psi_i, \epsilon_i\}$  from

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{KS}}(\mathbf{x})\right)\psi_i(\mathbf{x}) = \epsilon_i\psi_i(\mathbf{x})$$

so that  $\rho(\mathbf{x}) = \sum_{i=1}^A |\psi_i(\mathbf{x})|^2$  and

$$T_{\text{KS}}[\rho(\mathbf{x})] = \sum_{i=1}^A \langle \psi_i | -\frac{\hbar^2}{2m}\nabla_i^2 | \psi_i \rangle = \sum_{i=1}^A \epsilon_i - \int d^3x \rho(\mathbf{x}) V_{\text{KS}}(\mathbf{x})$$

- Local density approximation:  $E_{xc}[\rho(\mathbf{x})] \approx \int d^3x \mathcal{E}_{xc}(\rho(\mathbf{x}))$ 
  - fit  $\mathcal{E}_{xc}(\rho)$  to Monte Carlo calculation of uniform electron gas



- in practice, use parametric formulas for energy density, e.g.,

$$\mathcal{E}_{xc}(\rho)/\rho = -0.458/r_s - 0.0666G(r_s/11.4)$$

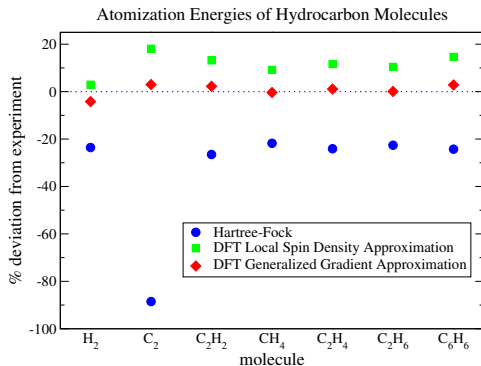
$$\text{with } G(x) = \frac{1}{2} \left\{ (1+x)^3 \log(1+x^{-1}) - x^2 + \frac{1}{2}x - \frac{1}{3} \right\}$$

- just like “naive” Hartree approach with additional potential:

$$v_{xc}(\mathbf{x}) = \left. \frac{d[\mathcal{E}_{xc}(\rho)]}{d\rho} \right|_{\rho=\rho(\mathbf{x})}$$

# Density Functional Theory (DFT)

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



e.g., van Leeuwen–Baerends GGA

$$v_{xc}(\mathbf{r}) = -\beta\rho^{1/3}(\mathbf{r}) \frac{x^2(\mathbf{r})}{1 + 3\beta x(\mathbf{r}) \sinh^{-1}(x(\mathbf{r}))}$$

$$\text{with } x = |\nabla\rho|/\rho^{4/3}$$

# Quotes From the DFT Literature

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“To many, the success of DFT appeared somewhat miraculous, and maybe even unjust and unjustified. Unjust in view of the easy achievement of accuracy that was so hard to come by in the wave function based methods. And unjustified it appeared to those who doubted the soundness of the theoretical foundations. ”

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## *Meta-Generalized Gradient Approximation* (Perdew et al., 1999)

“Some say that ‘there is no systematic way to construct density functional approximations.’ But there are more or less systematic ways, and the approach taken ... here is one of the former.”

## Preview of DFT as Effective Action

- Recall ordinary thermodynamics with  $N$  particles at  $T = 0$
- Use a chemical potential  $\mu$  as source to change  $\langle \hat{N} \rangle$

$$\Omega(\mu) = -kT \ln Z(\mu) \quad \text{and} \quad N = - \left( \frac{\partial \Omega}{\partial \mu} \right)_{TV}$$

- *Invert* to find  $\mu(N)$ , Legendre transform to  $F(N)$

$$F(N) = \Omega(\mu(N)) + \mu(N)N$$

$\implies$  This is our energy function!

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- Generalize to spatially dependent chemical potential  $J(\mathbf{x})$

$$Z(\mu) \longrightarrow Z[J(\mathbf{x})] \quad \text{and} \quad \mu N = \mu \int \psi^\dagger \psi \longrightarrow \int J(\mathbf{x}) \psi^\dagger \psi(\mathbf{x})$$

- LT from  $\ln Z[J(\mathbf{x})]$  to  $\Gamma[\rho(\mathbf{x})]$ , where  $\rho = \langle \psi^\dagger \psi \rangle_J \implies$  DFT!

# Outline

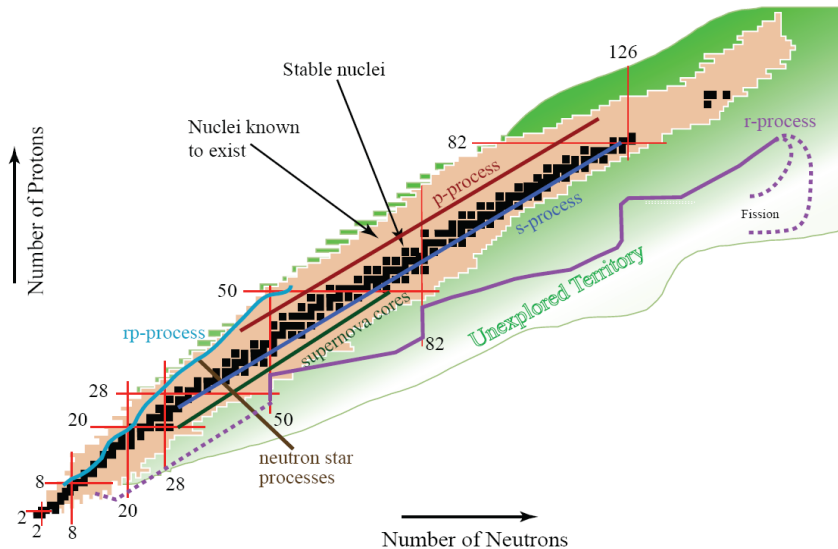
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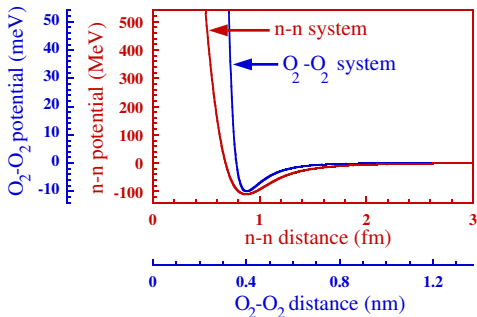
Summary I

# Table of the Nuclides



# Nuclear and Cold Atom Many-Body Problems

- Lennard-Jones and nucleon-nucleon potentials

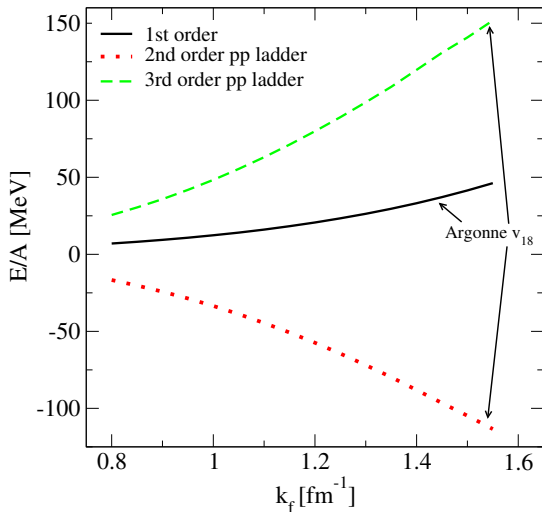


[figure borrowed from J. Dobaczewski]

- Are there universal features of such many-body systems?
- How can we deal with “hard cores” in many-body systems?

# Nuclear Matter in Low-Order Perturbation Theory

- Standard Argonne  $v_{18}$  potential
- Brueckner ladders order-by-order
- 1st order is Hartree-Fock  $\implies$  unbound!
- Repulsive core  $\implies$  series diverges



# Hartree-Fock Wave Function

- Best single Slater determinant in variational sense

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

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

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

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- Solve self-consistently; somewhat tricky because non-local  
 $\implies$  much simpler if  $v(\mathbf{x}, \mathbf{y}) \propto \delta(\mathbf{x} - \mathbf{y})$



# Skyrme Hartree-Fock Energy Functionals

- Skyrme: Do Hartree-Fock with  $V_2^{\text{Skyrme}} + V_3^{\text{Skyrme}}$ , where
$$\langle \mathbf{k} | V_2^{\text{Skyrme}} | \mathbf{k}' \rangle = t_0 + \frac{1}{2} t_1 (\mathbf{k}^2 + \mathbf{k}'^2) + t_2 \mathbf{k} \cdot \mathbf{k}' + iW_0 (\sigma_1 + \sigma_2) \cdot \mathbf{k} \times \mathbf{k}'$$

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- Motivates Skyrme energy density functional (for  $N = Z$ ):

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

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

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

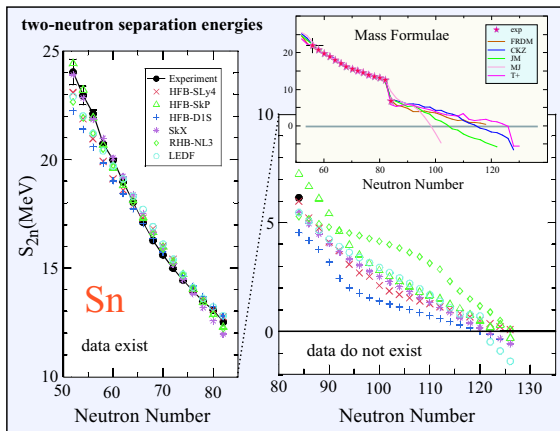
$$\left( -\nabla \frac{1}{2M^*(\mathbf{x})} \nabla + U(\mathbf{x}) + \frac{3}{4} W_0 \nabla \rho \cdot \frac{1}{i} \nabla \times \sigma \right) \phi_i(\mathbf{x}) = \epsilon_i \phi_i(\mathbf{x}),$$

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

- Iterate until  $\phi_i$ 's and  $\epsilon_i$ 's are self-consistent

# Problems with Extrapolations

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



# Questions and Criticisms of Skyrme HF

- Typical [e.g., SkIII] model parameters (in units of MeV-fm<sup>n</sup>):  
 $t_0 = -1129$     $t_1 = 395$     $t_2 = -95$     $t_3 = 14000$     $W_0 = 120$ 
  - These seem large; is there an expansion parameter?
  - Where does  $\rho^{2+\alpha}$  come from? Why not  $\rho^{2+\beta}$ ?
  - Parameter Fitting [von Neumann via Fermi via Dyson]:  
*“With four parameters I can fit an elephant,  
and with five I can make him wiggle his trunk.”*

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- Skyrme HF is only mean-field; too simple for NN correlations
  - Law of the Conservation of Difficulty  
*“Difficulty in a solution to a problem is always conserved  
regardless of the technique used in the solution.”*
  - How do we improve the approach? Is pairing treated correctly?

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*“Difficulty in a solution to a problem is always conserved  
regardless of the technique used in the solution.”*
  - How do we improve the approach? Is pairing treated correctly?
- How does Skyrme HF relate to NN (and NNN) forces?

# (Nuclear) Many-Body Physics: “Old” Approach




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One Hamiltonian for all problems and energy/length scales (not QCD!)

For nuclear structure, protons and neutrons with a *local* potential fit to NN data

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# (Nuclear) Many-Body Physics: “Old” Approach

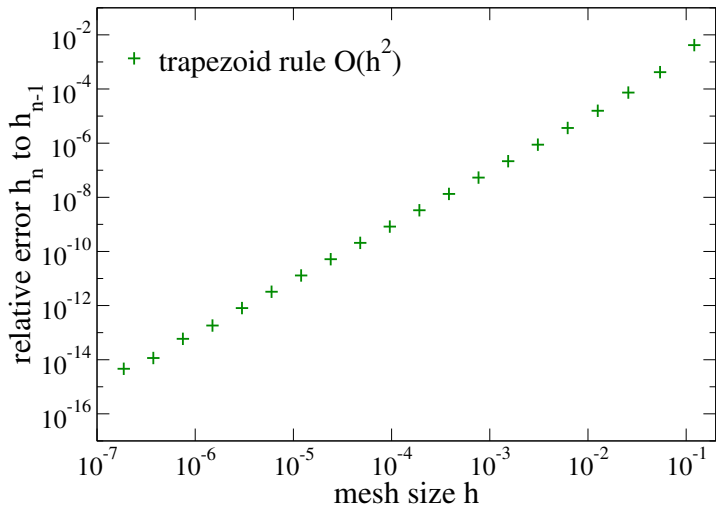
One Hamiltonian for all problems and energy/length scales (not QCD!)	For nuclear structure, protons and neutrons with a <i>local</i> potential fit to NN data
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Two-body data may be sufficient; many-body forces as last resort	Let phenomenology dictate whether three-body forces are needed (answer: yes!)
Avoid (hide) divergences	Add “form factor” to suppress high-energy intermediate states; don’t consider cutoff dependence
Choose approximations by “art”	Use physical arguments (often handwaving) to justify the subset of diagrams used

# Why Use EFT For Many-Body Physics?

- Systematic calculations with error estimates
- Reliable, model independent **extrapolation**
- Analogy between EFT and basic numerical analysis
  - naive error analysis: pick a method and reduce the mesh size (e.g., increase grid points) until the error is “acceptable”
  - sophisticated error analysis: understand scaling and sources of error (e.g., algorithm vs. round-off errors)  
⇒ **Does it work as well as it should?**
  - **representation dependence** ⇒ **not all are equally effective!**
  - extrapolation: completeness of an expansion basis
- Quantum mechanics makes EFT trickier!

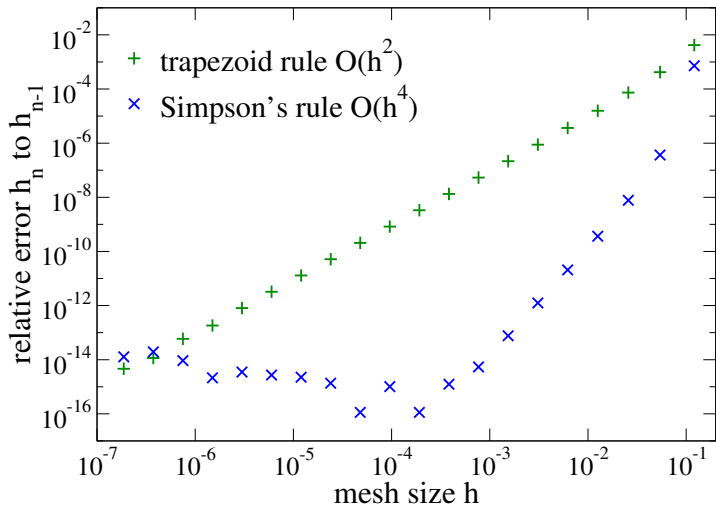
# Error Plots in Numerical Analysis

## Numerical Integration



# Error Plots in Numerical Analysis

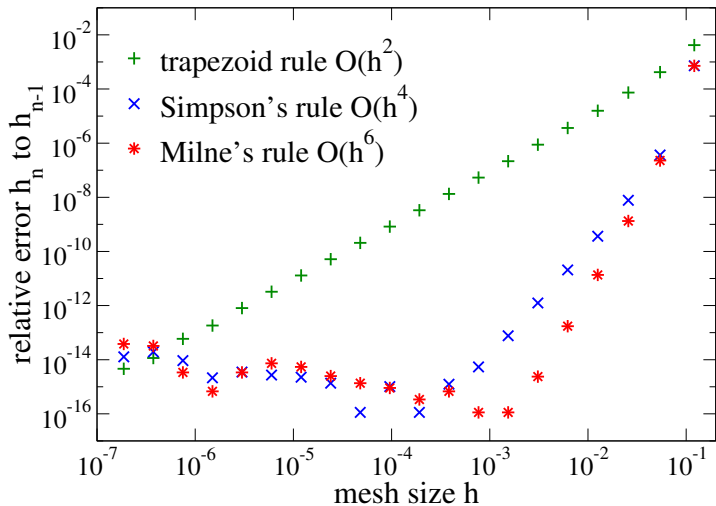
## Numerical Integration





# Error Plots in Numerical Analysis

## Numerical Integration



# The Representation Can Make A Difference!

- E.g., elliptic integral:

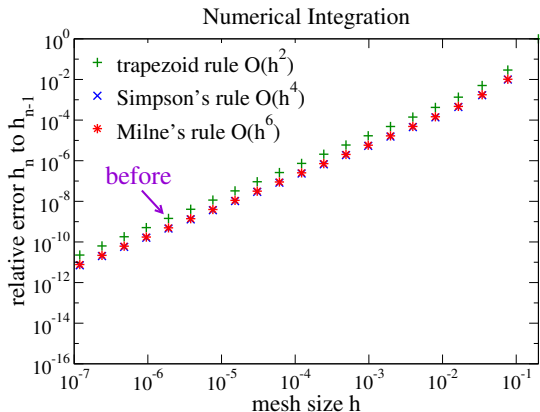
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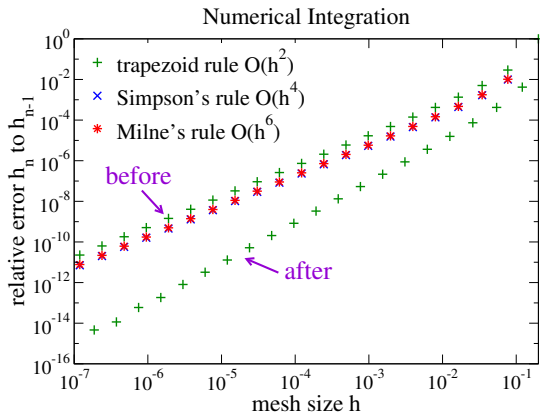
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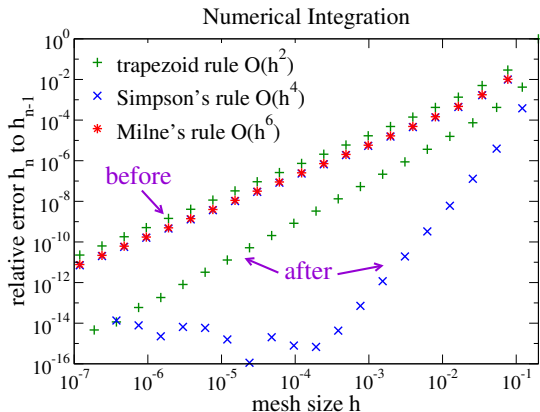
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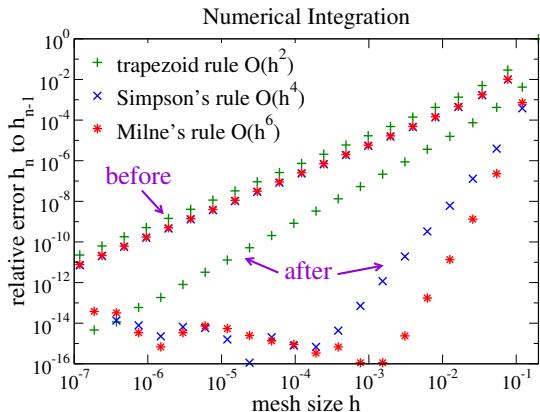
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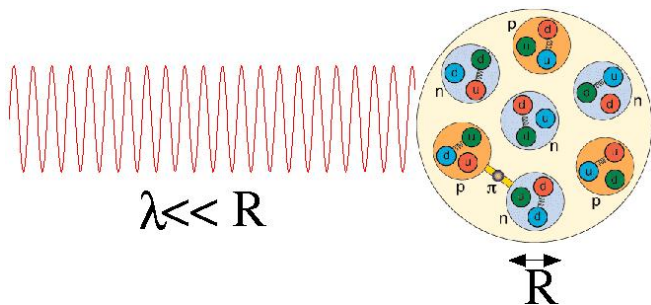
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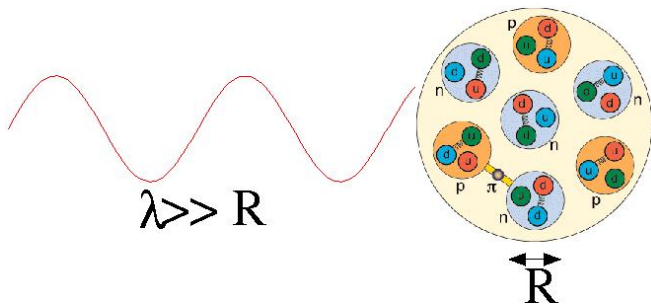
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# Principles of Effective Low-Energy Theories



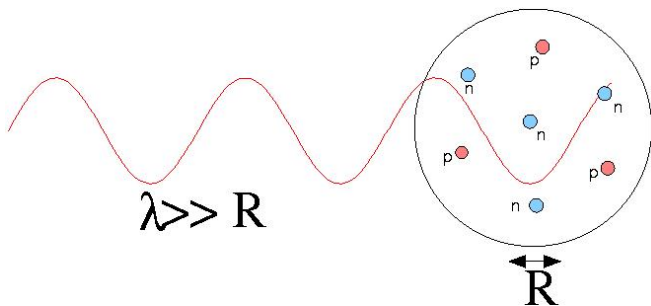
# Principles of Effective Low-Energy Theories



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

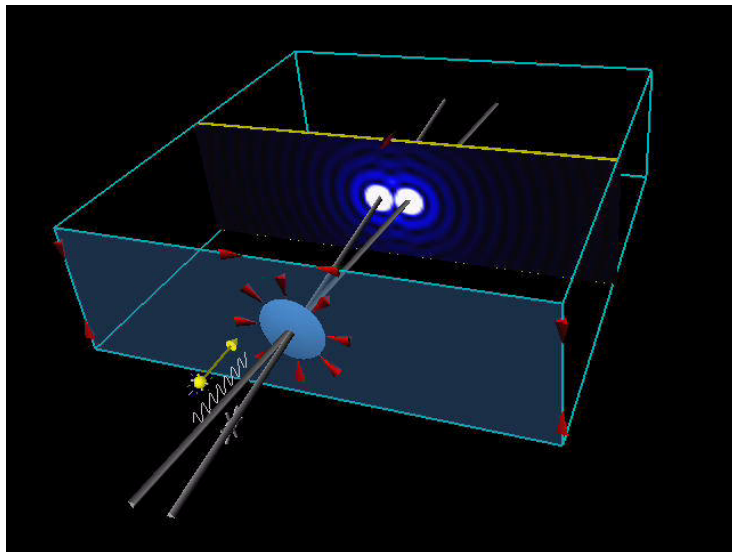


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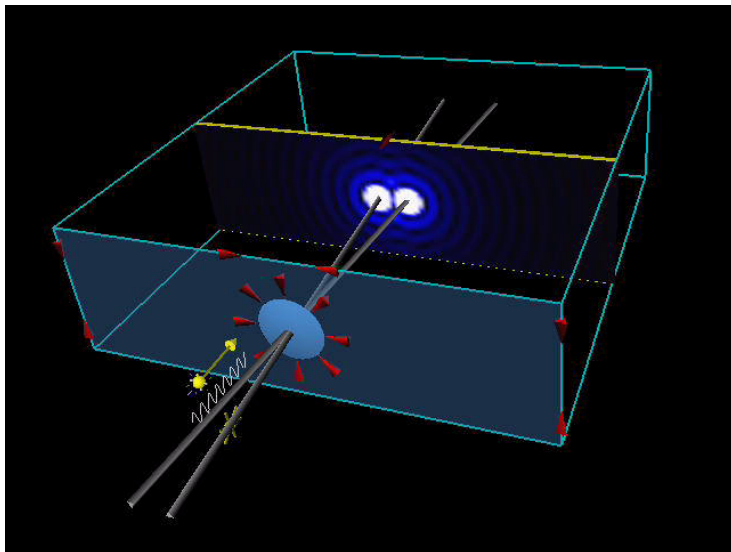


- If system is probed at low energies, fine details not resolved
  - use low-energy variables for low-energy processes
  - short-distance structure can be **replaced** by something simpler without distorting low-energy observables

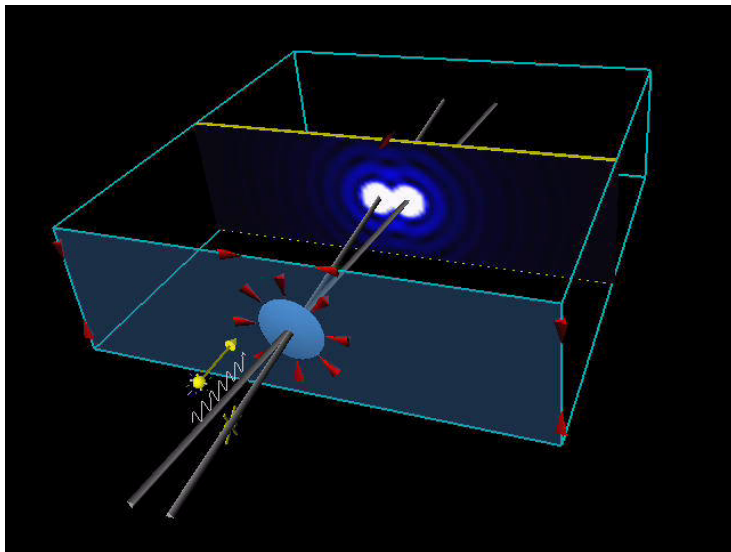
# Wavelength and Resolution



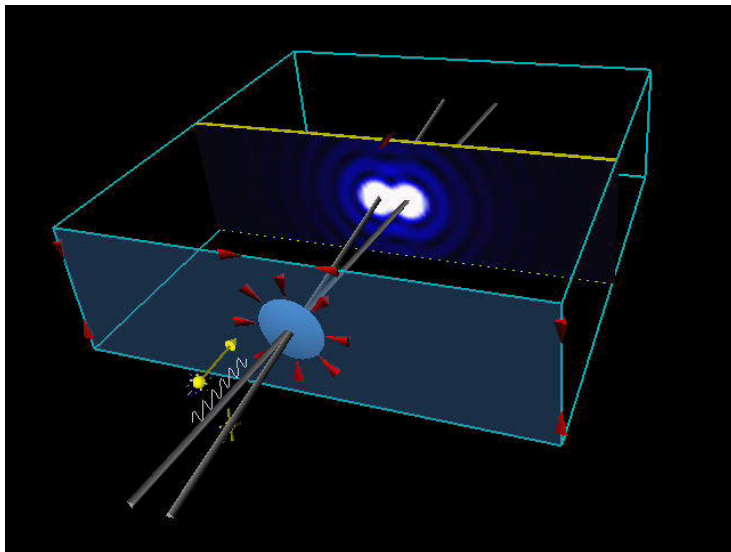
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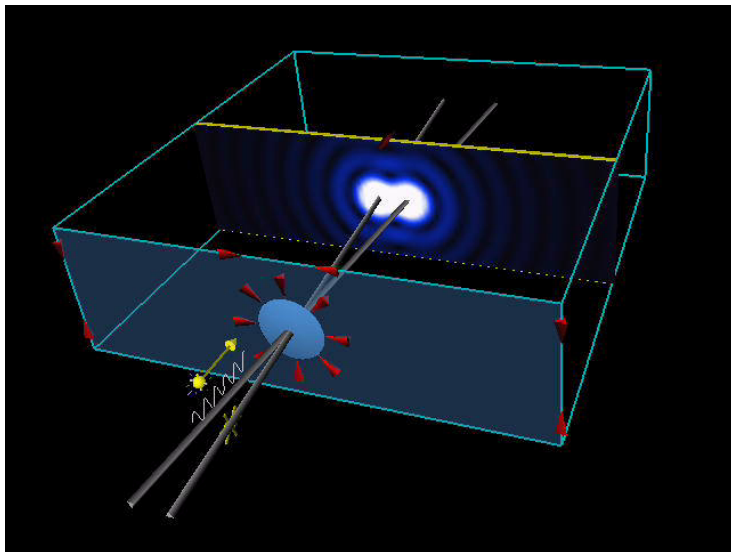
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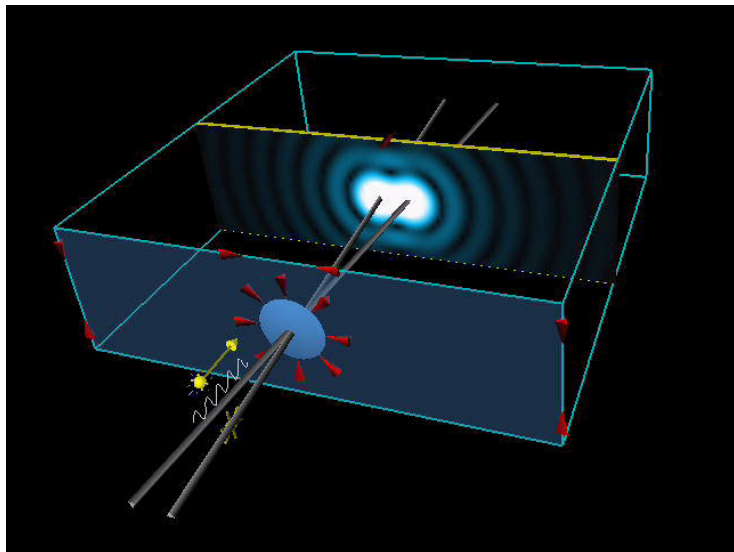
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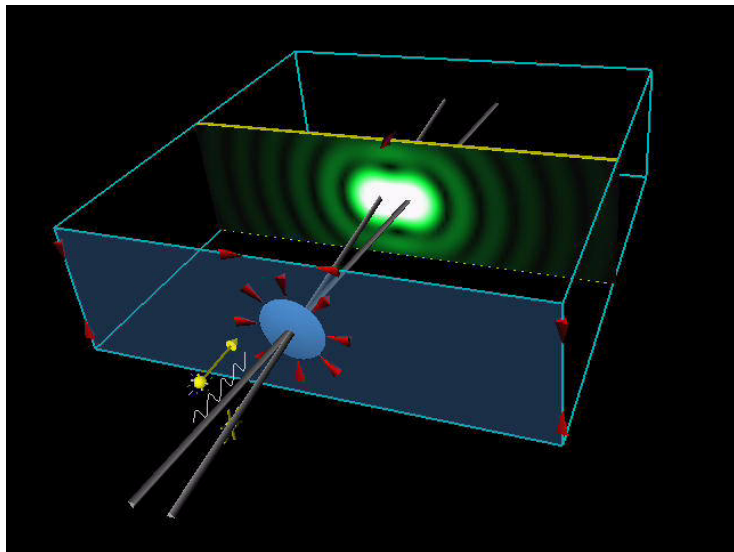
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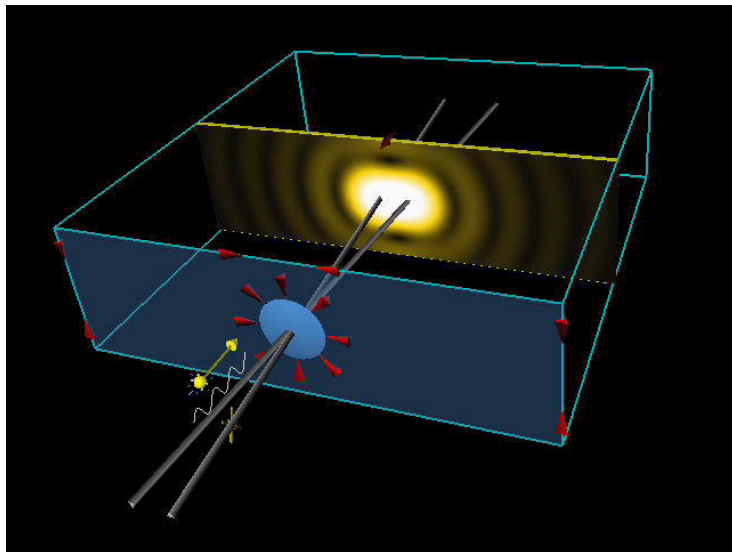


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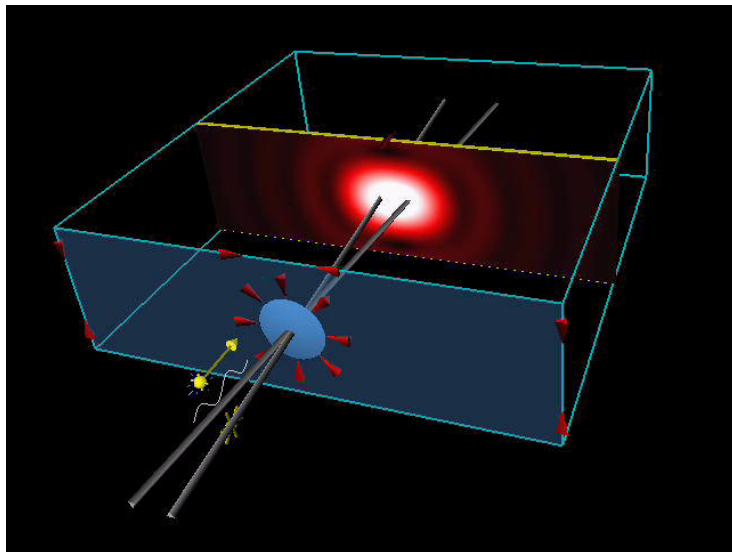




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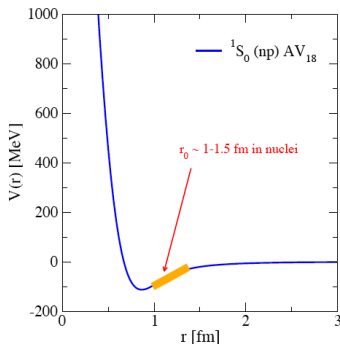


# Wavelength and Resolution



# Sources of Nonperturbative Physics for NN

- 1** Strong short-range repulsion (“hard core”)
- 2** Iterated tensor ( $S_{12}$ ) interaction
- 3** Near zero-energy bound states

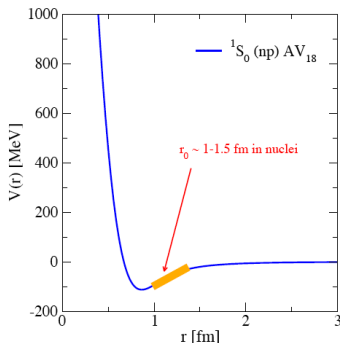


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- Consequences:

- In Coulomb DFT, Hartree-Fock gives dominate contribution  
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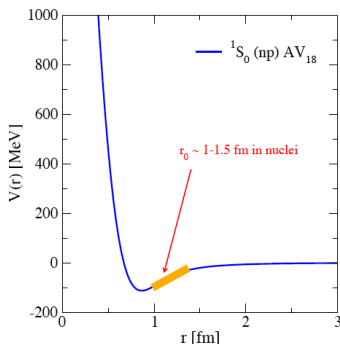
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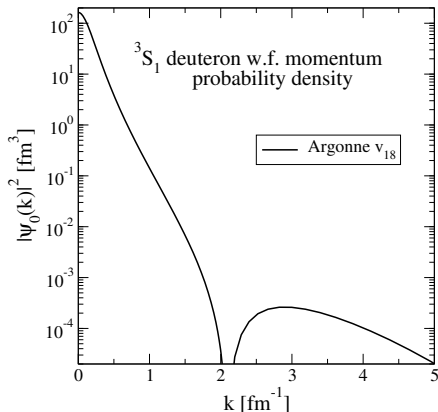
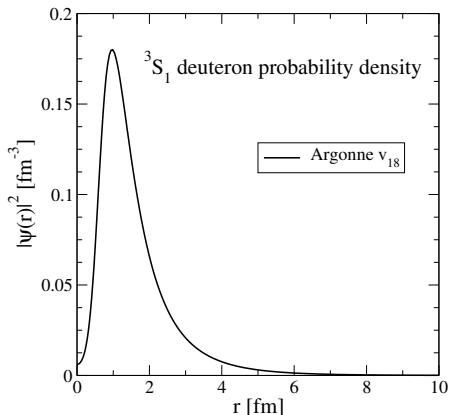
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- However . . .

- the first two depend on the *resolution*  $\implies$  *different cutoffs*
- third one is affected by Pauli blocking

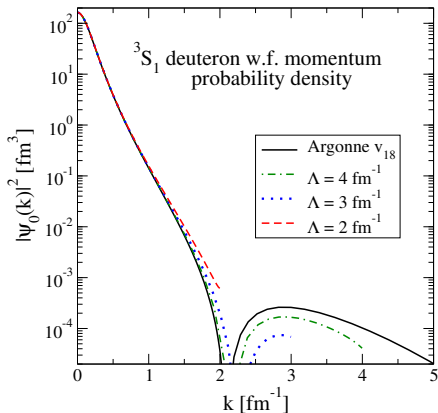
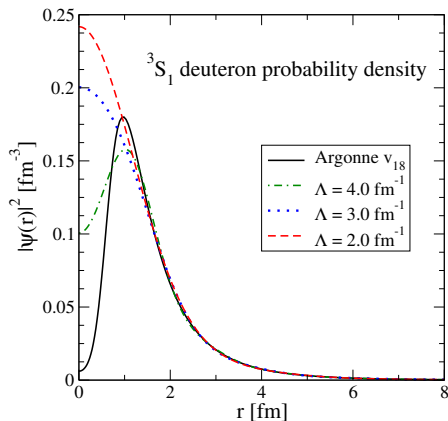


# The Deuteron (Bound np) at High Resolution



- Repulsive core  $\implies$  short-distance suppression  
 $\implies$  important high-momentum (small  $\lambda$ ) components
- Makes the many-body problem complicated!

# The Deuteron at Lower Resolutions

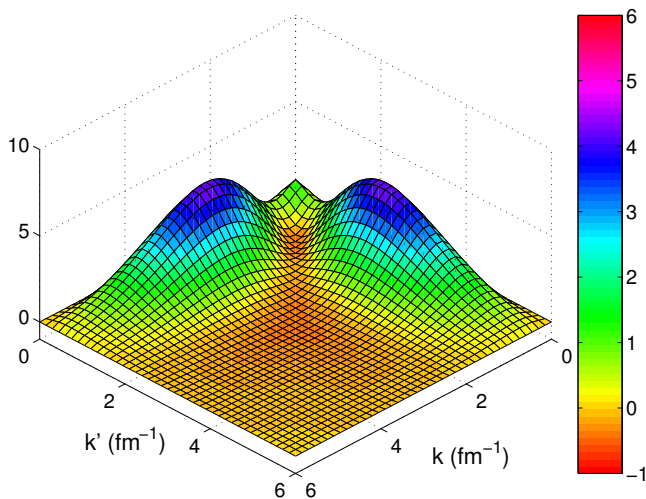


- Repulsive core  $\implies$  short-distance suppression / high-momentum components
- Low-momentum potential  $\implies$  much simpler wave function!

# The Deuteron at Different Resolutions

[more](#)

Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 6.0 \text{ fm}^{-1}$

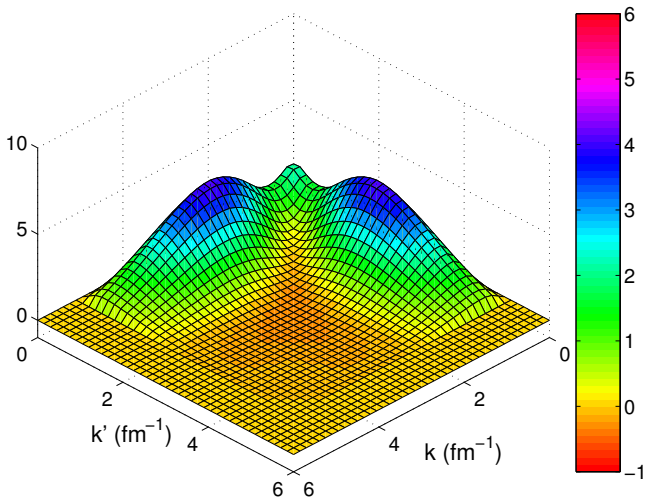




# The Deuteron at Different Resolutions

[more](#)

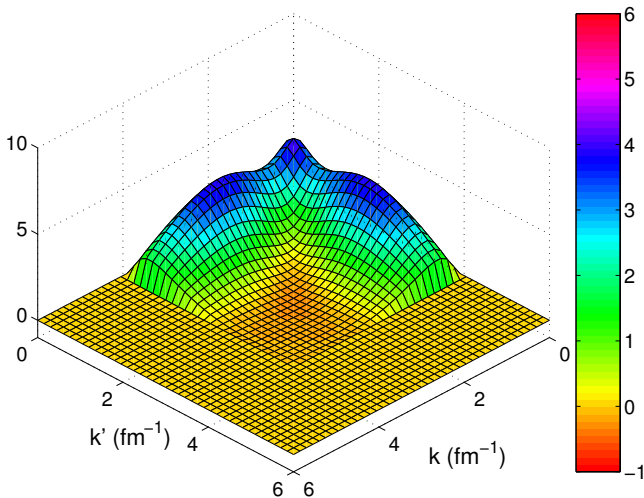
Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 5.0 \text{ fm}^{-1}$



# The Deuteron at Different Resolutions

[more](#)

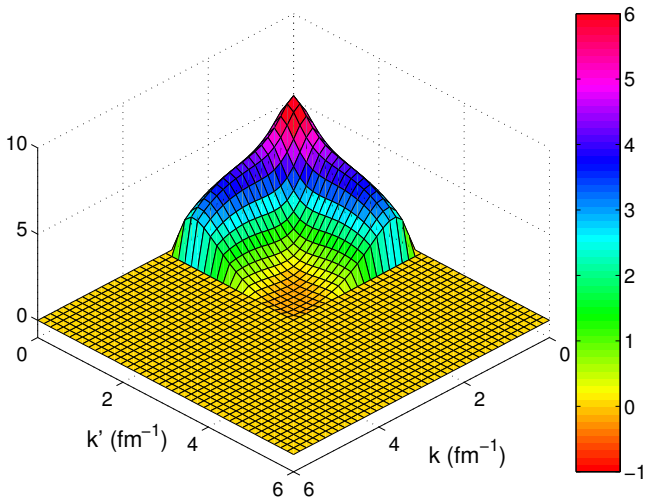
Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 4.0 \text{ fm}^{-1}$



# The Deuteron at Different Resolutions

[more](#)

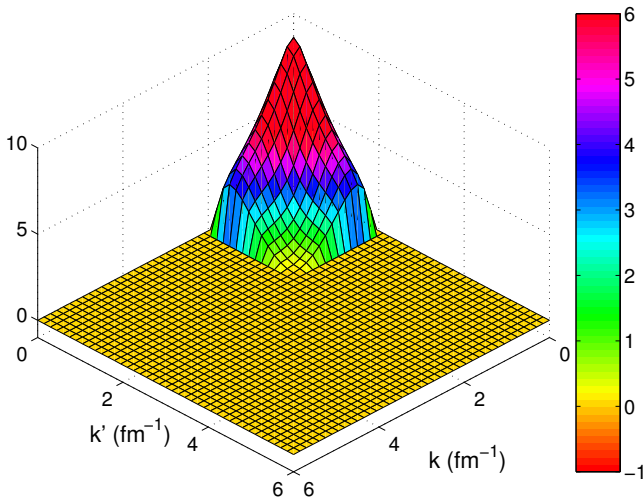
Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 3.0 \text{ fm}^{-1}$



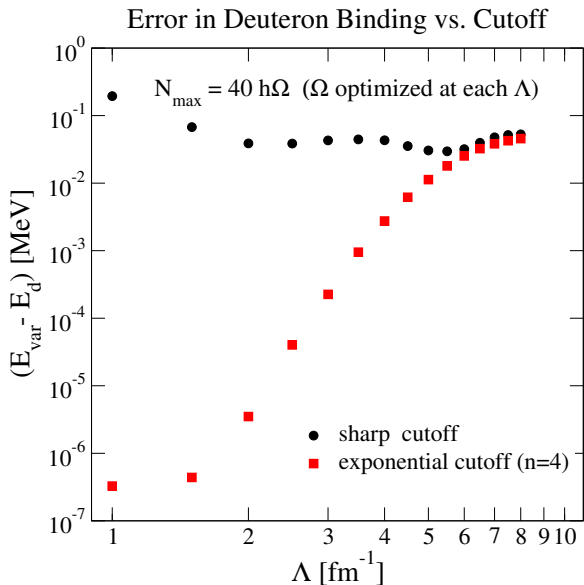
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[more](#)

Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 2.0 \text{ fm}^{-1}$

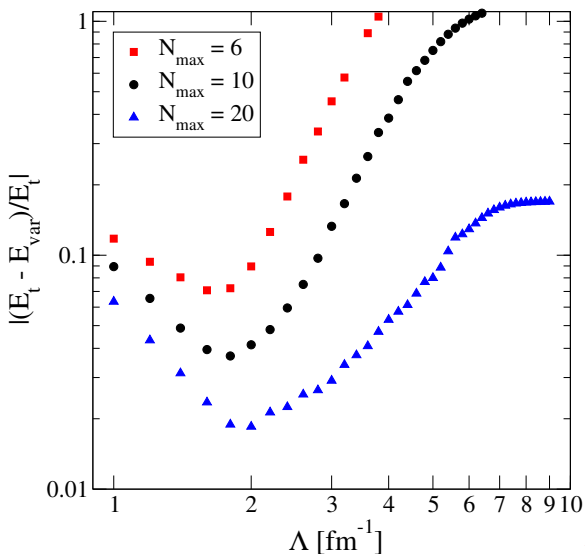


# Consequence for Basis Expansions [nucl-th/0602017]

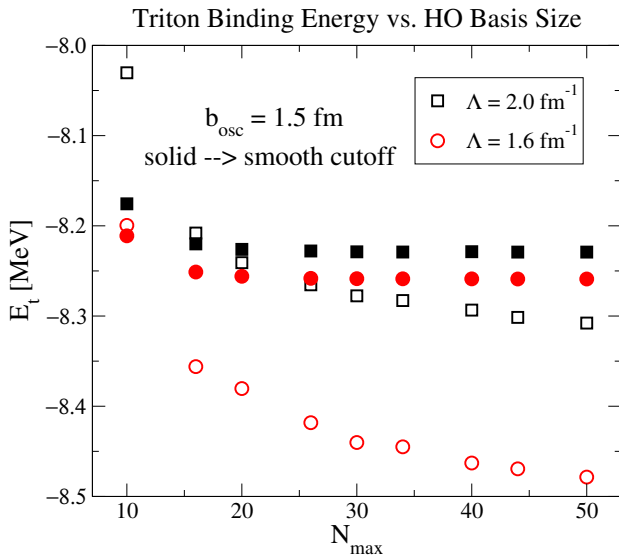


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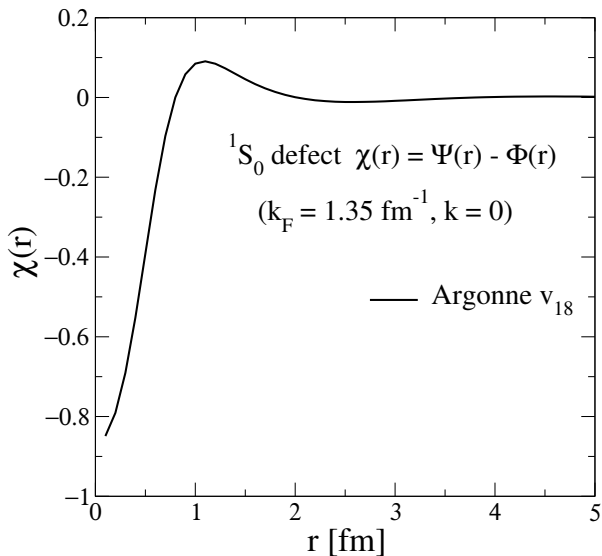
## Error in Triton Binding vs. Cutoff



# Consequence for Basis Expansions [nucl-th/0602017]

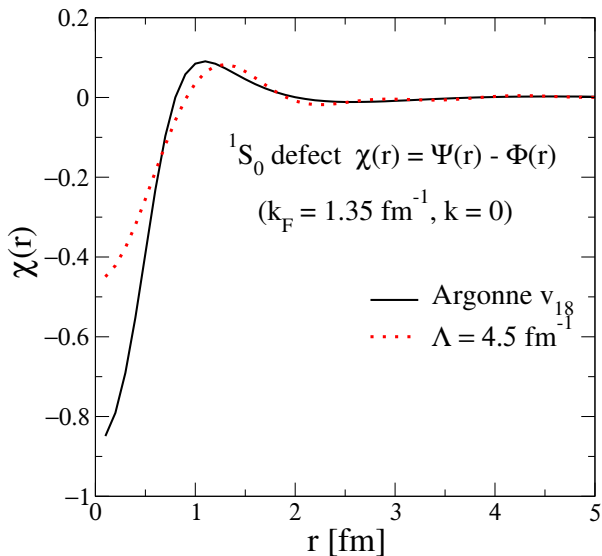


# Two-Body Correlations in Nuclear Matter?

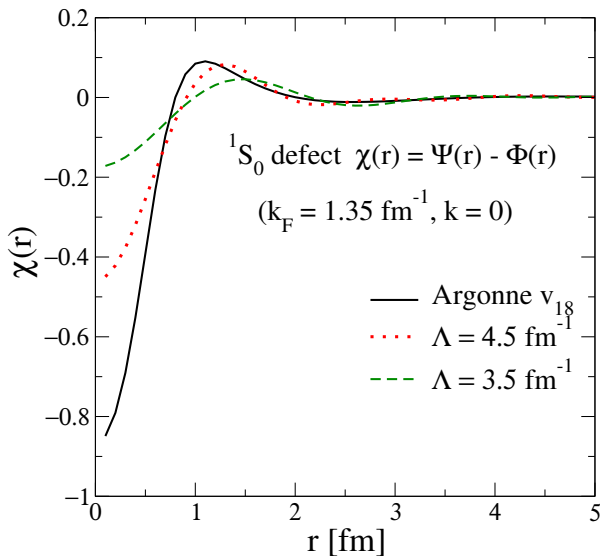




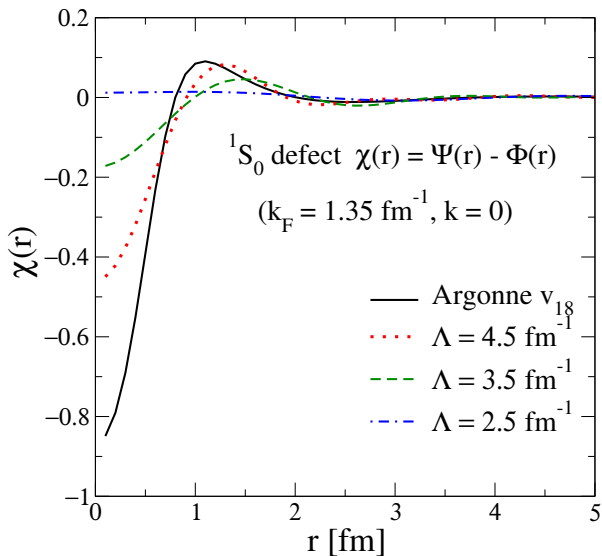
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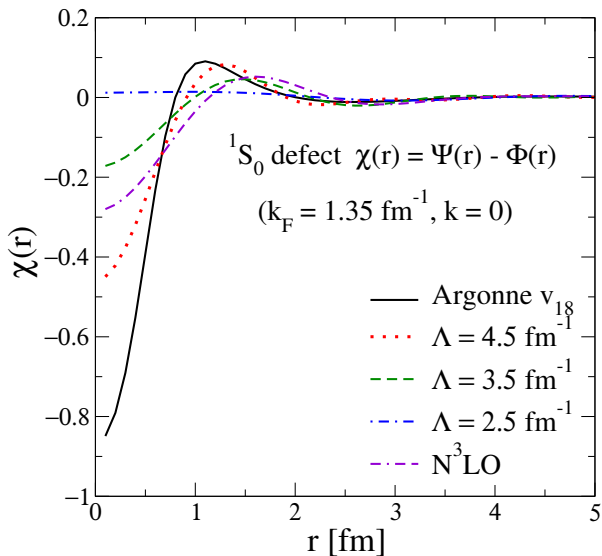
# Two-Body Correlations in Nuclear Matter?



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# Why is In-Medium $T$ Perturbative for $V_{\text{low } k}$ ?

- Phase space in pp-channel strongly suppressed:

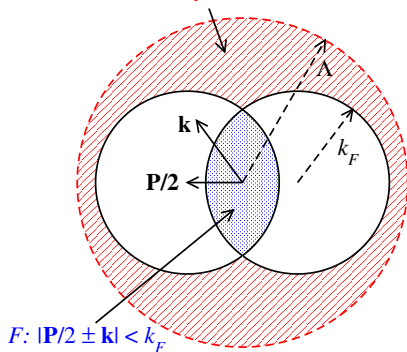
$$\int_{k_F}^{\infty} q^2 dq \frac{V_{NN}(k', q) V_{NN}(q, k)}{k^2 - q^2}$$

vs.

$$\int_{k_F}^{\Lambda} q^2 dq \frac{V_{\text{low } k}(k', q) V_{\text{low } k}(q, k)}{k^2 - q^2}$$

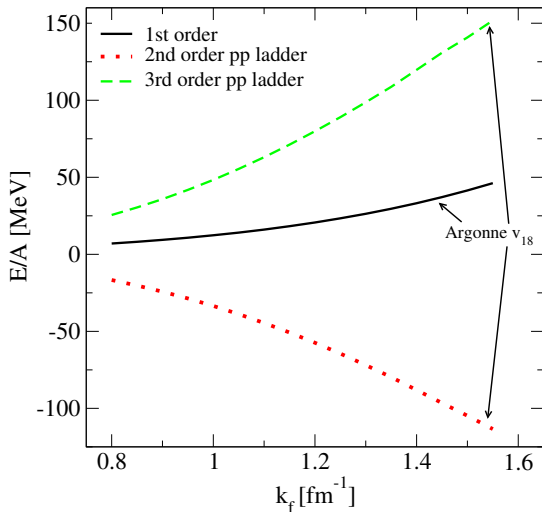
- Tames hard core, tensor, and bound state

$\Lambda$ :  $|P/2 \pm k| > k_F$  and  $|k| < \Lambda$



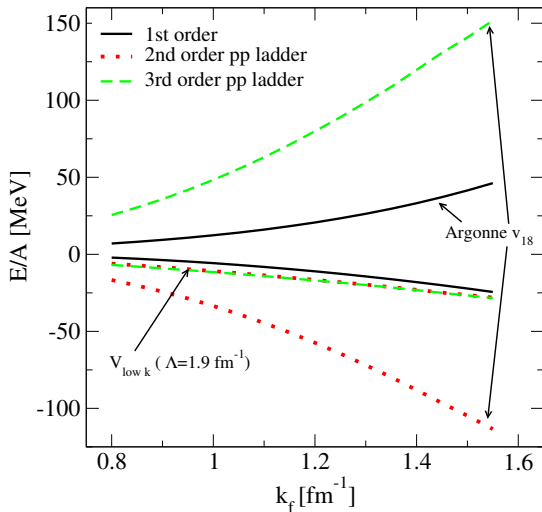
# Nuclear Matter with NN Ladders Only

- Brueckner ladders order-by-order
- Repulsive core  $\implies$  series diverges



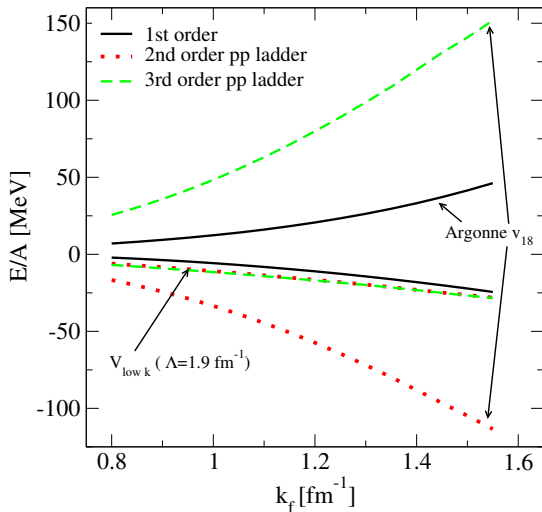
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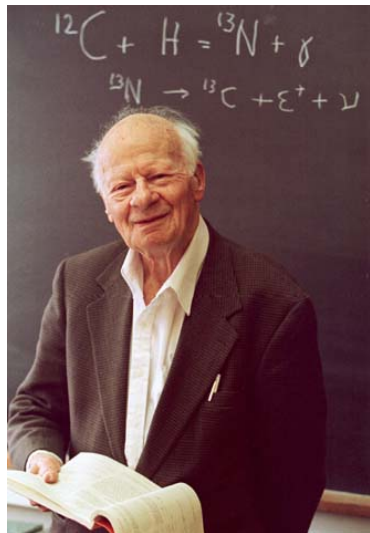
- Brueckner ladders order-by-order
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- $V_{\text{low}k}$  converges
- **No saturation in sight!**





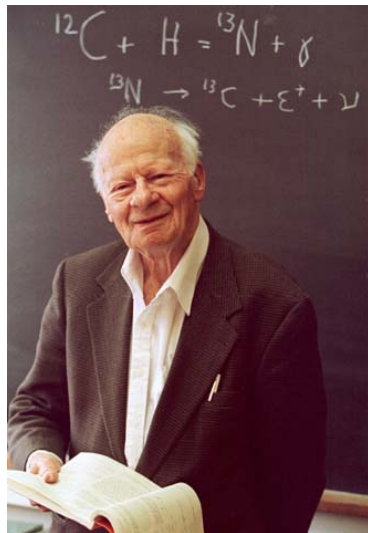
## Deja Vu All Over Again?

- 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 30+ years trying to solve accurately with “hard” potential



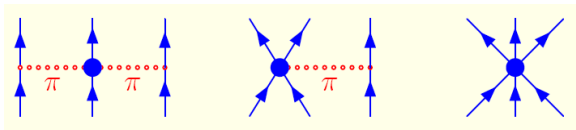
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- Next 30+ years trying to solve accurately with “hard” potential
- **But the story is not complete: three-nucleon forces (3NF)!**



# $V_{\text{low}k}$ with Chiral 3NF

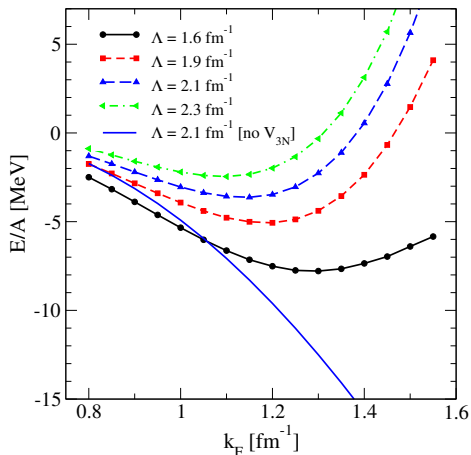
- Ideal: Start with chiral NN + 3NF EFT and run  $\Lambda \downarrow$



- Possible now: Run NN and **fit** 3NF EFT at each  $\Lambda$   
 Bogner, Nogga, Schwenk, Phys. Rev. C **70** (2004) 061002
  - two-pion-exchange  $c_i$ 's from NN PSA fit
  - two free parameters fit to  ${}^3\text{H}$  and  ${}^4\text{He}$  binding energies
  - ratio 2NF/3NF consistent with chiral counting

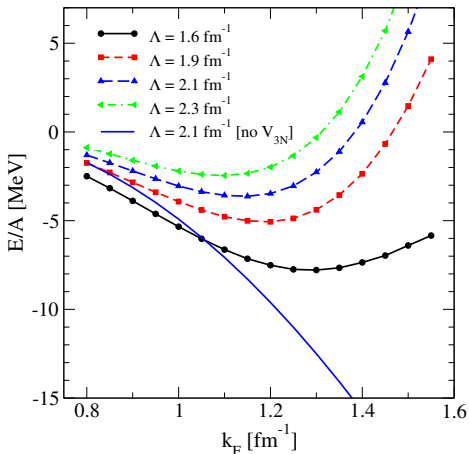
# (Approximate) Nuclear Matter with NN and NNN

## Hartree-Fock

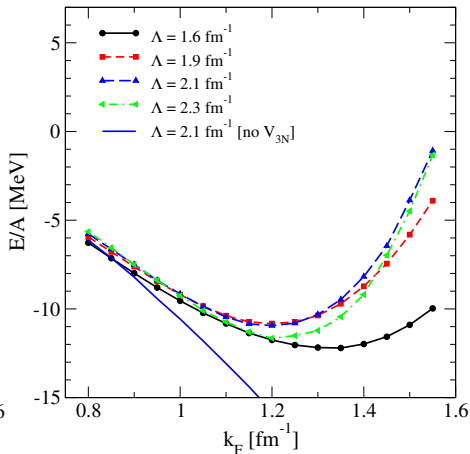


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## Hartree-Fock



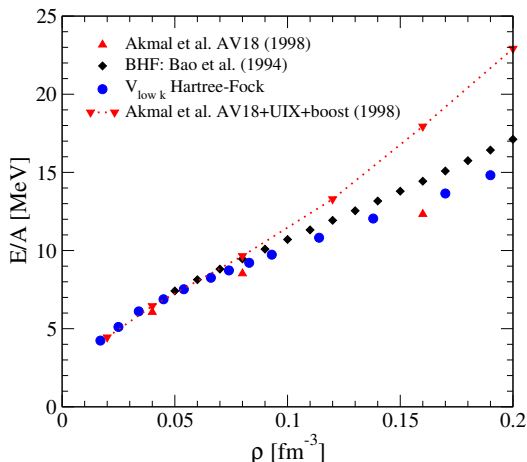
## " $\approx$ 2nd Order"



3-body out of control?

# Low-Momentum Potential for Neutron Matter

- Removing hard core  $\implies$  simpler many-body starting point for neutron matter [Schwenk, Friman, Brown]



- Simple Hartree-Fock (circles) matches best calculations!

# Outline

Overview of Fermion Many-Body Systems

Density Functional Theory for Coulomb Systems

DFT for Nuclei?  $\implies$  EFT and RG

## Summary I

# Bethe and Calculating Nuclear Matter

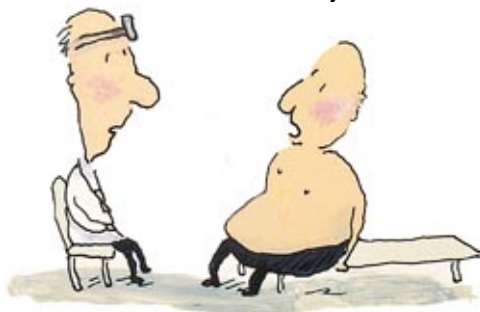
- Hans Bethe in review of nuclear matter (1971):

*“The theory must be such that it can deal with any nucleon-nucleon (NN) force, including hard or ‘soft’ core, tensor forces, and other complications. It ought not to be necessary to tailor the NN force for the sake of making the computation of nuclear matter (or finite nuclei) easier, but the force should be chosen on the basis of NN experiments (and possibly subsidiary experimental evidence, like the binding energy of  $H^3$ ).”*



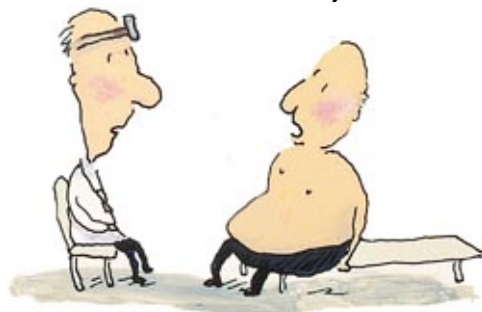
# EFT and RG Make Many-Body Physics Easier

- There's an old vaudeville joke about a doctor and patient ...



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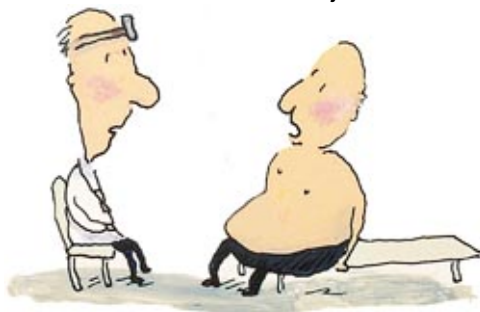
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**Patient:** Doctor, doctor, it hurts when I do this!

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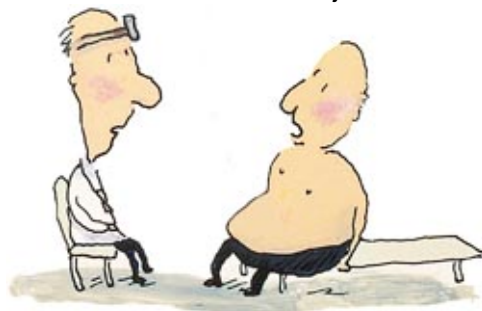


**Patient:** Doctor, doctor, it hurts when I do this!

**Doctor:** Then don't do that.

# EFT and RG Make Many-Body Physics Easier

- There's an old vaudeville joke about a doctor and patient ...



**Patient:** Doctor, doctor, it hurts when I do this!

**Doctor:** Then don't do that.

- Weinberg's Third Law of Progress in Theoretical Physics:  
*"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"*

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


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One Hamiltonian for all problems and energy/length scales

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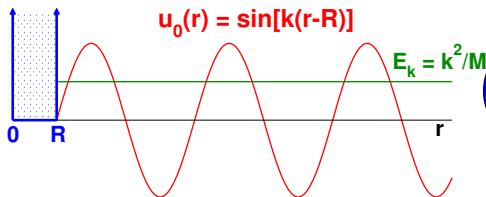
<p>One Hamiltonian for all problems and energy/length scales</p>	<p>Infinite # of low-energy potentials; different resolutions <math>\implies</math> different dof's and Hamiltonians</p>
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<p>Avoid divergences</p>	<p>Exploit divergences (cutoff dependence as tool)</p>

# (Nuclear) Many-Body Physics: “Blue” vs. “Green”

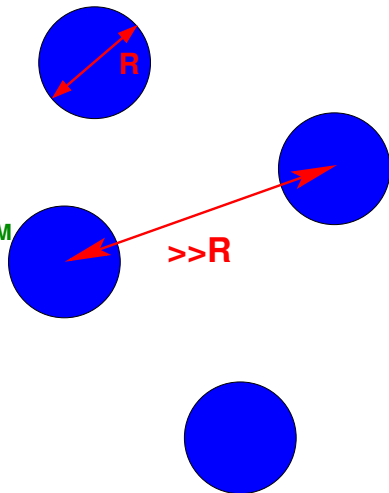
One Hamiltonian for all problems and energy/length scales	Infinite # of low-energy potentials; different resolutions $\implies$ different dof's and Hamiltonians
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Choose diagrams by “art”	Power counting determines diagrams and truncation error

# “Simple” Many-Body Problem: Hard Spheres

- Infinite potential at radius  $R$
- Scattering solutions are simple:



- What is the energy / particle and density profile of the trapped many-body system?



## Renormalization “Old” vs. “New”

### More Deuteron Variational

### Weinberg Eigenvalues

# Renormalization: “Old” vs. “New”


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Cutoff  $\Lambda$  is artificial variable;  
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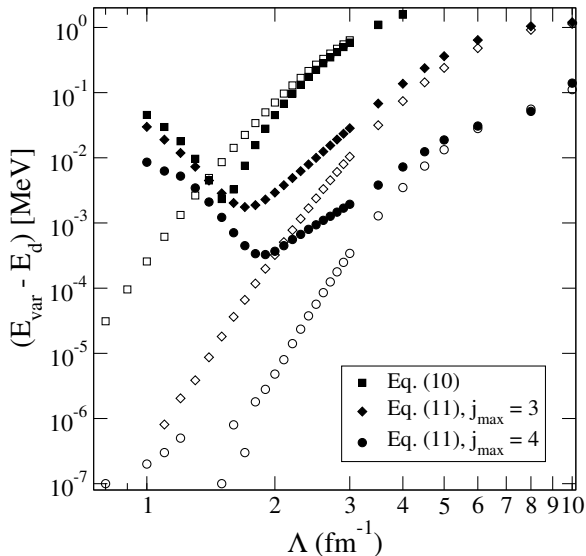
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<p>Renormalization is technical device to get rid of divergences in perturbation theory.</p>	<p>“Renormalization is an expression of the variation of the structure of physical interactions with changes in the scale of the phenomena being probed.”</p>
<p>Focus on the high-energy behavior and on ways of circumventing divergences</p>	<p>Focus on finite variation of physical interactions with finite changes of energy</p>
<p>Cutoff <math>\Lambda</math> is artificial variable; <math>\Lambda \rightarrow \infty</math> at end</p>	<p><math>\Lambda</math> is boundary of unknown/unresolved physics; keep <math>\Lambda</math> finite. Remove <math>\Lambda</math> dependence systematically</p>
<p>Non-renormalizable means no predictive power <math>\implies</math> renormalizable theories</p>	<p>Non-renormalizable <math>\implies</math> systematic expansion! Effective field theories</p>

# More Deuteron Variational Calculations



# Convergence of the Born Series for Scattering

- Consider whether the Born series converges for given  $E$

$$T(E) = V + V \frac{1}{E - H_0} V + V \frac{1}{E - H_0} V \frac{1}{E - H_0} V + \dots$$

- For fixed  $E$ , find (complex) eigenvalues  $\eta_\nu(E)$  [Weinberg]

$$\frac{1}{E - H_0} V |\Gamma_\nu\rangle = \eta_\nu |\Gamma_\nu\rangle \quad \implies \quad T(E) |\Gamma_\nu\rangle = V |\Gamma_\nu\rangle (1 + \eta_\nu + \eta_\nu^2 + \dots)$$

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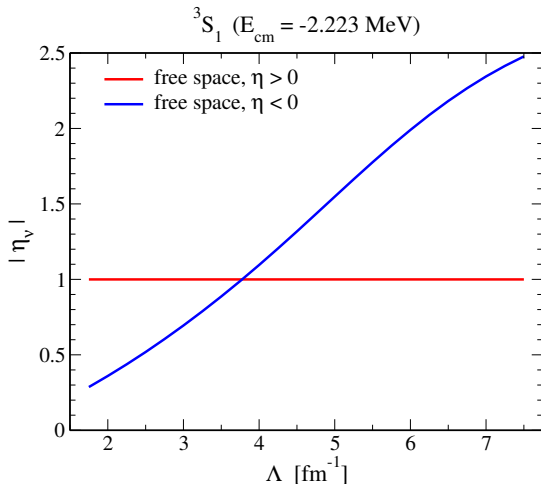
$\Longrightarrow T$  diverges if *any*  $|\eta_\nu(E)| \geq 1$

- For  $E < 0$ , same as finding  $\eta_\nu$  where  $V/\eta_\nu$  has bound state

$$(H_0 + V/\eta_\nu) |b\rangle = E |b\rangle \quad \text{with} \quad \eta_\nu > 0 \quad \text{or} \quad \eta_\nu < 0$$

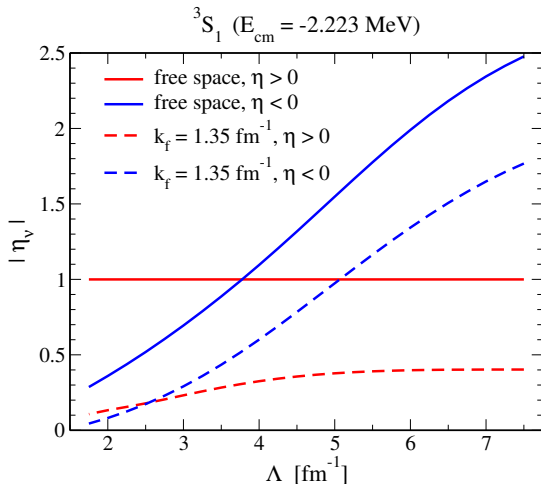
# Weinberg Eigenvalues as Function of Cutoff

- Deuteron  $\implies$  **attractive** eigenvalue  $\eta_\nu$ 
  - $\Lambda \downarrow \implies$  unchanged
- Hard core  $\implies$  **repulsive** eigenvalue  $\eta_\nu$ 
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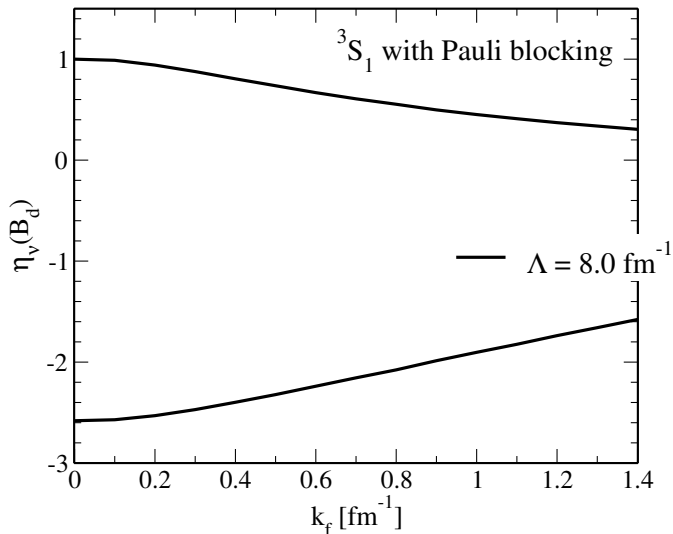


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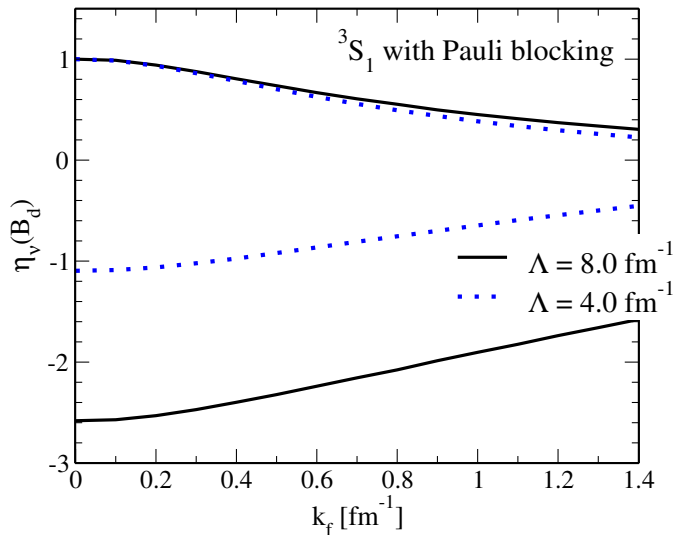
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- In medium: both reduced
  - $\eta_\nu \ll 1$  for  $\Lambda \approx 2 \text{ fm}^{-1}$ $\implies$  **perturbative (in pp)**



# Weinberg Eigenvalues as Function of Density

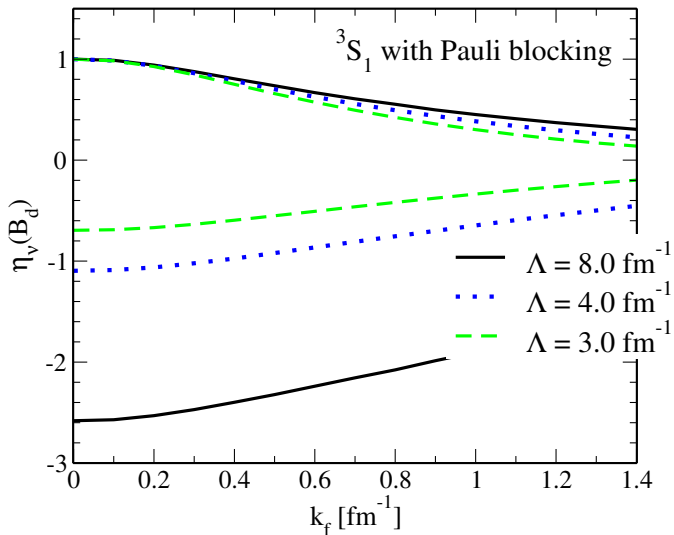


# Weinberg Eigenvalues as Function of Density

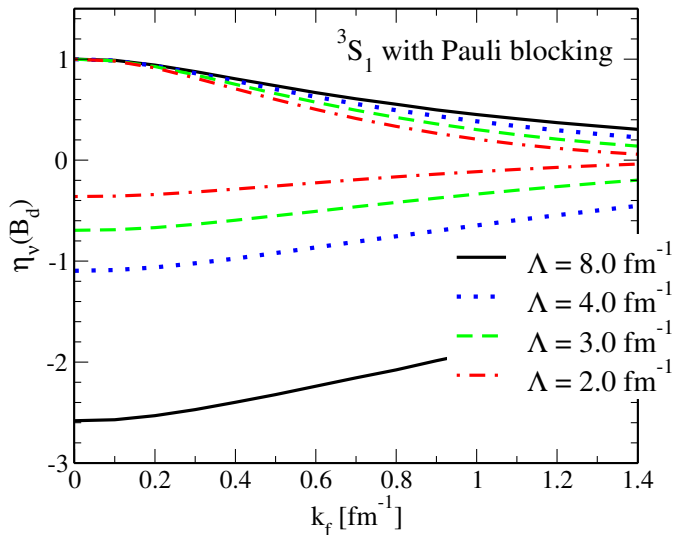




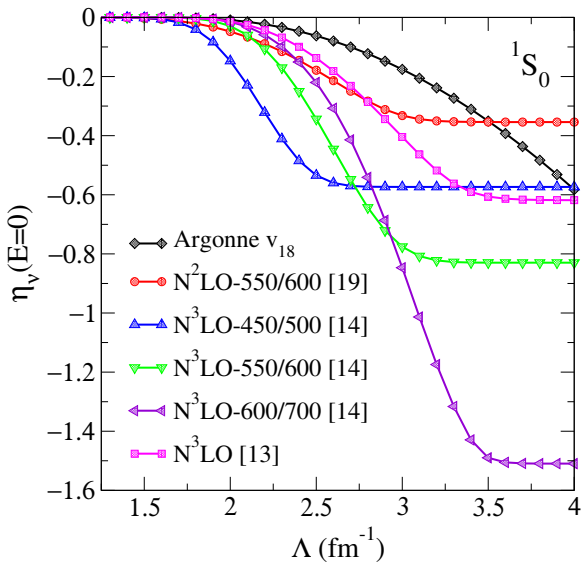
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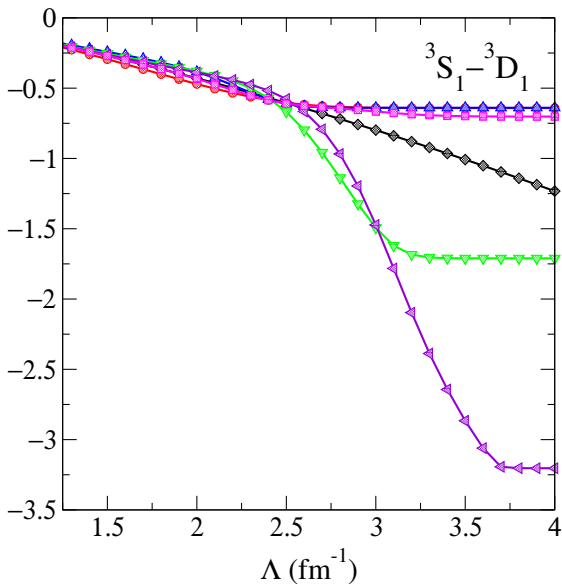
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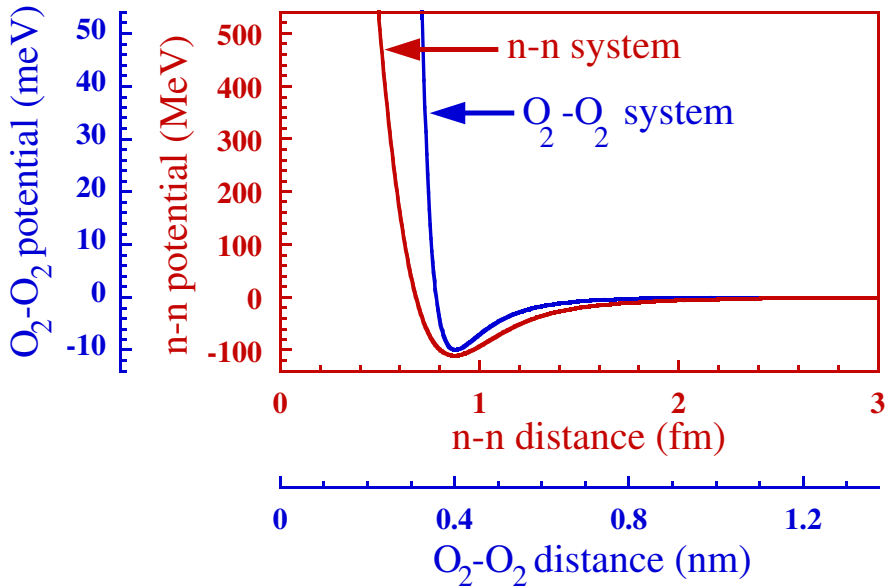


# Collapse of Weinberg Eigenvalues



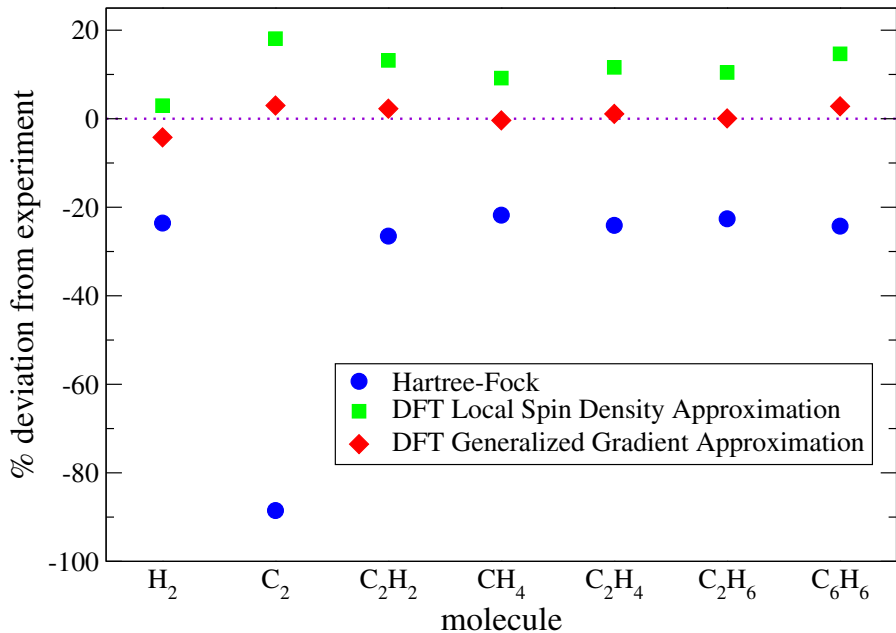
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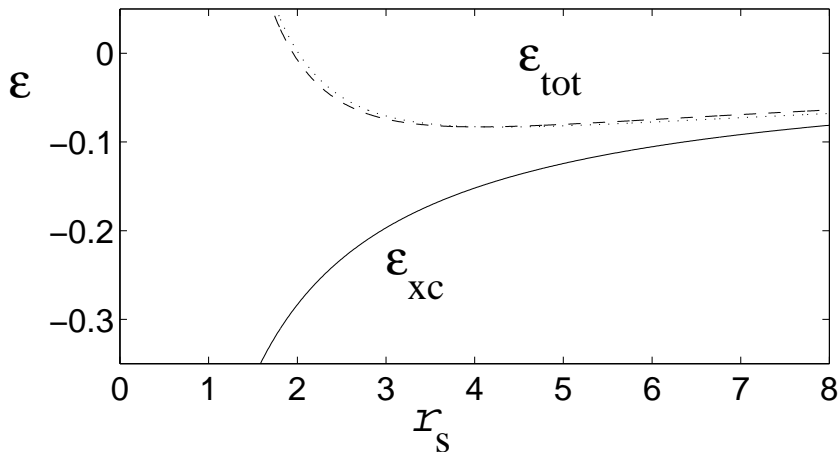
[figure borrowed from J. Dobaczewski]

# Atomization Energies of Hydrocarbon Molecules



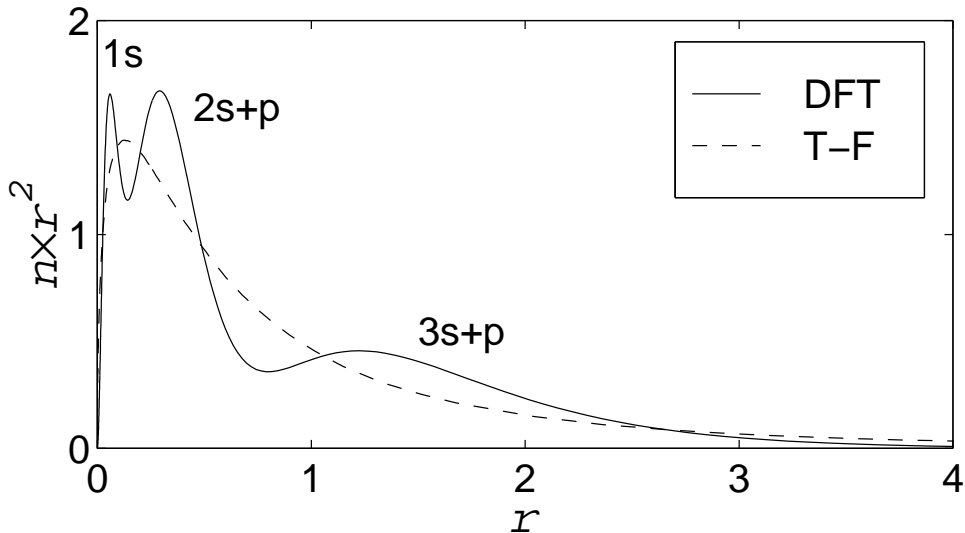
- Local density approximation

- fit  $\mathcal{E}_{\text{xc}}(\rho)$  to Monte Carlo cal



# Calculation of uniform electron gas

Ar  $Z=18$

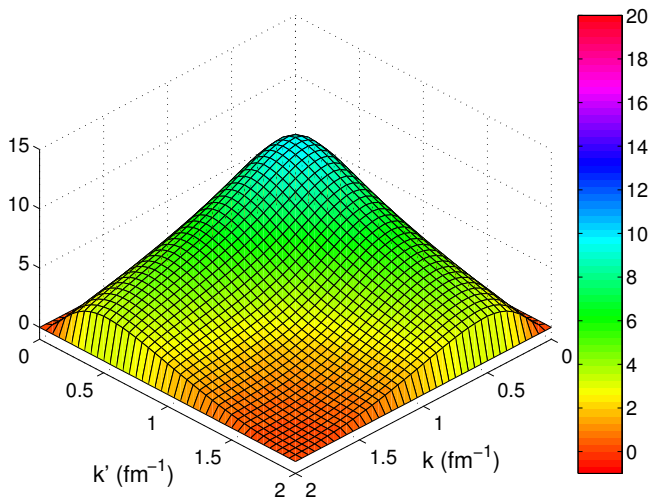




# The Deuteron at Different Resolutions

[back](#)

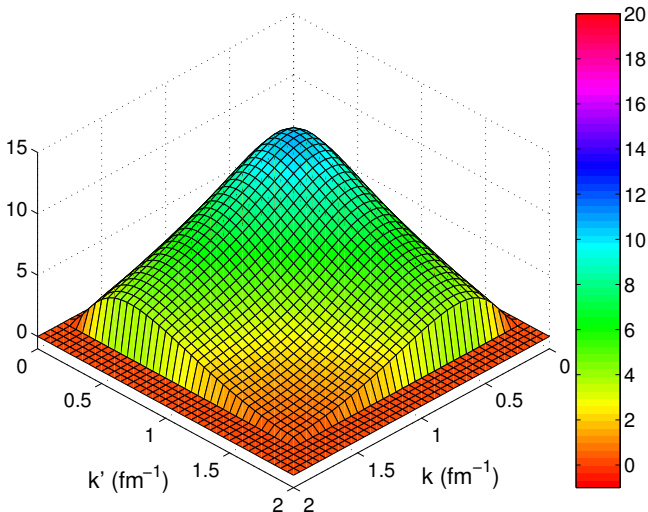
Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 2.0 \text{ fm}^{-1}$



# The Deuteron at Different Resolutions

[back](#)

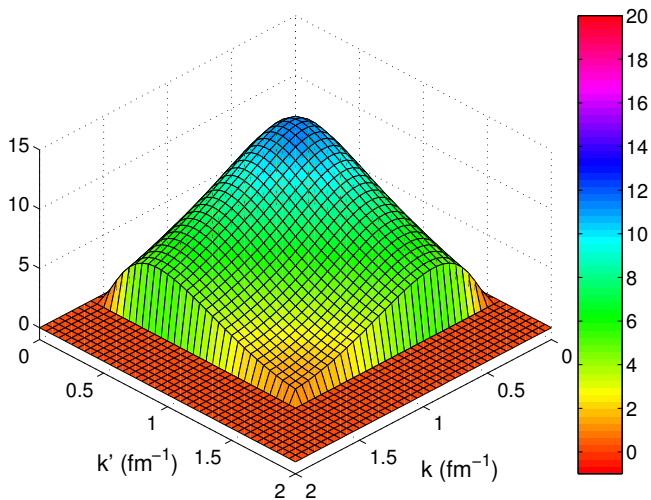
Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 1.8 \text{ fm}^{-1}$



# The Deuteron at Different Resolutions

[back](#)

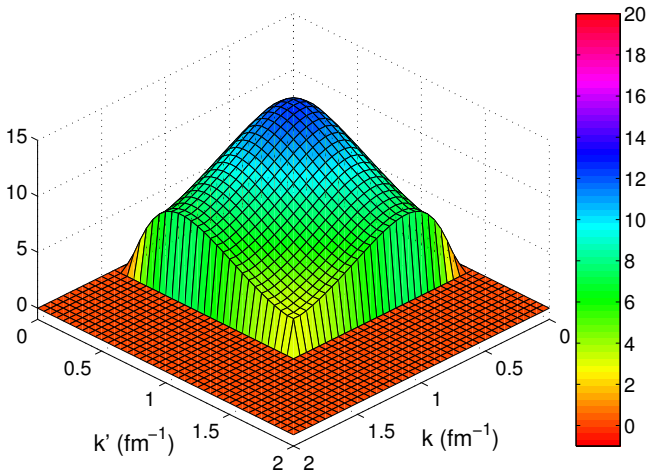
Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 1.6 \text{ fm}^{-1}$



# The Deuteron at Different Resolutions

[back](#)

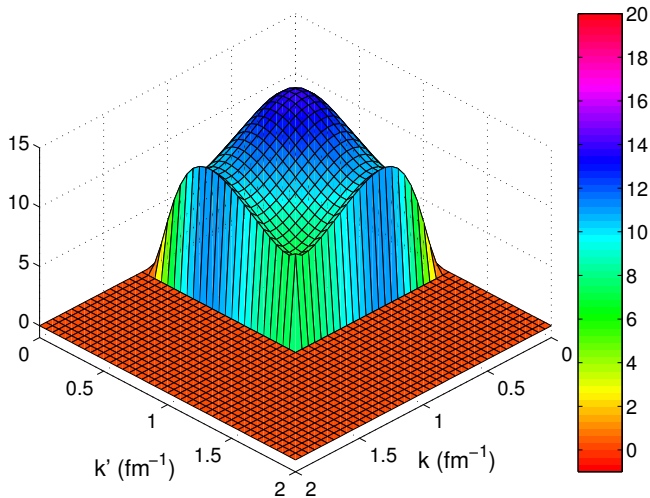
Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 1.4 \text{ fm}^{-1}$



# The Deuteron at Different Resolutions

[back](#)

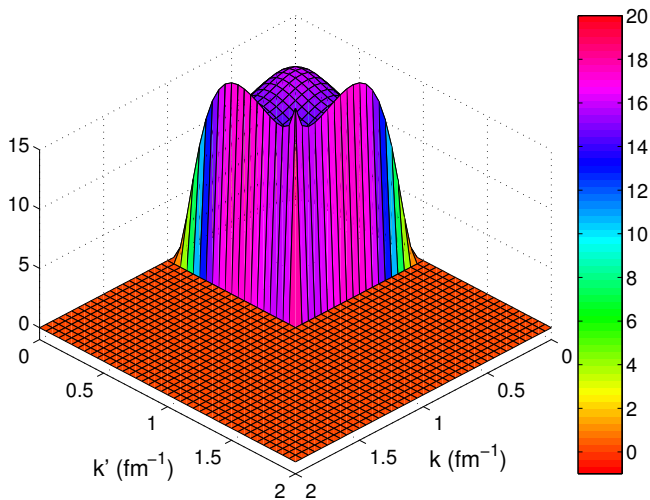
Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 1.2 \text{ fm}^{-1}$



# The Deuteron at Different Resolutions

[back](#)

Integrand of  $-\langle \psi_d | V_\Lambda | \psi_d \rangle$  for  $\Lambda = 1.0 \text{ fm}^{-1}$

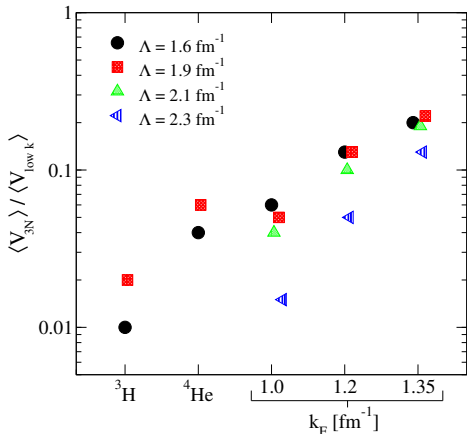


# Is Three-Body Contribution Out of Control?

back

- Saturation driven by 3NF
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- Chiral:  $\langle V_{3N} \rangle \sim (Q/\Lambda)^3 \langle V_{NN} \rangle$   
 $\implies$  consistent

Check ratios:



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- Power counting still needed with NN + 3N HF at LO
- Four-body contributions?

Check ratios:

